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(54) SOLUTION STRUCTURE OF IL-13 AND USES THEREOF

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Publication Classification

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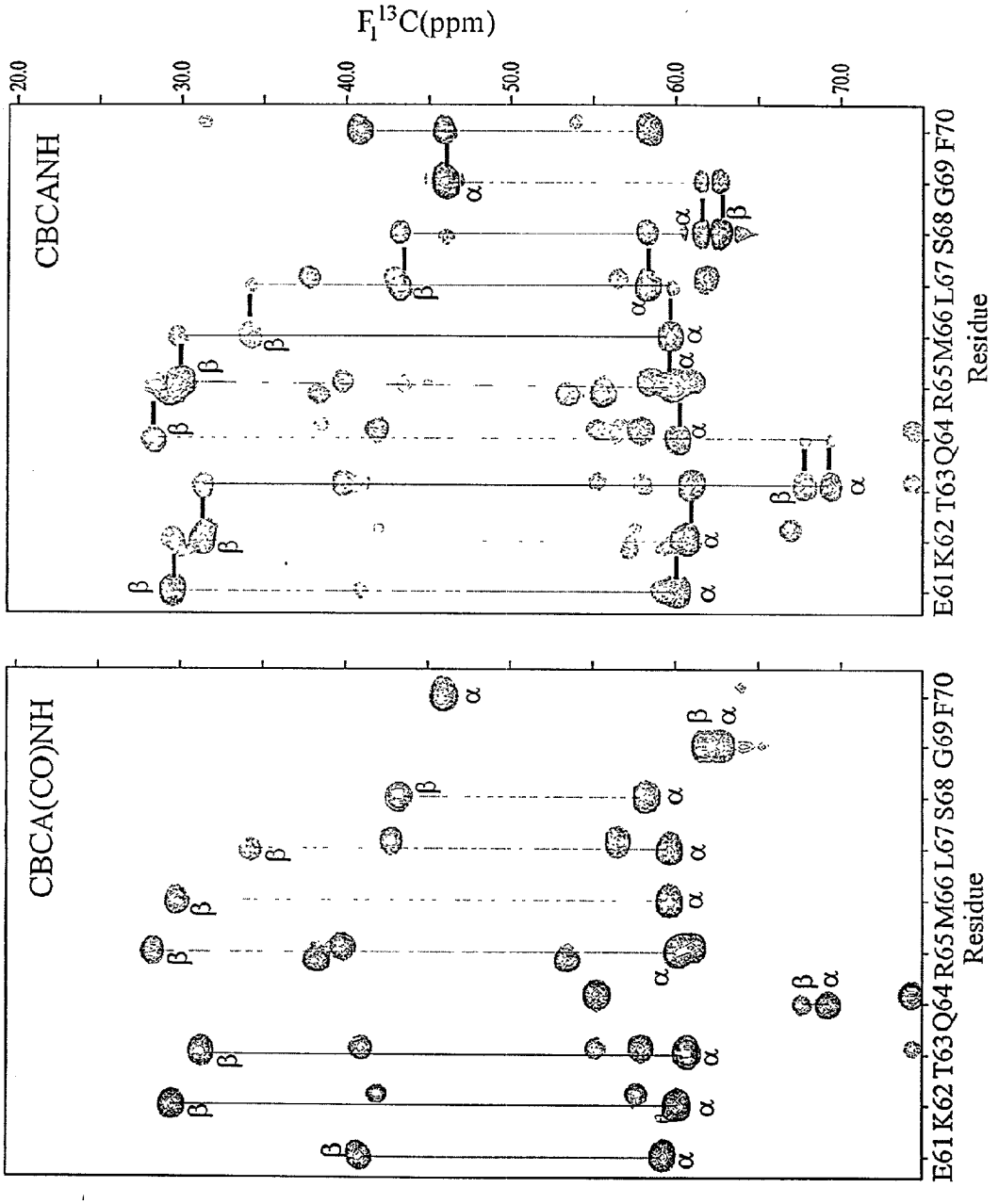
(52) **U.S. Cl.** **530/351**; 702/19

(57) ABSTRACT

The present invention relates to the three dimensional solution structure of interleukin-13 (IL-13), as well as the identification and characterization of various binding active sites of IL-13. Also provided for by the present invention are methods of utilizing the three dimensional structure for the design and selection of potent and selective agents that interact with IL-13.

	Atom No.	Atom Type	Res.	Res. No.	X	Y	Z	OCC.	B	
ATOM	1	CA	MET	1	21.496	5.345	13.553	1.00	2.00	IL13
ATOM	2	HA	MET	1	21.091	4.864	14.432	1.00	2.52	IL13
ATOM	3	CB	MET	1	22.712	6.191	13.945	1.00	2.41	IL13
ATOM	4	HB1	MET	1	22.407	6.959	14.639	1.00	2.85	IL13
ATOM	5	HB2	MET	1	23.132	6.649	13.061	1.00	2.73	IL13
ATOM	6	CG	MET	1	23.761	5.295	14.607	1.00	2.86	IL13
ATOM	7	HG1	MET	1	23.277	4.679	15.344	1.00	2.93	IL13
ATOM	8	HG2	MET	1	24.508	5.912	15.087	1.00	3.19	IL13
ATOM	9	SD	MET	1	24.548	4.261	13.331	1.00	3.84	IL13
ATOM	10	CE	MET	1	24.995	2.795	14.313	1.00	4.23	IL13
ATOM	11	HE1	MET	1	25.990	2.925	14.715	1.00	4.26	IL13
ATOM	12	HE2	MET	1	24.983	1.926	13.676	1.00	4.46	IL13
ATOM	13	HE3	MET	1	24.292	2.647	15.117	1.00	4.75	IL13
ATOM	14	C	MET	1	20.430	6.238	12.922	1.00	1.66	IL13
ATOM	15	O	MET	1	19.289	6.251	13.339	1.00	1.58	IL13
ATOM	16	N	MET	1	21.908	4.310	12.564	1.00	2.43	IL13
ATOM	17	HT1	MET	1	22.629	4.706	11.927	1.00	2.81	IL13
ATOM	18	HT2	MET	1	21.080	4.012	12.009	1.00	2.72	IL13
ATOM	19	HT3	MET	1	22.305	3.489	13.064	1.00	2.88	IL13
ATOM	20	N	GLY	2	20.790	6.979	11.911	1.00	1.55	IL13
ATOM	21	HN	GLY	2	21.714	6.947	11.585	1.00	1.70	IL13
ATOM	22	CA	GLY	2	19.795	7.862	11.244	1.00	1.31	IL13
ATOM	23	HA1	GLY	2	20.300	8.530	10.563	1.00	1.39	IL13
ATOM	24	HA2	GLY	2	19.269	8.435	11.993	1.00	1.36	IL13
ATOM	25	C	GLY	2	18.806	6.993	10.463	1.00	1.04	IL13
ATOM	26	O	GLY	2	18.998	5.801	10.328	1.00	1.02	IL13
ATOM	27	N	PRO	3	17.755	7.578	9.950	1.00	0.95	IL13
ATOM	28	CA	PRO	3	16.747	6.806	9.176	1.00	0.85	IL13
ATOM	29	HA	PRO	3	16.204	6.136	9.821	1.00	0.95	IL13
ATOM	30	CB	PRO	3	15.811	7.900	8.659	1.00	0.98	IL13
ATOM	31	HB1	PRO	3	14.804	7.704	8.996	1.00	1.10	IL13
ATOM	32	HB2	PRO	3	15.835	7.915	7.578	1.00	0.96	IL13
ATOM	33	CG	PRO	3	16.278	9.256	9.205	1.00	1.14	IL13
ATOM	34	HG1	PRO	3	15.487	9.704	9.787	1.00	1.29	IL13
ATOM	35	HG2	PRO	3	16.538	9.907	8.383	1.00	1.28	IL13
ATOM	36	CD	PRO	3	17.505	9.035	10.096	1.00	1.12	IL13
ATOM	37	HD2	PRO	3	18.347	9.613	9.737	1.00	1.24	IL13
ATOM	38	HD1	PRO	3	17.277	9.277	11.121	1.00	1.20	IL13
ATOM	39	C	PRO	3	17.385	6.040	8.014	1.00	0.72	IL13
ATOM	40	O	PRO	3	18.471	6.361	7.573	1.00	0.73	IL13
ATOM	41	N	VAL	4	16.727	5.032	7.512	1.00	0.68	IL13
ATOM	42	HN	VAL	4	15.854	4.782	7.876	1.00	0.75	IL13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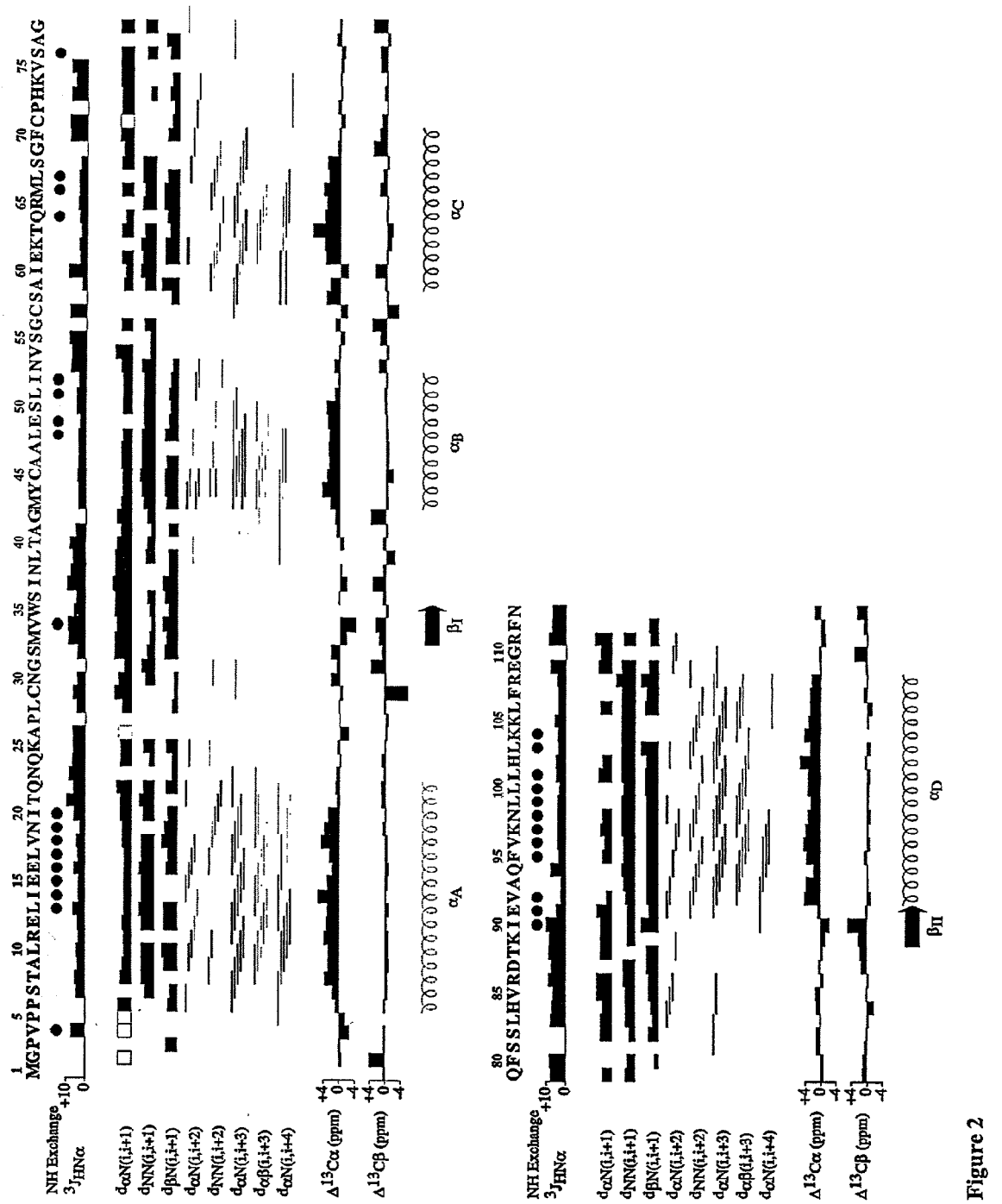
30.0
40.0
50.0
60.0
70.0
CBCANH
CBCA(CO)NH
E61 K62 T63 Q64 R65 M66 L67 S68 G69 F70
Residue

Figure 1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QFSSLHVRDTKIEVAQFVKNLLLHLKKLFREGRFN
NH Exchange
3JHNα
dαN(i,i+1)
dNN(i,i+1)
dβN(i,i+1)
dαN(i,i+2)
dNN(i,i+2)
dαN(i,i+3)
dαβ(i,i+3)
dαN(i,i+4)
Δ13Cα (ppm)
Δ13Cβ (ppm)
αA
βI
αB
αC
αD
βII

Figure 2

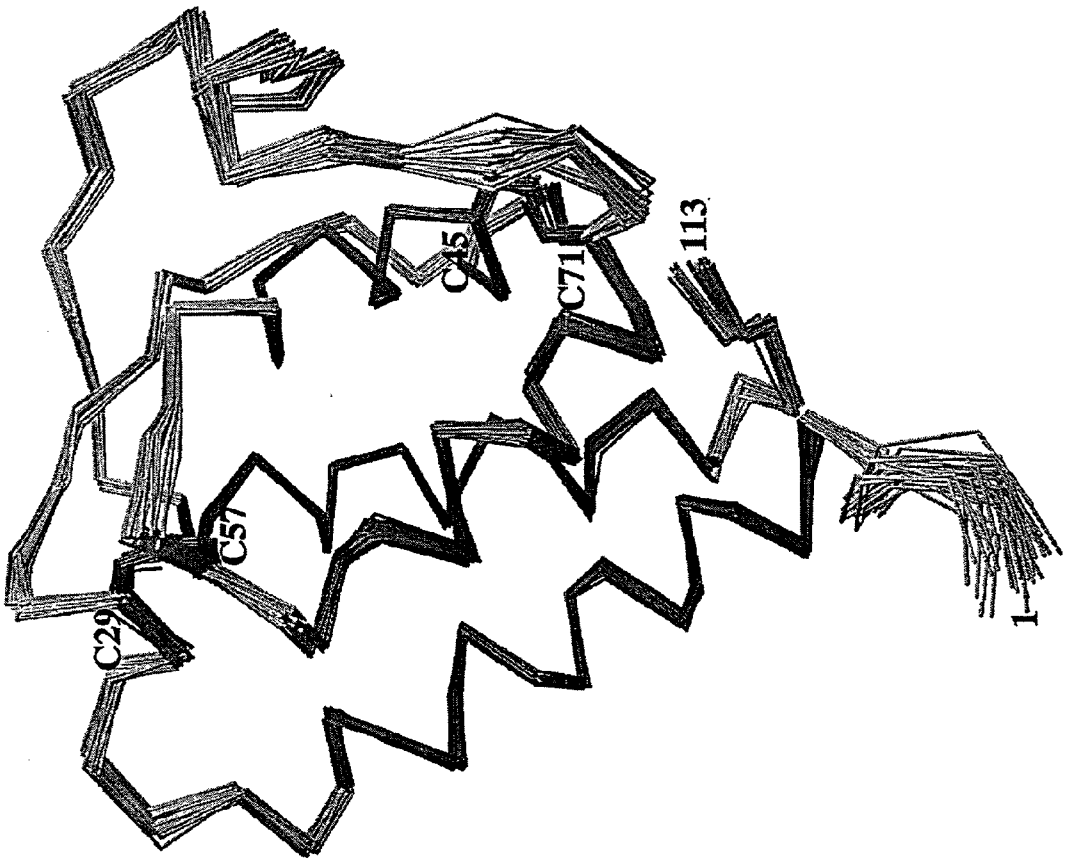
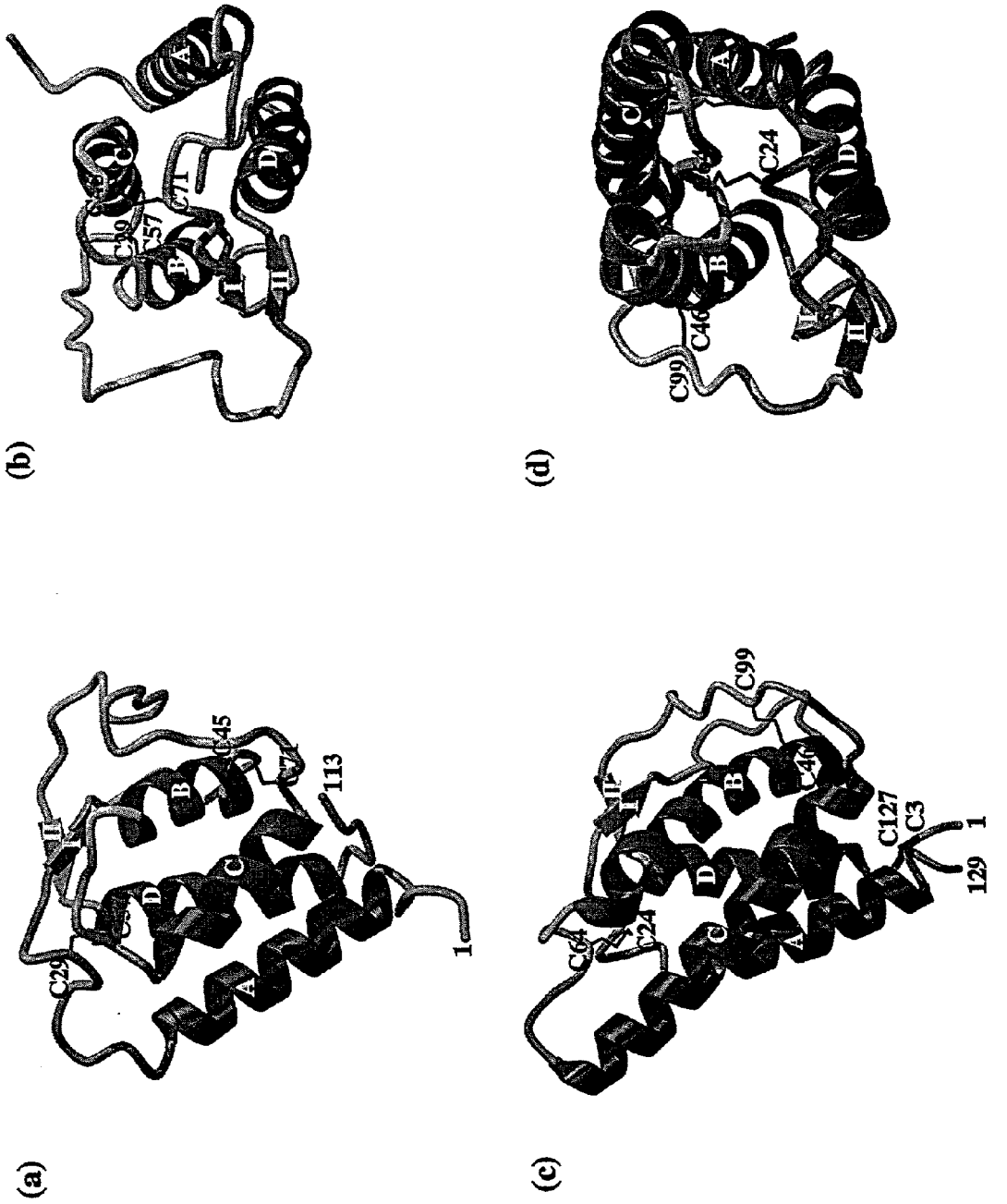


Figure 3


(b)
A
C
C39
C57
C71
B
D
I
II
(d)
A
C24
D
B
C46
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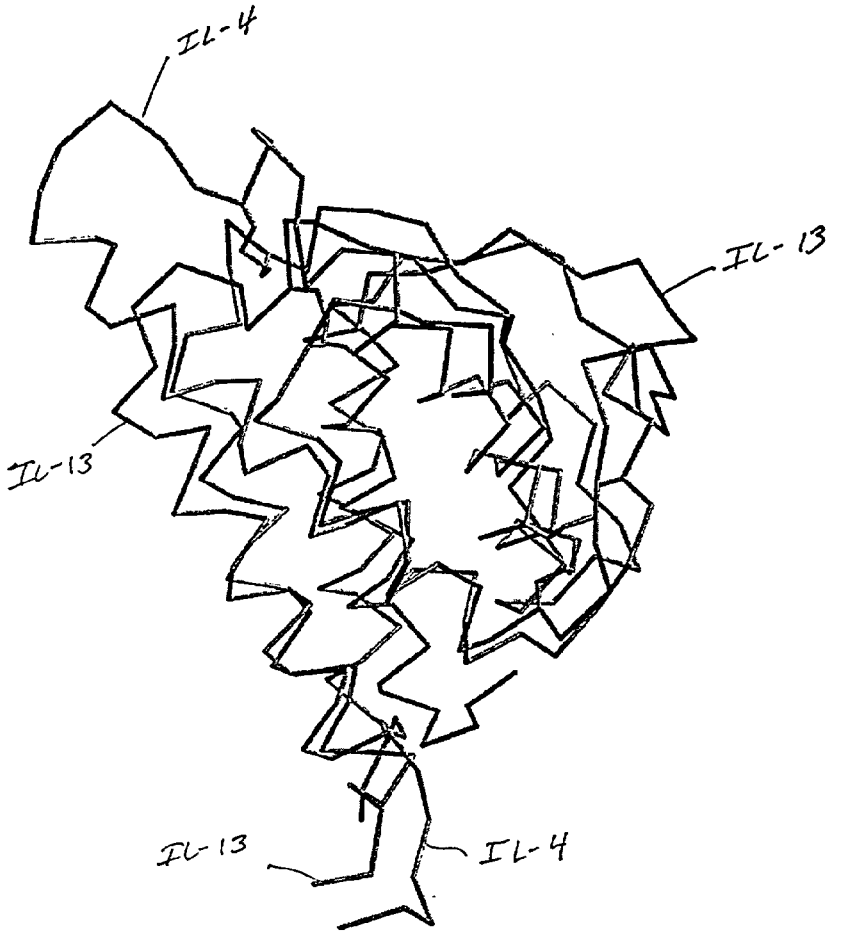
I
II
(a)
C29
II
I
B
C45
113
C
D
A
1
(c)
C99
II
I
B
C46
C127
C3
129
1
D
C64
C24
C
A

Figure 4

(a)



