Full wwPDB EM Validation Report ⓘ

Dec 8, 2024 – 09:57 am GMT

PDB ID	:	9F9S
EMDB ID	:	EMD-50259
Title	:	Yeast SDD1 Disome with Mbf1
Authors	:	Denk, T.; Beckmann, R.
Deposited on	:	2024-05-08
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

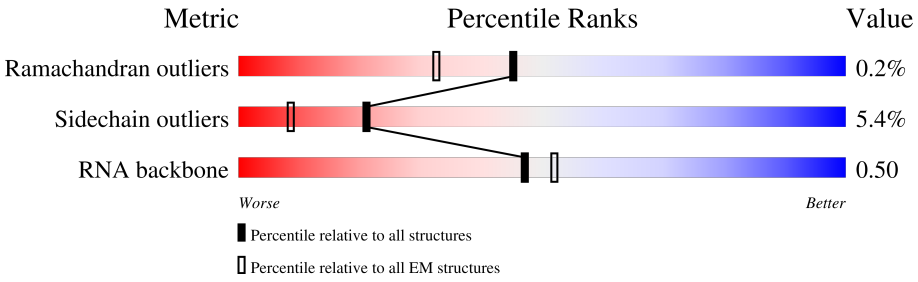
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



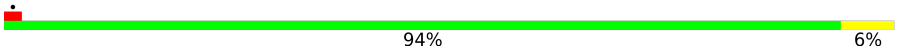
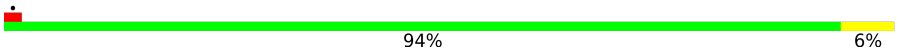
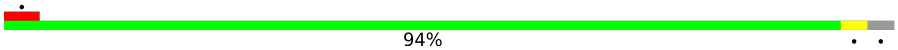
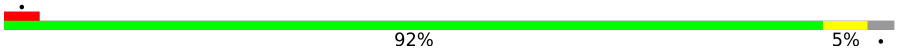
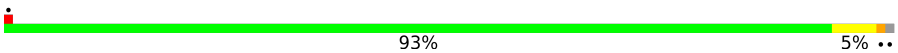
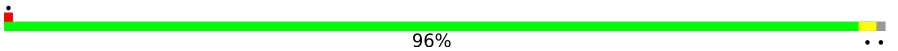
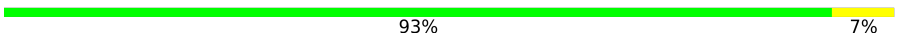
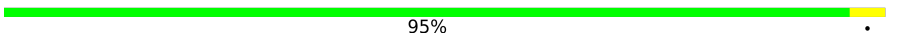
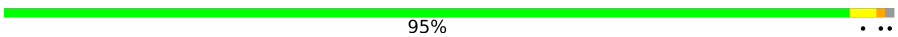
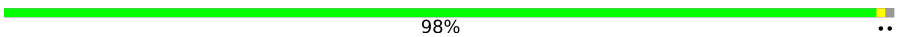
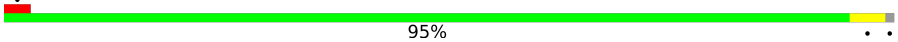
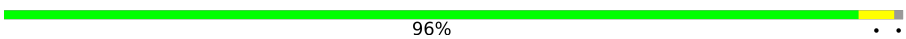
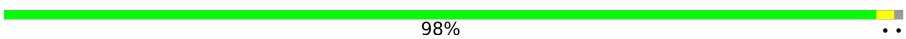
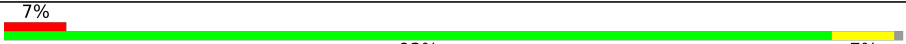
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	CC	233	5% · 94%
2	CM	41	17% 56% 39% 5%
3	CN	151	5% 85% 5% 10%
4	CP	76	5% 86% 13% ·
5	L1	3396	· 73% 18% · 8%
6	L2	158	· 82% 18% ·
6	M2	158	· 84% 16%
7	L3	121	88% 12%

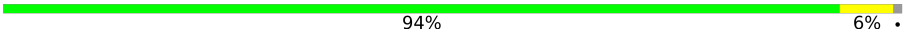
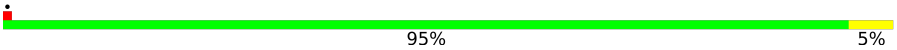
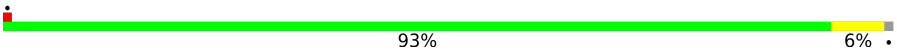
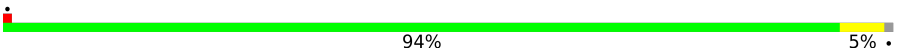
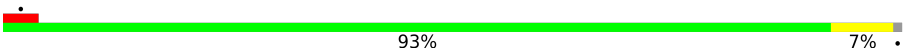
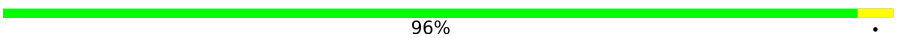
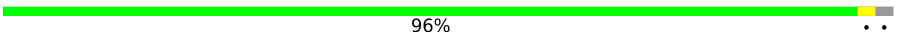
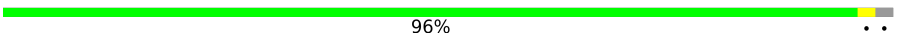
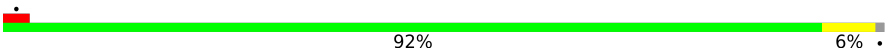
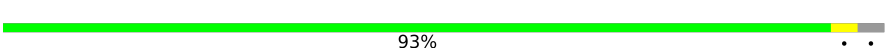
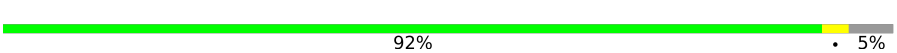
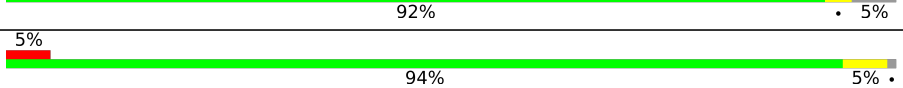
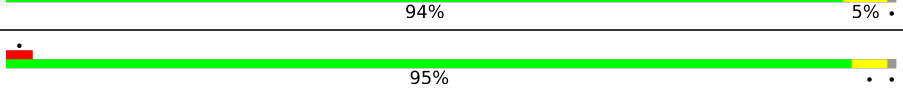
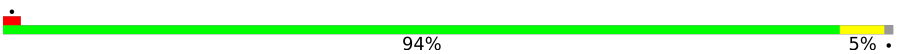
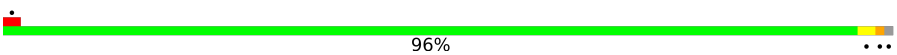
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	M3	121	
8	LA	176	
9	LB	244	
9	MB	244	
10	LC	256	
10	MC	256	
11	LD	191	
11	MD	191	
12	LE	221	
12	ME	221	
13	LF	174	
13	MF	174	
14	LG	199	
14	MG	199	
15	LH	138	
15	MH	138	
16	LI	204	
16	MI	204	
17	LJ	199	
17	MJ	199	
18	LK	184	
18	MK	184	
19	LL	186	
19	ML	186	
20	LM	189	

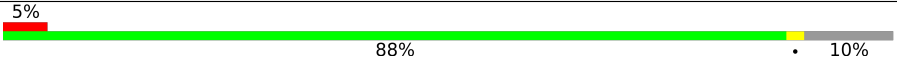
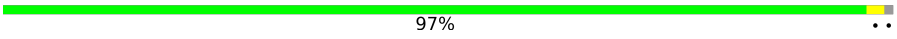
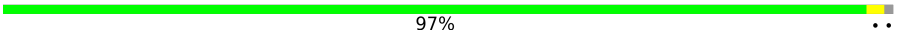
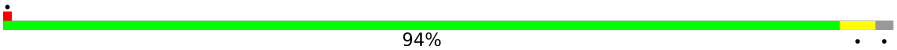
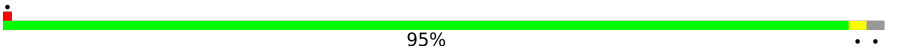
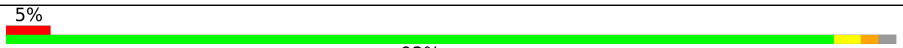
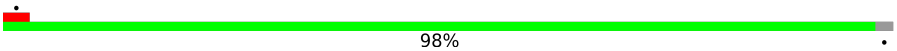
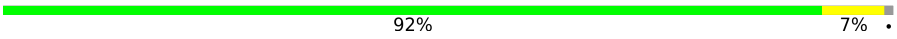
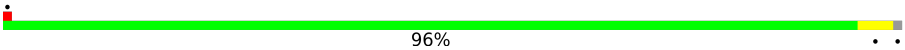
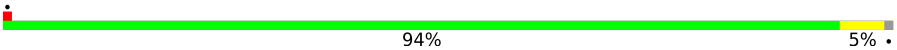
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
20	MM	189	
21	LN	172	
21	MN	172	
22	LO	160	
22	MO	160	
23	La	137	
23	Ma	137	
24	Lb	92	
24	Mb	92	
25	Lc	106	
25	Mc	106	
26	Ld	25	
26	Md	25	
27	Le	128	
27	Me	128	
28	Lf	51	
28	Mf	51	
29	Lg	78	
29	Mg	78	
30	Lh	88	
30	Mh	88	
31	Li	100	
31	Mi	100	
32	Lj	120	
32	Mj	120	

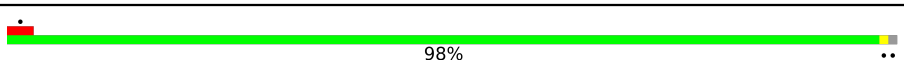
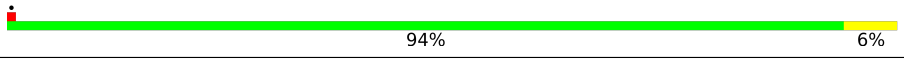
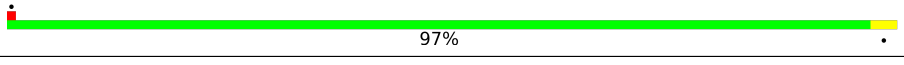
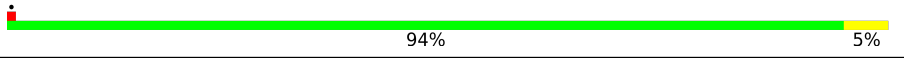
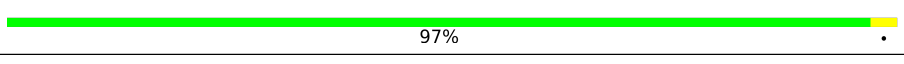
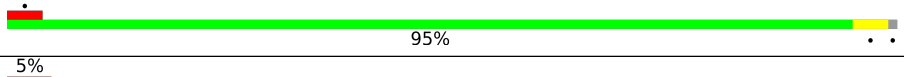
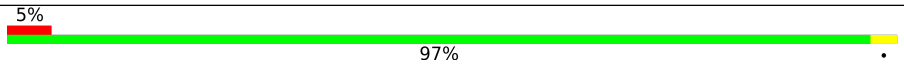
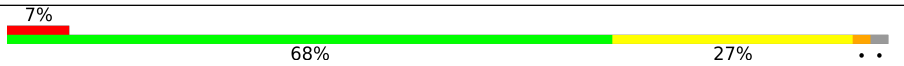
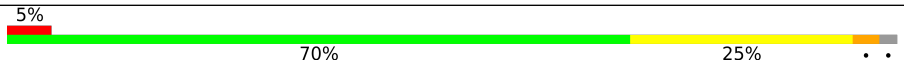
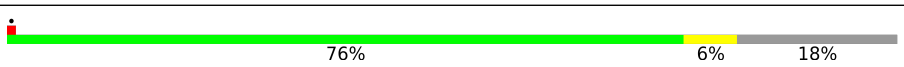
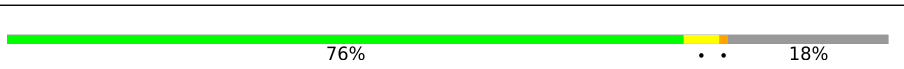
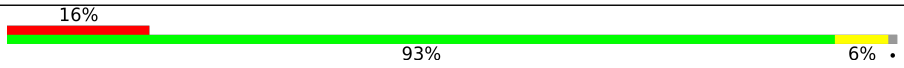
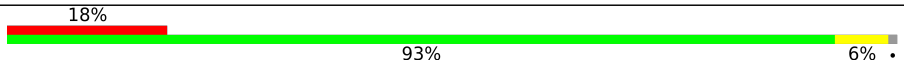
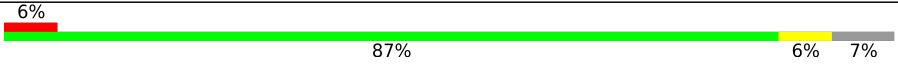
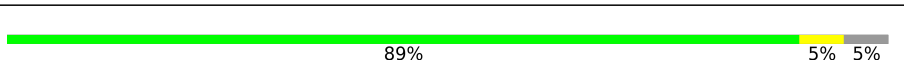
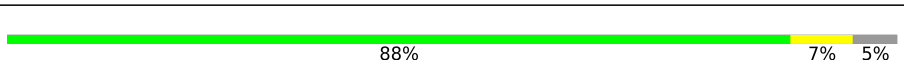
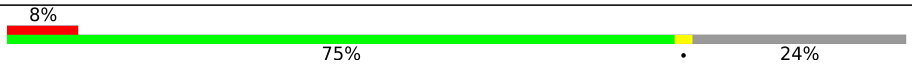
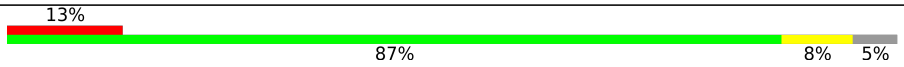
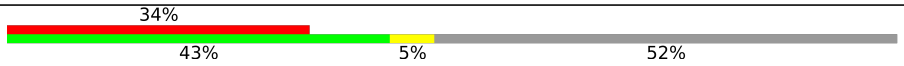
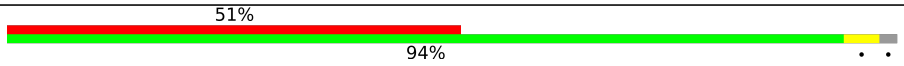
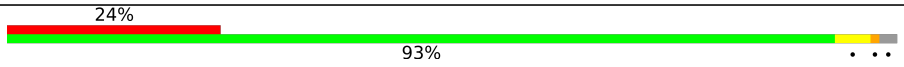
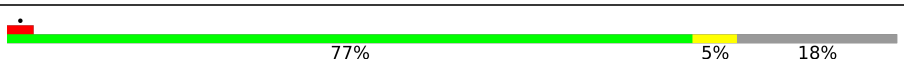
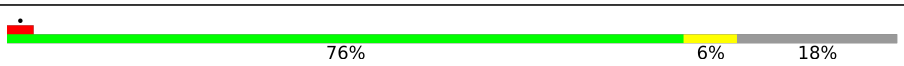
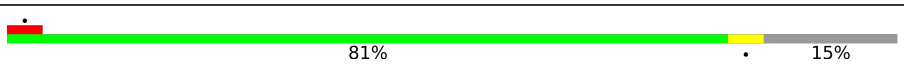
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	Lk	121	
33	Mk	121	
34	Ll	107	
34	Ml	107	
35	Lm	130	
35	Mm	130	
36	Ln	113	
36	Mn	113	
37	Lo	105	
37	Mo	105	
38	Lp	59	
38	Mp	59	
39	Lq	149	
39	Mq	149	
40	Lr	136	
40	Mr	136	
41	Ls	127	
41	Ms	127	
42	Lt	142	
42	Mt	142	
43	Lu	155	
43	Mu	155	
44	Lv	121	
44	Mv	121	
45	Lw	254	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
45	Mw	254	
46	Lx	387	
46	Mx	387	
47	Ly	362	
47	My	362	
48	Lz	297	
48	Mz	297	
49	R1	1800	
49	S1	1800	
50	RA	119	
50	SA	119	
51	RB	82	
51	SB	82	
52	SC	67	
53	RD	56	
53	SD	56	
54	RE	63	
54	SE	63	
55	RF	152	
55	SF	152	
56	RG	319	
56	SG	319	
57	Ra	252	
57	Sa	252	
58	Rb	255	

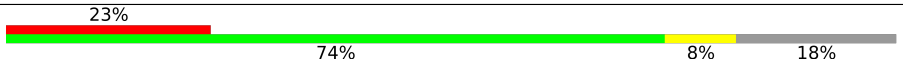
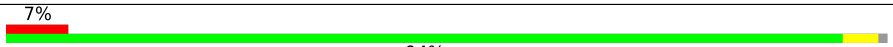
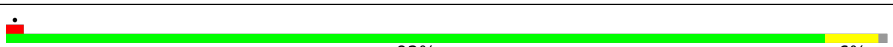
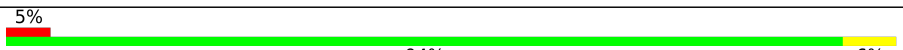
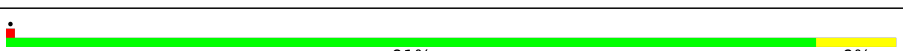
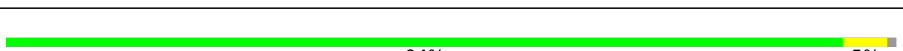
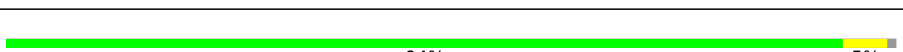
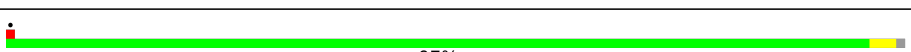
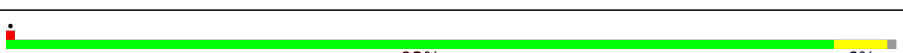
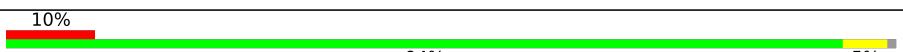
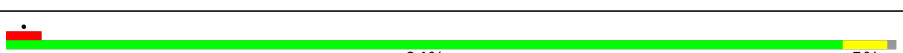
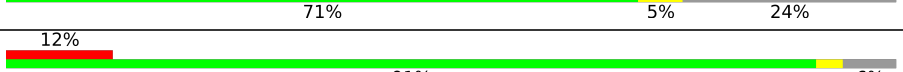
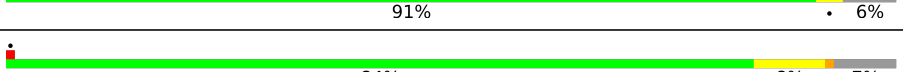
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	Sb	255	5% 80% 7% 11%
59	Rc	254	84% 15%
59	Sc	254	81% 15%
60	Rd	240	15% 85% 7% 7%
60	Sd	240	5% 87% 5% 8%
61	Re	261	96%
61	Se	261	94% 5%
62	Rf	225	12% 89% 8%
62	Sf	225	7% 88% 8%
63	Rg	236	9% 89% 8%
63	Sg	236	7% 90% 6%
64	Rh	190	22% 92% 5%
64	Sh	190	19% 89% 7%
65	Ri	200	92% 6%
65	Si	200	88% 6%
66	Rj	197	10% 89% 6%
66	Sj	197	87% 7% 7%
67	Rk	105	25% 82% 6% 12%
67	Sk	105	12% 73% 13% 12%
68	Rl	156	8% 88% 6% 6%
68	Sl	156	5% 87% 6% 8%
69	Rm	143	70% 80% 7% 13%
69	Sm	143	66% 73% 10% 15%
70	Rn	151	93% 5%
70	Sn	151	93% 7%

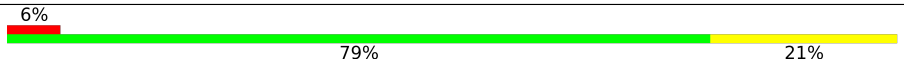
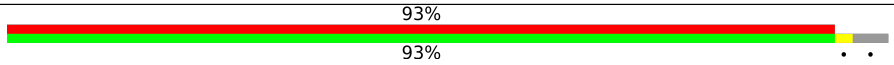
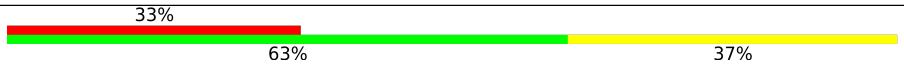
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
71	So	137	
72	Rp	142	
72	Sp	142	
73	Rq	143	
73	Sq	143	
74	Sr	136	
75	Rs	146	
75	Ss	146	
76	Rt	144	
76	St	144	
77	Ru	121	
77	Su	121	
78	Rv	87	
78	Sv	87	
79	Rw	130	
79	Sw	130	
80	Rx	145	
80	Sx	145	
81	Ry	135	
81	Sy	135	
82	Rz	108	
82	Sz	108	
83	RC	67	
84	Ro	138	
85	Rr	136	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
86	MA	176	
87	M1	3396	
88	DQ	77	
89	MQ	312	
90	MP	165	
91	DP	76	

2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 406583 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Uncharacterized protein YEL057C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CC	14	Total	C	N	O	S	0	0
			129	85	21	22	1		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CM	41	Total	C	N	O	P	0	0
			838	377	108	312	41		

- Molecule 3 is a protein called Multiprotein-bridging factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CN	136	Total	C	N	O	S	0	0
			1046	636	210	199	1		

- Molecule 4 is a RNA chain called tRNA P-site, stalled.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CP	76	Total	C	N	O	P	0	0
			1621	723	290	532	76		