(b)

```
            1         10         20         30         40         50         60
                ** ** +** +                                    *  **
IL-4          HKCDITLQEIIKTLNSLTEQK TLCTELTVTDIFAASKTTEKETFCRAATVLRQFYSHHEKDTRCL
IL-13     MGPVPPSTALRELIEELVNITQNQKAPLCNGSMVWSINL     TAGMYCAALESLINV
                    #  #
          1         10         20         30              40         50

            70         80         90         100              110        120
                   *-  ** **  ** **                                  +  ++
IL-4      GATAQQFHRHKQLIRFLKRLDRNLWGLAGLNSCP         VKEADQSTLENFLERLKTIMREKYSKCSS
IL-13                  SGCSAIEKTQRMLSGFCPHKVSAGQFSSLHVRDTKIEVAQFVKDLLLHLKKLFREGRFN
                             #  #                                          &   &
                          60         70         80         90         100        110
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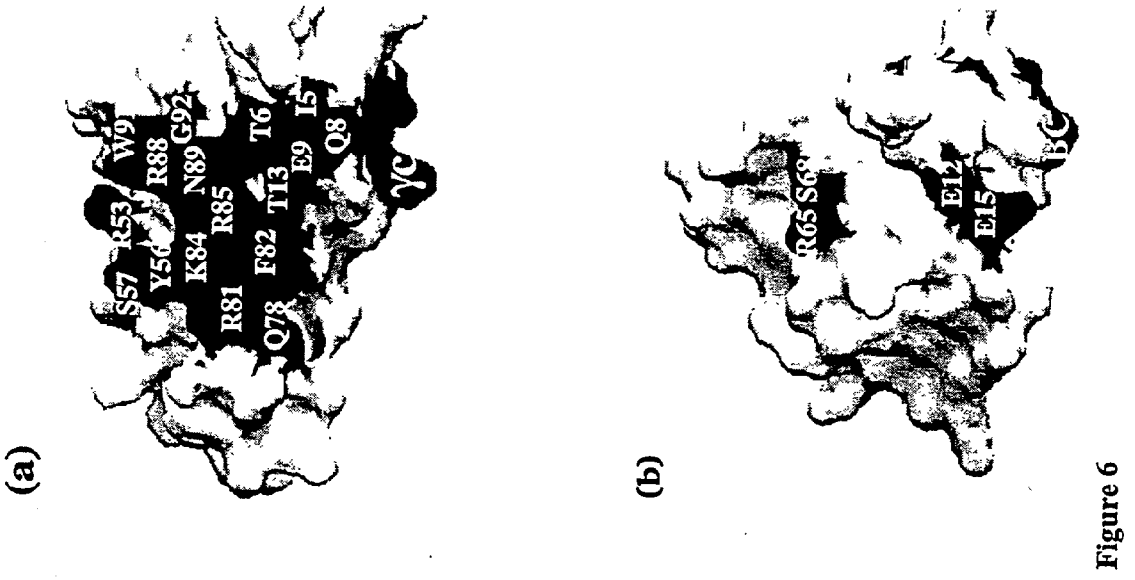
Figure 5


(a)
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R88
G92
T6
I5
N89
E9
Q8
R53
T13
R85
K84
F82
Y56
S57
R81
Q78
(b)
R65
S68
E12
E15

Figure 6

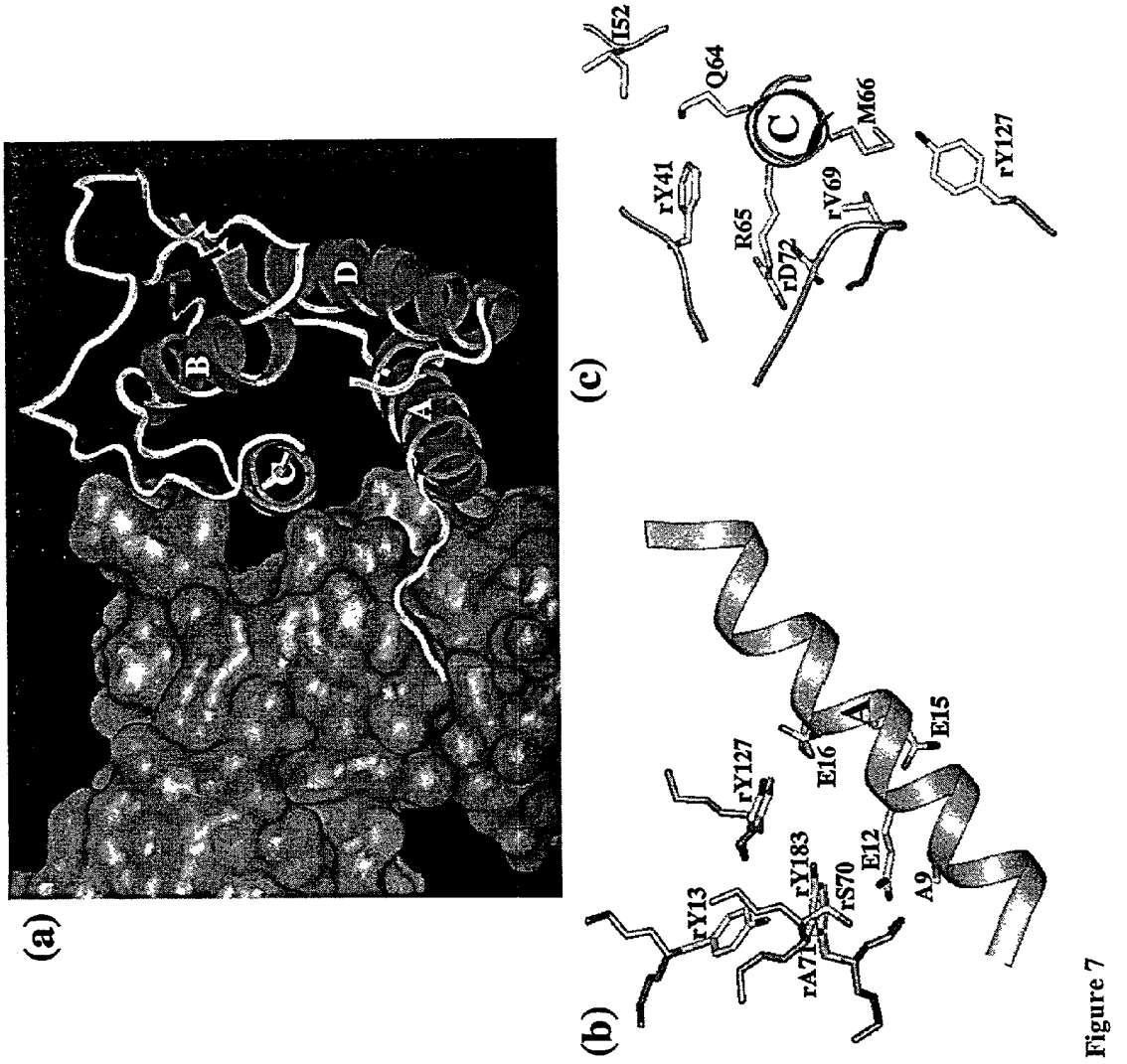
(a)
B
D
A
(c)
I52
Q64
M66
rY41
R65
rD72
rV69
rY127
(b)
rY127
E16
A
E15
rY13
rY183
rS70
E12
A9
rA7

Figure 7

Figure 8 (1/30)

		Atom Type	Res.	Res. No.	X	Y	Z	OCC.	B	
ATOM	1	CA	MET	1	21.496	5.345	13.553	1.00	2.00	IL13
ATOM	2	HA	MET	1	21.091	4.864	14.432	1.00	2.52	IL13
ATOM	3	CB	MET	1	22.712	6.191	13.945	1.00	2.41	IL13
ATOM	4	HB1	MET	1	22.407	6.959	14.639	1.00	2.85	IL13
ATOM	5	HB2	MET	1	23.132	6.649	13.061	1.00	2.73	IL13
ATOM	6	CG	MET	1	23.761	5.295	14.607	1.00	2.86	IL13
ATOM	7	HG1	MET	1	23.277	4.679	15.344	1.00	2.93	IL13
ATOM	8	HG2	MET	1	24.508	5.912	15.087	1.00	3.19	IL13
ATOM	9	SD	MET	1	24.548	4.261	13.331	1.00	3.84	IL13
ATOM	10	CE	MET	1	24.995	2.795	14.313	1.00	4.23	IL13
ATOM	11	HE1	MET	1	25.990	2.925	14.715	1.00	4.26	IL13
ATOM	12	HE2	MET	1	24.983	1.926	13.676	1.00	4.46	IL13
ATOM	13	HE3	MET	1	24.292	2.647	15.117	1.00	4.75	IL13
ATOM	14	C	MET	1	20.430	6.238	12.922	1.00	1.66	IL13
ATOM	15	O	MET	1	19.289	6.251	13.339	1.00	1.58	IL13
ATOM	16	N	MET	1	21.908	4.310	12.564	1.00	2.43	IL13
ATOM	17	HT1	MET	1	22.629	4.706	11.927	1.00	2.81	IL13
ATOM	18	HT2	MET	1	21.080	4.012	12.009	1.00	2.72	IL13
ATOM	19	HT3	MET	1	22.305	3.489	13.064	1.00	2.88	IL13
ATOM	20	N	GLY	2	20.790	6.979	11.911	1.00	1.55	IL13
ATOM	21	HN	GLY	2	21.714	6.947	11.585	1.00	1.70	IL13
ATOM	22	CA	GLY	2	19.795	7.862	11.244	1.00	1.31	IL13
ATOM	23	HA1	GLY	2	20.300	8.530	10.563	1.00	1.39	IL13
ATOM	24	HA2	GLY	2	19.269	8.435	11.993	1.00	1.36	IL13
ATOM	25	C	GLY	2	18.806	6.993	10.463	1.00	1.04	IL13
ATOM	26	O	GLY	2	18.998	5.801	10.328	1.00	1.02	IL13
ATOM	27	N	PRO	3	17.755	7.578	9.950	1.00	0.95	IL13
ATOM	28	CA	PRO	3	16.747	6.806	9.176	1.00	0.85	IL13
ATOM	29	HA	PRO	3	16.204	6.136	9.821	1.00	0.95	IL13
ATOM	30	CB	PRO	3	15.811	7.900	8.659	1.00	0.98	IL13
ATOM	31	HB1	PRO	3	14.804	7.704	8.996	1.00	1.10	IL13
ATOM	32	HB2	PRO	3	15.835	7.915	7.578	1.00	0.96	IL13
ATOM	33	CG	PRO	3	16.278	9.256	9.205	1.00	1.14	IL13
ATOM	34	HG1	PRO	3	15.487	9.704	9.787	1.00	1.29	IL13
ATOM	35	HG2	PRO	3	16.538	9.907	8.383	1.00	1.28	IL13
ATOM	36	CD	PRO	3	17.505	9.035	10.096	1.00	1.12	IL13
ATOM	37	HD2	PRO	3	18.347	9.613	9.737	1.00	1.24	IL13
ATOM	38	HD1	PRO	3	17.277	9.277	11.121	1.00	1.20	IL13
ATOM	39	C	PRO	3	17.385	6.040	8.014	1.00	0.72	IL13
ATOM	40	O	PRO	3	18.471	6.361	7.573	1.00	0.73	IL13
ATOM	41	N	VAL	4	16.727	5.032	7.512	1.00	0.68	IL13
ATOM	42	HN	VAL	4	15.854	4.782	7.876	1.00	0.75	IL13

Figure 8 (2/30)

ATOM	43	CA	VAL	4	17.314	4.262	6.384	1.00	0.62	IL13
ATOM	44	HA	VAL	4	18.361	4.131	6.574	1.00	0.69	IL13
ATOM	45	CB	VAL	4	16.621	2.893	6.285	1.00	0.70	IL13
ATOM	46	HB	VAL	4	16.900	2.425	5.355	1.00	0.84	IL13
ATOM	47	CG1	VAL	4	17.036	1.978	7.454	1.00	0.89	IL13
ATOM	48	HG11	VAL	4	16.887	0.947	7.167	1.00	1.47	IL13
ATOM	49	HG12	VAL	4	16.435	2.196	8.323	1.00	1.23	IL13
ATOM	50	HG13	VAL	4	18.077	2.131	7.694	1.00	1.44	IL13
ATOM	51	CG2	VAL	4	15.100	3.095	6.308	1.00	0.74	IL13
ATOM	52	HG21	VAL	4	14.792	3.464	7.275	1.00	1.24	IL13
ATOM	53	HG22	VAL	4	14.608	2.154	6.111	1.00	1.31	IL13
ATOM	54	HG23	VAL	4	14.824	3.810	5.550	1.00	1.29	IL13
ATOM	55	C	VAL	4	17.091	5.056	5.073	1.00	0.51	IL13
ATOM	56	O	VAL	4	16.097	5.744	4.949	1.00	0.50	IL13
ATOM	57	N	PRO	5	17.987	4.986	4.095	1.00	0.50	IL13
ATOM	58	CA	PRO	5	17.785	5.755	2.829	1.00	0.47	IL13
ATOM	59	HA	PRO	5	17.860	6.805	3.030	1.00	0.52	IL13
ATOM	60	CB	PRO	5	18.967	5.311	1.966	1.00	0.59	IL13
ATOM	61	HB1	PRO	5	19.546	6.173	1.672	1.00	0.63	IL13
ATOM	62	HB2	PRO	5	18.599	4.803	1.085	1.00	0.68	IL13
ATOM	63	CG	PRO	5	19.849	4.356	2.776	1.00	0.63	IL13
ATOM	64	HG1	PRO	5	20.839	4.775	2.874	1.00	0.70	IL13
ATOM	65	HG2	PRO	5	19.908	3.403	2.274	1.00	0.68	IL13
ATOM	66	CD	PRO	5	19.237	4.172	4.166	1.00	0.60	IL13
ATOM	67	HD2	PRO	5	19.014	3.129	4.352	1.00	0.61	IL13
ATOM	68	HD1	PRO	5	19.902	4.568	4.916	1.00	0.69	IL13
ATOM	69	C	PRO	5	16.460	5.406	2.122	1.00	0.38	IL13
ATOM	70	O	PRO	5	15.864	4.385	2.401	1.00	0.37	IL13
ATOM	71	N	PRO	6	15.999	6.235	1.201	1.00	0.41	IL13
ATOM	72	CA	PRO	6	14.731	5.944	0.473	1.00	0.39	IL13
ATOM	73	HA	PRO	6	13.897	5.931	1.150	1.00	0.41	IL13
ATOM	74	CB	PRO	6	14.603	7.132	-0.481	1.00	0.51	IL13
ATOM	75	HB1	PRO	6	13.721	7.702	-0.235	1.00	0.62	IL13
ATOM	76	HB2	PRO	6	14.531	6.770	-1.497	1.00	0.46	IL13
ATOM	77	CG	PRO	6	15.843	8.021	-0.339	1.00	0.63	IL13
ATOM	78	HG1	PRO	6	15.538	9.037	-0.137	1.00	0.78	IL13
ATOM	79	HG2	PRO	6	16.419	7.989	-1.253	1.00	0.68	IL13
ATOM	80	CD	PRO	6	16.690	7.503	0.825	1.00	0.57	IL13
ATOM	81	HD2	PRO	6	17.707	7.315	0.505	1.00	0.63	IL13
ATOM	82	HD1	PRO	6	16.662	8.205	1.642	1.00	0.64	IL13
ATOM	83	C	PRO	6	14.799	4.640	-0.325	1.00	0.31	IL13
ATOM	84	O	PRO	6	13.898	3.826	-0.285	1.00	0.29	IL13
ATOM	85	N	SER	7	15.858	4.443	-1.060	1.00	0.31	IL13
ATOM	86	HN	SER	7	16.568	5.116	-1.084	1.00	0.36	IL13
ATOM	87	CA	SER	7	15.978	3.199	-1.870	1.00	0.28	IL13
ATOM	88	HA	SER	7	15.138	3.128	-2.545	1.00	0.27	IL13
ATOM	89	CB	SER	7	17.276	3.242	-2.681	1.00	0.32	IL13
ATOM	90	HB1	SER	7	17.337	4.183	-3.212	1.00	0.35	IL13
ATOM	91	HB2	SER	7	17.285	2.431	-3.391	1.00	0.33	IL13
ATOM	92	OG	SER	7	18.384	3.106	-1.801	1.00	0.36	IL13
ATOM	93	HG	SER	7	18.070	3.240	-0.904	1.00	0.98	IL13
ATOM	94	C	SER	7	15.995	1.980	-0.948	1.00	0.26	IL13
ATOM	95	O	SER	7	15.399	0.967	-1.241	1.00	0.25	IL13
ATOM	96	N	THR	8	16.667	2.067	0.166	1.00	0.28	IL13
ATOM	97	HN	THR	8	17.141	2.895	0.391	1.00	0.31	IL13
ATOM	98	CA	THR	8	16.710	0.901	1.097	1.00	0.29	IL13
ATOM	99	HA	THR	8	16.998	0.016	0.548	1.00	0.31	IL13
ATOM	100	CB	THR	8	17.736	1.167	2.199	1.00	0.35	IL13
ATOM	101	HB	THR	8	17.465	2.068	2.730	1.00	0.35	IL13
ATOM	102	OG1	THR	8	19.018	1.332	1.614	1.00	0.40	IL13
ATOM	103	HG1	THR	8	19.007	0.911	0.751	1.00	0.90	IL13

Figure 8 (3/30)

ATOM	104	CG2	THR	8	17.763	-0.007	3.180	1.00	0.38	IL13
ATOM	105	HG21	THR	8	17.180	-0.824	2.782	1.00	1.07	IL13
ATOM	106	HG22	THR	8	17.346	0.306	4.126	1.00	1.15	IL13
ATOM	107	HG23	THR	8	18.783	-0.330	3.326	1.00	1.03	IL13
ATOM	108	C	THR	8	15.332	0.681	1.720	1.00	0.26	IL13
ATOM	109	O	THR	8	14.870	-0.434	1.849	1.00	0.27	IL13
ATOM	110	N	ALA	9	14.669	1.733	2.106	1.00	0.25	IL13
ATOM	111	HN	ALA	9	15.056	2.624	1.994	1.00	0.26	IL13
ATOM	112	CA	ALA	9	13.324	1.577	2.718	1.00	0.26	IL13
ATOM	113	HA	ALA	9	13.398	0.973	3.609	1.00	0.29	IL13
ATOM	114	CB	ALA	9	12.764	2.954	3.077	1.00	0.29	IL13
ATOM	115	HB1	ALA	9	12.549	3.502	2.172	1.00	0.97	IL13
ATOM	116	HB2	ALA	9	13.491	3.497	3.659	1.00	1.09	IL13
ATOM	117	HB3	ALA	9	11.857	2.837	3.651	1.00	1.09	IL13
ATOM	118	C	ALA	9	12.391	0.900	1.718	1.00	0.24	IL13
ATOM	119	O	ALA	9	11.593	0.055	2.071	1.00	0.26	IL13
ATOM	120	N	LEU	10	12.470	1.277	0.472	1.00	0.22	IL13
ATOM	121	HN	LEU	10	13.111	1.970	0.206	1.00	0.22	IL13
ATOM	122	CA	LEU	10	11.572	0.663	-0.540	1.00	0.22	IL13
ATOM	123	HA	LEU	10	10.556	0.808	-0.210	1.00	0.23	IL13
ATOM	124	CB	LEU	10	11.765	1.357	-1.898	1.00	0.22	IL13
ATOM	125	HB1	LEU	10	12.813	1.307	-2.191	1.00	0.23	IL13
ATOM	126	HB2	LEU	10	11.470	2.393	-1.813	1.00	0.29	IL13
ATOM	127	CG	LEU	10	10.908	0.674	-2.977	1.00	0.33	IL13
ATOM	128	HG	LEU	10	11.262	-0.330	-3.134	1.00	0.78	IL13
ATOM	129	CD1	LEU	10	9.435	0.641	-2.559	1.00	0.48	IL13
ATOM	130	HD11	LEU	10	8.827	0.475	-3.426	1.00	1.16	IL13
ATOM	131	HD12	LEU	10	9.164	1.582	-2.104	1.00	1.04	IL13
ATOM	132	HD13	LEU	10	9.272	-0.162	-1.858	1.00	1.13	IL13
ATOM	133	CD2	LEU	10	11.055	1.464	-4.277	1.00	0.82	IL13
ATOM	134	HD21	LEU	10	10.140	1.985	-4.515	1.00	1.40	IL13
ATOM	135	HD22	LEU	10	11.308	0.793	-5.080	1.00	1.41	IL13
ATOM	136	HD23	LEU	10	11.835	2.175	-4.147	1.00	1.37	IL13
ATOM	137	C	LEU	10	11.850	-0.841	-0.669	1.00	0.21	IL13
ATOM	138	O	LEU	10	10.943	-1.650	-0.638	1.00	0.23	IL13
ATOM	139	N	ARG	11	13.089	-1.225	-0.833	1.00	0.23	IL13
ATOM	140	HN	ARG	11	13.808	-0.561	-0.870	1.00	0.23	IL13
ATOM	141	CA	ARG	11	13.403	-2.678	-0.985	1.00	0.25	IL13
ATOM	142	HA	ARG	11	12.905	-3.074	-1.857	1.00	0.26	IL13
ATOM	143	CB	ARG	11	14.912	-2.861	-1.124	1.00	0.29	IL13
ATOM	144	HB1	ARG	11	15.135	-3.910	-1.256	1.00	0.32	IL13
ATOM	145	HB2	ARG	11	15.391	-2.502	-0.227	1.00	0.30	IL13
ATOM	146	CG	ARG	11	15.412	-2.078	-2.342	1.00	0.33	IL13
ATOM	147	HG1	ARG	11	15.013	-1.079	-2.314	1.00	0.68	IL13
ATOM	148	HG2	ARG	11	15.075	-2.570	-3.244	1.00	0.76	IL13
ATOM	149	CD	ARG	11	16.947	-2.016	-2.342	1.00	0.95	IL13
ATOM	150	HD1	ARG	11	17.313	-1.869	-1.337	1.00	1.64	IL13
ATOM	151	HD2	ARG	11	17.272	-1.195	-2.955	1.00	1.65	IL13
ATOM	152	NE	ARG	11	17.494	-3.285	-2.896	1.00	1.53	IL13
ATOM	153	HE	ARG	11	16.904	-4.056	-3.034	1.00	2.05	IL13
ATOM	154	CZ	ARG	11	18.753	-3.358	-3.225	1.00	2.18	IL13
ATOM	155	NH1	ARG	11	19.228	-4.449	-3.760	1.00	3.10	IL13
ATOM	156	HH11	ARG	11	18.625	-5.230	-3.919	1.00	3.51	IL13
ATOM	157	HH12	ARG	11	20.194	-4.503	-4.012	1.00	3.62	IL13
ATOM	158	NH2	ARG	11	19.542	-2.340	-3.008	1.00	2.48	IL13
ATOM	159	HH21	ARG	11	19.179	-1.507	-2.589	1.00	2.43	IL13
ATOM	160	HH22	ARG	11	20.508	-2.394	-3.257	1.00	3.15	IL13
ATOM	161	C	ARG	11	12.938	-3.421	0.259	1.00	0.25	IL13
ATOM	162	O	ARG	11	12.333	-4.472	0.182	1.00	0.27	IL13
ATOM	163	N	GLU	12	13.207	-2.876	1.410	1.00	0.25	IL13
ATOM	164	HN	GLU	12	13.689	-2.024	1.452	1.00	0.24	IL13

Figure 8 (4/30)

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ATOM    165  CA  GLU    12      12.767  -3.546   2.657  1.00  0.28      IL13
ATOM    166  HA  GLU    12      13.195  -4.538   2.698  1.00  0.30      IL13
ATOM    167  CB  GLU    12      13.220  -2.734   3.879  1.00  0.30      IL13
ATOM    168  HB1 GLU    12      12.729  -3.108   4.764  1.00  0.33      IL13
ATOM    169  HB2 GLU    12      12.960  -1.693   3.734  1.00  0.29      IL13
ATOM    170  CG  GLU    12      14.742  -2.854   4.052  1.00  0.34      IL13
ATOM    171  HG1 GLU    12      15.237  -2.259   3.299  1.00  0.83      IL13
ATOM    172  HG2 GLU    12      15.044  -3.886   3.950  1.00  0.89      IL13
ATOM    173  CD  GLU    12      15.143  -2.345   5.438  1.00  1.14      IL13
ATOM    174  OE1 GLU    12      14.373  -1.600   6.021  1.00  1.92      IL13
ATOM    175  OE2 GLU    12      16.208  -2.722   5.900  1.00  1.81      IL13
ATOM    176  C   GLU    12      11.245  -3.665   2.620  1.00  0.26      IL13
ATOM    177  O   GLU    12      10.679  -4.652   3.044  1.00  0.29      IL13
ATOM    178  N   LEU    13      10.577  -2.669   2.104  1.00  0.23      IL13
ATOM    179  HN  LEU    13      11.054  -1.885   1.758  1.00  0.22      IL13
ATOM    180  CA  LEU    13       9.092  -2.734   2.025  1.00  0.24      IL13
ATOM    181  HA  LEU    13       8.702  -3.011   2.992  1.00  0.27      IL13
ATOM    182  CB  LEU    13       8.549  -1.350   1.626  1.00  0.24      IL13
ATOM    183  HB1 LEU    13       9.008  -1.045   0.698  1.00  0.22      IL13
ATOM    184  HB2 LEU    13       8.802  -0.637   2.398  1.00  0.26      IL13
ATOM    185  CG  LEU    13       7.020  -1.380   1.450  1.00  0.27      IL13
ATOM    186  HG  LEU    13       6.753  -2.089   0.682  1.00  0.26      IL13
ATOM    187  CD1 LEU    13       6.337  -1.769   2.764  1.00  0.32      IL13
ATOM    188 HD11 LEU    13       5.302  -1.460   2.733  1.00  1.06      IL13
ATOM    189 HD12 LEU    13       6.832  -1.278   3.585  1.00  1.07      IL13
ATOM    190 HD13 LEU    13       6.385  -2.837   2.899  1.00  1.01      IL13
ATOM    191  CD2 LEU    13       6.537   0.012   1.036  1.00  0.31      IL13
ATOM    192 HD21 LEU    13       7.224   0.433   0.317  1.00  1.08      IL13
ATOM    193 HD22 LEU    13       6.491   0.650   1.906  1.00  1.03      IL13
ATOM    194 HD23 LEU    13       5.555  -0.065   0.593  1.00  1.07      IL13
ATOM    195  C   LEU    13       8.681  -3.789   0.983  1.00  0.22      IL13
ATOM    196  O   LEU    13       7.834  -4.621   1.239  1.00  0.23      IL13
ATOM    197  N   ILE    14       9.270  -3.765  -0.192  1.00  0.21      IL13
ATOM    198  HN  ILE    14       9.951  -3.089  -0.387  1.00  0.21      IL13
ATOM    199  CA  ILE    14       8.892  -4.776  -1.231  1.00  0.21      IL13
ATOM    200  HA  ILE    14       7.834  -4.688  -1.438  1.00  0.22      IL13
ATOM    201  CB  ILE    14       9.687  -4.543  -2.537  1.00  0.21      IL13
ATOM    202  HB  ILE    14      10.744  -4.523  -2.311  1.00  0.21      IL13
ATOM    203  CG1 ILE    14       9.269  -3.193  -3.152  1.00  0.23      IL13
ATOM    204 HG11 ILE    14       9.229  -2.449  -2.371  1.00  0.23      IL13
ATOM    205 HG12 ILE    14       8.291  -3.287  -3.600  1.00  0.23      IL13
ATOM    206  CG2 ILE    14       9.404  -5.688  -3.545  1.00  0.23      IL13
ATOM    207 HG21 ILE    14       8.615  -6.325  -3.180  1.00  1.06      IL13
ATOM    208 HG22 ILE    14      10.300  -6.273  -3.682  1.00  1.01      IL13
ATOM    209 HG23 ILE    14       9.102  -5.281  -4.494  1.00  1.03      IL13
ATOM    210  CD1 ILE    14      10.283  -2.743  -4.220  1.00  0.25      IL13
ATOM    211 HD11 ILE    14      10.050  -1.737  -4.529  1.00  1.05      IL13
ATOM    212 HD12 ILE    14      10.236  -3.389  -5.081  1.00  0.97      IL13
ATOM    213 HD13 ILE    14      11.279  -2.770  -3.806  1.00  1.12      IL13
ATOM    214  C   ILE    14       9.181  -6.183  -0.700  1.00  0.21      IL13
ATOM    215  O   ILE    14       8.358  -7.069  -0.803  1.00  0.22      IL13
ATOM    216  N   GLU    15      10.341  -6.411  -0.161  1.00  0.23      IL13
ATOM    217  HN  GLU    15      11.009  -5.697  -0.100  1.00  0.23      IL13
ATOM    218  CA  GLU    15      10.655  -7.780   0.326  1.00  0.25      IL13
ATOM    219  HA  GLU    15      10.594  -8.475  -0.497  1.00  0.26      IL13
ATOM    220  CB  GLU    15      12.066  -7.811   0.918  1.00  0.28      IL13
ATOM    221  HB1 GLU    15      12.231  -8.762   1.401  1.00  0.30      IL13
ATOM    222  HB2 GLU    15      12.170  -7.016   1.642  1.00  0.29      IL13
ATOM    223  CG  GLU    15      13.096  -7.625  -0.199  1.00  0.31      IL13
ATOM    224  HG1 GLU    15      13.058  -6.606  -0.555  1.00  0.85      IL13
ATOM    225  HG2 GLU    15      12.875  -8.300  -1.012  1.00  0.84      IL13
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Figure 8 (5/30)

ATOM	226	CD	GLU	15	14.495	-7.917	0.345	1.00	1.10	IL13
ATOM	227	OE1	GLU	15	14.911	-9.061	0.265	1.00	1.78	IL13
ATOM	228	OE2	GLU	15	15.126	-6.994	0.833	1.00	1.90	IL13
ATOM	229	C	GLU	15	9.649	-8.181	1.400	1.00	0.24	IL13
ATOM	230	O	GLU	15	9.203	-9.310	1.451	1.00	0.26	IL13
ATOM	231	N	GLU	16	9.286	-7.276	2.264	1.00	0.24	IL13
ATOM	232	HN	GLU	16	9.653	-6.369	2.214	1.00	0.24	IL13
ATOM	233	CA	GLU	16	8.312	-7.637	3.325	1.00	0.26	IL13
ATOM	234	HA	GLU	16	8.636	-8.552	3.798	1.00	0.28	IL13
ATOM	235	CB	GLU	16	8.249	-6.529	4.376	1.00	0.27	IL13
ATOM	236	HB1	GLU	16	7.912	-5.613	3.914	1.00	0.27	IL13
ATOM	237	HB2	GLU	16	9.229	-6.381	4.803	1.00	0.29	IL13
ATOM	238	CG	GLU	16	7.264	-6.937	5.474	1.00	0.32	IL13
ATOM	239	HG1	GLU	16	7.396	-7.983	5.708	1.00	0.84	IL13
ATOM	240	HG2	GLU	16	6.253	-6.770	5.129	1.00	0.80	IL13
ATOM	241	CD	GLU	16	7.517	-6.100	6.729	1.00	0.91	IL13
ATOM	242	OE1	GLU	16	6.858	-6.348	7.725	1.00	1.56	IL13
ATOM	243	OE2	GLU	16	8.370	-5.229	6.674	1.00	1.68	IL13
ATOM	244	C	GLU	16	6.922	-7.858	2.721	1.00	0.24	IL13
ATOM	245	O	GLU	16	6.259	-8.814	3.050	1.00	0.25	IL13
ATOM	246	N	LEU	17	6.473	-6.992	1.842	1.00	0.23	IL13
ATOM	247	HN	LEU	17	7.022	-6.223	1.582	1.00	0.23	IL13
ATOM	248	CA	LEU	17	5.113	-7.183	1.242	1.00	0.24	IL13
ATOM	249	HA	LEU	17	4.380	-7.173	2.027	1.00	0.25	IL13
ATOM	250	CB	LEU	17	4.806	-6.058	0.243	1.00	0.25	IL13
ATOM	251	HB1	LEU	17	3.920	-6.309	-0.322	1.00	0.27	IL13
ATOM	252	HB2	LEU	17	5.639	-5.955	-0.437	1.00	0.24	IL13
ATOM	253	CG	LEU	17	4.590	-4.727	0.975	1.00	0.27	IL13
ATOM	254	HG	LEU	17	5.405	-4.562	1.662	1.00	0.26	IL13
ATOM	255	CD1	LEU	17	4.550	-3.594	-0.051	1.00	0.30	IL13
ATOM	256	HD11	LEU	17	5.446	-3.620	-0.652	1.00	1.03	IL13
ATOM	257	HD12	LEU	17	4.487	-2.646	0.463	1.00	1.09	IL13
ATOM	258	HD13	LEU	17	3.685	-3.716	-0.687	1.00	1.06	IL13
ATOM	259	CD2	LEU	17	3.257	-4.733	1.744	1.00	0.32	IL13
ATOM	260	HD21	LEU	17	2.666	-3.884	1.432	1.00	1.11	IL13
ATOM	261	HD22	LEU	17	3.453	-4.660	2.803	1.00	0.95	IL13
ATOM	262	HD23	LEU	17	2.709	-5.640	1.542	1.00	1.12	IL13
ATOM	263	C	LEU	17	5.048	-8.518	0.503	1.00	0.23	IL13
ATOM	264	O	LEU	17	4.103	-9.269	0.639	1.00	0.25	IL13
ATOM	265	N	VAL	18	6.039	-8.815	-0.285	1.00	0.23	IL13
ATOM	266	HN	VAL	18	6.789	-8.193	-0.386	1.00	0.23	IL13
ATOM	267	CA	VAL	18	6.028	-10.095	-1.040	1.00	0.26	IL13
ATOM	268	HA	VAL	18	5.160	-10.130	-1.679	1.00	0.27	IL13
ATOM	269	CB	VAL	18	7.299	-10.177	-1.899	1.00	0.28	IL13
ATOM	270	HB	VAL	18	8.163	-9.982	-1.280	1.00	0.29	IL13
ATOM	271	CG1	VAL	18	7.430	-11.566	-2.531	1.00	0.32	IL13
ATOM	272	HG11	VAL	18	7.639	-12.300	-1.767	1.00	1.07	IL13
ATOM	273	HG12	VAL	18	8.239	-11.557	-3.248	1.00	1.07	IL13
ATOM	274	HG13	VAL	18	6.510	-11.817	-3.035	1.00	1.05	IL13
ATOM	275	CG2	VAL	18	7.223	-9.130	-3.011	1.00	0.29	IL13
ATOM	276	HG21	VAL	18	6.301	-9.254	-3.556	1.00	1.10	IL13
ATOM	277	HG22	VAL	18	8.058	-9.257	-3.684	1.00	1.02	IL13
ATOM	278	HG23	VAL	18	7.255	-8.142	-2.580	1.00	0.97	IL13
ATOM	279	C	VAL	18	5.987	-11.266	-0.051	1.00	0.26	IL13
ATOM	280	O	VAL	18	5.189	-12.170	-0.173	1.00	0.28	IL13
ATOM	281	N	ASN	19	6.852	-11.253	0.919	1.00	0.26	IL13
ATOM	282	HN	ASN	19	7.491	-10.513	0.989	1.00	0.26	IL13
ATOM	283	CA	ASN	19	6.904	-12.367	1.910	1.00	0.29	IL13
ATOM	284	HA	ASN	19	7.282	-13.254	1.427	1.00	0.32	IL13
ATOM	285	CB	ASN	19	7.853	-11.966	3.043	1.00	0.31	IL13
ATOM	286	HB1	ASN	19	7.290	-11.468	3.818	1.00	0.77	IL13

Figure 8 (6/30)

ATOM	287	HB2	ASN	19	8.605	-11.292	2.659	1.00	0.94	IL13
ATOM	288	CG	ASN	19	8.533	-13.205	3.631	1.00	1.16	IL13
ATOM	289	OD1	ASN	19	8.177	-14.323	3.316	1.00	1.93	IL13
ATOM	290	ND2	ASN	19	9.512	-13.048	4.480	1.00	1.89	IL13
ATOM	291	HD21	ASN	19	9.802	-12.146	4.733	1.00	2.20	IL13
ATOM	292	HD22	ASN	19	9.960	-13.831	4.862	1.00	2.51	IL13
ATOM	293	C	ASN	19	5.516	-12.659	2.499	1.00	0.29	IL13
ATOM	294	O	ASN	19	5.104	-13.798	2.587	1.00	0.32	IL13
ATOM	295	N	ILE	20	4.803	-11.655	2.932	1.00	0.28	IL13
ATOM	296	HN	ILE	20	5.155	-10.742	2.879	1.00	0.27	IL13
ATOM	297	CA	ILE	20	3.465	-11.910	3.545	1.00	0.29	IL13
ATOM	298	HA	ILE	20	3.555	-12.753	4.215	1.00	0.33	IL13
ATOM	299	CB	ILE	20	3.027	-10.686	4.366	1.00	0.32	IL13
ATOM	300	HB	ILE	20	2.050	-10.872	4.790	1.00	0.37	IL13
ATOM	301	CG1	ILE	20	2.973	-9.430	3.470	1.00	0.29	IL13
ATOM	302	HG11	ILE	20	2.522	-9.675	2.524	1.00	0.30	IL13
ATOM	303	HG12	ILE	20	3.966	-9.073	3.299	1.00	0.30	IL13
ATOM	304	CG2	ILE	20	4.042	-10.490	5.505	1.00	0.39	IL13
ATOM	305	HG21	ILE	20	4.363	-9.462	5.552	1.00	1.08	IL13
ATOM	306	HG22	ILE	20	4.900	-11.120	5.328	1.00	1.12	IL13
ATOM	307	HG23	ILE	20	3.584	-10.767	6.443	1.00	1.01	IL13
ATOM	308	CD1	ILE	20	2.143	-8.326	4.143	1.00	0.40	IL13
ATOM	309	HD11	ILE	20	2.116	-7.459	3.499	1.00	1.03	IL13
ATOM	310	HD12	ILE	20	2.584	-8.055	5.088	1.00	1.16	IL13
ATOM	311	HD13	ILE	20	1.137	-8.681	4.305	1.00	1.10	IL13
ATOM	312	C	ILE	20	2.412	-12.253	2.482	1.00	0.26	IL13
ATOM	313	O	ILE	20	1.337	-12.709	2.813	1.00	0.28	IL13
ATOM	314	N	THR	21	2.701	-12.031	1.219	1.00	0.24	IL13
ATOM	315	HN	THR	21	3.572	-11.654	0.975	1.00	0.24	IL13
ATOM	316	CA	THR	21	1.693	-12.340	0.151	1.00	0.25	IL13
ATOM	317	HA	THR	21	0.715	-12.425	0.593	1.00	0.27	IL13
ATOM	318	CB	THR	21	1.668	-11.203	-0.876	1.00	0.27	IL13
ATOM	319	HB	THR	21	1.036	-11.482	-1.706	1.00	0.30	IL13
ATOM	320	OG1	THR	21	2.984	-10.956	-1.346	1.00	0.28	IL13
ATOM	321	HG1	THR	21	3.160	-10.016	-1.254	1.00	0.90	IL13
ATOM	322	CG2	THR	21	1.105	-9.936	-0.229	1.00	0.29	IL13
ATOM	323	HG21	THR	21	1.795	-9.118	-0.377	1.00	1.02	IL13
ATOM	324	HG22	THR	21	0.965	-10.103	0.828	1.00	1.02	IL13
ATOM	325	HG23	THR	21	0.156	-9.692	-0.682	1.00	1.05	IL13
ATOM	326	C	THR	21	2.031	-13.661	-0.558	1.00	0.27	IL13
ATOM	327	O	THR	21	1.216	-14.199	-1.281	1.00	0.36	IL13
ATOM	328	N	GLN	22	3.211	-14.196	-0.373	1.00	0.27	IL13
ATOM	329	HN	GLN	22	3.868	-13.760	0.210	1.00	0.28	IL13
ATOM	330	CA	GLN	22	3.544	-15.483	-1.062	1.00	0.31	IL13
ATOM	331	HA	GLN	22	3.044	-15.508	-2.016	1.00	0.33	IL13
ATOM	332	CB	GLN	22	5.059	-15.619	-1.275	1.00	0.36	IL13
ATOM	333	HB1	GLN	22	5.284	-16.623	-1.603	1.00	0.41	IL13
ATOM	334	HB2	GLN	22	5.567	-15.428	-0.340	1.00	0.35	IL13
ATOM	335	CG	GLN	22	5.551	-14.621	-2.330	1.00	0.38	IL13
ATOM	336	HG1	GLN	22	5.733	-13.675	-1.862	1.00	0.88	IL13
ATOM	337	HG2	GLN	22	4.812	-14.501	-3.107	1.00	0.90	IL13
ATOM	338	CD	GLN	22	6.854	-15.129	-2.946	1.00	1.16	IL13
ATOM	339	OE1	GLN	22	7.597	-15.856	-2.317	1.00	1.92	IL13
ATOM	340	NE2	GLN	22	7.162	-14.774	-4.163	1.00	1.95	IL13
ATOM	341	HE21	GLN	22	6.560	-14.187	-4.668	1.00	2.31	IL13
ATOM	342	HE22	GLN	22	7.992	-15.094	-4.573	1.00	2.56	IL13
ATOM	343	C	GLN	22	3.060	-16.676	-0.236	1.00	0.33	IL13
ATOM	344	O	GLN	22	2.587	-17.655	-0.778	1.00	0.38	IL13
ATOM	345	N	ASN	23	3.195	-16.618	1.064	1.00	0.36	IL13
ATOM	346	HN	ASN	23	3.595	-15.828	1.480	1.00	0.38	IL13
ATOM	347	CA	ASN	23	2.763	-17.773	1.905	1.00	0.43	IL13

Figure 8 (7/30)

ATOM	348	HA	ASN	23	2.794	-18.678	1.316	1.00	0.46	IL13
ATOM	349	CB	ASN	23	3.685	-17.939	3.124	1.00	0.56	IL13
ATOM	350	HB1	ASN	23	3.807	-18.993	3.331	1.00	1.17	IL13
ATOM	351	HB2	ASN	23	3.232	-17.462	3.980	1.00	1.10	IL13
ATOM	352	CG	ASN	23	5.064	-17.317	2.870	1.00	1.45	IL13
ATOM	353	OD1	ASN	23	5.447	-17.067	1.744	1.00	2.30	IL13
ATOM	354	ND2	ASN	23	5.842	-17.073	3.890	1.00	2.11	IL13
ATOM	355	HD21	ASN	23	5.542	-17.289	4.798	1.00	2.24	IL13
ATOM	356	HD22	ASN	23	6.725	-16.672	3.749	1.00	2.87	IL13
ATOM	357	C	ASN	23	1.335	-17.550	2.400	1.00	0.42	IL13
ATOM	358	O	ASN	23	0.854	-18.264	3.257	1.00	0.53	IL13
ATOM	359	N	GLN	24	0.643	-16.576	1.874	1.00	0.37	IL13
ATOM	360	HN	GLN	24	1.033	-16.006	1.180	1.00	0.37	IL13
ATOM	361	CA	GLN	24	-0.751	-16.352	2.342	1.00	0.40	IL13
ATOM	362	HA	GLN	24	-0.802	-16.540	3.405	1.00	0.47	IL13
ATOM	363	CB	GLN	24	-1.186	-14.900	2.059	1.00	0.36	IL13
ATOM	364	HB1	GLN	24	-0.361	-14.237	2.268	1.00	0.38	IL13
ATOM	365	HB2	GLN	24	-2.016	-14.646	2.701	1.00	0.39	IL13
ATOM	366	CG	GLN	24	-1.611	-14.723	0.592	1.00	0.44	IL13
ATOM	367	HG1	GLN	24	-2.551	-15.225	0.418	1.00	0.71	IL13
ATOM	368	HG2	GLN	24	-0.854	-15.133	-0.059	1.00	0.92	IL13
ATOM	369	CD	GLN	24	-1.793	-13.232	0.296	1.00	1.19	IL13
ATOM	370	OE1	GLN	24	-1.568	-12.398	1.151	1.00	1.80	IL13
ATOM	371	NE2	GLN	24	-2.201	-12.859	-0.886	1.00	1.81	IL13
ATOM	372	HE21	GLN	24	-2.389	-13.532	-1.574	1.00	2.00	IL13
ATOM	373	HE22	GLN	24	-2.321	-11.907	-1.086	1.00	2.37	IL13
ATOM	374	C	GLN	24	-1.671	-17.329	1.615	1.00	0.52	IL13
ATOM	375	O	GLN	24	-1.666	-17.415	0.403	1.00	0.59	IL13
ATOM	376	N	LYS	25	-2.470	-18.055	2.339	1.00	0.65	IL13
ATOM	377	HN	LYS	25	-2.468	-17.966	3.315	1.00	0.67	IL13
ATOM	378	CA	LYS	25	-3.398	-19.012	1.679	1.00	0.84	IL13
ATOM	379	HA	LYS	25	-2.949	-19.389	0.772	1.00	0.87	IL13
ATOM	380	CB	LYS	25	-3.693	-20.172	2.635	1.00	1.01	IL13
ATOM	381	HB1	LYS	25	-4.143	-19.787	3.538	1.00	1.03	IL13
ATOM	382	HB2	LYS	25	-2.771	-20.678	2.881	1.00	1.00	IL13
ATOM	383	CG	LYS	25	-4.655	-21.159	1.971	1.00	1.23	IL13
ATOM	384	HG1	LYS	25	-4.233	-21.502	1.039	1.00	1.36	IL13
ATOM	385	HG2	LYS	25	-5.600	-20.671	1.780	1.00	1.32	IL13
ATOM	386	CD	LYS	25	-4.880	-22.356	2.896	1.00	1.64	IL13
ATOM	387	HD1	LYS	25	-5.123	-22.004	3.888	1.00	1.95	IL13
ATOM	388	HD2	LYS	25	-3.981	-22.954	2.935	1.00	1.94	IL13
ATOM	389	CE	LYS	25	-6.036	-23.202	2.360	1.00	2.05	IL13
ATOM	390	HE1	LYS	25	-6.288	-22.877	1.362	1.00	2.39	IL13
ATOM	391	HE2	LYS	25	-6.895	-23.085	3.004	1.00	2.56	IL13
ATOM	392	NZ	LYS	25	-5.632	-24.635	2.329	1.00	2.46	IL13
ATOM	393	HZ1	LYS	25	-6.012	-25.084	1.472	1.00	2.79	IL13
ATOM	394	HZ2	LYS	25	-6.008	-25.119	3.170	1.00	2.81	IL13
ATOM	395	HZ3	LYS	25	-4.595	-24.704	2.323	1.00	2.82	IL13
ATOM	396	C	LYS	25	-4.690	-18.269	1.349	1.00	0.87	IL13
ATOM	397	O	LYS	25	-4.904	-17.834	0.235	1.00	0.96	IL13
ATOM	398	N	ALA	26	-5.539	-18.103	2.320	1.00	0.92	IL13
ATOM	399	HN	ALA	26	-5.331	-18.449	3.212	1.00	1.00	IL13
ATOM	400	CA	ALA	26	-6.809	-17.365	2.090	1.00	0.95	IL13
ATOM	401	HA	ALA	26	-7.214	-17.632	1.125	1.00	1.08	IL13
ATOM	402	CB	ALA	26	-7.798	-17.741	3.195	1.00	1.11	IL13
ATOM	403	HB1	ALA	26	-8.008	-16.873	3.802	1.00	1.63	IL13
ATOM	404	HB2	ALA	26	-7.366	-18.515	3.813	1.00	1.48	IL13
ATOM	405	HB3	ALA	26	-8.713	-18.105	2.752	1.00	1.49	IL13
ATOM	406	C	ALA	26	-6.500	-15.862	2.134	1.00	0.70	IL13
ATOM	407	O	ALA	26	-5.406	-15.476	2.496	1.00	0.55	IL13
ATOM	408	N	PRO	27	-7.428	-15.006	1.771	1.00	0.71	IL13

Figure 8 (8/30)

ATOM	409	CA	PRO	27	-7.152	-13.545	1.800	1.00	0.56	IL13
ATOM	410	HA	PRO	27	-6.406	-13.286	1.067	1.00	0.61	IL13
ATOM	411	CB	PRO	27	-8.497	-12.936	1.403	1.00	0.65	IL13
ATOM	412	HB1	PRO	27	-8.366	-12.292	0.546	1.00	0.74	IL13
ATOM	413	HB2	PRO	27	-8.894	-12.364	2.230	1.00	0.57	IL13
ATOM	414	CG	PRO	27	-9.469	-14.068	1.045	1.00	0.88	IL13
ATOM	415	HG1	PRO	27	-9.731	-14.004	0.000	1.00	1.02	IL13
ATOM	416	HG2	PRO	27	-10.361	-13.982	1.649	1.00	0.93	IL13
ATOM	417	CD	PRO	27	-8.788	-15.413	1.319	1.00	0.93	IL13
ATOM	418	HD2	PRO	27	-9.318	-15.943	2.096	1.00	1.03	IL13
ATOM	419	HD1	PRO	27	-8.728	-16.001	0.418	1.00	1.07	IL13
ATOM	420	C	PRO	27	-6.725	-13.075	3.193	1.00	0.41	IL13
ATOM	421	O	PRO	27	-7.151	-13.612	4.196	1.00	0.54	IL13
ATOM	422	N	LEU	28	-5.882	-12.081	3.266	1.00	0.39	IL13
ATOM	423	HN	LEU	28	-5.543	-11.662	2.448	1.00	0.49	IL13
ATOM	424	CA	LEU	28	-5.429	-11.593	4.599	1.00	0.50	IL13
ATOM	425	HA	LEU	28	-4.926	-12.383	5.130	1.00	0.61	IL13
ATOM	426	CB	LEU	28	-4.476	-10.414	4.396	1.00	0.72	IL13
ATOM	427	HB1	LEU	28	-4.222	-9.984	5.353	1.00	0.86	IL13
ATOM	428	HB2	LEU	28	-4.968	-9.666	3.791	1.00	0.75	IL13
ATOM	429	CG	LEU	28	-3.202	-10.883	3.682	1.00	0.81	IL13
ATOM	430	HG	LEU	28	-3.490	-11.410	2.781	1.00	0.71	IL13
ATOM	431	CD1	LEU	28	-2.393	-9.627	3.277	1.00	1.06	IL13
ATOM	432	HD11	LEU	28	-1.335	-9.769	3.414	1.00	1.56	IL13
ATOM	433	HD12	LEU	28	-2.718	-8.789	3.873	1.00	1.35	IL13
ATOM	434	HD13	LEU	28	-2.587	-9.411	2.236	1.00	1.60	IL13
ATOM	435	CD2	LEU	28	-2.411	-11.856	4.610	1.00	0.91	IL13
ATOM	436	HD21	LEU	28	-2.728	-11.728	5.633	1.00	1.30	IL13
ATOM	437	HD22	LEU	28	-1.349	-11.689	4.547	1.00	1.42	IL13
ATOM	438	HD23	LEU	28	-2.619	-12.871	4.306	1.00	1.37	IL13
ATOM	439	C	LEU	28	-6.645	-11.120	5.394	1.00	0.43	IL13
ATOM	440	O	LEU	28	-6.866	-11.527	6.518	1.00	0.76	IL13
ATOM	441	N	CYS	29	-7.444	-10.276	4.806	1.00	0.39	IL13
ATOM	442	HN	CYS	29	-7.247	-9.974	3.896	1.00	0.65	IL13
ATOM	443	CA	CYS	29	-8.660	-9.781	5.507	1.00	0.40	IL13
ATOM	444	HA	CYS	29	-8.480	-9.757	6.572	1.00	0.51	IL13
ATOM	445	HB1	CYS	29	-9.954	-8.073	5.421	1.00	0.46	IL13
ATOM	446	HB2	CYS	29	-9.058	-8.377	3.933	1.00	0.40	IL13
ATOM	447	C	CYS	29	-9.822	-10.725	5.203	1.00	0.36	IL13
ATOM	448	O	CYS	29	-9.732	-11.569	4.333	1.00	0.36	IL13
ATOM	449	CB	CYS	29	-9.002	-8.375	5.012	1.00	0.40	IL13
ATOM	450	SG	CYS	29	-7.721	-7.214	5.546	1.00	0.47	IL13
ATOM	451	N	ASN	30	-10.914	-10.592	5.902	1.00	0.37	IL13
ATOM	452	HN	ASN	30	-10.974	-9.904	6.597	1.00	0.39	IL13
ATOM	453	CA	ASN	30	-12.072	-11.488	5.632	1.00	0.38	IL13
ATOM	454	HA	ASN	30	-11.742	-12.516	5.633	1.00	0.44	IL13
ATOM	455	CB	ASN	30	-13.140	-11.291	6.709	1.00	0.42	IL13
ATOM	456	HB1	ASN	30	-14.037	-11.820	6.427	1.00	0.86	IL13
ATOM	457	HB2	ASN	30	-13.359	-10.238	6.809	1.00	1.00	IL13
ATOM	458	CG	ASN	30	-12.627	-11.836	8.042	1.00	1.37	IL13
ATOM	459	OD1	ASN	30	-11.499	-12.279	8.137	1.00	2.17	IL13
ATOM	460	ND2	ASN	30	-13.417	-11.832	9.080	1.00	2.11	IL13
ATOM	461	HD21	ASN	30	-14.329	-11.482	9.000	1.00	2.37	IL13
ATOM	462	HD22	ASN	30	-13.098	-12.179	9.939	1.00	2.78	IL13
ATOM	463	C	ASN	30	-12.662	-11.142	4.265	1.00	0.32	IL13
ATOM	464	O	ASN	30	-13.838	-10.863	4.139	1.00	0.36	IL13
ATOM	465	N	GLY	31	-11.856	-11.151	3.241	1.00	0.31	IL13
ATOM	466	HN	GLY	31	-10.909	-11.373	3.362	1.00	0.38	IL13
ATOM	467	CA	GLY	31	-12.375	-10.815	1.887	1.00	0.29	IL13
ATOM	468	HA1	GLY	31	-13.270	-11.386	1.691	1.00	0.34	IL13
ATOM	469	HA2	GLY	31	-11.625	-11.049	1.145	1.00	0.31	IL13

Figure 8 (9/30)

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ATOM    470  C    GLY   31     -12.704  -9.324   1.831  1.00  0.23      IL13
ATOM    471  O    GLY   31     -13.507  -8.885   1.032  1.00  0.26      IL13
ATOM    472  N    SER   32     -12.086  -8.539   2.671  1.00  0.22      IL13
ATOM    473  HN   SER   32     -11.438  -8.909   3.306  1.00  0.26      IL13
ATOM    474  CA   SER   32     -12.365  -7.079   2.657  1.00  0.22      IL13
ATOM    475  HA   SER   32     -13.419  -6.910   2.820  1.00  0.26      IL13
ATOM    476  CB   SER   32     -11.563  -6.382   3.757  1.00  0.30      IL13
ATOM    477  HB1  SER   32     -11.751  -5.317   3.718  1.00  0.34      IL13
ATOM    478  HB2  SER   32     -10.512  -6.563   3.609  1.00  0.33      IL13
ATOM    479  OG   SER   32     -11.954  -6.899   5.022  1.00  0.35      IL13
ATOM    480  HG   SER   32     -12.317  -6.176   5.538  1.00  0.96      IL13
ATOM    481  C    SER   32     -11.968  -6.515   1.297  1.00  0.21      IL13
ATOM    482  O    SER   32     -11.072  -7.021   0.646  1.00  0.26      IL13
ATOM    483  N    MET   33     -12.640  -5.482   0.867  1.00  0.23      IL13
ATOM    484  HN   MET   33     -13.361  -5.110   1.417  1.00  0.27      IL13
ATOM    485  CA   MET   33     -12.331  -4.864  -0.453  1.00  0.25      IL13
ATOM    486  HA   MET   33     -11.541  -5.405  -0.949  1.00  0.28      IL13
ATOM    487  CB   MET   33     -13.585  -4.876  -1.324  1.00  0.35      IL13
ATOM    488  HB1  MET   33     -13.342  -4.451  -2.277  1.00  0.40      IL13
ATOM    489  HB2  MET   33     -14.361  -4.292  -0.853  1.00  0.38      IL13
ATOM    490  CG   MET   33     -14.072  -6.311  -1.530  1.00  0.40      IL13
ATOM    491  HG1  MET   33     -14.260  -6.768  -0.570  1.00  0.79      IL13
ATOM    492  HG2  MET   33     -13.318  -6.876  -2.057  1.00  0.93      IL13
ATOM    493  SD   MET   33     -15.605  -6.296  -2.500  1.00  0.89      IL13
ATOM    494  CE   MET   33     -14.871  -6.252  -4.158  1.00  0.67      IL13
ATOM    495  HE1  MET   33     -15.547  -5.748  -4.835  1.00  1.20      IL13
ATOM    496  HE2  MET   33     -14.704  -7.258  -4.505  1.00  1.32      IL13
ATOM    497  HE3  MET   33     -13.929  -5.726  -4.127  1.00  1.36      IL13
ATOM    498  C    MET   33     -11.895  -3.417  -0.228  1.00  0.21      IL13
ATOM    499  O    MET   33     -12.249  -2.807   0.762  1.00  0.22      IL13
ATOM    500  N    VAL   34     -11.135  -2.868  -1.143  1.00  0.19      IL13
ATOM    501  HN   VAL   34     -10.873  -3.389  -1.930  1.00  0.21      IL13
ATOM    502  CA   VAL   34     -10.671  -1.455  -1.005  1.00  0.18      IL13
ATOM    503  HA   VAL   34     -11.195  -0.971  -0.195  1.00  0.18      IL13
ATOM    504  CB   VAL   34      -9.170  -1.423  -0.726  1.00  0.19      IL13
ATOM    505  HB   VAL   34      -8.802  -0.416  -0.863  1.00  0.22      IL13
ATOM    506  CG1  VAL   34      -8.913  -1.864   0.712  1.00  0.25      IL13
ATOM    507  HG11 VAL   34      -9.447  -2.783   0.908  1.00  1.05      IL13
ATOM    508  HG12 VAL   34      -9.259  -1.096   1.384  1.00  1.04      IL13
ATOM    509  HG13 VAL   34      -7.855  -2.023   0.857  1.00  1.02      IL13
ATOM    510  CG2  VAL   34      -8.449  -2.366  -1.685  1.00  0.22      IL13
ATOM    511  HG21 VAL   34      -9.001  -2.430  -2.611  1.00  1.06      IL13
ATOM    512  HG22 VAL   34      -8.376  -3.347  -1.240  1.00  1.06      IL13
ATOM    513  HG23 VAL   34      -7.460  -1.984  -1.881  1.00  0.99      IL13
ATOM    514  C    VAL   34     -10.959  -0.703  -2.299  1.00  0.17      IL13
ATOM    515  O    VAL   34     -11.158  -1.291  -3.344  1.00  0.17      IL13
ATOM    516  N    TRP   35     -10.996   0.593  -2.231  1.00  0.18      IL13
ATOM    517  HN   TRP   35     -10.840   1.043  -1.373  1.00  0.20      IL13
ATOM    518  CA   TRP   35     -11.285   1.397  -3.445  1.00  0.19      IL13
ATOM    519  HA   TRP   35     -12.132   0.987  -3.961  1.00  0.19      IL13
ATOM    520  CB   TRP   35     -11.592   2.824  -3.029  1.00  0.22      IL13
ATOM    521  HB1  TRP   35     -11.669   3.443  -3.910  1.00  0.25      IL13
ATOM    522  HB2  TRP   35     -10.793   3.192  -2.403  1.00  0.24      IL13
ATOM    523  CG   TRP   35     -12.879   2.880  -2.270  1.00  0.25      IL13
ATOM    524  CD1  TRP   35     -13.006   2.711  -0.934  1.00  0.28      IL13
ATOM    525  HD1  TRP   35     -12.200   2.497  -0.248  1.00  0.29      IL13
ATOM    526  CD2  TRP   35     -14.215   3.149  -2.777  1.00  0.27      IL13
ATOM    527  NE1  TRP   35     -14.327   2.901  -0.584  1.00  0.33      IL13
ATOM    528  HE1  TRP   35     -14.680   2.850   0.327  1.00  0.37      IL13
ATOM    529  CE2  TRP   35     -15.116   3.158  -1.688  1.00  0.32      IL13
ATOM    530  CE3  TRP   35     -14.725   3.388  -4.063  1.00  0.28      IL13
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Figure 8 (10/30)

ATOM	531	HE3	TRP	35	-14.058	3.384	-4.913	1.00	0.26	IL13
ATOM	532	CZ2	TRP	35	-16.478	3.402	-1.867	1.00	0.37	IL13
ATOM	533	HZ2	TRP	35	-17.146	3.407	-1.018	1.00	0.42	IL13
ATOM	534	CZ3	TRP	35	-16.096	3.624	-4.250	1.00	0.33	IL13
ATOM	535	HZ3	TRP	35	-16.479	3.792	-5.245	1.00	0.35	IL13
ATOM	536	CH2	TRP	35	-16.971	3.632	-3.154	1.00	0.37	IL13
ATOM	537	HH2	TRP	35	-18.025	3.815	-3.304	1.00	0.42	IL13
ATOM	538	C	TRP	35	-10.073	1.404	-4.375	1.00	0.18	IL13
ATOM	539	O	TRP	35	-8.953	1.605	-3.948	1.00	0.19	IL13
ATOM	540	N	SER	36	-10.288	1.205	-5.646	1.00	0.20	IL13
ATOM	541	HN	SER	36	-11.200	1.058	-5.974	1.00	0.22	IL13
ATOM	542	CA	SER	36	-9.145	1.223	-6.600	1.00	0.21	IL13
ATOM	543	HA	SER	36	-8.354	0.589	-6.228	1.00	0.21	IL13
ATOM	544	CB	SER	36	-9.607	0.721	-7.968	1.00	0.26	IL13
ATOM	545	HB1	SER	36	-10.292	-0.106	-7.834	1.00	0.77	IL13
ATOM	546	HB2	SER	36	-8.756	0.389	-8.539	1.00	0.77	IL13
ATOM	547	OG	SER	36	-10.253	1.778	-8.662	1.00	0.97	IL13
ATOM	548	HG	SER	36	-9.584	2.419	-8.915	1.00	1.48	IL13
ATOM	549	C	SER	36	-8.635	2.660	-6.724	1.00	0.23	IL13
ATOM	550	O	SER	36	-9.387	3.603	-6.574	1.00	0.28	IL13
ATOM	551	N	ILE	37	-7.365	2.829	-6.992	1.00	0.21	IL13
ATOM	552	HN	ILE	37	-6.786	2.046	-7.102	1.00	0.21	IL13
ATOM	553	CA	ILE	37	-6.786	4.204	-7.124	1.00	0.24	IL13
ATOM	554	HA	ILE	37	-7.579	4.930	-7.209	1.00	0.28	IL13
ATOM	555	CB	ILE	37	-5.933	4.526	-5.893	1.00	0.24	IL13
ATOM	556	HB	ILE	37	-5.382	5.439	-6.067	1.00	0.28	IL13
ATOM	557	CG1	ILE	37	-4.950	3.368	-5.632	1.00	0.22	IL13
ATOM	558	HG11	ILE	37	-4.572	2.990	-6.568	1.00	0.23	IL13
ATOM	559	HG12	ILE	37	-5.463	2.575	-5.114	1.00	0.23	IL13
ATOM	560	CG2	ILE	37	-6.864	4.716	-4.686	1.00	0.28	IL13
ATOM	561	HG21	ILE	37	-6.296	5.046	-3.831	1.00	1.01	IL13
ATOM	562	HG22	ILE	37	-7.353	3.782	-4.454	1.00	1.07	IL13
ATOM	563	HG23	ILE	37	-7.611	5.459	-4.924	1.00	1.07	IL13
ATOM	564	CD1	ILE	37	-3.774	3.853	-4.778	1.00	0.27	IL13
ATOM	565	HD11	ILE	37	-4.131	4.212	-3.829	1.00	1.04	IL13
ATOM	566	HD12	ILE	37	-3.262	4.650	-5.295	1.00	1.04	IL13
ATOM	567	HD13	ILE	37	-3.087	3.034	-4.617	1.00	1.06	IL13
ATOM	568	C	ILE	37	-5.906	4.277	-8.372	1.00	0.25	IL13
ATOM	569	O	ILE	37	-5.613	3.279	-8.998	1.00	0.25	IL13
ATOM	570	N	ASN	38	-5.467	5.453	-8.725	1.00	0.27	IL13
ATOM	571	HN	ASN	38	-5.704	6.244	-8.196	1.00	0.29	IL13
ATOM	572	CA	ASN	38	-4.587	5.589	-9.916	1.00	0.30	IL13
ATOM	573	HA	ASN	38	-4.810	4.804	-10.623	1.00	0.31	IL13
ATOM	574	CB	ASN	38	-4.814	6.952	-10.570	1.00	0.35	IL13
ATOM	575	HB1	ASN	38	-3.889	7.305	-11.001	1.00	0.95	IL13
ATOM	576	HB2	ASN	38	-5.158	7.656	-9.825	1.00	0.94	IL13
ATOM	577	CG	ASN	38	-5.867	6.818	-11.670	1.00	1.36	IL13
ATOM	578	OD1	ASN	38	-6.893	7.467	-11.629	1.00	2.23	IL13
ATOM	579	ND2	ASN	38	-5.652	5.995	-12.659	1.00	2.07	IL13
ATOM	580	HD21	ASN	38	-4.823	5.473	-12.691	1.00	2.30	IL13
ATOM	581	HD22	ASN	38	-6.319	5.900	-13.371	1.00	2.78	IL13
ATOM	582	C	ASN	38	-3.132	5.475	-9.465	1.00	0.28	IL13
ATOM	583	O	ASN	38	-2.668	6.237	-8.640	1.00	0.28	IL13
ATOM	584	N	LEU	39	-2.409	4.524	-9.987	1.00	0.28	IL13
ATOM	585	HN	LEU	39	-2.800	3.911	-10.644	1.00	0.31	IL13
ATOM	586	CA	LEU	39	-0.992	4.366	-9.568	1.00	0.29	IL13
ATOM	587	HA	LEU	39	-0.909	4.555	-8.513	1.00	0.28	IL13
ATOM	588	CB	LEU	39	-0.509	2.942	-9.878	1.00	0.31	IL13
ATOM	589	HB1	LEU	39	0.559	2.890	-9.725	1.00	0.33	IL13
ATOM	590	HB2	LEU	39	-0.729	2.711	-10.909	1.00	0.34	IL13
ATOM	591	CG	LEU	39	-1.198	1.905	-8.971	1.00	0.32	IL13

Figure 8 (11/30)

ATOM	592	HG	LEU	39	-0.833	0.924	-9.243	1.00	0.37	IL13
ATOM	593	CD1	LEU	39	-0.841	2.153	-7.491	1.00	0.36	IL13
ATOM	594	HD11	LEU	39	-1.524	2.857	-7.043	1.00	1.03	IL13
ATOM	595	HD12	LEU	39	0.161	2.545	-7.429	1.00	1.09	IL13
ATOM	596	HD13	LEU	39	-0.890	1.218	-6.954	1.00	1.11	IL13
ATOM	597	CD2	LEU	39	-2.724	1.939	-9.194	1.00	0.31	IL13
ATOM	598	HD21	LEU	39	-3.145	0.986	-8.906	1.00	1.00	IL13
ATOM	599	HD22	LEU	39	-2.925	2.113	-10.240	1.00	1.09	IL13
ATOM	600	HD23	LEU	39	-3.180	2.722	-8.611	1.00	1.10	IL13
ATOM	601	C	LEU	39	-0.126	5.372	-10.331	1.00	0.31	IL13
ATOM	602	O	LEU	39	0.144	5.204	-11.504	1.00	0.34	IL13
ATOM	603	N	THR	40	0.308	6.417	-9.669	1.00	0.33	IL13
ATOM	604	HN	THR	40	0.070	6.526	-8.728	1.00	0.34	IL13
ATOM	605	CA	THR	40	1.157	7.445	-10.340	1.00	0.38	IL13
ATOM	606	HA	THR	40	1.581	7.035	-11.244	1.00	0.41	IL13
ATOM	607	CB	THR	40	0.296	8.661	-10.687	1.00	0.40	IL13
ATOM	608	HB	THR	40	0.911	9.420	-11.145	1.00	0.45	IL13
ATOM	609	OG1	THR	40	-0.290	9.177	-9.500	1.00	0.44	IL13
ATOM	610	HG1	THR	40	-1.018	8.601	-9.255	1.00	1.05	IL13
ATOM	611	CG2	THR	40	-0.805	8.246	-11.664	1.00	0.46	IL13
ATOM	612	HG21	THR	40	-0.386	7.610	-12.429	1.00	1.16	IL13
ATOM	613	HG22	THR	40	-1.231	9.127	-12.121	1.00	1.05	IL13
ATOM	614	HG23	THR	40	-1.575	7.709	-11.131	1.00	1.04	IL13
ATOM	615	C	THR	40	2.290	7.871	-9.399	1.00	0.45	IL13
ATOM	616	O	THR	40	3.287	7.188	-9.278	1.00	0.69	IL13
ATOM	617	N	ALA	41	2.141	8.998	-8.740	1.00	0.43	IL13
ATOM	618	HN	ALA	41	1.326	9.528	-8.863	1.00	0.54	IL13
ATOM	619	CA	ALA	41	3.207	9.488	-7.806	1.00	0.50	IL13
ATOM	620	HA	ALA	41	4.103	8.899	-7.928	1.00	0.57	IL13
ATOM	621	CB	ALA	41	3.522	10.951	-8.124	1.00	0.64	IL13
ATOM	622	HB1	ALA	41	3.079	11.216	-9.073	1.00	1.19	IL13
ATOM	623	HB2	ALA	41	4.592	11.086	-8.175	1.00	1.13	IL13
ATOM	624	HB3	ALA	41	3.116	11.582	-7.348	1.00	1.32	IL13
ATOM	625	C	ALA	41	2.728	9.383	-6.356	1.00	0.41	IL13
ATOM	626	O	ALA	41	3.272	8.637	-5.566	1.00	0.51	IL13
ATOM	627	N	GLY	42	1.716	10.126	-5.996	1.00	0.37	IL13
ATOM	628	HN	GLY	42	1.292	10.724	-6.646	1.00	0.47	IL13
ATOM	629	CA	GLY	42	1.207	10.071	-4.592	1.00	0.35	IL13
ATOM	630	HA1	GLY	42	0.464	10.841	-4.450	1.00	0.44	IL13
ATOM	631	HA2	GLY	42	2.027	10.231	-3.907	1.00	0.40	IL13
ATOM	632	C	GLY	42	0.574	8.704	-4.320	1.00	0.25	IL13
ATOM	633	O	GLY	42	-0.437	8.601	-3.653	1.00	0.26	IL13
ATOM	634	N	MET	43	1.152	7.654	-4.835	1.00	0.21	IL13
ATOM	635	HN	MET	43	1.962	7.755	-5.372	1.00	0.25	IL13
ATOM	636	CA	MET	43	0.578	6.301	-4.612	1.00	0.20	IL13
ATOM	637	HA	MET	43	-0.427	6.262	-5.005	1.00	0.23	IL13
ATOM	638	CB	MET	43	1.446	5.263	-5.319	1.00	0.28	IL13
ATOM	639	HB1	MET	43	1.006	4.284	-5.199	1.00	0.35	IL13
ATOM	640	HB2	MET	43	2.437	5.269	-4.890	1.00	0.32	IL13
ATOM	641	CG	MET	43	1.526	5.603	-6.802	1.00	0.33	IL13
ATOM	642	HG1	MET	43	2.141	6.481	-6.935	1.00	0.36	IL13
ATOM	643	HG2	MET	43	0.537	5.800	-7.172	1.00	0.46	IL13
ATOM	644	SD	MET	43	2.253	4.215	-7.707	1.00	0.72	IL13
ATOM	645	CE	MET	43	3.883	4.266	-6.925	1.00	0.36	IL13
ATOM	646	HE1	MET	43	3.847	3.730	-5.986	1.00	1.06	IL13
ATOM	647	HE2	MET	43	4.163	5.290	-6.743	1.00	1.16	IL13
ATOM	648	HE3	MET	43	4.610	3.807	-7.580	1.00	1.07	IL13
ATOM	649	C	MET	43	0.560	5.987	-3.120	1.00	0.19	IL13
ATOM	650	O	MET	43	-0.416	5.498	-2.597	1.00	0.21	IL13
ATOM	651	N	TYR	44	1.639	6.258	-2.438	1.00	0.18	IL13
ATOM	652	HN	TYR	44	2.416	6.647	-2.890	1.00	0.18	IL13

Figure 8 (12/30)

ATOM	653	CA	TYR	44	1.703	5.957	-0.979	1.00	0.20	IL13
ATOM	654	HA	TYR	44	1.626	4.892	-0.823	1.00	0.22	IL13
ATOM	655	CB	TYR	44	3.040	6.461	-0.427	1.00	0.21	IL13
ATOM	656	HB1	TYR	44	3.050	6.347	0.647	1.00	0.22	IL13
ATOM	657	HB2	TYR	44	3.161	7.504	-0.679	1.00	0.22	IL13
ATOM	658	CG	TYR	44	4.174	5.663	-1.026	1.00	0.22	IL13
ATOM	659	CD1	TYR	44	4.636	4.509	-0.383	1.00	0.23	IL13
ATOM	660	HD1	TYR	44	4.190	4.195	0.546	1.00	0.24	IL13
ATOM	661	CD2	TYR	44	4.757	6.074	-2.230	1.00	0.25	IL13
ATOM	662	HD2	TYR	44	4.401	6.965	-2.726	1.00	0.27	IL13
ATOM	663	CE1	TYR	44	5.683	3.767	-0.942	1.00	0.27	IL13
ATOM	664	HE1	TYR	44	6.038	2.877	-0.446	1.00	0.31	IL13
ATOM	665	CE2	TYR	44	5.805	5.333	-2.789	1.00	0.29	IL13
ATOM	666	HE2	TYR	44	6.257	5.652	-3.716	1.00	0.33	IL13
ATOM	667	CZ	TYR	44	6.268	4.179	-2.145	1.00	0.30	IL13
ATOM	668	OH	TYR	44	7.300	3.448	-2.696	1.00	0.35	IL13
ATOM	669	HH	TYR	44	7.474	3.796	-3.574	1.00	0.97	IL13
ATOM	670	C	TYR	44	0.566	6.670	-0.251	1.00	0.20	IL13
ATOM	671	O	TYR	44	-0.127	6.086	0.559	1.00	0.24	IL13
ATOM	672	N	CYS	45	0.368	7.926	-0.527	1.00	0.20	IL13
ATOM	673	HN	CYS	45	0.940	8.381	-1.180	1.00	0.20	IL13
ATOM	674	CA	CYS	45	-0.722	8.671	0.157	1.00	0.23	IL13
ATOM	675	HA	CYS	45	-0.643	8.518	1.221	1.00	0.28	IL13
ATOM	676	HB1	CYS	45	-1.437	10.691	0.265	1.00	0.34	IL13
ATOM	677	HB2	CYS	45	-0.577	10.305	-1.226	1.00	0.36	IL13
ATOM	678	C	CYS	45	-2.078	8.153	-0.316	1.00	0.18	IL13
ATOM	679	O	CYS	45	-2.934	7.820	0.479	1.00	0.18	IL13
ATOM	680	CB	CYS	45	-0.596	10.162	-0.155	1.00	0.28	IL13
ATOM	681	SG	CYS	45	0.939	10.796	0.566	1.00	0.58	IL13
ATOM	682	N	ALA	46	-2.286	8.076	-1.599	1.00	0.18	IL13
ATOM	683	HN	ALA	46	-1.587	8.343	-2.231	1.00	0.19	IL13
ATOM	684	CA	ALA	46	-3.592	7.570	-2.094	1.00	0.16	IL13
ATOM	685	HA	ALA	46	-4.385	8.204	-1.730	1.00	0.16	IL13
ATOM	686	CB	ALA	46	-3.596	7.568	-3.623	1.00	0.19	IL13
ATOM	687	HB1	ALA	46	-3.317	6.589	-3.981	1.00	1.05	IL13
ATOM	688	HB2	ALA	46	-2.889	8.299	-3.987	1.00	1.05	IL13
ATOM	689	HB3	ALA	46	-4.585	7.813	-3.981	1.00	1.00	IL13
ATOM	690	C	ALA	46	-3.794	6.147	-1.576	1.00	0.15	IL13
ATOM	691	O	ALA	46	-4.863	5.778	-1.125	1.00	0.15	IL13
ATOM	692	N	ALA	47	-2.767	5.347	-1.630	1.00	0.17	IL13
ATOM	693	HN	ALA	47	-1.914	5.667	-1.991	1.00	0.19	IL13
ATOM	694	CA	ALA	47	-2.889	3.950	-1.138	1.00	0.18	IL13
ATOM	695	HA	ALA	47	-3.701	3.469	-1.652	1.00	0.18	IL13
ATOM	696	CB	ALA	47	-1.584	3.187	-1.398	1.00	0.21	IL13
ATOM	697	HB1	ALA	47	-0.748	3.780	-1.066	1.00	1.06	IL13
ATOM	698	HB2	ALA	47	-1.487	2.984	-2.455	1.00	1.03	IL13
ATOM	699	HB3	ALA	47	-1.594	2.257	-0.851	1.00	0.99	IL13
ATOM	700	C	ALA	47	-3.174	3.951	0.361	1.00	0.17	IL13
ATOM	701	O	ALA	47	-3.928	3.139	0.859	1.00	0.18	IL13
ATOM	702	N	LEU	48	-2.553	4.833	1.090	1.00	0.17	IL13
ATOM	703	HN	LEU	48	-1.932	5.466	0.675	1.00	0.18	IL13
ATOM	704	CA	LEU	48	-2.768	4.854	2.560	1.00	0.18	IL13
ATOM	705	HA	LEU	48	-2.475	3.899	2.961	1.00	0.20	IL13
ATOM	706	CB	LEU	48	-1.893	5.953	3.178	1.00	0.19	IL13
ATOM	707	HB1	LEU	48	-2.160	6.905	2.742	1.00	0.19	IL13
ATOM	708	HB2	LEU	48	-0.858	5.740	2.958	1.00	0.22	IL13
ATOM	709	CG	LEU	48	-2.085	6.026	4.707	1.00	0.21	IL13
ATOM	710	HG	LEU	48	-3.120	6.242	4.931	1.00	0.22	IL13
ATOM	711	CD1	LEU	48	-1.703	4.670	5.343	1.00	0.25	IL13
ATOM	712	HD11	LEU	48	-2.542	3.995	5.271	1.00	1.00	IL13
ATOM	713	HD12	LEU	48	-1.451	4.792	6.384	1.00	1.05	IL13

Figure 8 (13/30)

ATOM	714	HD13	LEU	48	-0.861	4.250	4.815	1.00	1.09	IL13
ATOM	715	CD2	LEU	48	-1.203	7.177	5.246	1.00	0.24	IL13
ATOM	716	HD21	LEU	48	-1.772	8.095	5.224	1.00	0.98	IL13
ATOM	717	HD22	LEU	48	-0.331	7.288	4.621	1.00	0.99	IL13
ATOM	718	HD23	LEU	48	-0.889	6.983	6.259	1.00	1.14	IL13
ATOM	719	C	LEU	48	-4.240	5.110	2.888	1.00	0.17	IL13
ATOM	720	O	LEU	48	-4.853	4.353	3.606	1.00	0.19	IL13
ATOM	721	N	GLU	49	-4.815	6.165	2.380	1.00	0.16	IL13
ATOM	722	HN	GLU	49	-4.310	6.775	1.802	1.00	0.15	IL13
ATOM	723	CA	GLU	49	-6.242	6.447	2.708	1.00	0.17	IL13
ATOM	724	HA	GLU	49	-6.328	6.623	3.771	1.00	0.19	IL13
ATOM	725	CB	GLU	49	-6.724	7.693	1.958	1.00	0.17	IL13
ATOM	726	HB1	GLU	49	-6.245	8.568	2.371	1.00	0.19	IL13
ATOM	727	HB2	GLU	49	-7.795	7.785	2.071	1.00	0.19	IL13
ATOM	728	CG	GLU	49	-6.379	7.580	0.474	1.00	0.16	IL13
ATOM	729	HG1	GLU	49	-6.745	6.642	0.087	1.00	0.34	IL13
ATOM	730	HG2	GLU	49	-5.307	7.630	0.349	1.00	0.31	IL13
ATOM	731	CD	GLU	49	-7.039	8.736	-0.282	1.00	0.42	IL13
ATOM	732	OE1	GLU	49	-6.468	9.184	-1.261	1.00	1.23	IL13
ATOM	733	OE2	GLU	49	-8.110	9.150	0.129	1.00	1.20	IL13
ATOM	734	C	GLU	49	-7.108	5.250	2.334	1.00	0.17	IL13
ATOM	735	O	GLU	49	-8.086	4.955	2.993	1.00	0.20	IL13
ATOM	736	N	SER	50	-6.771	4.553	1.290	1.00	0.17	IL13
ATOM	737	HN	SER	50	-5.979	4.798	0.762	1.00	0.17	IL13
ATOM	738	CA	SER	50	-7.598	3.379	0.904	1.00	0.19	IL13
ATOM	739	HA	SER	50	-8.631	3.689	0.806	1.00	0.20	IL13
ATOM	740	CB	SER	50	-7.097	2.820	-0.427	1.00	0.21	IL13
ATOM	741	HB1	SER	50	-7.773	2.047	-0.768	1.00	0.98	IL13
ATOM	742	HB2	SER	50	-6.114	2.399	-0.296	1.00	1.01	IL13
ATOM	743	OG	SER	50	-7.035	3.869	-1.383	1.00	1.36	IL13
ATOM	744	HG	SER	50	-7.260	3.503	-2.241	1.00	1.92	IL13
ATOM	745	C	SER	50	-7.484	2.295	1.986	1.00	0.19	IL13
ATOM	746	O	SER	50	-8.453	1.653	2.339	1.00	0.21	IL13
ATOM	747	N	LEU	51	-6.304	2.087	2.509	1.00	0.19	IL13
ATOM	748	HN	LEU	51	-5.536	2.616	2.206	1.00	0.19	IL13
ATOM	749	CA	LEU	51	-6.117	1.045	3.565	1.00	0.21	IL13
ATOM	750	HA	LEU	51	-6.557	0.116	3.236	1.00	0.23	IL13
ATOM	751	CB	LEU	51	-4.620	0.843	3.816	1.00	0.23	IL13
ATOM	752	HB1	LEU	51	-4.479	0.202	4.673	1.00	0.25	IL13
ATOM	753	HB2	LEU	51	-4.161	1.802	4.008	1.00	0.25	IL13
ATOM	754	CG	LEU	51	-3.971	0.206	2.579	1.00	0.26	IL13
ATOM	755	HG	LEU	51	-4.207	0.803	1.709	1.00	0.26	IL13
ATOM	756	CD1	LEU	51	-2.454	0.168	2.762	1.00	0.30	IL13
ATOM	757	HD11	LEU	51	-2.198	-0.578	3.499	1.00	1.09	IL13
ATOM	758	HD12	LEU	51	-2.108	1.136	3.093	1.00	0.97	IL13
ATOM	759	HD13	LEU	51	-1.984	-0.079	1.821	1.00	1.03	IL13
ATOM	760	CD2	LEU	51	-4.491	-1.225	2.369	1.00	0.29	IL13
ATOM	761	HD21	LEU	51	-5.353	-1.202	1.719	1.00	1.01	IL13
ATOM	762	HD22	LEU	51	-4.767	-1.661	3.317	1.00	1.06	IL13
ATOM	763	HD23	LEU	51	-3.717	-1.823	1.912	1.00	1.03	IL13
ATOM	764	C	LEU	51	-6.795	1.496	4.860	1.00	0.22	IL13
ATOM	765	O	LEU	51	-7.314	0.697	5.615	1.00	0.25	IL13
ATOM	766	N	ILE	52	-6.793	2.773	5.121	1.00	0.22	IL13
ATOM	767	HN	ILE	52	-6.368	3.397	4.497	1.00	0.22	IL13
ATOM	768	CA	ILE	52	-7.435	3.288	6.363	1.00	0.25	IL13
ATOM	769	HA	ILE	52	-6.911	2.904	7.223	1.00	0.28	IL13
ATOM	770	CB	ILE	52	-7.367	4.827	6.348	1.00	0.26	IL13
ATOM	771	HB	ILE	52	-7.686	5.169	5.373	1.00	0.27	IL13
ATOM	772	CG1	ILE	52	-5.917	5.308	6.586	1.00	0.29	IL13
ATOM	773	HG11	ILE	52	-5.890	6.385	6.537	1.00	0.34	IL13
ATOM	774	HG12	ILE	52	-5.287	4.909	5.815	1.00	0.32	IL13

Figure 8 (14/30)

ATOM	775	CG2	ILE	52	-8.304	5.432	7.397	1.00	0.28	IL13
ATOM	776	HG21	ILE	52	-8.453	4.736	8.205	1.00	1.04	IL13
ATOM	777	HG22	ILE	52	-9.251	5.652	6.935	1.00	1.03	IL13
ATOM	778	HG23	ILE	52	-7.872	6.345	7.782	1.00	1.09	IL13
ATOM	779	CD1	ILE	52	-5.365	4.852	7.948	1.00	0.36	IL13
ATOM	780	HD11	ILE	52	-6.169	4.629	8.626	1.00	1.11	IL13
ATOM	781	HD12	ILE	52	-4.756	5.640	8.366	1.00	1.12	IL13
ATOM	782	HD13	ILE	52	-4.758	3.969	7.809	1.00	1.03	IL13
ATOM	783	C	ILE	52	-8.893	2.805	6.408	1.00	0.25	IL13
ATOM	784	O	ILE	52	-9.532	2.813	7.442	1.00	0.28	IL13
ATOM	785	N	ASN	53	-9.423	2.365	5.299	1.00	0.25	IL13
ATOM	786	HN	ASN	53	-8.895	2.349	4.474	1.00	0.25	IL13
ATOM	787	CA	ASN	53	-10.831	1.871	5.297	1.00	0.27	IL13
ATOM	788	HA	ASN	53	-11.423	2.470	5.973	1.00	0.30	IL13
ATOM	789	CB	ASN	53	-11.408	1.976	3.882	1.00	0.31	IL13
ATOM	790	HB1	ASN	53	-12.417	1.593	3.877	1.00	0.33	IL13
ATOM	791	HB2	ASN	53	-10.800	1.399	3.200	1.00	0.30	IL13
ATOM	792	CG	ASN	53	-11.420	3.441	3.443	1.00	0.36	IL13
ATOM	793	OD1	ASN	53	-10.381	4.024	3.206	1.00	1.09	IL13
ATOM	794	ND2	ASN	53	-12.560	4.064	3.320	1.00	1.20	IL13
ATOM	795	HD21	ASN	53	-13.399	3.593	3.507	1.00	1.99	IL13
ATOM	796	HD22	ASN	53	-12.577	5.002	3.039	1.00	1.23	IL13
ATOM	797	C	ASN	53	-10.859	0.407	5.754	1.00	0.26	IL13
ATOM	798	O	ASN	53	-11.892	-0.117	6.122	1.00	0.31	IL13
ATOM	799	N	VAL	54	-9.732	-0.255	5.740	1.00	0.23	IL13
ATOM	800	HN	VAL	54	-8.909	0.186	5.444	1.00	0.22	IL13
ATOM	801	CA	VAL	54	-9.695	-1.682	6.180	1.00	0.24	IL13
ATOM	802	HA	VAL	54	-10.655	-2.139	5.990	1.00	0.28	IL13
ATOM	803	CB	VAL	54	-8.604	-2.430	5.406	1.00	0.23	IL13
ATOM	804	HB	VAL	54	-7.639	-2.021	5.666	1.00	0.27	IL13
ATOM	805	CG1	VAL	54	-8.633	-3.922	5.755	1.00	0.28	IL13
ATOM	806	HG11	VAL	54	-8.191	-4.487	4.948	1.00	1.04	IL13
ATOM	807	HG12	VAL	54	-9.653	-4.244	5.901	1.00	1.06	IL13
ATOM	808	HG13	VAL	54	-8.069	-4.090	6.661	1.00	1.06	IL13
ATOM	809	CG2	VAL	54	-8.842	-2.252	3.908	1.00	0.26	IL13
ATOM	810	HG21	VAL	54	-8.029	-2.702	3.357	1.00	1.06	IL13
ATOM	811	HG22	VAL	54	-8.894	-1.199	3.681	1.00	1.02	IL13
ATOM	812	HG23	VAL	54	-9.772	-2.728	3.631	1.00	1.06	IL13
ATOM	813	C	VAL	54	-9.387	-1.739	7.677	1.00	0.29	IL13
ATOM	814	O	VAL	54	-8.376	-1.233	8.123	1.00	0.33	IL13
ATOM	815	N	SER	55	-10.256	-2.345	8.448	1.00	0.36	IL13
ATOM	816	HN	SER	55	-11.063	-2.737	8.052	1.00	0.38	IL13
ATOM	817	CA	SER	55	-10.037	-2.441	9.925	1.00	0.44	IL13
ATOM	818	HA	SER	55	-9.051	-2.083	10.178	1.00	0.45	IL13
ATOM	819	CB	SER	55	-11.084	-1.591	10.645	1.00	0.56	IL13
ATOM	820	HB1	SER	55	-11.048	-1.799	11.706	1.00	0.65	IL13
ATOM	821	HB2	SER	55	-12.065	-1.829	10.268	1.00	0.59	IL13
ATOM	822	OG	SER	55	-10.814	-0.215	10.409	1.00	0.59	IL13
ATOM	823	HG	SER	55	-10.717	-0.090	9.462	1.00	1.01	IL13
ATOM	824	C	SER	55	-10.172	-3.898	10.373	1.00	0.45	IL13
ATOM	825	O	SER	55	-10.970	-4.648	9.846	1.00	0.45	IL13
ATOM	826	N	GLY	56	-9.396	-4.300	11.346	1.00	0.48	IL13
ATOM	827	HN	GLY	56	-8.763	-3.674	11.754	1.00	0.51	IL13
ATOM	828	CA	GLY	56	-9.472	-5.706	11.841	1.00	0.50	IL13
ATOM	829	HA1	GLY	56	-10.436	-6.126	11.594	1.00	0.51	IL13
ATOM	830	HA2	GLY	56	-9.342	-5.714	12.913	1.00	0.54	IL13
ATOM	831	C	GLY	56	-8.373	-6.548	11.189	1.00	0.46	IL13
ATOM	832	O	GLY	56	-8.270	-7.734	11.434	1.00	0.77	IL13
ATOM	833	N	CYS	57	-7.555	-5.940	10.364	1.00	0.35	IL13
ATOM	834	HN	CYS	57	-7.667	-4.982	10.190	1.00	0.56	IL13
ATOM	835	CA	CYS	57	-6.452	-6.689	9.685	1.00	0.32	IL13

Figure 8 (15/30)

ATOM	836	HA	CYS	57	-6.568	-7.749	9.850	1.00	0.33	IL13
ATOM	837	HB1	CYS	57	-5.706	-6.951	7.691	1.00	0.32	IL13
ATOM	838	HB2	CYS	57	-6.369	-5.348	8.012	1.00	0.38	IL13
ATOM	839	C	CYS	57	-5.098	-6.236	10.242	1.00	0.34	IL13
ATOM	840	O	CYS	57	-4.529	-5.261	9.797	1.00	0.37	IL13
ATOM	841	CB	CYS	57	-6.498	-6.406	8.183	1.00	0.32	IL13
ATOM	842	SG	CYS	57	-8.093	-6.934	7.512	1.00	0.37	IL13
ATOM	843	N	SER	58	-4.576	-6.938	11.209	1.00	0.37	IL13
ATOM	844	HN	SER	58	-5.048	-7.724	11.554	1.00	0.37	IL13
ATOM	845	CA	SER	58	-3.255	-6.550	11.783	1.00	0.43	IL13
ATOM	846	HA	SER	58	-3.243	-5.485	11.967	1.00	0.44	IL13
ATOM	847	CB	SER	58	-3.025	-7.297	13.096	1.00	0.53	IL13
ATOM	848	HB1	SER	58	-3.118	-8.361	12.925	1.00	0.55	IL13
ATOM	849	HB2	SER	58	-3.758	-6.987	13.822	1.00	0.57	IL13
ATOM	850	OG	SER	58	-1.725	-6.994	13.585	1.00	0.61	IL13
ATOM	851	HG	SER	58	-1.504	-6.101	13.309	1.00	1.20	IL13
ATOM	852	C	SER	58	-2.143	-6.906	10.792	1.00	0.43	IL13
ATOM	853	O	SER	58	-1.110	-6.268	10.744	1.00	0.49	IL13
ATOM	854	N	ALA	59	-2.341	-7.931	10.011	1.00	0.43	IL13
ATOM	855	HN	ALA	59	-3.176	-8.439	10.074	1.00	0.43	IL13
ATOM	856	CA	ALA	59	-1.292	-8.343	9.037	1.00	0.50	IL13
ATOM	857	HA	ALA	59	-0.438	-8.730	9.573	1.00	0.59	IL13
ATOM	858	CB	ALA	59	-1.852	-9.436	8.123	1.00	0.51	IL13
ATOM	859	HB1	ALA	59	-1.795	-9.111	7.095	1.00	1.13	IL13
ATOM	860	HB2	ALA	59	-2.883	-9.629	8.382	1.00	1.19	IL13
ATOM	861	HB3	ALA	59	-1.275	-10.340	8.247	1.00	1.08	IL13
ATOM	862	C	ALA	59	-0.856	-7.143	8.189	1.00	0.47	IL13
ATOM	863	O	ALA	59	0.244	-7.120	7.671	1.00	0.61	IL13
ATOM	864	N	ILE	60	-1.710	-6.154	8.041	1.00	0.36	IL13
ATOM	865	HN	ILE	60	-2.590	-6.206	8.469	1.00	0.36	IL13
ATOM	866	CA	ILE	60	-1.354	-4.949	7.220	1.00	0.38	IL13
ATOM	867	HA	ILE	60	-0.439	-5.138	6.679	1.00	0.44	IL13
ATOM	868	CB	ILE	60	-2.475	-4.666	6.209	1.00	0.41	IL13
ATOM	869	HB	ILE	60	-2.209	-3.798	5.621	1.00	0.45	IL13
ATOM	870	CG1	ILE	60	-3.797	-4.399	6.941	1.00	0.41	IL13
ATOM	871	HG11	ILE	60	-3.681	-3.571	7.622	1.00	0.39	IL13
ATOM	872	HG12	ILE	60	-4.084	-5.278	7.492	1.00	0.41	IL13
ATOM	873	CG2	ILE	60	-2.644	-5.871	5.278	1.00	0.46	IL13
ATOM	874	HG21	ILE	60	-1.677	-6.305	5.069	1.00	1.18	IL13
ATOM	875	HG22	ILE	60	-3.099	-5.550	4.353	1.00	1.05	IL13
ATOM	876	HG23	ILE	60	-3.274	-6.610	5.750	1.00	1.04	IL13
ATOM	877	CD1	ILE	60	-4.883	-4.057	5.920	1.00	0.50	IL13
ATOM	878	HD11	ILE	60	-5.761	-3.699	6.436	1.00	1.16	IL13
ATOM	879	HD12	ILE	60	-5.134	-4.939	5.351	1.00	1.12	IL13
ATOM	880	HD13	ILE	60	-4.520	-3.289	5.253	1.00	1.14	IL13
ATOM	881	C	ILE	60	-1.147	-3.725	8.122	1.00	0.37	IL13
ATOM	882	O	ILE	60	-0.850	-2.647	7.647	1.00	0.32	IL13
ATOM	883	N	GLU	61	-1.300	-3.867	9.411	1.00	0.43	IL13
ATOM	884	HN	GLU	61	-1.542	-4.739	9.788	1.00	0.48	IL13
ATOM	885	CA	GLU	61	-1.106	-2.685	10.305	1.00	0.44	IL13
ATOM	886	HA	GLU	61	-1.841	-1.930	10.069	1.00	0.47	IL13
ATOM	887	CB	GLU	61	-1.259	-3.109	11.770	1.00	0.56	IL13
ATOM	888	HB1	GLU	61	-0.435	-2.716	12.346	1.00	1.22	IL13
ATOM	889	HB2	GLU	61	-1.259	-4.186	11.833	1.00	0.92	IL13
ATOM	890	CG	GLU	61	-2.574	-2.566	12.331	1.00	1.38	IL13
ATOM	891	HG1	GLU	61	-3.402	-2.974	11.772	1.00	1.87	IL13
ATOM	892	HG2	GLU	61	-2.580	-1.488	12.252	1.00	2.08	IL13
ATOM	893	CD	GLU	61	-2.704	-2.970	13.801	1.00	1.74	IL13
ATOM	894	OE1	GLU	61	-3.825	-3.056	14.275	1.00	2.22	IL13
ATOM	895	OE2	GLU	61	-1.680	-3.180	14.430	1.00	2.26	IL13
ATOM	896	C	GLU	61	0.296	-2.118	10.092	1.00	0.37	IL13

Figure 8 (16/30)

ATOM	897	O	GLU	61	0.477	-0.934	9.892	1.00	0.35	IL13
ATOM	898	N	LYS	62	1.286	-2.960	10.127	1.00	0.35	IL13
ATOM	899	HN	LYS	62	1.111	-3.911	10.284	1.00	0.38	IL13
ATOM	900	CA	LYS	62	2.683	-2.492	9.919	1.00	0.33	IL13
ATOM	901	HA	LYS	62	2.940	-1.768	10.679	1.00	0.37	IL13
ATOM	902	CB	LYS	62	3.621	-3.693	10.015	1.00	0.36	IL13
ATOM	903	HB1	LYS	62	4.630	-3.383	9.791	1.00	0.37	IL13
ATOM	904	HB2	LYS	62	3.309	-4.453	9.313	1.00	0.34	IL13
ATOM	905	CG	LYS	62	3.565	-4.253	11.438	1.00	0.43	IL13
ATOM	906	HG1	LYS	62	2.553	-4.544	11.673	1.00	0.58	IL13
ATOM	907	HG2	LYS	62	3.892	-3.493	12.133	1.00	0.49	IL13
ATOM	908	CD	LYS	62	4.485	-5.469	11.549	1.00	0.60	IL13
ATOM	909	HD1	LYS	62	5.504	-5.170	11.361	1.00	0.99	IL13
ATOM	910	HD2	LYS	62	4.186	-6.212	10.823	1.00	1.04	IL13
ATOM	911	CE	LYS	62	4.378	-6.058	12.956	1.00	1.13	IL13
ATOM	912	HE1	LYS	62	3.348	-6.306	13.164	1.00	1.74	IL13
ATOM	913	HE2	LYS	62	4.726	-5.334	13.678	1.00	1.68	IL13
ATOM	914	NZ	LYS	62	5.212	-7.289	13.043	1.00	1.84	IL13
ATOM	915	HZ1	LYS	62	4.630	-8.079	13.387	1.00	2.27	IL13
ATOM	916	HZ2	LYS	62	6.001	-7.127	13.702	1.00	2.23	IL13
ATOM	917	HZ3	LYS	62	5.587	-7.522	12.102	1.00	2.42	IL13
ATOM	918	C	LYS	62	2.798	-1.849	8.535	1.00	0.27	IL13
ATOM	919	O	LYS	62	3.480	-0.860	8.351	1.00	0.27	IL13
ATOM	920	N	THR	63	2.139	-2.411	7.557	1.00	0.24	IL13
ATOM	921	HN	THR	63	1.600	-3.212	7.728	1.00	0.26	IL13
ATOM	922	CA	THR	63	2.212	-1.846	6.179	1.00	0.21	IL13
ATOM	923	HA	THR	63	3.227	-1.899	5.815	1.00	0.21	IL13
ATOM	924	CB	THR	63	1.287	-2.655	5.257	1.00	0.22	IL13
ATOM	925	HB	THR	63	0.263	-2.526	5.573	1.00	0.24	IL13
ATOM	926	OG1	THR	63	1.637	-4.029	5.337	1.00	0.25	IL13
ATOM	927	HG1	THR	63	2.472	-4.149	4.879	1.00	0.93	IL13
ATOM	928	CG2	THR	63	1.428	-2.190	3.800	1.00	0.24	IL13
ATOM	929	HG21	THR	63	1.497	-1.115	3.753	1.00	1.00	IL13
ATOM	930	HG22	THR	63	0.565	-2.514	3.238	1.00	1.06	IL13
ATOM	931	HG23	THR	63	2.318	-2.624	3.373	1.00	1.06	IL13
ATOM	932	C	THR	63	1.746	-0.392	6.209	1.00	0.21	IL13
ATOM	933	O	THR	63	2.333	0.466	5.585	1.00	0.19	IL13
ATOM	934	N	GLN	64	0.697	-0.102	6.918	1.00	0.25	IL13
ATOM	935	HN	GLN	64	0.226	-0.804	7.414	1.00	0.27	IL13
ATOM	936	CA	GLN	64	0.211	1.299	6.955	1.00	0.28	IL13
ATOM	937	HA	GLN	64	-0.038	1.621	5.956	1.00	0.27	IL13
ATOM	938	CB	GLN	64	-1.033	1.386	7.841	1.00	0.35	IL13
ATOM	939	HB1	GLN	64	-1.339	2.417	7.934	1.00	0.38	IL13
ATOM	940	HB2	GLN	64	-0.805	0.985	8.816	1.00	0.38	IL13
ATOM	941	CG	GLN	64	-2.165	0.576	7.204	1.00	0.38	IL13
ATOM	942	HG1	GLN	64	-1.888	-0.469	7.183	1.00	0.82	IL13
ATOM	943	HG2	GLN	64	-2.336	0.923	6.196	1.00	0.87	IL13
ATOM	944	CD	GLN	64	-3.443	0.741	8.028	1.00	0.86	IL13
ATOM	945	OE1	GLN	64	-3.390	0.893	9.232	1.00	1.52	IL13
ATOM	946	NE2	GLN	64	-4.599	0.719	7.422	1.00	1.47	IL13
ATOM	947	HE21	GLN	64	-4.640	0.597	6.450	1.00	1.77	IL13
ATOM	948	HE22	GLN	64	-5.425	0.827	7.937	1.00	1.97	IL13
ATOM	949	C	GLN	64	1.317	2.192	7.515	1.00	0.28	IL13
ATOM	950	O	GLN	64	1.540	3.289	7.042	1.00	0.29	IL13
ATOM	951	N	ARG	65	2.021	1.729	8.510	1.00	0.31	IL13
ATOM	952	HN	ARG	65	1.831	0.839	8.872	1.00	0.33	IL13
ATOM	953	CA	ARG	65	3.121	2.552	9.086	1.00	0.35	IL13
ATOM	954	HA	ARG	65	2.724	3.504	9.401	1.00	0.38	IL13
ATOM	955	CB	ARG	65	3.727	1.830	10.291	1.00	0.43	IL13
ATOM	956	HB1	ARG	65	4.797	1.975	10.296	1.00	1.03	IL13
ATOM	957	HB2	ARG	65	3.509	0.773	10.218	1.00	0.97	IL13

Figure 8 (17/30)

ATOM	958	CG	ARG	65	3.132	2.382	11.588	1.00	1.34	IL13
ATOM	959	HG1	ARG	65	2.067	2.211	11.601	1.00	2.01	IL13
ATOM	960	HG2	ARG	65	3.330	3.443	11.653	1.00	1.99	IL13
ATOM	961	CD	ARG	65	3.776	1.676	12.781	1.00	1.54	IL13
ATOM	962	HD1	ARG	65	4.100	0.689	12.485	1.00	1.90	IL13
ATOM	963	HD2	ARG	65	3.058	1.595	13.583	1.00	1.84	IL13
ATOM	964	NE	ARG	65	4.952	2.466	13.244	1.00	2.29	IL13
ATOM	965	HE	ARG	65	5.326	3.170	12.673	1.00	2.82	IL13
ATOM	966	CZ	ARG	65	5.480	2.226	14.412	1.00	2.82	IL13
ATOM	967	NH1	ARG	65	6.503	2.925	14.822	1.00	3.77	IL13
ATOM	968	HH11	ARG	65	6.882	3.645	14.241	1.00	4.19	IL13
ATOM	969	HH12	ARG	65	6.908	2.740	15.718	1.00	4.29	IL13
ATOM	970	NH2	ARG	65	4.986	1.285	15.168	1.00	2.91	IL13
ATOM	971	HH21	ARG	65	4.203	0.749	14.852	1.00	2.65	IL13
ATOM	972	HH22	ARG	65	5.390	1.100	16.064	1.00	3.59	IL13
ATOM	973	C	ARG	65	4.220	2.785	8.044	1.00	0.30	IL13
ATOM	974	O	ARG	65	4.659	3.898	7.838	1.00	0.30	IL13
ATOM	975	N	MET	66	4.685	1.748	7.399	1.00	0.28	IL13
ATOM	976	HN	MET	66	4.334	0.852	7.585	1.00	0.29	IL13
ATOM	977	CA	MET	66	5.771	1.936	6.394	1.00	0.27	IL13
ATOM	978	HA	MET	66	6.626	2.384	6.879	1.00	0.30	IL13
ATOM	979	CB	MET	66	6.175	0.580	5.800	1.00	0.29	IL13
ATOM	980	HB1	MET	66	6.837	0.738	4.961	1.00	0.31	IL13
ATOM	981	HB2	MET	66	5.291	0.058	5.467	1.00	0.28	IL13
ATOM	982	CG	MET	66	6.899	-0.257	6.866	1.00	0.36	IL13
ATOM	983	HG1	MET	66	6.183	-0.590	7.604	1.00	0.41	IL13
ATOM	984	HG2	MET	66	7.656	0.343	7.348	1.00	0.41	IL13
ATOM	985	SD	MET	66	7.682	-1.701	6.099	1.00	0.66	IL13
ATOM	986	CE	MET	66	6.208	-2.742	5.953	1.00	0.39	IL13
ATOM	987	HE1	MET	66	6.487	-3.699	5.534	1.00	1.16	IL13
ATOM	988	HE2	MET	66	5.489	-2.267	5.308	1.00	1.13	IL13
ATOM	989	HE3	MET	66	5.772	-2.886	6.932	1.00	1.04	IL13
ATOM	990	C	MET	66	5.287	2.871	5.281	1.00	0.23	IL13
ATOM	991	O	MET	66	6.018	3.722	4.815	1.00	0.24	IL13
ATOM	992	N	LEU	67	4.059	2.732	4.860	1.00	0.20	IL13
ATOM	993	HN	LEU	67	3.479	2.047	5.255	1.00	0.21	IL13
ATOM	994	CA	LEU	67	3.534	3.628	3.788	1.00	0.20	IL13
ATOM	995	HA	LEU	67	4.159	3.547	2.916	1.00	0.21	IL13
ATOM	996	CB	LEU	67	2.093	3.237	3.435	1.00	0.21	IL13
ATOM	997	HB1	LEU	67	1.677	3.975	2.765	1.00	0.23	IL13
ATOM	998	HB2	LEU	67	1.505	3.210	4.340	1.00	0.23	IL13
ATOM	999	CG	LEU	67	2.052	1.851	2.762	1.00	0.20	IL13
ATOM	1000	HG	LEU	67	2.608	1.147	3.360	1.00	0.19	IL13
ATOM	1001	CD1	LEU	67	0.598	1.392	2.658	1.00	0.23	IL13
ATOM	1002	HD11	LEU	67	0.561	0.402	2.230	1.00	1.05	IL13
ATOM	1003	HD12	LEU	67	0.049	2.077	2.029	1.00	1.02	IL13
ATOM	1004	HD13	LEU	67	0.157	1.375	3.641	1.00	1.05	IL13
ATOM	1005	CD2	LEU	67	2.644	1.902	1.346	1.00	0.22	IL13
ATOM	1006	HD21	LEU	67	2.284	1.055	0.780	1.00	1.03	IL13
ATOM	1007	HD22	LEU	67	3.721	1.858	1.395	1.00	1.04	IL13
ATOM	1008	HD23	LEU	67	2.338	2.811	0.855	1.00	1.03	IL13
ATOM	1009	C	LEU	67	3.566	5.075	4.287	1.00	0.22	IL13
ATOM	1010	O	LEU	67	3.893	5.987	3.555	1.00	0.24	IL13
ATOM	1011	N	SER	68	3.226	5.293	5.529	1.00	0.25	IL13
ATOM	1012	HN	SER	68	2.964	4.544	6.105	1.00	0.26	IL13
ATOM	1013	CA	SER	68	3.239	6.681	6.071	1.00	0.29	IL13
ATOM	1014	HA	SER	68	2.543	7.287	5.512	1.00	0.31	IL13
ATOM	1015	CB	SER	68	2.826	6.666	7.544	1.00	0.35	IL13
ATOM	1016	HB1	SER	68	3.048	7.627	7.989	1.00	0.38	IL13
ATOM	1017	HB2	SER	68	3.372	5.898	8.065	1.00	0.34	IL13
ATOM	1018	OG	SER	68	1.433	6.394	7.636	1.00	0.39	IL13

Figure 8 (18/30)

ATOM	1019	HG	SER	68	1.306	5.715	8.302	1.00	0.95	IL13
ATOM	1020	C	SER	68	4.645	7.265	5.930	1.00	0.28	IL13
ATOM	1021	O	SER	68	4.815	8.435	5.650	1.00	0.31	IL13
ATOM	1022	N	GLY	69	5.655	6.462	6.119	1.00	0.27	IL13
ATOM	1023	HN	GLY	69	5.498	5.520	6.341	1.00	0.27	IL13
ATOM	1024	CA	GLY	69	7.048	6.979	5.988	1.00	0.29	IL13
ATOM	1025	HA1	GLY	69	7.742	6.153	6.011	1.00	0.31	IL13
ATOM	1026	HA2	GLY	69	7.260	7.653	6.806	1.00	0.31	IL13
ATOM	1027	C	GLY	69	7.192	7.724	4.657	1.00	0.29	IL13
ATOM	1028	O	GLY	69	7.963	8.655	4.536	1.00	0.32	IL13
ATOM	1029	N	PHE	70	6.452	7.322	3.658	1.00	0.27	IL13
ATOM	1030	HN	PHE	70	5.834	6.571	3.780	1.00	0.26	IL13
ATOM	1031	CA	PHE	70	6.535	8.006	2.333	1.00	0.31	IL13
ATOM	1032	HA	PHE	70	7.495	8.488	2.225	1.00	0.34	IL13
ATOM	1033	CB	PHE	70	6.342	6.976	1.218	1.00	0.31	IL13
ATOM	1034	HB1	PHE	70	6.292	7.485	0.267	1.00	0.32	IL13
ATOM	1035	HB2	PHE	70	5.420	6.438	1.385	1.00	0.32	IL13
ATOM	1036	CG	PHE	70	7.493	6.003	1.205	1.00	0.29	IL13
ATOM	1037	CD1	PHE	70	8.619	6.263	0.417	1.00	0.31	IL13
ATOM	1038	HD1	PHE	70	8.666	7.163	-0.178	1.00	0.33	IL13
ATOM	1039	CD2	PHE	70	7.430	4.837	1.975	1.00	0.30	IL13
ATOM	1040	HD2	PHE	70	6.560	4.639	2.585	1.00	0.32	IL13
ATOM	1041	CE1	PHE	70	9.683	5.355	0.397	1.00	0.32	IL13
ATOM	1042	HE1	PHE	70	10.552	5.556	-0.212	1.00	0.35	IL13
ATOM	1043	CE2	PHE	70	8.494	3.930	1.959	1.00	0.31	IL13
ATOM	1044	HE2	PHE	70	8.446	3.030	2.554	1.00	0.33	IL13
ATOM	1045	CZ	PHE	70	9.621	4.188	1.169	1.00	0.32	IL13
ATOM	1046	HZ	PHE	70	10.440	3.486	1.153	1.00	0.34	IL13
ATOM	1047	C	PHE	70	5.415	9.042	2.230	1.00	0.35	IL13
ATOM	1048	O	PHE	70	5.325	9.781	1.269	1.00	0.48	IL13
ATOM	1049	N	CYS	71	4.549	9.073	3.206	1.00	0.32	IL13
ATOM	1050	HN	CYS	71	4.643	8.447	3.954	1.00	0.32	IL13
ATOM	1051	CA	CYS	71	3.400	10.025	3.186	1.00	0.41	IL13
ATOM	1052	HA	CYS	71	3.548	10.775	2.427	1.00	0.48	IL13
ATOM	1053	HB1	CYS	71	1.888	8.589	3.684	1.00	0.87	IL13
ATOM	1054	HB2	CYS	71	2.319	8.624	1.976	1.00	0.91	IL13
ATOM	1055	C	CYS	71	3.247	10.669	4.583	1.00	0.41	IL13
ATOM	1056	O	CYS	71	2.523	10.158	5.413	1.00	0.53	IL13
ATOM	1057	CB	CYS	71	2.140	9.228	2.854	1.00	0.65	IL13
ATOM	1058	SG	CYS	71	0.780	10.365	2.534	1.00	1.28	IL13
ATOM	1059	N	PRO	72	3.943	11.757	4.866	1.00	0.46	IL13
ATOM	1060	CA	PRO	72	3.866	12.398	6.217	1.00	0.67	IL13
ATOM	1061	HA	PRO	72	4.241	11.720	6.964	1.00	0.76	IL13
ATOM	1062	CB	PRO	72	4.837	13.571	6.089	1.00	0.84	IL13
ATOM	1063	HB1	PRO	72	5.566	13.524	6.882	1.00	1.03	IL13
ATOM	1064	HB2	PRO	72	4.289	14.501	6.151	1.00	0.95	IL13
ATOM	1065	CG	PRO	72	5.549	13.483	4.737	1.00	0.73	IL13
ATOM	1066	HG1	PRO	72	6.581	13.207	4.886	1.00	0.79	IL13
ATOM	1067	HG2	PRO	72	5.496	14.440	4.237	1.00	0.84	IL13
ATOM	1068	CD	PRO	72	4.854	12.419	3.888	1.00	0.51	IL13
ATOM	1069	HD2	PRO	72	4.293	12.885	3.088	1.00	0.53	IL13
ATOM	1070	HD1	PRO	72	5.567	11.710	3.499	1.00	0.50	IL13
ATOM	1071	C	PRO	72	2.474	12.909	6.632	1.00	0.74	IL13
ATOM	1072	O	PRO	72	2.255	13.180	7.796	1.00	1.04	IL13
ATOM	1073	N	HIS	73	1.533	13.046	5.726	1.00	0.76	IL13
ATOM	1074	HN	HIS	73	1.711	12.824	4.788	1.00	0.86	IL13
ATOM	1075	CA	HIS	73	0.181	13.545	6.147	1.00	0.95	IL13
ATOM	1076	HA	HIS	73	0.293	14.167	7.024	1.00	1.18	IL13
ATOM	1077	CB	HIS	73	-0.462	14.382	5.033	1.00	1.53	IL13
ATOM	1078	HB1	HIS	73	0.296	14.992	4.563	1.00	2.36	IL13
ATOM	1079	HB2	HIS	73	-1.217	15.024	5.462	1.00	2.15	IL13

Figure 8 (19/30)

ATOM	1080	CG	HIS	73	-1.096	13.498	4.002	1.00	0.85	IL13
ATOM	1081	ND1	HIS	73	-2.428	13.115	4.063	1.00	0.78	IL13
ATOM	1082	HD1	HIS	73	-3.070	13.358	4.763	1.00	1.01	IL13
ATOM	1083	CD2	HIS	73	-0.596	12.937	2.861	1.00	1.00	IL13
ATOM	1084	HD2	HIS	73	0.425	13.033	2.520	1.00	1.15	IL13
ATOM	1085	CE1	HIS	73	-2.679	12.354	2.981	1.00	1.09	IL13
ATOM	1086	HE1	HIS	73	-3.640	11.916	2.757	1.00	1.38	IL13
ATOM	1087	NE2	HIS	73	-1.595	12.214	2.215	1.00	1.46	IL13
ATOM	1088	C	HIS	73	-0.707	12.353	6.509	1.00	0.64	IL13
ATOM	1089	O	HIS	73	-0.964	11.479	5.706	1.00	0.86	IL13
ATOM	1090	N	LYS	74	-1.148	12.313	7.738	1.00	0.59	IL13
ATOM	1091	HN	LYS	74	-0.901	13.027	8.361	1.00	0.83	IL13
ATOM	1092	CA	LYS	74	-1.996	11.185	8.217	1.00	0.72	IL13
ATOM	1093	HA	LYS	74	-1.567	10.245	7.903	1.00	0.91	IL13
ATOM	1094	CB	LYS	74	-2.058	11.238	9.744	1.00	1.15	IL13
ATOM	1095	HB1	LYS	74	-2.597	10.377	10.110	1.00	1.36	IL13
ATOM	1096	HB2	LYS	74	-2.565	12.140	10.053	1.00	1.22	IL13
ATOM	1097	CG	LYS	74	-0.637	11.225	10.314	1.00	1.42	IL13
ATOM	1098	HG1	LYS	74	-0.057	12.013	9.860	1.00	1.37	IL13
ATOM	1099	HG2	LYS	74	-0.174	10.271	10.107	1.00	1.61	IL13
ATOM	1100	CD	LYS	74	-0.695	11.447	11.826	1.00	2.06	IL13
ATOM	1101	HD1	LYS	74	-1.252	10.647	12.288	1.00	2.46	IL13
ATOM	1102	HD2	LYS	74	-1.180	12.391	12.031	1.00	2.40	IL13
ATOM	1103	CE	LYS	74	0.726	11.470	12.391	1.00	2.49	IL13
ATOM	1104	HE1	LYS	74	1.327	12.165	11.823	1.00	2.75	IL13
ATOM	1105	HE2	LYS	74	1.157	10.483	12.323	1.00	2.71	IL13
ATOM	1106	NZ	LYS	74	0.685	11.899	13.817	1.00	3.26	IL13
ATOM	1107	HZ1	LYS	74	1.599	11.693	14.268	1.00	3.58	IL13
ATOM	1108	HZ2	LYS	74	-0.071	11.383	14.312	1.00	3.72	IL13
ATOM	1109	HZ3	LYS	74	0.500	12.921	13.867	1.00	3.58	IL13
ATOM	1110	C	LYS	74	-3.410	11.324	7.655	1.00	0.55	IL13
ATOM	1111	O	LYS	74	-3.828	12.402	7.280	1.00	0.62	IL13
ATOM	1112	N	VAL	75	-4.139	10.237	7.592	1.00	0.50	IL13
ATOM	1113	HN	VAL	75	-3.767	9.385	7.901	1.00	0.64	IL13
ATOM	1114	CA	VAL	75	-5.532	10.282	7.054	1.00	0.38	IL13
ATOM	1115	HA	VAL	75	-5.851	11.306	6.942	1.00	0.36	IL13
ATOM	1116	CB	VAL	75	-5.559	9.592	5.691	1.00	0.51	IL13
ATOM	1117	HB	VAL	75	-5.335	8.543	5.815	1.00	1.15	IL13
ATOM	1118	CG1	VAL	75	-6.947	9.747	5.072	1.00	1.20	IL13
ATOM	1119	HG11	VAL	75	-7.354	8.772	4.847	1.00	1.80	IL13
ATOM	1120	HG12	VAL	75	-6.878	10.327	4.163	1.00	1.78	IL13
ATOM	1121	HG13	VAL	75	-7.592	10.253	5.771	1.00	1.72	IL13
ATOM	1122	CG2	VAL	75	-4.510	10.236	4.782	1.00	1.18	IL13
ATOM	1123	HG21	VAL	75	-3.522	9.998	5.150	1.00	1.79	IL13
ATOM	1124	HG22	VAL	75	-4.644	11.307	4.783	1.00	1.70	IL13
ATOM	1125	HG23	VAL	75	-4.619	9.859	3.776	1.00	1.71	IL13
ATOM	1126	C	VAL	75	-6.484	9.564	8.019	1.00	0.40	IL13
ATOM	1127	O	VAL	75	-6.238	8.447	8.431	1.00	0.54	IL13
ATOM	1128	N	SER	76	-7.574	10.196	8.374	1.00	0.36	IL13
ATOM	1129	HN	SER	76	-7.753	11.094	8.025	1.00	0.37	IL13
ATOM	1130	CA	SER	76	-8.548	9.553	9.306	1.00	0.43	IL13
ATOM	1131	HA	SER	76	-8.042	8.807	9.900	1.00	0.51	IL13
ATOM	1132	CB	SER	76	-9.156	10.610	10.228	1.00	0.53	IL13
ATOM	1133	HB1	SER	76	-8.364	11.191	10.678	1.00	1.15	IL13
ATOM	1134	HB2	SER	76	-9.728	10.128	11.003	1.00	1.20	IL13
ATOM	1135	OG	SER	76	-10.012	11.456	9.472	1.00	1.38	IL13
ATOM	1136	HG	SER	76	-10.285	12.183	10.037	1.00	1.78	IL13
ATOM	1137	C	SER	76	-9.668	8.888	8.501	1.00	0.39	IL13
ATOM	1138	O	SER	76	-9.847	9.151	7.329	1.00	0.38	IL13
ATOM	1139	N	ALA	77	-10.424	8.030	9.128	1.00	0.42	IL13
ATOM	1140	HN	ALA	77	-10.260	7.836	10.075	1.00	0.46	IL13

Figure 8 (20/30)

ATOM	1141	CA	ALA	77	-11.537	7.343	8.414	1.00	0.44	IL13
ATOM	1142	HA	ALA	77	-11.152	6.846	7.540	1.00	0.45	IL13
ATOM	1143	CB	ALA	77	-12.172	6.313	9.346	1.00	0.51	IL13
ATOM	1144	HB1	ALA	77	-12.773	5.627	8.768	1.00	1.11	IL13
ATOM	1145	HB2	ALA	77	-12.795	6.818	10.069	1.00	1.22	IL13
ATOM	1146	HB3	ALA	77	-11.395	5.766	9.859	1.00	1.09	IL13
ATOM	1147	C	ALA	77	-12.586	8.369	7.983	1.00	0.44	IL13
ATOM	1148	O	ALA	77	-13.584	8.024	7.383	1.00	0.53	IL13
ATOM	1149	N	GLY	78	-12.360	9.623	8.286	1.00	0.44	IL13
ATOM	1150	HN	GLY	78	-11.542	9.863	8.769	1.00	0.49	IL13
ATOM	1151	CA	GLY	78	-13.330	10.693	7.899	1.00	0.49	IL13
ATOM	1152	HA1	GLY	78	-13.558	11.298	8.762	1.00	0.55	IL13
ATOM	1153	HA2	GLY	78	-14.241	10.250	7.522	1.00	0.50	IL13
ATOM	1154	C	GLY	78	-12.708	11.579	6.817	1.00	0.47	IL13
ATOM	1155	O	GLY	78	-13.398	12.135	5.985	1.00	0.51	IL13
ATOM	1156	N	GLN	79	-11.410	11.721	6.825	1.00	0.45	IL13
ATOM	1157	HN	GLN	79	-10.871	11.267	7.506	1.00	0.45	IL13
ATOM	1158	CA	GLN	79	-10.749	12.578	5.799	1.00	0.45	IL13
ATOM	1159	HA	GLN	79	-11.437	13.339	5.464	1.00	0.49	IL13
ATOM	1160	CB	GLN	79	-9.513	13.237	6.399	1.00	0.50	IL13
ATOM	1161	HB1	GLN	79	-9.078	13.898	5.668	1.00	0.54	IL13
ATOM	1162	HB2	GLN	79	-8.798	12.472	6.665	1.00	0.49	IL13
ATOM	1163	CG	GLN	79	-9.906	14.031	7.649	1.00	0.57	IL13
ATOM	1164	HG1	GLN	79	-9.494	13.548	8.522	1.00	0.90	IL13
ATOM	1165	HG2	GLN	79	-10.982	14.058	7.731	1.00	1.10	IL13
ATOM	1166	CD	GLN	79	-9.366	15.463	7.564	1.00	1.52	IL13
ATOM	1167	OE1	GLN	79	-8.352	15.716	6.943	1.00	2.14	IL13
ATOM	1168	NE2	GLN	79	-10.006	16.420	8.177	1.00	2.15	IL13
ATOM	1169	HE21	GLN	79	-10.821	16.217	8.684	1.00	2.12	IL13
ATOM	1170	HE22	GLN	79	-9.674	17.340	8.131	1.00	2.89	IL13
ATOM	1171	C	GLN	79	-10.316	11.722	4.612	1.00	0.40	IL13
ATOM	1172	O	GLN	79	-9.644	10.728	4.776	1.00	0.40	IL13
ATOM	1173	N	PHE	80	-10.706	12.102	3.425	1.00	0.37	IL13
ATOM	1174	HN	PHE	80	-11.254	12.909	3.330	1.00	0.40	IL13
ATOM	1175	CA	PHE	80	-10.322	11.323	2.212	1.00	0.34	IL13
ATOM	1176	HA	PHE	80	-9.573	10.589	2.465	1.00	0.34	IL13
ATOM	1177	CB	PHE	80	-11.550	10.614	1.682	1.00	0.36	IL13
ATOM	1178	HB1	PHE	80	-11.296	10.108	0.773	1.00	0.37	IL13
ATOM	1179	HB2	PHE	80	-12.332	11.335	1.492	1.00	0.39	IL13
ATOM	1180	CG	PHE	80	-12.018	9.609	2.706	1.00	0.37	IL13
ATOM	1181	CD1	PHE	80	-13.211	9.823	3.404	1.00	0.42	IL13
ATOM	1182	HD1	PHE	80	-13.788	10.716	3.223	1.00	0.45	IL13
ATOM	1183	CD2	PHE	80	-11.262	8.457	2.948	1.00	0.38	IL13
ATOM	1184	HD2	PHE	80	-10.334	8.298	2.416	1.00	0.38	IL13
ATOM	1185	CE1	PHE	80	-13.653	8.879	4.340	1.00	0.45	IL13
ATOM	1186	HE1	PHE	80	-14.575	9.044	4.878	1.00	0.50	IL13
ATOM	1187	CE2	PHE	80	-11.700	7.515	3.885	1.00	0.42	IL13
ATOM	1188	HE2	PHE	80	-11.118	6.623	4.069	1.00	0.45	IL13
ATOM	1189	CZ	PHE	80	-12.898	7.724	4.579	1.00	0.45	IL13
ATOM	1190	HZ	PHE	80	-13.239	6.995	5.298	1.00	0.49	IL13
ATOM	1191	C	PHE	80	-9.754	12.258	1.141	1.00	0.35	IL13
ATOM	1192	O	PHE	80	-10.118	13.416	1.078	1.00	0.41	IL13
ATOM	1193	N	SER	81	-8.859	11.761	0.309	1.00	0.34	IL13
ATOM	1194	HN	SER	81	-8.585	10.824	0.396	1.00	0.33	IL13
ATOM	1195	CA	SER	81	-8.255	12.611	-0.771	1.00	0.39	IL13
ATOM	1196	HA	SER	81	-8.697	13.594	-0.747	1.00	0.43	IL13
ATOM	1197	CB	SER	81	-6.752	12.743	-0.527	1.00	0.45	IL13
ATOM	1198	HB1	SER	81	-6.335	13.444	-1.239	1.00	0.50	IL13
ATOM	1199	HB2	SER	81	-6.278	11.785	-0.650	1.00	0.50	IL13
ATOM	1200	OG	SER	81	-6.534	13.209	0.798	1.00	0.53	IL13
ATOM	1201	HG	SER	81	-7.324	13.673	1.083	1.00	0.98	IL13

Figure 8 (21/30)

ATOM	1202	C	SER	81	-8.487	12.001	-2.168	1.00	0.38	IL13
ATOM	1203	O	SER	81	-8.888	12.686	-3.087	1.00	0.47	IL13
ATOM	1204	N	SER	82	-8.188	10.736	-2.351	1.00	0.34	IL13
ATOM	1205	HN	SER	82	-7.828	10.207	-1.608	1.00	0.36	IL13
ATOM	1206	CA	SER	82	-8.338	10.113	-3.710	1.00	0.35	IL13
ATOM	1207	HA	SER	82	-8.255	10.882	-4.460	1.00	0.40	IL13
ATOM	1208	CB	SER	82	-7.212	9.099	-3.919	1.00	0.38	IL13
ATOM	1209	HB1	SER	82	-7.425	8.205	-3.347	1.00	0.39	IL13
ATOM	1210	HB2	SER	82	-6.279	9.520	-3.586	1.00	0.42	IL13
ATOM	1211	OG	SER	82	-7.116	8.782	-5.301	1.00	0.44	IL13
ATOM	1212	HG	SER	82	-7.678	8.022	-5.471	1.00	1.02	IL13
ATOM	1213	C	SER	82	-9.684	9.396	-3.881	1.00	0.34	IL13
ATOM	1214	O	SER	82	-9.986	8.895	-4.947	1.00	0.37	IL13
ATOM	1215	N	LEU	83	-10.489	9.317	-2.865	1.00	0.33	IL13
ATOM	1216	HN	LEU	83	-10.237	9.710	-2.003	1.00	0.33	IL13
ATOM	1217	CA	LEU	83	-11.792	8.603	-3.017	1.00	0.35	IL13
ATOM	1218	HA	LEU	83	-11.674	7.787	-3.711	1.00	0.37	IL13
ATOM	1219	CB	LEU	83	-12.222	8.048	-1.663	1.00	0.37	IL13
ATOM	1220	HB1	LEU	83	-13.237	7.693	-1.731	1.00	0.38	IL13
ATOM	1221	HB2	LEU	83	-12.174	8.825	-0.929	1.00	0.44	IL13
ATOM	1222	CG	LEU	83	-11.305	6.873	-1.274	1.00	0.54	IL13
ATOM	1223	HG	LEU	83	-10.558	6.709	-2.031	1.00	1.48	IL13
ATOM	1224	CD1	LEU	83	-10.609	7.114	0.056	1.00	1.30	IL13
ATOM	1225	HD11	LEU	83	-10.236	8.125	0.103	1.00	1.94	IL13
ATOM	1226	HD12	LEU	83	-9.781	6.424	0.154	1.00	1.80	IL13
ATOM	1227	HD13	LEU	83	-11.313	6.939	0.848	1.00	1.89	IL13
ATOM	1228	CD2	LEU	83	-12.157	5.631	-1.148	1.00	1.22	IL13
ATOM	1229	HD21	LEU	83	-12.626	5.434	-2.095	1.00	1.90	IL13
ATOM	1230	HD22	LEU	83	-12.916	5.784	-0.393	1.00	1.80	IL13
ATOM	1231	HD23	LEU	83	-11.525	4.807	-0.870	1.00	1.77	IL13
ATOM	1232	C	LEU	83	-12.864	9.549	-3.561	1.00	0.39	IL13
ATOM	1233	O	LEU	83	-14.041	9.376	-3.313	1.00	0.42	IL13
ATOM	1234	N	HIS	84	-12.471	10.539	-4.314	1.00	0.44	IL13
ATOM	1235	HN	HIS	84	-11.519	10.655	-4.512	1.00	0.46	IL13
ATOM	1236	CA	HIS	84	-13.474	11.482	-4.887	1.00	0.50	IL13
ATOM	1237	HA	HIS	84	-14.232	11.693	-4.149	1.00	0.54	IL13
ATOM	1238	CB	HIS	84	-12.775	12.780	-5.289	1.00	0.60	IL13
ATOM	1239	HB1	HIS	84	-13.513	13.518	-5.566	1.00	0.73	IL13
ATOM	1240	HB2	HIS	84	-12.115	12.594	-6.124	1.00	0.62	IL13
ATOM	1241	CG	HIS	84	-11.980	13.281	-4.120	1.00	0.60	IL13
ATOM	1242	ND1	HIS	84	-12.089	12.707	-2.866	1.00	0.53	IL13
ATOM	1243	HD1	HIS	84	-12.668	11.955	-2.621	1.00	0.71	IL13
ATOM	1244	CD2	HIS	84	-11.061	14.292	-3.994	1.00	0.90	IL13
ATOM	1245	HD2	HIS	84	-10.739	14.944	-4.792	1.00	1.24	IL13
ATOM	1246	CE1	HIS	84	-11.258	13.367	-2.046	1.00	0.52	IL13
ATOM	1247	HE1	HIS	84	-11.130	13.132	-1.005	1.00	0.53	IL13
ATOM	1248	NE2	HIS	84	-10.605	14.345	-2.680	1.00	0.80	IL13
ATOM	1249	C	HIS	84	-14.122	10.843	-6.120	1.00	0.45	IL13
ATOM	1250	O	HIS	84	-15.286	11.049	-6.401	1.00	0.46	IL13
ATOM	1251	N	VAL	85	-13.371	10.068	-6.854	1.00	0.47	IL13
ATOM	1252	HN	VAL	85	-12.437	9.919	-6.602	1.00	0.53	IL13
ATOM	1253	CA	VAL	85	-13.926	9.406	-8.073	1.00	0.48	IL13
ATOM	1254	HA	VAL	85	-14.563	10.098	-8.601	1.00	0.52	IL13
ATOM	1255	CB	VAL	85	-12.772	8.946	-8.983	1.00	0.59	IL13
ATOM	1256	HB	VAL	85	-12.990	7.956	-9.354	1.00	1.12	IL13
ATOM	1257	CG1	VAL	85	-12.584	9.899	-10.175	1.00	1.29	IL13
ATOM	1258	HG11	VAL	85	-12.847	10.909	-9.896	1.00	1.88	IL13
ATOM	1259	HG12	VAL	85	-13.209	9.577	-10.995	1.00	1.85	IL13
ATOM	1260	HG13	VAL	85	-11.550	9.876	-10.487	1.00	1.84	IL13
ATOM	1261	CG2	VAL	85	-11.474	8.904	-8.174	1.00	1.54	IL13
ATOM	1262	HG21	VAL	85	-11.188	9.909	-7.901	1.00	1.98	IL13

Figure 8 (22/30)

ATOM	1263	HG22	VAL	85	-10.693	8.459	-8.773	1.00	2.19	IL13
ATOM	1264	HG23	VAL	85	-11.624	8.316	-7.282	1.00	2.09	IL13
ATOM	1265	C	VAL	85	-14.759	8.193	-7.656	1.00	0.39	IL13
ATOM	1266	O	VAL	85	-14.532	7.596	-6.623	1.00	0.37	IL13
ATOM	1267	N	ARG	86	-15.732	7.832	-8.450	1.00	0.41	IL13
ATOM	1268	HN	ARG	86	-15.904	8.333	-9.274	1.00	0.47	IL13
ATOM	1269	CA	ARG	86	-16.588	6.667	-8.094	1.00	0.41	IL13
ATOM	1270	HA	ARG	86	-16.608	6.549	-7.021	1.00	0.41	IL13
ATOM	1271	CB	ARG	86	-18.009	6.905	-8.603	1.00	0.54	IL13
ATOM	1272	HB1	ARG	86	-18.613	6.032	-8.410	1.00	0.61	IL13
ATOM	1273	HB2	ARG	86	-17.981	7.095	-9.667	1.00	0.58	IL13
ATOM	1274	CG	ARG	86	-18.617	8.111	-7.887	1.00	0.60	IL13
ATOM	1275	HG1	ARG	86	-18.153	9.017	-8.249	1.00	0.64	IL13
ATOM	1276	HG2	ARG	86	-18.451	8.020	-6.823	1.00	0.68	IL13
ATOM	1277	CD	ARG	86	-20.118	8.162	-8.169	1.00	0.89	IL13
ATOM	1278	HD1	ARG	86	-20.635	7.514	-7.475	1.00	1.38	IL13
ATOM	1279	HD2	ARG	86	-20.307	7.829	-9.178	1.00	1.47	IL13
ATOM	1280	NE	ARG	86	-20.611	9.558	-8.007	1.00	1.58	IL13
ATOM	1281	HE	ARG	86	-20.049	10.229	-7.566	1.00	2.26	IL13
ATOM	1282	CZ	ARG	86	-21.786	9.889	-8.467	1.00	2.14	IL13
ATOM	1283	NH1	ARG	86	-22.212	11.116	-8.349	1.00	3.16	IL13
ATOM	1284	HH11	ARG	86	-21.638	11.805	-7.907	1.00	3.60	IL13
ATOM	1285	HH12	ARG	86	-23.114	11.368	-8.702	1.00	3.74	IL13
ATOM	1286	NH2	ARG	86	-22.536	8.989	-9.042	1.00	2.34	IL13
ATOM	1287	HH21	ARG	86	-22.210	8.047	-9.129	1.00	2.15	IL13
ATOM	1288	HH22	ARG	86	-23.438	9.240	-9.394	1.00	3.14	IL13
ATOM	1289	C	ARG	86	-16.034	5.392	-8.735	1.00	0.41	IL13
ATOM	1290	O	ARG	86	-16.653	4.800	-9.597	1.00	0.50	IL13
ATOM	1291	N	ASP	87	-14.882	4.955	-8.311	1.00	0.36	IL13
ATOM	1292	HN	ASP	87	-14.403	5.440	-7.606	1.00	0.34	IL13
ATOM	1293	CA	ASP	87	-14.301	3.709	-8.883	1.00	0.40	IL13
ATOM	1294	HA	ASP	87	-14.517	3.661	-9.941	1.00	0.50	IL13
ATOM	1295	CB	ASP	87	-12.786	3.694	-8.668	1.00	0.43	IL13
ATOM	1296	HB1	ASP	87	-12.414	2.693	-8.822	1.00	0.47	IL13
ATOM	1297	HB2	ASP	87	-12.563	4.010	-7.659	1.00	0.38	IL13
ATOM	1298	CG	ASP	87	-12.112	4.643	-9.661	1.00	0.56	IL13
ATOM	1299	OD1	ASP	87	-11.721	4.180	-10.720	1.00	1.13	IL13
ATOM	1300	OD2	ASP	87	-12.000	5.816	-9.347	1.00	1.34	IL13
ATOM	1301	C	ASP	87	-14.922	2.502	-8.178	1.00	0.34	IL13
ATOM	1302	O	ASP	87	-15.625	2.639	-7.197	1.00	0.31	IL13
ATOM	1303	N	THR	88	-14.666	1.321	-8.666	1.00	0.40	IL13
ATOM	1304	HN	THR	88	-14.093	1.231	-9.456	1.00	0.47	IL13
ATOM	1305	CA	THR	88	-15.237	0.105	-8.019	1.00	0.41	IL13
ATOM	1306	HA	THR	88	-16.154	0.355	-7.508	1.00	0.42	IL13
ATOM	1307	CB	THR	88	-15.492	-0.976	-9.083	1.00	0.54	IL13
ATOM	1308	HB	THR	88	-15.365	-1.949	-8.631	1.00	1.27	IL13
ATOM	1309	OG1	THR	88	-14.542	-0.827	-10.128	1.00	1.16	IL13
ATOM	1310	HG1	THR	88	-14.823	-1.375	-10.864	1.00	1.59	IL13
ATOM	1311	CG2	THR	88	-16.911	-0.879	-9.672	1.00	1.28	IL13
ATOM	1312	HG21	THR	88	-17.519	-1.676	-9.269	1.00	1.85	IL13
ATOM	1313	HG22	THR	88	-16.856	-0.983	-10.745	1.00	1.78	IL13
ATOM	1314	HG23	THR	88	-17.359	0.072	-9.433	1.00	1.93	IL13
ATOM	1315	C	THR	88	-14.235	-0.434	-7.001	1.00	0.33	IL13
ATOM	1316	O	THR	88	-13.046	-0.206	-7.101	1.00	0.32	IL13
ATOM	1317	N	LYS	89	-14.710	-1.141	-6.016	1.00	0.30	IL13
ATOM	1318	HN	LYS	89	-15.674	-1.298	-5.948	1.00	0.34	IL13
ATOM	1319	CA	LYS	89	-13.788	-1.688	-4.985	1.00	0.24	IL13
ATOM	1320	HA	LYS	89	-13.001	-0.985	-4.794	1.00	0.22	IL13
ATOM	1321	CB	LYS	89	-14.560	-1.961	-3.697	1.00	0.28	IL13
ATOM	1322	HB1	LYS	89	-13.877	-2.332	-2.958	1.00	0.27	IL13
ATOM	1323	HB2	LYS	89	-15.330	-2.694	-3.880	1.00	0.34	IL13

Figure 8 (23/30)

ATOM	1324	CG	LYS	89	-15.190	-0.677	-3.170	1.00	0.33	IL13
ATOM	1325	HG1	LYS	89	-15.876	-0.283	-3.905	1.00	0.37	IL13
ATOM	1326	HG2	LYS	89	-14.417	0.050	-2.967	1.00	0.32	IL13
ATOM	1327	CD	LYS	89	-15.953	-0.995	-1.880	1.00	0.41	IL13
ATOM	1328	HD1	LYS	89	-15.269	-1.393	-1.146	1.00	0.57	IL13
ATOM	1329	HD2	LYS	89	-16.724	-1.723	-2.088	1.00	0.72	IL13
ATOM	1330	CE	LYS	89	-16.589	0.282	-1.342	1.00	0.75	IL13
ATOM	1331	HE1	LYS	89	-16.951	0.871	-2.168	1.00	1.23	IL13
ATOM	1332	HE2	LYS	89	-15.850	0.840	-0.791	1.00	1.31	IL13
ATOM	1333	NZ	LYS	89	-17.723	-0.054	-0.438	1.00	1.49	IL13
ATOM	1334	HZ1	LYS	89	-18.331	0.782	-0.323	1.00	1.86	IL13
ATOM	1335	HZ2	LYS	89	-17.351	-0.343	0.490	1.00	2.05	IL13
ATOM	1336	HZ3	LYS	89	-18.277	-0.830	-0.848	1.00	2.04	IL13
ATOM	1337	C	LYS	89	-13.180	-3.003	-5.485	1.00	0.24	IL13
ATOM	1338	O	LYS	89	-13.777	-3.709	-6.274	1.00	0.28	IL13
ATOM	1339	N	ILE	90	-11.994	-3.327	-5.025	1.00	0.20	IL13
ATOM	1340	HN	ILE	90	-11.544	-2.731	-4.390	1.00	0.18	IL13
ATOM	1341	CA	ILE	90	-11.318	-4.591	-5.454	1.00	0.21	IL13
ATOM	1342	HA	ILE	90	-12.016	-5.212	-5.997	1.00	0.23	IL13
ATOM	1343	CB	ILE	90	-10.132	-4.243	-6.369	1.00	0.22	IL13
ATOM	1344	HB	ILE	90	-9.618	-5.152	-6.650	1.00	0.23	IL13
ATOM	1345	CG1	ILE	90	-9.159	-3.306	-5.631	1.00	0.20	IL13
ATOM	1346	HG11	ILE	90	-8.850	-3.762	-4.703	1.00	0.22	IL13
ATOM	1347	HG12	ILE	90	-9.652	-2.370	-5.421	1.00	0.23	IL13
ATOM	1348	CG2	ILE	90	-10.663	-3.550	-7.629	1.00	0.27	IL13
ATOM	1349	HG21	ILE	90	-10.280	-2.541	-7.675	1.00	1.04	IL13
ATOM	1350	HG22	ILE	90	-11.742	-3.524	-7.601	1.00	0.99	IL13
ATOM	1351	HG23	ILE	90	-10.339	-4.096	-8.503	1.00	1.07	IL13
ATOM	1352	CD1	ILE	90	-7.916	-3.041	-6.489	1.00	0.23	IL13
ATOM	1353	HD11	ILE	90	-7.070	-3.558	-6.060	1.00	1.05	IL13
ATOM	1354	HD12	ILE	90	-7.714	-1.981	-6.509	1.00	1.06	IL13
ATOM	1355	HD13	ILE	90	-8.079	-3.395	-7.495	1.00	1.03	IL13
ATOM	1356	C	ILE	90	-10.833	-5.357	-4.216	1.00	0.19	IL13
ATOM	1357	O	ILE	90	-10.688	-4.797	-3.148	1.00	0.18	IL13
ATOM	1358	N	GLU	91	-10.588	-6.632	-4.350	1.00	0.21	IL13
ATOM	1359	HN	GLU	91	-10.714	-7.067	-5.219	1.00	0.23	IL13
ATOM	1360	CA	GLU	91	-10.120	-7.431	-3.179	1.00	0.21	IL13
ATOM	1361	HA	GLU	91	-10.822	-7.322	-2.366	1.00	0.21	IL13
ATOM	1362	CB	GLU	91	-10.026	-8.907	-3.576	1.00	0.24	IL13
ATOM	1363	HB1	GLU	91	-9.593	-9.473	-2.766	1.00	0.25	IL13
ATOM	1364	HB2	GLU	91	-9.407	-9.004	-4.457	1.00	0.26	IL13
ATOM	1365	CG	GLU	91	-11.429	-9.439	-3.876	1.00	0.28	IL13
ATOM	1366	HG1	GLU	91	-11.812	-8.960	-4.765	1.00	0.80	IL13
ATOM	1367	HG2	GLU	91	-12.081	-9.224	-3.042	1.00	0.83	IL13
ATOM	1368	CD	GLU	91	-11.369	-10.951	-4.102	1.00	1.14	IL13
ATOM	1369	OE1	GLU	91	-12.164	-11.651	-3.497	1.00	1.86	IL13
ATOM	1370	OE2	GLU	91	-10.529	-11.383	-4.874	1.00	1.88	IL13
ATOM	1371	C	GLU	91	-8.745	-6.927	-2.733	1.00	0.19	IL13
ATOM	1372	O	GLU	91	-7.924	-6.549	-3.545	1.00	0.18	IL13
ATOM	1373	N	VAL	92	-8.485	-6.906	-1.450	1.00	0.19	IL13
ATOM	1374	HN	VAL	92	-9.161	-7.204	-0.802	1.00	0.20	IL13
ATOM	1375	CA	VAL	92	-7.160	-6.406	-0.982	1.00	0.19	IL13
ATOM	1376	HA	VAL	92	-7.056	-5.368	-1.251	1.00	0.18	IL13
ATOM	1377	CB	VAL	92	-7.037	-6.557	0.540	1.00	0.22	IL13
ATOM	1378	HB	VAL	92	-7.271	-7.578	0.813	1.00	0.24	IL13
ATOM	1379	CG1	VAL	92	-5.583	-6.248	0.948	1.00	0.24	IL13
ATOM	1380	HG11	VAL	92	-5.127	-5.620	0.196	1.00	1.06	IL13
ATOM	1381	HG12	VAL	92	-5.030	-7.172	1.020	1.00	1.00	IL13
ATOM	1382	HG13	VAL	92	-5.552	-5.744	1.900	1.00	1.07	IL13
ATOM	1383	CG2	VAL	92	-8.030	-5.600	1.231	1.00	0.24	IL13
ATOM	1384	HG21	VAL	92	-7.794	-5.502	2.280	1.00	1.05	IL13

Figure 8 (24/30)

ATOM	1385	HG22	VAL	92	-9.025	-5.999	1.137	1.00	0.98	IL13
ATOM	1386	HG23	VAL	92	-7.990	-4.630	0.760	1.00	1.08	IL13
ATOM	1387	C	VAL	92	-6.049	-7.219	-1.651	1.00	0.20	IL13
ATOM	1388	O	VAL	92	-5.043	-6.682	-2.073	1.00	0.19	IL13
ATOM	1389	N	ALA	93	-6.220	-8.507	-1.753	1.00	0.22	IL13
ATOM	1390	HN	ALA	93	-7.037	-8.922	-1.407	1.00	0.23	IL13
ATOM	1391	CA	ALA	93	-5.170	-9.346	-2.395	1.00	0.25	IL13
ATOM	1392	HA	ALA	93	-4.309	-9.403	-1.744	1.00	0.28	IL13
ATOM	1393	CB	ALA	93	-5.721	-10.754	-2.632	1.00	0.31	IL13
ATOM	1394	HB1	ALA	93	-6.083	-10.832	-3.646	1.00	1.05	IL13
ATOM	1395	HB2	ALA	93	-6.531	-10.943	-1.944	1.00	1.02	IL13
ATOM	1396	HB3	ALA	93	-4.936	-11.479	-2.473	1.00	1.10	IL13
ATOM	1397	C	ALA	93	-4.757	-8.720	-3.732	1.00	0.22	IL13
ATOM	1398	O	ALA	93	-3.592	-8.673	-4.067	1.00	0.24	IL13
ATOM	1399	N	GLN	94	-5.697	-8.229	-4.495	1.00	0.21	IL13
ATOM	1400	HN	GLN	94	-6.633	-8.267	-4.206	1.00	0.22	IL13
ATOM	1401	CA	GLN	94	-5.341	-7.599	-5.802	1.00	0.22	IL13
ATOM	1402	HA	GLN	94	-4.629	-8.225	-6.318	1.00	0.26	IL13
ATOM	1403	CB	GLN	94	-6.592	-7.433	-6.666	1.00	0.28	IL13
ATOM	1404	HB1	GLN	94	-6.437	-6.636	-7.377	1.00	0.78	IL13
ATOM	1405	HB2	GLN	94	-7.435	-7.193	-6.033	1.00	0.91	IL13
ATOM	1406	CG	GLN	94	-6.872	-8.734	-7.413	1.00	1.00	IL13
ATOM	1407	HG1	GLN	94	-7.031	-9.529	-6.703	1.00	1.55	IL13
ATOM	1408	HG2	GLN	94	-6.028	-8.972	-8.043	1.00	1.62	IL13
ATOM	1409	CD	GLN	94	-8.121	-8.569	-8.279	1.00	1.32	IL13
ATOM	1410	OE1	GLN	94	-9.017	-7.823	-7.939	1.00	1.59	IL13
ATOM	1411	NE2	GLN	94	-8.214	-9.236	-9.396	1.00	2.05	IL13
ATOM	1412	HE21	GLN	94	-7.488	-9.835	-9.671	1.00	2.51	IL13
ATOM	1413	HE22	GLN	94	-9.009	-9.139	-9.961	1.00	2.39	IL13
ATOM	1414	C	GLN	94	-4.722	-6.227	-5.562	1.00	0.19	IL13
ATOM	1415	O	GLN	94	-3.815	-5.811	-6.255	1.00	0.19	IL13
ATOM	1416	N	PHE	95	-5.210	-5.522	-4.590	1.00	0.17	IL13
ATOM	1417	HN	PHE	95	-5.945	-5.877	-4.048	1.00	0.19	IL13
ATOM	1418	CA	PHE	95	-4.662	-4.175	-4.302	1.00	0.17	IL13
ATOM	1419	HA	PHE	95	-4.797	-3.532	-5.159	1.00	0.19	IL13
ATOM	1420	CB	PHE	95	-5.401	-3.596	-3.105	1.00	0.18	IL13
ATOM	1421	HB1	PHE	95	-5.275	-4.250	-2.257	1.00	0.18	IL13
ATOM	1422	HB2	PHE	95	-6.450	-3.504	-3.340	1.00	0.19	IL13
ATOM	1423	CG	PHE	95	-4.834	-2.247	-2.780	1.00	0.19	IL13
ATOM	1424	CD1	PHE	95	-5.443	-1.091	-3.273	1.00	0.21	IL13
ATOM	1425	HD1	PHE	95	-6.329	-1.164	-3.886	1.00	0.22	IL13
ATOM	1426	CD2	PHE	95	-3.687	-2.155	-1.986	1.00	0.22	IL13
ATOM	1427	HD2	PHE	95	-3.219	-3.052	-1.606	1.00	0.23	IL13
ATOM	1428	CE1	PHE	95	-4.904	0.159	-2.970	1.00	0.23	IL13
ATOM	1429	HE1	PHE	95	-5.372	1.054	-3.345	1.00	0.26	IL13
ATOM	1430	CE2	PHE	95	-3.149	-0.906	-1.683	1.00	0.25	IL13
ATOM	1431	HE2	PHE	95	-2.264	-0.831	-1.069	1.00	0.29	IL13
ATOM	1432	CZ	PHE	95	-3.759	0.249	-2.176	1.00	0.25	IL13
ATOM	1433	HZ	PHE	95	-3.345	1.206	-1.948	1.00	0.29	IL13
ATOM	1434	C	PHE	95	-3.177	-4.285	-3.965	1.00	0.16	IL13
ATOM	1435	O	PHE	95	-2.357	-3.547	-4.473	1.00	0.17	IL13
ATOM	1436	N	VAL	96	-2.825	-5.199	-3.107	1.00	0.17	IL13
ATOM	1437	HN	VAL	96	-3.502	-5.783	-2.706	1.00	0.17	IL13
ATOM	1438	CA	VAL	96	-1.394	-5.355	-2.733	1.00	0.18	IL13
ATOM	1439	HA	VAL	96	-1.020	-4.424	-2.333	1.00	0.19	IL13
ATOM	1440	CB	VAL	96	-1.258	-6.457	-1.683	1.00	0.21	IL13
ATOM	1441	HB	VAL	96	-1.632	-7.386	-2.090	1.00	0.20	IL13
ATOM	1442	CG1	VAL	96	0.215	-6.625	-1.309	1.00	0.25	IL13
ATOM	1443	HG11	VAL	96	0.724	-7.173	-2.088	1.00	1.06	IL13
ATOM	1444	HG12	VAL	96	0.290	-7.167	-0.379	1.00	0.99	IL13
ATOM	1445	HG13	VAL	96	0.670	-5.652	-1.197	1.00	1.09	IL13

Figure 8 (25/30)

ATOM	1446	CG2	VAL	96	-2.063	-6.084	-0.438	1.00	0.24	IL13
ATOM	1447	HG21	VAL	96	-2.549	-6.966	-0.048	1.00	1.03	IL13
ATOM	1448	HG22	VAL	96	-2.809	-5.348	-0.699	1.00	1.01	IL13
ATOM	1449	HG23	VAL	96	-1.401	-5.677	0.311	1.00	1.07	IL13
ATOM	1450	C	VAL	96	-0.585	-5.745	-3.970	1.00	0.17	IL13
ATOM	1451	O	VAL	96	0.445	-5.169	-4.260	1.00	0.18	IL13
ATOM	1452	N	LYS	97	-1.040	-6.729	-4.694	1.00	0.17	IL13
ATOM	1453	HN	LYS	97	-1.869	-7.185	-4.436	1.00	0.18	IL13
ATOM	1454	CA	LYS	97	-0.295	-7.170	-5.903	1.00	0.19	IL13
ATOM	1455	HA	LYS	97	0.694	-7.493	-5.617	1.00	0.20	IL13
ATOM	1456	CB	LYS	97	-1.038	-8.334	-6.559	1.00	0.21	IL13
ATOM	1457	HB1	LYS	97	-0.569	-8.574	-7.502	1.00	0.23	IL13
ATOM	1458	HB2	LYS	97	-2.068	-8.057	-6.726	1.00	0.21	IL13
ATOM	1459	CG	LYS	97	-0.975	-9.552	-5.638	1.00	0.25	IL13
ATOM	1460	HG1	LYS	97	-1.416	-9.303	-4.686	1.00	0.24	IL13
ATOM	1461	HG2	LYS	97	0.057	-9.839	-5.493	1.00	0.26	IL13
ATOM	1462	CD	LYS	97	-1.743	-10.714	-6.274	1.00	0.31	IL13
ATOM	1463	HD1	LYS	97	-1.215	-11.056	-7.151	1.00	0.69	IL13
ATOM	1464	HD2	LYS	97	-2.730	-10.378	-6.557	1.00	0.71	IL13
ATOM	1465	CE	LYS	97	-1.866	-11.871	-5.274	1.00	0.68	IL13
ATOM	1466	HE1	LYS	97	-2.910	-12.072	-5.087	1.00	1.31	IL13
ATOM	1467	HE2	LYS	97	-1.379	-11.607	-4.348	1.00	1.39	IL13
ATOM	1468	NZ	LYS	97	-1.221	-13.089	-5.837	1.00	1.52	IL13
ATOM	1469	HZ1	LYS	97	-0.375	-12.817	-6.376	1.00	1.99	IL13
ATOM	1470	HZ2	LYS	97	-1.892	-13.577	-6.465	1.00	2.14	IL13
ATOM	1471	HZ3	LYS	97	-0.946	-13.725	-5.062	1.00	2.02	IL13
ATOM	1472	C	LYS	97	-0.184	-6.015	-6.896	1.00	0.18	IL13
ATOM	1473	O	LYS	97	0.878	-5.721	-7.383	1.00	0.19	IL13
ATOM	1474	N	ASP	98	-1.264	-5.349	-7.198	1.00	0.18	IL13
ATOM	1475	HN	ASP	98	-2.124	-5.589	-6.795	1.00	0.18	IL13
ATOM	1476	CA	ASP	98	-1.177	-4.225	-8.176	1.00	0.20	IL13
ATOM	1477	HA	ASP	98	-0.855	-4.601	-9.136	1.00	0.21	IL13
ATOM	1478	CB	ASP	98	-2.549	-3.563	-8.316	1.00	0.21	IL13
ATOM	1479	HB1	ASP	98	-2.451	-2.648	-8.880	1.00	0.23	IL13
ATOM	1480	HB2	ASP	98	-2.939	-3.339	-7.333	1.00	0.21	IL13
ATOM	1481	CG	ASP	98	-3.508	-4.507	-9.041	1.00	0.24	IL13
ATOM	1482	OD1	ASP	98	-4.705	-4.359	-8.858	1.00	1.07	IL13
ATOM	1483	OD2	ASP	98	-3.029	-5.359	-9.772	1.00	1.02	IL13
ATOM	1484	C	ASP	98	-0.177	-3.196	-7.664	1.00	0.19	IL13
ATOM	1485	O	ASP	98	0.616	-2.658	-8.412	1.00	0.21	IL13
ATOM	1486	N	LEU	99	-0.196	-2.930	-6.394	1.00	0.19	IL13
ATOM	1487	HN	LEU	99	-0.836	-3.384	-5.808	1.00	0.19	IL13
ATOM	1488	CA	LEU	99	0.764	-1.950	-5.828	1.00	0.20	IL13
ATOM	1489	HA	LEU	99	0.685	-1.041	-6.396	1.00	0.21	IL13
ATOM	1490	CB	LEU	99	0.388	-1.682	-4.353	1.00	0.23	IL13
ATOM	1491	HB1	LEU	99	0.398	-2.621	-3.820	1.00	0.22	IL13
ATOM	1492	HB2	LEU	99	-0.608	-1.267	-4.316	1.00	0.24	IL13
ATOM	1493	CG	LEU	99	1.364	-0.699	-3.668	1.00	0.25	IL13
ATOM	1494	HG	LEU	99	2.362	-1.040	-3.827	1.00	0.25	IL13
ATOM	1495	CD1	LEU	99	1.221	0.733	-4.220	1.00	0.29	IL13
ATOM	1496	HD11	LEU	99	1.867	1.398	-3.663	1.00	1.07	IL13
ATOM	1497	HD12	LEU	99	0.199	1.060	-4.119	1.00	1.07	IL13
ATOM	1498	HD13	LEU	99	1.508	0.762	-5.257	1.00	1.04	IL13
ATOM	1499	CD2	LEU	99	1.083	-0.682	-2.156	1.00	0.30	IL13
ATOM	1500	HD21	LEU	99	0.938	0.335	-1.822	1.00	1.07	IL13
ATOM	1501	HD22	LEU	99	1.922	-1.113	-1.632	1.00	0.98	IL13
ATOM	1502	HD23	LEU	99	0.194	-1.256	-1.944	1.00	1.05	IL13
ATOM	1503	C	LEU	99	2.194	-2.510	-5.966	1.00	0.19	IL13
ATOM	1504	O	LEU	99	3.118	-1.790	-6.277	1.00	0.20	IL13
ATOM	1505	N	LEU	100	2.379	-3.790	-5.742	1.00	0.19	IL13
ATOM	1506	HN	LEU	100	1.618	-4.355	-5.496	1.00	0.20	IL13

Figure 8 (26/30)

ATOM	1507	CA	LEU	100	3.751	-4.393	-5.853	1.00	0.20	IL13
ATOM	1508	HA	LEU	100	4.375	-4.001	-5.065	1.00	0.21	IL13
ATOM	1509	CB	LEU	100	3.647	-5.922	-5.698	1.00	0.22	IL13
ATOM	1510	HB1	LEU	100	2.937	-6.304	-6.413	1.00	0.23	IL13
ATOM	1511	HB2	LEU	100	3.305	-6.154	-4.700	1.00	0.24	IL13
ATOM	1512	CG	LEU	100	5.010	-6.597	-5.932	1.00	0.25	IL13
ATOM	1513	HG	LEU	100	5.337	-6.433	-6.948	1.00	0.28	IL13
ATOM	1514	CD1	LEU	100	6.049	-6.024	-4.962	1.00	0.30	IL13
ATOM	1515	HD11	LEU	100	6.819	-6.758	-4.779	1.00	0.99	IL13
ATOM	1516	HD12	LEU	100	5.568	-5.767	-4.030	1.00	1.06	IL13
ATOM	1517	HD13	LEU	100	6.492	-5.139	-5.394	1.00	1.09	IL13
ATOM	1518	CD2	LEU	100	4.860	-8.103	-5.694	1.00	0.27	IL13
ATOM	1519	HD21	LEU	100	5.815	-8.590	-5.826	1.00	0.96	IL13
ATOM	1520	HD22	LEU	100	4.152	-8.508	-6.402	1.00	0.93	IL13
ATOM	1521	HD23	LEU	100	4.502	-8.274	-4.691	1.00	0.96	IL13
ATOM	1522	C	LEU	100	4.384	-4.056	-7.209	1.00	0.20	IL13
ATOM	1523	O	LEU	100	5.546	-3.699	-7.278	1.00	0.21	IL13
ATOM	1524	N	LEU	101	3.656	-4.168	-8.288	1.00	0.21	IL13
ATOM	1525	HN	LEU	101	2.721	-4.463	-8.230	1.00	0.22	IL13
ATOM	1526	CA	LEU	101	4.275	-3.851	-9.611	1.00	0.23	IL13
ATOM	1527	HA	LEU	101	5.100	-4.523	-9.783	1.00	0.25	IL13
ATOM	1528	CB	LEU	101	3.249	-4.015	-10.741	1.00	0.26	IL13
ATOM	1529	HB1	LEU	101	3.545	-3.416	-11.588	1.00	0.29	IL13
ATOM	1530	HB2	LEU	101	2.287	-3.670	-10.387	1.00	0.30	IL13
ATOM	1531	CG	LEU	101	3.121	-5.488	-11.165	1.00	0.30	IL13
ATOM	1532	HG	LEU	101	2.315	-5.562	-11.883	1.00	0.35	IL13
ATOM	1533	CD1	LEU	101	4.423	-5.972	-11.852	1.00	0.43	IL13
ATOM	1534	HD11	LEU	101	5.035	-6.536	-11.168	1.00	1.19	IL13
ATOM	1535	HD12	LEU	101	4.986	-5.122	-12.204	1.00	1.09	IL13
ATOM	1536	HD13	LEU	101	4.164	-6.595	-12.695	1.00	1.08	IL13
ATOM	1537	CD2	LEU	101	2.768	-6.348	-9.942	1.00	0.47	IL13
ATOM	1538	HD21	LEU	101	3.651	-6.606	-9.377	1.00	1.17	IL13
ATOM	1539	HD22	LEU	101	2.269	-7.249	-10.266	1.00	1.14	IL13
ATOM	1540	HD23	LEU	101	2.106	-5.785	-9.319	1.00	1.09	IL13
ATOM	1541	C	LEU	101	4.792	-2.412	-9.618	1.00	0.22	IL13
ATOM	1542	O	LEU	101	5.886	-2.147	-10.071	1.00	0.23	IL13
ATOM	1543	N	HIS	102	4.026	-1.481	-9.130	1.00	0.22	IL13
ATOM	1544	HN	HIS	102	3.142	-1.706	-8.770	1.00	0.22	IL13
ATOM	1545	CA	HIS	102	4.497	-0.068	-9.129	1.00	0.22	IL13
ATOM	1546	HA	HIS	102	4.853	0.178	-10.120	1.00	0.23	IL13
ATOM	1547	CB	HIS	102	3.341	0.868	-8.777	1.00	0.23	IL13
ATOM	1548	HB1	HIS	102	3.731	1.819	-8.452	1.00	0.23	IL13
ATOM	1549	HB2	HIS	102	2.748	0.430	-7.988	1.00	0.24	IL13
ATOM	1550	CG	HIS	102	2.487	1.068	-9.996	1.00	0.25	IL13
ATOM	1551	ND1	HIS	102	2.719	2.088	-10.906	1.00	0.26	IL13
ATOM	1552	HD1	HIS	102	3.427	2.763	-10.851	1.00	0.26	IL13
ATOM	1553	CD2	HIS	102	1.406	0.379	-10.473	1.00	0.28	IL13
ATOM	1554	HD2	HIS	102	0.962	-0.479	-9.993	1.00	0.30	IL13
ATOM	1555	CE1	HIS	102	1.795	1.982	-11.877	1.00	0.29	IL13
ATOM	1556	HE1	HIS	102	1.734	2.645	-12.728	1.00	0.32	IL13
ATOM	1557	NE2	HIS	102	0.968	0.955	-11.663	1.00	0.30	IL13
ATOM	1558	C	HIS	102	5.644	0.127	-8.132	1.00	0.21	IL13
ATOM	1559	O	HIS	102	6.537	0.907	-8.362	1.00	0.22	IL13
ATOM	1560	N	LEU	103	5.631	-0.542	-7.015	1.00	0.21	IL13
ATOM	1561	HN	LEU	103	4.898	-1.162	-6.815	1.00	0.21	IL13
ATOM	1562	CA	LEU	103	6.738	-0.322	-6.032	1.00	0.22	IL13
ATOM	1563	HA	LEU	103	6.731	0.708	-5.715	1.00	0.23	IL13
ATOM	1564	CB	LEU	103	6.549	-1.233	-4.815	1.00	0.22	IL13
ATOM	1565	HB1	LEU	103	7.422	-1.192	-4.192	1.00	0.22	IL13
ATOM	1566	HB2	LEU	103	6.405	-2.248	-5.155	1.00	0.23	IL13
ATOM	1567	CG	LEU	103	5.326	-0.799	-4.008	1.00	0.23	IL13

Figure 8 (27/30)

ATOM	1568	HG	LEU	103	4.476	-0.809	-4.657	1.00	0.25	IL13
ATOM	1569	CD1	LEU	103	5.111	-1.782	-2.856	1.00	0.24	IL13
ATOM	1570	HD11	LEU	103	5.867	-1.620	-2.101	1.00	1.01	IL13
ATOM	1571	HD12	LEU	103	5.185	-2.793	-3.225	1.00	1.04	IL13
ATOM	1572	HD13	LEU	103	4.135	-1.627	-2.423	1.00	1.07	IL13
ATOM	1573	CD2	LEU	103	5.507	0.610	-3.431	1.00	0.24	IL13
ATOM	1574	HD21	LEU	103	4.964	0.688	-2.500	1.00	1.01	IL13
ATOM	1575	HD22	LEU	103	5.123	1.338	-4.130	1.00	1.04	IL13
ATOM	1576	HD23	LEU	103	6.548	0.799	-3.253	1.00	1.09	IL13
ATOM	1577	C	LEU	103	8.097	-0.634	-6.668	1.00	0.23	IL13
ATOM	1578	O	LEU	103	8.979	0.201	-6.690	1.00	0.25	IL13
ATOM	1579	N	LYS	104	8.287	-1.819	-7.181	1.00	0.23	IL13
ATOM	1580	HN	LYS	104	7.573	-2.492	-7.156	1.00	0.23	IL13
ATOM	1581	CA	LYS	104	9.609	-2.141	-7.796	1.00	0.26	IL13
ATOM	1582	HA	LYS	104	10.388	-1.899	-7.086	1.00	0.29	IL13
ATOM	1583	CB	LYS	104	9.693	-3.639	-8.133	1.00	0.32	IL13
ATOM	1584	HB1	LYS	104	9.590	-4.212	-7.224	1.00	0.36	IL13
ATOM	1585	HB2	LYS	104	10.654	-3.849	-8.578	1.00	0.37	IL13
ATOM	1586	CG	LYS	104	8.584	-4.045	-9.112	1.00	0.34	IL13
ATOM	1587	HG1	LYS	104	8.596	-3.396	-9.973	1.00	0.37	IL13
ATOM	1588	HG2	LYS	104	7.625	-3.976	-8.620	1.00	0.38	IL13
ATOM	1589	CD	LYS	104	8.824	-5.488	-9.567	1.00	0.46	IL13
ATOM	1590	HD1	LYS	104	9.183	-6.075	-8.735	1.00	1.13	IL13
ATOM	1591	HD2	LYS	104	9.561	-5.497	-10.357	1.00	1.30	IL13
ATOM	1592	CE	LYS	104	7.516	-6.088	-10.086	1.00	1.06	IL13
ATOM	1593	HE1	LYS	104	7.045	-5.392	-10.762	1.00	1.68	IL13
ATOM	1594	HE2	LYS	104	6.857	-6.285	-9.254	1.00	1.61	IL13
ATOM	1595	NZ	LYS	104	7.802	-7.362	-10.804	1.00	1.73	IL13
ATOM	1596	HZ1	LYS	104	8.139	-8.076	-10.127	1.00	2.10	IL13
ATOM	1597	HZ2	LYS	104	8.532	-7.196	-11.527	1.00	2.23	IL13
ATOM	1598	HZ3	LYS	104	6.933	-7.705	-11.261	1.00	2.20	IL13
ATOM	1599	C	LYS	104	9.816	-1.297	-9.057	1.00	0.24	IL13
ATOM	1600	O	LYS	104	10.925	-1.116	-9.520	1.00	0.25	IL13
ATOM	1601	N	LYS	105	8.755	-0.794	-9.624	1.00	0.24	IL13
ATOM	1602	HN	LYS	105	7.870	-0.962	-9.238	1.00	0.26	IL13
ATOM	1603	CA	LYS	105	8.881	0.025	-10.865	1.00	0.25	IL13
ATOM	1604	HA	LYS	105	9.361	-0.563	-11.632	1.00	0.27	IL13
ATOM	1605	CB	LYS	105	7.482	0.422	-11.338	1.00	0.28	IL13
ATOM	1606	HB1	LYS	105	7.055	1.126	-10.642	1.00	0.41	IL13
ATOM	1607	HB2	LYS	105	6.857	-0.456	-11.388	1.00	0.39	IL13
ATOM	1608	CG	LYS	105	7.560	1.068	-12.720	1.00	0.40	IL13
ATOM	1609	HG1	LYS	105	7.985	0.367	-13.422	1.00	0.53	IL13
ATOM	1610	HG2	LYS	105	8.180	1.952	-12.669	1.00	0.54	IL13
ATOM	1611	CD	LYS	105	6.149	1.451	-13.171	1.00	0.43	IL13
ATOM	1612	HD1	LYS	105	5.682	2.060	-12.413	1.00	0.83	IL13
ATOM	1613	HD2	LYS	105	5.566	0.553	-13.321	1.00	0.76	IL13
ATOM	1614	CE	LYS	105	6.220	2.235	-14.482	1.00	1.13	IL13
ATOM	1615	HE1	LYS	105	6.995	2.984	-14.413	1.00	1.64	IL13
ATOM	1616	HE2	LYS	105	5.271	2.717	-14.663	1.00	1.77	IL13
ATOM	1617	NZ	LYS	105	6.526	1.305	-15.605	1.00	1.85	IL13
ATOM	1618	HZ1	LYS	105	7.505	0.967	-15.518	1.00	2.28	IL13
ATOM	1619	HZ2	LYS	105	6.410	1.806	-16.510	1.00	2.37	IL13
ATOM	1620	HZ3	LYS	105	5.877	0.494	-15.571	1.00	2.31	IL13
ATOM	1621	C	LYS	105	9.713	1.289	-10.600	1.00	0.24	IL13
ATOM	1622	O	LYS	105	10.631	1.598	-11.333	1.00	0.25	IL13
ATOM	1623	N	LEU	106	9.397	2.027	-9.568	1.00	0.24	IL13
ATOM	1624	HN	LEU	106	8.649	1.767	-8.991	1.00	0.24	IL13
ATOM	1625	CA	LEU	106	10.169	3.274	-9.273	1.00	0.25	IL13
ATOM	1626	HA	LEU	106	10.164	3.910	-10.143	1.00	0.27	IL13
ATOM	1627	CB	LEU	106	9.544	4.021	-8.083	1.00	0.27	IL13
ATOM	1628	HB1	LEU	106	10.276	4.700	-7.671	1.00	0.29	IL13

Figure 8 (28/30)

ATOM	1629	HB2	LEU	106	9.267	3.304	-7.324	1.00	0.27	IL13
ATOM	1630	CG	LEU	106	8.292	4.822	-8.505	1.00	0.29	IL13
ATOM	1631	HG	LEU	106	7.727	5.070	-7.617	1.00	0.36	IL13
ATOM	1632	CD1	LEU	106	8.691	6.123	-9.210	1.00	0.34	IL13
ATOM	1633	HD11	LEU	106	8.505	6.957	-8.550	1.00	1.11	IL13
ATOM	1634	HD12	LEU	106	8.102	6.240	-10.107	1.00	1.05	IL13
ATOM	1635	HD13	LEU	106	9.738	6.097	-9.468	1.00	1.04	IL13
ATOM	1636	CD2	LEU	106	7.404	3.994	-9.441	1.00	0.32	IL13
ATOM	1637	HD21	LEU	106	7.858	3.926	-10.417	1.00	1.08	IL13
ATOM	1638	HD22	LEU	106	6.439	4.470	-9.531	1.00	1.06	IL13
ATOM	1639	HD23	LEU	106	7.276	3.010	-9.033	1.00	0.99	IL13
ATOM	1640	C	LEU	106	11.621	2.922	-8.932	1.00	0.24	IL13
ATOM	1641	O	LEU	106	12.514	3.730	-9.094	1.00	0.27	IL13
ATOM	1642	N	PHE	107	11.869	1.732	-8.455	1.00	0.23	IL13
ATOM	1643	HN	PHE	107	11.140	1.092	-8.322	1.00	0.22	IL13
ATOM	1644	CA	PHE	107	13.269	1.360	-8.101	1.00	0.24	IL13
ATOM	1645	HA	PHE	107	13.641	2.031	-7.340	1.00	0.24	IL13
ATOM	1646	CB	PHE	107	13.313	-0.081	-7.581	1.00	0.23	IL13
ATOM	1647	HB1	PHE	107	12.953	-0.753	-8.345	1.00	0.25	IL13
ATOM	1648	HB2	PHE	107	12.693	-0.166	-6.702	1.00	0.22	IL13
ATOM	1649	CG	PHE	107	14.737	-0.438	-7.228	1.00	0.25	IL13
ATOM	1650	CD1	PHE	107	15.308	0.083	-6.065	1.00	0.24	IL13
ATOM	1651	HD1	PHE	107	14.730	0.724	-5.424	1.00	0.23	IL13
ATOM	1652	CD2	PHE	107	15.487	-1.278	-8.061	1.00	0.33	IL13
ATOM	1653	HD2	PHE	107	15.047	-1.682	-8.961	1.00	0.37	IL13
ATOM	1654	CE1	PHE	107	16.625	-0.229	-5.728	1.00	0.27	IL13
ATOM	1655	HE1	PHE	107	17.058	0.183	-4.831	1.00	0.27	IL13
ATOM	1656	CE2	PHE	107	16.810	-1.596	-7.723	1.00	0.36	IL13
ATOM	1657	HE2	PHE	107	17.390	-2.245	-8.362	1.00	0.43	IL13
ATOM	1658	CZ	PHE	107	17.379	-1.070	-6.555	1.00	0.32	IL13
ATOM	1659	HZ	PHE	107	18.399	-1.313	-6.294	1.00	0.35	IL13
ATOM	1660	C	PHE	107	14.143	1.466	-9.348	1.00	0.27	IL13
ATOM	1661	O	PHE	107	15.270	1.916	-9.294	1.00	0.30	IL13
ATOM	1662	N	ARG	108	13.631	1.054	-10.470	1.00	0.30	IL13
ATOM	1663	HN	ARG	108	12.720	0.695	-10.490	1.00	0.29	IL13
ATOM	1664	CA	ARG	108	14.428	1.128	-11.722	1.00	0.36	IL13
ATOM	1665	HA	ARG	108	15.330	0.546	-11.606	1.00	0.38	IL13
ATOM	1666	CB	ARG	108	13.610	0.571	-12.887	1.00	0.42	IL13
ATOM	1667	HB1	ARG	108	14.195	0.628	-13.792	1.00	0.45	IL13
ATOM	1668	HB2	ARG	108	12.707	1.155	-13.004	1.00	0.42	IL13
ATOM	1669	CG	ARG	108	13.242	-0.890	-12.605	1.00	0.49	IL13
ATOM	1670	HG1	ARG	108	12.229	-0.938	-12.232	1.00	0.84	IL13
ATOM	1671	HG2	ARG	108	13.915	-1.298	-11.866	1.00	0.97	IL13
ATOM	1672	CD	ARG	108	13.342	-1.709	-13.894	1.00	0.83	IL13
ATOM	1673	HD1	ARG	108	14.375	-1.975	-14.069	1.00	1.48	IL13
ATOM	1674	HD2	ARG	108	12.976	-1.128	-14.726	1.00	1.52	IL13
ATOM	1675	NE	ARG	108	12.523	-2.945	-13.763	1.00	1.48	IL13
ATOM	1676	HE	ARG	108	12.183	-3.219	-12.885	1.00	2.04	IL13
ATOM	1677	CZ	ARG	108	12.247	-3.653	-14.822	1.00	2.17	IL13
ATOM	1678	NH1	ARG	108	11.510	-4.725	-14.720	1.00	3.13	IL13
ATOM	1679	HH11	ARG	108	11.155	-5.004	-13.828	1.00	3.49	IL13
ATOM	1680	HH12	ARG	108	11.301	-5.266	-15.534	1.00	3.72	IL13
ATOM	1681	NH2	ARG	108	12.716	-3.291	-15.984	1.00	2.50	IL13
ATOM	1682	HH21	ARG	108	13.285	-2.471	-16.060	1.00	2.36	IL13
ATOM	1683	HH22	ARG	108	12.508	-3.832	-16.799	1.00	3.27	IL13
ATOM	1684	C	ARG	108	14.804	2.583	-12.013	1.00	0.38	IL13
ATOM	1685	O	ARG	108	15.894	2.870	-12.467	1.00	0.43	IL13
ATOM	1686	N	GLU	109	13.911	3.505	-11.774	1.00	0.36	IL13
ATOM	1687	HN	GLU	109	13.032	3.260	-11.418	1.00	0.34	IL13
ATOM	1688	CA	GLU	109	14.232	4.932	-12.060	1.00	0.40	IL13
ATOM	1689	HA	GLU	109	14.874	4.985	-12.928	1.00	0.46	IL13

Figure 8 (29/30)

ATOM	1690	CB	GLU	109	12.941	5.706	-12.340	1.00	0.43	IL13
ATOM	1691	HB1	GLU	109	13.179	6.735	-12.566	1.00	0.47	IL13
ATOM	1692	HB2	GLU	109	12.300	5.667	-11.471	1.00	0.41	IL13
ATOM	1693	CG	GLU	109	12.220	5.080	-13.537	1.00	0.48	IL13
ATOM	1694	HG1	GLU	109	11.806	4.125	-13.246	1.00	0.96	IL13
ATOM	1695	HG2	GLU	109	12.921	4.937	-14.346	1.00	0.98	IL13
ATOM	1696	CD	GLU	109	11.088	6.002	-13.995	1.00	1.19	IL13
ATOM	1697	OE1	GLU	109	10.059	6.018	-13.340	1.00	1.94	IL13
ATOM	1698	OE2	GLU	109	11.269	6.674	-14.997	1.00	1.91	IL13
ATOM	1699	C	GLU	109	14.955	5.556	-10.861	1.00	0.39	IL13
ATOM	1700	O	GLU	109	15.375	6.695	-10.906	1.00	0.44	IL13
ATOM	1701	N	GLY	110	15.108	4.824	-9.789	1.00	0.35	IL13
ATOM	1702	HN	GLY	110	14.766	3.909	-9.764	1.00	0.34	IL13
ATOM	1703	CA	GLY	110	15.805	5.381	-8.601	1.00	0.36	IL13
ATOM	1704	HA1	GLY	110	16.827	5.614	-8.857	1.00	0.41	IL13
ATOM	1705	HA2	GLY	110	15.792	4.651	-7.804	1.00	0.34	IL13
ATOM	1706	C	GLY	110	15.094	6.653	-8.143	1.00	0.38	IL13
ATOM	1707	O	GLY	110	15.566	7.354	-7.270	1.00	0.42	IL13
ATOM	1708	N	ARG	111	13.954	6.950	-8.714	1.00	0.37	IL13
ATOM	1709	HN	ARG	111	13.585	6.366	-9.408	1.00	0.37	IL13
ATOM	1710	CA	ARG	111	13.214	8.172	-8.292	1.00	0.41	IL13
ATOM	1711	HA	ARG	111	13.907	8.895	-7.889	1.00	0.45	IL13
ATOM	1712	CB	ARG	111	12.468	8.783	-9.482	1.00	0.45	IL13
ATOM	1713	HB1	ARG	111	11.855	9.602	-9.139	1.00	0.46	IL13
ATOM	1714	HB2	ARG	111	11.839	8.029	-9.935	1.00	0.45	IL13
ATOM	1715	CG	ARG	111	13.471	9.298	-10.517	1.00	0.53	IL13
ATOM	1716	HG1	ARG	111	13.813	8.476	-11.128	1.00	0.57	IL13
ATOM	1717	HG2	ARG	111	14.315	9.750	-10.017	1.00	0.57	IL13
ATOM	1718	CD	ARG	111	12.791	10.338	-11.406	1.00	0.59	IL13
ATOM	1719	HD1	ARG	111	12.591	11.229	-10.825	1.00	1.02	IL13
ATOM	1720	HD2	ARG	111	11.862	9.944	-11.783	1.00	1.11	IL13
ATOM	1721	NE	ARG	111	13.688	10.669	-12.548	1.00	1.37	IL13
ATOM	1722	HE	ARG	111	14.617	10.356	-12.548	1.00	2.06	IL13
ATOM	1723	CZ	ARG	111	13.235	11.362	-13.555	1.00	1.93	IL13
ATOM	1724	NH1	ARG	111	14.015	11.632	-14.565	1.00	2.86	IL13
ATOM	1725	HH11	ARG	111	14.960	11.306	-14.567	1.00	3.27	IL13
ATOM	1726	HH12	ARG	111	13.668	12.165	-15.336	1.00	3.40	IL13
ATOM	1727	NH2	ARG	111	12.004	11.795	-13.546	1.00	2.21	IL13
ATOM	1728	HH21	ARG	111	11.409	11.594	-12.768	1.00	2.07	IL13
ATOM	1729	HH22	ARG	111	11.656	12.329	-14.316	1.00	2.98	IL13
ATOM	1730	C	ARG	111	12.217	7.785	-7.210	1.00	0.39	IL13
ATOM	1731	O	ARG	111	11.109	7.365	-7.480	1.00	0.41	IL13
ATOM	1732	N	PHE	112	12.617	7.917	-5.982	1.00	0.40	IL13
ATOM	1733	HN	PHE	112	13.519	8.250	-5.798	1.00	0.43	IL13
ATOM	1734	CA	PHE	112	11.724	7.555	-4.857	1.00	0.42	IL13
ATOM	1735	HA	PHE	112	11.069	6.749	-5.154	1.00	0.39	IL13
ATOM	1736	CB	PHE	112	12.602	7.102	-3.694	1.00	0.42	IL13
ATOM	1737	HB1	PHE	112	11.991	6.644	-2.931	1.00	0.44	IL13
ATOM	1738	HB2	PHE	112	13.131	7.949	-3.283	1.00	0.48	IL13
ATOM	1739	CG	PHE	112	13.586	6.090	-4.230	1.00	0.35	IL13
ATOM	1740	CD1	PHE	112	13.183	4.771	-4.427	1.00	0.29	IL13
ATOM	1741	HD1	PHE	112	12.177	4.475	-4.177	1.00	0.32	IL13
ATOM	1742	CD2	PHE	112	14.894	6.477	-4.556	1.00	0.38	IL13
ATOM	1743	HD2	PHE	112	15.208	7.499	-4.407	1.00	0.44	IL13
ATOM	1744	CE1	PHE	112	14.086	3.834	-4.945	1.00	0.25	IL13
ATOM	1745	HE1	PHE	112	13.783	2.822	-5.108	1.00	0.25	IL13
ATOM	1746	CE2	PHE	112	15.793	5.533	-5.074	1.00	0.35	IL13
ATOM	1747	HE2	PHE	112	16.797	5.824	-5.333	1.00	0.40	IL13
ATOM	1748	CZ	PHE	112	15.382	4.212	-5.265	1.00	0.28	IL13
ATOM	1749	HZ	PHE	112	16.067	3.478	-5.657	1.00	0.29	IL13
ATOM	1750	C	PHE	112	10.895	8.777	-4.466	1.00	0.50	IL13

Figure 8 (30/30)

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ATOM   1751  O    PHE  112      11.416   9.861  -4.294  1.00  0.58      IL13
ATOM   1752  N    ASN  113       9.605   8.613  -4.335  1.00  0.56      IL13
ATOM   1753  HN   ASN  113       9.210   7.729  -4.488  1.00  0.59      IL13
ATOM   1754  CA   ASN  113       8.723   9.766  -3.973  1.00  0.66      IL13
ATOM   1755  HA   ASN  113       7.711   9.412  -3.893  1.00  0.45      IL13
ATOM   1756  CB   ASN  113       9.175  10.406  -2.639  1.00  1.53      IL13
ATOM   1757  HB1  ASN  113       9.365  11.456  -2.803  1.00  1.93      IL13
ATOM   1758  HB2  ASN  113      10.085   9.935  -2.303  1.00  2.15      IL13
ATOM   1759  CG   ASN  113       8.110  10.258  -1.534  1.00  2.22      IL13
ATOM   1760  OD1  ASN  113       6.982   9.872  -1.773  1.00  2.71      IL13
ATOM   1761  ND2  ASN  113       8.433  10.567  -0.309  1.00  3.05      IL13
ATOM   1762  HD21 ASN  113       9.337  10.887  -0.106  1.00  3.25      IL13
ATOM   1763  HD22 ASN  113       7.771  10.481   0.409  1.00  3.76      IL13
ATOM   1764  C    ASN  113       8.790  10.818  -5.085  1.00  1.47      IL13
ATOM   1765  OT1  ASN  113       9.854  10.982  -5.660  1.00  2.22      IL13
ATOM   1766  OT2  ASN  113       7.774  11.441  -5.345  1.00  2.04      IL13
END
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Figure 9 (1/52)

		Atom Type	Res.	Res. No.	X	Y	Z	OCC.	B	
ATOM	1	N	PHE	1	20.579	9.023	-52.555	1.00	33.17	B
ATOM	2	HT1	PHE	1	20.041	9.506	-53.301	1.00	20.00	B
ATOM	3	HT2	PHE	1	20.394	8.001	-52.524	1.00	20.00	B
ATOM	4	HT3	PHE	1	20.315	9.368	-51.617	1.00	20.00	B
ATOM	5	CA	PHE	1	22.019	9.194	-52.721	1.00	32.84	B
ATOM	6	CB	PHE	1	22.460	10.575	-52.228	1.00	34.28	B
ATOM	7	CG	PHE	1	21.433	11.644	-52.419	1.00	35.34	B
ATOM	8	CD1	PHE	1	20.152	11.512	-51.865	1.00	35.27	B
ATOM	9	CD2	PHE	1	21.731	12.772	-53.167	1.00	35.42	B
ATOM	10	CE1	PHE	1	19.179	12.484	-52.055	1.00	35.22	B
ATOM	11	CE2	PHE	1	20.770	13.755	-53.363	1.00	36.91	B
ATOM	12	CZ	PHE	1	19.481	13.606	-52.802	1.00	36.75	B
ATOM	13	C	PHE	1	22.648	8.139	-51.836	1.00	31.55	B
ATOM	14	O	PHE	1	21.990	7.162	-51.466	1.00	31.36	B
ATOM	15	N	LYS	2	23.916	8.319	-51.496	1.00	30.59	B
ATOM	16	H	LYS	2	24.494	9.088	-51.789	1.00	20.00	B
ATOM	17	CA	LYS	2	24.575	7.369	-50.621	1.00	29.78	B
ATOM	18	CB	LYS	2	25.557	6.503	-51.412	1.00	30.27	B
ATOM	19	CG	LYS	2	25.884	5.154	-50.766	1.00	31.00	B
ATOM	20	CD	LYS	2	26.205	4.107	-51.833	1.00	29.94	B
ATOM	21	CE	LYS	2	24.976	3.784	-52.680	1.00	29.45	B
ATOM	22	NZ	LYS	2	25.285	2.926	-53.863	1.00	30.12	B
ATOM	23	HZ1	LYS	2	24.498	2.963	-54.539	1.00	20.00	B
ATOM	24	HZ2	LYS	2	26.149	3.268	-54.328	1.00	20.00	B
ATOM	25	HZ3	LYS	2	25.432	1.950	-53.528	1.00	20.00	B
ATOM	26	C	LYS	2	25.295	8.174	-49.568	1.00	29.00	B
ATOM	27	O	LYS	2	25.762	9.274	-49.846	1.00	28.91	B
ATOM	28	N	VAL	3	25.340	7.652	-48.350	1.00	29.17	B
ATOM	29	H	VAL	3	24.939	6.755	-48.162	1.00	20.00	B
ATOM	30	CA	VAL	3	26.024	8.328	-47.258	1.00	28.15	B
ATOM	31	CB	VAL	3	25.277	8.176	-45.890	1.00	26.36	B
ATOM	32	CG1	VAL	3	25.781	9.208	-44.922	1.00	26.58	B
ATOM	33	CG2	VAL	3	23.789	8.360	-46.053	1.00	23.90	B
ATOM	34	C	VAL	3	27.376	7.645	-47.167	1.00	28.03	B
ATOM	35	O	VAL	3	27.459	6.460	-46.880	1.00	28.16	B
ATOM	36	N	LEU	4	28.421	8.385	-47.488	1.00	29.44	B
ATOM	37	H	LEU	4	28.209	9.300	-47.816	1.00	20.00	B
ATOM	38	CA	LEU	4	29.782	7.889	-47.431	1.00	31.20	B
ATOM	39	CB	LEU	4	30.706	8.867	-48.123	1.00	31.44	B
ATOM	40	CG	LEU	4	31.020	8.551	-49.565	1.00	33.85	B
ATOM	41	CD1	LEU	4	31.590	9.796	-50.228	1.00	35.82	B
ATOM	42	CD2	LEU	4	32.003	7.390	-49.595	1.00	34.04	B
ATOM	43	C	LEU	4	30.259	7.722	-46.001	1.00	32.29	B
ATOM	44	O	LEU	4	30.808	6.682	-45.637	1.00	33.97	B
ATOM	45	N	GLN	5	30.093	8.774	-45.204	1.00	32.53	B
ATOM	46	H	GLN	5	29.460	9.484	-45.485	1.00	20.00	B
ATOM	47	CA	GLN	5	30.508	8.773	-43.802	1.00	32.30	B
ATOM	48	CB	GLN	5	31.397	10.006	-43.513	1.00	33.24	B
ATOM	49	CG	GLN	5	32.042	10.077	-42.096	1.00	35.76	B
ATOM	50	CD	GLN	5	31.534	11.246	-41.205	1.00	36.89	B
ATOM	51	OE1	GLN	5	30.996	11.023	-40.117	1.00	36.25	B
ATOM	52	NE2	GLN	5	31.734	12.481	-41.661	1.00	35.68	B
ATOM	53	HE21	GLN	5	31.968	12.702	-42.598	1.00	20.00	B

Figure 9 (2/52)

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ATOM     54 HE22 GLN     5      31.611  13.183 -40.941  1.00 20.00      B
ATOM     55  C   GLN     5      29.224   8.836 -42.983  1.00 30.86      B
ATOM     56  O   GLN     5      28.456   9.792 -43.138  1.00 31.32      B
ATOM     57  N   GLU     6      28.987   7.803 -42.166  1.00 29.22      B
ATOM     58  H   GLU     6      29.723   7.142 -42.032  1.00 20.00      B
ATOM     59  CA  GLU     6      27.823   7.700 -41.265  1.00 27.32      B
ATOM     60  CB  GLU     6      27.938   6.465 -40.374  1.00 29.67      B
ATOM     61  CG  GLU     6      27.714   5.134 -41.055  1.00 33.88      B
ATOM     62  CD  GLU     6      27.205   4.060 -40.091  1.00 35.92      B
ATOM     63  OE1 GLU     6      27.405   4.189 -38.854  1.00 35.32      B
ATOM     64  OE2 GLU     6      26.589   3.086 -40.581  1.00 37.28      B
ATOM     65  C   GLU     6      27.836   8.908 -40.346  1.00 23.37      B
ATOM     66  O   GLU     6      28.906   9.402 -40.014  1.00 22.89      B
ATOM     67  N   PRO     7      26.662   9.396 -39.918  1.00 21.16      B
ATOM     68  CD  PRO     7      25.283   9.042 -40.283  1.00 18.86      B
ATOM     69  CA  PRO     7      26.673  10.565 -39.032  1.00 19.38      B
ATOM     70  CB  PRO     7      25.183  10.853 -38.835  1.00 18.22      B
ATOM     71  CG  PRO     7      24.562  10.356 -40.090  1.00 16.16      B
ATOM     72  C   PRO     7      27.403  10.310 -37.699  1.00 20.30      B
ATOM     73  O   PRO     7      27.199   9.271 -37.061  1.00 20.82      B
ATOM     74  N   THR     8      28.282  11.232 -37.312  1.00 18.33      B
ATOM     75  H   THR     8      28.492  11.979 -37.941  1.00 20.00      B
ATOM     76  CA  THR     8      29.018  11.149 -36.054  1.00 17.62      B
ATOM     77  CB  THR     8      30.535  11.230 -36.268  1.00 18.65      B
ATOM     78  OG1 THR     8      30.821  12.200 -37.280  1.00 22.53      B
ATOM     79  HG1 THR     8      30.662  11.782 -38.135  1.00 20.00      B
ATOM     80  CG2 THR     8      31.099   9.903 -36.672  1.00 21.32      B
ATOM     81  C   THR     8      28.588  12.411 -35.333  1.00 17.19      B
ATOM     82  O   THR     8      28.596  13.495 -35.935  1.00 16.69      B
ATOM     83  N   CYS     9      28.214  12.288 -34.059  1.00 16.35      B
ATOM     84  H   CYS     9      28.261  11.391 -33.619  1.00 20.00      B
ATOM     85  CA  CYS     9      27.749  13.446 -33.298  1.00 15.64      B
ATOM     86  CB  CYS     9      26.267  13.288 -32.938  1.00 16.03      B
ATOM     87  SG  CYS     9      25.164  12.608 -34.210  1.00 14.01      B
ATOM     88  C   CYS     9      28.510  13.661 -31.997  1.00 14.28      B
ATOM     89  O   CYS     9      29.125  12.735 -31.468  1.00 13.76      B
ATOM     90  N   VAL    10      28.473  14.892 -31.503  1.00 13.22      B
ATOM     91  H   VAL    10      27.992  15.597 -32.029  1.00 20.00      B
ATOM     92  CA  VAL    10      29.090  15.249 -30.228  1.00 13.38      B
ATOM     93  CB  VAL    10      30.391  16.083 -30.379  1.00 12.62      B
ATOM     94  CG1 VAL    10      31.455  15.254 -31.079  1.00 14.09      B
ATOM     95  CG2 VAL    10      30.130  17.379 -31.131  1.00 12.23      B
ATOM     96  C   VAL    10      28.017  16.074 -29.527  1.00 14.42      B
ATOM     97  O   VAL    10      27.160  16.683 -30.194  1.00 14.30      B
ATOM     98  N   SER    11      28.050  16.079 -28.195  1.00 14.07      B
ATOM     99  H   SER    11      28.858  15.627 -27.810  1.00 20.00      B
ATOM    100  CA  SER    11      27.067  16.813 -27.395  1.00 13.23      B
ATOM    101  CB  SER    11      26.156  15.812 -26.686  1.00 13.26      B
ATOM    102  OG  SER    11      25.074  16.473 -26.065  1.00 13.07      B
ATOM    103  HG  SER    11      24.953  16.131 -25.176  1.00 20.00      B
ATOM    104  C   SER    11      27.697  17.757 -26.351  1.00 12.85      B
ATOM    105  O   SER    11      28.665  17.393 -25.676  1.00 12.00      B
ATOM    106  N   ASP    12      27.155  18.971 -26.226  1.00 13.64      B
ATOM    107  H   ASP    12      26.401  19.298 -26.807  1.00 20.00      B
ATOM    108  CA  ASP    12      27.666  19.915 -25.234  1.00 12.77      B
ATOM    109  CB  ASP    12      27.475  21.370 -25.700  1.00 11.29      B
ATOM    110  CG  ASP    12      26.034  21.849 -25.655  1.00 13.52      B
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Figure 9 (3/52)

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ATOM    111  OD1 ASP    12      25.123  21.077 -25.322  1.00 14.16      B
ATOM    112  OD2 ASP    12      25.811  23.038 -25.964  1.00 14.09      B
ATOM    113  C   ASP    12      27.028  19.656 -23.858  1.00 13.08      B
ATOM    114  O   ASP    12      27.258  20.392 -22.893  1.00 14.57      B
ATOM    115  N   TYR    13      26.202  18.612 -23.796  1.00 12.77      B
ATOM    116  H   TYR    13      25.751  18.375 -24.654  1.00 20.00      B
ATOM    117  CA  TYR    13      25.528  18.190 -22.575  1.00 12.61      B
ATOM    118  CB  TYR    13      26.543  17.691 -21.560  1.00 10.73      B
ATOM    119  CG  TYR    13      26.044  16.472 -20.862  1.00 11.80      B
ATOM    120  CD1 TYR    13      25.431  15.461 -21.588  1.00 10.53      B
ATOM    121  CE1 TYR    13      24.971  14.323 -20.976  1.00 11.01      B
ATOM    122  CD2 TYR    13      26.175  16.311 -19.473  1.00 11.22      B
ATOM    123  CE2 TYR    13      25.710  15.157 -18.839  1.00 10.70      B
ATOM    124  CZ  TYR    13      25.109  14.169 -19.609  1.00 11.82      B
ATOM    125  OH  TYR    13      24.659  12.999 -19.047  1.00 12.67      B
ATOM    126  HH  TYR    13      23.926  13.260 -18.483  1.00 20.00      B
ATOM    127  C   TYR    13      24.675  19.246 -21.910  1.00 13.82      B
ATOM    128  O   TYR    13      24.503  19.231 -20.701  1.00 14.05      B
ATOM    129  N   MET    14      24.123  20.154 -22.691  1.00 15.31      B
ATOM    130  H   MET    14      24.284  20.152 -23.680  1.00 20.00      B
ATOM    131  CA  MET    14      23.305  21.218 -22.132  1.00 17.26      B
ATOM    132  CB  MET    14      24.105  22.527 -22.070  1.00 19.76      B
ATOM    133  CG  MET    14      23.535  23.617 -21.163  1.00 21.01      B
ATOM    134  SD  MET    14      24.625  25.079 -21.094  1.00 26.14      B
ATOM    135  CE  MET    14      23.428  26.431 -21.405  1.00 27.19      B
ATOM    136  C   MET    14      22.097  21.354 -23.031  1.00 18.26      B
ATOM    137  O   MET    14      21.026  20.879 -22.683  1.00 19.43      B
ATOM    138  N   SER    15      22.287  21.897 -24.230  1.00 17.98      B
ATOM    139  H   SER    15      23.201  22.159 -24.531  1.00 20.00      B
ATOM    140  CA  SER    15      21.168  22.102 -25.154  1.00 16.21      B
ATOM    141  CB  SER    15      20.737  23.534 -25.009  1.00 16.57      B
ATOM    142  OG  SER    15      21.901  24.337 -25.138  1.00 21.55      B
ATOM    143  HG  SER    15      21.521  25.210 -25.062  1.00 20.00      B
ATOM    144  C   SER    15      21.392  21.819 -26.647  1.00 15.49      B
ATOM    145  O   SER    15      20.461  21.919 -27.435  1.00 16.57      B
ATOM    146  N   ILE    16      22.612  21.470 -27.044  1.00 16.38      B
ATOM    147  H   ILE    16      23.348  21.389 -26.370  1.00 20.00      B
ATOM    148  CA  ILE    16      22.916  21.217 -28.454  1.00 16.06      B
ATOM    149  CB  ILE    16      23.681  22.433 -29.082  1.00 17.01      B
ATOM    150  CG2 ILE    16      24.077  22.156 -30.522  1.00 17.41      B
ATOM    151  CG1 ILE    16      22.803  23.675 -29.052  1.00 18.41      B
ATOM    152  CD1 ILE    16      23.532  24.958 -29.453  1.00 21.06      B
ATOM    153  C   ILE    16      23.768  19.967 -28.675  1.00 14.01      B
ATOM    154  O   ILE    16      24.656  19.675 -27.877  1.00 13.85      B
ATOM    155  N   SER    17      23.473  19.239 -29.751  1.00 12.52      B
ATOM    156  H   SER    17      22.652  19.510 -30.250  1.00 20.00      B
ATOM    157  CA  SER    17      24.227  18.063 -30.171  1.00 12.77      B
ATOM    158  CB  SER    17      23.406  16.784 -30.008  1.00 12.79      B
ATOM    159  OG  SER    17      23.984  15.921 -29.051  1.00 15.46      B
ATOM    160  HG  SER    17      24.036  16.433 -28.245  1.00 20.00      B
ATOM    161  C   SER    17      24.477  18.330 -31.662  1.00 14.68      B
ATOM    162  O   SER    17      23.556  18.677 -32.403  1.00 15.73      B
ATOM    163  N   THR    18      25.717  18.217 -32.102  1.00 15.15      B
ATOM    164  H   THR    18      26.467  17.914 -31.518  1.00 20.00      B
ATOM    165  CA  THR    18      26.015  18.471 -33.501  1.00 16.44      B
ATOM    166  CB  THR    18      27.141  19.535 -33.656  1.00 18.07      B
ATOM    167  OG1 THR    18      26.665  20.792 -33.155  1.00 21.73      B
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Figure 9 (4/52)

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ATOM    168  HG1 THR    18      27.385  21.212 -32.697  1.00 20.00      B
ATOM    169  CG2 THR    18      27.547  19.728 -35.136  1.00 16.96      B
ATOM    170  C   THR    18      26.460  17.189 -34.146  1.00 16.63      B
ATOM    171  O   THR    18      27.325  16.497 -33.608  1.00 16.08      B
ATOM    172  N   CYS    19      25.847  16.870 -35.282  1.00 15.95      B
ATOM    173  H   CYS    19      25.193  17.531 -35.650  1.00 20.00      B
ATOM    174  CA  CYS    19      26.181  15.675 -36.045  1.00 16.17      B
ATOM    175  CB  CYS    19      24.943  14.799 -36.280  1.00 14.65      B
ATOM    176  SG  CYS    19      24.086  14.212 -34.798  1.00 17.71      B
ATOM    177  C   CYS    19      26.706  16.103 -37.405  1.00 16.73      B
ATOM    178  O   CYS    19      26.343  17.168 -37.908  1.00 17.56      B
ATOM    179  N   GLU    20      27.537  15.271 -38.012  1.00 18.17      B
ATOM    180  H   GLU    20      27.910  14.484 -37.513  1.00 20.00      B
ATOM    181  CA  GLU    20      28.051  15.562 -39.342  1.00 21.84      B
ATOM    182  CB  GLU    20      29.396  16.262 -39.258  1.00 24.96      B
ATOM    183  CG  GLU    20      30.340  15.583 -38.341  1.00 34.25      B
ATOM    184  CD  GLU    20      31.760  15.742 -38.786  1.00 39.61      B
ATOM    185  OE1 GLU    20      32.356  16.830 -38.547  1.00 41.98      B
ATOM    186  OE2 GLU    20      32.268  14.755 -39.382  1.00 41.40      B
ATOM    187  C   GLU    20      28.196  14.270 -40.130  1.00 20.48      B
ATOM    188  O   GLU    20      28.428  13.211 -39.546  1.00 21.25      B
ATOM    189  N   TRP    21      28.004  14.336 -41.444  1.00 20.33      B
ATOM    190  H   TRP    21      27.761  15.220 -41.848  1.00 20.00      B
ATOM    191  CA  TRP    21      28.158  13.150 -42.271  1.00 18.73      B
ATOM    192  CB  TRP    21      26.862  12.339 -42.328  1.00 16.79      B
ATOM    193  CG  TRP    21      25.678  13.020 -42.958  1.00 16.10      B
ATOM    194  CD2 TRP    21      24.746  13.911 -42.312  1.00 16.49      B
ATOM    195  CE2 TRP    21      23.778  14.271 -43.276  1.00 16.05      B
ATOM    196  CE3 TRP    21      24.634  14.434 -41.012  1.00 15.96      B
ATOM    197  CD1 TRP    21      25.244  12.883 -44.247  1.00 14.41      B
ATOM    198  NE1 TRP    21      24.106  13.629 -44.443  1.00 15.91      B
ATOM    199  HE1 TRP    21      23.600  13.665 -45.276  1.00 20.00      B
ATOM    200  CZ2 TRP    21      22.704  15.130 -42.980  1.00 16.39      B
ATOM    201  CZ3 TRP    21      23.564  15.287 -40.715  1.00 14.68      B
ATOM    202  CH2 TRP    21      22.616  15.626 -41.699  1.00 16.24      B
ATOM    203  C   TRP    21      28.612  13.513 -43.668  1.00 19.64      B
ATOM    204  O   TRP    21      28.747  14.689 -44.002  1.00 20.51      B
ATOM    205  N   LYS    22      28.872  12.500 -44.483  1.00 21.38      B
ATOM    206  H   LYS    22      28.765  11.574 -44.114  1.00 20.00      B
ATOM    207  CA  LYS    22      29.293  12.732 -45.856  1.00 24.41      B
ATOM    208  CB  LYS    22      30.802  12.552 -46.012  1.00 25.20      B
ATOM    209  CG  LYS    22      31.549  13.823 -45.689  1.00 30.60      B
ATOM    210  CD  LYS    22      33.048  13.607 -45.577  1.00 35.07      B
ATOM    211  CE  LYS    22      33.726  14.901 -45.113  1.00 36.85      B
ATOM    212  NZ  LYS    22      35.140  14.669 -44.660  1.00 38.67      B
ATOM    213  HZ1 LYS    22      35.555  15.585 -44.397  1.00 20.00      B
ATOM    214  HZ2 LYS    22      35.082  14.059 -43.819  1.00 20.00      B
ATOM    215  HZ3 LYS    22      35.672  14.208 -45.423  1.00 20.00      B
ATOM    216  C   LYS    22      28.577  11.817 -46.803  1.00 24.31      B
ATOM    217  O   LYS    22      28.558  10.610 -46.614  1.00 22.67      B
ATOM    218  N   MET    23      27.973  12.404 -47.822  1.00 26.71      B
ATOM    219  H   MET    23      28.116  13.389 -47.953  1.00 20.00      B
ATOM    220  CA  MET    23      27.271  11.634 -48.839  1.00 29.52      B
ATOM    221  CB  MET    23      25.918  12.281 -49.110  1.00 31.22      B
ATOM    222  CG  MET    23      25.118  12.420 -47.829  1.00 31.82      B
ATOM    223  SD  MET    23      23.394  12.490 -48.109  1.00 37.77      B
ATOM    224  CE  MET    23      23.036  10.768 -48.341  1.00 36.69      B
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Figure 9 (5/52)

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ATOM    225  C    MET    23      28.152  11.638 -50.083  1.00 30.25      B
ATOM    226  O    MET    23      29.035  12.492 -50.193  1.00 30.70      B
ATOM    227  N    ASN    24      27.971  10.673 -50.987  1.00 32.09      B
ATOM    228  H    ASN    24      27.166  10.080 -50.921  1.00 20.00      B
ATOM    229  CA   ASN    24      28.789  10.651 -52.210  1.00 33.10      B
ATOM    230  CB   ASN    24      29.147   9.220 -52.672  1.00 33.70      B
ATOM    231  CG   ASN    24      27.954   8.420 -53.176  1.00 35.07      B
ATOM    232  OD1  ASN    24      26.788   8.783 -52.983  1.00 36.20      B
ATOM    233  ND2  ASN    24      28.249   7.298 -53.817  1.00 34.71      B
ATOM    234  HD21 ASN    24      29.162   6.936 -54.008  1.00 20.00      B
ATOM    235  HD22 ASN    24      27.427   6.864 -54.176  1.00 20.00      B
ATOM    236  C    ASN    24      28.114  11.449 -53.322  1.00 32.84      B
ATOM    237  O    ASN    24      26.930  11.266 -53.636  1.00 33.89      B
ATOM    238  N    GLY    25      28.876  12.369 -53.888  1.00 31.91      B
ATOM    239  H    GLY    25      29.800  12.518 -53.551  1.00 20.00      B
ATOM    240  CA   GLY    25      28.345  13.217 -54.930  1.00 32.99      B
ATOM    241  C    GLY    25      27.734  14.456 -54.313  1.00 33.19      B
ATOM    242  O    GLY    25      27.199  14.405 -53.196  1.00 33.82      B
ATOM    243  N    PRO    26      27.826  15.602 -55.004  1.00 33.04      B
ATOM    244  CD   PRO    26      28.488  15.796 -56.304  1.00 32.93      B
ATOM    245  CA   PRO    26      27.266  16.869 -54.502  1.00 32.36      B
ATOM    246  CB   PRO    26      27.339  17.802 -55.719  1.00 31.98      B
ATOM    247  CG   PRO    26      27.630  16.868 -56.914  1.00 32.81      B
ATOM    248  C    PRO    26      25.847  16.726 -53.947  1.00 31.52      B
ATOM    249  O    PRO    26      25.024  15.995 -54.508  1.00 31.96      B
ATOM    250  N    THR    27      25.577  17.417 -52.840  1.00 31.62      B
ATOM    251  H    THR    27      26.229  18.053 -52.432  1.00 20.00      B
ATOM    252  CA   THR    27      24.267  17.355 -52.200  1.00 30.54      B
ATOM    253  CB   THR    27      24.251  16.342 -51.042  1.00 29.88      B
ATOM    254  OG1  THR    27      24.790  15.089 -51.474  1.00 32.49      B
ATOM    255  HG1  THR    27      24.891  14.587 -50.683  1.00 20.00      B
ATOM    256  CG2  THR    27      22.845  16.135 -50.560  1.00 30.89      B
ATOM    257  C    THR    27      23.934  18.682 -51.563  1.00 30.32      B
ATOM    258  O    THR    27      24.830  19.329 -51.015  1.00 31.25      B
ATOM    259  N    ASN    28      22.673  19.106 -51.658  1.00 29.73      B
ATOM    260  H    ASN    28      22.003  18.551 -52.132  1.00 20.00      B
ATOM    261  CA   ASN    28      22.244  20.326 -50.975  1.00 30.52      B
ATOM    262  CB   ASN    28      21.290  21.187 -51.794  1.00 32.02      B
ATOM    263  CG   ASN    28      20.754  22.373 -50.986  1.00 34.74      B
ATOM    264  OD1  ASN    28      21.047  22.510 -49.797  1.00 37.76      B
ATOM    265  ND2  ASN    28      19.957  23.219 -51.621  1.00 36.73      B
ATOM    266  HD21 ASN    28      19.689  23.137 -52.575  1.00 20.00      B
ATOM    267  HD22 ASN    28      19.632  23.985 -51.067  1.00 20.00      B
ATOM    268  C    ASN    28      21.505  19.844 -49.740  1.00 29.25      B
ATOM    269  O    ASN    28      20.296  19.598 -49.781  1.00 29.94      B
ATOM    270  N    CYS    29      22.244  19.727 -48.644  1.00 28.42      B
ATOM    271  H    CYS    29      23.173  20.111 -48.710  1.00 20.00      B
ATOM    272  CA   CYS    29      21.717  19.240 -47.387  1.00 26.43      B
ATOM    273  CB   CYS    29      22.776  19.378 -46.315  1.00 26.40      B
ATOM    274  SG   CYS    29      24.401  18.819 -46.907  1.00 27.35      B
ATOM    275  C    CYS    29      20.428  19.878 -46.936  1.00 25.70      B
ATOM    276  O    CYS    29      19.458  19.173 -46.753  1.00 25.56      B
ATOM    277  N    SER    30      20.390  21.202 -46.809  1.00 27.45      B
ATOM    278  H    SER    30      21.172  21.740 -47.123  1.00 20.00      B
ATOM    279  CA   SER    30      19.179  21.903 -46.342  1.00 28.21      B
ATOM    280  CB   SER    30      19.444  23.398 -46.219  1.00 28.69      B
ATOM    281  OG   SER    30      19.825  23.940 -47.459  1.00 33.68      B
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Figure 9 (6/52)

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ATOM    282  HG  SER    30      20.715  23.627 -47.617  1.00 20.00      B
ATOM    283  C   SER    30      17.865  21.710 -47.096  1.00 27.89      B
ATOM    284  O   SER    30      16.789  21.954 -46.537  1.00 29.02      B
ATOM    285  N   THR    31      17.930  21.290 -48.355  1.00 27.09      B
ATOM    286  H   THR    31      18.822  21.146 -48.788  1.00 20.00      B
ATOM    287  CA  THR    31      16.711  21.084 -49.131  1.00 25.85      B
ATOM    288  CB  THR    31      16.762  21.861 -50.476  1.00 26.30      B
ATOM    289  OG1 THR    31      17.833  21.350 -51.290  1.00 26.89      B
ATOM    290  HG1 THR    31      17.789  21.846 -52.095  1.00 20.00      B
ATOM    291  CG2 THR    31      16.982  23.360 -50.221  1.00 23.67      B
ATOM    292  C   THR    31      16.454  19.606 -49.416  1.00 25.24      B
ATOM    293  O   THR    31      15.309  19.171 -49.472  1.00 24.64      B
ATOM    294  N   GLU    32      17.517  18.827 -49.564  1.00 24.89      B
ATOM    295  H   GLU    32      18.432  19.241 -49.527  1.00 20.00      B
ATOM    296  CA  GLU    32      17.357  17.415 -49.862  1.00 26.91      B
ATOM    297  CB  GLU    32      18.526  16.938 -50.703  1.00 29.53      B
ATOM    298  CG  GLU    32      18.684  17.699 -51.998  1.00 34.62      B
ATOM    299  CD  GLU    32      19.687  17.041 -52.918  1.00 37.52      B
ATOM    300  OE1 GLU    32      20.912  17.238 -52.738  1.00 37.75      B
ATOM    301  OE2 GLU    32      19.239  16.311 -53.828  1.00 40.58      B
ATOM    302  C   GLU    32      17.203  16.467 -48.670  1.00 26.74      B
ATOM    303  O   GLU    32      16.434  15.495 -48.731  1.00 26.95      B
ATOM    304  N   LEU    33      17.923  16.753 -47.589  1.00 24.43      B
ATOM    305  H   LEU    33      18.448  17.607 -47.526  1.00 20.00      B
ATOM    306  CA  LEU    33      17.909  15.896 -46.414  1.00 21.98      B
ATOM    307  CB  LEU    33      19.352  15.544 -46.045  1.00 20.46      B
ATOM    308  CG  LEU    33      20.197  15.070 -47.227  1.00 20.05      B
ATOM    309  CD1 LEU    33      21.592  14.715 -46.781  1.00 19.45      B
ATOM    310  CD2 LEU    33      19.544  13.881 -47.873  1.00 19.02      B
ATOM    311  C   LEU    33      17.180  16.464 -45.195  1.00 21.11      B
ATOM    312  O   LEU    33      16.965  17.671 -45.073  1.00 20.62      B
ATOM    313  N   ARG    34      16.778  15.561 -44.311  1.00 20.39      B
ATOM    314  H   ARG    34      16.814  14.597 -44.589  1.00 20.00      B
ATOM    315  CA  ARG    34      16.096  15.904 -43.067  1.00 19.90      B
ATOM    316  CB  ARG    34      14.571  15.798 -43.205  1.00 19.70      B
ATOM    317  CG  ARG    34      13.900  16.978 -43.907  1.00 22.22      B
ATOM    318  CD  ARG    34      14.235  18.289 -43.223  1.00 23.56      B
ATOM    319  NE  ARG    34      13.662  19.474 -43.864  1.00 23.15      B
ATOM    320  HE  ARG    34      12.729  19.711 -43.614  1.00 20.00      B
ATOM    321  CZ  ARG    34      14.286  20.218 -44.777  1.00 22.13      B
ATOM    322  NH1 ARG    34      15.506  19.907 -45.198  1.00 19.51      B
ATOM    323 HH11 ARG    34      16.037  20.540 -45.781  1.00 20.00      B
ATOM    324 HH12 ARG    34      16.018  19.087 -44.919  1.00 20.00      B
ATOM    325  NH2 ARG    34      13.702  21.313 -45.231  1.00 21.66      B
ATOM    326 HH21 ARG    34      14.163  21.907 -45.898  1.00 20.00      B
ATOM    327 HH22 ARG    34      12.795  21.572 -44.922  1.00 20.00      B
ATOM    328  C   ARG    34      16.570  14.872 -42.047  1.00 19.95      B
ATOM    329  O   ARG    34      16.442  13.664 -42.285  1.00 21.04      B
ATOM    330  N   LEU    35      17.175  15.322 -40.949  1.00 18.33      B
ATOM    331  H   LEU    35      17.314  16.305 -40.779  1.00 20.00      B
ATOM    332  CA  LEU    35      17.606  14.370 -39.931  1.00 16.46      B
ATOM    333  CB  LEU    35      19.018  14.682 -39.379  1.00 13.60      B
ATOM    334  CG  LEU    35      19.680  13.703 -38.380  1.00 10.41      B
ATOM    335  CD1 LEU    35      20.037  12.387 -39.035  1.00  9.30      B
ATOM    336  CD2 LEU    35      20.932  14.320 -37.813  1.00 10.61      B
ATOM    337  C   LEU    35      16.568  14.470 -38.832  1.00 15.96      B
ATOM    338  O   LEU    35      16.404  15.522 -38.223  1.00 16.24      B
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Figure 9 (7/52)

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ATOM    339  N   LEU   36      15.819  13.388 -38.652  1.00 16.93      B
ATOM    340  H   LEU   36      16.069  12.558 -39.151  1.00 20.00      B
ATOM    341  CA  LEU   36      14.804  13.280 -37.611  1.00 16.01      B
ATOM    342  CB  LEU   36      13.629  12.434 -38.096  1.00 15.92      B
ATOM    343  CG  LEU   36      12.561  13.196 -38.887  1.00 18.33      B
ATOM    344  CD1 LEU   36      13.209  13.963 -40.014  1.00 18.38      B
ATOM    345  CD2 LEU   36      11.524  12.222 -39.425  1.00 17.94      B
ATOM    346  C   LEU   36      15.488  12.599 -36.429  1.00 14.91      B
ATOM    347  O   LEU   36      16.256  11.660 -36.605  1.00 13.94      B
ATOM    348  N   TYR   37      15.236  13.090 -35.227  1.00 14.63      B
ATOM    349  H   TYR   37      14.518  13.788 -35.151  1.00 20.00      B
ATOM    350  CA  TYR   37      15.849  12.511 -34.037  1.00 13.25      B
ATOM    351  CB  TYR   37      17.075  13.344 -33.624  1.00 12.38      B
ATOM    352  CG  TYR   37      16.803  14.811 -33.320  1.00 12.39      B
ATOM    353  CD1 TYR   37      16.604  15.739 -34.339  1.00 11.33      B
ATOM    354  CE1 TYR   37      16.362  17.069 -34.058  1.00 11.96      B
ATOM    355  CD2 TYR   37      16.753  15.262 -32.008  1.00 12.39      B
ATOM    356  CE2 TYR   37      16.513  16.588 -31.720  1.00 14.42      B
ATOM    357  CZ  TYR   37      16.318  17.491 -32.746  1.00 12.97      B
ATOM    358  OH  TYR   37      16.073  18.814 -32.431  1.00 13.87      B
ATOM    359  HH  TYR   37      15.510  18.845 -31.659  1.00 20.00      B
ATOM    360  C   TYR   37      14.810  12.445 -32.933  1.00 12.64      B
ATOM    361  O   TYR   37      14.014  13.364 -32.777  1.00 13.73      B
ATOM    362  N   GLN   38      14.788  11.353 -32.184  1.00 12.57      B
ATOM    363  H   GLN   38      15.354  10.596 -32.501  1.00 20.00      B
ATOM    364  CA  GLN   38      13.803  11.195 -31.107  1.00 11.27      B
ATOM    365  CB  GLN   38      12.596  10.434 -31.626  1.00 11.06      B
ATOM    366  CG  GLN   38      11.420  10.481 -30.691  1.00 11.42      B
ATOM    367  CD  GLN   38      10.169   9.942 -31.309  1.00 11.21      B
ATOM    368  OE1 GLN   38      10.097   9.740 -32.510  1.00 10.36      B
ATOM    369  NE2 GLN   38       9.169   9.706 -30.492  1.00 13.10      B
ATOM    370 HE21 GLN   38       9.301   9.868 -29.500  1.00 20.00      B
ATOM    371 HE22 GLN   38       8.271   9.421 -30.817  1.00 20.00      B
ATOM    372  C   GLN   38      14.345  10.472 -29.876  1.00 10.77      B
ATOM    373  O   GLN   38      15.042   9.465 -30.002  1.00 10.44      B
ATOM    374  N   LEU   39      14.046  10.995 -28.686  1.00 10.61      B
ATOM    375  H   LEU   39      13.536  11.862 -28.646  1.00 20.00      B
ATOM    376  CA  LEU   39      14.499  10.374 -27.456  1.00  8.93      B
ATOM    377  CB  LEU   39      14.122  11.239 -26.241  1.00  8.72      B
ATOM    378  CG  LEU   39      14.531  10.728 -24.841  1.00  7.53      B
ATOM    379  CD1 LEU   39      16.037  10.751 -24.676  1.00  4.93      B
ATOM    380  CD2 LEU   39      13.896  11.581 -23.771  1.00  5.75      B
ATOM    381  C   LEU   39      13.810   9.027 -27.363  1.00 10.38      B
ATOM    382  O   LEU   39      12.606   8.927 -27.597  1.00  9.22      B
ATOM    383  N   VAL   40      14.583   7.989 -27.053  1.00 11.32      B
ATOM    384  H   VAL   40      15.552   8.173 -26.890  1.00 20.00      B
ATOM    385  CA  VAL   40      14.045   6.633 -26.896  1.00 11.21      B
ATOM    386  CB  VAL   40      15.148   5.537 -27.107  1.00 10.19      B
ATOM    387  CG1 VAL   40      14.552   4.163 -27.001  1.00 10.88      B
ATOM    388  CG2 VAL   40      15.781   5.676 -28.475  1.00 10.72      B
ATOM    389  C   VAL   40      13.522   6.546 -25.468  1.00 13.71      B
ATOM    390  O   VAL   40      14.190   6.018 -24.576  1.00 15.73      B
ATOM    391  N   PHE   41      12.332   7.077 -25.255  1.00 14.67      B
ATOM    392  H   PHE   41      11.828   7.573 -25.980  1.00 20.00      B
ATOM    393  CA  PHE   41      11.692   7.091 -23.949  1.00 17.42      B
ATOM    394  CB  PHE   41      12.185   8.317 -23.151  1.00 15.54      B
ATOM    395  CG  PHE   41      11.633   8.407 -21.753  1.00 14.72      B
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Figure 9 (8/52)

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ATOM    396  CD1 PHE    41      11.955   7.444 -20.795  1.00 15.18      B
ATOM    397  CD2 PHE    41      10.789   9.462 -21.395  1.00 14.30      B
ATOM    398  CE1 PHE    41      11.441   7.520 -19.506  1.00 14.71      B
ATOM    399  CE2 PHE    41      10.262   9.556 -20.112  1.00 13.59      B
ATOM    400  CZ  PHE    41      10.589   8.588 -19.161  1.00 15.45      B
ATOM    401  C   PHE    41      10.194   7.173 -24.270  1.00 20.14      B
ATOM    402  O   PHE    41       9.808   7.758 -25.273  1.00 20.90      B
ATOM    403  N   LEU    42       9.349   6.577 -23.444  1.00 24.60      B
ATOM    404  H   LEU    42       9.724   6.255 -22.578  1.00 20.00      B
ATOM    405  CA  LEU    42       7.915   6.594 -23.719  1.00 28.73      B
ATOM    406  CB  LEU    42       7.144   5.947 -22.561  1.00 33.55      B
ATOM    407  CG  LEU    42       5.629   5.825 -22.778  1.00 37.60      B
ATOM    408  CD1 LEU    42       5.322   5.215 -24.170  1.00 36.88      B
ATOM    409  CD2 LEU    42       5.020   5.009 -21.608  1.00 38.78      B
ATOM    410  C   LEU    42       7.401   8.007 -23.989  1.00 28.11      B
ATOM    411  O   LEU    42       6.659   8.231 -24.951  1.00 29.36      B
ATOM    412  N   LEU    43       7.801   8.951 -23.139  1.00 26.47      B
ATOM    413  H   LEU    43       8.333   8.703 -22.336  1.00 20.00      B
ATOM    414  CA  LEU    43       7.409  10.351 -23.289  1.00 24.48      B
ATOM    415  CB  LEU    43       7.397  11.084 -21.935  1.00 23.94      B
ATOM    416  CG  LEU    43       6.433  10.756 -20.798  1.00 23.12      B
ATOM    417  CD1 LEU    43       6.631  11.816 -19.734  1.00 20.55      B
ATOM    418  CD2 LEU    43       4.992  10.761 -21.286  1.00 21.06      B
ATOM    419  C   LEU    43       8.430  11.049 -24.182  1.00 23.95      B
ATOM    420  O   LEU    43       9.488  11.454 -23.694  1.00 24.85      B
ATOM    421  N   SER    44       8.139  11.195 -25.470  1.00 21.89      B
ATOM    422  H   SER    44       7.242  10.957 -25.844  1.00 20.00      B
ATOM    423  CA  SER    44       9.068  11.862 -26.368  1.00 21.30      B
ATOM    424  CB  SER    44      10.219  10.936 -26.782  1.00 19.71      B
ATOM    425  OG  SER    44       9.769   9.905 -27.649  1.00 21.34      B
ATOM    426  HG  SER    44      10.523   9.323 -27.699  1.00 20.00      B
ATOM    427  C   SER    44       8.343  12.356 -27.602  1.00 21.71      B
ATOM    428  O   SER    44       7.188  12.006 -27.844  1.00 22.45      B
ATOM    429  N   GLU    45       9.040  13.164 -28.389  1.00 21.78      B
ATOM    430  H   GLU    45       9.889  13.593 -28.074  1.00 20.00      B
ATOM    431  CA  GLU    45       8.466  13.736 -29.581  1.00 21.05      B
ATOM    432  CB  GLU    45       7.999  15.161 -29.273  1.00 23.95      B
ATOM    433  CG  GLU    45       7.325  15.881 -30.423  1.00 31.83      B
ATOM    434  CD  GLU    45       6.630  17.155 -29.972  1.00 36.73      B
ATOM    435  OE1 GLU    45       5.739  17.043 -29.101  1.00 40.50      B
ATOM    436  OE2 GLU    45       6.965  18.257 -30.477  1.00 39.67      B
ATOM    437  C   GLU    45       9.510  13.744 -30.675  1.00 18.01      B
ATOM    438  O   GLU    45      10.641  14.120 -30.434  1.00 17.90      B
ATOM    439  N   ALA    46       9.121  13.292 -31.862  1.00 17.43      B
ATOM    440  H   ALA    46       8.129  13.216 -31.981  1.00 20.00      B
ATOM    441  CA  ALA    46       9.989  13.251 -33.034  1.00 15.82      B
ATOM    442  CB  ALA    46       9.272  12.543 -34.164  1.00 13.83      B
ATOM    443  C   ALA    46      10.301  14.694 -33.418  1.00 15.44      B
ATOM    444  O   ALA    46       9.397  15.528 -33.496  1.00 16.31      B
ATOM    445  N   HIS    47      11.579  14.999 -33.610  1.00 15.18      B
ATOM    446  H   HIS    47      12.273  14.314 -33.395  1.00 20.00      B
ATOM    447  CA  HIS    47      12.012  16.337 -33.972  1.00 15.35      B
ATOM    448  CB  HIS    47      12.959  16.886 -32.904  1.00 17.87      B
ATOM    449  CG  HIS    47      12.305  17.063 -31.570  1.00 20.19      B
ATOM    450  ND1 HIS    47      11.396  18.062 -31.313  1.00 21.32      B
ATOM    451  HD1 HIS    47      10.979  18.692 -31.930  1.00 20.00      B
ATOM    452  CD2 HIS    47      12.409  16.348 -30.426  1.00 21.45      B
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Figure 9 (9/52)

ATOM	453	NE2	HIS	47	11.554	16.921	-29.513	1.00	21.95	B
ATOM	454	CE1	HIS	47	10.955	17.953	-30.077	1.00	20.83	B
ATOM	455	C	HIS	47	12.727	16.236	-35.301	1.00	15.50	B
ATOM	456	O	HIS	47	13.250	15.171	-35.628	1.00	13.77	B
ATOM	457	N	THR	48	12.744	17.347	-36.048	1.00	15.63	B
ATOM	458	H	THR	48	12.297	18.164	-35.694	1.00	20.00	B
ATOM	459	CA	THR	48	13.367	17.448	-37.369	1.00	15.81	B
ATOM	460	CB	THR	48	12.362	17.856	-38.447	1.00	15.24	B
ATOM	461	OG1	THR	48	11.220	17.001	-38.393	1.00	14.89	B
ATOM	462	HG1	THR	48	10.449	17.488	-38.667	1.00	20.00	B
ATOM	463	CG2	THR	48	13.002	17.776	-39.817	1.00	13.51	B
ATOM	464	C	THR	48	14.431	18.518	-37.400	1.00	16.80	B
ATOM	465	O	THR	48	14.162	19.682	-37.107	1.00	18.14	B
ATOM	466	N	CYS	49	15.627	18.130	-37.802	1.00	17.03	B
ATOM	467	H	CYS	49	15.763	17.210	-38.145	1.00	20.00	B
ATOM	468	CA	CYS	49	16.745	19.043	-37.882	1.00	17.22	B
ATOM	469	CB	CYS	49	17.977	18.379	-37.263	1.00	16.55	B
ATOM	470	SG	CYS	49	19.519	19.333	-37.331	1.00	17.70	B
ATOM	471	C	CYS	49	16.939	19.280	-39.368	1.00	18.41	B
ATOM	472	O	CYS	49	16.878	18.336	-40.153	1.00	17.68	B
ATOM	473	N	ILE	50	17.097	20.535	-39.776	1.00	20.19	B
ATOM	474	H	ILE	50	17.199	21.240	-39.072	1.00	20.00	B
ATOM	475	CA	ILE	50	17.338	20.818	-41.189	1.00	21.85	B
ATOM	476	CB	ILE	50	16.446	22.008	-41.776	1.00	24.02	B
ATOM	477	CG2	ILE	50	15.994	22.972	-40.686	1.00	26.38	B
ATOM	478	CG1	ILE	50	17.197	22.710	-42.913	1.00	25.01	B
ATOM	479	CD1	ILE	50	16.352	23.686	-43.705	1.00	30.70	B
ATOM	480	C	ILE	50	18.833	21.094	-41.341	1.00	20.29	B
ATOM	481	O	ILE	50	19.350	22.068	-40.800	1.00	19.91	B
ATOM	482	N	PRO	51	19.552	20.205	-42.043	1.00	18.43	B
ATOM	483	CD	PRO	51	19.043	18.958	-42.640	1.00	17.07	B
ATOM	484	CA	PRO	51	20.992	20.343	-42.259	1.00	19.19	B
ATOM	485	CB	PRO	51	21.375	19.010	-42.897	1.00	17.56	B
ATOM	486	CG	PRO	51	20.151	18.567	-43.570	1.00	16.91	B
ATOM	487	C	PRO	51	21.469	21.536	-43.091	1.00	21.32	B
ATOM	488	O	PRO	51	20.690	22.223	-43.739	1.00	20.61	B
ATOM	489	N	GLU	52	22.769	21.764	-43.051	1.00	22.87	B
ATOM	490	H	GLU	52	23.341	21.207	-42.442	1.00	20.00	B
ATOM	491	CA	GLU	52	23.419	22.828	-43.795	1.00	25.85	B
ATOM	492	CB	GLU	52	23.732	24.007	-42.855	1.00	27.18	B
ATOM	493	CG	GLU	52	24.675	23.660	-41.700	1.00	28.52	B
ATOM	494	CD	GLU	52	25.196	24.883	-40.960	1.00	29.71	B
ATOM	495	OE1	GLU	52	24.397	25.561	-40.275	1.00	31.00	B
ATOM	496	OE2	GLU	52	26.416	25.162	-41.055	1.00	31.07	B
ATOM	497	C	GLU	52	24.709	22.166	-44.316	1.00	26.46	B
ATOM	498	O	GLU	52	25.157	21.173	-43.744	1.00	26.14	B
ATOM	499	N	ASN	53	25.294	22.668	-45.397	1.00	28.45	B
ATOM	500	H	ASN	53	24.913	23.476	-45.840	1.00	20.00	B
ATOM	501	CA	ASN	53	26.521	22.048	-45.922	1.00	30.18	B
ATOM	502	CB	ASN	53	26.702	22.367	-47.416	1.00	31.20	B
ATOM	503	CG	ASN	53	25.825	21.518	-48.321	1.00	31.72	B
ATOM	504	OD1	ASN	53	24.590	21.683	-48.359	1.00	31.71	B
ATOM	505	ND2	ASN	53	26.455	20.611	-49.068	1.00	29.88	B
ATOM	506	HD21	ASN	53	27.413	20.424	-48.863	1.00	20.00	B
ATOM	507	HD22	ASN	53	25.947	20.160	-49.797	1.00	20.00	B
ATOM	508	C	ASN	53	27.818	22.430	-45.215	1.00	31.00	B
ATOM	509	O	ASN	53	27.938	23.507	-44.627	1.00	31.23	B

Figure 9 (10/52)

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ATOM    510  N   ASN   54      28.787  21.525 -45.307  1.00 32.94      B
ATOM    511  H   ASN   54      28.531  20.668 -45.754  1.00 20.00      B
ATOM    512  CA  ASN   54      30.140  21.700 -44.775  1.00 34.71      B
ATOM    513  CB  ASN   54      30.281  20.990 -43.403  1.00 37.76      B
ATOM    514  CG  ASN   54      31.065  19.671 -43.454  1.00 42.89      B
ATOM    515  OD1 ASN   54      30.490  18.572 -43.501  1.00 45.91      B
ATOM    516  ND2 ASN   54      32.389  19.779 -43.430  1.00 43.90      B
ATOM    517  HD21 ASN  54      32.822  20.683 -43.460  1.00 20.00      B
ATOM    518  HD22 ASN  54      32.985  18.992 -43.310  1.00 20.00      B
ATOM    519  C   ASN   54      30.997  21.112 -45.924  1.00 34.74      B
ATOM    520  O   ASN   54      31.730  20.141 -45.799  1.00 36.67      B
ATOM    521  N   GLY   55      30.857  21.730 -47.086  1.00 33.09      B
ATOM    522  H   GLY   55      30.111  22.393 -47.144  1.00 20.00      B
ATOM    523  CA  GLY   55      31.548  21.260 -48.266  1.00 31.34      B
ATOM    524  C   GLY   55      30.422  20.832 -49.181  1.00 31.09      B
ATOM    525  O   GLY   55      29.273  20.735 -48.739  1.00 32.15      B
ATOM    526  N   GLY   56      30.728  20.564 -50.442  1.00 30.33      B
ATOM    527  H   GLY   56      31.681  20.623 -50.718  1.00 20.00      B
ATOM    528  CA  GLY   56      29.690  20.182 -51.380  1.00 27.99      B
ATOM    529  C   GLY   56      29.096  18.808 -51.178  1.00 28.44      B
ATOM    530  O   GLY   56      27.966  18.563 -51.608  1.00 28.58      B
ATOM    531  N   ALA   57      29.858  17.915 -50.543  1.00 27.60      B
ATOM    532  H   ALA   57      30.651  18.254 -50.044  1.00 20.00      B
ATOM    533  CA  ALA   57      29.421  16.543 -50.290  1.00 27.54      B
ATOM    534  CB  ALA   57      30.476  15.559 -50.820  1.00 25.92      B
ATOM    535  C   ALA   57      29.172  16.285 -48.798  1.00 27.85      B
ATOM    536  O   ALA   57      28.775  15.182 -48.408  1.00 28.00      B
ATOM    537  N   GLY   58      29.389  17.308 -47.974  1.00 27.42      B
ATOM    538  H   GLY   58      29.514  18.240 -48.306  1.00 20.00      B
ATOM    539  CA  GLY   58      29.209  17.159 -46.543  1.00 25.94      B
ATOM    540  C   GLY   58      28.048  17.928 -45.951  1.00 25.50      B
ATOM    541  O   GLY   58      27.722  19.039 -46.408  1.00 23.68      B
ATOM    542  N   CYS   59      27.460  17.346 -44.901  1.00 25.03      B
ATOM    543  H   CYS   59      27.844  16.484 -44.566  1.00 20.00      B
ATOM    544  CA  CYS   59      26.314  17.925 -44.201  1.00 24.02      B
ATOM    545  CB  CYS   59      25.055  17.099 -44.501  1.00 25.26      B
ATOM    546  SG  CYS   59      24.597  16.894 -46.266  1.00 24.53      B
ATOM    547  C   CYS   59      26.527  17.998 -42.681  1.00 24.03      B
ATOM    548  O   CYS   59      27.217  17.160 -42.094  1.00 24.62      B
ATOM    549  N   VAL   60      25.918  18.996 -42.047  1.00 22.89      B
ATOM    550  H   VAL   60      25.407  19.688 -42.567  1.00 20.00      B
ATOM    551  CA  VAL   60      26.018  19.199 -40.604  1.00 21.36      B
ATOM    552  CB  VAL   60      26.928  20.442 -40.266  1.00 21.99      B
ATOM    553  CG1 VAL   60      26.855  20.786 -38.789  1.00 21.80      B
ATOM    554  CG2 VAL   60      28.368  20.153 -40.615  1.00 21.77      B
ATOM    555  C   VAL   60      24.613  19.458 -40.060  1.00 20.52      B
ATOM    556  O   VAL   60      23.795  20.077 -40.734  1.00 19.23      B
ATOM    557  N   CYS   61      24.326  18.972 -38.858  1.00 19.36      B
ATOM    558  H   CYS   61      25.004  18.481 -38.312  1.00 20.00      B
ATOM    559  CA  CYS   61      23.026  19.215 -38.263  1.00 19.20      B
ATOM    560  CB  CYS   61      22.093  18.033 -38.450  1.00 18.65      B
ATOM    561  SG  CYS   61      20.468  18.618 -38.978  1.00 20.53      B
ATOM    562  C   CYS   61      23.159  19.489 -36.784  1.00 18.34      B
ATOM    563  O   CYS   61      23.927  18.832 -36.094  1.00 18.33      B
ATOM    564  N   HIS   62      22.394  20.457 -36.303  1.00 17.59      B
ATOM    565  H   HIS   62      21.782  20.946 -36.921  1.00 20.00      B
ATOM    566  CA  HIS   62      22.415  20.824 -34.907  1.00 16.74      B
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Figure 9 (11/52)

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ATOM    567  CB  HIS    62      22.590  22.332 -34.777  1.00 15.54      B
ATOM    568  CG  HIS    62      23.861  22.827 -35.392  1.00 15.75      B
ATOM    569  ND1 HIS    62      25.098  22.358 -35.007  1.00 17.59      B
ATOM    570  HD1 HIS    62      25.311  21.696 -34.311  1.00 20.00      B
ATOM    571  CD2 HIS    62      24.089  23.740 -36.362  1.00 15.43      B
ATOM    572  NE2 HIS    62      25.450  23.804 -36.547  1.00 18.49      B
ATOM    573  CE1 HIS    62      26.038  22.957 -35.718  1.00 17.24      B
ATOM    574  C   HIS    62      21.131  20.375 -34.230  1.00 17.54      B
ATOM    575  O   HIS    62      20.060  20.942 -34.471  1.00 18.20      B
ATOM    576  N   LEU    63      21.231  19.326 -33.417  1.00 16.41      B
ATOM    577  H   LEU    63      22.098  18.838 -33.446  1.00 20.00      B
ATOM    578  CA  LEU    63      20.076  18.805 -32.688  1.00 15.97      B
ATOM    579  CB  LEU    63      20.250  17.317 -32.334  1.00 14.77      B
ATOM    580  CG  LEU    63      20.891  16.367 -33.345  1.00 14.73      B
ATOM    581  CD1 LEU    63      20.642  14.958 -32.888  1.00 14.60      B
ATOM    582  CD2 LEU    63      20.306  16.561 -34.719  1.00 14.75      B
ATOM    583  C   LEU    63      19.948  19.608 -31.410  1.00 16.51      B
ATOM    584  O   LEU    63      20.948  19.920 -30.764  1.00 16.15      B
ATOM    585  N   LEU    64      18.718  19.942 -31.056  1.00 17.41      B
ATOM    586  H   LEU    64      17.958  19.690 -31.660  1.00 20.00      B
ATOM    587  CA  LEU    64      18.431  20.718 -29.859  1.00 18.26      B
ATOM    588  CB  LEU    64      17.477  21.869 -30.200  1.00 19.34      B
ATOM    589  CG  LEU    64      18.032  22.859 -31.220  1.00 19.99      B
ATOM    590  CD1 LEU    64      16.981  23.938 -31.556  1.00 19.08      B
ATOM    591  CD2 LEU    64      19.313  23.467 -30.647  1.00 19.65      B
ATOM    592  C   LEU    64      17.802  19.822 -28.810  1.00 17.90      B
ATOM    593  O   LEU    64      16.809  19.162 -29.091  1.00 17.87      B
ATOM    594  N   MET    65      18.388  19.800 -27.613  1.00 19.48      B
ATOM    595  H   MET    65      19.083  20.511 -27.472  1.00 20.00      B
ATOM    596  CA  MET    65      17.899  18.976 -26.501  1.00 19.50      B
ATOM    597  CB  MET    65      18.990  18.024 -25.963  1.00 21.17      B
ATOM    598  CG  MET    65      20.232  17.732 -26.855  1.00 21.80      B
ATOM    599  SD  MET    65      20.050  16.574 -28.243  1.00 25.21      B
ATOM    600  CE  MET    65      21.160  15.372 -27.852  1.00 25.58      B
ATOM    601  C   MET    65      17.508  19.942 -25.390  1.00 19.63      B
ATOM    602  O   MET    65      18.217  20.906 -25.145  1.00 20.63      B
ATOM    603  N   ASP    66      16.394  19.687 -24.718  1.00 20.34      B
ATOM    604  H   ASP    66      15.870  18.869 -24.937  1.00 20.00      B
ATOM    605  CA  ASP    66      15.921  20.544 -23.622  1.00 21.91      B
ATOM    606  CB  ASP    66      14.417  20.294 -23.427  1.00 25.95      B
ATOM    607  CG  ASP    66      13.906  20.757 -22.089  1.00 29.61      B
ATOM    608  OD1 ASP    66      14.228  21.890 -21.688  1.00 34.01      B
ATOM    609  OD2 ASP    66      13.174  19.979 -21.437  1.00 33.64      B
ATOM    610  C   ASP    66      16.701  20.339 -22.296  1.00 19.86      B
ATOM    611  O   ASP    66      16.884  21.279 -21.515  1.00 19.03      B
ATOM    612  N   ASP    67      17.145  19.107 -22.069  1.00 17.77      B
ATOM    613  H   ASP    67      16.796  18.397 -22.677  1.00 20.00      B
ATOM    614  CA  ASP    67      17.910  18.719 -20.895  1.00 15.71      B
ATOM    615  CB  ASP    67      16.979  18.551 -19.683  1.00 16.61      B
ATOM    616  CG  ASP    67      17.716  18.635 -18.347  1.00 16.56      B
ATOM    617  OD1 ASP    67      18.916  18.944 -18.320  1.00 15.83      B
ATOM    618  OD2 ASP    67      17.093  18.391 -17.299  1.00 16.13      B
ATOM    619  C   ASP    67      18.442  17.368 -21.326  1.00 15.22      B
ATOM    620  O   ASP    67      17.868  16.733 -22.212  1.00 17.15      B
ATOM    621  N   VAL    68      19.541  16.918 -20.752  1.00 13.90      B
ATOM    622  H   VAL    68      19.836  17.384 -19.915  1.00 20.00      B
ATOM    623  CA  VAL    68      20.062  15.617 -21.139  1.00 13.03      B
```