- Molecule 5 is a RNA chain called Saccharomyces cerevisiae S288C 25S ribosomal RNA (RDN25-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L1	3116	Total	C	N	O	P	0	0
			66660	29774	12025	21745	3116		

- Molecule 6 is a RNA chain called Saccharomyces cerevisiae S288C 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M2	158	Total 3353	C 1500	N 586	O 1109	P 158	0	0

- Molecule 7 is a RNA chain called Saccharomyces cerevisiae S288C 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L3	121	Total 2579	C 1152	N 461	O 845	P 121	0	0
7	M3	121	Total 2579	C 1152	N 461	O 845	P 121	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	LA	167	Total 1305	C 842	N 234	O 229	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LB	222	Total 1784	C 1151	N 324	O 308	S 1	0	0
9	MB	222	Total 1784	C 1151	N 324	O 308	S 1	0	0

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LC	233	Total 1804	C 1151	N 323	O 327	S 3	0	0
10	MC	233	Total 1804	C 1151	N 323	O 327	S 3	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LD	191	Total 1508	C 957	N 274	O 273	S 4	0	0
11	MD	191	Total 1518	C 963	N 274	O 277	S 4	0	0

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LE	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		
12	ME	215	Total	C	N	O	S	0	0
			1743	1102	331	303	7		

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LF	169	Total	C	N	O	S	0	0
			1350	846	253	247	4		
13	MF	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	LG	193	Total	C	N	O	0	0
			1543	962	315	266		
14	MG	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LH	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		
15	MH	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LI	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		
16	MI	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LJ	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
17	MJ	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	LK	183	Total	C	N	O	0	0
			1416	879	284	253		
18	MK	154	Total	C	N	O	0	0
			1222	761	237	224		

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LL	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		
19	ML	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	LM	188	Total	C	N	O	0	0
			1515	932	323	260		
20	MM	176	Total	C	N	O	0	0
			1423	875	308	240		

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LN	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		
21	MN	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LO	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		
22	MO	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 23 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	La	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		
23	Ma	129	Total	C	N	O	S	0	0
			963	607	180	169	7		

- Molecule 24 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Lb	91	Total	C	N	O	S	0	0
			694	429	138	121	6		
24	Mb	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 25 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Lc	103	Total	C	N	O	S	0	0
			824	517	167	135	5		
25	Mc	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 26 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ld	25	Total	C	N	O	S	0	0
			229	139	62	27	1		
26	Md	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 27 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Le	52	Total	C	N	O	S	0	0
			417	259	86	67	5		
27	Me	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 28 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Lf	50	Total	C	N	O	S	0	0
			436	272	97	65	2		
28	Mf	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 29 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Lg	77	Total	C	N	O	0	0
			612	391	115	106		
29	Mg	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 30 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lh	85	Total	C	N	O	S	0	0
			670	408	146	111	5		
30	Mh	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 31 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Li	99	Total	C	N	O	S	0	0
			766	478	154	132	2		
31	Mi	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 32 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lj	119	Total	C	N	O	S	0	0
			969	615	186	167	1		
32	Mj	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 33 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lk	106	Total	C	N	O	S	0	0
			836	519	171	142	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Mk	109	Total 861	C 533	N 175	O 149	S 4	0	0

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ll	106	Total 850	C 540	N 165	O 144	S 1	0	0
34	Ml	106	Total 850	C 540	N 165	O 144	S 1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lm	127	Total 1017	C 644	N 205	O 167	S 1	0	0
35	Mm	127	Total 1020	C 647	N 205	O 167	S 1	0	0

- Molecule 36 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ln	109	Total 876	C 556	N 167	O 152	S 1	0	0
36	Mn	109	Total 883	C 559	N 167	O 156	S 1	0	0

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lo	96	Total 737	C 476	N 123	O 137	S 1	0	0
37	Mo	97	Total 742	C 479	N 124	O 138	S 1	0	0

- Molecule 38 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Lp	58	Total 462	C 289	N 100	O 73	0	0
38	Mp	58	Total 462	C 289	N 100	O 73	0	0

- Molecule 39 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lq	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		
39	Mq	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 40 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	Lr	135	Total	C	N	O	0	0
			1092	710	202	180		
40	Mr	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 41 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Ls	125	Total	C	N	O	0	0
			984	620	191	173		
41	Ms	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 42 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lt	121	Total	C	N	O	S	0	0
			964	620	169	173	2		
42	Mt	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 43 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lu	126	Total	C	N	O	S	0	0
			836	525	165	145	1		
43	Mu	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 44 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	Lv	100	Total 796	C 516	N 131	O 149	0	0
44	Mv	97	Total 770	C 499	N 126	O 145	0	0

- Molecule 45 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lw	251	Total 1899	C 1182	N 385	O 331	S 1	0	0
45	Mw	252	Total 1914	C 1191	N 388	O 334	S 1	0	0

- Molecule 46 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lx	386	Total 3075	C 1950	N 584	O 533	S 8	0	0
46	Mx	386	Total 3075	C 1950	N 584	O 533	S 8	0	0

- Molecule 47 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ly	361	Total 2748	C 1729	N 522	O 494	S 3	0	0
47	My	361	Total 2748	C 1729	N 522	O 494	S 3	0	0

- Molecule 48 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lz	294	Total 2351	C 1484	N 410	O 455	S 2	0	0
48	Mz	296	Total 2375	C 1501	N 414	O 458	S 2	0	0

- Molecule 49 is a RNA chain called Saccharomyces cerevisiae S288C 18S ribosomal RNA (RDN18-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S1	1771	Total 37739	C 16872	N 6683	O 12413	P 1771	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
49	R1	1758	Total 37455	C 16745	N 6624	O 12328	P 1758	0	0

- Molecule 50 is a protein called Small ribosomal subunit protein eS26A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SA	97	Total 769	C 475	N 160	O 129	S 5	0	0
50	RA	97	Total 769	C 475	N 160	O 129	S 5	0	0

- Molecule 51 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SB	81	Total 610	C 382	N 110	O 113	S 5	0	0
51	RB	81	Total 610	C 382	N 110	O 113	S 5	0	0

- Molecule 52 is a protein called Small ribosomal subunit protein eS28B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SC	62	Total 486	C 300	N 95	O 90	S 1	0	0

- Molecule 53 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SD	53	Total 442	C 274	N 92	O 72	S 4	0	0
53	RD	53	Total 442	C 274	N 92	O 72	S 4	0	0

- Molecule 54 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SE	60	Total 472	C 298	N 97	O 76	S 1	0	0
54	RE	48	Total 385	C 246	N 77	O 62		0	0

- Molecule 55 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SF	73	Total	C	N	O	S	0	0
			556	352	105	95	4		
55	RF	72	Total	C	N	O	S	0	0
			547	347	104	92	4		

- Molecule 56 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SG	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		
56	RG	313	Total	C	N	O	S	0	0
			2403	1521	411	463	8		

- Molecule 57 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Sa	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		
57	Ra	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 58 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Sb	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		
58	Rb	216	Total	C	N	O	S	0	0
			1722	1091	312	315	4		

- Molecule 59 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Sc	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		
59	Rc	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 60 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Sd	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Rd	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 61 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Se	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		
61	Re	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 62 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Sf	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		
62	Rf	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 63 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sg	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		
63	Rg	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 64 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	Sh	184	Total	C	N	O	0	0
			1473	946	263	264		
64	Rh	185	Total	C	N	O	0	0
			1486	954	266	266		

- Molecule 65 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Si	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		
65	Ri	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 66 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sj	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		
66	Rj	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 67 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Sk	92	Total	C	N	O	S	0	0
			752	487	122	141	2		
67	Rk	92	Total	C	N	O	S	0	0
			741	478	121	140	2		

- Molecule 68 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Sl	144	Total	C	N	O	S	0	0
			1159	742	219	195	3		
68	Rl	146	Total	C	N	O	S	0	0
			1168	747	221	197	3		

- Molecule 69 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Sm	121	Total	C	N	O	S	0	0
			875	551	153	169	2		
69	Rm	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 70 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Sn	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		
70	Rn	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 71 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	So	127	Total	C	N	O	S	0	0
			926	569	185	169	3		

- Molecule 72 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sp	117	Total	C	N	O	S	0	0
			916	583	171	155	7		
72	Rp	119	Total	C	N	O	S	0	0
			939	595	176	161	7		

- Molecule 73 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	Sq	141	Total	C	N	O	0	0
			1105	708	203	194		
73	Rq	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 74 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sr	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 75 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Ss	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		
75	Rs	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 76 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	St	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		
76	Rt	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 77 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Su	100	Total	C	N	O	S	0	0
			797	506	144	146	1		
77	Ru	101	Total	C	N	O	S	0	0
			805	512	145	147	1		

- Molecule 78 is a protein called Small ribosomal subunit protein eS21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sv	87	Total	C	N	O	S	0	0
			673	415	125	131	2		
78	Rv	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 79 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sw	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		
79	Rw	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 80 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sx	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		
80	Rx	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 81 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	Sy	134	Total	C	N	O	0	0
			1073	676	208	189		
81	Ry	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 82 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Sz	82	Total	C	N	O	0	0
			651	416	123	112		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Rz	69	Total 558	C 357	N 103	O 98	0	0

- Molecule 83 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	RC	63	Total 497	C 306	N 99	O 91	S 1	0	0

- Molecule 84 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ro	128	Total 949	C 582	N 188	O 176	S 3	0	0

- Molecule 85 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Rr	125	Total 1000	C 625	N 188	O 185	S 2	0	0

- Molecule 86 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	MA	155	Total 1230	C 795	N 221	O 213	S 1	0	0

- Molecule 87 is a RNA chain called Saccharomyces cerevisiae S288C 18S ribosomal RNA (RDN18-1) with modifications.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	M1	3190	Total 68285	C 30524	N 12313	O 22258	P 3190	0	0

- Molecule 88 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	DQ	77	Total 1644	C 732	N 298	O 537	P 77	0	0

- Molecule 89 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	MQ	197	Total	C	N	O	S	0	0
			1531	980	266	281	4		

- Molecule 90 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	MP	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 91 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	DP	76	Total	C	N	O	P	0	0
			1638	736	294	533	75		

- Molecule 92 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
92	CP	1	Total	Mg	0
			1	1	
92	S1	84	Total	Mg	0
			84	84	
92	Sf	1	Total	Mg	0
			1	1	
92	Sx	1	Total	Mg	0
			1	1	
92	M1	194	Total	Mg	0
			194	194	
92	MK	1	Total	Mg	0
			1	1	
92	M3	4	Total	Mg	0
			4	4	
92	M2	3	Total	Mg	0
			3	3	
92	MM	1	Total	Mg	0
			1	1	
92	Mx	1	Total	Mg	0
			1	1	
92	Ma	1	Total	Mg	0
			1	1	
92	ME	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
92	MI	2	Total Mg 2 2	0

- Molecule 93 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
93	Lb	1	Total Zn 1 1	0
93	Lc	1	Total Zn 1 1	0
93	Le	1	Total Zn 1 1	0
93	Lh	1	Total Zn 1 1	0
93	Lk	1	Total Zn 1 1	0
93	SD	1	Total Zn 1 1	0
93	SF	1	Total Zn 1 1	0
93	RB	1	Total Zn 1 1	0
93	Mk	1	Total Zn 1 1	0
93	Mh	1	Total Zn 1 1	0
93	Me	1	Total Zn 1 1	0
93	Mc	1	Total Zn 1 1	0
93	Mb	1	Total Zn 1 1	0

- Molecule 94 is POTASSIUM ION (three-letter code: K) (formula: K).

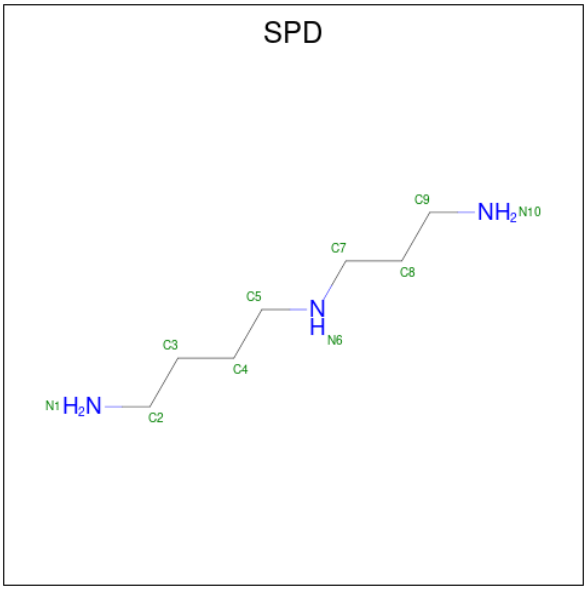
Mol	Chain	Residues	Atoms	AltConf
94	M1	11	Total K 11 11	0
94	Mw	1	Total K 1 1	0
94	ME	1	Total K 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
94	Mm	1	Total K 1 1	0
94	Mk	1	Total K 1 1	0
94	Mc	1	Total K 1 1	0

- Molecule 95 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



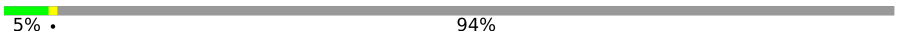
Mol	Chain	Residues	Atoms	AltConf
95	M1	1	Total C N 10 7 3	0
95	M1	1	Total C N 10 7 3	0
95	M1	1	Total C N 10 7 3	0

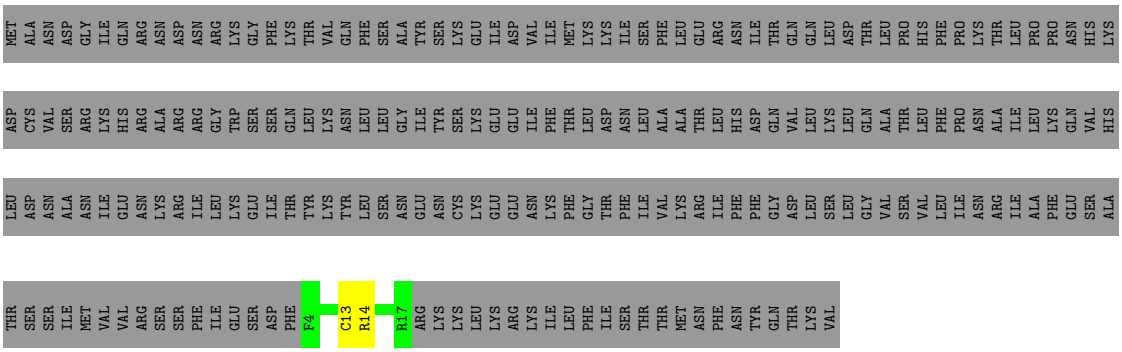
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Uncharacterized protein YEL057C

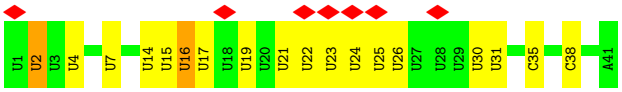
Chain CC:





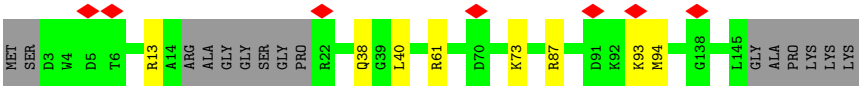
• Molecule 2: mRNA

Chain CM:



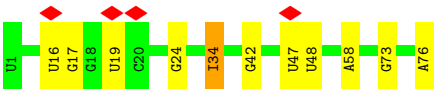
• Molecule 3: Multiprotein-bridging factor 1

Chain CN:



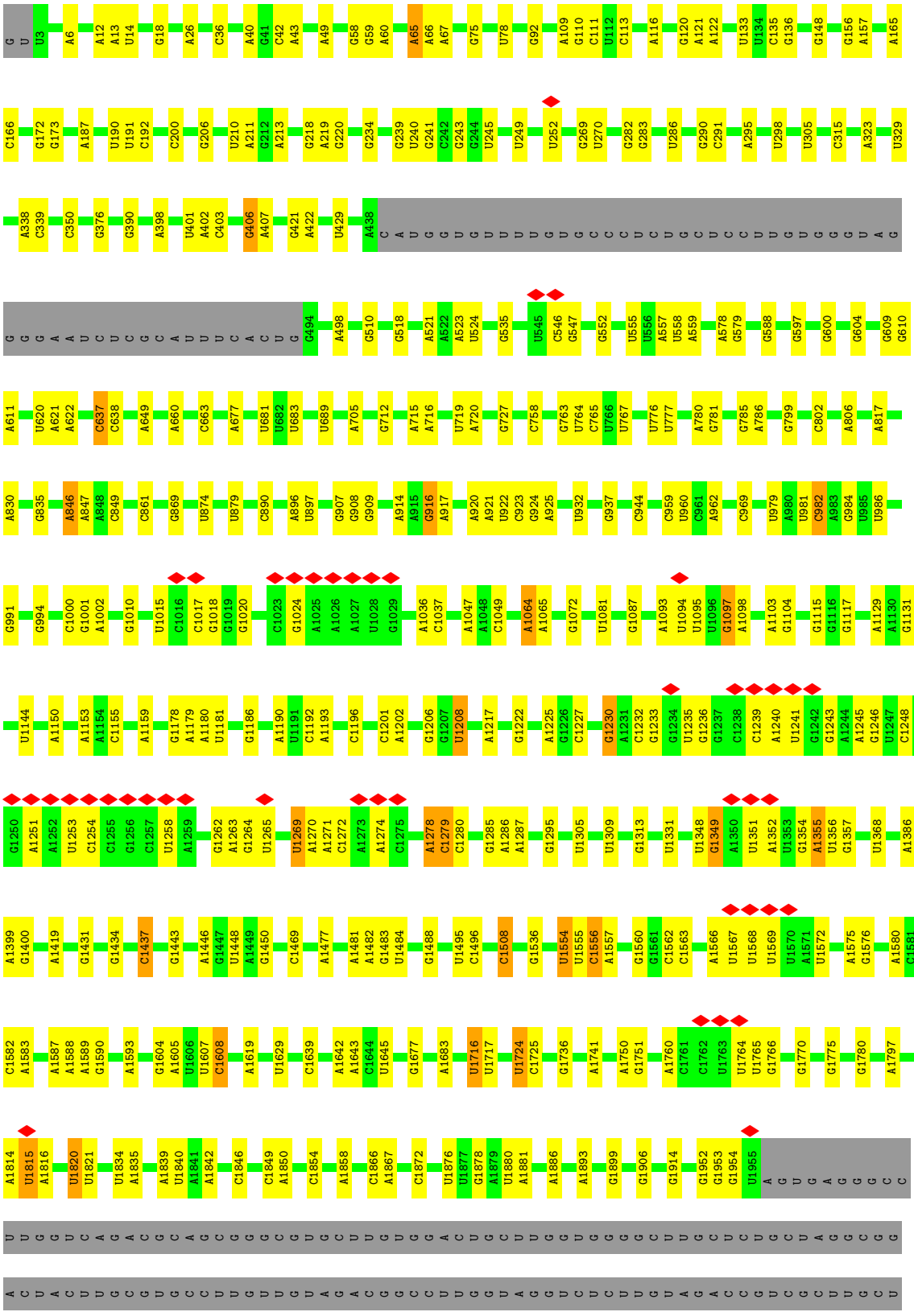
• Molecule 4: tRNA P-site, stalled

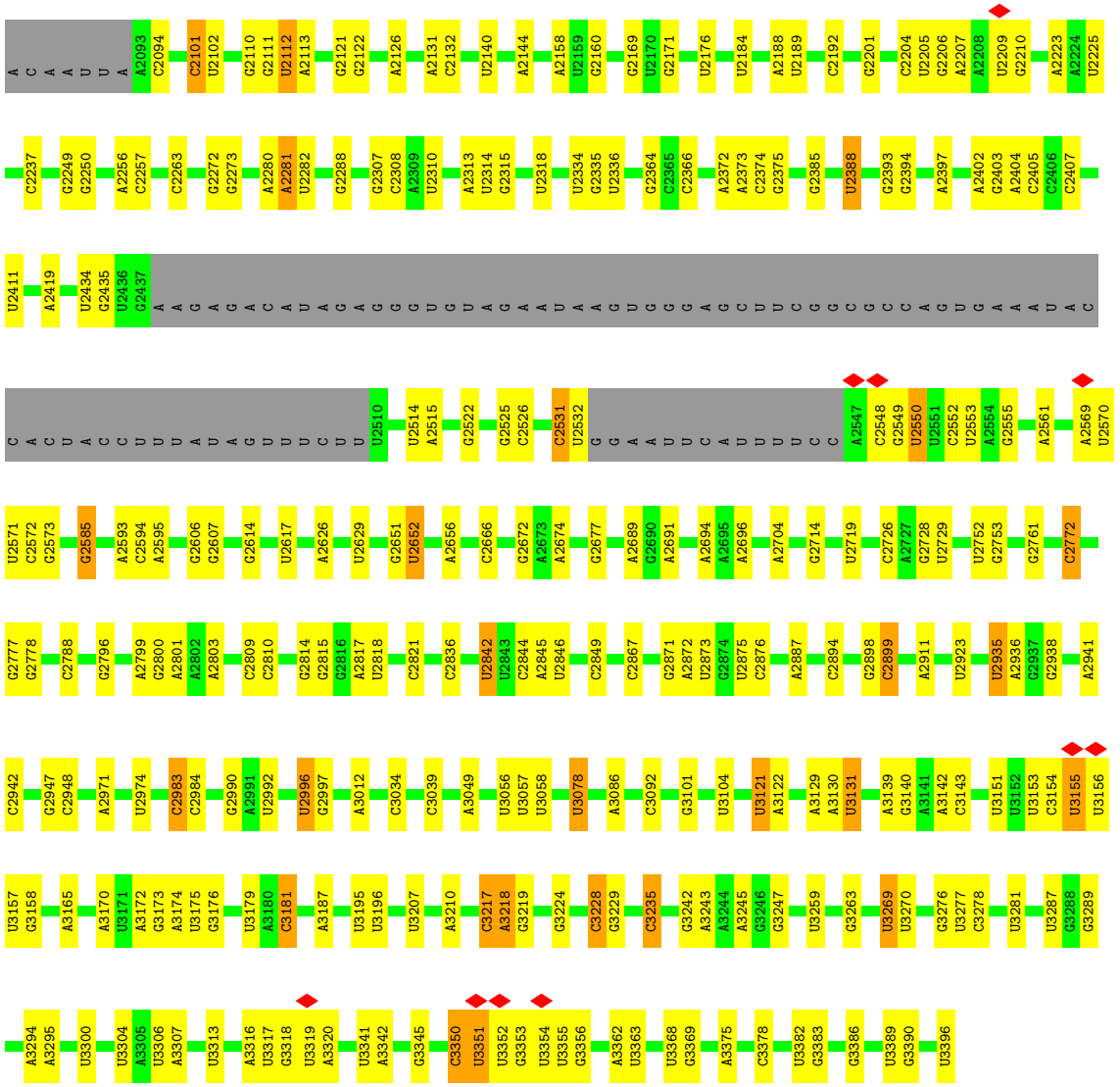
Chain CP:



• Molecule 5: Saccharomyces cerevisiae S288C 25S ribosomal RNA (RDN25-1)

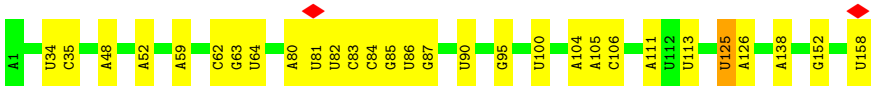
Chain L1:





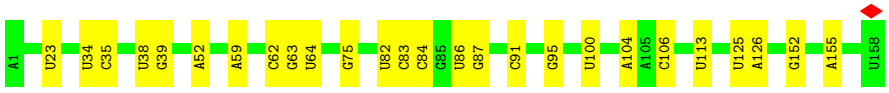
• Molecule 6: Saccharomyces cerevisiae S288C 5.8S ribosomal RNA

Chain L2:



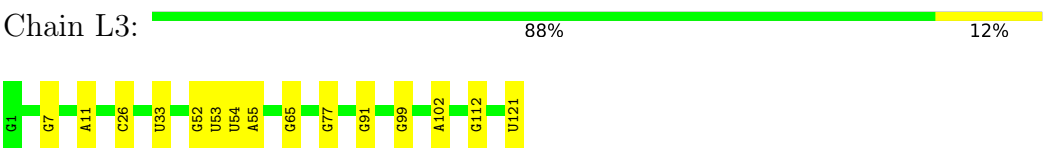
• Molecule 6: Saccharomyces cerevisiae S288C 5.8S ribosomal RNA

Chain M2:



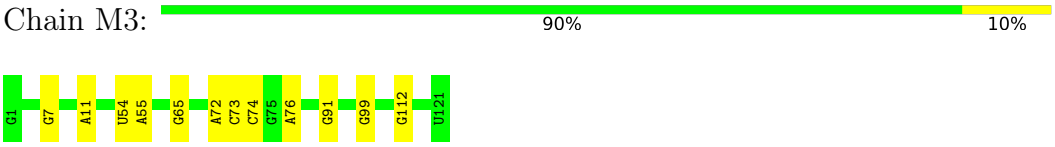
• Molecule 7: Saccharomyces cerevisiae S288C 5S ribosomal RNA

Chain L3:



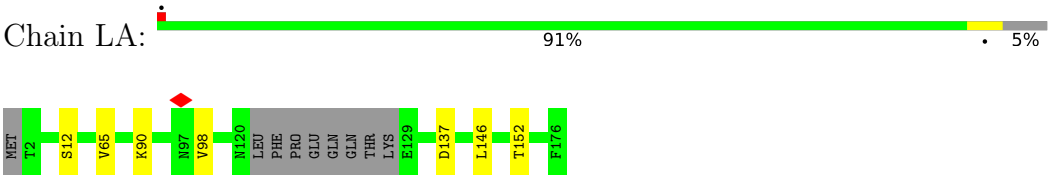
• Molecule 7: Saccharomyces cerevisiae S288C 5S ribosomal RNA

Chain M3:



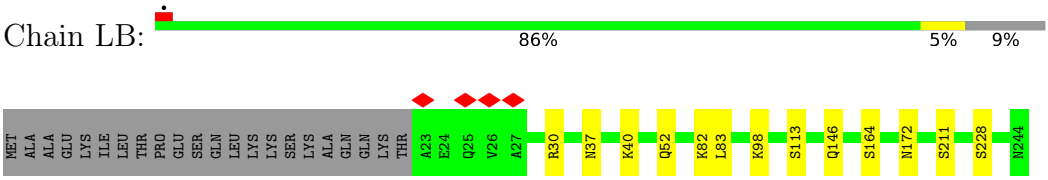
• Molecule 8: 60S ribosomal protein L6-B

Chain LA:



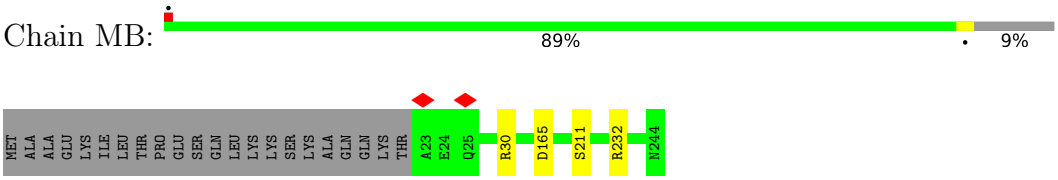
• Molecule 9: 60S ribosomal protein L7-A

Chain LB:



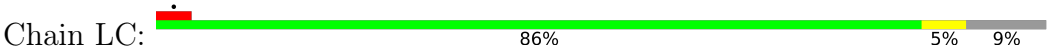
• Molecule 9: 60S ribosomal protein L7-A

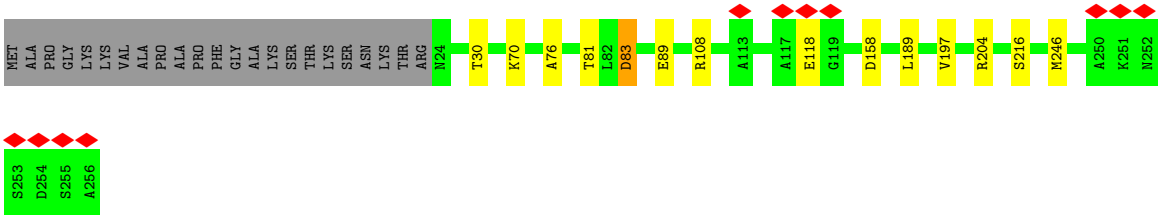
Chain MB:



• Molecule 10: 60S ribosomal protein L8-A

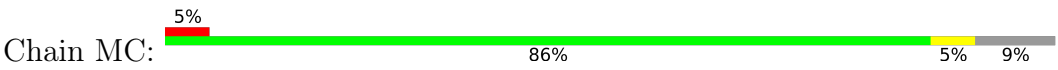
Chain LC:

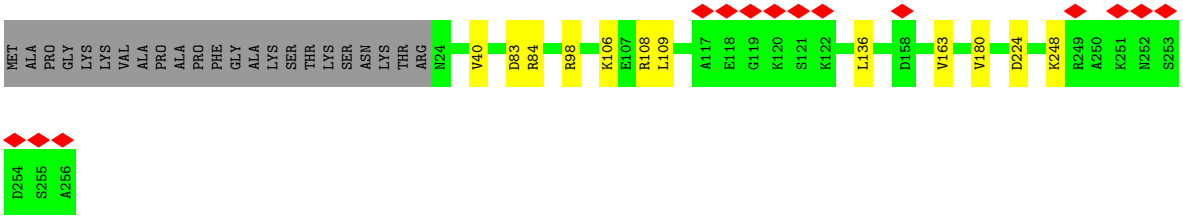




• Molecule 10: 60S ribosomal protein L8-A

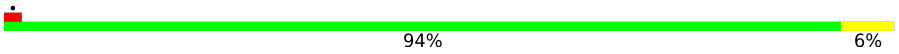
Chain MC:

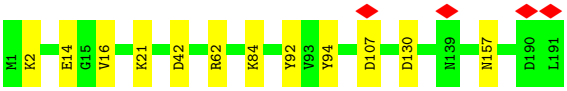




• Molecule 11: 60S ribosomal protein L9-A

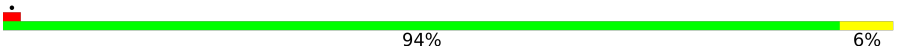
Chain LD:

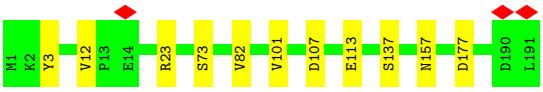




• Molecule 11: 60S ribosomal protein L9-A

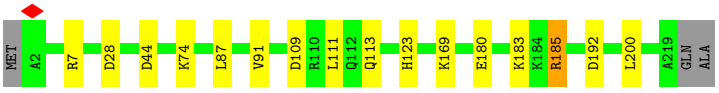
Chain MD:





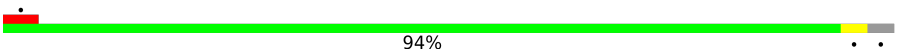
• Molecule 12: 60S ribosomal protein L10

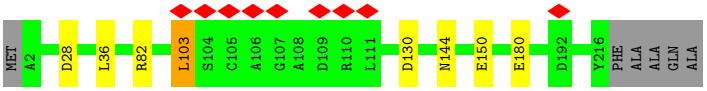
Chain LE:



• Molecule 12: 60S ribosomal protein L10

Chain ME:



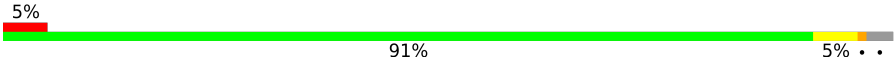


• Molecule 13: 60S ribosomal protein L11-A

Chain LF:

• Molecule 13: 60S ribosomal protein L11-A

Chain MF:

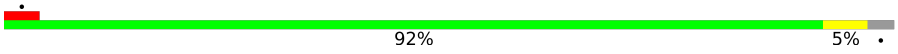


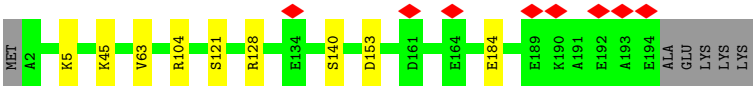
• Molecule 14: 60S ribosomal protein L13-A

Chain LG:

• Molecule 14: 60S ribosomal protein L13-A

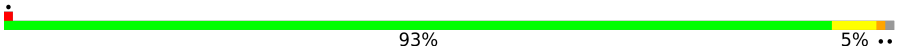
Chain MG:

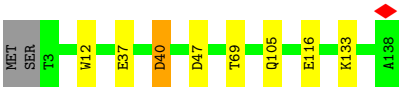




• Molecule 15: 60S ribosomal protein L14-A

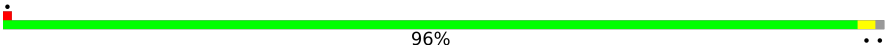
Chain LH:

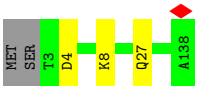




• Molecule 15: 60S ribosomal protein L14-A

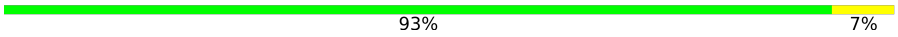
Chain MH:

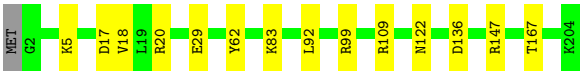




• Molecule 16: 60S ribosomal protein L15-A

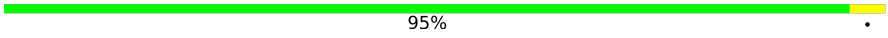
Chain LI:





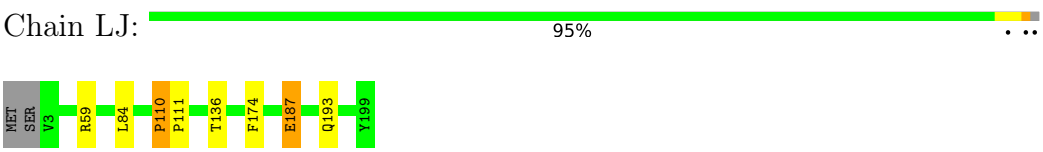
• Molecule 16: 60S ribosomal protein L15-A

Chain MI:



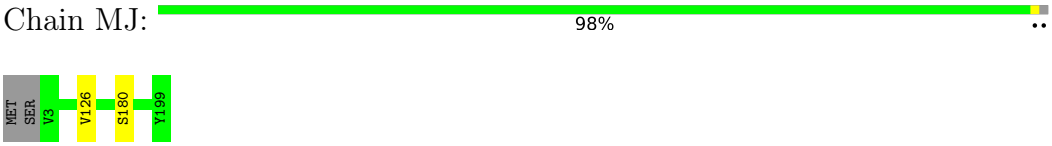
• Molecule 17: 60S ribosomal protein L16-A

Chain LJ:



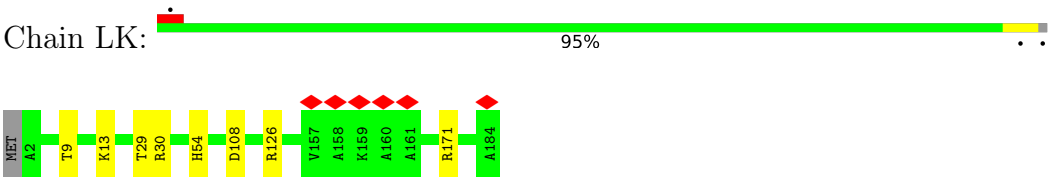
• Molecule 17: 60S ribosomal protein L16-A

Chain MJ:



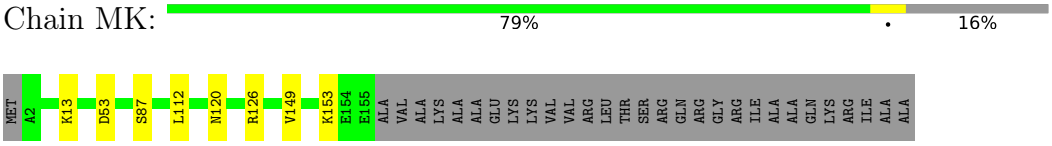
• Molecule 18: 60S ribosomal protein L17-A

Chain LK:



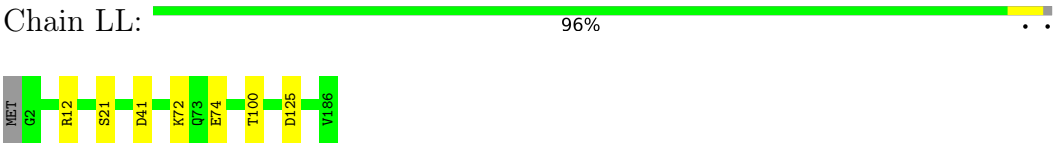
• Molecule 18: 60S ribosomal protein L17-A

Chain MK:



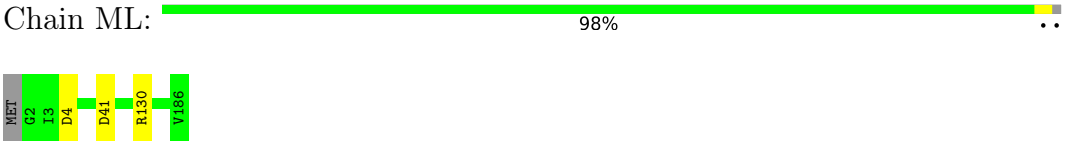
• Molecule 19: 60S ribosomal protein L18-A

Chain LL:



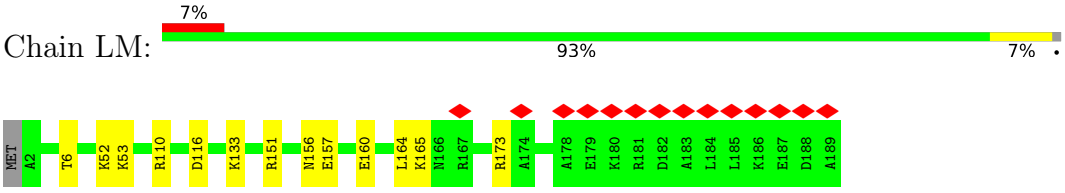
• Molecule 19: 60S ribosomal protein L18-A

Chain ML:



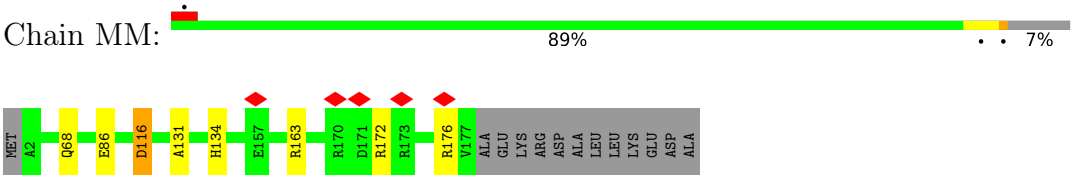
• Molecule 20: 60S ribosomal protein L19-A

Chain LM:



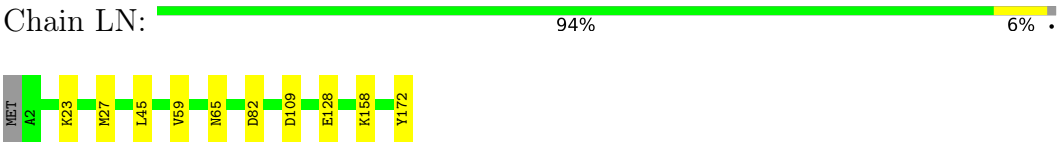
• Molecule 20: 60S ribosomal protein L19-A

Chain MM:



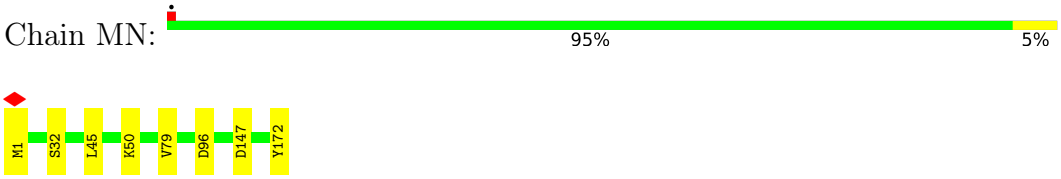
• Molecule 21: 60S ribosomal protein L20-A

Chain LN:



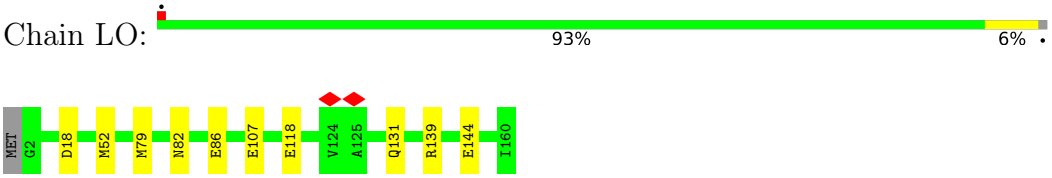
• Molecule 21: 60S ribosomal protein L20-A

Chain MN:



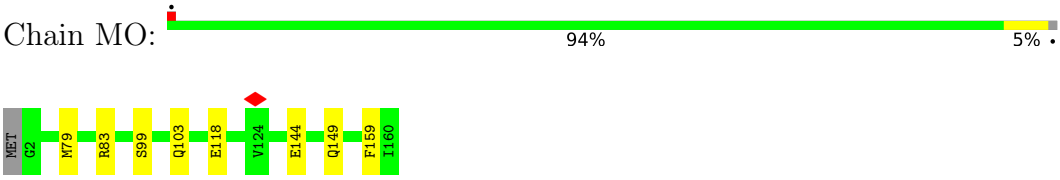
• Molecule 22: 60S ribosomal protein L21-A

Chain LO:



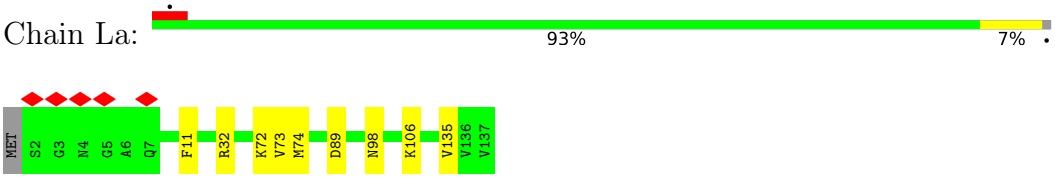
• Molecule 22: 60S ribosomal protein L21-A

Chain MO:



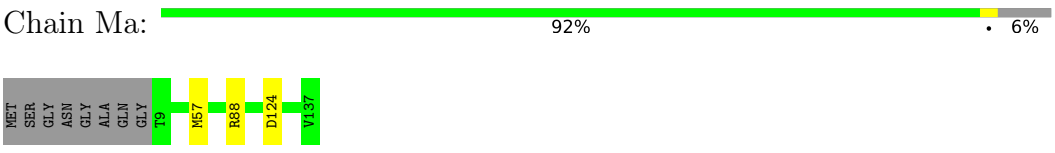
• Molecule 23: 60S ribosomal protein L23-A

Chain La:



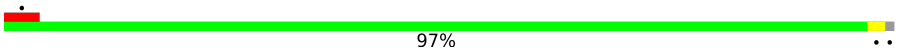
• Molecule 23: 60S ribosomal protein L23-A