Figure 9 (12/52)

ATOM	624	CB	VAL	68	21.107	15.756	-22.302	1.00	13.11	B
ATOM	625	CG1	VAL	68	22.305	16.514	-21.836	1.00	14.43	B
ATOM	626	CG2	VAL	68	21.503	14.379	-22.844	1.00	12.77	B
ATOM	627	C	VAL	68	20.675	14.939	-19.915	1.00	11.14	B
ATOM	628	O	VAL	68	21.302	15.599	-19.089	1.00	10.66	B
ATOM	629	N	VAL	69	20.427	13.639	-19.767	1.00	8.25	B
ATOM	630	H	VAL	69	19.802	13.197	-20.421	1.00	20.00	B
ATOM	631	CA	VAL	69	20.982	12.895	-18.661	1.00	7.42	B
ATOM	632	CB	VAL	69	19.896	12.396	-17.655	1.00	6.88	B
ATOM	633	CG1	VAL	69	19.133	13.559	-17.076	1.00	6.26	B
ATOM	634	CG2	VAL	69	18.950	11.408	-18.316	1.00	4.43	B
ATOM	635	C	VAL	69	21.745	11.712	-19.246	1.00	7.31	B
ATOM	636	O	VAL	69	21.701	11.444	-20.445	1.00	8.44	B
ATOM	637	N	SER	70	22.435	11.007	-18.371	1.00	8.15	B
ATOM	638	H	SER	70	22.415	11.342	-17.428	1.00	20.00	B
ATOM	639	CA	SER	70	23.266	9.861	-18.693	1.00	7.90	B
ATOM	640	CB	SER	70	23.767	9.262	-17.388	1.00	8.25	B
ATOM	641	OG	SER	70	24.514	8.089	-17.590	1.00	12.74	B
ATOM	642	HG	SER	70	25.041	8.076	-16.787	1.00	20.00	B
ATOM	643	C	SER	70	22.599	8.783	-19.505	1.00	7.30	B
ATOM	644	O	SER	70	23.141	8.330	-20.523	1.00	6.89	B
ATOM	645	N	ALA	71	21.415	8.373	-19.068	1.00	5.35	B
ATOM	646	H	ALA	71	20.935	8.907	-18.369	1.00	20.00	B
ATOM	647	CA	ALA	71	20.717	7.296	-19.752	1.00	5.54	B
ATOM	648	CB	ALA	71	19.634	6.745	-18.856	1.00	3.01	B
ATOM	649	C	ALA	71	20.129	7.641	-21.118	1.00	5.50	B
ATOM	650	O	ALA	71	19.809	6.753	-21.886	1.00	5.98	B
ATOM	651	N	ASP	72	19.989	8.920	-21.424	1.00	6.82	B
ATOM	652	H	ASP	72	20.185	9.676	-20.794	1.00	20.00	B
ATOM	653	CA	ASP	72	19.387	9.342	-22.675	1.00	7.33	B
ATOM	654	CB	ASP	72	19.299	10.848	-22.715	1.00	5.25	B
ATOM	655	CG	ASP	72	18.175	11.372	-21.871	1.00	5.06	B
ATOM	656	OD1	ASP	72	17.318	10.578	-21.463	1.00	5.25	B
ATOM	657	OD2	ASP	72	18.131	12.577	-21.617	1.00	3.46	B
ATOM	658	C	ASP	72	20.024	8.846	-23.943	1.00	8.33	B
ATOM	659	O	ASP	72	21.232	8.926	-24.124	1.00	8.13	B
ATOM	660	N	ASN	73	19.166	8.346	-24.825	1.00	11.34	B
ATOM	661	H	ASN	73	18.334	7.827	-24.744	1.00	20.00	B
ATOM	662	CA	ASN	73	19.552	7.825	-26.131	1.00	13.40	B
ATOM	663	CB	ASN	73	19.438	6.310	-26.166	1.00	15.69	B
ATOM	664	CG	ASN	73	20.735	5.648	-25.946	1.00	18.63	B
ATOM	665	OD1	ASN	73	21.504	5.455	-26.897	1.00	22.79	B
ATOM	666	ND2	ASN	73	21.019	5.298	-24.694	1.00	18.30	B
ATOM	667	HD21	ASN	73	20.425	5.389	-23.896	1.00	20.00	B
ATOM	668	HD22	ASN	73	21.952	4.959	-24.599	1.00	20.00	B
ATOM	669	C	ASN	73	18.605	8.386	-27.170	1.00	13.15	B
ATOM	670	O	ASN	73	17.417	8.524	-26.892	1.00	13.52	B
ATOM	671	N	TYR	74	19.129	8.660	-28.365	1.00	11.81	B
ATOM	672	H	TYR	74	20.115	8.543	-28.519	1.00	20.00	B
ATOM	673	CA	TYR	74	18.356	9.212	-29.464	1.00	10.42	B
ATOM	674	CB	TYR	74	18.874	10.621	-29.789	1.00	10.75	B
ATOM	675	CG	TYR	74	18.401	11.679	-28.807	1.00	11.02	B
ATOM	676	CD1	TYR	74	19.082	11.908	-27.604	1.00	11.25	B
ATOM	677	CE1	TYR	74	18.624	12.863	-26.681	1.00	12.30	B
ATOM	678	CD2	TYR	74	17.256	12.425	-29.070	1.00	8.57	B
ATOM	679	CE2	TYR	74	16.785	13.371	-28.174	1.00	11.99	B
ATOM	680	CZ	TYR	74	17.473	13.592	-26.974	1.00	14.49	B

Figure 9 (13/52)

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ATOM    681  OH  TYR    74      16.988  14.534 -26.092  1.00 11.42      B
ATOM    682  HH  TYR    74      16.158  14.890 -26.406  1.00 20.00      B
ATOM    683  C   TYR    74      18.404   8.351 -30.727  1.00 10.93      B
ATOM    684  O   TYR    74      19.455   7.845 -31.100  1.00 10.39      B
ATOM    685  N   THR    75      17.254   8.157 -31.360  1.00  9.85      B
ATOM    686  H   THR    75      16.454   8.703 -31.106  1.00 20.00      B
ATOM    687  CA  THR    75      17.202   7.424 -32.614  1.00 10.56      B
ATOM    688  CB  THR    75      15.848   6.702 -32.833  1.00  9.16      B
ATOM    689  OG1 THR    75      15.701   5.658 -31.865  1.00 13.37      B
ATOM    690  HG1 THR    75      15.835   6.112 -31.039  1.00 20.00      B
ATOM    691  CG2 THR    75      15.777   6.074 -34.229  1.00 10.36      B
ATOM    692  C   THR    75      17.338   8.533 -33.651  1.00  9.88      B
ATOM    693  O   THR    75      16.648   9.546 -33.557  1.00 10.86      B
ATOM    694  N   LEU    76      18.233   8.344 -34.611  1.00  9.63      B
ATOM    695  H   LEU    76      18.740   7.499 -34.744  1.00 20.00      B
ATOM    696  CA  LEU    76      18.478   9.319 -35.673  1.00  9.47      B
ATOM    697  CB  LEU    76      19.961   9.710 -35.666  1.00  9.47      B
ATOM    698  CG  LEU    76      20.624  10.819 -34.836  1.00  9.62      B
ATOM    699  CD1 LEU    76      19.991  11.063 -33.493  1.00  9.96      B
ATOM    700  CD2 LEU    76      22.060  10.410 -34.664  1.00  9.98      B
ATOM    701  C   LEU    76      18.120   8.663 -37.023  1.00  9.83      B
ATOM    702  O   LEU    76      18.612   7.579 -37.322  1.00  8.08      B
ATOM    703  N   ASP    77      17.254   9.312 -37.813  1.00 10.64      B
ATOM    704  H   ASP    77      16.900  10.189 -37.511  1.00 20.00      B
ATOM    705  CA  ASP    77      16.819   8.824 -39.123  1.00  9.34      B
ATOM    706  CB  ASP    77      15.315   8.550 -39.158  1.00 10.92      B
ATOM    707  CG  ASP    77      14.885   7.460 -38.198  1.00 12.78      B
ATOM    708  OD1 ASP    77      15.615   6.466 -38.047  1.00 11.03      B
ATOM    709  OD2 ASP    77      13.805   7.589 -37.590  1.00 14.77      B
ATOM    710  C   ASP    77      17.088   9.902 -40.155  1.00 10.18      B
ATOM    711  O   ASP    77      16.493  10.954 -40.085  1.00  9.17      B
ATOM    712  N   LEU    78      18.006   9.639 -41.081  1.00 11.73      B
ATOM    713  H   LEU    78      18.311   8.681 -41.040  1.00 20.00      B
ATOM    714  CA  LEU    78      18.339  10.549 -42.178  1.00 11.33      B
ATOM    715  CB  LEU    78      19.801  10.360 -42.598  1.00  9.44      B
ATOM    716  CG  LEU    78      20.315  11.349 -43.652  1.00 10.82      B
ATOM    717  CD1 LEU    78      20.129  12.796 -43.153  1.00  8.65      B
ATOM    718  CD2 LEU    78      21.779  11.062 -43.948  1.00  7.68      B
ATOM    719  C   LEU    78      17.421  10.201 -43.366  1.00 12.55      B
ATOM    720  O   LEU    78      17.575   9.150 -43.977  1.00 11.81      B
ATOM    721  N   TRP    79      16.457  11.068 -43.661  1.00 14.44      B
ATOM    722  H   TRP    79      16.369  11.900 -43.107  1.00 20.00      B
ATOM    723  CA  TRP    79      15.518  10.880 -44.767  1.00 14.97      B
ATOM    724  CB  TRP    79      14.085  11.184 -44.336  1.00 14.82      B
ATOM    725  CG  TRP    79      13.477  10.233 -43.363  1.00 15.53      B
ATOM    726  CD2 TRP    79      12.663   9.105 -43.672  1.00 14.37      B
ATOM    727  CE2 TRP    79      12.275   8.520 -42.445  1.00 14.22      B
ATOM    728  CE3 TRP    79      12.215   8.533 -44.869  1.00 14.99      B
ATOM    729  CD1 TRP    79      13.557  10.285 -41.996  1.00 15.45      B
ATOM    730  NE1 TRP    79      12.838   9.260 -41.442  1.00 14.43      B
ATOM    731  HE1 TRP    79      12.740   9.089 -40.475  1.00 20.00      B
ATOM    732  CZ2 TRP    79      11.460   7.394 -42.380  1.00 14.97      B
ATOM    733  CZ3 TRP    79      11.407   7.416 -44.809  1.00 15.48      B
ATOM    734  CH2 TRP    79      11.034   6.854 -43.571  1.00 17.93      B
ATOM    735  C   TRP    79      15.809  11.847 -45.904  1.00 15.72      B
ATOM    736  O   TRP    79      16.233  12.977 -45.678  1.00 14.64      B
ATOM    737  N   ALA    80      15.539  11.392 -47.121  1.00 17.05      B
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Figure 9 (14/52)

ATOM	738	H	ALA	80	15.329	10.412	-47.228	1.00	20.00	B
ATOM	739	CA	ALA	80	15.677	12.196	-48.336	1.00	17.62	B
ATOM	740	CB	ALA	80	16.711	11.600	-49.256	1.00	17.67	B
ATOM	741	C	ALA	80	14.291	12.029	-48.931	1.00	17.97	B
ATOM	742	O	ALA	80	13.978	10.973	-49.486	1.00	19.33	B
ATOM	743	N	GLY	81	13.451	13.046	-48.801	1.00	19.20	B
ATOM	744	H	GLY	81	13.799	13.842	-48.298	1.00	20.00	B
ATOM	745	CA	GLY	81	12.097	12.935	-49.297	1.00	21.79	B
ATOM	746	C	GLY	81	11.379	11.801	-48.595	1.00	25.06	B
ATOM	747	O	GLY	81	10.938	11.943	-47.455	1.00	28.06	B
ATOM	748	N	GLN	82	11.254	10.658	-49.261	1.00	27.45	B
ATOM	749	H	GLN	82	11.668	10.566	-50.165	1.00	20.00	B
ATOM	750	CA	GLN	82	10.571	9.531	-48.636	1.00	28.91	B
ATOM	751	CB	GLN	82	9.244	9.253	-49.334	1.00	32.38	B
ATOM	752	CG	GLN	82	8.269	10.410	-49.223	1.00	37.38	B
ATOM	753	CD	GLN	82	6.841	9.984	-49.449	1.00	40.04	B
ATOM	754	OE1	GLN	82	6.552	8.791	-49.578	1.00	41.34	B
ATOM	755	NE2	GLN	82	5.931	10.956	-49.494	1.00	40.56	B
ATOM	756	HE21	GLN	82	6.140	11.921	-49.377	1.00	20.00	B
ATOM	757	HE22	GLN	82	4.990	10.674	-49.662	1.00	20.00	B
ATOM	758	C	GLN	82	11.395	8.269	-48.597	1.00	27.54	B
ATOM	759	O	GLN	82	10.847	7.176	-48.438	1.00	26.56	B
ATOM	760	N	GLN	83	12.705	8.427	-48.749	1.00	25.45	B
ATOM	761	H	GLN	83	13.063	9.356	-48.859	1.00	20.00	B
ATOM	762	CA	GLN	83	13.634	7.312	-48.706	1.00	24.68	B
ATOM	763	CB	GLN	83	14.521	7.302	-49.949	1.00	25.72	B
ATOM	764	CG	GLN	83	13.759	7.423	-51.276	1.00	30.02	B
ATOM	765	CD	GLN	83	14.665	7.338	-52.520	1.00	30.19	B
ATOM	766	OE1	GLN	83	14.843	6.257	-53.085	1.00	31.12	B
ATOM	767	NE2	GLN	83	15.212	8.477	-52.954	1.00	28.74	B
ATOM	768	HE21	GLN	83	15.048	9.333	-52.466	1.00	20.00	B
ATOM	769	HE22	GLN	83	15.669	8.481	-53.838	1.00	20.00	B
ATOM	770	C	GLN	83	14.523	7.451	-47.461	1.00	23.05	B
ATOM	771	O	GLN	83	15.243	8.432	-47.303	1.00	21.67	B
ATOM	772	N	LEU	84	14.447	6.469	-46.572	1.00	22.07	B
ATOM	773	H	LEU	84	13.854	5.692	-46.780	1.00	20.00	B
ATOM	774	CA	LEU	84	15.244	6.439	-45.349	1.00	19.53	B
ATOM	775	CB	LEU	84	14.708	5.352	-44.414	1.00	21.12	B
ATOM	776	CG	LEU	84	14.596	5.507	-42.894	1.00	19.90	B
ATOM	777	CD1	LEU	84	14.332	4.136	-42.317	1.00	19.41	B
ATOM	778	CD2	LEU	84	15.839	6.090	-42.307	1.00	18.28	B
ATOM	779	C	LEU	84	16.648	6.060	-45.802	1.00	18.65	B
ATOM	780	O	LEU	84	16.869	4.938	-46.259	1.00	19.27	B
ATOM	781	N	LEU	85	17.595	6.974	-45.664	1.00	17.16	B
ATOM	782	H	LEU	85	17.321	7.865	-45.306	1.00	20.00	B
ATOM	783	CA	LEU	85	18.955	6.713	-46.102	1.00	16.53	B
ATOM	784	CB	LEU	85	19.615	8.023	-46.537	1.00	15.21	B
ATOM	785	CG	LEU	85	18.817	8.952	-47.457	1.00	16.32	B
ATOM	786	CD1	LEU	85	19.666	10.176	-47.635	1.00	18.12	B
ATOM	787	CD2	LEU	85	18.465	8.306	-48.825	1.00	15.07	B
ATOM	788	C	LEU	85	19.848	6.031	-45.079	1.00	17.61	B
ATOM	789	O	LEU	85	20.793	5.336	-45.448	1.00	20.38	B
ATOM	790	N	TRP	86	19.568	6.254	-43.796	1.00	16.42	B
ATOM	791	H	TRP	86	18.828	6.878	-43.533	1.00	20.00	B
ATOM	792	CA	TRP	86	20.367	5.699	-42.707	1.00	14.17	B
ATOM	793	CB	TRP	86	21.692	6.467	-42.596	1.00	11.59	B
ATOM	794	CG	TRP	86	22.567	6.063	-41.445	1.00	12.77	B

Figure 9 (15/52)

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ATOM    795  CD2 TRP    86      22.591   6.659 -40.139  1.00 11.60      B
ATOM    796  CE2 TRP    86      23.563   5.966 -39.379  1.00 10.17      B
ATOM    797  CE3 TRP    86      21.890   7.709 -39.533  1.00 11.42      B
ATOM    798  CD1 TRP    86      23.499   5.066 -41.428  1.00 12.74      B
ATOM    799  NE1 TRP    86      24.103   4.998 -40.187  1.00 12.15      B
ATOM    800  HE1 TRP    86      24.855   4.400 -39.926  1.00 20.00      B
ATOM    801  CZ2 TRP    86      23.847   6.291 -38.050  1.00  9.27      B
ATOM    802  CZ3 TRP    86      22.176   8.034 -38.204  1.00 10.25      B
ATOM    803  CH2 TRP    86      23.148   7.324 -37.483  1.00  9.10      B
ATOM    804  C   TRP    86      19.552   5.871 -41.425  1.00 13.50      B
ATOM    805  O   TRP    86      18.849   6.864 -41.253  1.00 13.08      B
ATOM    806  N   LYS    87      19.681   4.909 -40.520  1.00 14.43      B
ATOM    807  H   LYS    87      20.289   4.119 -40.640  1.00 20.00      B
ATOM    808  CA  LYS    87      18.972   4.906 -39.248  1.00 12.56      B
ATOM    809  CB  LYS    87      17.812   3.938 -39.377  1.00 13.18      B
ATOM    810  CG  LYS    87      16.947   3.729 -38.188  1.00 13.54      B
ATOM    811  CD  LYS    87      15.756   2.900 -38.643  1.00 13.00      B
ATOM    812  CE  LYS    87      14.635   3.014 -37.665  1.00 15.38      B
ATOM    813  NZ  LYS    87      14.110   4.377 -37.594  1.00 12.88      B
ATOM    814  HZ1 LYS    87      13.252   4.565 -37.049  1.00 20.00      B
ATOM    815  HZ2 LYS    87      14.866   5.040 -37.280  1.00 20.00      B
ATOM    816  HZ3 LYS    87      14.007   4.763 -38.557  1.00 20.00      B
ATOM    817  C   LYS    87      19.982   4.429 -38.218  1.00 11.44      B
ATOM    818  O   LYS    87      20.601   3.391 -38.413  1.00  9.81      B
ATOM    819  N   GLY    88      20.177   5.213 -37.155  1.00 13.03      B
ATOM    820  H   GLY    88      19.695   6.083 -37.110  1.00 20.00      B
ATOM    821  CA  GLY    88      21.117   4.854 -36.096  1.00 11.91      B
ATOM    822  C   GLY    88      20.765   5.462 -34.746  1.00 10.44      B
ATOM    823  O   GLY    88      19.661   5.971 -34.563  1.00 10.34      B
ATOM    824  N   SER    89      21.696   5.418 -33.800  1.00 10.13      B
ATOM    825  H   SER    89      22.598   5.078 -34.059  1.00 20.00      B
ATOM    826  CA  SER    89      21.434   5.962 -32.465  1.00 10.81      B
ATOM    827  CB  SER    89      21.084   4.849 -31.460  1.00  9.83      B
ATOM    828  OG  SER    89      22.217   4.057 -31.170  1.00 13.93      B
ATOM    829  HG  SER    89      22.936   4.434 -31.680  1.00 20.00      B
ATOM    830  C   SER    89      22.574   6.785 -31.919  1.00  9.77      B
ATOM    831  O   SER    89      23.727   6.600 -32.286  1.00 10.13      B
ATOM    832  N   PHE    90      22.243   7.697 -31.028  1.00  9.33      B
ATOM    833  H   PHE    90      21.272   7.893 -30.935  1.00 20.00      B
ATOM    834  CA  PHE    90      23.245   8.561 -30.444  1.00  9.70      B
ATOM    835  CB  PHE    90      23.254   9.907 -31.161  1.00  7.89      B
ATOM    836  CG  PHE    90      24.204  10.907 -30.561  1.00  7.33      B
ATOM    837  CD1 PHE    90      25.522  10.561 -30.296  1.00  5.24      B
ATOM    838  CD2 PHE    90      23.772  12.190 -30.250  1.00  6.62      B
ATOM    839  CE1 PHE    90      26.382  11.476 -29.748  1.00  7.50      B
ATOM    840  CE2 PHE    90      24.635  13.116 -29.699  1.00  6.97      B
ATOM    841  CZ  PHE    90      25.933  12.759 -29.442  1.00  7.31      B
ATOM    842  C   PHE    90      22.982   8.790 -28.959  1.00  9.95      B
ATOM    843  O   PHE    90      21.911   9.262 -28.587  1.00 10.72      B
ATOM    844  N   LYS    91      23.995   8.482 -28.152  1.00  8.15      B
ATOM    845  H   LYS    91      24.812   8.197 -28.660  1.00 20.00      B
ATOM    846  CA  LYS    91      23.994   8.633 -26.697  1.00  8.19      B
ATOM    847  CB  LYS    91      24.601   7.371 -26.058  1.00  9.16      B
ATOM    848  CG  LYS    91      24.687   7.427 -24.567  1.00 14.20      B
ATOM    849  CD  LYS    91      24.567   6.048 -23.959  1.00 16.65      B
ATOM    850  CE  LYS    91      23.796   6.114 -22.656  1.00 17.64      B
ATOM    851  NZ  LYS    91      23.716   4.774 -22.053  1.00 21.33      B
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Figure 9 (16/52)