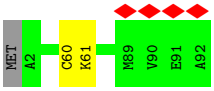
Chain Ma:



• Molecule 24: 60S ribosomal protein L43-A

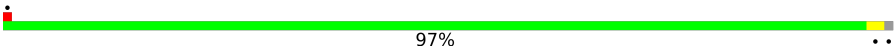
Chain Lb:

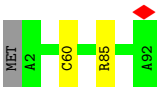




• Molecule 24: 60S ribosomal protein L43-A

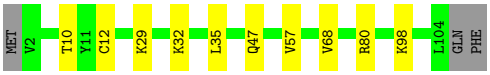
Chain Mb:





• Molecule 25: 60S ribosomal protein L42-A

Chain Lc:

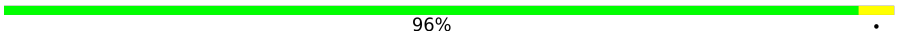


• Molecule 25: 60S ribosomal protein L42-A

Chain Mc:

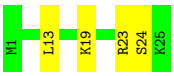
• Molecule 26: 60S ribosomal protein L41-A

Chain Ld:



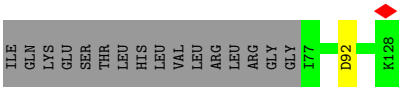
• Molecule 26: 60S ribosomal protein L41-A

Chain Md:



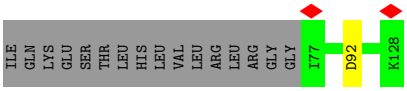
• Molecule 27: Ubiquitin-60S ribosomal protein L40

Chain Le:



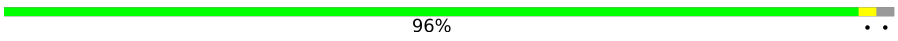
• Molecule 27: Ubiquitin-60S ribosomal protein L40

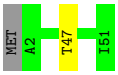
Chain Me:



• Molecule 28: 60S ribosomal protein L39

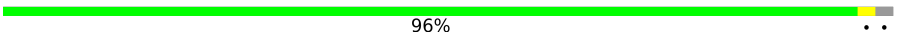
Chain Lf:

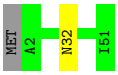




• Molecule 28: 60S ribosomal protein L39

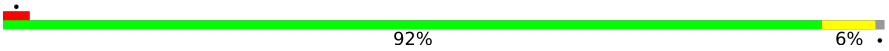
Chain Mf:

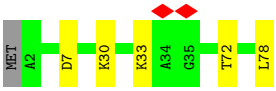




• Molecule 29: 60S ribosomal protein L38

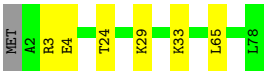
Chain Lg:





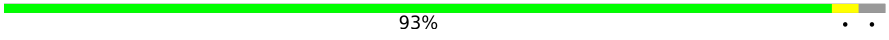
• Molecule 29: 60S ribosomal protein L38

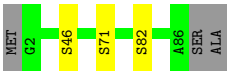
Chain Mg:



• Molecule 30: 60S ribosomal protein L37-A

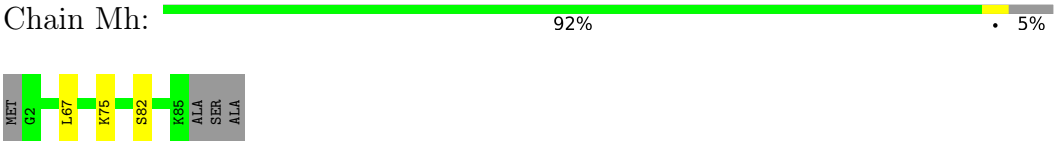
Chain Lh:





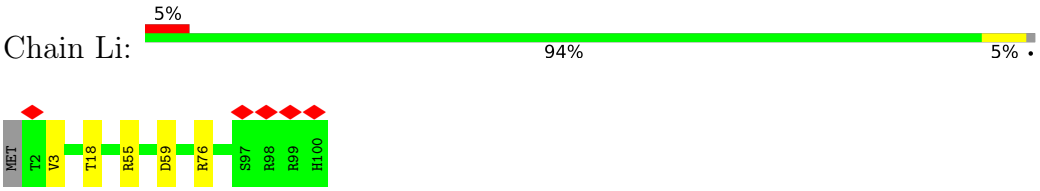
• Molecule 30: 60S ribosomal protein L37-A

Chain Mh:



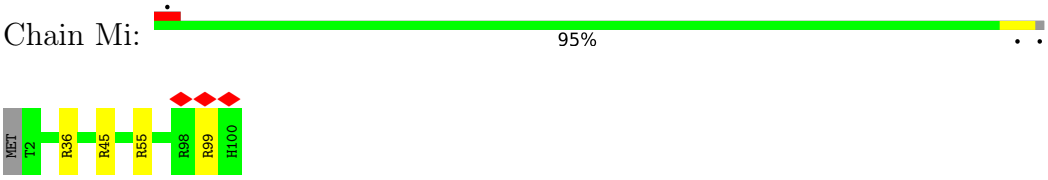
• Molecule 31: 60S ribosomal protein L36-A

Chain Li:



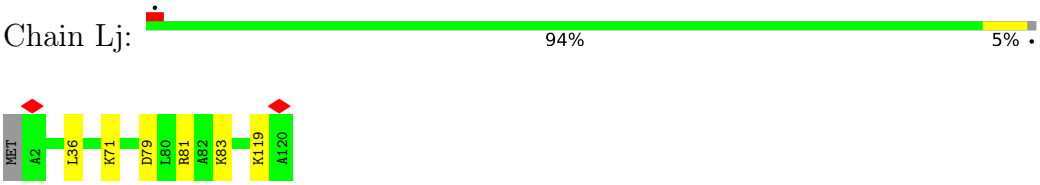
• Molecule 31: 60S ribosomal protein L36-A

Chain Mi:



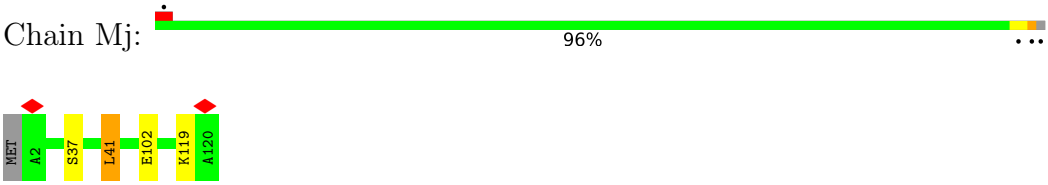
• Molecule 32: 60S ribosomal protein L35-A

Chain Lj:



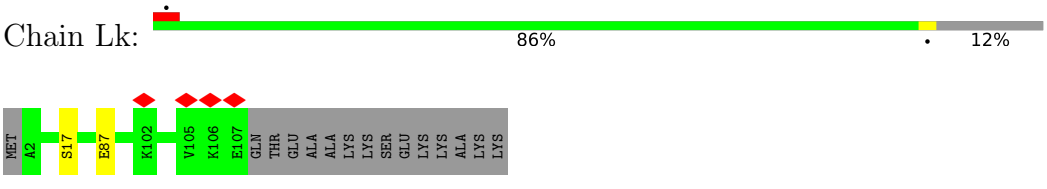
• Molecule 32: 60S ribosomal protein L35-A

Chain Mj:



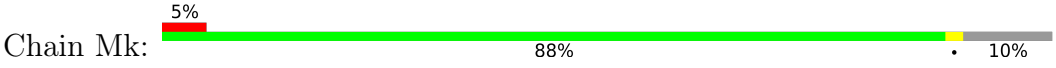
• Molecule 33: 60S ribosomal protein L34-A

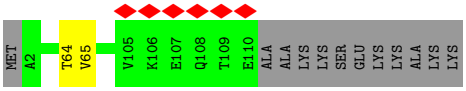
Chain Lk:



• Molecule 33: 60S ribosomal protein L34-A

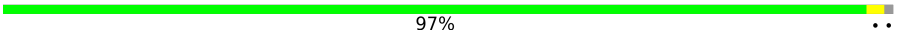
Chain Mk:





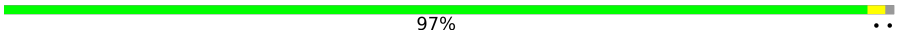
• Molecule 34: 60S ribosomal protein L33-A

Chain Ll:



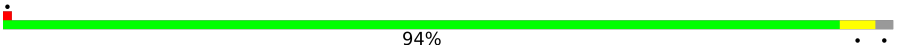
• Molecule 34: 60S ribosomal protein L33-A

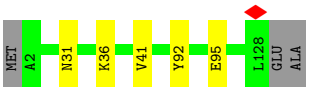
Chain Ml:



• Molecule 35: 60S ribosomal protein L32

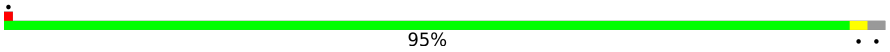
Chain Lm:

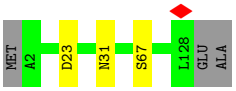




• Molecule 35: 60S ribosomal protein L32

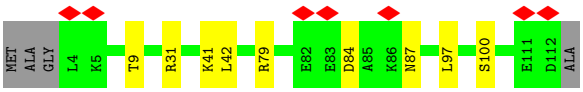
Chain Mm:





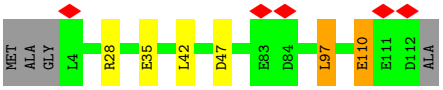
• Molecule 36: 60S ribosomal protein L31-A

Chain Ln:



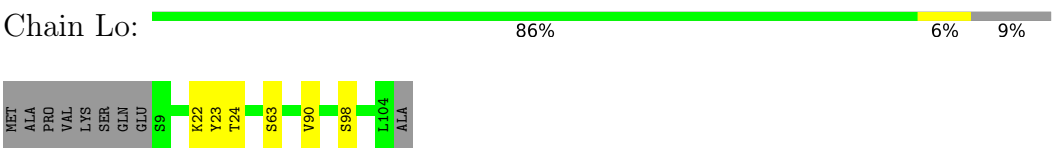
• Molecule 36: 60S ribosomal protein L31-A

Chain Mn:



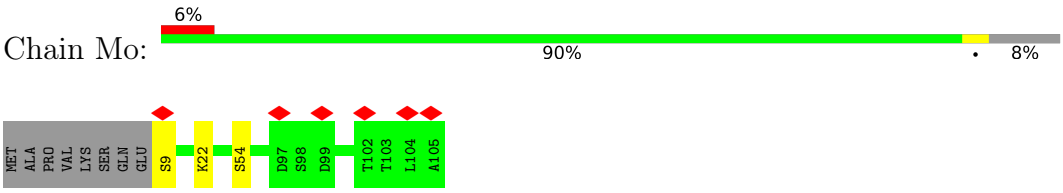
• Molecule 37: 60S ribosomal protein L30

Chain Lo:



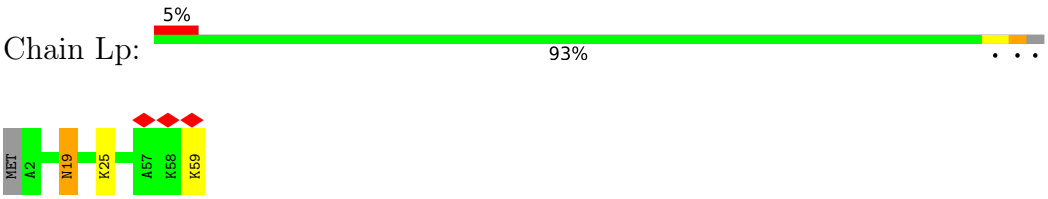
• Molecule 37: 60S ribosomal protein L30

Chain Mo:



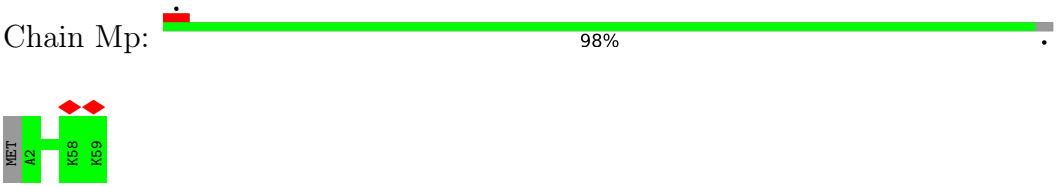
• Molecule 38: 60S ribosomal protein L29

Chain Lp:



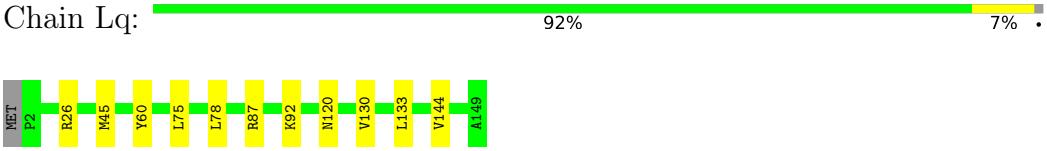
• Molecule 38: 60S ribosomal protein L29

Chain Mp:



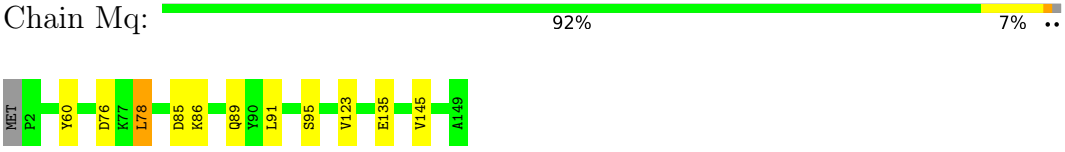
• Molecule 39: 60S ribosomal protein L28

Chain Lq:



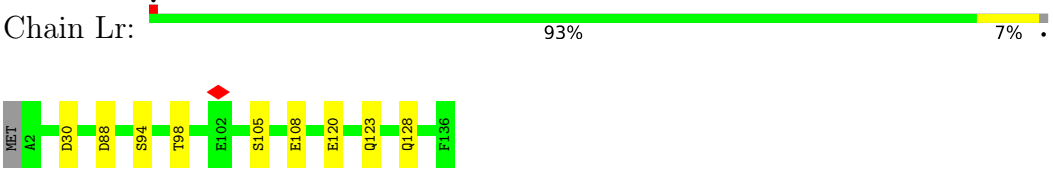
• Molecule 39: 60S ribosomal protein L28

Chain Mq:



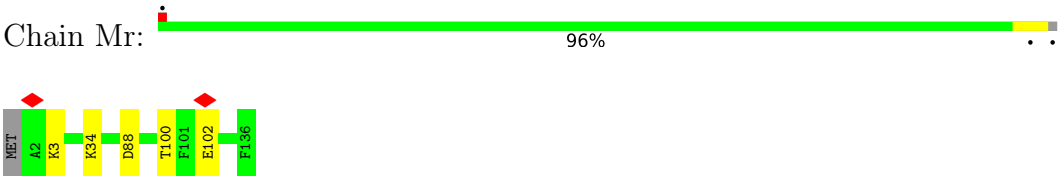
• Molecule 40: 60S ribosomal protein L27-A

Chain Lr:



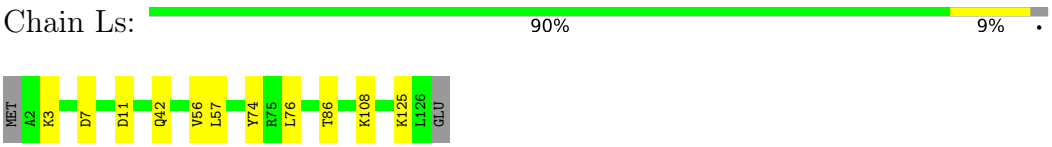
• Molecule 40: 60S ribosomal protein L27-A

Chain Mr:



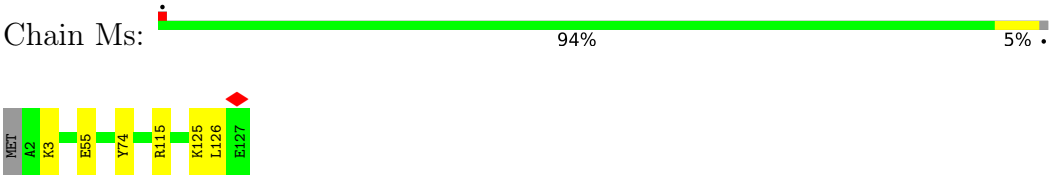
• Molecule 41: 60S ribosomal protein L26-A

Chain Ls:



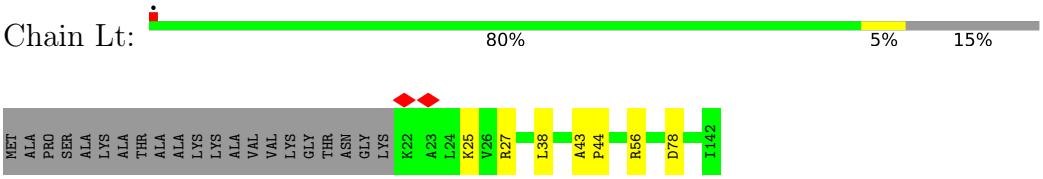
• Molecule 41: 60S ribosomal protein L26-A

Chain Ms:



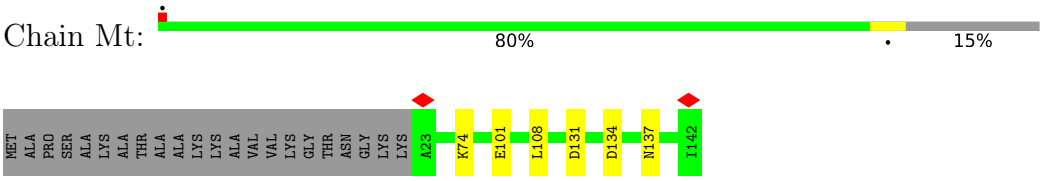
• Molecule 42: 60S ribosomal protein L25

Chain Lt:



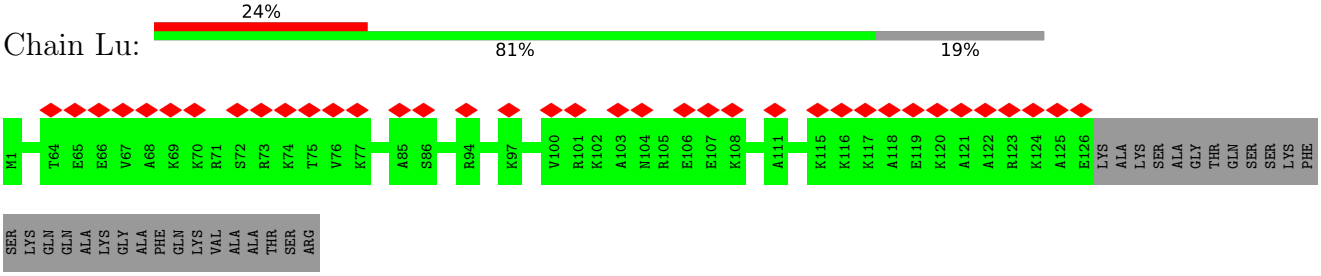
• Molecule 42: 60S ribosomal protein L25

Chain Mt:



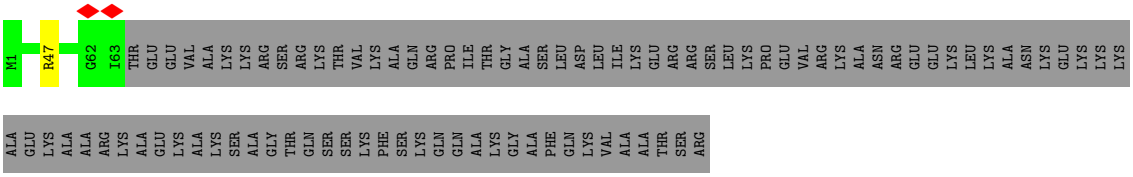
• Molecule 43: 60S ribosomal protein L24-A

Chain Lu:

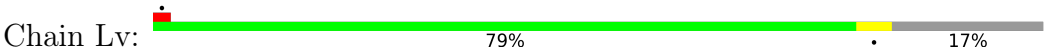


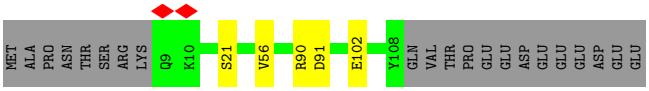
• Molecule 43: 60S ribosomal protein L24-A

Chain Mu:

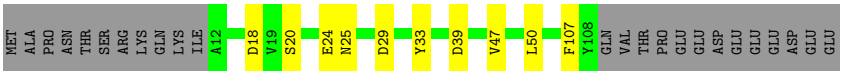


• Molecule 44: 60S ribosomal protein L22-A

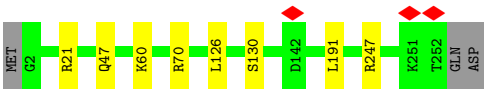




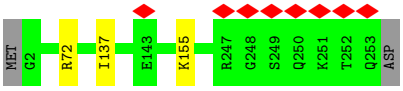
• Molecule 44: 60S ribosomal protein L22-A



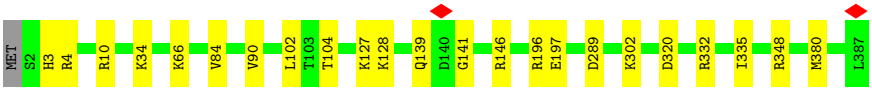
• Molecule 45: 60S ribosomal protein L2-A



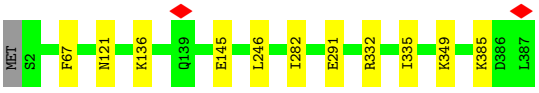
• Molecule 45: 60S ribosomal protein L2-A