ATOM	852	HZ1	LYS	91	23.026	4.806	-21.281	1.00	20.00	B
ATOM	853	HZ2	LYS	91	23.458	4.078	-22.772	1.00	20.00	B
ATOM	854	HZ3	LYS	91	24.666	4.554	-21.695	1.00	20.00	B
ATOM	855	C	LYS	91	24.854	9.859	-26.358	1.00	5.41	B
ATOM	856	O	LYS	91	26.071	9.794	-26.374	1.00	6.73	B
ATOM	857	N	PRO	92	24.227	11.010	-26.101	1.00	5.56	B
ATOM	858	CD	PRO	92	22.775	11.264	-26.170	1.00	3.39	B
ATOM	859	CA	PRO	92	24.945	12.239	-25.772	1.00	5.52	B
ATOM	860	CB	PRO	92	23.811	13.159	-25.330	1.00	5.86	B
ATOM	861	CG	PRO	92	22.709	12.753	-26.241	1.00	3.00	B
ATOM	862	C	PRO	92	26.062	12.137	-24.719	1.00	7.25	B
ATOM	863	O	PRO	92	27.181	12.617	-24.936	1.00	7.31	B
ATOM	864	N	SER	93	25.765	11.465	-23.608	1.00	9.44	B
ATOM	865	H	SER	93	24.892	10.983	-23.585	1.00	20.00	B
ATOM	866	CA	SER	93	26.702	11.343	-22.492	1.00	10.05	B
ATOM	867	CB	SER	93	26.016	10.631	-21.350	1.00	10.12	B
ATOM	868	OG	SER	93	25.624	9.345	-21.766	1.00	10.96	B
ATOM	869	HG	SER	93	24.922	9.078	-21.171	1.00	20.00	B
ATOM	870	C	SER	93	28.017	10.647	-22.797	1.00	11.72	B
ATOM	871	O	SER	93	28.995	10.759	-22.052	1.00	12.32	B
ATOM	872	N	GLU	94	28.049	9.909	-23.892	1.00	13.08	B
ATOM	873	H	GLU	94	27.277	9.821	-24.527	1.00	20.00	B
ATOM	874	CA	GLU	94	29.265	9.230	-24.252	1.00	13.78	B
ATOM	875	CB	GLU	94	28.942	7.821	-24.719	1.00	13.65	B
ATOM	876	CG	GLU	94	28.358	7.041	-23.588	1.00	21.82	B
ATOM	877	CD	GLU	94	28.186	5.568	-23.893	1.00	26.79	B
ATOM	878	OE1	GLU	94	28.257	5.203	-25.087	1.00	27.72	B
ATOM	879	OE2	GLU	94	27.968	4.782	-22.933	1.00	26.22	B
ATOM	880	C	GLU	94	30.017	9.987	-25.318	1.00	12.27	B
ATOM	881	O	GLU	94	31.048	9.530	-25.767	1.00	16.13	B
ATOM	882	N	HIS	95	29.505	11.128	-25.755	1.00	10.44	B
ATOM	883	H	HIS	95	28.592	11.394	-25.437	1.00	20.00	B
ATOM	884	CA	HIS	95	30.196	11.880	-26.793	1.00	9.71	B
ATOM	885	CB	HIS	95	29.533	11.626	-28.145	1.00	9.49	B
ATOM	886	CG	HIS	95	29.521	10.183	-28.518	1.00	10.37	B
ATOM	887	ND1	HIS	95	30.592	9.562	-29.136	1.00	10.94	B
ATOM	888	HD1	HIS	95	31.418	10.017	-29.401	1.00	20.00	B
ATOM	889	CD2	HIS	95	28.609	9.207	-28.304	1.00	12.02	B
ATOM	890	NE2	HIS	95	29.133	8.035	-28.785	1.00	11.55	B
ATOM	891	CE1	HIS	95	30.336	8.280	-29.285	1.00	10.24	B
ATOM	892	C	HIS	95	30.189	13.330	-26.455	1.00	9.28	B
ATOM	893	O	HIS	95	29.934	14.173	-27.307	1.00	10.84	B
ATOM	894	N	VAL	96	30.491	13.622	-25.196	1.00	9.36	B
ATOM	895	H	VAL	96	30.944	12.901	-24.678	1.00	20.00	B
ATOM	896	CA	VAL	96	30.493	14.989	-24.724	1.00	8.40	B
ATOM	897	CB	VAL	96	30.379	15.055	-23.189	1.00	6.95	B
ATOM	898	CG1	VAL	96	30.463	16.512	-22.717	1.00	5.76	B
ATOM	899	CG2	VAL	96	29.064	14.469	-22.749	1.00	5.79	B
ATOM	900	C	VAL	96	31.720	15.779	-25.134	1.00	8.91	B
ATOM	901	O	VAL	96	32.839	15.331	-24.943	1.00	10.27	B
ATOM	902	N	LYS	97	31.482	16.950	-25.722	1.00	9.88	B
ATOM	903	H	LYS	97	30.521	17.146	-25.893	1.00	20.00	B
ATOM	904	CA	LYS	97	32.515	17.903	-26.097	1.00	12.34	B
ATOM	905	CB	LYS	97	32.546	18.177	-27.607	1.00	15.14	B
ATOM	906	CG	LYS	97	33.585	19.230	-27.979	1.00	16.49	B
ATOM	907	CD	LYS	97	33.581	19.577	-29.445	1.00	15.49	B
ATOM	908	CE	LYS	97	34.668	20.582	-29.716	1.00	15.85	B

Figure 9 (17/52)

ATOM	909	NZ	LYS	97	34.593	21.123	-31.088	1.00 20.39	B
ATOM	910	HZ1	LYS	97	35.425	21.740	-31.278	1.00 20.00	B
ATOM	911	HZ2	LYS	97	34.557	20.356	-31.788	1.00 20.00	B
ATOM	912	HZ3	LYS	97	33.751	21.715	-31.216	1.00 20.00	B
ATOM	913	C	LYS	97	31.941	19.121	-25.387	1.00 11.39	B
ATOM	914	O	LYS	97	30.865	19.598	-25.751	1.00 9.79	B
ATOM	915	N	PRO	98	32.621	19.617	-24.338	1.00 10.24	B
ATOM	916	CD	PRO	98	33.756	19.073	-23.568	1.00 10.73	B
ATOM	917	CA	PRO	98	32.028	20.778	-23.675	1.00 12.39	B
ATOM	918	CB	PRO	98	32.723	20.805	-22.300	1.00 10.03	B
ATOM	919	CG	PRO	98	34.022	20.165	-22.541	1.00 11.90	B
ATOM	920	C	PRO	98	32.029	22.129	-24.359	1.00 12.99	B
ATOM	921	O	PRO	98	32.831	22.417	-25.246	1.00 13.23	B
ATOM	922	N	ARG	99	31.078	22.946	-23.930	1.00 13.88	B
ATOM	923	H	ARG	99	30.492	22.621	-23.185	1.00 20.00	B
ATOM	924	CA	ARG	99	30.910	24.297	-24.390	1.00 12.95	B
ATOM	925	CB	ARG	99	29.683	24.868	-23.699	1.00 15.79	B
ATOM	926	CG	ARG	99	29.043	26.036	-24.379	1.00 23.15	B
ATOM	927	CD	ARG	99	27.738	26.421	-23.691	1.00 28.32	B
ATOM	928	NE	ARG	99	26.606	25.559	-24.039	1.00 32.23	B
ATOM	929	HE	ARG	99	26.747	24.607	-24.342	1.00 20.00	B
ATOM	930	CZ	ARG	99	25.339	25.977	-24.080	1.00 34.15	B
ATOM	931	NH1	ARG	99	25.033	27.243	-23.793	1.00 34.78	B
ATOM	932	HH11	ARG	99	24.092	27.567	-23.902	1.00 20.00	B
ATOM	933	HH12	ARG	99	25.714	27.880	-23.438	1.00 20.00	B
ATOM	934	NH2	ARG	99	24.371	25.131	-24.408	1.00 34.85	B
ATOM	935	HH21	ARG	99	23.384	25.329	-24.430	1.00 20.00	B
ATOM	936	HH22	ARG	99	24.609	24.185	-24.693	1.00 20.00	B
ATOM	937	C	ARG	99	32.187	25.030	-23.953	1.00 13.41	B
ATOM	938	O	ARG	99	32.777	24.700	-22.917	1.00 12.29	B
ATOM	939	N	ALA	100	32.611	26.023	-24.733	1.00 12.40	B
ATOM	940	H	ALA	100	31.989	26.336	-25.453	1.00 20.00	B
ATOM	941	CA	ALA	100	33.828	26.777	-24.430	1.00 10.93	B
ATOM	942	CB	ALA	100	34.405	27.370	-25.715	1.00 9.18	B
ATOM	943	C	ALA	100	33.614	27.901	-23.403	1.00 11.77	B
ATOM	944	O	ALA	100	32.544	28.527	-23.396	1.00 13.94	B
ATOM	945	N	PRO	101	34.600	28.131	-22.491	1.00 10.02	B
ATOM	946	CD	PRO	101	35.834	27.350	-22.261	1.00 8.14	B
ATOM	947	CA	PRO	101	34.482	29.194	-21.496	1.00 7.80	B
ATOM	948	CB	PRO	101	35.751	29.041	-20.666	1.00 7.70	B
ATOM	949	CG	PRO	101	36.134	27.640	-20.828	1.00 6.61	B
ATOM	950	C	PRO	101	34.523	30.494	-22.292	1.00 8.99	B
ATOM	951	O	PRO	101	35.087	30.536	-23.387	1.00 10.15	B
ATOM	952	N	GLY	102	33.947	31.554	-21.750	1.00 8.41	B
ATOM	953	H	GLY	102	33.599	31.479	-20.814	1.00 20.00	B
ATOM	954	CA	GLY	102	33.964	32.818	-22.450	1.00 8.84	B
ATOM	955	C	GLY	102	34.150	33.944	-21.464	1.00 8.68	B
ATOM	956	O	GLY	102	34.434	33.707	-20.296	1.00 9.22	B
ATOM	957	N	ASN	103	33.995	35.167	-21.939	1.00 7.00	B
ATOM	958	H	ASN	103	33.794	35.319	-22.905	1.00 20.00	B
ATOM	959	CA	ASN	103	34.129	36.358	-21.111	1.00 9.51	B
ATOM	960	CB	ASN	103	33.080	36.385	-19.974	1.00 9.75	B
ATOM	961	CG	ASN	103	31.642	36.382	-20.480	1.00 9.21	B
ATOM	962	OD1	ASN	103	31.361	36.738	-21.624	1.00 9.30	B
ATOM	963	ND2	ASN	103	30.724	35.961	-19.622	1.00 9.93	B
ATOM	964	HD21	ASN	103	31.002	35.632	-18.715	1.00 20.00	B
ATOM	965	HD22	ASN	103	29.770	36.012	-19.910	1.00 20.00	B

Figure 9 (18/52)

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ATOM    966  C   ASN  103      35.520  36.483 -20.502  1.00 10.58      B
ATOM    967  O   ASN  103      35.691  37.088 -19.440  1.00 11.61      B
ATOM    968  N   LEU  104      36.511  35.914 -21.172  1.00 10.97      B
ATOM    969  H   LEU  104      36.309  35.651 -22.109  1.00 20.00      B
ATOM    970  CA  LEU  104      37.887  35.978 -20.696  1.00 11.51      B
ATOM    971  CB  LEU  104      38.758  35.033 -21.529  1.00 11.33      B
ATOM    972  CG  LEU  104      40.272  35.176 -21.398  1.00 15.00      B
ATOM    973  CD1 LEU  104      40.753  34.682 -20.024  1.00 14.27      B
ATOM    974  CD2 LEU  104      40.922  34.362 -22.471  1.00 14.96      B
ATOM    975  C   LEU  104      38.467  37.400 -20.760  1.00 11.74      B
ATOM    976  O   LEU  104      38.637  37.961 -21.846  1.00 12.16      B
ATOM    977  N   THR  105      38.752  37.978 -19.596  1.00 12.98      B
ATOM    978  H   THR  105      38.502  37.494 -18.756  1.00 20.00      B
ATOM    979  CA  THR  105      39.357  39.303 -19.509  1.00 12.46      B
ATOM    980  CB  THR  105      38.385  40.400 -19.032  1.00 10.73      B
ATOM    981  OG1 THR  105      37.830  40.055 -17.757  1.00 10.05      B
ATOM    982  HG1 THR  105      37.310  39.267 -17.911  1.00 20.00      B
ATOM    983  CG2 THR  105      37.290  40.590 -20.032  1.00  8.58      B
ATOM    984  C   THR  105      40.542  39.267 -18.556  1.00 15.49      B
ATOM    985  O   THR  105      40.675  38.338 -17.754  1.00 14.77      B
ATOM    986  N   VAL  106      41.383  40.295 -18.651  1.00 17.30      B
ATOM    987  H   VAL  106      41.146  41.092 -19.208  1.00 20.00      B
ATOM    988  CA  VAL  106      42.594  40.434 -17.840  1.00 19.11      B
ATOM    989  CB  VAL  106      43.854  40.523 -18.757  1.00 18.08      B
ATOM    990  CG1 VAL  106      44.941  41.316 -18.114  1.00 19.51      B
ATOM    991  CG2 VAL  106      44.384  39.162 -19.029  1.00 18.62      B
ATOM    992  C   VAL  106      42.457  41.712 -17.009  1.00 20.83      B
ATOM    993  O   VAL  106      41.974  42.729 -17.501  1.00 22.72      B
ATOM    994  N   HIS  107      42.881  41.670 -15.756  1.00 22.29      B
ATOM    995  H   HIS  107      43.290  40.831 -15.396  1.00 20.00      B
ATOM    996  CA  HIS  107      42.770  42.838 -14.897  1.00 23.81      B
ATOM    997  CB  HIS  107      42.177  42.412 -13.559  1.00 25.88      B
ATOM    998  CG  HIS  107      41.593  43.538 -12.763  1.00 29.87      B
ATOM    999  ND1 HIS  107      41.546  43.530 -11.382  1.00 30.67      B
ATOM   1000  HD1 HIS  107      41.877  42.804 -10.816  1.00 20.00      B
ATOM   1001  CD2 HIS  107      41.035  44.714 -13.148  1.00 30.23      B
ATOM   1002  NE2 HIS  107      40.667  45.382 -12.005  1.00 29.39      B
ATOM   1003  CE1 HIS  107      40.989  44.648 -10.953  1.00 28.79      B
ATOM   1004  C   HIS  107      44.162  43.424 -14.709  1.00 24.81      B
ATOM   1005  O   HIS  107      45.147  42.673 -14.613  1.00 25.53      B
ATOM   1006  N   ASP  112      53.354  43.590  -9.367  1.00 39.53      B
ATOM   1007  H   ASP  112      53.576  44.527  -9.122  1.00 20.00      B
ATOM   1008  CA  ASP  112      52.350  42.818  -8.654  1.00 37.88      B
ATOM   1009  CB  ASP  112      51.175  43.726  -8.247  1.00 39.79      B
ATOM   1010  CG  ASP  112      51.068  44.992  -9.099  1.00 40.68      B
ATOM   1011  OD1 ASP  112      51.022  44.891 -10.341  1.00 41.08      B
ATOM   1012  OD2 ASP  112      51.024  46.098  -8.519  1.00 42.48      B
ATOM   1013  C   ASP  112      51.846  41.606  -9.443  1.00 37.03      B
ATOM   1014  O   ASP  112      52.583  41.011 -10.250  1.00 35.64      B
ATOM   1015  N   THR  113      50.595  41.232  -9.182  1.00 35.50      B
ATOM   1016  H   THR  113      49.949  41.913  -8.853  1.00 20.00      B
ATOM   1017  CA  THR  113      49.983  40.091  -9.837  1.00 34.44      B
ATOM   1018  CB  THR  113      48.923  39.397  -8.929  1.00 35.48      B
ATOM   1019  OG1 THR  113      48.646  38.079  -9.432  1.00 38.30      B
ATOM   1020  HG1 THR  113      48.123  38.195 -10.217  1.00 20.00      B
ATOM   1021  CG2 THR  113      47.601  40.188  -8.923  1.00 36.95      B
ATOM   1022  C   THR  113      49.286  40.520 -11.103  1.00 31.10      B
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Figure 9 (19/52)

ATOM	1023	O	THR	113	49.134	41.712	-11.392	1.00 32.78	B
ATOM	1024	N	LEU	114	48.850	39.511	-11.839	1.00 28.33	B
ATOM	1025	H	LEU	114	49.217	38.609	-11.610	1.00 20.00	B
ATOM	1026	CA	LEU	114	48.120	39.655	-13.080	1.00 23.23	B
ATOM	1027	CB	LEU	114	49.002	39.161	-14.219	1.00 24.57	B
ATOM	1028	CG	LEU	114	48.462	39.024	-15.622	1.00 23.23	B
ATOM	1029	CD1	LEU	114	48.670	40.318	-16.406	1.00 21.77	B
ATOM	1030	CD2	LEU	114	49.205	37.872	-16.254	1.00 24.04	B
ATOM	1031	C	LEU	114	46.958	38.700	-12.838	1.00 20.32	B
ATOM	1032	O	LEU	114	47.156	37.574	-12.405	1.00 16.73	B
ATOM	1033	N	LEU	115	45.746	39.157	-13.083	1.00 18.68	B
ATOM	1034	H	LEU	115	45.613	40.070	-13.472	1.00 20.00	B
ATOM	1035	CA	LEU	115	44.593	38.314	-12.857	1.00 17.55	B
ATOM	1036	CB	LEU	115	43.740	38.932	-11.753	1.00 16.30	B
ATOM	1037	CG	LEU	115	42.491	38.165	-11.343	1.00 16.68	B
ATOM	1038	CD1	LEU	115	42.875	36.867	-10.682	1.00 16.13	B
ATOM	1039	CD2	LEU	115	41.676	39.026	-10.419	1.00 15.79	B
ATOM	1040	C	LEU	115	43.756	38.092	-14.120	1.00 16.99	B
ATOM	1041	O	LEU	115	43.347	39.044	-14.792	1.00 17.21	B
ATOM	1042	N	LEU	116	43.527	36.833	-14.455	1.00 14.63	B
ATOM	1043	H	LEU	116	43.892	36.117	-13.864	1.00 20.00	B
ATOM	1044	CA	LEU	116	42.712	36.510	-15.604	1.00 15.00	B
ATOM	1045	CB	LEU	116	43.398	35.457	-16.487	1.00 15.38	B
ATOM	1046	CG	LEU	116	44.490	35.843	-17.508	1.00 15.43	B
ATOM	1047	CD1	LEU	116	45.708	36.355	-16.788	1.00 17.78	B
ATOM	1048	CD2	LEU	116	44.899	34.622	-18.321	1.00 16.84	B
ATOM	1049	C	LEU	116	41.415	35.955	-15.042	1.00 14.93	B
ATOM	1050	O	LEU	116	41.431	35.231	-14.052	1.00 13.43	B
ATOM	1051	N	THR	117	40.292	36.283	-15.662	1.00 14.27	B
ATOM	1052	H	THR	117	40.263	36.939	-16.419	1.00 20.00	B
ATOM	1053	CA	THR	117	39.025	35.774	-15.178	1.00 14.21	B
ATOM	1054	CB	THR	117	38.400	36.770	-14.175	1.00 17.16	B
ATOM	1055	OG1	THR	117	37.356	36.115	-13.448	1.00 24.71	B
ATOM	1056	HG1	THR	117	36.567	36.079	-13.975	1.00 20.00	B
ATOM	1057	CG2	THR	117	37.837	37.978	-14.866	1.00 14.58	B
ATOM	1058	C	THR	117	38.093	35.473	-16.350	1.00 12.04	B
ATOM	1059	O	THR	117	38.119	36.174	-17.354	1.00 11.54	B
ATOM	1060	N	TRP	118	37.278	34.429	-16.219	1.00 10.62	B
ATOM	1061	H	TRP	118	37.264	33.903	-15.361	1.00 20.00	B
ATOM	1062	CA	TRP	118	36.371	34.010	-17.286	1.00 10.29	B
ATOM	1063	CB	TRP	118	37.097	33.057	-18.247	1.00 9.20	B
ATOM	1064	CG	TRP	118	37.601	31.805	-17.572	1.00 9.25	B
ATOM	1065	CD2	TRP	118	38.842	31.636	-16.869	1.00 8.33	B
ATOM	1066	CE2	TRP	118	38.874	30.308	-16.399	1.00 6.52	B
ATOM	1067	CE3	TRP	118	39.936	32.489	-16.591	1.00 8.52	B
ATOM	1068	CD1	TRP	118	36.956	30.596	-17.501	1.00 7.24	B
ATOM	1069	NE1	TRP	118	37.711	29.707	-16.799	1.00 7.69	B
ATOM	1070	HE1	TRP	118	37.423	28.799	-16.569	1.00 20.00	B
ATOM	1071	CZ2	TRP	118	39.941	29.800	-15.668	1.00 7.21	B
ATOM	1072	CZ3	TRP	118	41.007	31.981	-15.866	1.00 7.25	B
ATOM	1073	CH2	TRP	118	40.999	30.645	-15.411	1.00 7.76	B
ATOM	1074	C	TRP	118	35.135	33.321	-16.709	1.00 9.67	B
ATOM	1075	O	TRP	118	35.063	33.085	-15.507	1.00 8.43	B
ATOM	1076	N	SER	119	34.169	32.993	-17.570	1.00 10.41	B
ATOM	1077	H	SER	119	34.286	33.254	-18.524	1.00 20.00	B
ATOM	1078	CA	SER	119	32.924	32.346	-17.136	1.00 9.64	B
ATOM	1079	CB	SER	119	31.718	32.937	-17.864	1.00 9.32	B

Figure 9 (20/52)

ATOM	1080	OG	SER	119	31.553	34.298	-17.589	1.00	10.84	B
ATOM	1081	HG	SER	119	31.840	34.440	-16.689	1.00	20.00	B
ATOM	1082	C	SER	119	32.871	30.844	-17.382	1.00	8.46	B
ATOM	1083	O	SER	119	33.345	30.352	-18.400	1.00	6.60	B
ATOM	1084	N	ASN	120	32.323	30.122	-16.416	1.00	8.08	B
ATOM	1085	H	ASN	120	31.985	30.606	-15.612	1.00	20.00	B
ATOM	1086	CA	ASN	120	32.092	28.689	-16.567	1.00	10.60	B
ATOM	1087	CB	ASN	120	31.557	28.071	-15.263	1.00	9.79	B
ATOM	1088	CG	ASN	120	31.284	26.585	-15.393	1.00	10.26	B
ATOM	1089	OD1	ASN	120	30.703	26.117	-16.375	1.00	13.59	B
ATOM	1090	ND2	ASN	120	31.715	25.833	-14.409	1.00	9.93	B
ATOM	1091	HD21	ASN	120	32.184	26.279	-13.646	1.00	20.00	B
ATOM	1092	HD22	ASN	120	31.582	24.850	-14.300	1.00	20.00	B
ATOM	1093	C	ASN	120	30.948	28.756	-17.586	1.00	10.50	B
ATOM	1094	O	ASN	120	29.975	29.498	-17.389	1.00	9.94	B
ATOM	1095	N	PRO	121	31.036	27.990	-18.673	1.00	9.90	B
ATOM	1096	CD	PRO	121	32.064	27.039	-19.133	1.00	9.71	B
ATOM	1097	CA	PRO	121	29.936	28.091	-19.629	1.00	10.80	B
ATOM	1098	CB	PRO	121	30.571	27.560	-20.917	1.00	9.39	B
ATOM	1099	CG	PRO	121	31.441	26.458	-20.412	1.00	8.72	B
ATOM	1100	C	PRO	121	28.647	27.363	-19.264	1.00	11.70	B
ATOM	1101	O	PRO	121	27.681	27.467	-19.982	1.00	12.79	B
ATOM	1102	N	TYR	122	28.621	26.625	-18.160	1.00	13.10	B
ATOM	1103	H	TYR	122	29.337	26.707	-17.467	1.00	20.00	B
ATOM	1104	CA	TYR	122	27.420	25.882	-17.772	1.00	12.62	B
ATOM	1105	CB	TYR	122	27.784	24.443	-17.438	1.00	11.34	B
ATOM	1106	CG	TYR	122	28.273	23.670	-18.624	1.00	11.47	B
ATOM	1107	CD1	TYR	122	27.379	22.992	-19.433	1.00	10.62	B
ATOM	1108	CE1	TYR	122	27.811	22.277	-20.522	1.00	12.46	B
ATOM	1109	CD2	TYR	122	29.630	23.612	-18.940	1.00	10.42	B
ATOM	1110	CE2	TYR	122	30.076	22.899	-20.031	1.00	10.31	B
ATOM	1111	CZ	TYR	122	29.154	22.231	-20.817	1.00	12.32	B
ATOM	1112	OH	TYR	122	29.563	21.503	-21.905	1.00	14.64	B
ATOM	1113	HH	TYR	122	28.856	20.904	-22.137	1.00	20.00	B
ATOM	1114	C	TYR	122	26.758	26.492	-16.563	1.00	13.69	B
ATOM	1115	O	TYR	122	27.433	27.137	-15.755	1.00	13.94	B
ATOM	1116	N	PRO	123	25.423	26.330	-16.436	1.00	13.07	B
ATOM	1117	CD	PRO	123	24.479	25.767	-17.412	1.00	12.16	B
ATOM	1118	CA	PRO	123	24.719	26.883	-15.274	1.00	13.11	B
ATOM	1119	CB	PRO	123	23.247	26.867	-15.708	1.00	13.29	B
ATOM	1120	CG	PRO	123	23.167	25.727	-16.643	1.00	11.20	B
ATOM	1121	C	PRO	123	25.003	25.975	-14.087	1.00	14.05	B
ATOM	1122	O	PRO	123	25.422	24.827	-14.269	1.00	13.38	B
ATOM	1123	N	PRO	124	24.778	26.473	-12.852	1.00	16.35	B
ATOM	1124	CD	PRO	124	24.284	27.828	-12.538	1.00	17.71	B
ATOM	1125	CA	PRO	124	25.017	25.725	-11.613	1.00	17.33	B
ATOM	1126	CB	PRO	124	24.445	26.654	-10.534	1.00	18.16	B
ATOM	1127	CG	PRO	124	24.721	28.007	-11.088	1.00	17.03	B
ATOM	1128	C	PRO	124	24.418	24.333	-11.530	1.00	18.56	B
ATOM	1129	O	PRO	124	25.033	23.435	-10.962	1.00	19.53	B
ATOM	1130	N	ASP	125	23.230	24.151	-12.096	1.00	19.56	B
ATOM	1131	H	ASP	125	22.748	24.854	-12.620	1.00	20.00	B
ATOM	1132	CA	ASP	125	22.561	22.856	-12.032	1.00	19.50	B
ATOM	1133	CB	ASP	125	21.045	23.039	-11.986	1.00	22.69	B
ATOM	1134	CG	ASP	125	20.490	23.754	-13.209	1.00	26.88	B
ATOM	1135	OD1	ASP	125	21.264	24.373	-13.991	1.00	28.76	B
ATOM	1136	OD2	ASP	125	19.248	23.701	-13.374	1.00	26.76	B

Figure 9 (21/52)

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ATOM   1137  C   ASP  125      22.909  21.831 -13.091  1.00 17.83      B
ATOM   1138  O   ASP  125      22.325  20.740 -13.095  1.00 16.29      B
ATOM   1139  N   ASN  126      23.829  22.169 -13.994  1.00 15.06      B
ATOM   1140  H   ASN  126      24.212  23.086 -13.944  1.00 20.00      B
ATOM   1141  CA  ASN  126      24.233  21.213 -15.017  1.00 13.78      B
ATOM   1142  CB  ASN  126      24.916  21.917 -16.195  1.00 13.44      B
ATOM   1143  CG  ASN  126      25.204  20.967 -17.366  1.00 11.95      B
ATOM   1144  OD1 ASN  126      26.113  20.138 -17.316  1.00 12.17      B
ATOM   1145  ND2 ASN  126      24.428  21.091 -18.408  1.00 14.74      B
ATOM   1146 HD21 ASN  126      23.709  21.774 -18.500  1.00 20.00      B
ATOM   1147 HD22 ASN  126      24.515  20.363 -19.093  1.00 20.00      B
ATOM   1148  C   ASN  126      25.194  20.215 -14.381  1.00 13.62      B
ATOM   1149  O   ASN  126      26.060  20.601 -13.602  1.00 15.17      B
ATOM   1150  N   TYR  127      25.065  18.937 -14.716  1.00 12.58      B
ATOM   1151  H   TYR  127      24.275  18.682 -15.275  1.00 20.00      B
ATOM   1152  CA  TYR  127      25.939  17.915 -14.157  1.00 11.52      B
ATOM   1153  CB  TYR  127      25.550  16.528 -14.705  1.00  9.45      B
ATOM   1154  CG  TYR  127      24.212  15.988 -14.241  1.00  9.26      B
ATOM   1155  CD1 TYR  127      23.905  15.912 -12.887  1.00 10.15      B
ATOM   1156  CE1 TYR  127      22.687  15.360 -12.437  1.00 11.38      B
ATOM   1157  CD2 TYR  127      23.279  15.481 -15.152  1.00  9.94      B
ATOM   1158  CE2 TYR  127      22.046  14.919 -14.716  1.00 10.54      B
ATOM   1159  CZ  TYR  127      21.766  14.842 -13.351  1.00 11.32      B
ATOM   1160  OH  TYR  127      20.616  14.214 -12.877  1.00  7.46      B
ATOM   1161  HH  TYR  127      20.204  14.642 -12.131  1.00 20.00      B
ATOM   1162  C   TYR  127      27.425  18.182 -14.446  1.00 13.13      B
ATOM   1163  O   TYR  127      28.302  17.702 -13.713  1.00 13.07      B
ATOM   1164  N   LEU  128      27.725  18.914 -15.523  1.00 14.20      B
ATOM   1165  H   LEU  128      26.967  19.040 -16.156  1.00 20.00      B
ATOM   1166  CA  LEU  128      29.130  19.204 -15.858  1.00 15.59      B
ATOM   1167  CB  LEU  128      29.303  19.598 -17.333  1.00 13.89      B
ATOM   1168  CG  LEU  128      29.078  18.576 -18.456  1.00 14.98      B
ATOM   1169  CD1 LEU  128      29.600  19.133 -19.763  1.00 11.93      B
ATOM   1170  CD2 LEU  128      29.788  17.285 -18.134  1.00 13.17      B
ATOM   1171  C   LEU  128      29.769  20.287 -15.000  1.00 16.08      B
ATOM   1172  O   LEU  128      30.933  20.199 -14.681  1.00 16.18      B
ATOM   1173  N   TYR  129      29.000  21.303 -14.634  1.00 19.38      B
ATOM   1174  H   TYR  129      28.027  21.153 -14.824  1.00 20.00      B
ATOM   1175  CA  TYR  129      29.475  22.446 -13.840  1.00 22.33      B
ATOM   1176  CB  TYR  129      28.295  23.035 -13.027  1.00 21.40      B
ATOM   1177  CG  TYR  129      28.533  24.411 -12.421  1.00 20.78      B
ATOM   1178  CD1 TYR  129      28.359  25.565 -13.175  1.00 20.29      B
ATOM   1179  CE1 TYR  129      28.554  26.833 -12.617  1.00 22.10      B
ATOM   1180  CD2 TYR  129      28.914  24.559 -11.086  1.00 22.27      B
ATOM   1181  CE2 TYR  129      29.115  25.823 -10.519  1.00 23.02      B
ATOM   1182  CZ  TYR  129      28.931  26.952 -11.291  1.00 22.15      B
ATOM   1183  OH  TYR  129      29.114  28.198 -10.752  1.00 21.59      B
ATOM   1184  HH  TYR  129      29.128  28.148  -9.803  1.00 20.00      B
ATOM   1185  C   TYR  129      30.687  22.205 -12.914  1.00 24.21      B
ATOM   1186  O   TYR  129      31.715  22.883 -13.046  1.00 25.71      B
ATOM   1187  N   ASN  130      30.562  21.230 -12.010  1.00 25.07      B
ATOM   1188  H   ASN  130      29.772  20.621 -12.091  1.00 20.00      B
ATOM   1189  CA  ASN  130      31.594  20.899 -11.020  1.00 26.55      B
ATOM   1190  CB  ASN  130      30.937  20.319  -9.762  1.00 30.80      B
ATOM   1191  CG  ASN  130      30.518  18.843  -9.949  1.00 36.07      B
ATOM   1192  OD1 ASN  130      31.283  17.917  -9.632  1.00 39.13      B
ATOM   1193  ND2 ASN  130      29.313  18.622 -10.491  1.00 38.22      B
```

Figure 9 (22/52)

```
ATOM   1194 HD21 ASN   130      28.607  19.301 -10.677  1.00 20.00      B
ATOM   1195 HD22 ASN   130      29.085  17.665 -10.675  1.00 20.00      B
ATOM   1196  C   ASN   130      32.653  19.897 -11.481  1.00 25.26      B
ATOM   1197  O   ASN   130      33.483  19.456 -10.677  1.00 26.12      B
ATOM   1198  N   HIS   131      32.619  19.514 -12.752  1.00 22.77      B
ATOM   1199  H   HIS   131      31.826  19.792 -13.269  1.00 20.00      B
ATOM   1200  CA  HIS   131      33.576  18.543 -13.273  1.00 20.21      B
ATOM   1201  CB  HIS   131      32.835  17.373 -13.921  1.00 19.88      B
ATOM   1202  CG  HIS   131      32.228  16.448 -12.924  1.00 21.58      B
ATOM   1203  ND1 HIS   131      30.891  16.501 -12.564  1.00 24.26      B
ATOM   1204  HD1 HIS   131      30.208  17.084 -12.965  1.00 20.00      B
ATOM   1205  CD2 HIS   131      32.770  15.473 -12.160  1.00 22.22      B
ATOM   1206  NE2 HIS   131      31.781  14.966 -11.362  1.00 20.93      B
ATOM   1207  CE1 HIS   131      30.653  15.610 -11.626  1.00 23.09      B
ATOM   1208  C   HIS   131      34.575  19.135 -14.236  1.00 18.88      B
ATOM   1209  O   HIS   131      35.431  18.422 -14.745  1.00 18.62      B
ATOM   1210  N   LEU   132      34.481  20.442 -14.454  1.00 17.77      B
ATOM   1211  H   LEU   132      33.861  20.959 -13.866  1.00 20.00      B
ATOM   1212  CA  LEU   132      35.363  21.145 -15.387  1.00 16.50      B
ATOM   1213  CB  LEU   132      34.704  22.464 -15.829  1.00 16.00      B
ATOM   1214  CG  LEU   132      33.471  22.489 -16.754  1.00 13.49      B
ATOM   1215  CD1 LEU   132      33.342  23.898 -17.319  1.00 11.57      B
ATOM   1216  CD2 LEU   132      33.620  21.490 -17.909  1.00 12.74      B
ATOM   1217  C   LEU   132      36.799  21.447 -14.925  1.00 16.09      B
ATOM   1218  O   LEU   132      37.017  21.843 -13.793  1.00 16.98      B
ATOM   1219  N   THR   133      37.767  21.220 -15.815  1.00 16.11      B
ATOM   1220  H   THR   133      37.456  20.863 -16.696  1.00 20.00      B
ATOM   1221  CA  THR   133      39.167  21.528 -15.580  1.00 13.57      B
ATOM   1222  CB  THR   133      40.140  20.363 -15.830  1.00 14.81      B
ATOM   1223  OG1 THR   133      39.913  19.342 -14.872  1.00 19.77      B
ATOM   1224  HG1 THR   133      40.373  18.566 -15.163  1.00 20.00      B
ATOM   1225  CG2 THR   133      41.610  20.842 -15.678  1.00 15.66      B
ATOM   1226  C   THR   133      39.441  22.491 -16.694  1.00 11.54      B
ATOM   1227  O   THR   133      39.136  22.213 -17.843  1.00 11.61      B
ATOM   1228  N   TYR   134      40.033  23.613 -16.353  1.00  9.84      B
ATOM   1229  H   TYR   134      40.151  23.787 -15.375  1.00 20.00      B
ATOM   1230  CA  TYR   134      40.364  24.632 -17.312  1.00  8.85      B
ATOM   1231  CB  TYR   134      40.056  25.974 -16.714  1.00  6.59      B
ATOM   1232  CG  TYR   134      38.598  26.171 -16.405  1.00  6.58      B
ATOM   1233  CD1 TYR   134      37.659  26.372 -17.430  1.00  5.35      B
ATOM   1234  CE1 TYR   134      36.308  26.638 -17.140  1.00  5.42      B
ATOM   1235  CD2 TYR   134      38.158  26.229 -15.093  1.00  4.22      B
ATOM   1236  CE2 TYR   134      36.832  26.492 -14.800  1.00  7.24      B
ATOM   1237  CZ  TYR   134      35.918  26.700 -15.821  1.00  6.57      B
ATOM   1238  OH  TYR   134      34.635  27.003 -15.461  1.00 10.26      B
ATOM   1239  HH  TYR   134      34.319  26.330 -14.849  1.00 20.00      B
ATOM   1240  C   TYR   134      41.834  24.596 -17.657  1.00 10.23      B
ATOM   1241  O   TYR   134      42.665  24.263 -16.806  1.00  9.14      B
ATOM   1242  N   ALA   135      42.156  24.925 -18.904  1.00  9.99      B
ATOM   1243  H   ALA   135      41.411  25.148 -19.532  1.00 20.00      B
ATOM   1244  CA  ALA   135      43.546  25.010 -19.331  1.00 11.04      B
ATOM   1245  CB  ALA   135      43.878  23.944 -20.370  1.00 10.32      B
ATOM   1246  C   ALA   135      43.653  26.396 -19.937  1.00 12.65      B
ATOM   1247  O   ALA   135      42.956  26.702 -20.919  1.00 12.57      B
ATOM   1248  N   VAL   136      44.470  27.251 -19.315  1.00 12.70      B
ATOM   1249  H   VAL   136      44.955  26.904 -18.509  1.00 20.00      B
ATOM   1250  CA  VAL   136      44.693  28.611 -19.788  1.00 11.52      B
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Figure 9 (23/52)

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ATOM   1251  CB  VAL   136      44.747  29.610 -18.634  1.00 11.39      B
ATOM   1252  CG1 VAL   136      44.639  31.028 -19.174  1.00 12.78      B
ATOM   1253  CG2 VAL   136      43.615  29.332 -17.641  1.00 11.84      B
ATOM   1254  C   VAL   136      46.024  28.655 -20.526  1.00 13.97      B
ATOM   1255  O   VAL   136      47.061  28.249 -20.004  1.00 14.55      B
ATOM   1256  N   ASN   137      45.993  29.135 -21.754  1.00 16.06      B
ATOM   1257  H   ASN   137      45.066  29.301 -22.082  1.00 20.00      B
ATOM   1258  CA  ASN   137      47.198  29.214 -22.556  1.00 17.11      B
ATOM   1259  CB  ASN   137      46.922  28.591 -23.930  1.00 17.07      B
ATOM   1260  CG  ASN   137      48.165  28.475 -24.799  1.00 17.68      B
ATOM   1261  OD1 ASN   137      48.047  28.263 -25.996  1.00 16.64      B
ATOM   1262  ND2 ASN   137      49.353  28.587 -24.206  1.00 18.63      B
ATOM   1263 HD21 ASN   137      49.516  28.533 -23.214  1.00 20.00      B
ATOM   1264 HD22 ASN   137      50.184  28.637 -24.762  1.00 20.00      B
ATOM   1265  C   ASN   137      47.622  30.684 -22.673  1.00 18.52      B
ATOM   1266  O   ASN   137      46.801  31.567 -22.956  1.00 19.16      B
ATOM   1267  N   ILE   138      48.889  30.944 -22.375  1.00 18.30      B
ATOM   1268  H   ILE   138      49.512  30.229 -22.057  1.00 20.00      B
ATOM   1269  CA  ILE   138      49.459  32.282 -22.447  1.00 19.01      B
ATOM   1270  CB  ILE   138      49.941  32.758 -21.063  1.00 20.56      B
ATOM   1271  CG2 ILE   138      50.704  34.056 -21.172  1.00 21.92      B
ATOM   1272  CG1 ILE   138      48.746  32.951 -20.134  1.00 22.40      B
ATOM   1273  CD1 ILE   138      48.389  31.720 -19.354  1.00 24.03      B
ATOM   1274  C   ILE   138      50.665  32.169 -23.367  1.00 19.42      B
ATOM   1275  O   ILE   138      51.332  31.140 -23.377  1.00 18.60      B
ATOM   1276  N   TRP   139      50.949  33.209 -24.140  1.00 21.69      B
ATOM   1277  H   TRP   139      50.406  34.051 -24.158  1.00 20.00      B
ATOM   1278  CA  TRP   139      52.100  33.178 -25.050  1.00 22.86      B
ATOM   1279  CB  TRP   139      51.791  32.299 -26.267  1.00 20.59      B
ATOM   1280  CG  TRP   139      50.883  32.908 -27.291  1.00 19.28      B
ATOM   1281  CD2 TRP   139      49.466  32.754 -27.382  1.00 17.88      B
ATOM   1282  CE2 TRP   139      49.047  33.426 -28.543  1.00 17.86      B
ATOM   1283  CE3 TRP   139      48.519  32.102 -26.599  1.00 16.95      B
ATOM   1284  CD1 TRP   139      51.252  33.672 -28.364  1.00 18.44      B
ATOM   1285  NE1 TRP   139      50.157  33.982 -29.118  1.00 18.38      B
ATOM   1286  HE1 TRP   139      50.220  34.565 -29.903  1.00 20.00      B
ATOM   1287  CZ2 TRP   139      47.706  33.479 -28.940  1.00 17.95      B
ATOM   1288  CZ3 TRP   139      47.185  32.154 -26.993  1.00 17.13      B
ATOM   1289  CH2 TRP   139      46.793  32.833 -28.157  1.00 17.36      B
ATOM   1290  C   TRP   139      52.459  34.582 -25.488  1.00 24.42      B
ATOM   1291  O   TRP   139      51.565  35.420 -25.638  1.00 24.38      B
ATOM   1292  N   SER   140      53.751  34.862 -25.675  1.00 27.89      B
ATOM   1293  H   SER   140      54.500  34.189 -25.609  1.00 20.00      B
ATOM   1294  CA  SER   140      54.150  36.215 -26.080  1.00 30.05      B
ATOM   1295  CB  SER   140      55.663  36.455 -25.942  1.00 30.19      B
ATOM   1296  OG  SER   140      56.425  35.689 -26.849  1.00 34.47      B
ATOM   1297  HG  SER   140      57.363  35.759 -26.669  1.00 20.00      B
ATOM   1298  C   SER   140      53.682  36.442 -27.500  1.00 31.64      B
ATOM   1299  O   SER   140      54.073  35.729 -28.429  1.00 31.10      B
ATOM   1300  N   GLU   141      52.789  37.414 -27.632  1.00 33.38      B
ATOM   1301  H   GLU   141      52.604  37.983 -26.837  1.00 20.00      B
ATOM   1302  CA  GLU   141      52.202  37.758 -28.908  1.00 35.66      B
ATOM   1303  CB  GLU   141      51.439  39.060 -28.786  1.00 34.71      B
ATOM   1304  CG  GLU   141      50.715  39.387 -30.050  1.00 36.31      B
ATOM   1305  CD  GLU   141      50.096  40.744 -30.021  1.00 36.84      B
ATOM   1306  OE1 GLU   141      49.532  41.117 -28.981  1.00 36.68      B
ATOM   1307  OE2 GLU   141      50.172  41.425 -31.050  1.00 38.64      B
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Figure 9 (24/52)

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ATOM   1308  C    GLU   141      53.302  37.922 -29.920  1.00 36.91      B
ATOM   1309  O    GLU   141      53.249  37.365 -31.024  1.00 37.66      B
ATOM   1310  N    ASN   142      54.295  38.700 -29.505  1.00 39.05      B
ATOM   1311  H    ASN   142      54.197  39.062 -28.582  1.00 20.00      B
ATOM   1312  CA   ASN   142      55.470  39.026 -30.281  1.00 41.29      B
ATOM   1313  CB   ASN   142      56.294  40.107 -29.563  1.00 43.51      B
ATOM   1314  CG   ASN   142      55.427  41.103 -28.753  1.00 45.34      B
ATOM   1315  OD1  ASN   142      54.292  41.419 -29.114  1.00 46.39      B
ATOM   1316  ND2  ASN   142      55.985  41.594 -27.645  1.00 45.81      B
ATOM   1317  HD21 ASN   142      56.914  41.344 -27.378  1.00 20.00      B
ATOM   1318  HD22 ASN   142      55.478  42.273 -27.119  1.00 20.00      B
ATOM   1319  C    ASN   142      56.325  37.791 -30.444  1.00 42.36      B
ATOM   1320  O    ASN   142      57.393  37.696 -29.838  1.00 44.37      B
ATOM   1321  N    ASP   143      55.835  36.854 -31.262  1.00 42.80      B
ATOM   1322  H    ASP   143      54.996  37.103 -31.730  1.00 20.00      B
ATOM   1323  CA   ASP   143      56.476  35.562 -31.598  1.00 42.35      B
ATOM   1324  CB   ASP   143      57.994  35.709 -31.806  1.00 43.89      B
ATOM   1325  CG   ASP   143      58.370  36.903 -32.700  1.00 45.79      B
ATOM   1326  OD1  ASP   143      57.477  37.556 -33.274  1.00 48.26      B
ATOM   1327  OD2  ASP   143      59.581  37.173 -32.796  1.00 45.79      B
ATOM   1328  C    ASP   143      56.217  34.498 -30.523  1.00 41.29      B
ATOM   1329  O    ASP   143      56.870  34.499 -29.481  1.00 42.29      B
ATOM   1330  N    PRO   144      55.269  33.610 -30.758  1.00 41.03      B
ATOM   1331  CD   PRO   144      54.341  33.558 -31.909  1.00 41.66      B
ATOM   1332  CA   PRO   144      54.943  32.529 -29.798  1.00 39.84      B
ATOM   1333  CB   PRO   144      53.662  31.939 -30.389  1.00 40.12      B
ATOM   1334  CG   PRO   144      53.872  32.105 -31.893  1.00 39.76      B
ATOM   1335  C    PRO   144      56.048  31.504 -29.474  1.00 38.40      B
ATOM   1336  O    PRO   144      57.141  31.909 -29.054  1.00 37.83      B
ATOM   1337  N    ALA   145      55.785  30.173 -29.617  1.00 37.41      B
ATOM   1338  H    ALA   145      54.897  29.936 -29.997  1.00 20.00      B
ATOM   1339  CA   ALA   145      56.766  29.089 -29.306  1.00 35.63      B
ATOM   1340  CB   ALA   145      58.031  29.187 -30.196  1.00 34.67      B
ATOM   1341  C    ALA   145      57.162  29.136 -27.822  1.00 34.90      B
ATOM   1342  O    ALA   145      57.530  28.110 -27.215  1.00 35.74      B
ATOM   1343  N    ASP   146      57.040  30.323 -27.239  1.00 33.03      B
ATOM   1344  H    ASP   146      56.724  31.213 -27.534  1.00 20.00      B
ATOM   1345  CA   ASP   146      57.338  30.538 -25.859  1.00 33.05      B
ATOM   1346  CB   ASP   146      58.188  31.795 -25.684  1.00 34.21      B
ATOM   1347  CG   ASP   146      58.418  32.141 -24.218  1.00 36.68      B
ATOM   1348  OD1  ASP   146      58.894  31.260 -23.473  1.00 39.35      B
ATOM   1349  OD2  ASP   146      58.109  33.285 -23.827  1.00 38.60      B
ATOM   1350  C    ASP   146      55.958  30.737 -25.256  1.00 31.57      B
ATOM   1351  O    ASP   146      55.367  31.831 -25.333  1.00 31.25      B
ATOM   1352  N    PHE   147      55.438  29.655 -24.686  1.00 28.45      B
ATOM   1353  H    PHE   147      56.062  28.873 -24.636  1.00 20.00      B
ATOM   1354  CA   PHE   147      54.125  29.677 -24.075  1.00 25.77      B
ATOM   1355  CB   PHE   147      53.135  29.038 -25.035  1.00 23.74      B
ATOM   1356  CG   PHE   147      53.403  27.600 -25.264  1.00 22.44      B
ATOM   1357  CD1  PHE   147      54.425  27.200 -26.118  1.00 22.91      B
ATOM   1358  CD2  PHE   147      52.660  26.625 -24.609  1.00 21.69      B
ATOM   1359  CE1  PHE   147      54.711  25.856 -26.320  1.00 20.85      B
ATOM   1360  CE2  PHE   147      52.930  25.274 -24.800  1.00 23.32      B
ATOM   1361  CZ   PHE   147      53.969  24.892 -25.661  1.00 23.53      B
ATOM   1362  C    PHE   147      54.102  28.894 -22.775  1.00 24.26      B
ATOM   1363  O    PHE   147      55.071  28.220 -22.426  1.00 23.49      B
ATOM   1364  N    ARG   148      52.979  28.998 -22.073  1.00 22.93      B
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Figure 9 (25/52)

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ATOM   1365  H   ARG   148      52.336  29.702 -22.378  1.00 20.00      B
ATOM   1366  CA  ARG   148      52.738  28.264 -20.839  1.00 21.26      B
ATOM   1367  CB  ARG   148      53.021  29.122 -19.615  1.00 21.95      B
ATOM   1368  CG  ARG   148      54.461  29.300 -19.281  1.00 23.54      B
ATOM   1369  CD  ARG   148      54.575  30.140 -18.030  1.00 25.22      B
ATOM   1370  NE  ARG   148      55.910  30.713 -17.878  1.00 25.17      B
ATOM   1371  HE  ARG   148      56.631  30.190 -18.334  1.00 20.00      B
ATOM   1372  CZ  ARG   148      56.171  31.876 -17.283  1.00 26.60      B
ATOM   1373  NH1 ARG   148      55.201  32.628 -16.766  1.00 25.32      B
ATOM   1374 HH11 ARG   148      55.380  33.508 -16.329  1.00 20.00      B
ATOM   1375 HH12 ARG   148      54.251  32.316 -16.853  1.00 20.00      B
ATOM   1376  NH2 ARG   148      57.419  32.292 -17.201  1.00 28.32      B
ATOM   1377 HH21 ARG   148      57.646  33.203 -16.841  1.00 20.00      B
ATOM   1378 HH22 ARG   148      58.180  31.743 -17.545  1.00 20.00      B
ATOM   1379  C   ARG   148      51.261  27.871 -20.816  1.00 19.71      B
ATOM   1380  O   ARG   148      50.417  28.561 -21.390  1.00 17.52      B
ATOM   1381  N   ILE   149      50.967  26.747 -20.172  1.00 19.49      B
ATOM   1382  H   ILE   149      51.696  26.241 -19.705  1.00 20.00      B
ATOM   1383  CA  ILE   149      49.597  26.267 -20.006  1.00 19.96      B
ATOM   1384  CB  ILE   149      49.345  24.916 -20.738  1.00 21.11      B
ATOM   1385  CG2 ILE   149      47.974  24.368 -20.378  1.00 20.93      B
ATOM   1386  CG1 ILE   149      49.398  25.120 -22.250  1.00 21.11      B
ATOM   1387  CD1 ILE   149      49.558  23.831 -23.037  1.00 24.23      B
ATOM   1388  C   ILE   149      49.406  26.076 -18.500  1.00 18.17      B
ATOM   1389  O   ILE   149      50.215  25.413 -17.852  1.00 18.21      B
ATOM   1390  N   TYR   150      48.373  26.704 -17.942  1.00 17.09      B
ATOM   1391  H   TYR   150      47.741  27.213 -18.532  1.00 20.00      B
ATOM   1392  CA  TYR   150      48.078  26.595 -16.514  1.00 14.82      B
ATOM   1393  CB  TYR   150      47.908  27.983 -15.882  1.00 13.05      B
ATOM   1394  CG  TYR   150      49.123  28.892 -15.836  1.00 11.42      B
ATOM   1395  CD1 TYR   150      49.606  29.503 -16.978  1.00 11.60      B
ATOM   1396  CE1 TYR   150      50.682  30.373 -16.918  1.00 12.58      B
ATOM   1397  CD2 TYR   150      49.751  29.179 -14.627  1.00 13.39      B
ATOM   1398  CE2 TYR   150      50.826  30.045 -14.548  1.00 10.95      B
ATOM   1399  CZ  TYR   150      51.287  30.641 -15.692  1.00 13.07      B
ATOM   1400  OH  TYR   150      52.346  31.511 -15.575  1.00 15.33      B
ATOM   1401  HH  TYR   150      52.087  32.311 -16.033  1.00 20.00      B
ATOM   1402  C   TYR   150      46.756  25.838 -16.336  1.00 14.49      B
ATOM   1403  O   TYR   150      45.738  26.242 -16.899  1.00 14.71      B
ATOM   1404  N   ASN   151      46.763  24.741 -15.583  1.00 13.53      B
ATOM   1405  H   ASN   151      47.576  24.490 -15.061  1.00 20.00      B
ATOM   1406  CA  ASN   151      45.524  23.995 -15.342  1.00 13.33      B
ATOM   1407  CB  ASN   151      45.756  22.499 -15.103  1.00 12.47      B
ATOM   1408  CG  ASN   151      46.243  21.759 -16.339  1.00 13.84      B
ATOM   1409  OD1 ASN   151      46.141  22.256 -17.454  1.00 15.61      B
ATOM   1410  ND2 ASN   151      46.784  20.564 -16.137  1.00 10.94      B
ATOM   1411 HD21 ASN   151      46.907  20.123 -15.248  1.00 20.00      B
ATOM   1412 HD22 ASN   151      47.101  20.141 -16.980  1.00 20.00      B
ATOM   1413  C   ASN   151      44.902  24.581 -14.096  1.00 13.84      B
ATOM   1414  O   ASN   151      45.572  24.723 -13.054  1.00 14.00      B
ATOM   1415  N   VAL   152      43.622  24.913 -14.215  1.00 14.45      B
ATOM   1416  H   VAL   152      43.124  24.671 -15.046  1.00 20.00      B
ATOM   1417  CA  VAL   152      42.824  25.492 -13.151  1.00 14.83      B
ATOM   1418  CB  VAL   152      42.310  26.894 -13.575  1.00 13.85      B
ATOM   1419  CG1 VAL   152      41.573  27.565 -12.413  1.00 13.57      B
ATOM   1420  CG2 VAL   152      43.469  27.761 -14.021  1.00 13.72      B
ATOM   1421  C   VAL   152      41.628  24.553 -12.905  1.00 17.31      B
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Figure 9 (26/52)

ATOM	1422	O	VAL	152	41.088	23.993	-13.858	1.00	16.78	B
ATOM	1423	N	THR	153	41.214	24.373	-11.649	1.00	18.40	B
ATOM	1424	H	THR	153	41.639	24.938	-10.944	1.00	20.00	B
ATOM	1425	CA	THR	153	40.078	23.496	-11.338	1.00	19.90	B
ATOM	1426	CB	THR	153	40.173	22.944	-9.893	1.00	18.69	B
ATOM	1427	OG1	THR	153	39.858	23.978	-8.951	1.00	19.37	B
ATOM	1428	HG1	THR	153	40.634	24.515	-8.825	1.00	20.00	B
ATOM	1429	CG2	THR	153	41.578	22.456	-9.623	1.00	19.73	B
ATOM	1430	C	THR	153	38.717	24.188	-11.525	1.00	20.39	B
ATOM	1431	O	THR	153	38.645	25.388	-11.719	1.00	20.83	B
ATOM	1432	N	TYR	154	37.643	23.411	-11.447	1.00	23.58	B
ATOM	1433	H	TYR	154	37.776	22.425	-11.523	1.00	20.00	B
ATOM	1434	CA	TYR	154	36.260	23.896	-11.601	1.00	26.00	B
ATOM	1435	CB	TYR	154	35.279	22.726	-11.331	1.00	28.59	B
ATOM	1436	CG	TYR	154	35.200	22.340	-9.852	1.00	29.43	B
ATOM	1437	CD1	TYR	154	36.226	21.615	-9.251	1.00	30.23	B
ATOM	1438	CE1	TYR	154	36.203	21.310	-7.885	1.00	31.31	B
ATOM	1439	CD2	TYR	154	34.115	22.740	-9.050	1.00	29.24	B
ATOM	1440	CE2	TYR	154	34.073	22.439	-7.679	1.00	30.62	B
ATOM	1441	CZ	TYR	154	35.124	21.717	-7.099	1.00	31.96	B
ATOM	1442	OH	TYR	154	35.147	21.429	-5.740	1.00	30.60	B
ATOM	1443	HH	TYR	154	34.356	21.741	-5.321	1.00	20.00	B
ATOM	1444	C	TYR	154	35.821	25.077	-10.714	1.00	25.96	B
ATOM	1445	O	TYR	154	35.177	26.008	-11.181	1.00	26.60	B
ATOM	1446	N	LEU	155	36.189	25.009	-9.437	1.00	25.88	B
ATOM	1447	H	LEU	155	36.767	24.242	-9.158	1.00	20.00	B
ATOM	1448	CA	LEU	155	35.783	25.960	-8.410	1.00	24.56	B
ATOM	1449	CB	LEU	155	36.552	25.673	-7.120	1.00	25.28	B
ATOM	1450	CG	LEU	155	35.936	26.283	-5.854	1.00	28.67	B
ATOM	1451	CD1	LEU	155	34.474	25.844	-5.674	1.00	26.45	B
ATOM	1452	CD2	LEU	155	36.765	25.858	-4.673	1.00	30.14	B
ATOM	1453	C	LEU	155	35.807	27.448	-8.671	1.00	23.26	B
ATOM	1454	O	LEU	155	34.800	28.143	-8.477	1.00	23.51	B
ATOM	1455	N	GLU	156	36.960	27.950	-9.068	1.00	22.74	B
ATOM	1456	H	GLU	156	37.732	27.345	-9.229	1.00	20.00	B
ATOM	1457	CA	GLU	156	37.100	29.373	-9.302	1.00	21.52	B
ATOM	1458	CB	GLU	156	37.969	29.955	-8.162	1.00	24.48	B
ATOM	1459	CG	GLU	156	38.605	31.340	-8.360	1.00	29.10	B
ATOM	1460	CD	GLU	156	37.722	32.515	-7.977	1.00	31.18	B
ATOM	1461	OE1	GLU	156	36.577	32.305	-7.512	1.00	32.78	B
ATOM	1462	OE2	GLU	156	38.195	33.661	-8.145	1.00	32.95	B
ATOM	1463	C	GLU	156	37.688	29.625	-10.692	1.00	19.66	B
ATOM	1464	O	GLU	156	38.818	29.238	-10.994	1.00	19.26	B
ATOM	1465	N	PRO	157	36.900	30.246	-11.576	1.00	18.57	B
ATOM	1466	CD	PRO	157	35.497	30.662	-11.386	1.00	18.32	B
ATOM	1467	CA	PRO	157	37.357	30.547	-12.932	1.00	18.16	B
ATOM	1468	CB	PRO	157	36.037	30.638	-13.708	1.00	17.46	B
ATOM	1469	CG	PRO	157	35.149	31.326	-12.721	1.00	16.25	B
ATOM	1470	C	PRO	157	38.190	31.856	-12.974	1.00	16.99	B
ATOM	1471	O	PRO	157	37.720	32.901	-13.429	1.00	17.47	B
ATOM	1472	N	SER	158	39.415	31.794	-12.452	1.00	17.20	B
ATOM	1473	H	SER	158	39.714	30.955	-11.982	1.00	20.00	B
ATOM	1474	CA	SER	158	40.344	32.919	-12.454	1.00	16.67	B
ATOM	1475	CB	SER	158	40.054	33.920	-11.336	1.00	17.24	B
ATOM	1476	OG	SER	158	40.204	33.335	-10.060	1.00	20.45	B
ATOM	1477	HG	SER	158	39.356	33.413	-9.603	1.00	20.00	B
ATOM	1478	C	SER	158	41.740	32.336	-12.305	1.00	16.21	B

Figure 9 (27/52)

ATOM	1479	O	SER	158	41.904	31.164	-11.951	1.00	14.94	B
ATOM	1480	N	LEU	159	42.750	33.147	-12.593	1.00	16.93	B
ATOM	1481	H	LEU	159	42.542	34.078	-12.904	1.00	20.00	B
ATOM	1482	CA	LEU	159	44.135	32.702	-12.547	1.00	15.45	B
ATOM	1483	CB	LEU	159	44.530	32.100	-13.912	1.00	12.87	B
ATOM	1484	CG	LEU	159	46.030	31.904	-14.167	1.00	12.76	B
ATOM	1485	CD1	LEU	159	46.522	30.739	-13.338	1.00	13.15	B
ATOM	1486	CD2	LEU	159	46.315	31.649	-15.619	1.00	12.19	B
ATOM	1487	C	LEU	159	45.010	33.905	-12.265	1.00	15.89	B
ATOM	1488	O	LEU	159	45.027	34.845	-13.052	1.00	16.27	B
ATOM	1489	N	ARG	160	45.713	33.870	-11.136	1.00	17.67	B
ATOM	1490	H	ARG	160	45.695	33.040	-10.581	1.00	20.00	B
ATOM	1491	CA	ARG	160	46.642	34.923	-10.716	1.00	18.31	B
ATOM	1492	CB	ARG	160	46.580	35.136	-9.198	1.00	19.70	B
ATOM	1493	CG	ARG	160	45.266	35.685	-8.692	1.00	23.78	B
ATOM	1494	CD	ARG	160	45.190	35.707	-7.163	1.00	28.26	B
ATOM	1495	NE	ARG	160	44.208	36.682	-6.684	1.00	32.99	B
ATOM	1496	HE	ARG	160	44.609	37.526	-6.320	1.00	20.00	B
ATOM	1497	CZ	ARG	160	42.886	36.548	-6.794	1.00	35.52	B
ATOM	1498	NH1	ARG	160	42.363	35.470	-7.365	1.00	36.77	B
ATOM	1499	HH11	ARG	160	41.376	35.273	-7.403	1.00	20.00	B
ATOM	1500	HH12	ARG	160	42.973	34.799	-7.782	1.00	20.00	B
ATOM	1501	NH2	ARG	160	42.078	37.500	-6.339	1.00	36.63	B
ATOM	1502	HH21	ARG	160	41.083	37.380	-6.363	1.00	20.00	B
ATOM	1503	HH22	ARG	160	42.440	38.366	-5.993	1.00	20.00	B
ATOM	1504	C	ARG	160	48.046	34.476	-11.084	1.00	17.32	B
ATOM	1505	O	ARG	160	48.511	33.439	-10.619	1.00	15.99	B
ATOM	1506	N	ILE	161	48.709	35.252	-11.928	1.00	19.47	B
ATOM	1507	H	ILE	161	48.316	36.137	-12.190	1.00	20.00	B
ATOM	1508	CA	ILE	161	50.064	34.967	-12.369	1.00	19.75	B
ATOM	1509	CB	ILE	161	50.150	34.955	-13.895	1.00	19.01	B
ATOM	1510	CG2	ILE	161	51.585	34.700	-14.337	1.00	19.21	B
ATOM	1511	CG1	ILE	161	49.182	33.930	-14.479	1.00	18.04	B
ATOM	1512	CD1	ILE	161	49.122	33.978	-16.010	1.00	15.54	B
ATOM	1513	C	ILE	161	51.002	36.081	-11.897	1.00	20.80	B
ATOM	1514	O	ILE	161	50.648	37.254	-11.925	1.00	20.82	B
ATOM	1515	N	ALA	162	52.193	35.710	-11.458	1.00	22.84	B
ATOM	1516	H	ALA	162	52.436	34.746	-11.526	1.00	20.00	B
ATOM	1517	CA	ALA	162	53.180	36.700	-11.049	1.00	24.31	B
ATOM	1518	CB	ALA	162	53.793	36.319	-9.705	1.00	23.51	B
ATOM	1519	C	ALA	162	54.258	36.685	-12.140	1.00	25.80	B
ATOM	1520	O	ALA	162	54.376	37.637	-12.908	1.00	26.27	B
ATOM	1521	N	ALA	163	55.001	35.567	-12.192	1.00	27.99	B
ATOM	1522	H	ALA	163	54.680	34.844	-11.597	1.00	20.00	B
ATOM	1523	CA	ALA	163	56.133	35.285	-13.104	1.00	28.16	B
ATOM	1524	CB	ALA	163	55.773	34.132	-14.043	1.00	26.62	B
ATOM	1525	C	ALA	163	56.727	36.447	-13.904	1.00	28.31	B
ATOM	1526	O	ALA	163	57.296	36.237	-14.985	1.00	29.08	B
ATOM	1527	N	GLY	169	58.754	43.060	-20.701	1.00	31.29	B
ATOM	1528	H	GLY	169	59.507	42.663	-21.222	1.00	20.00	B
ATOM	1529	CA	GLY	169	58.224	44.085	-21.585	1.00	31.25	B
ATOM	1530	C	GLY	169	57.520	43.567	-22.841	1.00	32.25	B
ATOM	1531	O	GLY	169	57.205	44.344	-23.741	1.00	33.28	B
ATOM	1532	N	ILE	170	57.256	42.267	-22.918	1.00	31.92	B
ATOM	1533	H	ILE	170	57.250	41.799	-22.035	1.00	20.00	B
ATOM	1534	CA	ILE	170	56.580	41.686	-24.081	1.00	32.21	B
ATOM	1535	CB	ILE	170	56.877	40.161	-24.174	1.00	32.40	B

Figure 9 (28/52)

ATOM	1536	CG2	ILE	170	56.438	39.620	-25.497	1.00	33.80	B
ATOM	1537	CG1	ILE	170	58.376	39.892	-24.000	1.00	34.08	B
ATOM	1538	CD1	ILE	170	58.743	38.410	-23.891	1.00	32.15	B
ATOM	1539	C	ILE	170	55.058	41.866	-23.900	1.00	31.46	B
ATOM	1540	O	ILE	170	54.599	42.337	-22.851	1.00	33.53	B
ATOM	1541	N	SER	171	54.272	41.543	-24.920	1.00	29.70	B
ATOM	1542	H	SER	171	54.601	41.261	-25.817	1.00	20.00	B
ATOM	1543	CA	SER	171	52.817	41.607	-24.783	1.00	27.84	B
ATOM	1544	CB	SER	171	52.187	42.489	-25.860	1.00	28.59	B
ATOM	1545	OG	SER	171	52.393	41.953	-27.158	1.00	32.58	B
ATOM	1546	HG	SER	171	51.570	41.636	-27.518	1.00	20.00	B
ATOM	1547	C	SER	171	52.395	40.139	-24.944	1.00	26.21	B
ATOM	1548	O	SER	171	52.944	39.427	-25.800	1.00	25.32	B
ATOM	1549	N	TYR	172	51.474	39.674	-24.100	1.00	23.96	B
ATOM	1550	H	TYR	172	51.080	40.346	-23.472	1.00	20.00	B
ATOM	1551	CA	TYR	172	51.036	38.284	-24.146	1.00	20.22	B
ATOM	1552	CB	TYR	172	51.222	37.642	-22.780	1.00	20.56	B
ATOM	1553	CG	TYR	172	52.669	37.565	-22.382	1.00	22.63	B
ATOM	1554	CD1	TYR	172	53.305	38.623	-21.715	1.00	21.12	B
ATOM	1555	CE1	TYR	172	54.674	38.551	-21.391	1.00	21.41	B
ATOM	1556	CD2	TYR	172	53.426	36.440	-22.706	1.00	22.25	B
ATOM	1557	CE2	TYR	172	54.768	36.364	-22.393	1.00	24.11	B
ATOM	1558	CZ	TYR	172	55.386	37.413	-21.744	1.00	22.92	B
ATOM	1559	OH	TYR	172	56.731	37.278	-21.514	1.00	24.55	B
ATOM	1560	HH	TYR	172	57.089	36.603	-22.083	1.00	20.00	B
ATOM	1561	C	TYR	172	49.601	38.145	-24.545	1.00	19.09	B
ATOM	1562	O	TYR	172	48.837	39.080	-24.447	1.00	18.96	B
ATOM	1563	N	ARG	173	49.248	36.970	-25.029	1.00	19.19	B
ATOM	1564	H	ARG	173	49.975	36.288	-25.117	1.00	20.00	B
ATOM	1565	CA	ARG	173	47.877	36.687	-25.370	1.00	17.23	B
ATOM	1566	CB	ARG	173	47.716	36.344	-26.846	1.00	21.16	B
ATOM	1567	CG	ARG	173	47.818	37.540	-27.783	1.00	23.88	B
ATOM	1568	CD	ARG	173	47.131	37.231	-29.102	1.00	27.17	B
ATOM	1569	NE	ARG	173	47.820	37.792	-30.267	1.00	29.90	B
ATOM	1570	HE	ARG	173	48.364	38.619	-30.053	1.00	20.00	B
ATOM	1571	CZ	ARG	173	47.715	37.297	-31.498	1.00	29.32	B
ATOM	1572	NH1	ARG	173	46.951	36.238	-31.735	1.00	29.92	B
ATOM	1573	HH11	ARG	173	46.892	35.826	-32.645	1.00	20.00	B
ATOM	1574	HH12	ARG	173	46.403	35.837	-31.004	1.00	20.00	B
ATOM	1575	NH2	ARG	173	48.371	37.865	-32.493	1.00	31.46	B
ATOM	1576	HH21	ARG	173	48.297	37.578	-33.448	1.00	20.00	B
ATOM	1577	HH22	ARG	173	48.992	38.637	-32.275	1.00	20.00	B
ATOM	1578	C	ARG	173	47.494	35.497	-24.510	1.00	15.34	B
ATOM	1579	O	ARG	173	48.349	34.710	-24.117	1.00	12.85	B
ATOM	1580	N	ALA	174	46.212	35.377	-24.206	1.00	13.85	B
ATOM	1581	H	ALA	174	45.591	36.094	-24.524	1.00	20.00	B
ATOM	1582	CA	ALA	174	45.735	34.275	-23.399	1.00	13.08	B
ATOM	1583	CB	ALA	174	45.557	34.745	-21.969	1.00	13.54	B
ATOM	1584	C	ALA	174	44.412	33.744	-23.917	1.00	12.66	B
ATOM	1585	O	ALA	174	43.575	34.513	-24.392	1.00	11.93	B
ATOM	1586	N	ARG	175	44.243	32.427	-23.851	1.00	12.51	B
ATOM	1587	H	ARG	175	44.974	31.891	-23.429	1.00	20.00	B
ATOM	1588	CA	ARG	175	42.983	31.763	-24.218	1.00	12.17	B
ATOM	1589	CB	ARG	175	42.991	31.083	-25.615	1.00	13.30	B
ATOM	1590	CG	ARG	175	44.224	31.194	-26.474	1.00	16.81	B
ATOM	1591	CD	ARG	175	44.784	29.812	-26.819	1.00	15.49	B
ATOM	1592	NE	ARG	175	44.409	29.321	-28.141	1.00	16.77	B

Figure 9 (29/52)

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ATOM   1593  HE  ARG   175      43.492  29.615 -28.424  1.00 20.00      B
ATOM   1594  CZ  ARG   175      45.126  28.454 -28.863  1.00 16.34      B
ATOM   1595  NH1 ARG   175      46.279  27.963 -28.431  1.00 13.87      B
ATOM   1596 HH11 ARG   175      46.750  27.184 -28.845  1.00 20.00      B
ATOM   1597 HH12 ARG   175      46.746  28.383 -27.639  1.00 20.00      B
ATOM   1598  NH2 ARG   175      44.663  28.033 -30.018  1.00 16.34      B
ATOM   1599 HH21 ARG   175      45.174  27.377 -30.576  1.00 20.00      B
ATOM   1600 HH22 ARG   175      43.792  28.359 -30.405  1.00 20.00      B
ATOM   1601  C   ARG   175      42.744  30.686 -23.147  1.00 10.72      B
ATOM   1602  O   ARG   175      43.675  30.325 -22.412  1.00  8.98      B
ATOM   1603  N   VAL   176      41.511  30.178 -23.068  1.00  8.47      B
ATOM   1604  H   VAL   176      40.749  30.563 -23.602  1.00 20.00      B
ATOM   1605  CA  VAL   176      41.157  29.152 -22.097  1.00  6.24      B
ATOM   1606  CB  VAL   176      40.554  29.794 -20.792  1.00  4.58      B
ATOM   1607  CG1 VAL   176      39.288  30.504 -21.092  1.00  3.58      B
ATOM   1608  CG2 VAL   176      40.319  28.753 -19.729  1.00  3.00      B
ATOM   1609  C   VAL   176      40.159  28.165 -22.682  1.00  7.31      B
ATOM   1610  O   VAL   176      39.237  28.560 -23.405  1.00  9.24      B
ATOM   1611  N   ARG   177      40.367  26.876 -22.417  1.00  7.48      B
ATOM   1612  H   ARG   177      41.119  26.635 -21.800  1.00 20.00      B
ATOM   1613  CA  ARG   177      39.433  25.845 -22.853  1.00  7.13      B
ATOM   1614  CB  ARG   177      39.991  25.019 -24.001  1.00  6.96      B
ATOM   1615  CG  ARG   177      41.181  24.176 -23.678  1.00  7.54      B
ATOM   1616  CD  ARG   177      41.683  23.549 -24.955  1.00  7.90      B
ATOM   1617  NE  ARG   177      42.907  22.782 -24.753  1.00 11.37      B
ATOM   1618  HE  ARG   177      43.243  22.856 -23.806  1.00 20.00      B
ATOM   1619  CZ  ARG   177      43.489  22.045 -25.700  1.00 12.34      B
ATOM   1620  NH1 ARG   177      42.970  21.980 -26.924  1.00 10.60      B
ATOM   1621 HH11 ARG   177      43.377  21.424 -27.651  1.00 20.00      B
ATOM   1622 HH12 ARG   177      42.130  22.491 -27.147  1.00 20.00      B
ATOM   1623  NH2 ARG   177      44.573  21.339 -25.421  1.00 11.48      B
ATOM   1624 HH21 ARG   177      44.965  20.686 -26.068  1.00 20.00      B
ATOM   1625 HH22 ARG   177      45.051  21.445 -24.542  1.00 20.00      B
ATOM   1626  C   ARG   177      39.177  24.974 -21.654  1.00  5.68      B
ATOM   1627  O   ARG   177      39.806  25.154 -20.635  1.00  7.55      B
ATOM   1628  N   ALA   178      38.291  24.003 -21.768  1.00  6.95      B
ATOM   1629  H   ALA   178      37.734  23.881 -22.596  1.00 20.00      B
ATOM   1630  CA  ALA   178      37.972  23.155 -20.621  1.00  9.25      B
ATOM   1631  CB  ALA   178      36.876  23.838 -19.782  1.00  9.92      B
ATOM   1632  C   ALA   178      37.497  21.775 -21.026  1.00 10.53      B
ATOM   1633  O   ALA   178      37.018  21.576 -22.130  1.00 12.74      B
ATOM   1634  N   TRP   179      37.636  20.813 -20.133  1.00 11.65      B
ATOM   1635  H   TRP   179      38.011  21.026 -19.227  1.00 20.00      B
ATOM   1636  CA  TRP   179      37.171  19.467 -20.412  1.00 12.80      B
ATOM   1637  CB  TRP   179      38.287  18.609 -21.032  1.00 14.13      B
ATOM   1638  CG  TRP   179      39.275  18.070 -20.100  1.00 16.50      B
ATOM   1639  CD2 TRP   179      39.521  16.682 -19.835  1.00 18.42      B
ATOM   1640  CE2 TRP   179      40.512  16.623 -18.828  1.00 18.91      B
ATOM   1641  CE3 TRP   179      38.996  15.478 -20.347  1.00 19.84      B
ATOM   1642  CD1 TRP   179      40.105  18.775 -19.286  1.00 16.56      B
ATOM   1643  NE1 TRP   179      40.848  17.915 -18.519  1.00 17.86      B
ATOM   1644  HE1 TRP   179      41.513  18.219 -17.863  1.00 20.00      B
ATOM   1645  CZ2 TRP   179      40.993  15.404 -18.314  1.00 20.35      B
ATOM   1646  CZ3 TRP   179      39.466  14.274 -19.842  1.00 19.75      B
ATOM   1647  CH2 TRP   179      40.460  14.246 -18.829  1.00 20.98      B
ATOM   1648  C   TRP   179      36.659  18.927 -19.089  1.00 12.50      B
ATOM   1649  O   TRP   179      36.808  19.597 -18.058  1.00 11.41      B
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Figure 9 (30/52)

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ATOM   1650  N   ALA  180      35.990  17.776 -19.122  1.00 12.16      B
ATOM   1651  H   ALA  180      35.859  17.282 -19.981  1.00 20.00      B
ATOM   1652  CA  ALA  180      35.448  17.174 -17.898  1.00 12.63      B
ATOM   1653  CB  ALA  180      33.910  17.306 -17.831  1.00 10.22      B
ATOM   1654  C   ALA  180      35.846  15.727 -17.805  1.00 14.46      B
ATOM   1655  O   ALA  180      35.211  14.864 -18.391  1.00 15.27      B
ATOM   1656  N   GLN  181      36.911  15.477 -17.060  1.00 16.28      B
ATOM   1657  H   GLN  181      37.278  16.279 -16.585  1.00 20.00      B
ATOM   1658  CA  GLN  181      37.452  14.135 -16.858  1.00 18.50      B
ATOM   1659  CB  GLN  181      38.487  14.168 -15.746  1.00 22.08      B
ATOM   1660  CG  GLN  181      38.951  12.795 -15.306  1.00 29.30      B
ATOM   1661  CD  GLN  181      39.650  12.829 -13.958  1.00 35.23      B
ATOM   1662  OE1 GLN  181      40.225  13.851 -13.561  1.00 35.68      B
ATOM   1663  NE2 GLN  181      39.595  11.715 -13.238  1.00 37.91      B
ATOM   1664 HE21 GLN  181      39.099  10.902 -13.551  1.00 20.00      B
ATOM   1665 HE22 GLN  181      39.971  11.752 -12.316  1.00 20.00      B
ATOM   1666  C   GLN  181      36.441  13.048 -16.524  1.00 17.39      B
ATOM   1667  O   GLN  181      36.452  11.998 -17.133  1.00 17.34      B
ATOM   1668  N   ALA  182      35.578  13.304 -15.549  1.00 16.09      B
ATOM   1669  H   ALA  182      35.567  14.239 -15.187  1.00 20.00      B
ATOM   1670  CA  ALA  182      34.595  12.327 -15.118  1.00 16.00      B
ATOM   1671  CB  ALA  182      33.795  12.874 -13.997  1.00 14.79      B
ATOM   1672  C   ALA  182      33.672  11.876 -16.240  1.00 17.55      B
ATOM   1673  O   ALA  182      33.192  10.748 -16.209  1.00 18.34      B
ATOM   1674  N   TYR  183      33.402  12.751 -17.211  1.00 17.78      B
ATOM   1675  H   TYR  183      33.906  13.607 -17.294  1.00 20.00      B
ATOM   1676  CA  TYR  183      32.544  12.391 -18.336  1.00 18.79      B
ATOM   1677  CB  TYR  183      31.610  13.554 -18.701  1.00 16.68      B
ATOM   1678  CG  TYR  183      30.420  13.628 -17.770  1.00 15.41      B
ATOM   1679  CD1 TYR  183      30.530  14.232 -16.522  1.00 14.31      B
ATOM   1680  CE1 TYR  183      29.465  14.256 -15.649  1.00 14.83      B
ATOM   1681  CD2 TYR  183      29.206  13.049 -18.118  1.00 14.38      B
ATOM   1682  CE2 TYR  183      28.136  13.066 -17.246  1.00 14.52      B
ATOM   1683  CZ  TYR  183      28.277  13.668 -16.012  1.00 15.12      B
ATOM   1684  OH  TYR  183      27.236  13.661 -15.117  1.00 17.70      B
ATOM   1685  HH  TYR  183      26.474  13.204 -15.463  1.00 20.00      B
ATOM   1686  C   TYR  183      33.364  11.945 -19.540  1.00 19.75      B
ATOM   1687  O   TYR  183      32.831  11.724 -20.634  1.00 20.80      B
ATOM   1688  N   ASN  184      34.673  11.824 -19.325  1.00 20.66      B
ATOM   1689  H   ASN  184      35.053  12.009 -18.423  1.00 20.00      B
ATOM   1690  CA  ASN  184      35.614  11.385 -20.356  1.00 21.34      B
ATOM   1691  CB  ASN  184      35.402   9.892 -20.661  1.00 24.67      B
ATOM   1692  CG  ASN  184      36.707   9.155 -20.836  1.00 30.04      B
ATOM   1693  OD1 ASN  184      37.694   9.721 -21.324  1.00 32.80      B
ATOM   1694  ND2 ASN  184      36.738   7.887 -20.415  1.00 34.51      B
ATOM   1695 HD21 ASN  184      35.981   7.486 -19.910  1.00 20.00      B
ATOM   1696 HD22 ASN  184      37.557   7.368 -20.626  1.00 20.00      B
ATOM   1697  C   ASN  184      35.423  12.194 -21.622  1.00 18.54      B
ATOM   1698  O   ASN  184      35.285  11.634 -22.696  1.00 19.83      B
ATOM   1699  N   THR  185      35.415  13.513 -21.490  1.00 15.77      B
ATOM   1700  H   THR  185      35.557  13.871 -20.569  1.00 20.00      B
ATOM   1701  CA  THR  185      35.184  14.379 -22.638  1.00 14.20      B
ATOM   1702  CB  THR  185      34.516  15.719 -22.232  1.00 13.05      B
ATOM   1703  OG1 THR  185      35.500  16.580 -21.636  1.00 11.51      B
ATOM   1704  HG1 THR  185      35.779  17.087 -22.401  1.00 20.00      B
ATOM   1705  CG2 THR  185      33.364  15.497 -21.287  1.00  7.21      B
ATOM   1706  C   THR  185      36.418  14.771 -23.422  1.00 14.09      B
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Figure 9 (31/52)

ATOM	1707	O	THR	185	37.555	14.570	-22.981	1.00	15.49	B
ATOM	1708	N	THR	186	36.172	15.324	-24.604	1.00	12.27	B
ATOM	1709	H	THR	186	35.207	15.488	-24.822	1.00	20.00	B
ATOM	1710	CA	THR	186	37.242	15.863	-25.419	1.00	12.56	B
ATOM	1711	CB	THR	186	36.852	15.885	-26.912	1.00	12.86	B
ATOM	1712	OG1	THR	186	35.461	16.176	-27.033	1.00	12.96	B
ATOM	1713	HG1	THR	186	34.994	15.344	-27.126	1.00	20.00	B
ATOM	1714	CG2	THR	186	37.137	14.562	-27.565	1.00	12.85	B
ATOM	1715	C	THR	186	37.373	17.314	-24.893	1.00	11.35	B
ATOM	1716	O	THR	186	36.629	17.716	-23.982	1.00	12.16	B
ATOM	1717	N	TRP	187	38.313	18.084	-25.436	1.00	10.49	B
ATOM	1718	H	TRP	187	38.808	17.742	-26.227	1.00	20.00	B
ATOM	1719	CA	TRP	187	38.473	19.472	-25.034	1.00	7.96	B
ATOM	1720	CB	TRP	187	39.834	20.001	-25.448	1.00	6.78	B
ATOM	1721	CG	TRP	187	40.958	19.550	-24.599	1.00	10.39	B
ATOM	1722	CD2	TRP	187	41.330	20.076	-23.314	1.00	11.86	B
ATOM	1723	CE2	TRP	187	42.520	19.415	-22.922	1.00	12.10	B
ATOM	1724	CE3	TRP	187	40.784	21.044	-22.460	1.00	11.30	B
ATOM	1725	CD1	TRP	187	41.901	18.608	-24.916	1.00	11.19	B
ATOM	1726	NE1	TRP	187	42.842	18.527	-23.915	1.00	11.86	B
ATOM	1727	HE1	TRP	187	43.573	17.872	-23.857	1.00	20.00	B
ATOM	1728	CZ2	TRP	187	43.168	19.697	-21.722	1.00	10.15	B
ATOM	1729	CZ3	TRP	187	41.430	21.323	-21.272	1.00	11.40	B
ATOM	1730	CH2	TRP	187	42.612	20.654	-20.912	1.00	11.68	B
ATOM	1731	C	TRP	187	37.437	20.343	-25.714	1.00	8.82	B
ATOM	1732	O	TRP	187	36.978	20.044	-26.815	1.00	9.63	B
ATOM	1733	N	SER	188	37.057	21.428	-25.062	1.00	8.57	B
ATOM	1734	H	SER	188	37.235	21.503	-24.084	1.00	20.00	B
ATOM	1735	CA	SER	188	36.144	22.359	-25.676	1.00	7.27	B
ATOM	1736	CB	SER	188	35.603	23.328	-24.620	1.00	6.07	B
ATOM	1737	OG	SER	188	36.578	24.303	-24.245	1.00	5.97	B
ATOM	1738	HG	SER	188	36.704	24.909	-24.970	1.00	20.00	B
ATOM	1739	C	SER	188	37.029	23.133	-26.674	1.00	9.19	B
ATOM	1740	O	SER	188	38.258	22.964	-26.708	1.00	9.09	B
ATOM	1741	N	GLU	189	36.401	23.968	-27.486	1.00	9.94	B
ATOM	1742	H	GLU	189	35.427	24.137	-27.361	1.00	20.00	B
ATOM	1743	CA	GLU	189	37.102	24.832	-28.413	1.00	10.44	B
ATOM	1744	CB	GLU	189	36.101	25.545	-29.328	1.00	11.73	B
ATOM	1745	CG	GLU	189	35.460	24.660	-30.379	1.00	13.36	B
ATOM	1746	CD	GLU	189	36.460	24.226	-31.416	1.00	15.85	B
ATOM	1747	OE1	GLU	189	37.002	25.117	-32.102	1.00	16.88	B
ATOM	1748	OE2	GLU	189	36.711	23.007	-31.541	1.00	16.39	B
ATOM	1749	C	GLU	189	37.702	25.867	-27.486	1.00	10.96	B
ATOM	1750	O	GLU	189	37.275	25.978	-26.350	1.00	12.52	B
ATOM	1751	N	TRP	190	38.669	26.643	-27.963	1.00	12.94	B
ATOM	1752	H	TRP	190	38.777	26.637	-28.955	1.00	20.00	B
ATOM	1753	CA	TRP	190	39.288	27.694	-27.159	1.00	12.42	B
ATOM	1754	CB	TRP	190	40.607	28.162	-27.811	1.00	13.35	B
ATOM	1755	CG	TRP	190	41.764	27.192	-27.696	1.00	14.17	B
ATOM	1756	CD2	TRP	190	42.570	26.941	-26.528	1.00	13.87	B
ATOM	1757	CE2	TRP	190	43.522	25.962	-26.885	1.00	14.03	B
ATOM	1758	CE3	TRP	190	42.577	27.451	-25.222	1.00	13.06	B
ATOM	1759	CD1	TRP	190	42.257	26.379	-28.680	1.00	13.33	B
ATOM	1760	NE1	TRP	190	43.307	25.643	-28.200	1.00	14.21	B
ATOM	1761	HE1	TRP	190	43.786	24.954	-28.707	1.00	20.00	B
ATOM	1762	CZ2	TRP	190	44.484	25.478	-25.977	1.00	14.67	B
ATOM	1763	CZ3	TRP	190	43.535	26.971	-24.315	1.00	12.71	B

Figure 9 (32/52)