• Molecule 46: 60S ribosomal protein L3

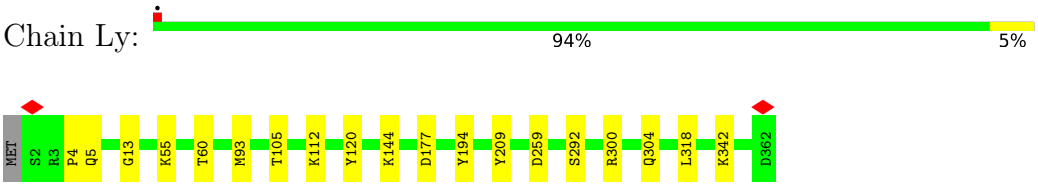


• Molecule 46: 60S ribosomal protein L3



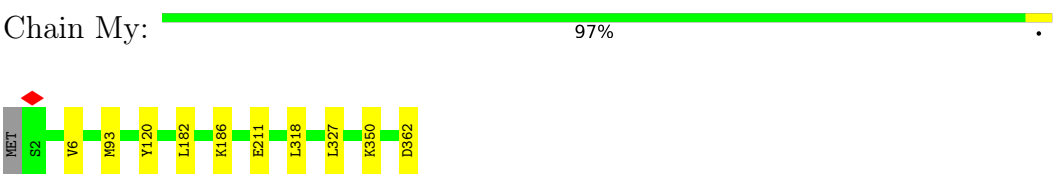
• Molecule 47: 60S ribosomal protein L4-A

Chain Ly:



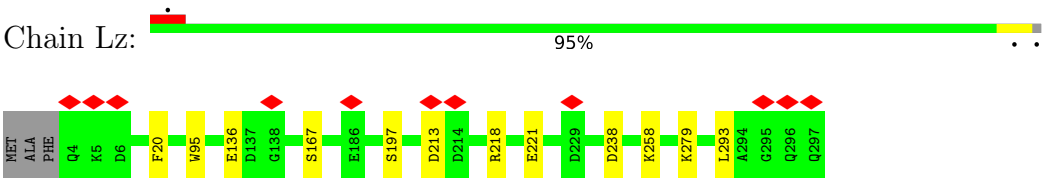
• Molecule 47: 60S ribosomal protein L4-A

Chain My:



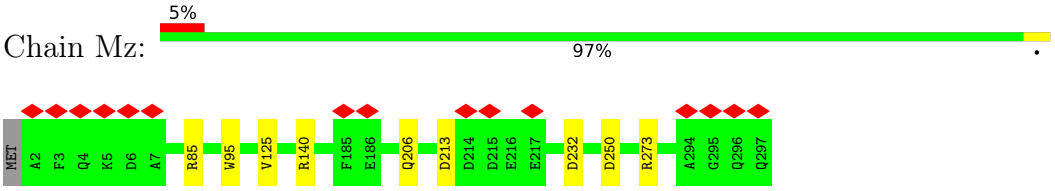
• Molecule 48: 60S ribosomal protein L5

Chain Lz:



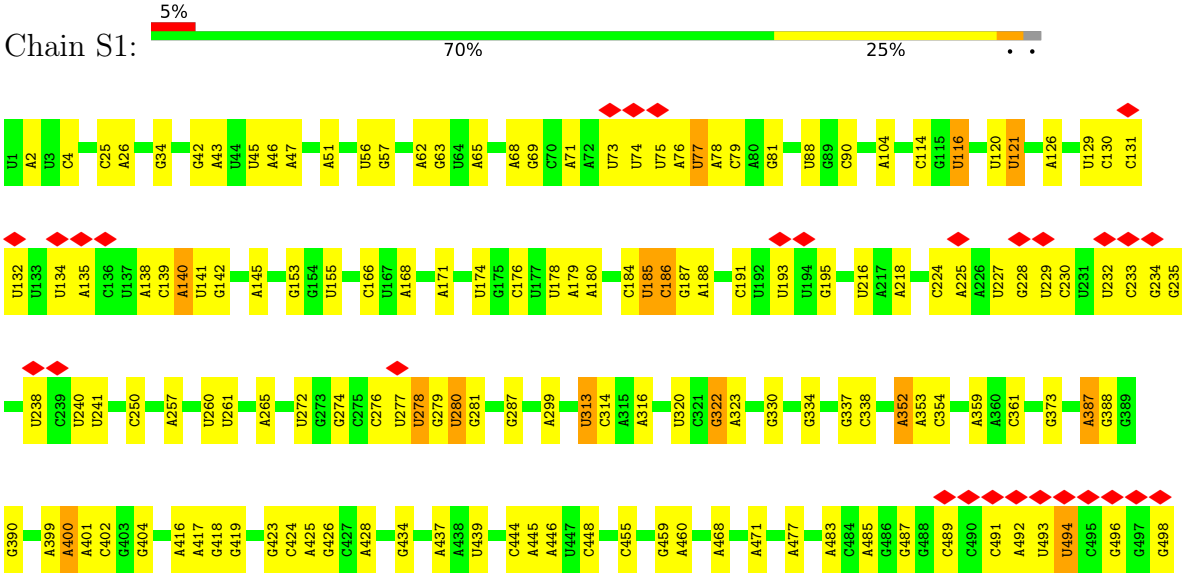
• Molecule 48: 60S ribosomal protein L5

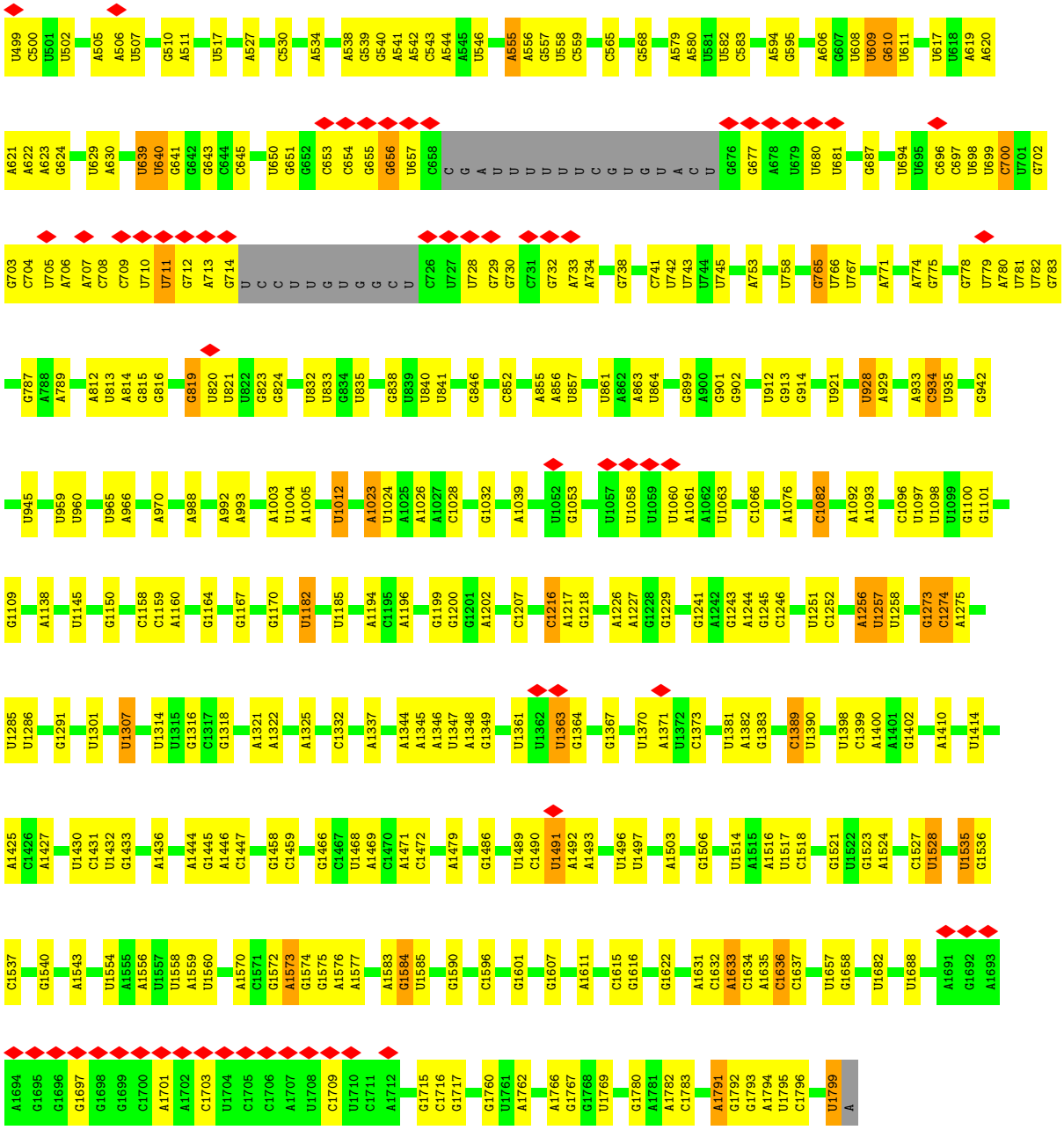
Chain Mz:



• Molecule 49: Saccharomyces cerevisiae S288C 18S ribosomal RNA (RDN18-1)

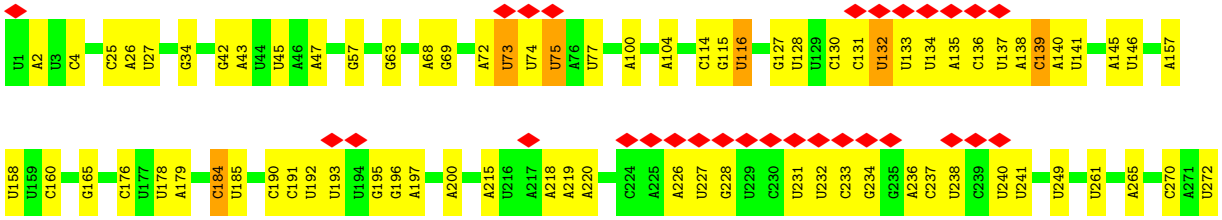
Chain S1:

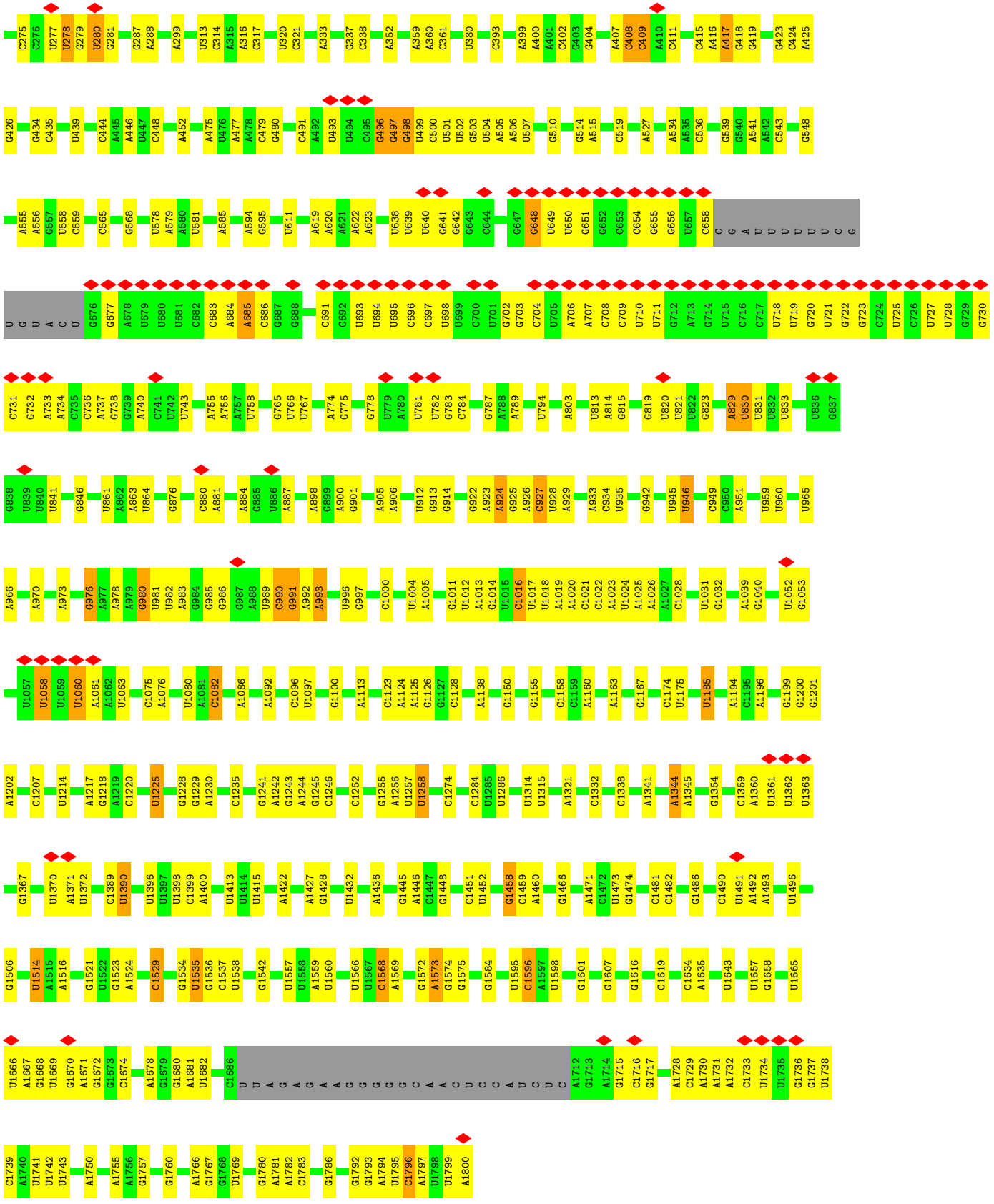




• Molecule 49: Saccharomyces cerevisiae S288C 18S ribosomal RNA (RDN18-1)

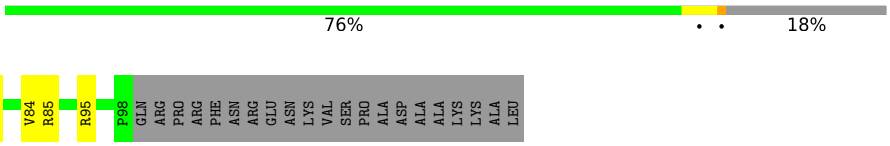
Chain R1:





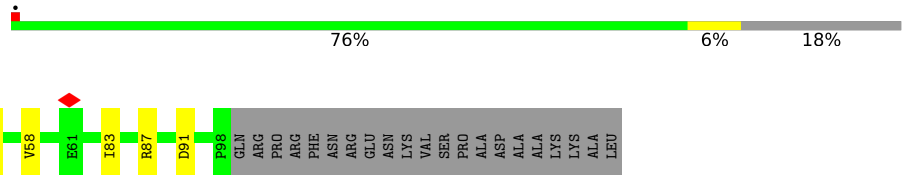
• Molecule 50: Small ribosomal subunit protein eS26A

Chain SA:



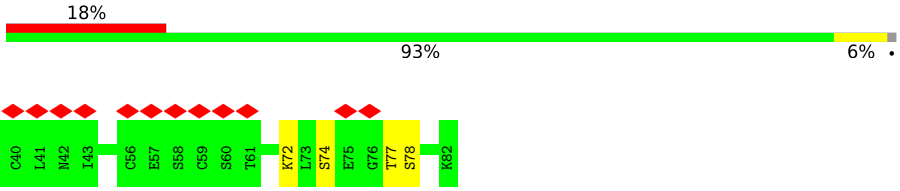
• Molecule 50: Small ribosomal subunit protein eS26A

Chain RA:



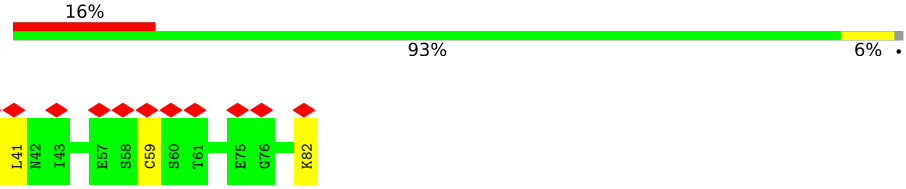
• Molecule 51: 40S ribosomal protein S27-A

Chain SB:



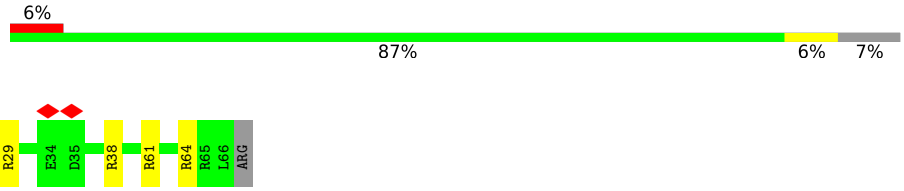
• Molecule 51: 40S ribosomal protein S27-A

Chain RB:



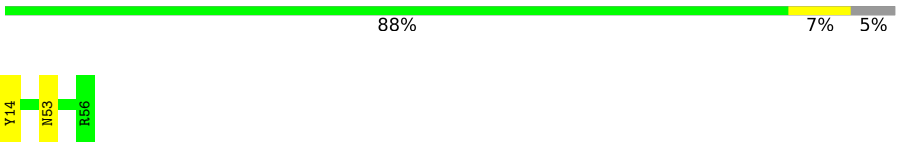
• Molecule 52: Small ribosomal subunit protein eS28B

Chain SC:



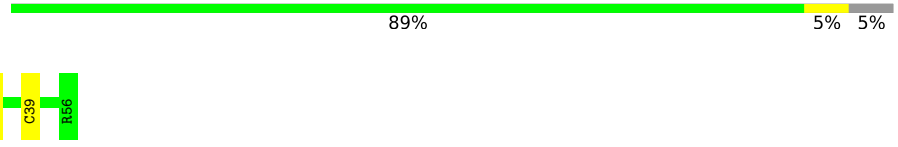
• Molecule 53: Small ribosomal subunit protein uS14A

Chain SD:



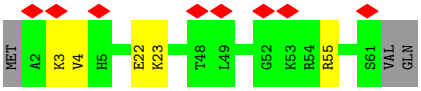
• Molecule 53: Small ribosomal subunit protein uS14A

Chain RD:



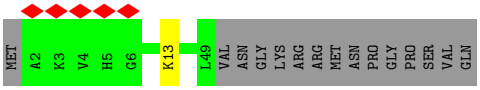
• Molecule 54: 40S ribosomal protein S30-A

Chain SE:



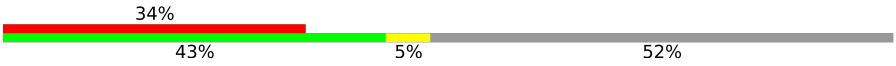
• Molecule 54: 40S ribosomal protein S30-A

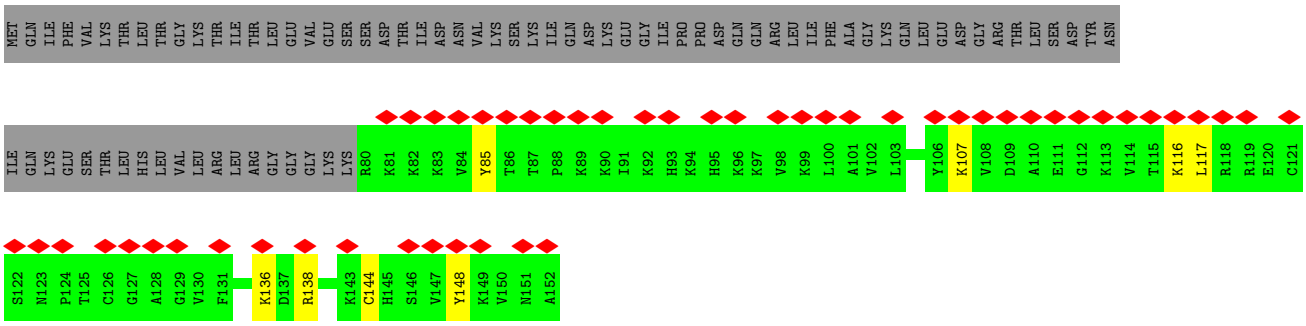
Chain RE:



• Molecule 55: Ubiquitin

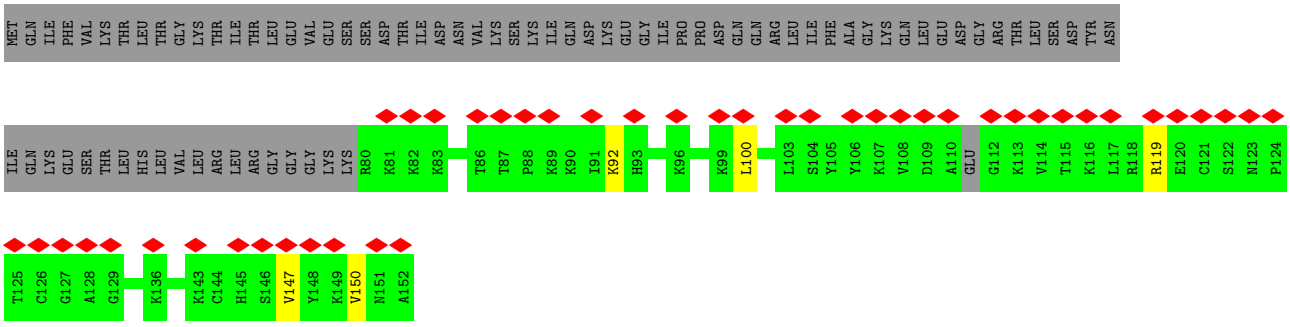
Chain SF:





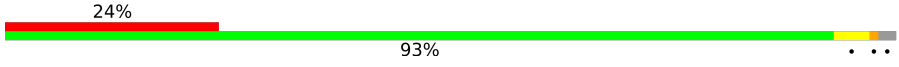
• Molecule 55: Ubiquitin

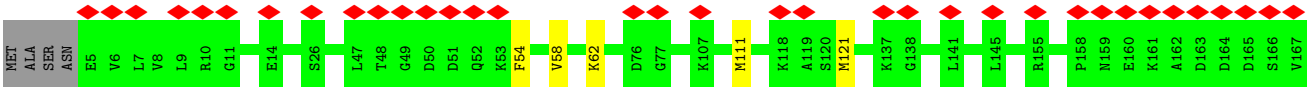
Chain RF:

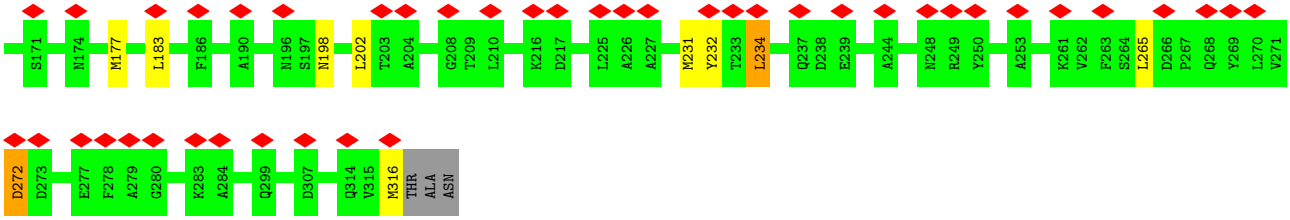


• Molecule 56: Guanine nucleotide-binding protein subunit beta-like protein

Chain SG:

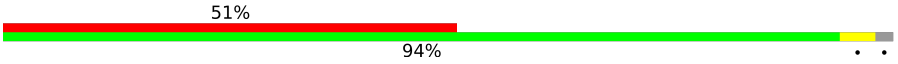


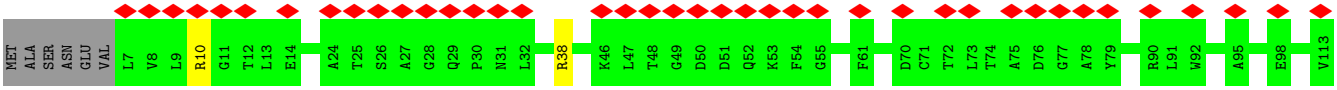


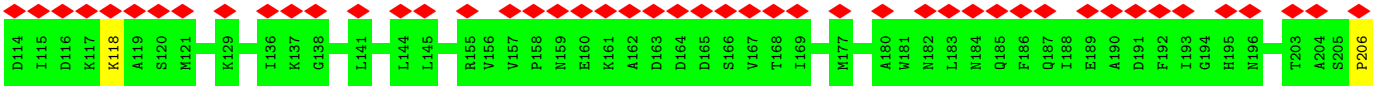


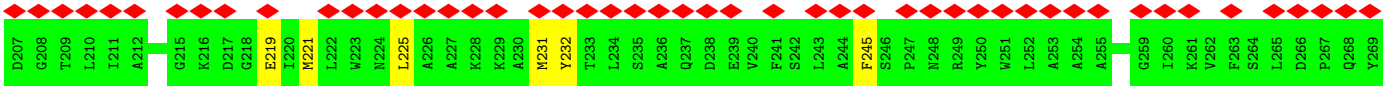
• Molecule 56: Guanine nucleotide-binding protein subunit beta-like protein

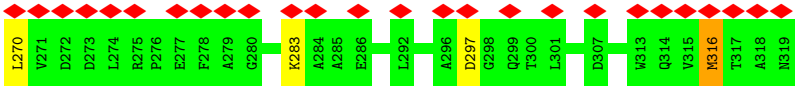
Chain RG:





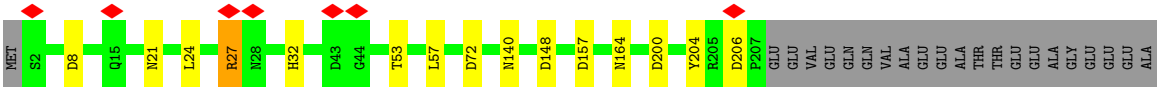






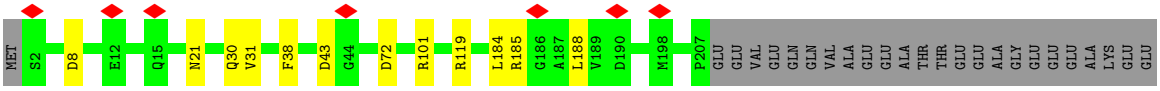
• Molecule 57: 40S ribosomal protein S0-A

Chain Sa:



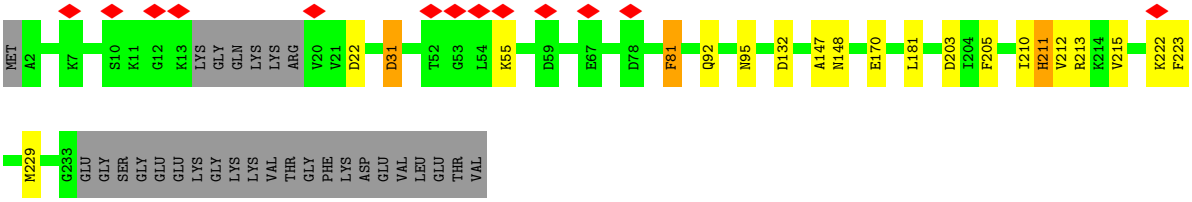
• Molecule 57: 40S ribosomal protein S0-A

Chain Ra:

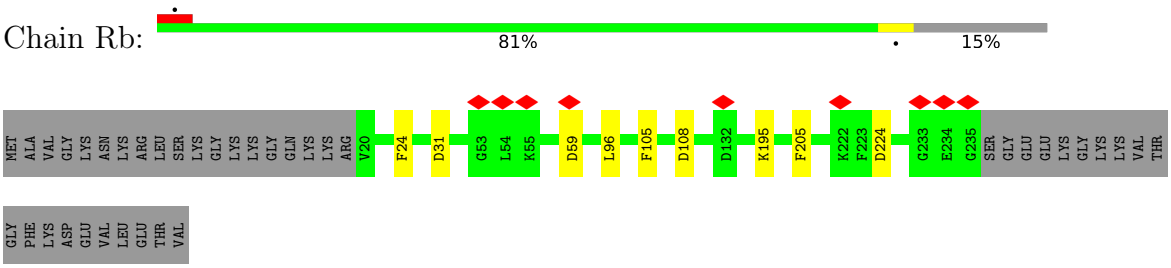


• Molecule 58: 40S ribosomal protein S1-A

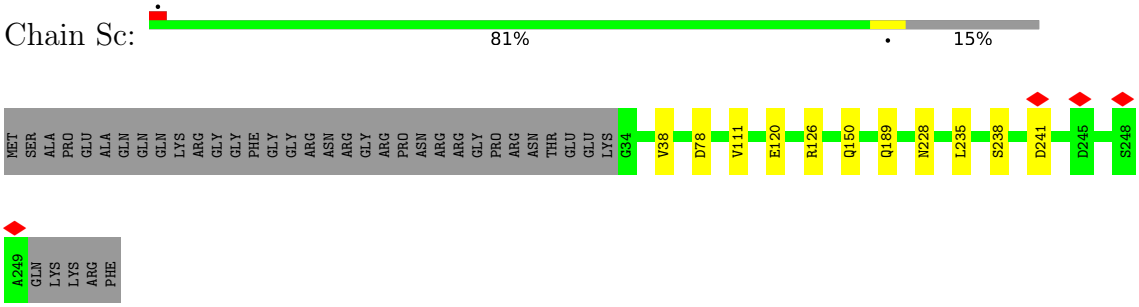
Chain Sb:



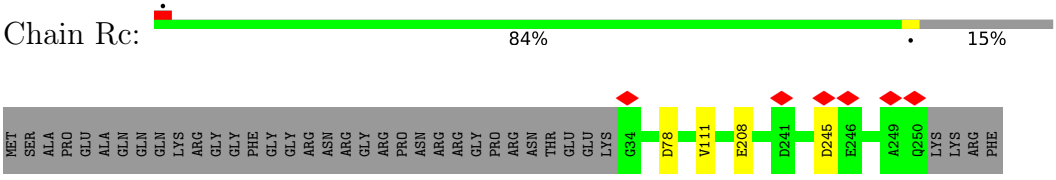
• Molecule 58: 40S ribosomal protein S1-A



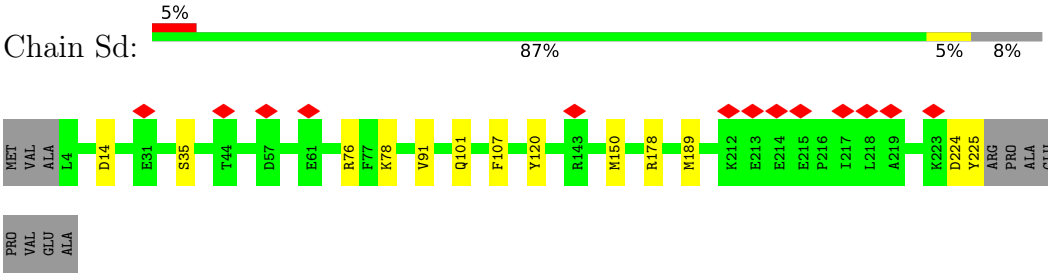
• Molecule 59: 40S ribosomal protein S2



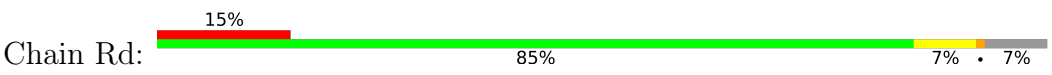
• Molecule 59: 40S ribosomal protein S2

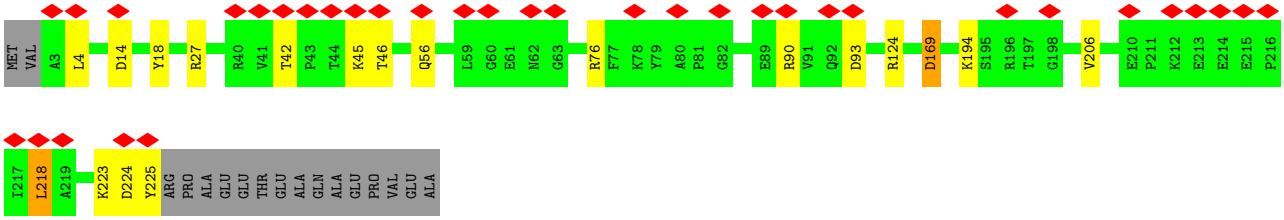


• Molecule 60: Small ribosomal subunit protein uS3



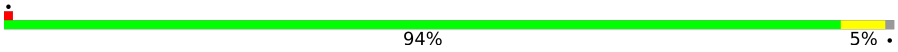
• Molecule 60: Small ribosomal subunit protein uS3

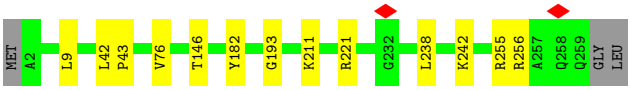




• Molecule 61: 40S ribosomal protein S4-A

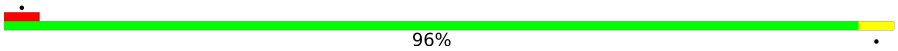
Chain Se:

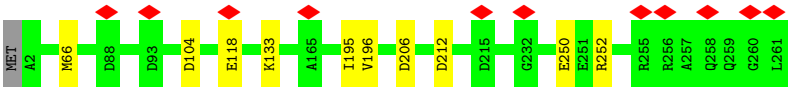




• Molecule 61: 40S ribosomal protein S4-A

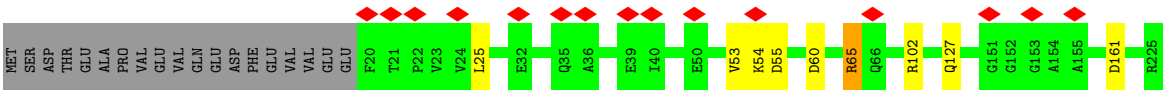
Chain Re:





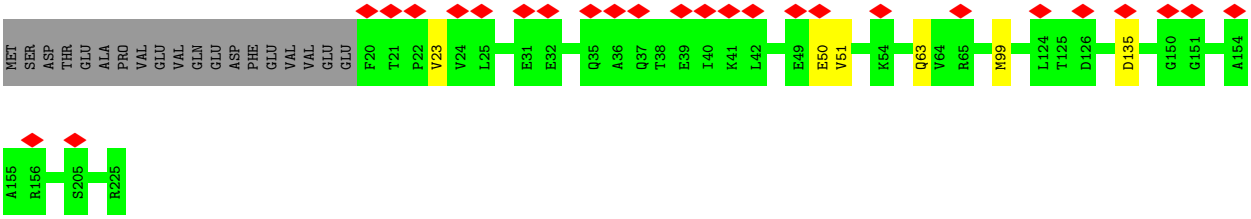
• Molecule 62: 40S ribosomal protein S5

Chain Sf:



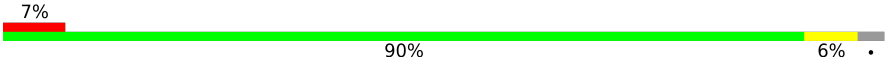
• Molecule 62: 40S ribosomal protein S5

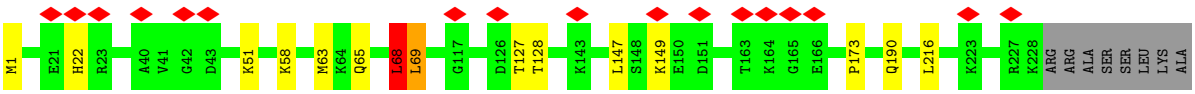
Chain Rf:



• Molecule 63: 40S ribosomal protein S6-A

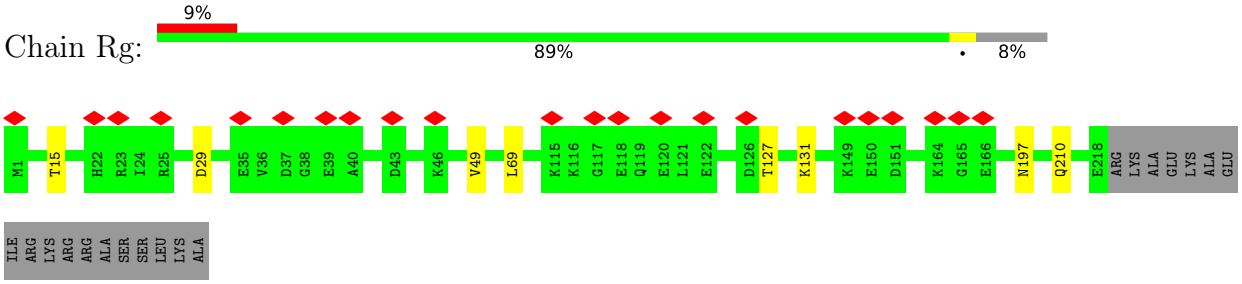
Chain Sg:





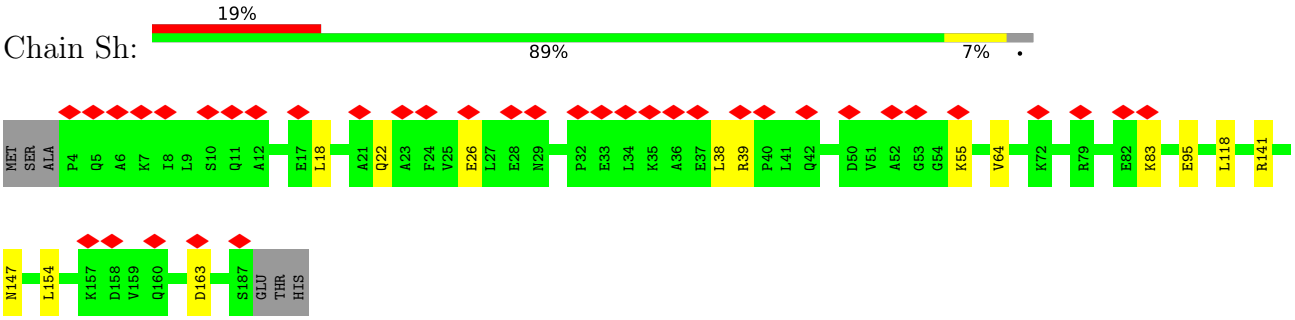
• Molecule 63: 40S ribosomal protein S6-A

Chain Rg:



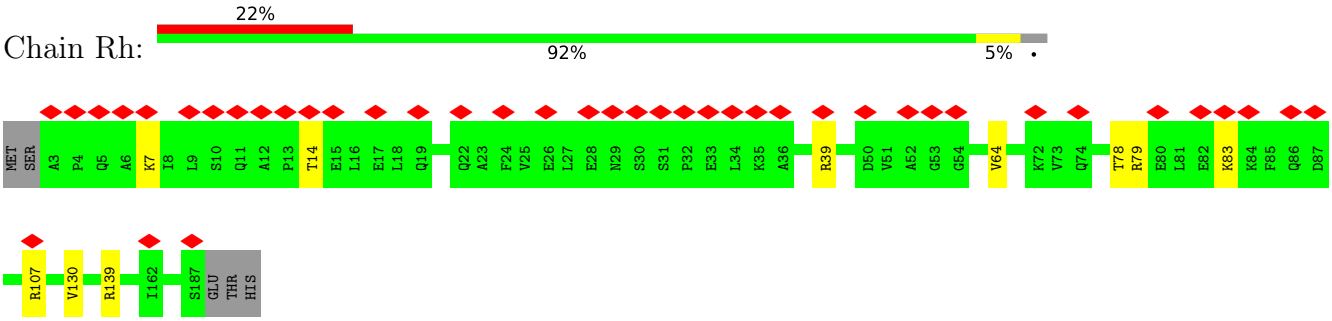
• Molecule 64: 40S ribosomal protein S7-A

Chain Sh:



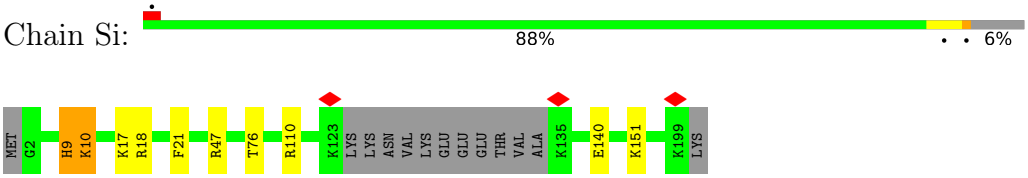
• Molecule 64: 40S ribosomal protein S7-A

Chain Rh:



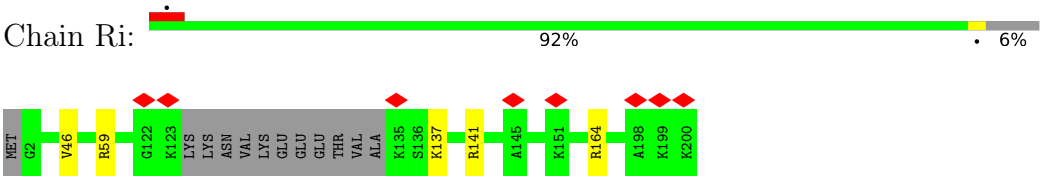
• Molecule 65: 40S ribosomal protein S8-A

Chain Si:



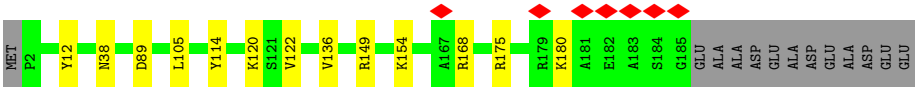
• Molecule 65: 40S ribosomal protein S8-A

Chain Ri:

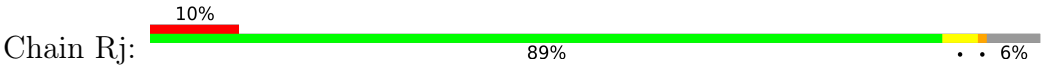


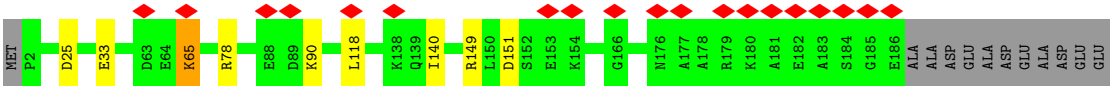
• Molecule 66: 40S ribosomal protein S9-A

Chain Sj:

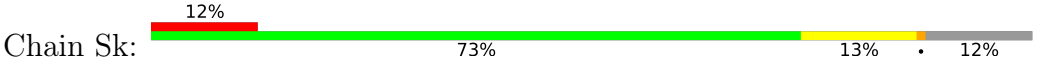


• Molecule 66: 40S ribosomal protein S9-A

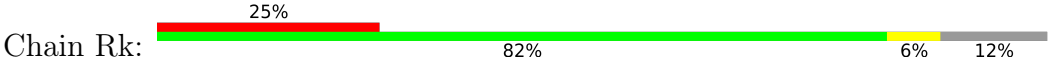


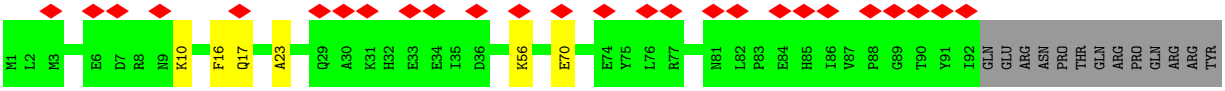


• Molecule 67: 40S ribosomal protein S10-A

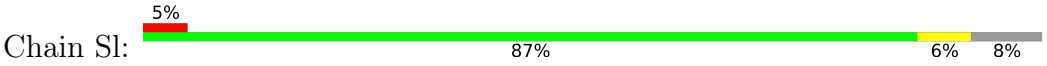


• Molecule 67: 40S ribosomal protein S10-A

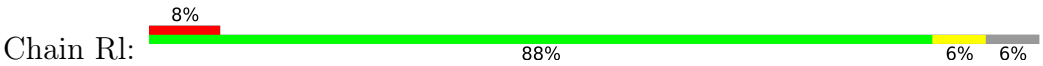


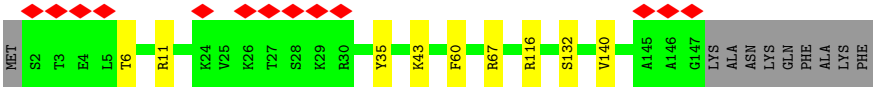


• Molecule 68: 40S ribosomal protein S11-A

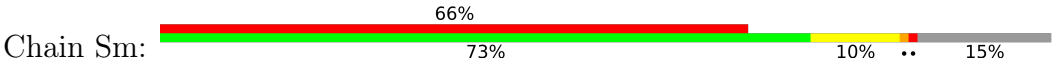


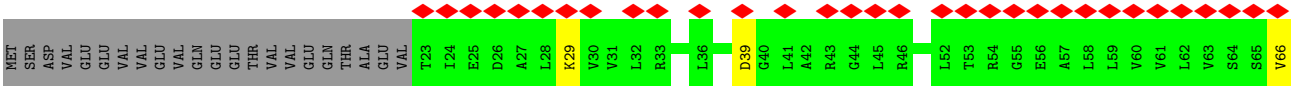
• Molecule 68: 40S ribosomal protein S11-A

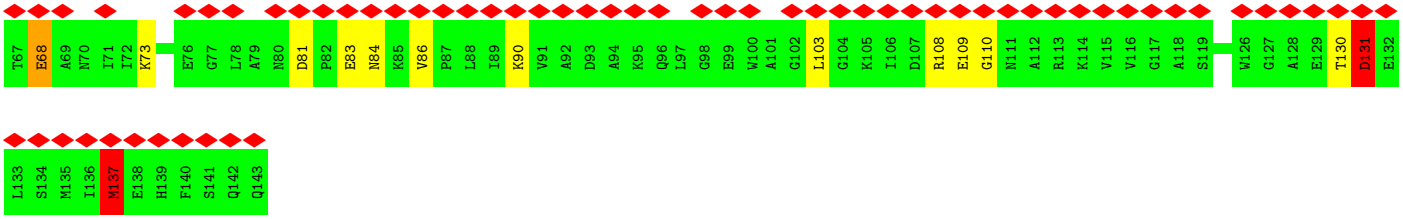




• Molecule 69: 40S ribosomal protein S12

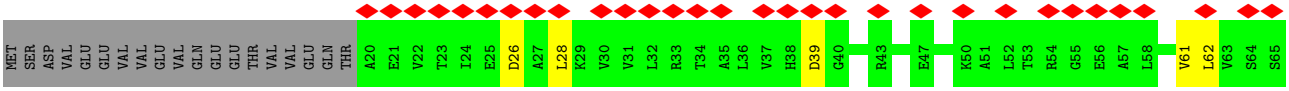


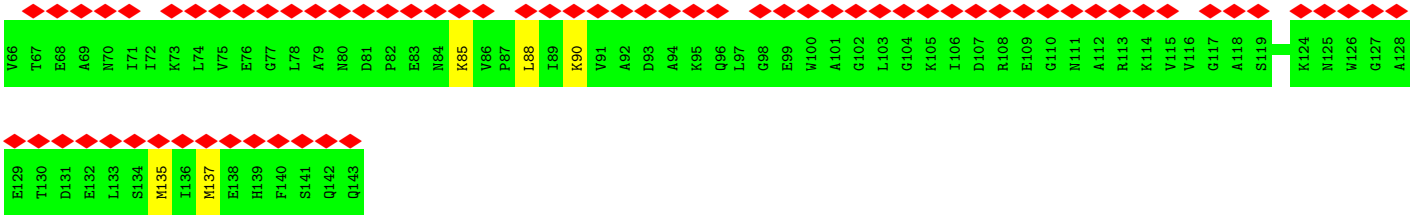




• Molecule 69: 40S ribosomal protein S12

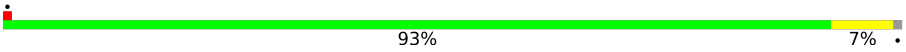
Chain Rm:





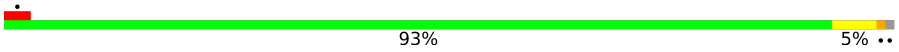
• Molecule 70: 40S ribosomal protein S13

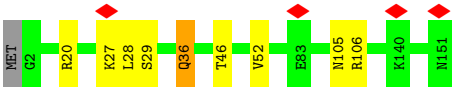
Chain Sn:



• Molecule 70: 40S ribosomal protein S13

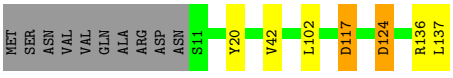
Chain Rn:





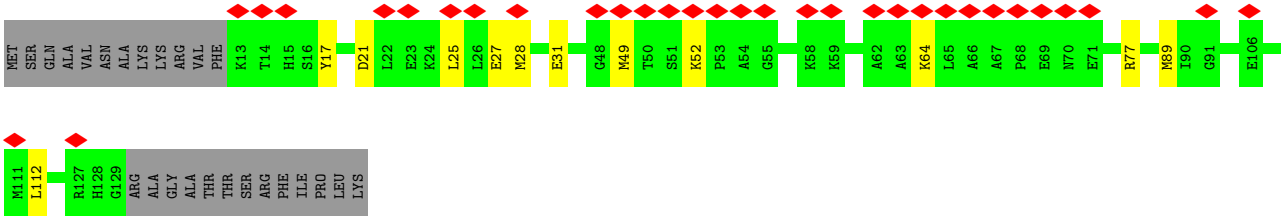
• Molecule 71: 40S ribosomal protein S14-A

Chain So:

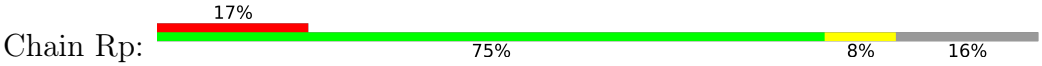


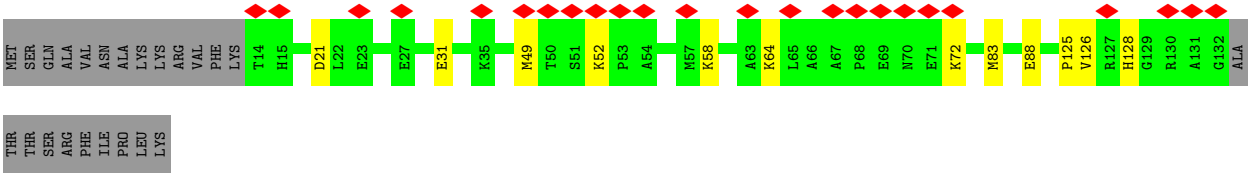
• Molecule 72: 40S ribosomal protein S15

Chain Sp:

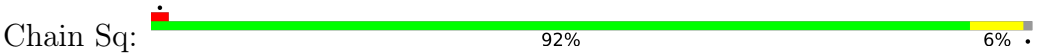


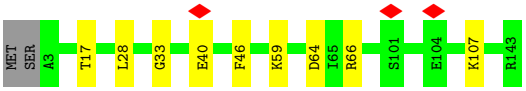
• Molecule 72: 40S ribosomal protein S15



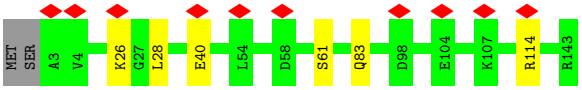


• Molecule 73: 40S ribosomal protein S16-A

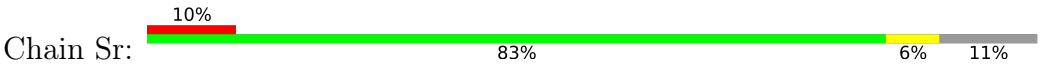


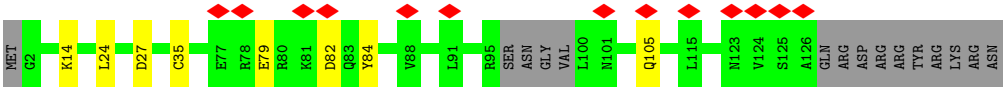


• Molecule 73: 40S ribosomal protein S16-A

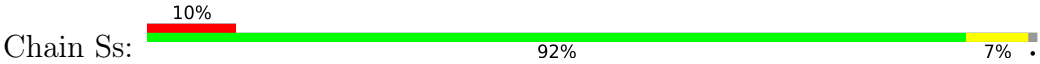


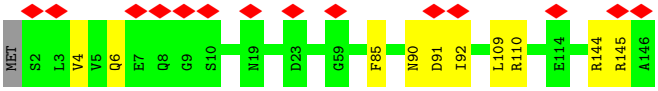
• Molecule 74: 40S ribosomal protein S17-B





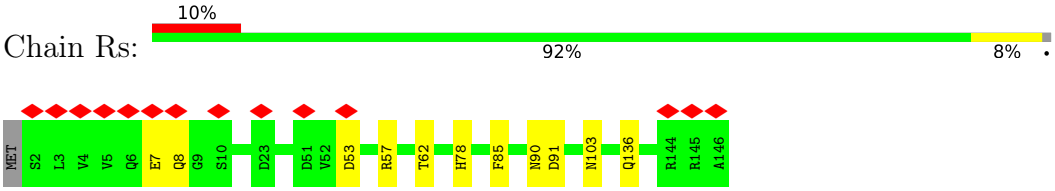
• Molecule 75: 40S ribosomal protein S18-A





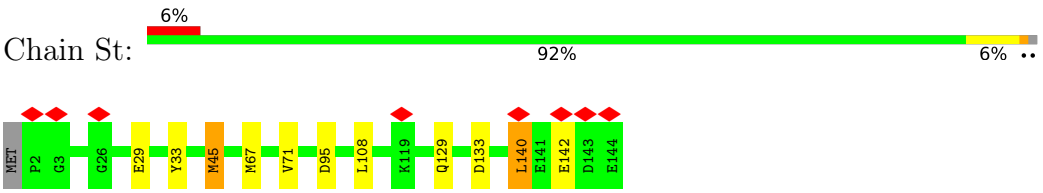
• Molecule 75: 40S ribosomal protein S18-A

Chain Rs:



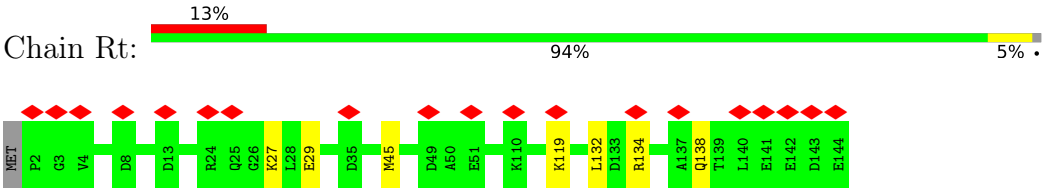
• Molecule 76: 40S ribosomal protein S19-A

Chain St:



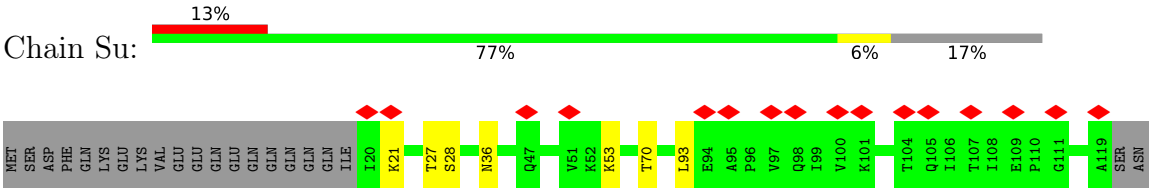
• Molecule 76: 40S ribosomal protein S19-A

Chain Rt:



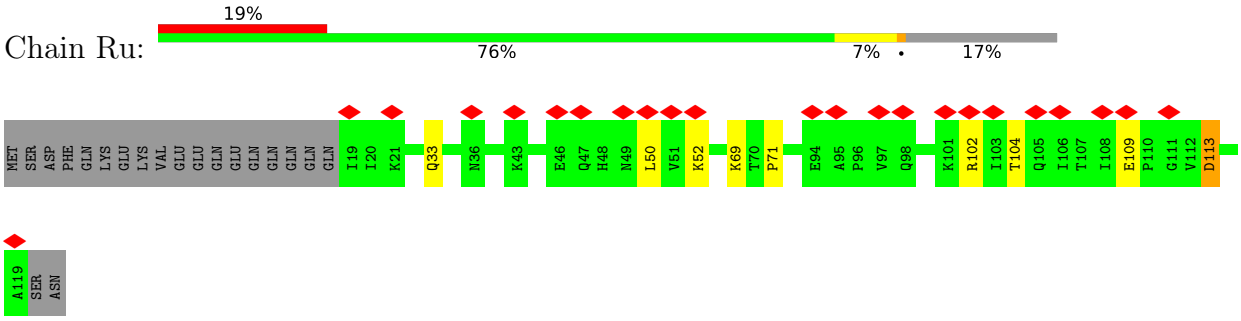
• Molecule 77: Small ribosomal subunit protein uS10

Chain Su:



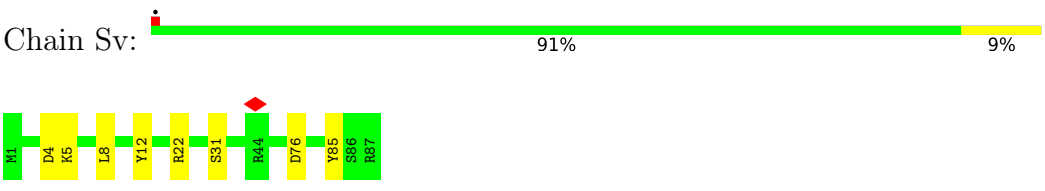
• Molecule 77: Small ribosomal subunit protein uS10

Chain Ru:



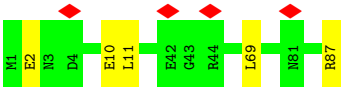
• Molecule 78: Small ribosomal subunit protein eS21A

Chain Sv:



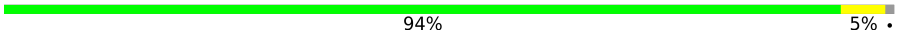
• Molecule 78: Small ribosomal subunit protein eS21A

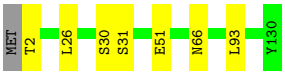
Chain Rv:



• Molecule 79: 40S ribosomal protein S22-A

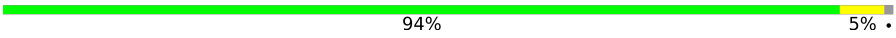
Chain Sw:

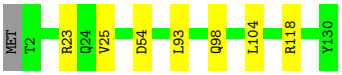




• Molecule 79: 40S ribosomal protein S22-A

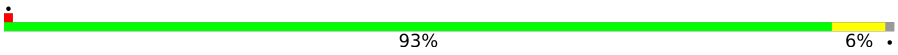
Chain Rw:

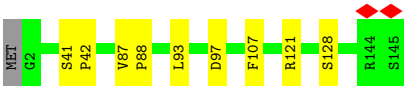




• Molecule 80: 40S ribosomal protein S23-A

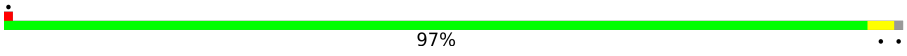
Chain Sx:





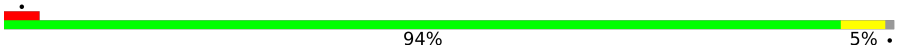
• Molecule 80: 40S ribosomal protein S23-A

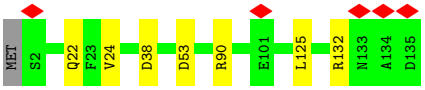
Chain Rx:



• Molecule 81: 40S ribosomal protein S24-A

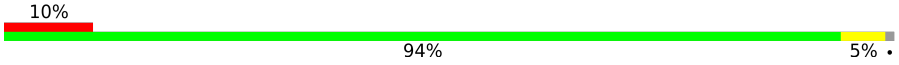
Chain Sy:

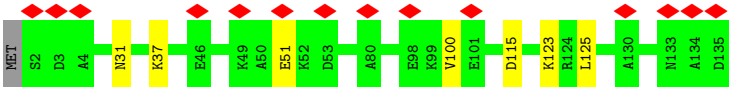




• Molecule 81: 40S ribosomal protein S24-A

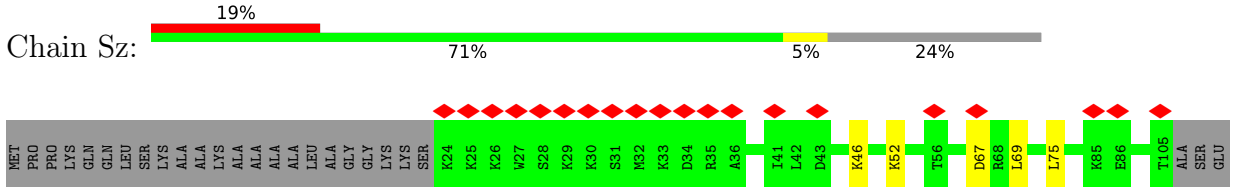
Chain Ry:





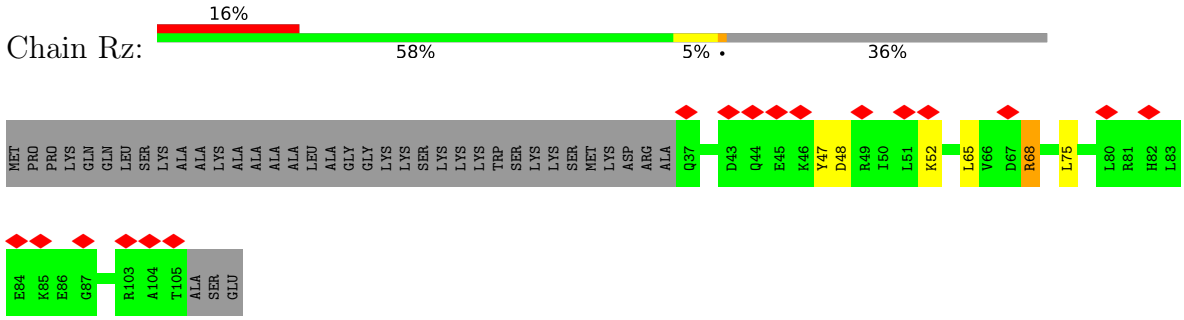
• Molecule 82: 40S ribosomal protein S25-A

Chain Sz:



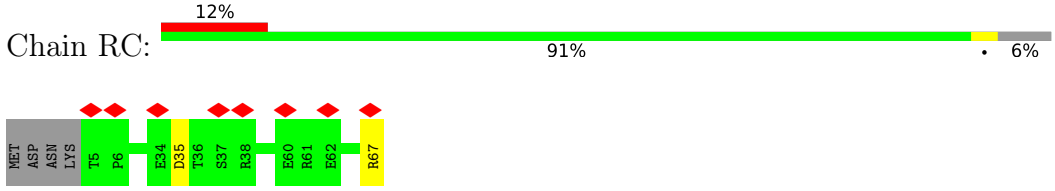
• Molecule 82: 40S ribosomal protein S25-A

Chain Rz:



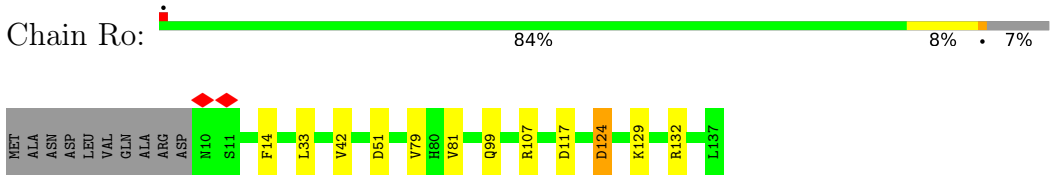
• Molecule 83: 40S ribosomal protein S28-A

Chain RC:



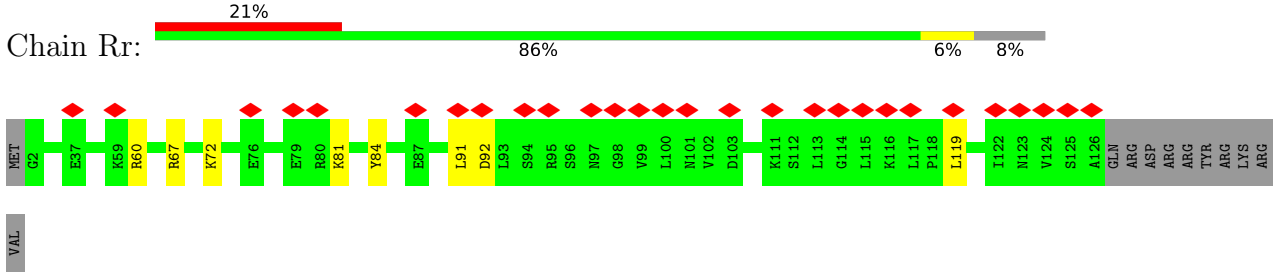
• Molecule 84: 40S ribosomal protein S14-B