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ATOM   1764  CH2 TRP   190      44.472  25.995 -24.701  1.00 13.47      B
ATOM   1765  C   TRP   190      38.328  28.899 -27.073  1.00 12.16      B
ATOM   1766  O   TRP   190      37.488  29.125 -27.973  1.00 12.32      B
ATOM   1767  N   SER   191      38.434  29.650 -25.988  1.00  8.82      B
ATOM   1768  H   SER   191      39.058  29.431 -25.242  1.00 20.00      B
ATOM   1769  CA  SER   191      37.640  30.844 -25.846  1.00 10.25      B
ATOM   1770  CB  SER   191      37.705  31.363 -24.394  1.00 11.62      B
ATOM   1771  OG  SER   191      39.026  31.784 -24.047  1.00  8.39      B
ATOM   1772  HG  SER   191      39.052  32.720 -24.243  1.00 20.00      B
ATOM   1773  C   SER   191      38.322  31.882 -26.743  1.00  7.95      B
ATOM   1774  O   SER   191      39.438  31.670 -27.230  1.00  8.66      B
ATOM   1775  N   PRO   192      37.653  33.002 -26.999  1.00  5.02      B
ATOM   1776  CD  PRO   192      36.244  33.328 -26.725  1.00  4.85      B
ATOM   1777  CA  PRO   192      38.293  34.023 -27.826  1.00  9.69      B
ATOM   1778  CB  PRO   192      37.246  35.143 -27.862  1.00  6.80      B
ATOM   1779  CG  PRO   192      35.953  34.382 -27.778  1.00  4.99      B
ATOM   1780  C   PRO   192      39.510  34.422 -26.997  1.00 11.81      B
ATOM   1781  O   PRO   192      39.449  34.374 -25.759  1.00 13.09      B
ATOM   1782  N   SER   193      40.609  34.808 -27.635  1.00 13.86      B
ATOM   1783  H   SER   193      40.582  34.865 -28.630  1.00 20.00      B
ATOM   1784  CA  SER   193      41.781  35.173 -26.856  1.00 16.38      B
ATOM   1785  CB  SER   193      43.054  34.639 -27.531  1.00 16.64      B
ATOM   1786  OG  SER   193      43.318  35.343 -28.704  1.00 19.00      B
ATOM   1787  HG  SER   193      42.944  36.216 -28.586  1.00 20.00      B
ATOM   1788  C   SER   193      41.868  36.671 -26.580  1.00 16.48      B
ATOM   1789  O   SER   193      41.379  37.492 -27.357  1.00 18.35      B
ATOM   1790  N   THR   194      42.479  37.019 -25.458  1.00 16.20      B
ATOM   1791  H   THR   194      42.915  36.316 -24.897  1.00 20.00      B
ATOM   1792  CA  THR   194      42.624  38.404 -25.043  1.00 16.68      B
ATOM   1793  CB  THR   194      41.855  38.644 -23.687  1.00 17.77      B
ATOM   1794  OG1 THR   194      41.785  40.052 -23.412  1.00 19.37      B
ATOM   1795  HG1 THR   194      41.745  40.163 -22.467  1.00 20.00      B
ATOM   1796  CG2 THR   194      42.558  37.940 -22.514  1.00 16.01      B
ATOM   1797  C   THR   194      44.125  38.704 -24.902  1.00 18.42      B
ATOM   1798  O   THR   194      44.944  37.806 -25.068  1.00 18.67      B
ATOM   1799  N   LYS   195      44.498  39.947 -24.589  1.00 21.30      B
ATOM   1800  H   LYS   195      43.819  40.648 -24.358  1.00 20.00      B
ATOM   1801  CA  LYS   195      45.910  40.292 -24.458  1.00 23.46      B
ATOM   1802  CB  LYS   195      46.502  40.563 -25.834  1.00 27.09      B
ATOM   1803  CG  LYS   195      46.035  41.838 -26.518  1.00 30.42      B
ATOM   1804  CD  LYS   195      46.745  41.952 -27.858  1.00 31.80      B
ATOM   1805  CE  LYS   195      46.494  43.275 -28.557  1.00 33.61      B
ATOM   1806  NZ  LYS   195      47.437  43.417 -29.712  1.00 35.31      B
ATOM   1807  HZ1 LYS   195      47.690  44.398 -29.931  1.00 20.00      B
ATOM   1808  HZ2 LYS   195      48.320  42.902 -29.449  1.00 20.00      B
ATOM   1809  HZ3 LYS   195      47.110  42.919 -30.555  1.00 20.00      B
ATOM   1810  C   LYS   195      46.216  41.478 -23.557  1.00 24.05      B
ATOM   1811  O   LYS   195      45.346  42.307 -23.292  1.00 22.84      B
ATOM   1812  N   TRP   196      47.472  41.545 -23.108  1.00 26.42      B
ATOM   1813  H   TRP   196      48.129  40.835 -23.376  1.00 20.00      B
ATOM   1814  CA  TRP   196      47.973  42.614 -22.230  1.00 27.20      B
ATOM   1815  CB  TRP   196      47.767  42.245 -20.745  1.00 25.08      B
ATOM   1816  CG  TRP   196      48.671  41.123 -20.244  1.00 23.98      B
ATOM   1817  CD2 TRP   196      48.451  39.697 -20.366  1.00 23.52      B
ATOM   1818  CE2 TRP   196      49.580  39.048 -19.800  1.00 22.81      B
ATOM   1819  CE3 TRP   196      47.415  38.911 -20.908  1.00 21.10      B
ATOM   1820  CD1 TRP   196      49.886  41.262 -19.616  1.00 23.08      B
```

Figure 9 (33/52)

ATOM	1821	NE1	TRP	196	50.434	40.024	-19.355	1.00	24.19	B
ATOM	1822	HE1	TRP	196	51.303	39.925	-18.902	1.00	20.00	B
ATOM	1823	CZ2	TRP	196	49.698	37.659	-19.753	1.00	22.06	B
ATOM	1824	CZ3	TRP	196	47.535	37.527	-20.859	1.00	21.00	B
ATOM	1825	CH2	TRP	196	48.671	36.916	-20.289	1.00	22.21	B
ATOM	1826	C	TRP	196	49.475	42.831	-22.481	1.00	28.61	B
ATOM	1827	O	TRP	196	50.132	42.000	-23.129	1.00	27.91	B
ATOM	1828	N	HIS	197	50.024	43.936	-21.970	1.00	30.93	B
ATOM	1829	H	HIS	197	49.542	44.489	-21.294	1.00	20.00	B
ATOM	1830	CA	HIS	197	51.452	44.206	-22.131	1.00	32.67	B
ATOM	1831	CB	HIS	197	51.701	45.641	-22.608	1.00	35.18	B
ATOM	1832	CG	HIS	197	53.109	45.866	-23.070	1.00	38.67	B
ATOM	1833	ND1	HIS	197	53.494	45.714	-24.391	1.00	39.27	B
ATOM	1834	HD1	HIS	197	52.929	45.402	-25.121	1.00	20.00	B
ATOM	1835	CD2	HIS	197	54.241	46.158	-22.387	1.00	39.93	B
ATOM	1836	NE2	HIS	197	55.276	46.166	-23.289	1.00	39.98	B
ATOM	1837	CE1	HIS	197	54.797	45.896	-24.493	1.00	39.91	B
ATOM	1838	C	HIS	197	52.197	43.972	-20.821	1.00	32.34	B
ATOM	1839	OCT1	HIS	197	52.101	44.784	-19.904	1.00	32.44	B
ATOM	1840	OCT2	HIS	197	52.798	42.919	-20.670	1.00	20.00	B
ATOM	1841	N	MET	1	32.308	7.680	-24.248	1.00	2.15	IL13
ATOM	1842	HT1	MET	1	33.299	7.779	-23.948	1.00	2.51	IL13
ATOM	1843	HT2	MET	1	31.732	7.351	-23.447	1.00	2.72	IL13
ATOM	1844	HT3	MET	1	31.954	8.603	-24.574	1.00	2.41	IL13
ATOM	1845	CA	MET	1	32.219	6.691	-25.361	1.00	1.64	IL13
ATOM	1846	CB	MET	1	33.583	6.301	-25.912	1.00	2.11	IL13
ATOM	1847	CG	MET	1	33.935	7.301	-27.012	1.00	2.56	IL13
ATOM	1848	SD	MET	1	35.506	6.929	-27.794	1.00	3.65	IL13
ATOM	1849	CE	MET	1	35.391	8.116	-29.145	1.00	4.14	IL13
ATOM	1850	C	MET	1	31.321	5.536	-24.942	1.00	1.43	IL13
ATOM	1851	O	MET	1	30.143	5.514	-25.237	1.00	1.40	IL13
ATOM	1852	N	GLY	2	31.858	4.576	-24.246	1.00	1.38	IL13
ATOM	1853	H	GLY	2	32.829	4.551	-24.049	1.00	20.00	IL13
ATOM	1854	CA	GLY	2	31.011	3.442	-23.812	1.00	1.26	IL13
ATOM	1855	C	GLY	2	30.053	3.972	-22.738	1.00	0.96	IL13
ATOM	1856	O	GLY	2	30.376	4.925	-22.055	1.00	0.86	IL13
ATOM	1857	N	PRO	3	28.888	3.394	-22.576	1.00	0.91	IL13
ATOM	1858	CD	PRO	3	28.549	2.040	-23.080	1.00	1.14	IL13
ATOM	1859	CA	PRO	3	27.943	3.900	-21.553	1.00	0.76	IL13
ATOM	1860	CB	PRO	3	27.002	2.665	-21.328	1.00	0.90	IL13
ATOM	1861	CG	PRO	3	27.121	1.794	-22.586	1.00	1.12	IL13
ATOM	1862	C	PRO	3	28.643	4.135	-20.214	1.00	0.62	IL13
ATOM	1863	O	PRO	3	29.795	3.792	-20.042	1.00	0.69	IL13
ATOM	1864	N	VAL	4	27.971	4.720	-19.266	1.00	0.60	IL13
ATOM	1865	H	VAL	4	27.073	5.111	-19.444	1.00	20.00	IL13
ATOM	1866	CA	VAL	4	28.629	4.968	-17.955	1.00	0.63	IL13
ATOM	1867	CB	VAL	4	27.952	6.108	-17.176	1.00	0.83	IL13
ATOM	1868	CG1	VAL	4	28.110	7.430	-17.929	1.00	1.27	IL13
ATOM	1869	CG2	VAL	4	26.490	5.812	-16.840	1.00	1.12	IL13
ATOM	1870	C	VAL	4	28.653	3.646	-17.160	1.00	0.50	IL13
ATOM	1871	O	VAL	4	27.645	2.970	-17.102	1.00	0.47	IL13
ATOM	1872	N	PRO	5	29.757	3.247	-16.541	1.00	0.49	IL13
ATOM	1873	CD	PRO	5	31.043	3.930	-16.540	1.00	0.60	IL13
ATOM	1874	CA	PRO	5	29.748	1.971	-15.779	1.00	0.45	IL13
ATOM	1875	CB	PRO	5	31.147	2.014	-15.136	1.00	0.56	IL13
ATOM	1876	CG	PRO	5	32.014	2.858	-16.068	1.00	0.64	IL13
ATOM	1877	C	PRO	5	28.607	1.949	-14.751	1.00	0.35	IL13

Figure 9 (34/52)

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ATOM   1878  O   PRO   5      28.018   2.973 -14.464  1.00  0.32      IL13
ATOM   1879  N   PRO   6      28.283   0.804 -14.201  1.00  0.38      IL13
ATOM   1880  CD  PRO   6      28.839  -0.513 -14.511  1.00  0.53      IL13
ATOM   1881  CA  PRO   6      27.178   0.717 -13.203  1.00  0.34      IL13
ATOM   1882  CB  PRO   6      27.028  -0.795 -12.985  1.00  0.45      IL13
ATOM   1883  CG  PRO   6      28.374  -1.408 -13.369  1.00  0.56      IL13
ATOM   1884  C   PRO   6      27.466   1.517 -11.928  1.00  0.28      IL13
ATOM   1885  O   PRO   6      26.635   2.263 -11.449  1.00  0.25      IL13
ATOM   1886  N   SER   7      28.631   1.355 -11.374  1.00  0.27      IL13
ATOM   1887  H   SER   7      29.314   0.698 -11.690  1.00 20.00      IL13
ATOM   1888  CA  SER   7      28.978   2.090 -10.125  1.00  0.25      IL13
ATOM   1889  CB  SER   7      30.360   1.697  -9.625  1.00  0.29      IL13
ATOM   1890  OG  SER   7      30.945   0.736 -10.513  1.00  0.33      IL13
ATOM   1891  HG  SER   7      31.081  -0.029  -9.961  1.00  1.03      IL13
ATOM   1892  C   SER   7      28.955   3.597 -10.385  1.00  0.25      IL13
ATOM   1893  O   SER   7      28.519   4.373  -9.558  1.00  0.24      IL13
ATOM   1894  N   THR   8      29.430   4.017 -11.524  1.00  0.28      IL13
ATOM   1895  H   THR   8      29.893   3.392 -12.152  1.00 20.00      IL13
ATOM   1896  CA  THR   8      29.447   5.475 -11.834  1.00  0.31      IL13
ATOM   1897  CB  THR   8      30.287   5.656 -13.099  1.00  0.37      IL13
ATOM   1898  OG1 THR   8      31.511   4.911 -12.977  1.00  0.41      IL13
ATOM   1899  HG1 THR   8      32.148   5.478 -12.551  1.00  0.89      IL13
ATOM   1900  CG2 THR   8      30.578   7.114 -13.449  1.00  0.46      IL13
ATOM   1901  C   THR   8      28.014   5.977 -11.998  1.00  0.27      IL13
ATOM   1902  O   THR   8      27.669   7.058 -11.564  1.00  0.28      IL13
ATOM   1903  N   ALA   9      27.177   5.201 -12.626  1.00  0.27      IL13
ATOM   1904  H   ALA   9      27.395   4.296 -12.991  1.00 20.00      IL13
ATOM   1905  CA  ALA   9      25.768   5.633 -12.825  1.00  0.27      IL13
ATOM   1906  CB  ALA   9      24.982   4.572 -13.597  1.00  0.30      IL13
ATOM   1907  C   ALA   9      25.098   5.850 -11.467  1.00  0.22      IL13
ATOM   1908  O   ALA   9      24.398   6.823 -11.263  1.00  0.23      IL13
ATOM   1909  N   LEU  10      25.296   4.954 -10.537  1.00  0.21      IL13
ATOM   1910  H   LEU  10      25.937   4.212 -10.755  1.00 20.00      IL13
ATOM   1911  CA  LEU  10      24.656   5.124  -9.203  1.00  0.19      IL13
ATOM   1912  CB  LEU  10      24.853   3.880  -8.334  1.00  0.20      IL13
ATOM   1913  CG  LEU  10      23.820   3.788  -7.205  1.00  0.23      IL13
ATOM   1914  CD1 LEU  10      22.390   3.719  -7.743  1.00  0.58      IL13
ATOM   1915  CD2 LEU  10      24.109   2.632  -6.249  1.00  0.64      IL13
ATOM   1916  C   LEU  10      25.188   6.400  -8.543  1.00  0.19      IL13
ATOM   1917  O   LEU  10      24.430   7.247  -8.114  1.00  0.19      IL13
ATOM   1918  N   ARG  11      26.482   6.538  -8.442  1.00  0.21      IL13
ATOM   1919  H   ARG  11      27.077   5.787  -8.739  1.00 20.00      IL13
ATOM   1920  CA  ARG  11      27.039   7.753  -7.788  1.00  0.24      IL13
ATOM   1921  CB  ARG  11      28.537   7.505  -7.955  1.00  0.30      IL13
ATOM   1922  CG  ARG  11      29.577   8.277  -7.163  1.00  0.35      IL13
ATOM   1923  CD  ARG  11      30.654   8.792  -8.120  1.00  0.67      IL13
ATOM   1924  NE  ARG  11      30.197  10.033  -8.732  1.00  1.37      IL13
ATOM   1925  HE  ARG  11      29.900  10.781  -8.126  1.00  2.02      IL13
ATOM   1926  CZ  ARG  11      30.105  10.291 -10.042  1.00  1.95      IL13
ATOM   1927  NH1 ARG  11      29.703  11.490 -10.432  1.00  2.95      IL13
ATOM   1928 HH11 ARG  11      29.324  12.119  -9.733  1.00  3.44      IL13
ATOM   1929 HH12 ARG  11      29.738  11.784 -11.390  1.00  3.44      IL13
ATOM   1930  NH2 ARG  11      30.384   9.363 -10.939  1.00  2.13      IL13
ATOM   1931 HH21 ARG  11      30.702   8.459 -10.663  1.00  2.06      IL13
ATOM   1932 HH22 ARG  11      30.235   9.581 -11.905  1.00  2.81      IL13
ATOM   1933  C   ARG  11      26.590   8.993  -8.552  1.00  0.24      IL13
ATOM   1934  O   ARG  11      26.185   9.977  -7.967  1.00  0.24      IL13
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Figure 9 (35/52)

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ATOM   1935  N   GLU   12      26.628   8.952  -9.852  1.00  0.25      IL13
ATOM   1936  H   GLU   12      26.956   8.132 -10.315  1.00 20.00      IL13
ATOM   1937  CA  GLU   12      26.166  10.127 -10.629  1.00  0.27      IL13
ATOM   1938  CB  GLU   12      26.267   9.894 -12.156  1.00  0.30      IL13
ATOM   1939  CG  GLU   12      27.646   9.916 -12.837  1.00  0.34      IL13
ATOM   1940  CD  GLU   12      27.638   9.423 -14.294  1.00  1.17      IL13
ATOM   1941  OE1 GLU   12      28.693   9.519 -14.928  1.00  1.86      IL13
ATOM   1942  OE2 GLU   12      26.610   8.939 -14.793  1.00  1.96      IL13
ATOM   1943  C   GLU   12      24.667  10.313 -10.383  1.00  0.25      IL13
ATOM   1944  O   GLU   12      24.170  11.422 -10.332  1.00  0.26      IL13
ATOM   1945  N   LEU   13      23.942   9.238 -10.211  1.00  0.22      IL13
ATOM   1946  H   LEU   13      24.370   8.340 -10.185  1.00 20.00      IL13
ATOM   1947  CA  LEU   13      22.478   9.359  -9.948  1.00  0.22      IL13
ATOM   1948  CB  LEU   13      21.826   7.972 -10.051  1.00  0.23      IL13
ATOM   1949  CG  LEU   13      20.332   7.855  -9.737  1.00  0.26      IL13
ATOM   1950  CD1 LEU   13      19.459   8.370 -10.876  1.00  0.31      IL13
ATOM   1951  CD2 LEU   13      19.952   6.423  -9.367  1.00  0.31      IL13
ATOM   1952  C   LEU   13      22.261   9.930  -8.537  1.00  0.19      IL13
ATOM   1953  O   LEU   13      21.461  10.823  -8.337  1.00  0.20      IL13
ATOM   1954  N   ILE   14      22.973   9.426  -7.558  1.00  0.18      IL13
ATOM   1955  H   ILE   14      23.782   8.906  -7.813  1.00 20.00      IL13
ATOM   1956  CA  ILE   14      22.809   9.946  -6.164  1.00  0.17      IL13
ATOM   1957  CB  ILE   14      23.723   9.142  -5.237  1.00  0.17      IL13
ATOM   1958  CG2 ILE   14      23.743   9.738  -3.829  1.00  0.19      IL13
ATOM   1959  CG1 ILE   14      23.264   7.683  -5.206  1.00  0.18      IL13
ATOM   1960  CD1 ILE   14      24.379   6.722  -4.794  1.00  0.21      IL13
ATOM   1961  C   ILE   14      23.152  11.437  -6.142  1.00  0.18      IL13
ATOM   1962  O   ILE   14      22.423  12.242  -5.598  1.00  0.18      IL13
ATOM   1963  N   GLU   15      24.271  11.808  -6.692  1.00  0.21      IL13
ATOM   1964  H   GLU   15      24.901  11.156  -7.124  1.00 20.00      IL13
ATOM   1965  CA  GLU   15      24.671  13.241  -6.650  1.00  0.24      IL13
ATOM   1966  CB  GLU   15      26.075  13.388  -7.234  1.00  0.27      IL13
ATOM   1967  CG  GLU   15      27.112  12.695  -6.330  1.00  0.30      IL13
ATOM   1968  CD  GLU   15      28.171  11.950  -7.135  1.00  0.87      IL13
ATOM   1969  OE1 GLU   15      29.093  11.387  -6.541  1.00  1.48      IL13
ATOM   1970  OE2 GLU   15      28.077  11.900  -8.362  1.00  1.66      IL13
ATOM   1971  C   GLU   15      23.620  14.111  -7.334  1.00  0.23      IL13
ATOM   1972  O   GLU   15      23.310  15.190  -6.870  1.00  0.24      IL13
ATOM   1973  N   GLU   16      23.065  13.674  -8.426  1.00  0.22      IL13
ATOM   1974  H   GLU   16      23.415  12.873  -8.911  1.00 20.00      IL13
ATOM   1975  CA  GLU   16      22.047  14.518  -9.103  1.00  0.23      IL13
ATOM   1976  CB  GLU   16      21.606  13.725 -10.324  1.00  0.25      IL13
ATOM   1977  CG  GLU   16      20.838  12.402 -10.622  1.00  0.29      IL13
ATOM   1978  CD  GLU   16      19.392  12.330 -10.119  1.00  1.02      IL13
ATOM   1979  OE1 GLU   16      18.665  13.328 -10.129  1.00  1.72      IL13
ATOM   1980  OE2 GLU   16      19.013  11.276  -9.612  1.00  1.82      IL13
ATOM   1981  C   GLU   16      20.738  14.535  -8.297  1.00  0.21      IL13
ATOM   1982  O   GLU   16      20.127  15.570  -8.136  1.00  0.22      IL13
ATOM   1983  N   LEU   17      20.305  13.411  -7.786  1.00  0.20      IL13
ATOM   1984  H   LEU   17      20.656  12.561  -8.191  1.00 20.00      IL13
ATOM   1985  CA  LEU   17      19.033  13.400  -6.997  1.00  0.19      IL13
ATOM   1986  CB  LEU   17      18.690  12.019  -6.425  1.00  0.22      IL13
ATOM   1987  CG  LEU   17      17.458  11.344  -7.038  1.00  0.24      IL13
ATOM   1988  CD1 LEU   17      17.023  10.124  -6.226  1.00  0.28      IL13
ATOM   1989  CD2 LEU   17      16.310  12.317  -7.313  1.00  0.30      IL13
ATOM   1990  C   LEU   17      19.171  14.327  -5.786  1.00  0.19      IL13
ATOM   1991  O   LEU   17      18.286  15.101  -5.479  1.00  0.19      IL13
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Figure 9 (36/52)

ATOM	1992	N	VAL	18	20.272	14.246	-5.095	1.00	0.20	IL13
ATOM	1993	H	VAL	18	21.000	13.650	-5.445	1.00	20.00	IL13
ATOM	1994	CA	VAL	18	20.475	15.111	-3.898	1.00	0.21	IL13
ATOM	1995	CB	VAL	18	21.806	14.816	-3.181	1.00	0.25	IL13
ATOM	1996	CG1	VAL	18	22.011	15.721	-1.960	1.00	0.28	IL13
ATOM	1997	CG2	VAL	18	21.933	13.354	-2.772	1.00	0.26	IL13
ATOM	1998	C	VAL	18	20.466	16.579	-4.337	1.00	0.21	IL13
ATOM	1999	O	VAL	18	19.791	17.409	-3.764	1.00	0.23	IL13
ATOM	2000	N	ASN	19	21.225	16.899	-5.342	1.00	0.22	IL13
ATOM	2001	H	ASN	19	21.663	16.198	-5.912	1.00	20.00	IL13
ATOM	2002	CA	ASN	19	21.305	18.310	-5.822	1.00	0.24	IL13
ATOM	2003	CB	ASN	19	22.218	18.525	-7.023	1.00	0.27	IL13
ATOM	2004	CG	ASN	19	22.696	19.966	-6.955	1.00	1.29	IL13
ATOM	2005	OD1	ASN	19	22.316	20.735	-6.073	1.00	2.08	IL13
ATOM	2006	ND2	ASN	19	23.578	20.278	-7.907	1.00	1.98	IL13
ATOM	2007	HD21	ASN	19	23.963	19.590	-8.531	1.00	2.18	IL13
ATOM	2008	HD22	ASN	19	23.823	21.243	-8.004	1.00	2.66	IL13
ATOM	2009	C	ASN	19	19.911	18.916	-6.036	1.00	0.23	IL13
ATOM	2010	O	ASN	19	19.649	20.037	-5.646	1.00	0.26	IL13
ATOM	2011	N	ILE	20	19.032	18.213	-6.693	1.00	0.22	IL13
ATOM	2012	H	ILE	20	19.300	17.316	-7.058	1.00	20.00	IL13
ATOM	2013	CA	ILE	20	17.681	18.783	-6.979	1.00	0.24	IL13
ATOM	2014	CB	ILE	20	17.005	18.078	-8.167	1.00	0.27	IL13
ATOM	2015	CG2	ILE	20	17.890	18.235	-9.408	1.00	0.33	IL13
ATOM	2016	CG1	ILE	20	16.689	16.603	-7.891	1.00	0.24	IL13
ATOM	2017	CD1	ILE	20	15.917	15.925	-9.025	1.00	0.32	IL13
ATOM	2018	C	ILE	20	16.770	18.799	-5.737	1.00	0.23	IL13
ATOM	2019	O	ILE	20	15.749	19.459	-5.751	1.00	0.27	IL13
ATOM	2020	N	THR	21	17.104	18.091	-4.679	1.00	0.20	IL13
ATOM	2021	H	THR	21	17.957	17.565	-4.699	1.00	20.00	IL13
ATOM	2022	CA	THR	21	16.212	18.092	-3.463	1.00	0.24	IL13
ATOM	2023	CB	THR	21	15.883	16.663	-3.019	1.00	0.26	IL13
ATOM	2024	OG1	THR	21	17.035	15.807	-3.044	1.00	0.27	IL13
ATOM	2025	HG1	THR	21	17.352	15.767	-3.951	1.00	0.95	IL13
ATOM	2026	CG2	THR	21	14.787	16.084	-3.912	1.00	0.25	IL13
ATOM	2027	C	THR	21	16.779	18.994	-2.359	1.00	0.28	IL13
ATOM	2028	O	THR	21	16.084	19.332	-1.422	1.00	0.44	IL13
ATOM	2029	N	GLN	22	18.020	19.389	-2.439	1.00	0.25	IL13
ATOM	2030	H	GLN	22	18.611	19.093	-3.195	1.00	20.00	IL13
ATOM	2031	CA	GLN	22	18.573	20.263	-1.361	1.00	0.31	IL13
ATOM	2032	CB	GLN	22	20.100	20.156	-1.278	1.00	0.37	IL13
ATOM	2033	CG	GLN	22	20.847	20.477	-2.579	1.00	0.43	IL13
ATOM	2034	CD	GLN	22	22.229	20.996	-2.254	1.00	1.18	IL13
ATOM	2035	OE1	GLN	22	22.568	21.258	-1.098	1.00	1.91	IL13
ATOM	2036	NE2	GLN	22	23.015	21.176	-3.316	1.00	1.89	IL13
ATOM	2037	HE21	GLN	22	22.673	21.059	-4.250	1.00	2.18	IL13
ATOM	2038	HE22	GLN	22	23.983	21.404	-3.240	1.00	2.50	IL13
ATOM	2039	C	GLN	22	18.148	21.720	-1.582	1.00	0.34	IL13
ATOM	2040	O	GLN	22	17.881	22.437	-0.637	1.00	0.42	IL13
ATOM	2041	N	ASN	23	18.086	22.168	-2.810	1.00	0.37	IL13
ATOM	2042	H	ASN	23	18.342	21.553	-3.561	1.00	20.00	IL13
ATOM	2043	CA	ASN	23	17.680	23.585	-3.069	1.00	0.48	IL13
ATOM	2044	CB	ASN	23	18.603	24.267	-4.065	1.00	0.64	IL13
ATOM	2045	CG	ASN	23	19.655	24.904	-3.189	1.00	1.34	IL13
ATOM	2046	OD1	ASN	23	19.354	25.441	-2.132	1.00	2.08	IL13
ATOM	2047	ND2	ASN	23	20.900	24.788	-3.632	1.00	2.13	IL13
ATOM	2048	HD21	ASN	23	21.157	24.323	-4.476	1.00	2.40	IL13

Figure 9 (37/52)

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ATOM   2049 HD22 ASN   23      21.577  25.220  -3.037  1.00  2.82      IL13
ATOM   2050  C   ASN   23      16.188  23.652  -3.385  1.00  0.43      IL13
ATOM   2051  O   ASN   23      15.673  24.696  -3.733  1.00  0.50      IL13
ATOM   2052  N   GLN   24      15.480  22.559  -3.289  1.00  0.36      IL13
ATOM   2053  H   GLN   24      15.904  21.728  -2.935  1.00 20.00      IL13
ATOM   2054  CA  GLN   24      14.032  22.618  -3.618  1.00  0.36      IL13
ATOM   2055  CB  GLN   24      13.399  21.226  -3.889  1.00  0.34      IL13
ATOM   2056  CG  GLN   24      13.338  20.243  -2.694  1.00  0.39      IL13
ATOM   2057  CD  GLN   24      12.267  19.157  -2.793  1.00  1.17      IL13
ATOM   2058  OE1 GLN   24      12.430  18.031  -2.301  1.00  1.85      IL13
ATOM   2059  NE2 GLN   24      11.122  19.550  -3.374  1.00  1.75      IL13
ATOM   2060 HE21 GLN   24      10.974  20.444  -3.802  1.00  1.89      IL13
ATOM   2061 HE22 GLN   24      10.407  18.861  -3.381  1.00  2.36      IL13
ATOM   2062  C   GLN   24      13.291  23.275  -2.461  1.00  0.43      IL13
ATOM   2063  O   GLN   24      13.415  22.875  -1.321  1.00  0.47      IL13
ATOM   2064  N   LYS   25      12.505  24.264  -2.747  1.00  0.52      IL13
ATOM   2065  H   LYS   25      12.487  24.570  -3.695  1.00 20.00      IL13
ATOM   2066  CA  LYS   25      11.729  24.919  -1.667  1.00  0.66      IL13
ATOM   2067  CB  LYS   25      11.583  26.406  -2.016  1.00  0.79      IL13
ATOM   2068  CG  LYS   25      10.697  27.248  -1.092  1.00  0.96      IL13
ATOM   2069  CD  LYS   25      10.485  28.635  -1.697  1.00  1.27      IL13
ATOM   2070  CE  LYS   25       9.360  29.429  -1.035  1.00  1.72      IL13
ATOM   2071  NZ  LYS   25       9.201  30.692  -1.769  1.00  2.61      IL13
ATOM   2072  HZ1 LYS   25       8.228  31.039  -1.659  1.00  3.05      IL13
ATOM   2073  HZ2 LYS   25       9.391  30.501  -2.775  1.00  3.06      IL13
ATOM   2074  HZ3 LYS   25       9.879  31.395  -1.414  1.00  2.98      IL13
ATOM   2075  C   LYS   25      10.393  24.188  -1.548  1.00  0.68      IL13
ATOM   2076  O   LYS   25      10.195  23.357  -0.687  1.00  0.79      IL13
ATOM   2077  N   ALA   26       9.491  24.477  -2.440  1.00  0.68      IL13
ATOM   2078  H   ALA   26       9.798  24.879  -3.294  1.00 20.00      IL13
ATOM   2079  CA  ALA   26       8.166  23.797  -2.440  1.00  0.70      IL13
ATOM   2080  CB  ALA   26       7.183  24.632  -3.270  1.00  0.81      IL13
ATOM   2081  C   ALA   26       8.344  22.413  -3.073  1.00  0.55      IL13
ATOM   2082  O   ALA   26       9.266  22.219  -3.840  1.00  0.46      IL13
ATOM   2083  N   PRO   27       7.483  21.453  -2.794  1.00  0.56      IL13
ATOM   2084  CD  PRO   27       6.340  21.502  -1.883  1.00  0.70      IL13
ATOM   2085  CA  PRO   27       7.631  20.118  -3.422  1.00  0.47      IL13
ATOM   2086  CB  PRO   27       6.282  19.459  -3.125  1.00  0.55      IL13
ATOM   2087  CG  PRO   27       5.871  20.054  -1.779  1.00  0.70      IL13
ATOM   2088  C   PRO   27       7.942  20.245  -4.916  1.00  0.38      IL13
ATOM   2089  O   PRO   27       7.551  21.199  -5.557  1.00  0.43      IL13
ATOM   2090  N   LEU   28       8.664  19.317  -5.470  1.00  0.36      IL13
ATOM   2091  H   LEU   28       8.927  18.499  -4.965  1.00 20.00      IL13
ATOM   2092  CA  LEU   28       9.014  19.428  -6.914  1.00  0.37      IL13
ATOM   2093  CB  LEU   28       9.889  18.247  -7.345  1.00  0.45      IL13
ATOM   2094  CG  LEU   28      11.258  18.193  -6.660  1.00  0.50      IL13
ATOM   2095  CD1 LEU   28      11.967  16.862  -6.911  1.00  0.62      IL13
ATOM   2096  CD2 LEU   28      12.139  19.383  -7.044  1.00  0.50      IL13
ATOM   2097  C   LEU   28       7.726  19.461  -7.745  1.00  0.35      IL13
ATOM   2098  O   LEU   28       7.533  20.337  -8.565  1.00  0.59      IL13
ATOM   2099  N   CYS   29       6.835  18.534  -7.529  1.00  0.35      IL13
ATOM   2100  H   CYS   29       6.958  17.965  -6.720  1.00 20.00      IL13
ATOM   2101  CA  CYS   29       5.553  18.543  -8.299  1.00  0.35      IL13
ATOM   2102  CB  CYS   29       5.113  17.094  -8.371  1.00  0.36      IL13
ATOM   2103  SG  CYS   29       5.376  16.268  -6.780  1.00  0.36      IL13
ATOM   2104  C   CYS   29       4.515  19.380  -7.548  1.00  0.34      IL13
ATOM   2105  O   CYS   29       4.766  19.871  -6.467  1.00  0.35      IL13
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Figure 9 (38/52)

ATOM	2106	N	ASN	30	3.337	19.518	-8.098	1.00	0.35	IL13
ATOM	2107	H	ASN	30	3.263	19.241	-9.055	1.00	20.00	IL13
ATOM	2108	CA	ASN	30	2.266	20.291	-7.402	1.00	0.39	IL13
ATOM	2109	CB	ASN	30	1.100	20.642	-8.314	1.00	0.46	IL13
ATOM	2110	CG	ASN	30	1.641	21.588	-9.352	1.00	1.49	IL13
ATOM	2111	OD1	ASN	30	2.346	22.556	-9.079	1.00	2.37	IL13
ATOM	2112	ND2	ASN	30	1.376	21.193	-10.599	1.00	2.17	IL13
ATOM	2113	HD21	ASN	30	0.734	20.455	-10.802	1.00	2.26	IL13
ATOM	2114	HD22	ASN	30	1.841	21.666	-11.347	1.00	2.98	IL13
ATOM	2115	C	ASN	30	1.813	19.521	-6.159	1.00	0.35	IL13
ATOM	2116	O	ASN	30	0.650	19.531	-5.809	1.00	0.41	IL13
ATOM	2117	N	GLY	31	2.701	18.828	-5.505	1.00	0.29	IL13
ATOM	2118	H	GLY	31	3.672	18.810	-5.657	1.00	20.00	IL13
ATOM	2119	CA	GLY	31	2.284	18.040	-4.317	1.00	0.29	IL13
ATOM	2120	C	GLY	31	1.806	16.674	-4.801	1.00	0.26	IL13
ATOM	2121	O	GLY	31	1.024	16.007	-4.154	1.00	0.30	IL13
ATOM	2122	N	SER	32	2.275	16.257	-5.948	1.00	0.23	IL13
ATOM	2123	H	SER	32	2.822	16.835	-6.546	1.00	20.00	IL13
ATOM	2124	CA	SER	32	1.857	14.938	-6.490	1.00	0.22	IL13
ATOM	2125	CB	SER	32	2.434	14.735	-7.882	1.00	0.26	IL13
ATOM	2126	OG	SER	32	2.175	15.925	-8.639	1.00	0.33	IL13
ATOM	2127	HG	SER	32	2.490	15.730	-9.519	1.00	0.95	IL13
ATOM	2128	C	SER	32	2.256	13.847	-5.505	1.00	0.20	IL13
ATOM	2129	O	SER	32	3.254	13.960	-4.817	1.00	0.23	IL13
ATOM	2130	N	MET	33	1.475	12.803	-5.428	1.00	0.22	IL13
ATOM	2131	H	MET	33	0.689	12.742	-6.036	1.00	20.00	IL13
ATOM	2132	CA	MET	33	1.779	11.686	-4.490	1.00	0.26	IL13
ATOM	2133	CB	MET	33	0.597	11.427	-3.557	1.00	0.36	IL13
ATOM	2134	CG	MET	33	0.192	12.644	-2.724	1.00	0.41	IL13
ATOM	2135	SD	MET	33	-1.246	12.296	-1.698	1.00	1.07	IL13
ATOM	2136	CE	MET	33	-0.428	11.352	-0.401	1.00	0.51	IL13
ATOM	2137	C	MET	33	2.104	10.433	-5.300	1.00	0.22	IL13
ATOM	2138	O	MET	33	1.652	10.282	-6.419	1.00	0.23	IL13
ATOM	2139	N	VAL	34	2.893	9.545	-4.745	1.00	0.20	IL13
ATOM	2140	H	VAL	34	3.203	9.600	-3.793	1.00	20.00	IL13
ATOM	2141	CA	VAL	34	3.268	8.294	-5.473	1.00	0.19	IL13
ATOM	2142	CB	VAL	34	4.744	8.282	-5.872	1.00	0.20	IL13
ATOM	2143	CG1	VAL	34	4.926	8.583	-7.349	1.00	0.24	IL13
ATOM	2144	CG2	VAL	34	5.588	9.178	-4.970	1.00	0.24	IL13
ATOM	2145	C	VAL	34	3.028	7.086	-4.571	1.00	0.19	IL13
ATOM	2146	O	VAL	34	2.924	7.207	-3.369	1.00	0.18	IL13
ATOM	2147	N	TRP	35	2.916	5.927	-5.156	1.00	0.21	IL13
ATOM	2148	H	TRP	35	3.296	5.821	-6.079	1.00	20.00	IL13
ATOM	2149	CA	TRP	35	2.648	4.697	-4.359	1.00	0.22	IL13
ATOM	2150	CB	TRP	35	2.191	3.574	-5.299	1.00	0.28	IL13
ATOM	2151	CG	TRP	35	1.058	4.027	-6.201	1.00	0.32	IL13
ATOM	2152	CD2	TRP	35	-0.359	3.873	-5.984	1.00	0.35	IL13
ATOM	2153	CE2	TRP	35	-1.031	4.441	-7.121	1.00	0.42	IL13
ATOM	2154	CE3	TRP	35	-1.110	3.299	-4.935	1.00	0.34	IL13
ATOM	2155	CD1	TRP	35	1.167	4.671	-7.448	1.00	0.37	IL13
ATOM	2156	NE1	TRP	35	-0.058	4.918	-7.995	1.00	0.43	IL13
ATOM	2157	HE1	TRP	35	-0.221	5.249	-8.912	1.00	0.48	IL13
ATOM	2158	CZ2	TRP	35	-2.440	4.417	-7.184	1.00	0.48	IL13
ATOM	2159	CZ3	TRP	35	-2.519	3.284	-5.012	1.00	0.39	IL13
ATOM	2160	CH2	TRP	35	-3.179	3.839	-6.130	1.00	0.46	IL13
ATOM	2161	C	TRP	35	3.888	4.263	-3.579	1.00	0.21	IL13
ATOM	2162	O	TRP	35	4.967	4.141	-4.123	1.00	0.24	IL13

Figure 9 (39/52)

ATOM	2163	N	SER	36	3.730	3.984	-2.313	1.00	0.20	IL13
ATOM	2164	H	SER	36	2.860	4.175	-1.853	1.00	20.00	IL13
ATOM	2165	CA	SER	36	4.885	3.505	-1.505	1.00	0.23	IL13
ATOM	2166	CB	SER	36	4.520	3.702	-0.015	1.00	0.26	IL13
ATOM	2167	OG	SER	36	4.942	2.634	0.843	1.00	1.09	IL13
ATOM	2168	HG	SER	36	4.330	1.926	0.660	1.00	1.63	IL13
ATOM	2169	C	SER	36	5.203	2.071	-1.941	1.00	0.25	IL13
ATOM	2170	O	SER	36	4.308	1.289	-2.198	1.00	0.33	IL13
ATOM	2171	N	ILE	37	6.462	1.732	-2.049	1.00	0.21	IL13
ATOM	2172	H	ILE	37	7.164	2.357	-1.713	1.00	20.00	IL13
ATOM	2173	CA	ILE	37	6.849	0.354	-2.497	1.00	0.22	IL13
ATOM	2174	CB	ILE	37	7.426	0.415	-3.921	1.00	0.21	IL13
ATOM	2175	CG2	ILE	37	6.333	0.723	-4.953	1.00	0.24	IL13
ATOM	2176	CG1	ILE	37	8.545	1.464	-3.968	1.00	0.20	IL13
ATOM	2177	CD1	ILE	37	9.449	1.363	-5.190	1.00	0.21	IL13
ATOM	2178	C	ILE	37	7.921	-0.226	-1.569	1.00	0.23	IL13
ATOM	2179	O	ILE	37	8.485	0.466	-0.743	1.00	0.24	IL13
ATOM	2180	N	ASN	38	8.216	-1.493	-1.713	1.00	0.25	IL13
ATOM	2181	H	ASN	38	7.797	-1.973	-2.485	1.00	20.00	IL13
ATOM	2182	CA	ASN	38	9.263	-2.120	-0.856	1.00	0.27	IL13
ATOM	2183	CB	ASN	38	8.950	-3.593	-0.649	1.00	0.32	IL13
ATOM	2184	CG	ASN	38	9.570	-4.017	0.657	1.00	1.18	IL13
ATOM	2185	OD1	ASN	38	10.774	-3.967	0.849	1.00	2.04	IL13
ATOM	2186	ND2	ASN	38	8.682	-4.466	1.542	1.00	1.86	IL13
ATOM	2187	HD21	ASN	38	7.702	-4.378	1.341	1.00	2.18	IL13
ATOM	2188	HD22	ASN	38	9.005	-4.869	2.397	1.00	2.47	IL13
ATOM	2189	C	ASN	38	10.616	-1.894	-1.528	1.00	0.24	IL13
ATOM	2190	O	ASN	38	10.823	-2.268	-2.664	1.00	0.23	IL13
ATOM	2191	N	LEU	39	11.523	-1.248	-0.856	1.00	0.25	IL13
ATOM	2192	H	LEU	39	11.333	-1.005	0.088	1.00	20.00	IL13
ATOM	2193	CA	LEU	39	12.838	-0.964	-1.490	1.00	0.25	IL13
ATOM	2194	CB	LEU	39	13.415	0.364	-0.975	1.00	0.29	IL13
ATOM	2195	CG	LEU	39	12.748	1.667	-1.451	1.00	0.31	IL13
ATOM	2196	CD1	LEU	39	12.606	1.717	-2.970	1.00	0.35	IL13
ATOM	2197	CD2	LEU	39	11.435	1.993	-0.736	1.00	0.34	IL13
ATOM	2198	C	LEU	39	13.798	-2.139	-1.278	1.00	0.26	IL13
ATOM	2199	O	LEU	39	14.623	-2.100	-0.385	1.00	0.28	IL13
ATOM	2200	N	THR	40	13.722	-3.164	-2.103	1.00	0.25	IL13
ATOM	2201	H	THR	40	12.988	-3.156	-2.782	1.00	20.00	IL13
ATOM	2202	CA	THR	40	14.666	-4.321	-1.959	1.00	0.27	IL13
ATOM	2203	CB	THR	40	13.810	-5.527	-1.571	1.00	0.28	IL13
ATOM	2204	OG1	THR	40	12.641	-5.563	-2.403	1.00	0.27	IL13
ATOM	2205	HG1	THR	40	11.999	-4.972	-2.013	1.00	0.88	IL13
ATOM	2206	CG2	THR	40	13.431	-5.535	-0.090	1.00	0.31	IL13
ATOM	2207	C	THR	40	15.394	-4.578	-3.286	1.00	0.27	IL13
ATOM	2208	O	THR	40	16.553	-4.245	-3.439	1.00	0.29	IL13
ATOM	2209	N	ALA	41	14.707	-5.162	-4.242	1.00	0.26	IL13
ATOM	2210	H	ALA	41	13.747	-5.367	-4.036	1.00	20.00	IL13
ATOM	2211	CA	ALA	41	15.326	-5.448	-5.578	1.00	0.27	IL13
ATOM	2212	CB	ALA	41	15.219	-6.937	-5.918	1.00	0.30	IL13
ATOM	2213	C	ALA	41	14.651	-4.610	-6.668	1.00	0.25	IL13
ATOM	2214	O	ALA	41	15.256	-3.768	-7.302	1.00	0.30	IL13
ATOM	2215	N	GLY	42	13.390	-4.871	-6.892	1.00	0.25	IL13
ATOM	2216	H	GLY	42	12.936	-5.524	-6.291	1.00	20.00	IL13
ATOM	2217	CA	GLY	42	12.615	-4.147	-7.944	1.00	0.27	IL13
ATOM	2218	C	GLY	42	12.624	-2.638	-7.699	1.00	0.22	IL13
ATOM	2219	O	GLY	42	11.972	-1.900	-8.401	1.00	0.24	IL13

Figure 9 (40/52)

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ATOM   2220  N   MET   43      13.325  -2.184  -6.697  1.00  0.20      IL13
ATOM   2221  H   MET   43      13.866  -2.769  -6.113  1.00 20.00      IL13
ATOM   2222  CA  MET   43      13.355  -0.723  -6.376  1.00  0.26      IL13
ATOM   2223  CB  MET   43      14.641  -0.339  -5.641  1.00  0.36      IL13
ATOM   2224  CG  MET   43      14.990  -1.152  -4.408  1.00  0.33      IL13
ATOM   2225  SD  MET   43      16.640  -0.792  -3.789  1.00  0.86      IL13
ATOM   2226  CE  MET   43      17.542  -1.506  -5.175  1.00  0.40      IL13
ATOM   2227  C   MET   43      13.395   0.130  -7.653  1.00  0.21      IL13
ATOM   2228  O   MET   43      12.545   0.968  -7.869  1.00  0.22      IL13
ATOM   2229  N   TYR   44      14.376  -0.066  -8.491  1.00  0.21      IL13
ATOM   2230  H   TYR   44      14.985  -0.833  -8.286  1.00 20.00      IL13
ATOM   2231  CA  TYR   44      14.459   0.750  -9.739  1.00  0.21      IL13
ATOM   2232  CB  TYR   44      15.724   0.378 -10.526  1.00  0.25      IL13
ATOM   2233  CG  TYR   44      16.971   0.343  -9.658  1.00  0.28      IL13
ATOM   2234  CD1 TYR   44      17.582   1.549  -9.253  1.00  0.30      IL13
ATOM   2235  CE1 TYR   44      18.763   1.496  -8.488  1.00  0.36      IL13
ATOM   2236  CD2 TYR   44      17.509  -0.911  -9.295  1.00  0.34      IL13
ATOM   2237  CE2 TYR   44      18.687  -0.962  -8.528  1.00  0.40      IL13
ATOM   2238  CZ  TYR   44      19.304   0.242  -8.132  1.00  0.40      IL13
ATOM   2239  OH  TYR   44      20.467   0.194  -7.378  1.00  0.47      IL13
ATOM   2240  HH  TYR   44      20.990   0.957  -7.608  1.00  1.00      IL13
ATOM   2241  C   TYR   44      13.209   0.539 -10.594  1.00  0.19      IL13
ATOM   2242  O   TYR   44      12.599   1.474 -11.073  1.00  0.20      IL13
ATOM   2243  N   CYS   45      12.848  -0.690 -10.808  1.00  0.20      IL13
ATOM   2244  H   CYS   45      13.237  -1.416 -10.250  1.00 20.00      IL13
ATOM   2245  CA  CYS   45      11.662  -1.002 -11.653  1.00  0.22      IL13
ATOM   2246  CB  CYS   45      11.679  -2.494 -11.993  1.00  0.26      IL13
ATOM   2247  SG  CYS   45      13.355  -3.129 -12.298  1.00  0.54      IL13
ATOM   2248  C   CYS   45      10.363  -0.608 -10.952  1.00  0.18      IL13
ATOM   2249  O   CYS   45       9.535   0.089 -11.503  1.00  0.19      IL13
ATOM   2250  N   ALA   46      10.181  -1.044  -9.746  1.00  0.18      IL13
ATOM   2251  H   ALA   46      10.664  -1.879  -9.534  1.00 20.00      IL13
ATOM   2252  CA  ALA   46       8.939  -0.696  -9.011  1.00  0.17      IL13
ATOM   2253  CB  ALA   46       8.914  -1.341  -7.625  1.00  0.20      IL13
ATOM   2254  C   ALA   46       8.866   0.823  -8.891  1.00  0.16      IL13
ATOM   2255  O   ALA   46       7.821   1.431  -9.044  1.00  0.15      IL13
ATOM   2256  N   ALA   47       9.976   1.444  -8.629  1.00  0.17      IL13
ATOM   2257  H   ALA   47      10.808   0.913  -8.517  1.00 20.00      IL13
ATOM   2258  CA  ALA   47       9.980   2.918  -8.513  1.00  0.17      IL13
ATOM   2259  CB  ALA   47      11.300   3.553  -8.069  1.00  0.19      IL13
ATOM   2260  C   ALA   47       9.615   3.540  -9.858  1.00  0.16      IL13
ATOM   2261  O   ALA   47       8.913   4.513  -9.928  1.00  0.16      IL13
ATOM   2262  N   LEU   48      10.104   3.003 -10.931  1.00  0.16      IL13
ATOM   2263  H   LEU   48      10.821   2.307 -10.825  1.00 20.00      IL13
ATOM   2264  CA  LEU   48       9.806   3.621 -12.250  1.00  0.17      IL13
ATOM   2265  CB  LEU   48      10.557   2.856 -13.348  1.00  0.18      IL13
ATOM   2266  CG  LEU   48      10.433   3.424 -14.766  1.00  0.20      IL13
ATOM   2267  CD1 LEU   48      10.910   4.873 -14.860  1.00  0.24      IL13
ATOM   2268  CD2 LEU   48      11.145   2.533 -15.786  1.00  0.23      IL13
ATOM   2269  C   LEU   48       8.293   3.641 -12.505  1.00  0.16      IL13
ATOM   2270  O   LEU   48       7.748   4.657 -12.886  1.00  0.17      IL13
ATOM   2271  N   GLU   49       7.602   2.554 -12.316  1.00  0.15      IL13
ATOM   2272  H   GLU   49       8.063   1.706 -12.047  1.00 20.00      IL13
ATOM   2273  CA  GLU   49       6.132   2.581 -12.578  1.00  0.16      IL13
ATOM   2274  CB  GLU   49       5.507   1.183 -12.415  1.00  0.18      IL13
ATOM   2275  CG  GLU   49       5.579   0.600 -10.999  1.00  0.17      IL13
ATOM   2276  CD  GLU   49       4.985  -0.788 -10.928  1.00  0.55      IL13
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Figure 9 (41/52)

ATOM	2277	OE1	GLU	49	5.720	-1.761	-11.076	1.00	1.32	IL13
ATOM	2278	OE2	GLU	49	3.788	-0.922	-10.692	1.00	1.28	IL13
ATOM	2279	C	GLU	49	5.448	3.616	-11.681	1.00	0.15	IL13
ATOM	2280	O	GLU	49	4.523	4.284	-12.096	1.00	0.17	IL13
ATOM	2281	N	SER	50	5.883	3.771	-10.460	1.00	0.15	IL13
ATOM	2282	H	SER	50	6.637	3.196	-10.144	1.00	20.00	IL13
ATOM	2283	CA	SER	50	5.229	4.781	-9.577	1.00	0.16	IL13
ATOM	2284	CB	SER	50	5.918	4.695	-8.207	1.00	0.18	IL13
ATOM	2285	OG	SER	50	5.002	4.944	-7.128	1.00	1.27	IL13
ATOM	2286	HG	SER	50	5.365	4.459	-6.379	1.00	1.71	IL13
ATOM	2287	C	SER	50	5.423	6.183	-10.175	1.00	0.16	IL13
ATOM	2288	O	SER	50	4.502	6.971	-10.252	1.00	0.17	IL13
ATOM	2289	N	LEU	51	6.613	6.483	-10.619	1.00	0.17	IL13
ATOM	2290	H	LEU	51	7.329	5.775	-10.572	1.00	20.00	IL13
ATOM	2291	CA	LEU	51	6.887	7.816	-11.240	1.00	0.19	IL13
ATOM	2292	CB	LEU	51	8.387	8.083	-11.418	1.00	0.21	IL13
ATOM	2293	CG	LEU	51	9.116	8.590	-10.161	1.00	0.23	IL13
ATOM	2294	CD1	LEU	51	8.340	9.700	-9.450	1.00	0.26	IL13
ATOM	2295	CD2	LEU	51	9.516	7.483	-9.189	1.00	0.21	IL13
ATOM	2296	C	LEU	51	6.136	7.951	-12.572	1.00	0.20	IL13
ATOM	2297	O	LEU	51	5.778	9.040	-12.975	1.00	0.22	IL13
ATOM	2298	N	ILE	52	5.879	6.870	-13.256	1.00	0.20	IL13
ATOM	2299	H	ILE	52	6.194	5.973	-12.951	1.00	20.00	IL13
ATOM	2300	CA	ILE	52	5.139	6.982	-14.550	1.00	0.22	IL13
ATOM	2301	CB	ILE	52	4.971	5.561	-15.151	1.00	0.24	IL13
ATOM	2302	CG2	ILE	52	3.975	5.477	-16.319	1.00	0.26	IL13
ATOM	2303	CG1	ILE	52	6.289	4.909	-15.589	1.00	0.27	IL13
ATOM	2304	CD1	ILE	52	6.723	5.193	-17.030	1.00	0.29	IL13
ATOM	2305	C	ILE	52	3.772	7.620	-14.282	1.00	0.22	IL13
ATOM	2306	O	ILE	52	3.128	8.134	-15.176	1.00	0.25	IL13
ATOM	2307	N	ASN	53	3.319	7.582	-13.059	1.00	0.22	IL13
ATOM	2308	H	ASN	53	3.817	7.015	-12.396	1.00	20.00	IL13
ATOM	2309	CA	ASN	53	1.990	8.174	-12.734	1.00	0.23	IL13
ATOM	2310	CB	ASN	53	1.547	7.663	-11.377	1.00	0.26	IL13
ATOM	2311	CG	ASN	53	0.719	6.416	-11.426	1.00	0.30	IL13
ATOM	2312	OD1	ASN	53	-0.116	6.229	-10.544	1.00	1.09	IL13
ATOM	2313	ND2	ASN	53	0.950	5.580	-12.445	1.00	1.12	IL13
ATOM	2314	HD21	ASN	53	1.785	5.614	-13.008	1.00	1.91	IL13
ATOM	2315	HD22	ASN	53	0.294	4.869	-12.675	1.00	1.14	IL13
ATOM	2316	C	ASN	53	2.131	9.676	-12.463	1.00	0.23	IL13
ATOM	2317	O	ASN	53	1.155	10.397	-12.422	1.00	0.27	IL13
ATOM	2318	N	VAL	54	3.332	10.156	-12.271	1.00	0.20	IL13
ATOM	2319	H	VAL	54	4.144	9.630	-12.486	1.00	20.00	IL13
ATOM	2320	CA	VAL	54	3.510	11.612	-11.996	1.00	0.22	IL13
ATOM	2321	CB	VAL	54	4.673	11.868	-11.036	1.00	0.21	IL13
ATOM	2322	CG1	VAL	54	4.804	13.350	-10.682	1.00	0.25	IL13
ATOM	2323	CG2	VAL	54	4.489	11.049	-9.767	1.00	0.20	IL13
ATOM	2324	C	VAL	54	3.702	12.371	-13.312	1.00	0.27	IL13
ATOM	2325	O	VAL	54	4.665	12.161	-14.023	1.00	0.29	IL13
ATOM	2326	N	SER	55	2.784	13.250	-13.631	1.00	0.34	IL13
ATOM	2327	H	SER	55	2.024	13.432	-13.011	1.00	20.00	IL13
ATOM	2328	CA	SER	55	2.883	14.041	-14.897	1.00	0.42	IL13
ATOM	2329	CB	SER	55	1.621	13.750	-15.705	1.00	0.50	IL13
ATOM	2330	OG	SER	55	1.416	12.325	-15.678	1.00	0.54	IL13
ATOM	2331	HG	SER	55	2.256	11.939	-15.449	1.00	1.04	IL13
ATOM	2332	C	SER	55	3.222	15.502	-14.582	1.00	0.41	IL13
ATOM	2333	O	SER	55	3.334	15.896	-13.437	1.00	0.39	IL13

Figure 9 (42/52)

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ATOM   2334  N   GLY   56       3.364  16.306 -15.599  1.00  0.47      IL13
ATOM   2335  H   GLY   56       3.279  15.967 -16.534  1.00 20.00      IL13
ATOM   2336  CA  GLY   56       3.674  17.753 -15.395  1.00  0.51      IL13
ATOM   2337  C   GLY   56       4.783  17.943 -14.357  1.00  0.44      IL13
ATOM   2338  O   GLY   56       4.653  18.726 -13.438  1.00  0.45      IL13
ATOM   2339  N   CYS   57       5.882  17.260 -14.510  1.00  0.39      IL13
ATOM   2340  H   CYS   57       5.983  16.565 -15.222  1.00 20.00      IL13
ATOM   2341  CA  CYS   57       7.007  17.433 -13.548  1.00  0.35      IL13
ATOM   2342  CB  CYS   57       6.946  16.366 -12.467  1.00  0.34      IL13
ATOM   2343  SG  CYS   57       5.534  16.540 -11.357  1.00  0.32      IL13
ATOM   2344  C   CYS   57       8.328  17.249 -14.297  1.00  0.36      IL13
ATOM   2345  O   CYS   57       8.821  16.149 -14.449  1.00  0.37      IL13
ATOM   2346  N   SER   58       8.895  18.316 -14.786  1.00  0.40      IL13
ATOM   2347  H   SER   58       8.411  19.183 -14.849  1.00 20.00      IL13
ATOM   2348  CA  SER   58      10.172  18.203 -15.546  1.00  0.46      IL13
ATOM   2349  CB  SER   58      10.388  19.457 -16.378  1.00  0.56      IL13
ATOM   2350  OG  SER   58       9.152  19.711 -17.079  1.00  0.61      IL13
ATOM   2351  HG  SER   58       9.410  19.599 -17.999  1.00  1.06      IL13
ATOM   2352  C   SER   58      11.332  17.825 -14.612  1.00  0.45      IL13
ATOM   2353  O   SER   58      12.251  17.127 -14.993  1.00  0.49      IL13
ATOM   2354  N   ALA   59      11.312  18.322 -13.407  1.00  0.43      IL13
ATOM   2355  H   ALA   59      10.553  18.936 -13.226  1.00 20.00      IL13
ATOM   2356  CA  ALA   59      12.425  18.053 -12.440  1.00  0.46      IL13
ATOM   2357  CB  ALA   59      12.076  18.608 -11.059  1.00  0.48      IL13
ATOM   2358  C   ALA   59      12.739  16.553 -12.300  1.00  0.43      IL13
ATOM   2359  O   ALA   59      13.840  16.200 -11.925  1.00  0.57      IL13
ATOM   2360  N   ILE   60      11.794  15.679 -12.565  1.00  0.33      IL13
ATOM   2361  H   ILE   60      10.987  15.973 -13.077  1.00 20.00      IL13
ATOM   2362  CA  ILE   60      12.048  14.203 -12.409  1.00  0.33      IL13
ATOM   2363  CB  ILE   60      11.052  13.554 -11.441  1.00  0.38      IL13
ATOM   2364  CG2 ILE   60      11.268  14.125 -10.035  1.00  0.58      IL13
ATOM   2365  CG1 ILE   60       9.610  13.750 -11.917  1.00  0.53      IL13
ATOM   2366  CD1 ILE   60       8.588  13.070 -11.011  1.00  0.51      IL13
ATOM   2367  C   ILE   60      12.032  13.500 -13.769  1.00  0.31      IL13
ATOM   2368  O   ILE   60      12.216  12.303 -13.860  1.00  0.29      IL13
ATOM   2369  N   GLU   61      11.807  14.221 -14.828  1.00  0.36      IL13
ATOM   2370  H   GLU   61      11.683  15.212 -14.747  1.00 20.00      IL13
ATOM   2371  CA  GLU   61      11.778  13.569 -16.167  1.00  0.40      IL13
ATOM   2372  CB  GLU   61      11.289  14.432 -17.332  1.00  0.50      IL13
ATOM   2373  CG  GLU   61       9.752  14.431 -17.478  1.00  1.31      IL13
ATOM   2374  CD  GLU   61       9.148  13.033 -17.669  1.00  1.91      IL13
ATOM   2375  OE1 GLU   61       9.429  12.357 -18.661  1.00  2.46      IL13
ATOM   2376  OE2 GLU   61       8.355  12.614 -16.827  1.00  2.50      IL13
ATOM   2377  C   GLU   61      13.117  12.888 -16.393  1.00  0.35      IL13
ATOM   2378  O   GLU   61      13.193  11.731 -16.754  1.00  0.36      IL13
ATOM   2379  N   LYS   62      14.176  13.602 -16.163  1.00  0.33      IL13
ATOM   2380  H   LYS   62      14.003  14.566 -15.980  1.00 20.00      IL13
ATOM   2381  CA  LYS   62      15.523  13.019 -16.337  1.00  0.34      IL13
ATOM   2382  CB  LYS   62      16.377  14.066 -15.621  1.00  0.37      IL13
ATOM   2383  CG  LYS   62      16.181  15.561 -15.892  1.00  0.44      IL13
ATOM   2384  CD  LYS   62      16.883  16.438 -14.842  1.00  0.51      IL13
ATOM   2385  CE  LYS   62      18.418  16.464 -14.918  1.00  0.75      IL13
ATOM   2386  NZ  LYS   62      18.868  17.047 -16.194  1.00  1.53      IL13
ATOM   2387  HZ1 LYS   62      19.893  17.013 -16.336  1.00  2.02      IL13
ATOM   2388  HZ2 LYS   62      18.379  16.568 -16.970  1.00  2.09      IL13
ATOM   2389  HZ3 LYS   62      18.531  18.024 -16.370  1.00  2.02      IL13
ATOM   2390  C   LYS   62      15.658  11.823 -15.391  1.00  0.29      IL13
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Figure 9 (43/52)

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ATOM   2391  O   LYS   62      16.216  10.800 -15.740  1.00  0.31      IL13
ATOM   2392  N   THR   63      15.132  11.940 -14.198  1.00  0.25      IL13
ATOM   2393  H   THR   63      14.806  12.839 -13.910  1.00 20.00      IL13
ATOM   2394  CA  THR   63      15.216  10.806 -13.234  1.00  0.23      IL13
ATOM   2395  CB  THR   63      14.659  11.211 -11.879  1.00  0.24      IL13
ATOM   2396  OG1 THR   63      14.791  12.624 -11.657  1.00  0.28      IL13
ATOM   2397  HG1 THR   63      15.714  12.885 -11.771  1.00  0.92      IL13
ATOM   2398  CG2 THR   63      15.311  10.408 -10.752  1.00  0.27      IL13
ATOM   2399  C   THR   63      14.515   9.590 -13.841  1.00  0.22      IL13
ATOM   2400  O   THR   63      14.996   8.482 -13.752  1.00  0.23      IL13
ATOM   2401  N   GLN   64      13.383   9.783 -14.458  1.00  0.23      IL13
ATOM   2402  H   GLN   64      13.044  10.721 -14.599  1.00 20.00      IL13
ATOM   2403  CA  GLN   64      12.665   8.622 -15.048  1.00  0.26      IL13
ATOM   2404  CB  GLN   64      11.411   9.070 -15.789  1.00  0.30      IL13
ATOM   2405  CG  GLN   64      10.094   8.615 -15.161  1.00  0.32      IL13
ATOM   2406  CD  GLN   64       9.012   8.720 -16.216  1.00  0.72      IL13
ATOM   2407  OE1 GLN   64       8.467   7.731 -16.705  1.00  1.45      IL13
ATOM   2408  NE2 GLN   64       8.769   9.957 -16.615  1.00  1.27      IL13
ATOM   2409  HE21 GLN  64       9.195  10.804 -16.287  1.00  1.76      IL13
ATOM   2410  HE22 GLN  64       8.108  10.189 -17.325  1.00  1.60      IL13
ATOM   2411  C   GLN   64      13.583   7.890 -16.013  1.00  0.27      IL13
ATOM   2412  O   GLN   64      13.619   6.675 -16.053  1.00  0.29      IL13
ATOM   2413  N   ARG   65      14.314   8.610 -16.805  1.00  0.28      IL13
ATOM   2414  H   ARG   65      14.269   9.608 -16.684  1.00 20.00      IL13
ATOM   2415  CA  ARG   65      15.209   7.943 -17.781  1.00  0.32      IL13
ATOM   2416  CB  ARG   65      15.570   8.398 -19.305  1.00  0.39      IL13
ATOM   2417  CG  ARG   65      16.637   7.575 -20.242  1.00  1.28      IL13
ATOM   2418  CD  ARG   65      16.563   6.961 -21.771  1.00  1.60      IL13
ATOM   2419  NE  ARG   65      17.353   7.509 -23.013  1.00  2.23      IL13
ATOM   2420  HE  ARG   65      18.228   7.032 -23.111  1.00  2.66      IL13
ATOM   2421  CZ  ARG   65      17.164   8.820 -23.632  1.00  2.84      IL13
ATOM   2422  NH1 ARG   65      18.150  10.103 -24.741  1.00  3.74      IL13
ATOM   2423  HH11 ARG  65      18.097  11.079 -24.477  1.00  4.09      IL13
ATOM   2424  HH12 ARG  65      18.712   9.948 -25.543  1.00  4.29      IL13
ATOM   2425  NH2 ARG   65      16.028   8.973 -22.861  1.00  3.05      IL13
ATOM   2426  HH21 ARG  65      15.257   8.349 -22.829  1.00  2.87      IL13
ATOM   2427  HH22 ARG  65      16.014   9.814 -22.292  1.00  3.75      IL13
ATOM   2428  C   ARG   65      16.373   7.261 -17.056  1.00  0.30      IL13
ATOM   2429  O   ARG   65      16.706   6.127 -17.340  1.00  0.31      IL13
ATOM   2430  N   MET   66      16.996   7.923 -16.118  1.00  0.29      IL13
ATOM   2431  H   MET   66      16.701   8.849 -15.861  1.00 20.00      IL13
ATOM   2432  CA  MET   66      18.120   7.268 -15.397  1.00  0.29      IL13
ATOM   2433  CB  MET   66      18.820   8.252 -14.466  1.00  0.33      IL13
ATOM   2434  CG  MET   66      19.696   9.204 -15.284  1.00  0.38      IL13
ATOM   2435  SD  MET   66      20.555  10.456 -14.318  1.00  0.83      IL13
ATOM   2436  CE  MET   66      19.110  11.353 -13.717  1.00  0.47      IL13
ATOM   2437  C   MET   66      17.579   6.012 -14.712  1.00  0.27      IL13
ATOM   2438  O   MET   66      18.229   4.988 -14.673  1.00  0.28      IL13
ATOM   2439  N   LEU   67      16.373   6.070 -14.210  1.00  0.26      IL13
ATOM   2440  H   LEU   67      15.941   6.966 -14.117  1.00 20.00      IL13
ATOM   2441  CA  LEU   67      15.780   4.859 -13.578  1.00  0.27      IL13
ATOM   2442  CB  LEU   67      14.401   5.145 -12.981  1.00  0.28      IL13
ATOM   2443  CG  LEU   67      14.435   6.013 -11.721  1.00  0.28      IL13
ATOM   2444  CD1 LEU   67      13.026   6.412 -11.281  1.00  0.30      IL13
ATOM   2445  CD2 LEU   67      15.225   5.355 -10.586  1.00  0.29      IL13
ATOM   2446  C   LEU   67      15.676   3.751 -14.633  1.00  0.28      IL13
ATOM   2447  O   LEU   67      15.928   2.593 -14.359  1.00  0.30      IL13
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Figure 9 (44/52)

ATOM	2448	N	SER	68	15.306	4.098	-15.840	1.00	0.30	IL13
ATOM	2449	H	SER	68	15.072	5.065	-15.969	1.00	20.00	IL13
ATOM	2450	CA	SER	68	15.186	3.068	-16.912	1.00	0.33	IL13
ATOM	2451	CB	SER	68	14.845	3.721	-18.239	1.00	0.36	IL13
ATOM	2452	OG	SER	68	13.558	4.335	-18.218	1.00	0.39	IL13
ATOM	2453	HG	SER	68	13.398	4.693	-17.338	1.00	0.89	IL13
ATOM	2454	C	SER	68	16.545	2.397	-17.121	1.00	0.32	IL13
ATOM	2455	O	SER	68	16.638	1.203	-17.321	1.00	0.35	IL13
ATOM	2456	N	GLY	69	17.601	3.162	-17.073	1.00	0.30	IL13
ATOM	2457	H	GLY	69	17.481	4.139	-16.870	1.00	20.00	IL13
ATOM	2458	CA	GLY	69	18.958	2.577	-17.269	1.00	0.31	IL13
ATOM	2459	C	GLY	69	19.144	1.367	-16.348	1.00	0.31	IL13
ATOM	2460	O	GLY	69	19.848	0.433	-16.675	1.00	0.35	IL13
ATOM	2461	N	PHE	70	18.516	1.372	-15.202	1.00	0.29	IL13
ATOM	2462	H	PHE	70	18.058	2.215	-14.910	1.00	20.00	IL13
ATOM	2463	CA	PHE	70	18.658	0.214	-14.270	1.00	0.33	IL13
ATOM	2464	CB	PHE	70	18.663	0.674	-12.811	1.00	0.34	IL13
ATOM	2465	CG	PHE	70	19.779	1.650	-12.514	1.00	0.31	IL13
ATOM	2466	CD1	PHE	70	21.079	1.167	-12.251	1.00	0.35	IL13
ATOM	2467	CD2	PHE	70	19.494	3.033	-12.485	1.00	0.30	IL13
ATOM	2468	CE1	PHE	70	22.108	2.079	-11.944	1.00	0.37	IL13
ATOM	2469	CE2	PHE	70	20.521	3.946	-12.181	1.00	0.32	IL13
ATOM	2470	CZ	PHE	70	21.817	3.459	-11.907	1.00	0.34	IL13
ATOM	2471	C	PHE	70	17.499	-0.752	-14.495	1.00	0.38	IL13
ATOM	2472	O	PHE	70	17.460	-1.837	-13.950	1.00	0.49	IL13
ATOM	2473	N	CYS	71	16.542	-0.339	-15.274	1.00	0.36	IL13
ATOM	2474	H	CYS	71	16.498	0.628	-15.503	1.00	20.00	IL13
ATOM	2475	CA	CYS	71	15.348	-1.187	-15.533	1.00	0.44	IL13
ATOM	2476	CB	CYS	71	14.188	-0.695	-14.660	1.00	0.62	IL13
ATOM	2477	SG	CYS	71	12.553	-1.247	-15.227	1.00	1.27	IL13
ATOM	2478	C	CYS	71	14.984	-1.085	-17.031	1.00	0.45	IL13
ATOM	2479	O	CYS	71	14.116	-0.323	-17.406	1.00	0.54	IL13
ATOM	2480	N	PRO	72	15.682	-1.805	-17.888	1.00	0.54	IL13
ATOM	2481	CD	PRO	72	16.765	-2.721	-17.552	1.00	0.60	IL13
ATOM	2482	CA	PRO	72	15.450	-1.727	-19.367	1.00	0.73	IL13
ATOM	2483	CB	PRO	72	16.573	-2.612	-19.927	1.00	1.03	IL13
ATOM	2484	CG	PRO	72	17.614	-2.736	-18.815	1.00	0.85	IL13
ATOM	2485	C	PRO	72	14.064	-2.158	-19.898	1.00	0.75	IL13
ATOM	2486	O	PRO	72	13.861	-2.107	-21.096	1.00	0.98	IL13
ATOM	2487	N	HIS	73	13.106	-2.554	-19.075	1.00	0.73	IL13
ATOM	2488	H	HIS	73	13.189	-2.496	-18.078	1.00	20.00	IL13
ATOM	2489	CA	HIS	73	11.766	-2.936	-19.660	1.00	0.93	IL13
ATOM	2490	CB	HIS	73	11.127	-4.160	-18.981	1.00	1.33	IL13
ATOM	2491	CG	HIS	73	10.483	-3.837	-17.650	1.00	0.81	IL13
ATOM	2492	ND1	HIS	73	9.209	-3.410	-17.516	1.00	0.78	IL13
ATOM	2493	HD1	HIS	73	8.545	-3.279	-18.224	1.00	1.13	IL13
ATOM	2494	CD2	HIS	73	11.059	-3.938	-16.382	1.00	1.29	IL13
ATOM	2495	NE2	HIS	73	10.107	-3.565	-15.493	1.00	1.64	IL13
ATOM	2496	CE1	HIS	73	8.970	-3.244	-16.177	1.00	1.12	IL13
ATOM	2497	C	HIS	73	10.858	-1.711	-19.659	1.00	0.73	IL13
ATOM	2498	O	HIS	73	10.866	-0.904	-18.750	1.00	0.80	IL13
ATOM	2499	N	LYS	74	10.110	-1.554	-20.708	1.00	0.77	IL13
ATOM	2500	H	LYS	74	10.050	-2.325	-21.339	1.00	20.00	IL13
ATOM	2501	CA	LYS	74	9.220	-0.374	-20.850	1.00	0.80	IL13
ATOM	2502	CB	LYS	74	8.848	-0.103	-22.305	1.00	1.16	IL13
ATOM	2503	CG	LYS	74	10.025	0.269	-23.203	1.00	1.46	IL13
ATOM	2504	CD	LYS	74	9.515	0.703	-24.576	1.00	2.02	IL13

Figure 9 (45/52)

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ATOM   2505  CE  LYS    74      10.627   1.032 -25.570  1.00  2.44      IL13
ATOM   2506  NZ  LYS    74      10.006   1.494 -26.818  1.00  2.84      IL13
ATOM   2507  HZ1 LYS    74      10.691   1.437 -27.604  1.00  3.17      IL13
ATOM   2508  HZ2 LYS    74       9.709   2.486 -26.710  1.00  3.06      IL13
ATOM   2509  HZ3 LYS    74       9.169   0.892 -26.976  1.00  3.27      IL13
ATOM   2510  C   LYS    74       7.940  -0.541 -20.036  1.00  0.59      IL13
ATOM   2511  O   LYS    74       7.283  -1.561 -20.093  1.00  0.71      IL13
ATOM   2512  N   VAL    75       7.587   0.476 -19.291  1.00  0.56      IL13
ATOM   2513  H   VAL    75       8.132   1.314 -19.247  1.00 20.00      IL13
ATOM   2514  CA  VAL    75       6.348   0.430 -18.466  1.00  0.40      IL13
ATOM   2515  CB  VAL    75       6.647   0.831 -17.012  1.00  0.54      IL13
ATOM   2516  CG1 VAL    75       5.429   0.605 -16.114  1.00  1.14      IL13
ATOM   2517  CG2 VAL    75       7.893   0.141 -16.457  1.00  0.90      IL13
ATOM   2518  C   VAL    75       5.332   1.408 -19.053  1.00  0.40      IL13
ATOM   2519  O   VAL    75       5.631   2.562 -19.291  1.00  0.53      IL13
ATOM   2520  N   SER    76       4.130   0.953 -19.266  1.00  0.39      IL13
ATOM   2521  H   SER    76       3.868   0.147 -18.737  1.00 20.00      IL13
ATOM   2522  CA  SER    76       3.077   1.846 -19.816  1.00  0.45      IL13
ATOM   2523  CB  SER    76       2.250   1.085 -20.844  1.00  0.57      IL13
ATOM   2524  OG  SER    76       1.448   2.006 -21.581  1.00  1.46      IL13
ATOM   2525  HG  SER    76       2.029   2.765 -21.662  1.00  1.93      IL13
ATOM   2526  C   SER    76       2.211   2.343 -18.668  1.00  0.41      IL13
ATOM   2527  O   SER    76       2.066   1.686 -17.656  1.00  0.41      IL13
ATOM   2528  N   ALA    77       1.629   3.492 -18.813  1.00  0.41      IL13
ATOM   2529  H   ALA    77       1.879   4.068 -19.588  1.00 20.00      IL13
ATOM   2530  CA  ALA    77       0.767   4.022 -17.730  1.00  0.41      IL13
ATOM   2531  CB  ALA    77       0.236   5.410 -18.091  1.00  0.46      IL13
ATOM   2532  C   ALA    77      -0.410   3.073 -17.519  1.00  0.42      IL13
ATOM   2533  O   ALA    77      -1.171   3.213 -16.584  1.00  0.46      IL13
ATOM   2534  N   GLY    78      -0.559   2.109 -18.387  1.00  0.46      IL13
ATOM   2535  H   GLY    78       0.050   1.989 -19.157  1.00 20.00      IL13
ATOM   2536  CA  GLY    78      -1.681   1.137 -18.255  1.00  0.52      IL13
ATOM   2537  C   GLY    78      -1.159  -0.166 -17.650  1.00  0.54      IL13
ATOM   2538  O   GLY    78      -1.854  -0.836 -16.912  1.00  0.62      IL13
ATOM   2539  N   GLN    79       0.057  -0.534 -17.960  1.00  0.53      IL13
ATOM   2540  H   GLN    79       0.676   0.198 -18.236  1.00 20.00      IL13
ATOM   2541  CA  GLN    79       0.614  -1.800 -17.406  1.00  0.58      IL13
ATOM   2542  CB  GLN    79       1.485  -2.478 -18.467  1.00  0.72      IL13
ATOM   2543  CG  GLN    79       0.710  -2.753 -19.766  1.00  0.86      IL13
ATOM   2544  CD  GLN    79       1.557  -3.521 -20.768  1.00  1.67      IL13
ATOM   2545  OE1 GLN    79       1.671  -3.174 -21.941  1.00  2.17      IL13
ATOM   2546  NE2 GLN    79       2.126  -4.622 -20.256  1.00  2.42      IL13
ATOM   2547 HE21 GLN    79       2.003  -4.904 -19.304  1.00  2.56      IL13
ATOM   2548 HE22 GLN    79       2.646  -5.204 -20.879  1.00  3.09      IL13
ATOM   2549  C   GLN    79       1.405  -1.515 -16.130  1.00  0.46      IL13
ATOM   2550  O   GLN    79       2.407  -0.827 -16.146  1.00  0.47      IL13
ATOM   2551  N   PHE    80       0.949  -2.054 -15.029  1.00  0.46      IL13
ATOM   2552  H   PHE    80       0.175  -2.677 -15.099  1.00 20.00      IL13
ATOM   2553  CA  PHE    80       1.640  -1.854 -13.722  1.00  0.38      IL13
ATOM   2554  CB  PHE    80       0.713  -1.227 -12.682  1.00  0.39      IL13
ATOM   2555  CG  PHE    80       0.411   0.199 -13.072  1.00  0.38      IL13
ATOM   2556  CD1 PHE    80      -0.924   0.566 -13.341  1.00  0.43      IL13
ATOM   2557  CD2 PHE    80       1.466   1.136 -13.161  1.00  0.36      IL13
ATOM   2558  CE1 PHE    80      -1.212   1.893 -13.708  1.00  0.44      IL13
ATOM   2559  CE2 PHE    80       1.180   2.462 -13.532  1.00  0.38      IL13
ATOM   2560  CZ  PHE    80      -0.157   2.824 -13.800  1.00  0.41      IL13
ATOM   2561  C   PHE    80       2.174  -3.201 -13.223  1.00  0.40      IL13
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Figure 9 (46/52)

ATOM	2562	O	PHE	80	1.680	-4.240	-13.615	1.00	0.46	IL13
ATOM	2563	N	SER	81	3.187	-3.190	-12.377	1.00	0.38	IL13
ATOM	2564	H	SER	81	3.624	-2.316	-12.143	1.00	20.00	IL13
ATOM	2565	CA	SER	81	3.770	-4.476	-11.866	1.00	0.42	IL13
ATOM	2566	CB	SER	81	5.169	-4.692	-12.438	1.00	0.48	IL13
ATOM	2567	OG	SER	81	5.052	-4.777	-13.864	1.00	0.57	IL13
ATOM	2568	HG	SER	81	4.994	-3.870	-14.155	1.00	1.04	IL13
ATOM	2569	C	SER	81	3.697	-4.573	-10.331	1.00	0.41	IL13
ATOM	2570	O	SER	81	3.370	-5.618	-9.804	1.00	0.48	IL13
ATOM	2571	N	SER	82	4.029	-3.524	-9.607	1.00	0.39	IL13
ATOM	2572	H	SER	82	4.291	-2.661	-10.046	1.00	20.00	IL13
ATOM	2573	CA	SER	82	4.007	-3.608	-8.103	1.00	0.40	IL13
ATOM	2574	CB	SER	82	5.309	-2.950	-7.610	1.00	0.47	IL13
ATOM	2575	OG	SER	82	5.431	-2.984	-6.184	1.00	0.57	IL13
ATOM	2576	HG	SER	82	6.311	-3.301	-6.008	1.00	1.11	IL13
ATOM	2577	C	SER	82	2.759	-2.944	-7.514	1.00	0.36	IL13
ATOM	2578	O	SER	82	2.557	-2.967	-6.317	1.00	0.38	IL13
ATOM	2579	N	LEU	83	1.923	-2.349	-8.315	1.00	0.35	IL13
ATOM	2580	H	LEU	83	2.176	-2.208	-9.280	1.00	20.00	IL13
ATOM	2581	CA	LEU	83	0.714	-1.692	-7.740	1.00	0.35	IL13
ATOM	2582	CB	LEU	83	0.241	-0.581	-8.682	1.00	0.39	IL13
ATOM	2583	CG	LEU	83	0.794	0.830	-8.449	1.00	0.53	IL13
ATOM	2584	CD1	LEU	83	2.318	0.914	-8.329	1.00	1.29	IL13
ATOM	2585	CD2	LEU	83	0.270	1.774	-9.531	1.00	1.01	IL13
ATOM	2586	C	LEU	83	-0.399	-2.730	-7.579	1.00	0.37	IL13
ATOM	2587	O	LEU	83	-1.569	-2.404	-7.598	1.00	0.41	IL13
ATOM	2588	N	HIS	84	-0.047	-3.976	-7.408	1.00	0.40	IL13
ATOM	2589	H	HIS	84	0.909	-4.196	-7.223	1.00	20.00	IL13
ATOM	2590	CA	HIS	84	-1.094	-5.019	-7.228	1.00	0.45	IL13
ATOM	2591	CB	HIS	84	-0.482	-6.407	-7.432	1.00	0.55	IL13
ATOM	2592	CG	HIS	84	-0.492	-6.779	-8.898	1.00	0.57	IL13
ATOM	2593	ND1	HIS	84	0.559	-6.663	-9.736	1.00	0.45	IL13
ATOM	2594	HD1	HIS	84	1.465	-6.341	-9.535	1.00	0.61	IL13
ATOM	2595	CD2	HIS	84	-1.569	-7.321	-9.605	1.00	0.90	IL13
ATOM	2596	NE2	HIS	84	-1.159	-7.535	-10.879	1.00	0.79	IL13
ATOM	2597	CE1	HIS	84	0.150	-7.125	-10.958	1.00	0.48	IL13
ATOM	2598	C	HIS	84	-1.668	-4.868	-5.819	1.00	0.42	IL13
ATOM	2599	O	HIS	84	-2.866	-4.885	-5.617	1.00	0.44	IL13
ATOM	2600	N	VAL	85	-0.813	-4.671	-4.853	1.00	0.42	IL13
ATOM	2601	H	VAL	85	0.151	-4.558	-5.091	1.00	20.00	IL13
ATOM	2602	CA	VAL	85	-1.288	-4.460	-3.454	1.00	0.43	IL13
ATOM	2603	CB	VAL	85	-0.188	-4.810	-2.445	1.00	0.50	IL13
ATOM	2604	CG1	VAL	85	-0.085	-6.329	-2.304	1.00	1.31	IL13
ATOM	2605	CG2	VAL	85	1.166	-4.192	-2.809	1.00	1.32	IL13
ATOM	2606	C	VAL	85	-1.751	-3.021	-3.344	1.00	0.38	IL13
ATOM	2607	O	VAL	85	-1.233	-2.151	-4.017	1.00	0.36	IL13
ATOM	2608	N	ARG	86	-2.712	-2.756	-2.506	1.00	0.41	IL13
ATOM	2609	H	ARG	86	-2.929	-3.429	-1.806	1.00	20.00	IL13
ATOM	2610	CA	ARG	86	-3.185	-1.360	-2.371	1.00	0.41	IL13
ATOM	2611	CB	ARG	86	-4.700	-1.291	-2.182	1.00	0.54	IL13
ATOM	2612	CG	ARG	86	-5.511	-1.491	-3.469	1.00	0.61	IL13
ATOM	2613	CD	ARG	86	-6.158	-2.871	-3.634	1.00	1.34	IL13
ATOM	2614	NE	ARG	86	-5.223	-3.918	-4.048	1.00	2.05	IL13
ATOM	2615	HE	ARG	86	-4.645	-3.768	-4.863	1.00	2.39	IL13
ATOM	2616	CZ	ARG	86	-5.286	-5.141	-3.482	1.00	2.79	IL13
ATOM	2617	NH1	ARG	86	-4.628	-6.140	-4.062	1.00	3.68	IL13
ATOM	2618	HH11	ARG	86	-4.082	-5.940	-4.890	1.00	3.91	IL13

Figure 9 (47/52)

ATOM	2619	HH12	ARG	86	-4.654	-7.081	-3.728	1.00	4.31	IL13
ATOM	2620	NH2	ARG	86	-5.983	-5.338	-2.361	1.00	3.06	IL13
ATOM	2621	HH21	ARG	86	-6.472	-4.572	-1.941	1.00	2.79	IL13
ATOM	2622	HH22	ARG	86	-6.026	-6.231	-1.912	1.00	3.81	IL13
ATOM	2623	C	ARG	86	-2.454	-0.699	-1.218	1.00	0.39	IL13
ATOM	2624	O	ARG	86	-2.865	-0.751	-0.076	1.00	0.47	IL13
ATOM	2625	N	ASP	87	-1.374	-0.062	-1.536	1.00	0.33	IL13
ATOM	2626	H	ASP	87	-1.034	-0.109	-2.474	1.00	20.00	IL13
ATOM	2627	CA	ASP	87	-0.583	0.645	-0.505	1.00	0.36	IL13
ATOM	2628	CB	ASP	87	0.913	0.474	-0.709	1.00	0.39	IL13
ATOM	2629	CG	ASP	87	1.214	-0.865	-0.081	1.00	0.46	IL13
ATOM	2630	OD1	ASP	87	0.962	-1.019	1.114	1.00	1.12	IL13
ATOM	2631	OD2	ASP	87	1.651	-1.762	-0.792	1.00	1.24	IL13
ATOM	2632	C	ASP	87	-1.078	2.084	-0.424	1.00	0.33	IL13
ATOM	2633	O	ASP	87	-1.919	2.502	-1.196	1.00	0.32	IL13
ATOM	2634	N	THR	88	-0.565	2.845	0.493	1.00	0.35	IL13
ATOM	2635	H	THR	88	0.258	2.505	0.955	1.00	20.00	IL13
ATOM	2636	CA	THR	88	-1.005	4.260	0.616	1.00	0.34	IL13
ATOM	2637	CB	THR	88	-1.131	4.643	2.103	1.00	0.40	IL13
ATOM	2638	OG1	THR	88	-2.095	3.782	2.741	1.00	1.37	IL13
ATOM	2639	HG1	THR	88	-1.850	2.890	2.528	1.00	1.79	IL13
ATOM	2640	CG2	THR	88	-1.521	6.107	2.341	1.00	1.45	IL13
ATOM	2641	C	THR	88	-0.039	5.137	-0.180	1.00	0.28	IL13
ATOM	2642	O	THR	88	1.138	4.851	-0.260	1.00	0.29	IL13
ATOM	2643	N	LYS	89	-0.511	6.197	-0.776	1.00	0.27	IL13
ATOM	2644	H	LYS	89	-1.444	6.490	-0.585	1.00	20.00	IL13
ATOM	2645	CA	LYS	89	0.425	7.050	-1.558	1.00	0.24	IL13
ATOM	2646	CB	LYS	89	-0.321	7.772	-2.681	1.00	0.31	IL13
ATOM	2647	CG	LYS	89	-0.814	6.769	-3.726	1.00	0.40	IL13
ATOM	2648	CD	LYS	89	-1.605	7.380	-4.886	1.00	0.53	IL13
ATOM	2649	CE	LYS	89	-0.810	8.346	-5.768	1.00	0.80	IL13
ATOM	2650	NZ	LYS	89	0.285	7.670	-6.487	1.00	1.41	IL13
ATOM	2651	HZ1	LYS	89	0.825	7.075	-5.833	1.00	1.98	IL13
ATOM	2652	HZ2	LYS	89	0.932	8.386	-6.891	1.00	1.89	IL13
ATOM	2653	HZ3	LYS	89	-0.085	7.054	-7.239	1.00	1.77	IL13
ATOM	2654	C	LYS	89	1.147	8.003	-0.611	1.00	0.23	IL13
ATOM	2655	O	LYS	89	0.654	8.328	0.452	1.00	0.25	IL13
ATOM	2656	N	ILE	90	2.311	8.451	-1.002	1.00	0.20	IL13
ATOM	2657	H	ILE	90	2.725	8.096	-1.829	1.00	20.00	IL13
ATOM	2658	CA	ILE	90	3.094	9.395	-0.154	1.00	0.21	IL13
ATOM	2659	CB	ILE	90	4.304	8.703	0.498	1.00	0.22	IL13
ATOM	2660	CG2	ILE	90	3.836	7.694	1.553	1.00	0.25	IL13
ATOM	2661	CG1	ILE	90	5.218	8.036	-0.540	1.00	0.24	IL13
ATOM	2662	CD1	ILE	90	6.514	7.495	0.066	1.00	0.25	IL13
ATOM	2663	C	ILE	90	3.572	10.563	-1.020	1.00	0.20	IL13
ATOM	2664	O	ILE	90	3.599	10.478	-2.232	1.00	0.19	IL13
ATOM	2665	N	GLU	91	3.936	11.652	-0.411	1.00	0.21	IL13
ATOM	2666	H	GLU	91	4.047	11.613	0.585	1.00	20.00	IL13
ATOM	2667	CA	GLU	91	4.397	12.828	-1.199	1.00	0.21	IL13
ATOM	2668	CB	GLU	91	4.647	14.001	-0.307	1.00	0.25	IL13
ATOM	2669	CG	GLU	91	3.334	14.527	0.227	1.00	0.32	IL13
ATOM	2670	CD	GLU	91	3.705	15.819	0.869	1.00	0.96	IL13
ATOM	2671	OE1	GLU	91	4.048	16.739	0.135	1.00	1.66	IL13
ATOM	2672	OE2	GLU	91	3.689	15.883	2.088	1.00	1.69	IL13
ATOM	2673	C	GLU	91	5.701	12.489	-1.927	1.00	0.19	IL13
ATOM	2674	O	GLU	91	6.542	11.775	-1.416	1.00	0.20	IL13
ATOM	2675	N	VAL	92	5.869	12.988	-3.124	1.00	0.19	IL13

Figure 9 (48/52)

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ATOM   2676  H   VAL   92       5.054  13.386  -3.539  1.00 20.00      IL13
ATOM   2677  CA  VAL   92       7.112  12.685  -3.894  1.00  0.18      IL13
ATOM   2678  CB  VAL   92       7.088  13.361  -5.278  1.00  0.20      IL13
ATOM   2679  CG1 VAL   92       8.397  13.189  -6.057  1.00  0.22      IL13
ATOM   2680  CG2 VAL   92       5.920  12.828  -6.110  1.00  0.22      IL13
ATOM   2681  C   VAL   92       8.345  13.091  -3.080  1.00  0.18      IL13
ATOM   2682  O   VAL   92       9.327  12.377  -3.030  1.00  0.19      IL13
ATOM   2683  N   ALA   93       8.305  14.230  -2.447  1.00  0.19      IL13
ATOM   2684  H   ALA   93       7.443  14.732  -2.424  1.00 20.00      IL13
ATOM   2685  CA  ALA   93       9.479  14.679  -1.644  1.00  0.20      IL13
ATOM   2686  CB  ALA   93       9.118  15.900  -0.797  1.00  0.24      IL13
ATOM   2687  C   ALA   93       9.952  13.542  -0.728  1.00  0.18      IL13
ATOM   2688  O   ALA   93      11.135  13.312  -0.569  1.00  0.18      IL13
ATOM   2689  N   GLN   94       9.038  12.825  -0.132  1.00  0.18      IL13
ATOM   2690  H   GLN   94       8.065  12.958  -0.320  1.00 20.00      IL13
ATOM   2691  CA  GLN   94       9.435  11.700   0.769  1.00  0.18      IL13
ATOM   2692  CB  GLN   94       8.272  11.310   1.672  1.00  0.23      IL13
ATOM   2693  CG  GLN   94       7.713  12.463   2.510  1.00  1.06      IL13
ATOM   2694  CD  GLN   94       6.564  11.909   3.319  1.00  1.45      IL13
ATOM   2695  OE1 GLN   94       5.778  11.108   2.828  1.00  1.85      IL13
ATOM   2696  NE2 GLN   94       6.560  12.282   4.603  1.00  2.09      IL13
ATOM   2697 HE21 GLN   94       7.127  13.049   4.911  1.00  2.44      IL13
ATOM   2698 HE22 GLN   94       5.997  11.765   5.247  1.00  2.51      IL13
ATOM   2699  C   GLN   94       9.883  10.508  -0.060  1.00  0.16      IL13
ATOM   2700  O   GLN   94      10.806   9.799   0.288  1.00  0.15      IL13
ATOM   2701  N   PHE   95       9.220  10.272  -1.145  1.00  0.16      IL13
ATOM   2702  H   PHE   95       8.484  10.901  -1.411  1.00 20.00      IL13
ATOM   2703  CA  PHE   95       9.576   9.115  -1.994  1.00  0.15      IL13
ATOM   2704  CB  PHE   95       8.645   9.025  -3.199  1.00  0.16      IL13
ATOM   2705  CG  PHE   95       8.755   7.680  -3.885  1.00  0.16      IL13
ATOM   2706  CD1 PHE   95       7.986   6.596  -3.407  1.00  0.17      IL13
ATOM   2707  CD2 PHE   95       9.615   7.532  -4.995  1.00  0.18      IL13
ATOM   2708  CE1 PHE   95       8.070   5.348  -4.054  1.00  0.18      IL13
ATOM   2709  CE2 PHE   95       9.702   6.284  -5.641  1.00  0.20      IL13
ATOM   2710  CZ  PHE   95       8.925   5.206  -5.167  1.00  0.18      IL13
ATOM   2711  C   PHE   95      11.034   9.236  -2.431  1.00  0.13      IL13
ATOM   2712  O   PHE   95      11.798   8.294  -2.346  1.00  0.14      IL13
ATOM   2713  N   VAL   96      11.429  10.388  -2.895  1.00  0.14      IL13
ATOM   2714  H   VAL   96      10.758  11.135  -2.862  1.00 20.00      IL13
ATOM   2715  CA  VAL   96      12.841  10.566  -3.332  1.00  0.14      IL13
ATOM   2716  CB  VAL   96      12.996  11.969  -3.935  1.00  0.16      IL13
ATOM   2717  CG1 VAL   96      14.455  12.342  -4.202  1.00  0.19      IL13
ATOM   2718  CG2 VAL   96      12.133  12.111  -5.191  1.00  0.19      IL13
ATOM   2719  C   VAL   96      13.769  10.379  -2.130  1.00  0.13      IL13
ATOM   2720  O   VAL   96      14.767   9.691  -2.212  1.00  0.15      IL13
ATOM   2721  N   LYS   97      13.462  10.989  -1.016  1.00  0.13      IL13
ATOM   2722  H   LYS   97      12.566  11.418  -0.897  1.00 20.00      IL13
ATOM   2723  CA  LYS   97      14.353  10.834   0.166  1.00  0.14      IL13
ATOM   2724  CB  LYS   97      13.900  11.814   1.254  1.00  0.18      IL13
ATOM   2725  CG  LYS   97      14.084  13.249   0.729  1.00  0.22      IL13
ATOM   2726  CD  LYS   97      13.328  14.340   1.502  1.00  0.34      IL13
ATOM   2727  CE  LYS   97      13.406  15.734   0.851  1.00  0.60      IL13
ATOM   2728  NZ  LYS   97      12.952  15.688  -0.545  1.00  1.65      IL13
ATOM   2729  HZ1 LYS   97      12.044  15.188  -0.621  1.00  2.19      IL13
ATOM   2730  HZ2 LYS   97      13.679  15.171  -1.066  1.00  2.21      IL13
ATOM   2731  HZ3 LYS   97      12.867  16.650  -0.938  1.00  2.14      IL13
ATOM   2732  C   LYS   97      14.443   9.362   0.569  1.00  0.14      IL13
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Figure 9 (49/52)

ATOM	2733	O	LYS	97	15.513	8.841	0.788	1.00	0.14	IL13
ATOM	2734	N	ASP	98	13.338	8.679	0.655	1.00	0.14	IL13
ATOM	2735	H	ASP	98	12.461	9.057	0.370	1.00	20.00	IL13
ATOM	2736	CA	ASP	98	13.402	7.248	1.053	1.00	0.16	IL13
ATOM	2737	CB	ASP	98	12.099	6.525	1.379	1.00	0.17	IL13
ATOM	2738	CG	ASP	98	12.562	5.270	2.105	1.00	0.19	IL13
ATOM	2739	OD1	ASP	98	12.780	5.325	3.313	1.00	1.11	IL13
ATOM	2740	OD2	ASP	98	12.782	4.260	1.445	1.00	1.07	IL13
ATOM	2741	C	ASP	98	14.251	6.485	0.037	1.00	0.16	IL13
ATOM	2742	O	ASP	98	15.042	5.632	0.388	1.00	0.17	IL13
ATOM	2743	N	LEU	99	14.102	6.794	-1.216	1.00	0.15	IL13
ATOM	2744	H	LEU	99	13.416	7.496	-1.437	1.00	20.00	IL13
ATOM	2745	CA	LEU	99	14.900	6.101	-2.264	1.00	0.16	IL13
ATOM	2746	CB	LEU	99	14.379	6.501	-3.649	1.00	0.17	IL13
ATOM	2747	CG	LEU	99	15.038	5.791	-4.836	1.00	0.19	IL13
ATOM	2748	CD1	LEU	99	14.857	4.273	-4.788	1.00	0.24	IL13
ATOM	2749	CD2	LEU	99	14.569	6.378	-6.169	1.00	0.23	IL13
ATOM	2750	C	LEU	99	16.393	6.454	-2.090	1.00	0.15	IL13
ATOM	2751	O	LEU	99	17.257	5.630	-2.307	1.00	0.16	IL13
ATOM	2752	N	LEU	100	16.701	7.667	-1.697	1.00	0.15	IL13
ATOM	2753	H	LEU	100	15.942	8.318	-1.635	1.00	20.00	IL13
ATOM	2754	CA	LEU	100	18.137	8.068	-1.512	1.00	0.15	IL13
ATOM	2755	CB	LEU	100	18.169	9.521	-1.053	1.00	0.15	IL13
ATOM	2756	CG	LEU	100	19.501	10.216	-1.290	1.00	0.19	IL13
ATOM	2757	CD1	LEU	100	19.864	10.245	-2.778	1.00	0.28	IL13
ATOM	2758	CD2	LEU	100	19.508	11.601	-0.646	1.00	0.19	IL13
ATOM	2759	C	LEU	100	18.828	7.134	-0.505	1.00	0.16	IL13
ATOM	2760	O	LEU	100	19.941	6.693	-0.728	1.00	0.18	IL13
ATOM	2761	N	LEU	101	18.197	6.834	0.601	1.00	0.16	IL13
ATOM	2762	H	LEU	101	17.242	7.138	0.722	1.00	20.00	IL13
ATOM	2763	CA	LEU	101	18.865	5.942	1.601	1.00	0.17	IL13
ATOM	2764	CB	LEU	101	18.007	5.756	2.858	1.00	0.20	IL13
ATOM	2765	CG	LEU	101	18.064	6.905	3.877	1.00	0.22	IL13
ATOM	2766	CD1	LEU	101	19.506	7.262	4.246	1.00	0.32	IL13
ATOM	2767	CD2	LEU	101	17.246	8.132	3.470	1.00	0.29	IL13
ATOM	2768	C	LEU	101	19.170	4.587	0.964	1.00	0.18	IL13
ATOM	2769	O	LEU	101	20.232	4.030	1.154	1.00	0.20	IL13
ATOM	2770	N	HIS	102	18.260	4.051	0.210	1.00	0.16	IL13
ATOM	2771	H	HIS	102	17.372	4.496	0.055	1.00	20.00	IL13
ATOM	2772	CA	HIS	102	18.518	2.734	-0.426	1.00	0.18	IL13
ATOM	2773	CB	HIS	102	17.269	1.884	-0.697	1.00	0.18	IL13
ATOM	2774	CG	HIS	102	17.347	0.704	0.261	1.00	0.19	IL13
ATOM	2775	ND1	HIS	102	16.467	-0.310	0.343	1.00	0.21	IL13
ATOM	2776	HD1	HIS	102	15.614	-0.427	-0.141	1.00	0.22	IL13
ATOM	2777	CD2	HIS	102	18.349	0.447	1.199	1.00	0.20	IL13
ATOM	2778	NE2	HIS	102	18.077	-0.722	1.826	1.00	0.22	IL13
ATOM	2779	CE1	HIS	102	16.899	-1.187	1.305	1.00	0.22	IL13
ATOM	2780	C	HIS	102	19.580	2.846	-1.527	1.00	0.18	IL13
ATOM	2781	O	HIS	102	20.396	1.975	-1.680	1.00	0.21	IL13
ATOM	2782	N	LEU	103	19.571	3.881	-2.320	1.00	0.17	IL13
ATOM	2783	H	LEU	103	18.837	4.559	-2.282	1.00	20.00	IL13
ATOM	2784	CA	LEU	103	20.586	3.956	-3.422	1.00	0.18	IL13
ATOM	2785	CB	LEU	103	20.407	5.236	-4.240	1.00	0.17	IL13
ATOM	2786	CG	LEU	103	19.058	5.361	-4.945	1.00	0.18	IL13
ATOM	2787	CD1	LEU	103	18.891	6.745	-5.571	1.00	0.18	IL13
ATOM	2788	CD2	LEU	103	18.815	4.235	-5.951	1.00	0.20	IL13
ATOM	2789	C	LEU	103	22.015	3.905	-2.870	1.00	0.20	IL13

Figure 9 (50/52)

ATOM	2790	O	LEU	103	22.800	3.064	-3.262	1.00	0.22	IL13
ATOM	2791	N	LYS	104	22.379	4.796	-1.989	1.00	0.20	IL13
ATOM	2792	H	LYS	104	21.653	5.410	-1.687	1.00	20.00	IL13
ATOM	2793	CA	LYS	104	23.778	4.773	-1.465	1.00	0.23	IL13
ATOM	2794	CB	LYS	104	24.063	5.922	-0.519	1.00	0.27	IL13
ATOM	2795	CG	LYS	104	24.543	7.201	-1.186	1.00	0.32	IL13
ATOM	2796	CD	LYS	104	24.358	8.420	-0.285	1.00	0.39	IL13
ATOM	2797	CE	LYS	104	22.922	8.959	-0.286	1.00	1.13	IL13
ATOM	2798	NZ	LYS	104	21.952	7.948	0.152	1.00	1.86	IL13
ATOM	2799	HZ1	LYS	104	21.735	7.243	-0.584	1.00	2.28	IL13
ATOM	2800	HZ2	LYS	104	21.052	8.399	0.385	1.00	2.28	IL13
ATOM	2801	HZ3	LYS	104	22.351	7.438	0.961	1.00	2.38	IL13
ATOM	2802	C	LYS	104	24.027	3.505	-0.643	1.00	0.22	IL13
ATOM	2803	O	LYS	104	25.156	3.104	-0.435	1.00	0.24	IL13
ATOM	2804	N	LYS	105	22.989	2.868	-0.177	1.00	0.23	IL13
ATOM	2805	H	LYS	105	22.069	3.146	-0.456	1.00	20.00	IL13
ATOM	2806	CA	LYS	105	23.177	1.625	0.629	1.00	0.26	IL13
ATOM	2807	CB	LYS	105	21.800	1.177	1.140	1.00	0.31	IL13
ATOM	2808	CG	LYS	105	21.604	0.012	2.130	1.00	0.47	IL13
ATOM	2809	CD	LYS	105	21.940	-1.421	1.687	1.00	0.55	IL13
ATOM	2810	CE	LYS	105	21.483	-1.852	0.286	1.00	0.96	IL13
ATOM	2811	NZ	LYS	105	20.038	-2.023	0.141	1.00	1.85	IL13
ATOM	2812	HZ1	LYS	105	19.546	-1.392	0.799	1.00	2.40	IL13
ATOM	2813	HZ2	LYS	105	19.789	-3.006	0.364	1.00	2.38	IL13
ATOM	2814	HZ3	LYS	105	19.773	-1.782	-0.839	1.00	2.20	IL13
ATOM	2815	C	LYS	105	23.812	0.534	-0.247	1.00	0.25	IL13
ATOM	2816	O	LYS	105	24.749	-0.128	0.154	1.00	0.28	IL13
ATOM	2817	N	LEU	106	23.305	0.341	-1.437	1.00	0.23	IL13
ATOM	2818	H	LEU	106	22.614	0.984	-1.781	1.00	20.00	IL13
ATOM	2819	CA	LEU	106	23.873	-0.713	-2.335	1.00	0.25	IL13
ATOM	2820	CB	LEU	106	23.154	-0.774	-3.689	1.00	0.26	IL13
ATOM	2821	CG	LEU	106	21.847	-1.568	-3.798	1.00	0.30	IL13
ATOM	2822	CD1	LEU	106	22.007	-3.009	-3.311	1.00	0.38	IL13
ATOM	2823	CD2	LEU	106	20.653	-0.843	-3.183	1.00	0.33	IL13
ATOM	2824	C	LEU	106	25.333	-0.383	-2.662	1.00	0.24	IL13
ATOM	2825	O	LEU	106	26.128	-1.262	-2.928	1.00	0.27	IL13
ATOM	2826	N	PHE	107	25.694	0.873	-2.668	1.00	0.23	IL13
ATOM	2827	H	PHE	107	25.045	1.600	-2.442	1.00	20.00	IL13
ATOM	2828	CA	PHE	107	27.100	1.229	-3.007	1.00	0.24	IL13
ATOM	2829	CB	PHE	107	27.279	2.749	-3.017	1.00	0.25	IL13
ATOM	2830	CG	PHE	107	28.135	3.165	-4.191	1.00	0.27	IL13
ATOM	2831	CD1	PHE	107	27.517	3.799	-5.290	1.00	0.25	IL13
ATOM	2832	CD2	PHE	107	29.525	2.914	-4.179	1.00	0.34	IL13
ATOM	2833	CE1	PHE	107	28.296	4.178	-6.399	1.00	0.29	IL13
ATOM	2834	CE2	PHE	107	30.306	3.293	-5.289	1.00	0.38	IL13
ATOM	2835	CZ	PHE	107	29.682	3.918	-6.389	1.00	0.35	IL13
ATOM	2836	C	PHE	107	28.045	0.560	-2.008	1.00	0.29	IL13
ATOM	2837	O	PHE	107	29.114	0.105	-2.362	1.00	0.33	IL13
ATOM	2838	N	ARG	108	27.666	0.507	-0.763	1.00	0.31	IL13
ATOM	2839	H	ARG	108	26.765	0.847	-0.491	1.00	20.00	IL13
ATOM	2840	CA	ARG	108	28.554	-0.124	0.253	1.00	0.37	IL13
ATOM	2841	CB	ARG	108	28.022	-0.180	1.687	1.00	0.42	IL13
ATOM	2842	CG	ARG	108	26.922	0.738	2.209	1.00	0.50	IL13
ATOM	2843	CD	ARG	108	26.604	0.200	3.605	1.00	0.93	IL13
ATOM	2844	NE	ARG	108	25.313	0.626	4.142	1.00	1.52	IL13
ATOM	2845	HE	ARG	108	25.169	1.597	4.334	1.00	2.07	IL13
ATOM	2846	CZ	ARG	108	24.376	-0.314	4.400	1.00	2.11	IL13

Figure 9 (51/52)

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ATOM   2847  NH1 ARG   108      23.313   0.011   5.135  1.00  3.04      IL13
ATOM   2848 HH11 ARG   108      23.249   0.920   5.548  1.00  3.45      IL13
ATOM   2849 HH12 ARG   108      22.564  -0.634   5.304  1.00  3.57      IL13
ATOM   2850  NH2 ARG   108      24.503  -1.555   3.932  1.00  2.35      IL13
ATOM   2851 HH21 ARG   108      25.256  -1.791   3.294  1.00  2.25      IL13
ATOM   2852 HH22 ARG   108      23.876  -2.308   4.123  1.00  3.05      IL13
ATOM   2853  C   ARG   108      28.809  -1.586  -0.106  1.00  0.38      IL13
ATOM   2854  O   ARG   108      29.904  -2.087   0.044  1.00  0.43      IL13
ATOM   2855  N   GLU   109      27.811  -2.282  -0.575  1.00  0.37      IL13
ATOM   2856  H   GLU   109      26.870  -1.941  -0.561  1.00 20.00      IL13
ATOM   2857  CA  GLU   109      28.021  -3.710  -0.929  1.00  0.43      IL13
ATOM   2858  CB  GLU   109      26.711  -4.504  -0.874  1.00  0.47      IL13
ATOM   2859  CG  GLU   109      25.994  -4.508   0.486  1.00  0.52      IL13
ATOM   2860  CD  GLU   109      25.177  -3.243   0.689  1.00  1.05      IL13
ATOM   2861  OE1 GLU   109      24.296  -2.973  -0.116  1.00  1.84      IL13
ATOM   2862  OE2 GLU   109      25.404  -2.524   1.657  1.00  1.66      IL13
ATOM   2863  C   GLU   109      28.631  -3.773  -2.327  1.00  0.42      IL13
ATOM   2864  O   GLU   109      29.043  -4.815  -2.796  1.00  0.50      IL13
ATOM   2865  N   GLY   110      28.714  -2.647  -2.983  1.00  0.34      IL13
ATOM   2866  H   GLY   110      28.309  -1.820  -2.603  1.00 20.00      IL13
ATOM   2867  CA  GLY   110      29.322  -2.607  -4.341  1.00  0.35      IL13
ATOM   2868  C   GLY   110      28.487  -3.433  -5.310  1.00  0.37      IL13
ATOM   2869  O   GLY   110      28.890  -3.672  -6.431  1.00  0.40      IL13
ATOM   2870  N   ARG   111      27.327  -3.865  -4.894  1.00  0.40      IL13
ATOM   2871  H   ARG   111      26.998  -3.615  -3.986  1.00 20.00      IL13
ATOM   2872  CA  ARG   111      26.468  -4.675  -5.801  1.00  0.45      IL13
ATOM   2873  CB  ARG   111      25.887  -5.965  -5.217  1.00  0.55      IL13
ATOM   2874  CG  ARG   111      25.825  -6.851  -6.462  1.00  0.67      IL13
ATOM   2875  CD  ARG   111      25.108  -8.204  -6.466  1.00  0.90      IL13
ATOM   2876  NE  ARG   111      24.928  -8.551  -7.879  1.00  1.61      IL13
ATOM   2877  HE  ARG   111      25.745  -8.844  -8.380  1.00  2.14      IL13
ATOM   2878  CZ  ARG   111      23.881  -7.926  -8.468  1.00  2.15      IL13
ATOM   2879  NH1 ARG   111      24.001  -7.348  -9.659  1.00  3.02      IL13
ATOM   2880 HH11 ARG   111      24.842  -7.376 -10.199  1.00  3.39      IL13
ATOM   2881 HH12 ARG   111      23.217  -6.811 -10.010  1.00  3.51      IL13
ATOM   2882  NH2 ARG   111      22.730  -7.844  -7.824  1.00  2.33      IL13
ATOM   2883 HH21 ARG   111      22.572  -8.330  -6.972  1.00  2.16      IL13
ATOM   2884 HH22 ARG   111      21.998  -7.246  -8.196  1.00  3.00      IL13
ATOM   2885  C   ARG   111      25.439  -3.768  -6.454  1.00  0.41      IL13
ATOM   2886  O   ARG   111      24.496  -3.336  -5.830  1.00  0.45      IL13
ATOM   2887  N   PHE   112      25.613  -3.478  -7.706  1.00  0.40      IL13
ATOM   2888  H   PHE   112      26.353  -3.940  -8.198  1.00 20.00      IL13
ATOM   2889  CA  PHE   112      24.645  -2.598  -8.402  1.00  0.42      IL13
ATOM   2890  CB  PHE   112      25.391  -1.677  -9.375  1.00  0.40      IL13
ATOM   2891  CG  PHE   112      26.496  -0.991  -8.599  1.00  0.33      IL13
ATOM   2892  CD1 PHE   112      26.174   0.064  -7.717  1.00  0.30      IL13
ATOM   2893  CD2 PHE   112      27.824  -1.455  -8.728  1.00  0.35      IL13
ATOM   2894  CE1 PHE   112      27.181   0.620  -6.906  1.00  0.27      IL13
ATOM   2895  CE2 PHE   112      28.830  -0.902  -7.913  1.00  0.33      IL13
ATOM   2896  CZ  PHE   112      28.494   0.113  -6.992  1.00  0.29      IL13
ATOM   2897  C   PHE   112      23.572  -3.455  -9.050  1.00  0.52      IL13
ATOM   2898  O   PHE   112      23.863  -4.451  -9.681  1.00  0.61      IL13
ATOM   2899  N   ASN   113      22.334  -3.085  -8.878  1.00  0.61      IL13
ATOM   2900  H   ASN   113      22.122  -2.372  -8.221  1.00 20.00      IL13
ATOM   2901  CA  ASN   113      21.228  -3.885  -9.467  1.00  0.73      IL13
ATOM   2902  CB  ASN   113      21.002  -3.668 -10.973  1.00  1.73      IL13
ATOM   2903  CG  ASN   113      19.504  -3.733 -11.231  1.00  2.37      IL13
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Figure 9 (52/52)

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ATOM   2904  OD1 ASN   113      18.698  -3.861 -10.313  1.00  2.85       IL13
ATOM   2905  ND2 ASN   113      19.161  -3.567 -12.512  1.00  3.08       IL13
ATOM   2906 HD21 ASN   113      19.854  -3.595 -13.225  1.00  3.21       IL13
ATOM   2907 HD22 ASN   113      18.191  -3.423 -12.738  1.00  3.76       IL13
ATOM   2908  C   ASN   113      21.363  -5.348  -9.029  1.00  1.60       IL13
ATOM   2909 OCT1 ASN   113      21.350  -5.621  -7.832  1.00  2.31       IL13
ATOM   2910 OCT2 ASN   113      21.520  -6.239  -9.861  1.00  2.23       IL13
END
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SOLUTION STRUCTURE OF IL-13 AND USES THEREOF

CROSS REFERENCE TO RELATED APPLICATION

[0001] This application claims the benefit of U.S. Provisional Application No. 60/296,607 filed Jun. 7, 2001.

FIELD OF THE INVENTION

[0002] The present invention relates to the three dimensional solution structure of human IL-13. This structure is critical for the design and selection of potent and selective agents that interact with IL-13.

BACKGROUND OF THE INVENTION

[0003] Interleukin-13 (IL-13) is a pleiotropic cytokine with roles in atopy, asthma, allergy and inflammatory response (For reviews see: Corry, 1999; De Vries, 1998; Finkelman et al., 1999; Shirakawa et al., 2000; Wills-Karp et al., 1998). IL-13 is produced by activated T cells and promotes B cell proliferation, induces B cells to produce IgE, down regulates the production of proinflamatory cytokines, increases expression of VCAM-1 on endothelial cells, enhances the expression of class II MHC antigens and various adhesion molecules on monocytes. IL-13 mediates these functions through an interaction with its receptor on hematopoietic and other cell types, but currently no functional receptors have been identified on T cells. The signaling human IL-13 receptor (IL-13 R) is a heterodimer composed of the interleukin-4 receptor α chain (IL-4Rα) and the IL-13 binding chain. Two IL-13 binding domains that are 27% homologous have been identified, IL-13Rα1 and IL-13Rα2. IL-13Rα2 demonstrates an approximate 100-fold higher affinity for IL-13 relative to IL-13Rα1 in the absence of IL-4Rα, but has been identified only in the serum and urine of mice. The association of IL-13 with its receptor induces the activation of STAT6 (signal transducer and activation of transcription 6) and Janus-family kinase (JAK1, JAK2, TYK2) through a binding interaction with the IL-4Rα chain.

[0004] IL-13 is located in a cluster of genes on chromosome 5 encoding IL-3, IL-4, IL-5, IL-9 and GM-CSF. IL-13 shares many functional properties with IL-4 as a result of the common IL-4Rα component in their receptors (Callard et al., 1996; Gessner and Rollinghoff, 2000). IL-4 exhibits a high affinity to IL-4Rα chain (K_d=20-300 pM), where this complex recruits the common γ chain (γ_c) of IL-4R to form the signaling complex. Similarly, IL-13 binds to the IL-13 binding chain (IL-13 Rα1) with relatively high affinity (K_d~4 nM) in the absence of the IL-4Rα chain, where an increase of affinity to IL-R occurs in the presence of IL-4Rα (K_d~50 pM). IL-13 does not bind IL-4Rα in the absence of the IL-13 binding chain. As a result, IL-4 exhibits binding to both IL-4R and IL-13R due to the existence of the IL-4Rα chain in both receptors, but IL-13 does not bind IL-4R because of the absence of the IL-13 binding chain (Callard et al., 1996). The cross-reactivity of IL-4 with both IL-4R and IL-13R is further promoted by the antagonistic activity of the IL-4 Y124D mutant (De Vries, 1994). The IL-4 Y124D mutant still maintains the ability to bind IL-4Rα, but is deficient in its ability to induce a signal through interaction with the γ_c chain. Since the γ_c chain is not present in IL-13R, IL-13 does not induce the proliferation and differentiation of T cells or the activation of JAK-3 kinase, which associates with the γ_c chain of IL-4R.

[0005] IL-13 and IL-4 are both members of the short chain four-helix bundle cytokine family (Sprang and Bazan, 1993), where both solution and crystal structures have been previously determined for IL-4 (Powers et al., 1992; Powers et al., 1993; Smith et al., 1992; Walter et al., 1992; Wlodaver et al., 1992). Despite the relatively low (25%) sequence homology between IL-13 and IL-4, a similarity in the overall topology between the two proteins is expected. A combination of mutational and kinetic analysis has identified a distinct site on the IL-4 structure associated with IL-4Rα binding and a second site associated with signaling through the γ_c chain (Kruse et al., 1993; Letzelter et al., 1998; Wang et al., 1997). Recently, the X-ray structure of IL-4 complexed with the ectodomain of IL-4Rα has been determined, which further defines the IL-4-IL-4Rα interface (Hage et al., 1999).

[0006] Despite the abundance of structural information on the IL-4 receptor system, structural information for IL-13, IL-13R or the complex is currently lacking. The present invention provides a high-resolution solution structure of human IL-13 by heteronuclear multidimensional NMR.

SUMMARY OF THE INVENTION

[0007] The present invention relates to the three dimensional structure of IL-13, and more specifically, to the solution structure of IL-13, as determined using spectroscopy and various computer modeling techniques.

[0008] Particularly, the invention is further directed to the identification, characterization and three dimensional structure of an active site of IL-13 that provides an attractive target for the rational design of potent and selective agents that interact with IL-13.

[0009] Accordingly, the present invention provides a solution comprising IL-13. The three dimensional solution structure of IL-13 is provided by the relative atomic structural coordinates of **FIG. 8**, as obtained from spectroscopy data.

[0010] Also provided by the present invention is an active site of IL-13, wherein said active site is characterized by a three dimensional structure comprising the relative structural coordinates of amino acid residues A9, E12, E15, E16 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

[0011] Also provided for by the present invention is an active site of IL-13, wherein said active site is characterized by a three dimensional structure comprising the relative structural coordinates of amino acid residues 152, Q64, R65 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

[0012] The solution coordinates of IL-13 or portions thereof (such as the active sites), as provided by this invention may be stored in a machine-readable form on a machine-readable storage medium, e.g. a computer hard drive, diskette, DAT tape, etc., for display as a three-dimensional shape or for other uses involving computer-assisted manipulation of, or computation based on, the

structural coordinates or the three-dimensional structures they define. By way of example, the data defining the three dimensional structure of IL-13 as set forth in **FIG. 8** or **9** may be stored in a machine-readable storage medium, and may be displayed as a graphical three-dimensional representation of the relevant structural coordinates, typically using a computer capable of reading the data from said storage medium and programmed with instructions for creating the representation from such data.

[**0013**] Accordingly, the present invention provides a machine, such as a computer, programmed in memory with the coordinates of IL-13 or portions thereof, together with a program capable of converting the coordinates into a three dimensional graphical representation of the structural coordinates on a display connected to the machine. A machine having a memory containing such data aids in the rational design or selection of inhibitors of IL-13 binding or activity, including the evaluation of the ability of a particular chemical entity to favorably associate with IL-13 as disclosed herein, as well as in the modeling of compounds, proteins, complexes, etc. related by structural or sequence homology to IL-13.

[**0014**] The present invention is additionally directed to a method of determining the three dimensional structure of a molecule or molecular complex whose structure is unknown, comprising the steps of first obtaining crystals or a solution of the molecule or molecular complex whose structure is unknown, and then generating X-ray diffraction data from the crystallized molecule or molecular complex and/or generating NMR data from the solution of the molecule or molecular complex. The generated diffraction or spectroscopy data from the molecule or molecular complex can then be compared with the solution coordinates or three dimensional structure of IL-13 as disclosed herein, and the three dimensional structure of the unknown molecule or molecular complex conformed to the IL-13 structure using standard techniques such as molecular replacement analysis, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques, and computer homology modeling. Alternatively, a three dimensional model of the unknown molecule may be generated by generating a sequence alignment between IL-13 and the unknown molecule, based on any or all of amino acid sequence identity, secondary structure elements or tertiary folds, and then generating by computer modeling a three dimensional structure for the molecule using the three dimensional structure of, and sequence alignment with, IL-13.

[**0015**] The present invention further provides a method for identifying an agent that interacts with IL-13, comprising the steps of: (a) generating a three dimensional model of IL-13 using the relative structural coordinates of the amino acids of **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å; and (b) employing said three-dimensional model to design an agent that interacts with IL-13.

[**0016**] Finally, the present invention provides agents that designed or selected using the methods disclosed herein. Additional objects of the present invention will be apparent from the description which follows.

BRIEF DESCRIPTION OF THE FIGURES

[**0017**] **FIG. 1** represents strip plots taken from the CBCA-(CO)NH and CBCANH spectra for the amides of residues E61 through F70 of IL-13. Each amide correlates with the C^{α} and C^{β} of the preceding residue in the CBCA(CO)NH spectra and with both its intraresidue C^{α} and C^{β} and the C^{α} and C^{β} of the preceding residue in the CBCANH spectra. Interresidue (i−1) correlations are indicated with the observed interresidue connectivities marked by a solid line. Negative contours are indicated by dashed lines.

[**0018**] **FIG. 2** is a summary of the sequential and medium range NOEs involving the NH, H^{α} and H^{β} protons, the amide exchange and $^{3}J_{HN\alpha}$ coupling constant data, and the $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ secondary chemical shifts observed for IL-13 with the secondary structure deduced from this data. The thickness of the lines reflects the strength of the NOEs. Amide protons still present after exchange to D_2O are indicated by closed circles. The open boxes on the same line as the $H^{\alpha}(i)$–NH(i+1) NOEs represents the sequential NOE between the H^{α} proton of residue i and the $C^{\delta}H$ proton of the i+1 proline and is indicative of a trans proline.

[**0019**] **FIG. 3** is a best-fit superposition of the backbone atoms (N,C,C') of the 30 best structures determined for IL-13 for residues 1-113. The helices are shown as dark grey. The two disulfide bonds are shown between residues C29 and C57, and C45 and C71, respectively.

[**0020**] **FIG. 4**(*a*) is a ribbon diagram of the NMR structure of IL-13 colored by secondary structure (same view as **FIG. 2**). **FIG. 4**(*c*) is a ribbon diagram of the NMR structure of IL-4 (1BBN) (Powers et al., 1992; Powers et al., 1993). The view is the same as IL-13 based on the alignment of the common secondary structure elements and disulfide bonds. FIGS. **4**(*b*) and 4(d) represent the top view of the IL-13 and IL-4 NMR ribbon diagram, respectively, illustrating the helix packing and orientation. The secondary structure elements and cysteines involved in disulfide bonds are labeled and are similar to **FIG. 2**.

[**0021**] **FIG. 5**(*a*) is the best-fit superposition of the backbone atoms (N, C, C') of the IL-13 and IL-4 restrained minimized average NMR structures (Powers et al., 1992; Powers et al., 1993). **FIG. 5**(*b*) is the sequence alignment of IL-13 with IL-4 based on the common secondary structure elements and disulfide bonds. The IL-4 mutational data and residues involved in the IL-4Rα binding site based on the IL-4/IL4Rα X-ray structure (PDB ID:11AR) (Hage et al., 1999) are indicated on top of the sequence. The IL-13 mutational data is indicated on the bottom of the sequence. IL-4 residues involved in the IL-4Rα and the $_{\gamma C}$ binding sites identified by mutational analysis are labeled with (*) and (+), respectively. IL-4 residues identified as part of the IL-4Rα binding site from the X-ray structure without corresponding mutational data are labeled with (−). IL-13 residues involved in the IL-4Rα and the IL-13 binding chain binding sites identified by mutational analysis are labeled with (#) and (&), respectively. The IL-4 sequence numbering is on top and the IL-13 sequence numbering is on the bottom.

[**0022**] FIGS. **6**(*a*) and 6(b) represent a GRASP molecular surface of the IL-4 and IL-13 NMR structures, respectively, where residues identified from mutational analysis that correlate with IL-4Rα affinity are shown. Residues proposed to interact with either the $_{\gamma C}$ or IL-13 binding chain (BC) are also shown. Residues in the IL-4Rα binding sites that were mutated are labeled.

[**0023**] **FIG. 7**(*a*) represents the IL-13/IL-4Rα model based on the IL-4/IL-4Rα X-ray structure (Hage et al.,

1999). IL-13 replaced IL-4 in the IL-4/IL-4Rα X-ray structure by overlaying IL-13 onto IL-4 based on the common secondary structure elements and cysteins (see **FIG. 4**). IL-4Rα is shown as a molecular surface and IL-13 as a ribbon diagram, where the helices are labeled as A, B, C and D. Only the IL-13/IL-4Rα interface is illustrated. The secondary structure elements are labeled. **FIG. 7**(*b*) is an expanded view of the IL-13/IL-4Rα binding site indicating the interaction with helix α_A from IL-13. **FIG. 7**(*c*) is an expanded view of the IL-13/IL-4Rα binding site illustrating the interaction with helix α_C from IL-13. The side-chains for critical residues based on the IL-4/IL-4Rα X-ray structure and mutational data are shown and labeled. Residues from IL-4Rα are labeled with the prefix 'r'.

[**0024**] **FIG. 8** lists the atomic structure coordinates for the restrained minimized mean structure of IL-13 as derived by multidimensional NMR spectroscopy. "Atom type" refers to the atom whose coordinates are being measured. "Residue" refers to the type of residue of which each measured atom is a part—i.e., amino acid, cofactor, ligand or solvent. The "x, y and z" coordinates indicate the Cartesian coordinates of each measured atom's location (Å).

[**0025**] **FIG. 9** provides the coordinates of the IL-13/IL-4Rα receptor model. "Atom type" refers to the atom whose coordinates are being measured. "Residue" refers to the type of residue of which each measured atom is a part—i.e., amino acid, cofactor, ligand or solvent. The "x, y and z" coordinates indicate the Cartesian coordinates of each measured atom's location (Å).

DETAILED DESCRIPTION OF THE INVENTION

[**0026**] As used herein, the following terms and phrases shall have the meanings set forth below:

[**0027**] Unless otherwise noted, "IL-13" includes the amino acid sequence of **FIG. 2**, including conservative substitutions thereof.

[**0028**] Unless otherwise indicated, "protein" or "molecule" shall include a protein, protein domain, polypeptide or peptide.

[**0029**] "Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using x-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original set provided in **FIG. 8** or **9** by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of **FIG. 8** or **9**.

[**0030**] An "agent" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound or drug.

[**0031**] "Root mean square deviation" is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates described herein. The present invention includes all embodiments comprising conservative substitutions of the noted amino acid residues resulting in same structural coordinates within the stated root mean square deviation.

[**0032**] "Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic), and includes substitutions having an inconsequential effect on the three dimensional structure of IL-13 with respect to the use of said structure for the identification and design of agents that interact with IL-13, for molecular replacement analyses and/or for homology modeling.

[**0033**] An "active site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug) via various covalent and/or non-covalent binding forces. As such, an active site of the present invention may include, for example, the actual site of receptor binding to IL-13, as well as accessory binding sites adjacent to the actual site of receptor binding that nonetheless may affect IL-13 upon interaction or association with a particular agent, either by direct interference with the actual site of receptor binding or by indirectly affecting the steric conformation or charge potential of IL-13 and thereby preventing or reducing receptor binding to IL-13 at the actual site of receptor binding. As used herein, "active site" also includes the receptor site of self association, as well as other binding sites present on IL-13.

[**0034**] A "IL-13 complex" refers to a co-complex of a molecule comprising IL-13 in bound association with a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, small molecule, compound or drug, either by covalent or non-covalent binding forces. A non-limiting example of a IL-13 complex includes the receptor, IL-4Rα bound to IL-13.

[**0035**] The present invention relates to the three dimensional structure of IL-13, and more specifically, to the solution structure of IL-13 as determined using multidimensional NMR spectroscopy and various computer modeling techniques. The structural coordinates of IL-13 in its unbound configuration (**FIG. 8**) or bound configuration (**FIG. 9**) are useful for a number of applications, including, but not limited to, the characterization of a three dimensional structure of IL-13, as well as the visualization, identification and characterization of IL-13 active sites, including the site of receptor binding to IL-13. The active site structures may then be used to predict the orientation and binding affinity of a designed or selected agent that interacts with IL-13 or of an IL-13 complex. Accordingly, the invention is also directed to the three dimensional structure of an IL-13 active site, including but not limited to the receptor binding site.

[**0036**] As used herein, the IL-13 in solution comprises amino acid 1-113 of **FIG. 2**, including conservative substitutions. Preferably, the IL-13 in solution is either unlabeled, ^{15}N enriched or ^{15}N, ^{13}C enriched, and is preferably biologically active. In addition, the secondary structure of the

IL-13 in the solution of the present invention comprises four alpha helices αA, αB, αC and αD, and two beta strands β1 and β2, wherein αA comprises amino acid residues P6-Q22 of IL-13, β1 comprises M33-W35 of IL-13, αB comprises amino acid residues M43-152 of IL-13, αC comprises amino acid residues A59-F70 of IL-13, β2 comprises amino acid residues K89-E91 of IL-13, and αD comprises amino acid residues V92-R108 of IL-13. In the most preferred embodiment, the IL-13 in the solution of the present invention is characterized by a three dimensional structure comprising the complete structural coordinates of the amino acids according to **FIG. 8**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å (or more preferably, not more than 1.0 Å, and most preferably, not more than 0.5 Å).

[**0037**] Molecular modeling methods known in the art may be used to identify an active site or binding pocket of IL-13 or of an IL-13 complex. Specifically, the solution structural coordinates provided by the present invention may be used to characterize a three dimensional structure of the IL-13 molecule or molecular complex. From such a structure, putative active sites may be computationally visualized, identified and characterized based on the surface structure of the molecule, surface charge, steric arrangement, the presence of reactive amino acids, regions of hydrophobicity or hydrophilicity, etc. Such putative active sites may be further refined using chemical shift perturbations of spectra generated from various and distinct IL-13 complexes, competitive and non-competitive inhibition experiments, and/or by the generation and characterization of IL-13 or ligand mutants to identify critical residues or characteristics of the active site.

[**0038**] The identification of putative active sites of a molecule or molecular complex is of great importance, as most often the biological activity of a molecule or molecular complex results from the interaction between an agent and one or more active sites of the molecule or molecular complex. Accordingly, the active sites of a molecule or molecular complex are the best targets to use in the design or selection of inhibitors that affect the activity of the molecule or molecular complex.

[**0039**] The present invention is directed to an active site of IL-13 or complex, that, as a result of its shape, reactivity, charge potential, etc., favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug). Preferably, the present invention is directed to an active site of IL-13 that is characterized by the three dimensional structure comprising the relative structural coordinates of amino acid residues A9, E12, E15, E16 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å, preferably not more than 1.0 Å, and most preferably not more than 0.5 Å. In another embodiment, the active site of IL-13 is characterized by the three dimensional structure comprising the relative structural coordinates of amino acid residues 152, Q64, R65 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å, preferably not more than 1.0 Å, and most preferably not more than 0.5 Å.

[**0040**] In order to use the structural coordinates generated for a solution structure of the present invention as set forth in **FIG. 8** or **9**, it is often necessary to display the relevant coordinates as, or convert them to, a three dimensional shape or graphical representation, or to otherwise manipulate them. For example, a three dimensional representation of the structural coordinates is often used in rational drug design, molecular replacement analysis, homology modeling, and mutation analysis. This is typically accomplished using any of a wide variety of commercially available software programs capable of generating three dimensional graphical representations of molecules or portions thereof from a set of structural coordinates. Examples of said commercially available software programs include, without limitation, the following: GRID (Oxford University, Oxford, UK); MCSS (Molecular Simulations, San Diego, Calif.); AUTODOCK (Scripps Research Institute, La Jolla, Calif.); DOCK (University of California, San Francisco, Calif.); Flo99 (Thistlesoft, Morris Township, N.J.); Ludi (Molecular Simulations, San Diego, Calif.); QUANTA (Molecular Simulations, San Diego, Calif.); Insight (Molecular Simulations, San Diego, Calif.); SYBYL (TRIPOS, Inc., St. Louis. MO); and LEAPFROG (TRIPOS, Inc., St. Louis, Mo.).

[**0041**] For storage, transfer and use with such programs, a machine, such as a computer, is provided for that produces a three dimensional representation of the IL-13, a portion thereof (such as an active site or a binding site), or a IL-13 complex. The machine of the present invention comprises a machine-readable data storage medium comprising a data storage material encoded with machine-readable data. Machine-readable storage media comprising data storage material include conventional computer hard drives, floppy disks, DAT tape, CD-ROM, and other magnetic, magneto-optical, optical, floptical and other media which may be adapted for use with a computer. The machine of the present invention also comprises a working memory for storing instructions for processing the machine-readable data, as well as a central processing unit (CPU) coupled to the working memory and to the machine-readable data storage medium for the purpose of processing the machine-readable data into the desired three dimensional representation. Finally, the machine of the present invention further comprises a display connected to the CPU so that the three dimensional representation may be visualized by the user. Accordingly, when used with a machine programmed with instructions for using said data, e.g., a computer loaded with one or more programs of the sort identified above, the machine provided for herein is capable of displaying a graphical three-dimensional representation of any of the molecules or molecular complexes, or portions of molecules of molecular complexes, described herein.

[**0042**] In one embodiment of the invention, the machine-readable data comprises the relative structural coordinates of amino acid residues A9, E12, E15, E16 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å, or preferably, not more than 1.0 Å, or more preferably not more than 0.5 Å. In an alternate embodiment, the machine-readable data further comprises the relative structural coordinates of amino acid residues 152, Q64, R65 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone

atoms of said amino acids of not more than 1.5 Å, preferably not more than 1.0 Å, and most preferably not more than 0.5 Å.

[0043] The structural coordinates of the present invention permit the use of various molecular design and analysis techniques in order to (i) solve the three dimensional structures of related molecules, molecular complexes or IIL-13, and (ii) to design, select, and synthesize chemical agents capable of favorably associating or interacting with an active site of an IL-13 molecule, or molecular complex, wherein said chemical agents potentially act as inhibitors, activators, agonists or antagonists of IL-13 or IL-13 binding to a protein, including, but not limited to, a receptor of IL-13 such as IL-4Rα.

[0044] More specifically, the present invention provides a method for determining the molecular structure of a molecule or molecular complex whose structure is unknown, comprising the steps of obtaining a solution of the molecule or molecular complex whose structure is unknown, and then generating NMR data from the solution of the molecule or molecular complex. The NMR data from the molecule or molecular complex whose structure is unknown is then compared to the solution structure data obtained from the IL-13 solutions of the present invention. Then, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques are used to conform the three dimensional structure determined from the IL-13 solution of the present invention to the NMR data from the solution molecule or molecular complex. Alternatively, molecular replacement may be used to conform the IL-13 solution structure of the present invention to x-ray diffraction data from crystals of the unknown molecule or molecular complex.

[0045] Molecular replacement uses a molecule having a known structure as a starting point to model the structure of an unknown crystalline sample. This technique is based on the principle that two molecules which have similar structures, orientations and positions will diffract x-rays similarly. A corresponding approach to molecular replacement is applicable to modeling an unknown solution structure using NMR technology. The NMR spectra and resulting analysis of the NMR data for two similar structures will be essentially identical for regions of the proteins that are structurally conserved, where the NMR analysis consists of obtaining the NMR resonance assignments and the structural constraint assignments, which may contain hydrogen bond, distance, dihedral angle, coupling constant, chemical shift and dipolar coupling constant constraints. The observed differences in the NMR spectra of the two structures will highlight the differences between the two structures and identify the corresponding differences in the structural constraints. The structure determination process for the unknown structure is then based on modifying the NMR constraints from the known structure to be consistent with the observed spectral differences between the NMR spectra.

[0046] Accordingly, in one non-limiting embodiment of the invention, the resonance assignments for the IL-13 solution provide the starting point for resonance assignments of IL-13 in a new IL-13:"unsolved agent" complex. Chemical shift perturbances in two dimensional $^{15}N/^{1}H$ spectra can be observed and compared between the IL-13 solution and the new IL-13:agent complex. In this way, the affected residues may be correlated with the three dimensional structure of IL-13 as provided by the relevant structural coordinates of **FIG. 8** or **9**. This effectively identifies the region of the IL-13:agent complex that has incurred a structural change relative to the native IL-13 structure. The ^{1}H, ^{15}N, ^{13}C and ^{13}CO NMR resonance assignments corresponding to both the sequential backbone and side-chain amino acid assignments of IL-13 may then be obtained and the three dimensional structure of the new IL-13:agent complex may be generated using standard 2D, 3D and 4D triple resonance NMR techniques and NMR assignment methodology, using the IL-13 solution structure, resonance assignments and structural constraints as a reference. Various computer fitting analyses of the new agent with the three dimensional model of IL-13 may be performed in order to generate an initial three dimensional model of the new agent complexed with IL-13, and the resulting three dimensional model may be refined using standard experimental constraints and energy minimization techniques in order to position and orient the new agent in association with the three dimensional structure of IL-13.

[0047] The present invention further provides that the structural coordinates of the present invention may be used with standard homology modeling techniques in order to determine the unknown three-dimensional structure of a molecule or molecular complex. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related protein molecules, molecular complexes or parts thereof (i.e., active sites). Homology modeling may be conducted by fitting common or homologous portions of the protein whose three dimensional structure is to be solved to the three dimensional structure of homologous structural elements in the known molecule, specifically using the relevant (i.e., homologous) structural coordinates provided by **FIG. 8** or **9** herein. Homology may be determined using amino acid sequence identity, homologous secondary structure elements, and/or homologous tertiary folds. Homology modeling can include rebuilding part or all of a three dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved.

[0048] Accordingly, a three dimensional structure for the unknown molecule or molecular complex may be generated using the three dimensional structure of the IL-13 molecule of the present invention, refined using a number of techniques well known in the art, and then used in the same fashion as the structural coordinates of the present invention, for instance, in applications involving molecular replacement analysis, homology modeling, and rational drug design.

[0049] Determination of the three dimensional structure of IL-13, its binding site to a receptor, and other binding sites, is critical to the rational identification and/or design of agents that may act as inhibitors, activators, agonists or antagonists of IL-13. This is advantageous over conventional drug assay techniques, in which the only way to identify such an agent is to screen thousands of test compounds until an agent having the desired inhibitory effect on a target compound is identified. Necessarily, such conventional screening methods are expensive, time consuming, and do not elucidate the method of action of the identified agent on the target compound.

[0050] However, advancing X-ray, spectroscopic and computer modeling technologies allow researchers to visu-

alize the three dimensional structure of a targeted compound (i.e., of IL-13). Using such a three dimensional structure, researchers identify putative binding sites and then identify or design agents to interact with these binding sites. These agents are then screened for an inhibitory effect upon the target molecule. In this manner, not only are the number of agents to be screened for the desired activity greatly reduced, but the mechanism of action on the target compound is better understood.

[0051] Accordingly, the present invention further provides a method for identifying an agent that interacts with IL-13, comprising the steps of generating the three dimensional structure of IL-13 as defined by the relative structural coordinates of **FIG. 8** or **9**, and using that three dimensional structure to identify, design or select an agent that interacts with IL-13. The inhibitor may be selected by screening an appropriate database, may be designed de novo by analyzing the steric configurations and charge potentials of an empty IL-13 or IL-13 complex active site in conjunction with the appropriate software programs, or may be designed using characteristics of known agents in order to create "hybrid" agents.

[0052] An agent that interacts or associates with an active site of IL-13 or an IL-13 complex may be identified by determining an active site from the three dimensional structure of IL-13, and performing computer fitting analyses to identify an agent which interacts or associates with said active site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the putative active site and the identified agent, by (a) generating a three dimensional model of the putative active site of a molecule or molecular complex using homology modeling or the atomic structural coordinates of the active site, and (b) determining the degree of association between the putative active site and the identified agent. The degree of association may be determined computationally by any number of commercially available software programs, or may be determined experimentally using standard binding assays.

[0053] Three dimensional models of the putative active site may be generated using any one of a number of methods known in the art, and include, but are not limited to, homology modeling as well as computer analysis of raw structural coordinate data generated using crystallographic or spectroscopy techniques. Computer programs used to generate such three dimensional models and/or perform the necessary fitting analyses include, but are not limited to: GRID (Oxford University, Oxford, UK), MCSS (Molecular Simulations, San Diego, Calif.), AUTODOCK (Scripps Research Institute, La Jolla, Calif.), DOCK (University of California, San Francisco, Calif.), Flo99 (Thistlesoft, Morris Township, N.J.), Ludi (Molecular Simulations, San Diego, Calif.), QUANTA (Molecular Simulations, San Diego, Calif.), Insight (Molecular Simulations, San Diego, Calif.), SYBYL (TRIPOS, Inc., St. Louis. MO) and LEAPFROG (TRIPOS, Inc., St. Louis, Mo.).

[0054] In the preferred embodiment, the method of the present invention includes the use of an active site characterized by the three dimensional structure comprising the relative structural coordinates of amino acid residues A9, E12, E15, E16 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å, preferably not more than 1.0 Å, and most preferably not more than 0.5 Å. In another embodiment, the active site is characterized by the three dimensional structure comprising the relative structural coordinates of amino acid residues 152, Q64, R65 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å, preferably not more than 1.0 Å, and most preferably not more than 0.5 Å. It is understood that the method of the present invention includes additional embodiments comprising conservative substitutions of the noted amino acids which result in the same structural coordinates of the corresponding residues in **FIG. 8** or **9** within the stated root mean square deviation.

[0055] The effect of such an agent identified by computer fitting analyses on IL-13 or the IL-13 complex may be further evaluated computationally, or experimentally by competitive binding experiments or by contacting the identified agent with IL-13 (or a IL-13 complex) and measuring the effect of the agent on the target's biological activity. Standard assays may be performed and the results analyzed to determine whether the agent is an activator, inhibitor, agonist or antagonist of IL-13 activity (e.g., the agent may reduce or prevent binding affinity between IL-13 and a relevant binding protein).

[0056] An agent designed or selected to interact with IL-13 preferably is capable of both physically and structurally associating with IL-13 via various covalent and/or non-covalent molecular interactions, and of assuming a three dimensional configuration and orientation that complements the relevant active site of IL-13.

[0057] Accordingly, using these criteria, the structural coordinates of the IL-13 molecule as disclosed herein, and/or structural coordinates derived therefrom using molecular replacement or homology modeling, agents may be designed to increase either or both of the potency and selectivity of known inhibitors, either by modifying the structure of known inhibitors or by designing new agents de novo via computational inspection of the three dimensional configuration and electrostatic potential of a IL-13 active site.

[0058] Accordingly, in one embodiment of the invention, the structural coordinates of **FIG. 8** or **9** of the present invention, or structural coordinates derived therefrom using molecular replacement or homology modeling techniques as discussed above, are used to screen a database for agents that may act as potential activators, inhibitors, agonists or antagonists of IL-13 activity. Specifically, the obtained structural coordinates of the present invention are read into a software package and the three dimensional structure is analyzed graphically. A number of computational software packages may be used for the analysis of structural coordinates, including, but not limited to, Sybyl (Tripos Associates), QUANTA and XPLOR (Brunger, A. T., (1994) *X-Plor* 3.851: *a system for X-ray Crystallography and NMR. Xplor Version* 3.851 New Haven, Conn.: Yale University Press). Additional software programs check for the correctness of the coordinates with regard to features such as bond and atom types. If necessary, the three dimensional structure is modified and then energy minimized using the appropriate software until all of the structural parameters are at their equilibrium/optimal values. The energy minimized structure is superimposed against the original structure to make sure

there are no significant deviations between the original and the energy minimized coordinates.

[0059] The energy minimized coordinates of IL-13 bound to a "solved" agent are then analyzed and the interactions between the solved ligand and IL-13 are identified. The final IL-13 structure is modified by graphically removing the solved agent so that only IL-13 and a few residues of the solved agent are left for analysis of the binding site cavity. QSAR and SAR analysis and/or conformational analysis may be carried out to determine how other inhibitors compare to the solved inhibitor. The solved agent may be docked into the uncomplexed structure's binding site to be used as a template for data base searching, using software to create excluded volume and distance restrained queries for the searches. Structures qualifying as hits are then screened for activity using standard assays and other methods known in the art.

[0060] Further, once the specific interaction is determined between the solved agent, docking studies with different agents allow for the generation of initial models of new agents bound to IL-13. The integrity of these new models may be evaluated a number of ways, including constrained conformational analysis using molecular dynamics methods (i.e., where both IL-13 and the bound agent are allowed to sample different three dimensional conformational states until the most favorable state is reached or found to exist between the protein and the bound agent). The final structure as proposed by the molecular dynamics analysis is analyzed visually to make sure that the model is in accord with known experimental SAR based on measured binding affinities. Once models are obtained of the original solved agent bound to IL-13 and computer models of other molecules bound to IL-13, strategies are determined for designing modifications into the inhibitors to improve their activity and/or enhance their selectivity.

[0061] Once an IL-13 binding agent has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analyzed for efficiency of fit IL-13 by the same computer methods described in detail above.

[0062] With respect to agonist/antagonist design, there are a number of computational software packages that may be used for the analysis of protein NMR structures. In this case, the software packages Sybyl v.6.4+ to v.6.5+ from Tripos Associates and QUANTA97 (Version 97.1003) an CPLOR (Version 3.840) from MSI may be used. Once the coordinates have been determined by NMR a number of steps may be taken as listed below:

[0063] 1. The original coordinates are read into the software package and the structure(3D) is analyzed graphically. In addition, programs within QUANTA check for the correctness of the NMR coordinates with regard to features such as bond and atom types.

[0064] 2. The modified (if necessary) structure is energy minimized using the QUANTA/CHARMm until all the structural parameters are at their equilibrium/optimal values.

[0065] 3. The energy minimized structure is superimposed against the original NMR structure to ensure there are no significant deviations between the original and minimized coordinates.

[0066] 4. The protein-native complex is analyzed, the interactions between the native ligand and the protein are identified. The uncomplexed structure binding site is compared to the complexed structure's binding site for areas which may be exploited by a potential agonist/antagonist.

[0067] 5. The final protein structure bound to the native ligand is modified by removing the native ligand so only the protein and a few residues of the natural ligand are left for analysis of the binding site cavity. The natural ligand residues are docked into the uncomplexed structure's binding site to be used as templates for SYBYL/UNITY database searching.

[0068] 6. SYBYL/UNITY is used to create excluded volume and distance constrained queries for searching structural databases. Structural qualifying as 'hits' are screened for activity.

[0069] 7. Once specific ligand-protein interactions are determined between new ligands and the protein structure, docking studies may be carried out between the different series of in-house ligands and IL-13. This part gives us the initial modeled complexes of new ligands with IL-13.

[0070] To check for the integrity of the modeled new IL-13-ligand complexes, different procedures may be used. In this case, constrained conformational analysis is carried out using molecular dynamic methods. In this modeling process, both protein and the complexed ligand are allowed to sample different 3D conformational states until the most favorable state is reached or found to exist between protein and inhibitor. The final structure as proposed by the molecular dynamics analysis is analyzed visually to make sure the modeled complex is in accord with known experimental SAR based on measured binding affinities.

[0071] Furthermore, agonist/antagonist design may take advantage of either the IL-13 binding chain or IL-4Rα binding states. Additionally, details of the IL-13/IL-4Rα interface may be used to design ligands that effectively bind to either IL-13 or IL-4Rα in this binding region. Also, conformational changes in IL-4 upon binding the IL-13 binding chain that are required to recruit IL-4Rα may be utilized in designing ligands that either inhibit or promote this structural change to affect the inherent IL-13 activity. Once computer models of the native ligand and/or other ligands bound to IL-13 have been determined, modifications can be designed into ligands to improve binding and/or activity based upon the models.

[0072] Various molecular analysis and rational drug design techniques are further disclosed in U.S. Pat. Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published as WO 99/09148, the contents of which are hereby incorporated by reference.

[0073] The present invention may be better understood by reference to the following non-limiting Examples. The following Examples are presented in order to more fully

illustrate the preferred embodiments of the invention, and should in no way be construed as limiting the scope of the present invention.

EXAMPLE 1

[0074] A. Methods and Methods.

[0075] The uniform ^{15}N and ^{13}C labeled 113 amino acid IL-13 was obtained as follows. The cDNA encoding the mature secreted portion of IL-13 was reconstructed with silent changes that optimized *E. coli* codon usage and increased AT content at the 5-prime end. The gene was subcloned into the T7-lac vector pRSET for expression in *Escherichia coli* BL21(DE3). Growth and expression were at 37°, in shake flasks with minimal medium supplemented with ^{13}C-glucose and/or ^{15}N-ammonium sulfate. The protein was essentially completely insoluble. Cells were broken with a microfluidizer and insoluble IL-13 was collected and dissolved at about 2 mg/ml in 50 mM CHES (pH 9), 6 M guanidine-HCl, 1 mM EDTA, 20 mM DTT. The solution was diluted 20-fold into 50 mM CHES (pH 9), 3 M guanidine-HCl 100 mM NaCl, 1 mM oxidized glutathione and dialyzed twice against 10 volumes of 50 mM CHES (pH 9), 100 mM NaCl and once against 10 volumes of 20 mM MES (pH 6). Following clarification by centrifugation, IL-13 was adsorbed to SP-Sepharose and eluted with a gradient of NaCl in MES buffer. Final purification was by size-exclusion chromatography in 40 mM sodium phosphate, 40 mM NaCl on Superdex 75.

[0076] The NMR samples contained 1 mM of IL-13 in a buffer containing 40 mM sodium Phosphate, 2 mM NaN_3, 40 m M NaCl, in either 90% H2O/10% D20 or 100% D20 at pH 6.0. All NMR spectra were recorded at 25° C. on a Bruker DRX 600 spectrometer equipped with a triple-resonance gradient probe. Spectra were processed using the NMRPipe software package (Delaglio et al., 1995) and analyzed with PIPP(Garrett et al., 1991).

[0077] The assignments of the ^{1}H, ^{15}N, ^{13}Co, and ^{13}C resonances were based on the following experiments: CBCA(CO)NH, CBCANH, C(CO)NH, HC(CO)NH, HNHB, HNCO, HNHA, HNCA and HCCH-COSY (for reviews see (Bax et al., 1994; Clore and Gronenbom, 1994). The accuracy of the IL-13 NMR assignments was further confirmed during the structure calculation and by sequential NOEs in the ^{15}N-edited NOESY-HMQC spectra and by NOEs between the β-strands observed in the ^{13}C-edited NOESY-HMQC and ^{15}N-edited NOESY-HMQC spectra.

[0078] The present structure is based on the experimental distance and torsional angle restraints determined from the following series of spectra: HNHA (Vuister and Bax, 1993), HNHB (Archer et al., 1991), HACAHB-COSY (Grzesiek et al., 1995), 3D ^{15}N- (Marion et al., 1989; Zuiderweg and Fesik, 1989) and ^{13}C-edited NOESY (Ikura et al., 1990; Zuiderweg et al., 1990). The ^{15}N-edited NOESY, and ^{13}C-edited NOESY experiments were collected with 100 ms and 120 ms mixing times, respectively.

[0079] The β-methylene stereospecific assignments and χ1 torsion angle restraints were obtained primarily from a qualitative estimate of the magnitude of $^{3}J_{\alpha\beta}$ coupling constants from the HACAHB-COSY experiment (Grzesiek et al., 1995) and $^{3}J_{N\beta}$ coupling constants from the HNHB experiment (Archer et al., 1991). Val γ-methyl stereospecific assignments were made from the relative inte nsity of intraresidue NH-CγH and CαH-CγH NOEs (Zuiderweg et al., 1985). Leu and Ile χ2 torsion angle restraints and Leu δ-methyl stereospecific assignments were obtained primarily from ^{13}C-^{13}C-long range coupling constants (Bax and Pochapsky, 1992) and the relative intensity of intra-molecular NOEs (Powers et al., 1993). The ϕ and ψ torsion angle restraints were obtained from $^{3}J_{NH\alpha}$ coupling constants measured from the HNHA experiment (Vuister and Bax, 1993) and from chemical shift analysis using the TALOS program (Cornilescu et al., 1999). The minimum ranges employed for the ϕ, ψ, and χ torsion angle restraints were ±30°, ±50°, and ±20°, respectively. The NOEs assigned from the 3D ^{15}N- and ^{13}C-edited NOESY experiments were classified into strong, medium, weak and very weak corresponding to interproton distance restraints where non-stereospecifically assignments were corrected appropriately for center averaging (Wuthrich et al., 1983).

[0080] The structures were calculated using the hybrid distance geometry-dynamical simulated annealing method of Nilges et al., (1988c) with minor modifications (Clore et al., 1990) using the program XPLOR (Brunger, 1993), adapted to incorporate pseudopotentials for $^{3}J_{NH\alpha}$ coupling constants (Garrett et al., 1994), secondary $^{13}C^{\alpha}/^{13}C^{\beta}$ chemical shift restraints (Kuszewski et al., 1995) radius of gyration (Kuszewski et al., 1999), and a conformational database potential (Kuszewski et al., 1996; Kuszewski et al., 1997). The target function that is minimized during restrained minimization and simulated annealing comprises only quadratic harmonic terms for covalent geometry, ^{3}JNHα coupling constants and secondary $^{13}C^{\alpha}/^{13}C^{\beta}$ chemical shift restraints, square-well quadratic potentials for the experimental distance, radius of gyration and torsion angle restraints, and a quartic van der Waals term for non-bonded contacts. All peptide bonds were constrained to be planar and trans. There were no hydrogen-bonding, electrostatic, or 6-12 Lennard-Jones empirical potential energy terms in the target function. The radius of gyration can be predicted with reasonable accuracy on the basis of the number of residues using a relationship determined empirically from the analysis of high-resolution x-ray structures (Kuszewski et al., 1996). The force constant for the conformational database and radius of gyration potentials were kept relatively low throughout the simulation to allow the experimental distance and torsional angle restraints to be the predominant influences on the resulting structures. The force constant for the NOE and dihedral restraints was 30 times and ten times stronger then the force constants used for the conformational database and radium gyration potentials, respectively.

[0081] Overlay of the IL-3 solution structure with free IL-4 and IL-4 in the IL-4/IL4Rα complex was accomplished with Quanta (Molecular Simulations, Inc., San Diego, Calif.). Minimization of the IL-3 side-chains to remove steric clashes was accomplished with CHARMM (Molecular Simulations, Inc., San Diego, Calif.). Measurement of the interhelical angles and axial distances in the IL-13 and IL-4 structures was determined using INTERHLX.

[0082] Atomic coordinates for the 30 final simulated annealing structures and the restrained minimized mean structure and the NMR chemical shift assignments of IL-13 have been deposited in the RCSB Protein Data Bank (PDB ID: 1ijz and 1iko) and the BioMagResBank (BMRB-5004), respectively.

[0083] B. Results and Discussion

[0084] 1. IL-13 NMR Structure

[0085] Nearly complete backbone and side-chain ^{1}H, ^{15}N, ^{13}C, and ^{13}CO assignments have been obtained for IL-13 that enabled the determination of a high-resolution solution structure for the protein by NMR (**FIG. 1**). The IL-13 structure is well defined by the NMR data, where a total of 2848 constraints were used to refine the structure (**FIG. 2**). This is evident by a best fit superposition of the backbone atoms shown in **FIG. 3**, where the atomic r.m.s. distribution of the 30 simulated annealing structures about the mean coordinate positions for residues 1-113 is 0.43 (±0.04) Å for the backbone atoms (Table 1). All of the backbone torsion angles for non-glycine residues lie within expected regions of the Ramachandran plot where 89.9% of the residues lie within the most favored region of the Ramachandran ϕ, ψ plot, 9.1% in the additionally allowed region and 1.0% in the generously allowed region. The high quality of the IL-13 NMR structure is also evident by the results of the PROCHECK analysis, where an overall G-factor of 0.15, a hydrogen bond energy of 0.90 and only 1.8 bad contacts per 100 residues were determined. The calculated PROCHECK parameters for IL-13 are comparable to values obtainable with ~1 Å X-ray structures and implies a relatively high quality for the structure, but does not infer an inherent resolution (Laskowski et al., 1996).

[0086] The IL-13 protein adopts the expected left-handed four-helical bundle with up-up-down-down connectivities previously observed for IL-4 and similar cytokines. The four helical regions correspond to residues 6-22 (α_A); 43-52 (α_B); 59-70 (α_C) and 92-108 (α_D). The observed angles and axial separation between the four antiparallel helical pairs, α_A-α_C, α_C-α_B, α_B-α_D and α_D-α_A, are −161.7° and 11.3 Å, −147.7° and 9.2 Å, −165.1° and 12.7 Å, and −150.3° and 9.8 Å, respectively. The corresponding values between the two parallel helical pairs, α_A-α_B and α_C-α_D, are 37.0° and 16.4 Å, and 33.4° and 14.2 Å, respectively. In addition, a short β-sheet region was observed in the IL-13 structure which corresponds to residues 33-35 (β_1) and 89-91 (β_2). Additionally, distinct Cβ chemical shifts (~42 ppm) for three Cys residues confirmed the presence of two disulfide bonds in the IL-13 structure. The C^{β} chemical shift for C29 was anomalous, where the chemical shift (34 ppm) was in-between typical values for both oxidized and reduced forms. The further identification of the C29-C57 and C45-C71 disulfide bonds was determined by distinct intermolecular NOEs that were identified during the IL-13 structure calculation. In particular, C29 H^{α} to C57 H^{β}, C29 H^{β} to C57 H^{β} NOEs and C45 H^{α} to C71 H^{β}, C45 H^{β} to C71 H^{β} NOEs defined the C29-C57 and C45-C71 disulfide bonds, respectively.

[0087] An interesting observation for the IL-13 structure is the presence of chemical shift heterogeneity in the 2D ^{1}H-^{15}N HSQC spectra for residues in the structural vicinity of C29. In addition to residues sequential to C29 and C57, A93 and residues sequential to A93 also exhibited multiple ^{1}H-^{15}N HSQC peaks. Except for the backbone NH resonance assignments, the remainder of the spin-system chemical shifts assignments for these residues were essentially identical. More importantly, the 3D ^{15}N-edited NOESY spectra exhibited identical NOE patterns and relative intensities for the multiple backbone NH diagonal peaks. Therefore, the chemical shift multiplicity observed in the 2D ^{1}H-^{15}N HSQC spectra suggests a local conformational heterogeneity in the vicinity of C29, where the IL-13 structural change is within the resolution of the structure and the limits of detection for an NOE intensity change. A probable source for the structural heterogeneity is the presence of multiple conformations for the side-chain dihedral angles that comprise the C29-C57 disulfide bond. The C^{α}-C^{α} distance separation for the two cysteins involved in a disulfide bond are directly dependent on the side-chain dihedral angles (Richardson, 1981). A distance range of 4.4 to 6.8 Å for the C^{α}-C^{α} separation is observed for typical values of dihedral angles observed in a disulfide bond, but distance changes of only 0.1-0.2 Å is common between pairs of side-chain conformations. Most likely, a smaller distance change is the source of the heterogeneity present in IL-13 where the different side-chain conformations result in C29 being slightly closer to either C57 or A93. The conformational heterogeneity centered on C29 may also explain the anomalous Cβ chemical shift for this residue.

[0088] Another feature of the IL-13 structure is the presence of three long loops connecting the four helices. The shortest loop connects helices α_B, and α_C and comprises residues N53 to S58. The two long overhand connections are comprised of residues N23 to G42, which connects helices α_A with α_B, and residues C71 to E91, which connects α_C with α_D. These loops come in close contact to form the short β-sheet. Additionally, the C29-C57 disulfide bond connects the AB loop to the BC loop. The combination of the short β-sheet and the disulfide bond results in regions of these loops being relatively well defined. Further stability of the long loops occurs from long-range intermolecular NOEs that result in packing of parts of the loop against the helical bundle.

[0089] An another interesting feature of the IL-13 structure is the location of the C45-C71 disulfide bond, which effectively connects the N-terminus of α_B with the C-terminus of α_C. Since the α_B and α_C helices are also connected by the short BC loop, which is further stabilized by the C29-C57 disulfide bond, the orientation of the α_B and α_C helices is extensively defined by covalent connectivity. The end result is a closed loop connecting the α_B and α_C helices.

[0090] 2. Comparison of the IL-13 and IL-4 Solution Structures

[0091] An abundance of structural information for IL-4 has been previously determined by both NMR and X-ray crystallography where a reasonable consensus was obtained for the IL-4 structure (Smith et al., 1994). Therefore, a single solution structure of IL-4 (PDB ID: 1BBN) was used to simplify the comparison between the solution structure of IL-13 with IL-4 (Powers et al., 1992; Powers et al., 1993). Ribbon diagrams for both the IL-13 and IL-4 restrained minimized solution structures are shown in **FIG. 4**. While the overall folding topology of the two proteins is quite similar, there are obvious distinctions between the two structures. A primary distinction is the overall size difference between the two proteins. IL-4 contains a total of 129 residues compared to 113 for IL-13. This results in the extension of the IL-4 structure by ~12 Å along the long axis relative to IL-13. Consistent with the overall size difference, are variations in the helix lengths between the IL-4 and IL-13 structures. The length of the four helices in IL-4

corresponds to 17, 23, 26 and 16 residues for helices α_A, α_B, α_C and α_D, respectively. Conversely, in IL-13 helices α_A, α_B, α_C and α_D have lengths of 17, 10, 12 and 17 residues, respectively. Clearly, the most pronounced distinction is between helices α_B and α_C, where the IL-4 helices are more than double the length of IL-13. Interestingly, a similar difference in the loop regions between the helices was not seen. The length of the AB, BC and CD loops between IL-4 and IL-13 are identical or nearly identical, where the loops in IL-13 are longer by one to two residues. Similarly, the length of the short β-sheet that comprises part of loops AB and CD are essentially identical. Another distinction between the two protein structures is the number and location of the disulfide bonds. IL-4 has a total of three disulfide bonds that connect the N- and C-terminus (C3-C127), the AB and BC loops (C24-C64), and helix α_B to loop CD (C46-C99). Conversely, IL-13 contains only two disulfide bonds that connect the AB and BC loops (C29-C57) and helix α_B to helix α_C (C45-C71).

[**0092**] A 25% sequence homology exists between IL-13 and IL-4; however, optimal superposition of the two proteins is determined mainly by alignment of shared secondary structure elements. An overlay of the IL-13 and IL-4 solution structures based on the common secondary structure elements and Cys residues yielded a backbone r.m.s. of 1.44 Å. The sequential alignment based on the shared secondary structure elements and Cys residues along with the overlay of the backbone atoms for IL-13 with IL-4 is illustrated in **FIG. 5**. In general, there is a good agreement in the superposition between the IL-13 and IL-4 structures including the loop regions. Nevertheless, there exist some distinct differences between the two proteins in the relative orientations and packing of the four-helix bundle, where aB and aD exhibit the largest changes. This is exemplified by an observed 20° difference in the interhelical angle between helices α_B-α_D and changes in opposite directions in the axial separation for helices α_A-α_B and α_C-α_D. The α_A-α_B axial separation decreases from 16.4 Å to 12.6 Å between IL-13 and IL-4, respectively. Conversely, the α_C-α_D axial separation increases from 14.2 Å to 16.7 Å between IL-13 and IL-4. Since α_B in IL-13 is the shortest helix and half the length of α_B in IL-4, the observed structural changes may be attributed to this change in helix length. Furthermore, the relative orientation of α_B in IL-13 is also defined by the disulfide bonds at both the N- and C-terminal ends of the helix. Comparison of IL-13 with IL-4 indicates that only a partial spatial alignment of the conserved cysteins occurs, further contributing to the perturbation in α_B. There is a good agreement with the relative orientation of C57 from IL-13 with C46 from IL-4. To a lesser extent, the positioning of C29 from IL-13 agrees with C24 from IL-4. But, there is essentially no correlation between the other members of the disulfide pairs. This difference results from the shorter α_B and α_C helices in IL-13 and that C99 resides within the CD loop in IL-4 compared to C71 being located in helix C for IL-13. Despite the highlighted differences between IL-13 and IL-4, it is important to stress that the overlap of the protein folds for the two proteins is quite similar.

[**0093**] 3. Implication for IL-13 Receptor Binding

[**0094**] The recent X-ray crystal structure of IL-4 complexed to the IL-4 receptor α chain has provided insight into cytokine-receptor interactions. Furthermore, an abundance of prior mutational work provides additional information pertaining to the characteristics of the cytokine-receptor interactions. A strong overlap in functionality exists for both IL-13 and IL-4 that is further exemplified by the fact that both receptors contain the same IL-4 chain. Therefore, the combination of the observed similarity in the protein folds, mutational data and the IL-4/receptor complex provides a framework to investigate the interaction of IL-13 with its receptor.

[**0095**] A combination of mutational and kinetic analysis has identified a distinct site on the IL-4 structure associated with IL-4Rα binding and a second site associated with signaling through the γc chain (Wang et al., 1997, Kruse et al., 1993, Letzelter et al., 1998). The IL-4Rα binding site on IL-4 is associated with amino acids that comprise a surface formed by helices A (15, E9, T13) and C (K77, R81, K84, R85 R88, N89, W91). The second site associated with signaling through the γc chain corresponds to residues in helices A (I11, N15) and D (R121, Y124, S125). Similar mutational work on IL-13 that alters its reactivity to IL-13R has also identified amino acids in helices A (E12, E15), C (R65, S68) and D (R108, F112), based on the predicted secondary structure for IL-13 (Thompson et al., 1999, Oshima et al., 2000). The results of the mutational analysis were mapped onto a GRASP surface for both IL-4 and IL-13 (**FIGS. 6*a*** and **6*c***). This analysis identifies the potential IL-13 binding chain and IL-4Rα binding sites on IL-13, which are consistent with the IL-4 binding sites.

[**0096**] The X-ray structure of IL-4 complexed to IL-4Rα confirmed the previous mutational data in identifying the α-chain binding site on IL-4 while further elucidating the specifics of the protein-receptor interaction (Hage et al., 1999). The face of helices α_A and α_C from IL-4 are almost perpendicular to the L-shaped structure of IL-4Rα. Contact residues from IL-4 are predominately polar and charged residues while the complementary receptor epitope is composed of clusters of polar residues surrounded by hydrophobic residues. Three distinct clusters of residues are described where E9 and R88 from IL-4 are focal points in clusters I and II, respectively, where these residues are involved in hydrogen bonds and ionic bonds with numerous IL-4Rα residues. A number of additional IL-4 residues proximal to E9 and R88 complete the IL-4-receptor interface. The third cluster is described as primarily an electrostatic interaction that does not significantly contribute to the binding affinity, but facilitates complex formation. An overlay of the backbone atoms of IL-13 with IL-4 based primarily on a correlation of secondary structure elements provided a mechanism to establish a structure-based sequence alignment. This structure-based sequence alignment of IL-13 with IL-4 is shown in **FIG. 4**, where both the mutational data and the key contact residues from the IL-4/receptor X-ray structure is summarized. Again, there is a clear consistency between the IL-4 mutational and structure contact data, where the IL-13 mutational data correlates well with this information. The overlay of the IL-13 structure with IL-4 may then be used in a similar manner to create a model of IL-13 complexed with IL-4Rα.

[**0097**] By creating a best-fit superposition of IL-13 with IL-4 in the IL-4/IL-4Rα complex, a simple model of IL-13 complexed with IL-4Rα is obtained. An overlay of the IL-13 NMR structure with IL-4 from the IL-4/receptor X-ray structure based on the common secondary structure elements and Cys residues yielded a backbone r.m.s. of 1.55 Å.

Additional refinement of the IL-13/IL-4Rα complex was limited to minimization of the IL-13 side-chain conformations to remove obvious steric clashes between IL-13 and IL-4Rα.

[0098] The IL-13/IL-4Rα model is illustrated in **FIG. 7**. It is readily apparent that the general interaction of IL-13 closely mimics the IL-4/IL-4Rα complex. Particularly, helices α_A and α_C pack approximately perpendicular against IL-4Rα (**FIG. 7A**). Furthermore, the framework of the IL-13 side-chain interactions with IL-4Rα mimics the network of interactions observed in the IL-4/IL-4Rα complex. In particular, E12 from IL-13 is positioned to mimic the bonding network of E9 from IL-4 with Y13, Y183 and S70 from IL-4Rα (**FIG. 7B**). Similarly, R65 from IL-13 is reasonably positioned to form a potential salt bridge with D72 from IL-4R (**FIG. 7C**). This interaction is comparable to the interaction of R88 from IL-4 with D72 from IL-4Rα. Distinctions between the IL-13/IL-4Rα model relative to the IL-4/IL-4Rα X-ray structure becomes apparent when comparison of the binding network that complement the E12 and R65 interaction with IL-4Rα is made. By reference to IL-4, residues proximal to E12 that are predicted to interact with IL-4Rα consist of IL-13 residues A9, E15, E16 and M66. These residues would correlate with T6, K12, T13 and N89 from IL-4 and interact with S70, Y183, Y127 and A71, respectively (**FIG. 7B**). Correspondingly, residues near R65 that are predicted to bind IL-4Rα comprises IL-13 residues 152, Q64 and M66 which correlate with IL-4 residues R53, N89 and W91. These IL-4 residues were shown to interact with F41 and V69 from IL-4R (**FIG. 7C**). While some comparable interactions are potentially present in the IL-13/IL-4α models, these interactions are clearly not optimal. Also, there exist some polarity or charge changes that would be predicted to have a detrimental affect on the affinity of IL-13 with IL-4Rα. This is also evident by comparison of the GRASP surfaces for IL-4 and IL-13 colored by electrostatic potential (not shown). A distinct surface is presented to IL-4Rα by the two proteins, where IL-4 presents a relatively higher negative charged surface compared to IL-13. Conversely, the IL-13 surface is more hydrophobic compared to IL-4 with some positive charge characteristics. This analysis implies that while some key interactions consistent with the IL-4/IL-4R complex are present, the IL-13/IL-4Rα model predicts that some re-arrangement of the IL-13 interaction with IL-4Rα is required to optimize the secondary interactions and accommodate the residue substitutions between IL-13 and IL-4.

[0099] The apparent sub-optimal interface between IL-13 and IL-4Rα based on the IL-4/IL-4Rα complex appears consistent with both the experimental affinity of IL-13 with IL-4Rα and the assembly mechanism of IL-4 with IL-4R. A sequential order of binding of IL-4 to IL-4R has been previously proposed (Kondo et al., 1993, Russell et al., 1993). First, IL-4 binds the IL-4Rα chain with high affinity (K_d=20-300 pM). The resulting complex then recruits the common γC chain to form the signaling heterodimer. Upon complex formation with IL-4Rα chain, IL-4 incurs a conformational change localized in the putative γC chain binding site (Wang et al., Kruse et al., Letzelter et al., Hage et al.). Presumably, the observed IL-4 conformational change is required to bind the γC chain binding. A similar mechanism appears consistent with the interaction of IL-13 with its receptor.

[0100] IL-13 does not bind IL-4R or the IL-4Rα chain in the absence of the IL-13 binding chain (Zurawski et al., 1993), but binds to the IL-13 binding chain (IL-13Rα1) with relatively high affinity (K_d~4 nM). Following the sequential binding mechanism proposed for IL-4, IL-13 would appear to first bind the IL-13 binding chain. The resulting complex then recruits the IL-4Rα chain to from the signaling heterodimer. Upon complex formation with the IL-13 binding chain, IL-13 would presumably incur a conformational change that would allow it to bind IL-4Rα. Again, this conformational change would probably resemble the change observed with IL-4 and result in a subtle re-arrangement in IL-13 helices α_A and α_C. Since the IL-13/IL-4Rα model reveals that the basic interaction network consistent with the IL-4/IL-4Rα is present, presumably only a modest modification in the helical packing would establish a comparable binding interface with IL-4/IL-4Rα complex and improve the affinity of IL-13 with IL-4Rα.

TABLE 1

Structural Statistics and Atomic r.m.s. Differences

	<SA>	$\overline{(SA)}_r$
A. Structural Statistics		
r.m.s. deviations from experimental distance restraints (Å)[a]		
all (2248)	0.014 ± 0.002	0.016
interresidue sequential (|i-j| = 1) (624)	0.011 ± 0.004	0.012
interresidue short range (1 < |i-j| < 5) (607)	0.015 ± 0.003	0.018
interresidue long-range (|i-j| > 5) (530)	0.016 ± 0.002	0.021
intraresidue (437)	0.007 ± 0.004	0.005
H-bonds (50)[b]	0.031 ± 0.006	0.026
r.m.s. deviation from exptl dihedral restraints (deg) (299)[c,d]	0.221 ± 0.053	0.186
r.m.s. deviation from exptl C^α restraints (ppm) (104)	0.95 ± 0.03	0.94
r.m.s. deviation from exptl C^β restraints (ppm) (101)	0.78 ± 0.04	0.78
r.m.s. deviation from $^3J_{NH\alpha}$ restraints (Hz) (96)	0.61 ± 0.02	0.58
F_{NOE} (kcal mol^{-1})[d]	22.3 ± 5.9	28.5
F_{tor} (kcal mol^{-1})[d]	0.95 ± 0.46	0.64
F_{repel} (kcal mol^{-1})[d]	22.5 ± 2.1	14.4
F_{L-J} (kcal mol^{-1})[e]	−423 ± 8	−408
deviations from idealized covalent geometry		
bonds (Å) (1783)	0.003 ± 0	0.004
angles (deg) (3240)	0.455 ± 0.011	0.523
impropers (deg) (901)[f]	0.437 ± 0.039	0.396
PROCHECK[g]		
Overall G-Factor	0.19 ± 0.02	0.15
% Residues in most favorable region of Ramachandran plot	90.5 ± 1.4	89.9
% Residues in disallowed region of Ramachandran plot	0.0 ± 0.0	0.0
H-bond energy	0.85 ± 0.06	0.90
Number of bad contacts/100 residues	2.6 ± 1.5	1.8

TABLE 1-continued

Structural Statistics and Atomic r.m.s. Differences
B. Atomic r.m.s. Differences (Å)

	Residues 1–113		secondary structure[h]		ordered side chain
	backbone atoms	all atoms	backbone atoms	all atoms	all atoms
<SA> vs $\overline{SA}$	0.43 ± 0.04	0.81 ± 0.06	0.22 ± 0.03	0.65 ± 0.06	0.47 ± 0.04
<SA> vs $\overline{(SA)_r}$	0.45 ± 0.04	0.90 ± 0.07	0.24 ± 0.03	0.73 ± 0.08	0.51 ± 0.04
$\overline{(SA)_r}$ vs $\overline{SA}$	0.15	0.38	0.10	0.32	0.20

[0101] The notation of the structures is as follows: <SA> are the final 30 simulated annealing structures; $\overline{SA}$ is the mean structure obtained by averaging the coordinates of the individual SA structures best fit to each; and $(\overline{SA})_r$ is the restrained minimized mean structure obtained by restrained minimization of the mean structure $\overline{SA}$ (Nilges et al., 1988). The number of terms for the various restraints is given in parentheses. a None of the structures exhibited distance violations greater than 0.2 Å or dihedral angle violations greater than 1°. b For backbone NH—CO hydrogen bond there are two restraints: $r_{NH—O}$=1.5-2.3 Å and $r_{N—O}$=2.5-3.3 Å. All hydrogen bonds involve slowly exchanging NH protons. c The torsion angle restraints comprise 104 ϕ, 105 ψ, 66 χ1, and 24 χ2 restraints. d The values of the square-well NOE (F_{NOE}) and torsion angle (F_{tor}) potentials [cf. eqs 2 and 3 in Clore et al., (1986)] are calculated with force constants of 50 kcal mol^{-1} $Å^{-2}$ and 200 kcal mol^{-1} rad^{-2}, respectively. The value of the quartic van der Waals repulsion term (F_{rep}) [cf. eq 5 in Nilges et al. (1988)] is calculated with a force constant of 4 kcal mol^{-1} $Å^{-4}$ with the hard-sphere van der Waals radius set to 0.8 times the standard values used in the CHARMM (Brooks et al., 1983) emperical energy function (Nilges et al., 1988, Nilges et al., 1988, Nilges et al., 1988). e E_{L-J} is the Lennard-Jones-van der Waals energy calculated with the CHARMM emperical energy function and is not included in the target function for simulated annealing or restrained minimization. f The improper torsion restraints serve to maintain planarity and chirality. g These were calculated using the PROCHECK program (Laskowski et al., 1996). h The residues in the regular secondary structure are: 6-22 (α_A), 43-52(α_B), 59-70(α_C), 92-108(α_D), 33-35(β_1) and 89-91(β_{II}).

REFERENCES

[0102] Archer, S. J., Ikura, M. Torchia, D. A., and Bax, A. (1991). An alternative 3D NMR technique for correlating backbone nitrogen-15 with side chain Hα resonances in larger proteins, J Magn Reson 95, 636-641.

[0103] Bax, A., and Pochapsky, S. S. (1992). Optimized Recording of Heteronuclear Multidimensional NMR Spectra Using Pulsed Field Gradients, Journal of Magnetic Resonance 99, 638-643.

[0104] Bax, A., Vuister, G. W., Grzesiek, S., and Delaglio (1994). Measurement of homo- and heteronuclear J couplings from quantitative J correlation, Methods Enzymol 239, 79-105.

[0105] Brooks, B. R., Bruccoleri, R. E., Olafson, B. D., States, D. J., Swaminathan, S., and Karplus, M. (1983). CHARMM: a program for macromolecular energy, minimization, and dynamics calculations, J Comput Chem 4, 187-217.

[0106] Brunger, A. T. (1993). X-PLOR Version 3.1 Manual (New Haven, Conn., Yale University). Callard, R. E., Matthews, D. J., and Hibbert, L. (1996). IL-4 and IL-13 receptors: are they one and the same?, Immunol Today 17, 108-110.

[0107] Clore, G. M., Appella, E., Yamada, M., Matsushima, K., and Gronenbom, A. M. (1990). Three-dimensional structure of interleukin 8 in solution, Biochemistry 29, 1689-1696.

[0108] Clore, G. M., and Gronenborn, A. M. (1994). Multidimensional heteronuclear nuclear magnetic resonance of proteins, Methods Enzymol 239, 349-362.

[0109] Clore, G. M., Nilges, M., Sukumaran, D. K., Bruenger, A. T., Karplus, M., and Gronenborn, A. M. (1986). The three-dimensional structure of α1-purothionin in solution: combined use of nuclear magnetic resonance, distance geometry and restrained molecular dynamics, EMBO J 5, 2729-2735.

[0110] Cornilescu, G., Delaglio, F., and Bax, A. (1999). Protein backbone angle restraints from searching a database for chemical shift and sequence homology, J Biomol NMR 13, 289-302.

[0111] Corry, D. B. (1999). IL-13 in allergy: home at last, Curr Opin Immunol 11, 610-614.

[0112] De Vries, J. E. (1994). Inhibition of IL-4- and IL-13-induced IgE synthesis by an IL-4 mutant protein, Arb Paul Ehrlich Inst 87, 275-282.

[0113] De Vries, J. E. (1998). The role of IL-13 and its receptor in allergy and inflammatory responses, J Allergy Clin Immunol 102, 165-169.

[0114] Delaglio, F., Grzesiek, S., Vuister, G. W., Zhu, G., Pfeifer, J., and Bax, A. (1995). NMRPipe: A multidimensional spectral processing system based on UNIX pipes, J Biomol NMR 6, 277-293.

[0115] Finkelman, F. D., Wynn, T. A., Donaldson, D. D., and Urban, J. F., Jr. (1999). The role of IL-13 in helminth-induced inflammation and protective immunity against nematode infections, Curr Opin Immunol 11, 420-426.

[0116] Garrett, D. S., Kuszewski, J., Hancock, T. J., Lodi, P. J., Vuister, G. W., Gronenbom, A. M., and Clore, G. M. (1994). The impact of direct refinement against three-bond HN—CH coupling constants on protein structure determination by NMR, J Magn Reson, Ser B 104, 99-103.

[0117] Garrett, D. S., Powers, R., Gronenbom, A. M., and Clore, G. M. (1991). A common sense approach to peak picking in two-, three-, and four-dimensional spectra using automatic computer analysis of contour diagrams, J Magn Reson 95, 214-220.

[0118] Gessner, A., and Rollinghoff, M. (2000). Biologic functions and signaling of the interleukin-4 receptor complexes, Immunobiology 201, 285-307.

[0119] Grzesiek, S., Kuboniwa, H., Hinck, A. P., and Bax, A. (1995). Multiple-Quantum Line Narrowing for Measurement of Hα.-Hβ J Couplings in Isotopically Enriched Proteins, J Am Chem Soc 117, 5312-5315.

[0120] Hage, T., Sebald, W., and Reinemer, P. (1999). Crystal structure of the interleukin-4/receptor a chain complex reveals a mosaic binding interface, Cell 97, 271-281.

[0121] Ikura, M., Kay, L. E., Tschudin, R., and Bax, A. (1990). Three-dimensional NOESY-HMQC spectroscopy of a carbon-13-labeled protein, J Magn Reson 86, 204-209.

[0122] Kondo, M., Takeshita, T., Ishii, N., Nakamura, M., Watanabe, S., Arai, K., and Sugamura, K. (1993). Sharing of the interleukin-2 (IL-2) receptor g chain between receptors for IL-2 and IL-4, Science 262, 1874-1877.

[0123] Kruse, N., Shen, B. J., Arnold, S., Tony, H. P., Mueller, T., and Sebald, W. (1993). Two distinct functional sites of human interleukin 4 are identified by variants impaired in either receptor binding or receptor activation, Embo J 12, 5121-5129.

[0124] Kuszewski, J., Gronenbom, A. M., and Clore, G. M. (1996). Improving the quality of NMR and crystallographic protein structures by means of a conformational database potential derived from structure databases, Protein Sci 5, 1067-1080.

[0125] Kuszewski, J., Gronenbom, A. M., and Clore, G. M. (1997). Improvements and extensions in the conformational database potential for the refinement of NMR and x-ray structures of proteins and nucleic acids, J Magn Reson 125, 171-177.

[0126] Kuszewski, J., Gronenbom, A. M., and Clore, G. M. (1999). Improving the Packing and Accuracy of NMR Structures with a Pseudopotential for the Radius of Gyration, J Am Chem Soc 121, 2337-2338.

[0127] Kuszewski, J., Qin, J., Gronenbom, A. M., and Clore, G. M. (1995). The impact of direct refinement against 13Cα and 13Cβ chemical shifts on protein structure determination by NMR, J Magn Reson, Ser B 106, 92-96.

[0128] Laskowski, R., Rullmannn, J., MacArthur, M., Kaptein, R., and J M, T. (1996). AQUA and PROCHECK-NMR: programs for checking the quality of protein structures solved by NMR., Biomol NMR 8, 477-486.

[0129] Letzelter, F., Wang, Y., and Sebald, W. (1998). The interleukin-4 site-2 epitope determining binding of the common receptor g chain, Eur J Biochem 257, 11-20.

[0130] Marion, D., Driscoll, P. C., Kay, L. E., Wingfield, P. T., Bax, A., Gronenbom, A. M., and Clore, G. M. (1989). Overcoming the overlap problem in the assignment of proton NMR spectra of larger proteins by use of three-dimensional heteronuclear proton-nitrogen-15 Hartmann-Hahn-multiple quantum coherence and nuclear Overhauser-multiple quantum coherence spectroscopy: application to interleukin 1β, Biochemistry 28, 6150-6156.

[0131] Nilges, M., Clore, G. M., and Gronenbom, A. M. (1988a). Determination of three-dimensional structures of proteins from interproton distance data by dynamical simulated annealing from a random array of atoms. Circumventing problems associated with folding, Febs Lett 239, 129-136.

[0132] Nilges, M., Clore, G. M., and Gronenborn, A. M. (1988b). Determination of three-dimensional structures of proteins from interproton distance data by hybrid distance geometry-dynamical stimulated annealing calculations, Febs Lett 229, 317-324.

[0133] Nilges, M., Gronenbom, A. M., Bruenger, A. T., and Clore, G. M. (1988c). Determination of three-dimensional structures of proteins by simulated annealing with interproton distance restraints. Application to crambin, potato carboxypeptidase inhibitor and barley serine proteinase inhibitor 2, Protein Eng 2, 27-38.

[0134] Oshima, Y., Joshi, B. H., and Puri, R. K. (2000). Conversion of interleukin-13 into a high affinity agonist by a single amino acid substitution, J Biol Chem 275, 14375-14380.

[0135] Powers, R., Garrett, D. S., March, C. J., Frieden, E. A., Gronenbom, A. M., and Clore, G. M. (1992). Three-dimensional solution structure of human interleukin-4 by multidimensional heteronuclear magnetic resonance spectroscopy, Science 256, 1673-1677.

[0136] Powers, R., Garrett, D. S., March, C. J., Frieden, E. A., Gronenborn, A. M., and Clore, G. M. (1993). The high-resolution, three-dimensional solution structure of human interleukin-4 determined by multidimensional heteronuclear magnetic resonance spectroscopy, Biochemistry 32, 6744-6762.

[0137] Russell, S. M., Keegan, A. D., Harada, N., Nakamura, Y., Noguchi, M., Leland, P., Friedmann, M. C., Miyajima, A., Puri, R. K., and et al. (1993). Interleukin-2 receptor g chain: a functional component of the interleukin-4 receptor, Science 262, 1880-1883.

[0138] Shirakawa, T. T., Deichmann, K. A. K. A., Izuhara, K. K., Mao, X. Q. X. Q., Adra, C. N. C. N., and Hopkin, J. M. J. M. (2000). Atopy and asthma: genetic variants of IL-4 and IL-13 signaling, Immunol Today 21, 60-64.

[0139] Smith, L. J., Redfield, C., Boyd, J., Lawrence, G. M. P., Edwards, R. G., Smith, R. A. G., and Dobson, C. M. (1992). Human interleukin 4. The solution structure of a four-helix bundle protein, J Mol Biol 224, 899-904.

[0140] Smith, L. J., Redfield, C., Smith, R. A. G., Dobson, C. M., Clore, G. M., Gronenbom, A. M., Walter, M. R., Naganbushan, T. L., and Wlodawer, A. (1994). Comparison of four independently determined structures of human recombinant interleukin-4, Nat Struct Biol 1, 301-310.

[0141] Sprang, S. R., and Bazan, J. F. (1993). Cytokine structural taxonomy and mechanisms of receptor engagement, Curr Opin Struct Biol 3, 815-827.

[0142] Thompson, J. P., and Debinski, W. (1999). Mutants of interleukin 13 with altered reactivity toward interleukin 13 receptors, J Biol Chem 274, 29944-29950.

[0143] Vuister, G. W., and Bax, A. (1993). Quantitative J correlation: a new approach for measuring homonuclear three-bond J(HNHα) coupling constants in ^{15}N-enriched proteins, J Am Chem Soc 115, 7772-7777.

[0144] Walter, M. R., Cook, W. J., Zhao, B. G., Cameron, R. P., Jr., Ealick, S. E., Walter, R. L., Jr., Reichert, P., Nagabhushan, T. L., Trotta, P. P., and Bugg, C. E. (1992). Crystal structure of recombinant human interleukin-4, J Biol Chem 267, 20371-20376.

[0145] Wang, Y., Shen, B. -J., and Sebald, W. (1997). A mixed-charge pair in human interleukin 4 dominates high-affinity interaction with the receptor a chain, Proc Natl Acad Sci U S A 94, 1657-1662.

[0146] Wills-Karp, M., Luyimbazi, J., Xu, X., Schofield, B., Neben, T. Y., Karp, C. L., and Donaldson, D. D. (1998). Interleukin-13: central mediator of allergic asthma, Science 282, 2258-2261.

[0147] Wlodaver, A., Pavlovsky, A., and Gustchina, A. (1992). Crystal structure of human recombinant interleukin-4 at 2.25 A resolution, FEBS Lett 309, 59-64.

[0148] Wuthrich, K., Billeter, M., and Braun, W. (1983). Pseudo-structures for the 20 Common Amino Acids for Use in Studies of Protein Conformation by Measurements of Intramolecular Proton-Proton Distance Constraints with Nuclear Magnetic Resonance., J Mol Biol 169, 949-996.

[0149] Zulderweg, E. R. P., Boelens, R., and Kaptein, R. (1985). Stereospecific assignments of proton-NMR methyl lines and conformation of valyl residues in the lac repressor headpiece, Biopolymers 24, 601-611.

[0150] Zuiderweg, E. R. P., and Fesik, S. W. (1989). Heteronuclear three-dimensional NMR spectroscopy of the inflammatory protein C5a, Biochemistry 28, 2387-2391.

[0151] Zuiderweg, E. R. P., McIntosh, L. P., Dahlquist, F. W., and Fesik, S. W. (1990). Three-dimensional carbon-13-resolved proton NOE spectroscopy of uniformly carbon-13-labeled proteins for the NMR assignment and structure determination of larger molecules, J Magn Reson 86, 210-216.

[0152] Zurawski, S. M., Vega, F., Jr., Huyghe, B., and Zurawski, G. (1993). Receptors for interleukin-13 and interleukin-4 are complex and share a novel component that functions in signal transduction, Embo J 12, 2663-2670.

[0153] All publications mentioned herein above, whether to issued patents, pending applications, published articles, protein structure deposits, or otherwise, are hereby incorporated by reference in their entirety. While the foregoing invention has been described in some detail for purposes of clarity and understanding, it will be appreciated by one skilled in the art from a reading of the disclosure that various changes in form and detail can be made without departing from the true scope of the invention in the appended claims.

What is claimed is:

1. A solution comprising interleukin-13 (IL-13), wherein IL-13 comprises amino acid residues 1-113 of **FIG. 2**, IL-13 is either unlabeled, ^{15}N enriched or ^{15}N,^{13}C enriched, IL-13 comprises four alpha helices αA, αB, αC and αD, and two beta strands β1 and β2, and αA comprises amino acid residues P6-Q22 of IL-13, β1 comprises M33-W35 of IL-13, αB comprises amino acid residues M43-152 of IL-13, αC comprises amino acid residues A59-F70 of IL-13, β2 comprises amino acid residues K89-E91 of IL-13, and αD comprises amino acid residues V92-R108 of IL-13.

2. The solution of claim 1, wherein IL-13 has the structure defined by the relative structural coordinates according to **FIG. 8**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

3. The solution of claim 1, wherein IL-13 has the structure defined by the relative structural coordinates according to **FIG. 8**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.0 Å.

4. The solution of claim 1, wherein IL-13 has the structure defined by the relative structural coordinates according to **FIG. 8**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 0.5 Å.

5. A structural model of IL-13 comprising the relative structural coordinates according to **FIG. 8** or **9** of IL-13, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

6. The model of claim 5, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 1.0 Å.

7. The model of claim 5, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 0.5 Å.

8. An active site of IL-13, wherein said active site is characterized by a three dimensional structure comprising the relative structural coordinates of amino acid residues A9, E12, E15, E16 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

9. The active site of claim 8, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 1.0 Å.

10. The active site of claim 8, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 0.5 Å.

11. An active site of IL-13, wherein said active site is characterized by a three dimensional structure comprising the relative structural coordinates of amino acid residues I52, Q64, R65 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

12. The active site of claim 11, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 1.0 Å.

13. The active site of claim 11, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 0.5 Å.

14. A method for designing an agent that interacts with IL-13, comprising the steps of:

(a) generating a three dimensional model of IL-13 using the relative structural coordinates of the amino acids of **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å; and

(b) employing said three-dimensional model to design an agent that interacts with IL-13.

15. The method of claim 14, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 1.0 Å.

16. The method of claim 14, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 0.5 Å.

17. The method of claim 14, wherein the agent is designed using an active site of IL-13.

18. The method of claim 17, wherein the active site comprises the relative structural coordinates of amino acid residues A9, E12, E15, E16 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

19. The method of claim 18, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 1.0 Å.

20. The method of claim 18, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 0.5 Å.

21. The method of claim 17, wherein the active site comprises the relative structural coordinates of amino acid residues I52, Q64, R65 and M66 of IL-13 according to **FIG. 8** or **9**, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

22. The method of claim 21, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 1.0 Å.

23. The method of claim 21, wherein the ± a root mean square deviation from the conserved backbone atoms of said amino acids is not more than 0.5 Å.

24. The method according to claim 14, wherein the step of employing the three dimensional structure to design an agent comprises the steps of:

(a) identifying chemical entities or fragments capable of associating with IL-13; and

(b) assembling the identified chemical entities or fragments into a single molecule to provide the structure of the agent.

25. The method according to claim 14, wherein the agent is designed de novo.

26. The method according to claim 14, wherein the agent is designed from a known agent.

27. The method of claim 14, further comprising the step of obtaining or synthesizing the agent.

28. The method of claim 27, wherein the agent obtained or synthesized in is contacted with IL-13 in order to determine the effect the agent has on IL-13.

29. An agent designed by the method of claim **14**.

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