Chain Ro:



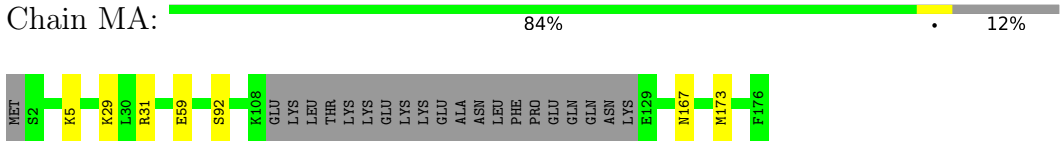
• Molecule 85: 40S ribosomal protein S17-A

Chain Rr:



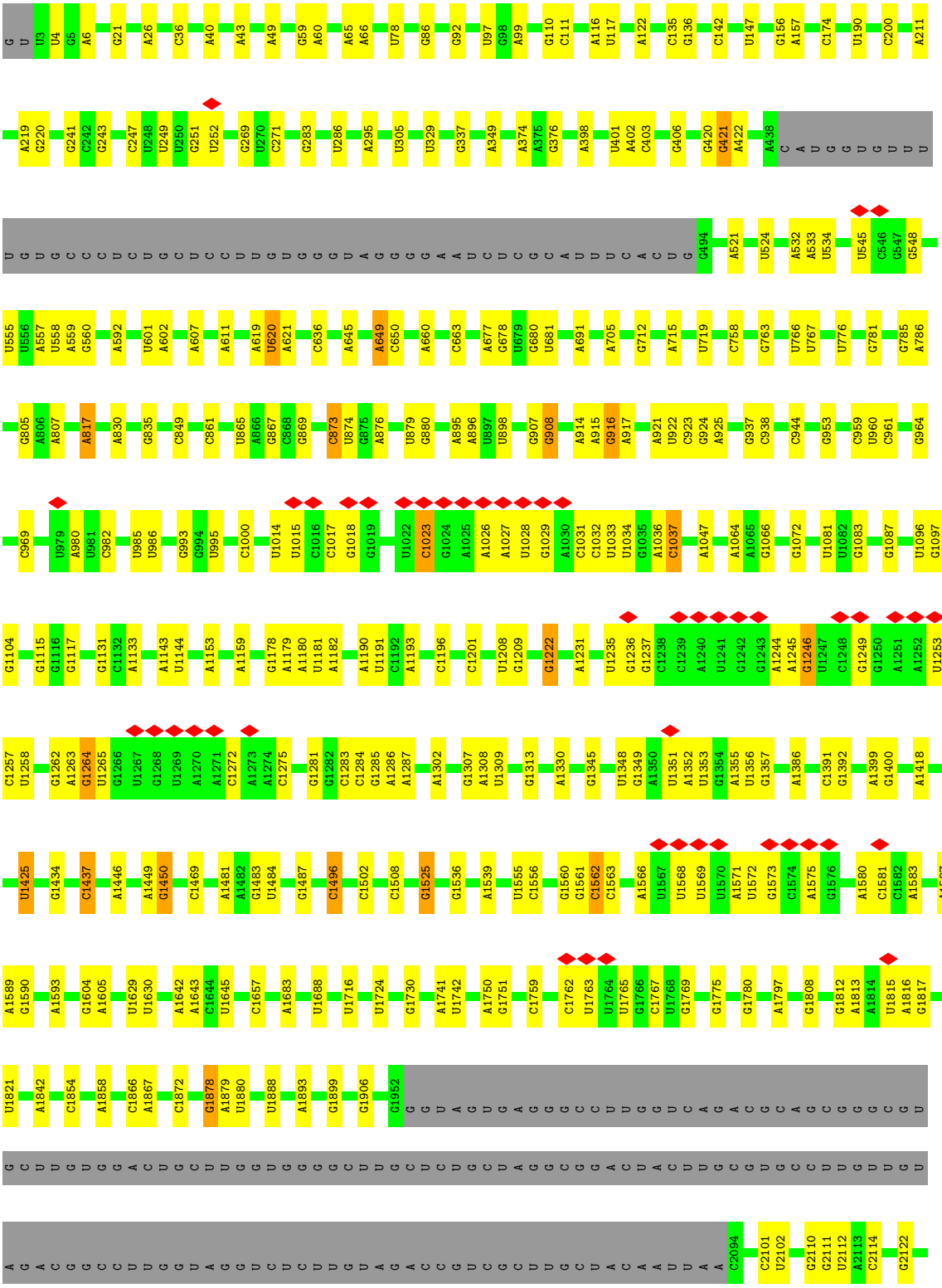
• Molecule 86: 60S ribosomal protein L6-A

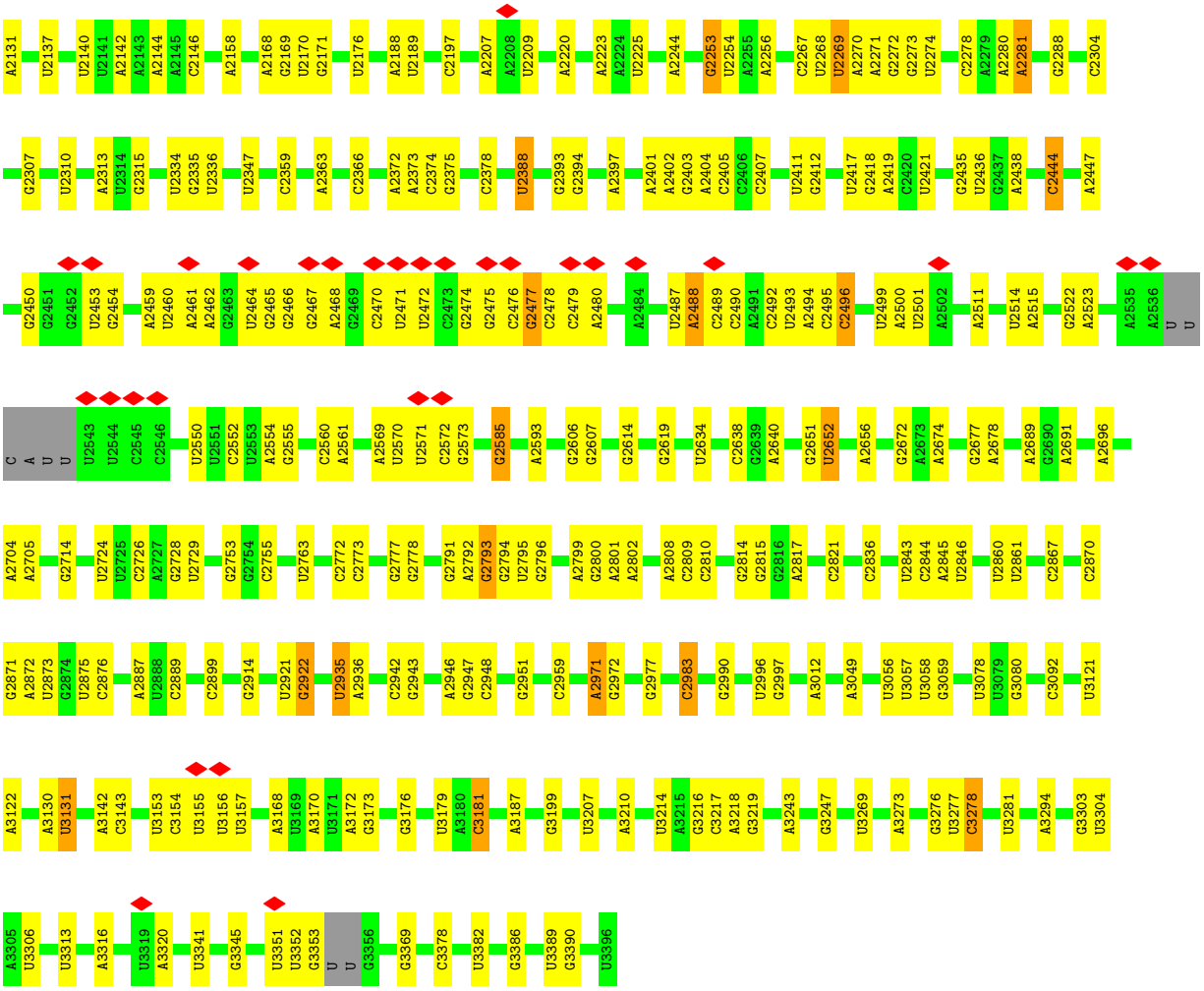
Chain MA:



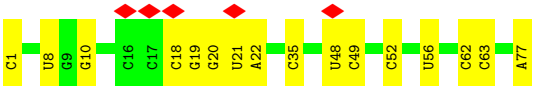
• Molecule 87: Saccharomyces cerevisiae S288C 18S ribosomal RNA (RDN18-1) with modifications

Chain M1:

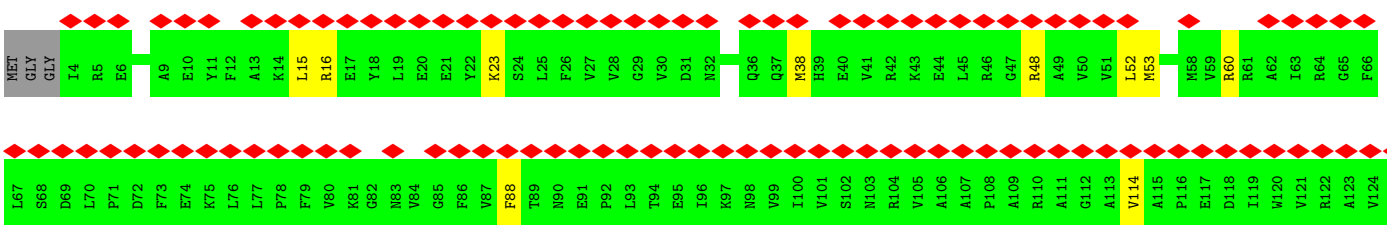


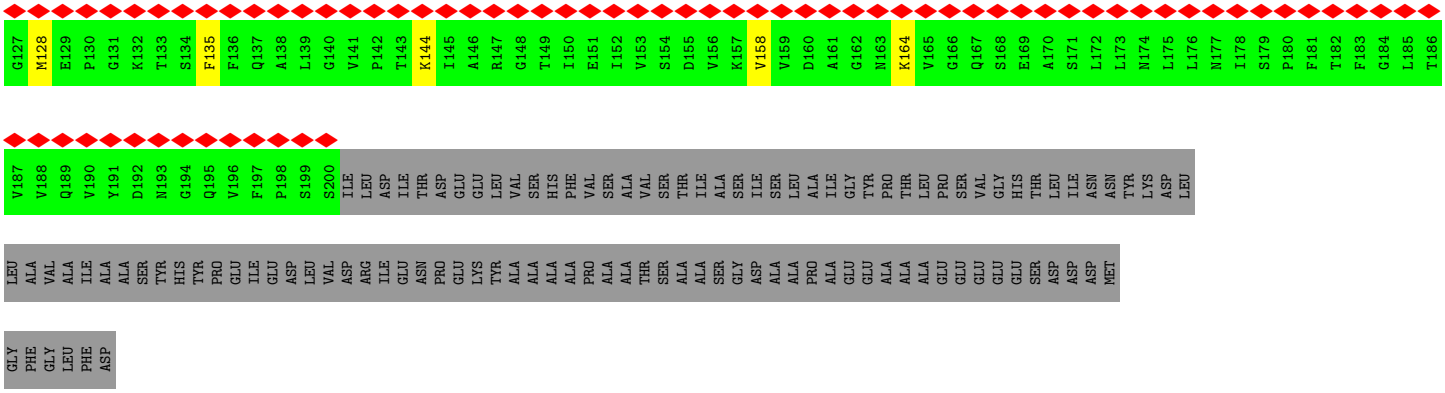


• Molecule 88: tRNA



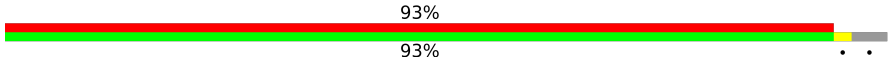
• Molecule 89: 60S acidic ribosomal protein P0

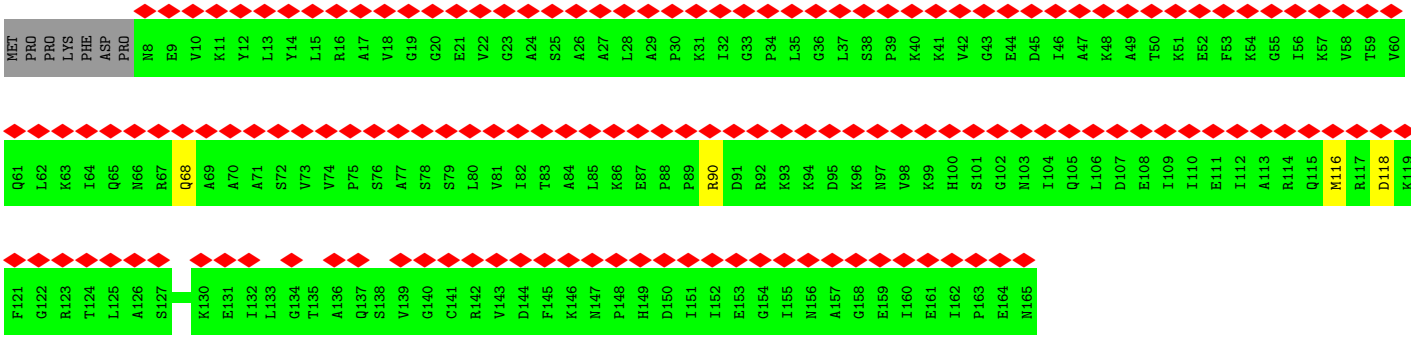




• Molecule 90: 60S ribosomal protein L12-A

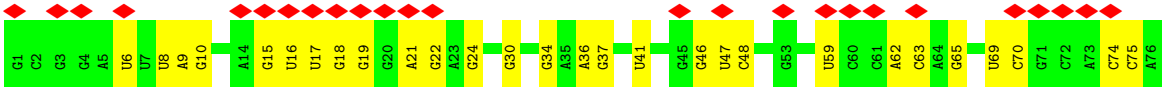
Chain MP:





• Molecule 91: tRNA

Chain DP:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	189911	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.6	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.572	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.44	Depositor
Map size (Å)	655.21497, 655.21497, 655.21497	wwPDB
Map dimensions	627, 627, 627	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 5MC, MG, A2M, OMC, OMU, SPD, 1MA, OMG, ZN, UR3, YYG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	CC	0.36	0/132	0.69	0/175
2	CM	0.41	0/927	1.14	11/1434 (0.8%)
3	CN	0.26	0/1053	0.59	0/1414
4	CP	0.47	3/1810 (0.2%)	0.86	0/2817
5	L1	0.74	0/74617	0.96	192/116334 (0.2%)
6	L2	0.72	0/3746	0.94	8/5832 (0.1%)
6	M2	0.69	0/3746	0.88	2/5832 (0.0%)
7	L3	0.60	0/2883	0.89	2/4491 (0.0%)
7	M3	0.59	0/2883	0.88	0/4491
8	LA	0.35	0/1327	0.56	0/1791
9	LB	0.39	0/1821	0.56	0/2451
9	MB	0.35	0/1821	0.53	0/2451
10	LC	0.36	0/1836	0.59	1/2481 (0.0%)
10	MC	0.33	0/1836	0.57	2/2481 (0.1%)
11	LD	0.34	0/1529	0.59	0/2060
11	MD	0.33	0/1539	0.56	0/2073
12	LE	0.38	0/1801	0.64	1/2416 (0.0%)
12	ME	0.35	0/1779	0.59	1/2386 (0.0%)
13	LF	0.36	0/1371	0.73	2/1838 (0.1%)
13	MF	0.33	0/1374	0.65	1/1842 (0.1%)
14	LG	0.36	0/1568	0.63	0/2106
14	MG	0.36	0/1568	0.61	0/2106
15	LH	0.33	0/1068	0.60	1/1438 (0.1%)
15	MH	0.33	0/1068	0.54	0/1438
16	LI	0.39	0/1757	0.65	1/2354 (0.0%)
16	MI	0.39	0/1757	0.61	0/2354
17	LJ	0.39	0/1585	0.57	1/2128 (0.0%)
17	MJ	0.36	0/1585	0.55	0/2128
18	LK	0.37	0/1439	0.64	1/1938 (0.1%)
18	MK	0.38	0/1245	0.57	0/1676
19	LL	0.37	0/1465	0.63	1/1965 (0.1%)
19	ML	0.34	0/1465	0.62	1/1965 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	LM	0.35	0/1532	0.64	2/2043 (0.1%)
20	MM	0.33	0/1440	0.63	1/1921 (0.1%)
21	LN	0.39	0/1473	0.65	1/1980 (0.1%)
21	MN	0.38	0/1481	0.59	0/1990
22	LO	0.40	0/1300	0.61	0/1743
22	MO	0.36	0/1300	0.59	0/1743
23	La	0.38	0/1018	0.61	0/1369
23	Ma	0.35	0/978	0.60	0/1316
24	Lb	0.37	0/701	0.65	0/934
24	Mb	0.33	0/701	0.61	0/934
25	Lc	0.40	0/836	0.66	0/1104
25	Mc	0.35	0/831	0.60	0/1097
26	Ld	0.34	0/230	0.69	0/296
26	Md	0.34	0/234	0.86	0/300
27	Le	0.35	0/423	0.70	1/562 (0.2%)
27	Me	0.32	0/423	0.55	0/562
28	Lf	0.37	0/443	0.66	0/588
28	Mf	0.35	0/443	0.72	0/588
29	Lg	0.33	0/618	0.71	1/826 (0.1%)
29	Mg	0.33	0/618	0.64	0/826
30	Lh	0.39	0/685	0.62	0/908
30	Mh	0.39	0/680	0.65	0/901
31	Li	0.32	0/772	0.60	0/1026
31	Mi	0.31	0/778	0.61	0/1034
32	Lj	0.35	0/978	0.57	0/1301
32	Mj	0.34	0/978	0.59	1/1301 (0.1%)
33	Lk	0.37	0/846	0.60	0/1130
33	Mk	0.35	0/871	0.59	0/1164
34	Ll	0.42	0/868	0.58	0/1168
34	Ml	0.39	0/868	0.59	0/1168
35	Lm	0.37	0/1038	0.59	0/1390
35	Mm	0.35	0/1041	0.54	0/1394
36	Ln	0.37	0/890	0.63	2/1196 (0.2%)
36	Mn	0.38	0/897	0.73	3/1205 (0.2%)
37	Lo	0.39	0/745	0.56	0/1001
37	Mo	0.35	0/750	0.53	0/1008
38	Lp	0.34	0/473	0.66	1/629 (0.2%)
38	Mp	0.30	0/473	0.52	0/629
39	Lq	0.39	0/1204	0.65	1/1612 (0.1%)
39	Mq	0.37	0/1204	0.61	1/1612 (0.1%)
40	Lr	0.38	0/1118	0.59	0/1497
40	Mr	0.34	0/1118	0.56	0/1497
41	Ls	0.34	0/995	0.60	0/1329

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	Ms	0.35	0/1004	0.64	1/1341 (0.1%)
42	Lt	0.38	0/979	0.64	2/1321 (0.2%)
42	Mt	0.38	0/974	0.66	1/1314 (0.1%)
43	Lu	0.33	0/850	0.60	0/1152
43	Mu	0.34	0/533	0.58	0/707
44	Lv	0.34	0/812	0.64	2/1099 (0.2%)
44	Mv	0.38	0/786	0.82	3/1065 (0.3%)
45	Lw	0.39	0/1933	0.63	0/2598
45	Mw	0.37	0/1948	0.59	0/2617
46	Lx	0.40	0/3146	0.63	0/4228
46	Mx	0.35	0/3146	0.58	0/4228
47	Ly	0.38	0/2800	0.58	0/3790
47	My	0.34	0/2800	0.57	1/3790 (0.0%)
48	Lz	0.33	0/2400	0.61	2/3239 (0.1%)
48	Mz	0.31	0/2425	0.56	1/3271 (0.0%)
49	R1	0.47	0/41891	0.99	183/65273 (0.3%)
49	S1	0.57	0/42211	0.98	151/65773 (0.2%)
50	RA	0.31	0/782	0.73	2/1047 (0.2%)
50	SA	0.34	0/782	0.71	0/1047
51	RB	0.31	0/620	0.68	0/838
51	SB	0.33	0/620	0.68	1/838 (0.1%)
52	SC	0.38	0/488	0.78	0/656
53	RD	0.29	0/452	0.55	0/600
53	SD	0.35	0/452	0.63	0/600
54	RE	0.47	0/391	0.70	0/520
54	SE	0.33	0/480	0.68	0/639
55	RF	0.29	0/557	0.62	0/749
55	SF	0.30	0/567	0.69	0/764
56	RG	0.26	0/2456	0.57	2/3343 (0.1%)
56	SG	0.30	0/2436	0.69	4/3318 (0.1%)
57	Ra	0.33	0/1623	0.65	1/2222 (0.0%)
57	Sa	0.35	0/1644	0.70	3/2249 (0.1%)
58	Rb	0.29	0/1748	0.56	1/2352 (0.0%)
58	Sb	0.34	0/1823	0.73	5/2447 (0.2%)
59	Rc	0.32	0/1665	0.54	0/2263
59	Sc	0.37	0/1656	0.64	1/2251 (0.0%)
60	Rd	0.30	0/1759	0.66	3/2368 (0.1%)
60	Sd	0.30	0/1754	0.59	1/2361 (0.0%)
61	Re	0.30	0/2109	0.58	0/2839
61	Se	0.34	0/2097	0.65	1/2823 (0.0%)
62	Rf	0.29	0/1629	0.63	0/2202
62	Sf	0.30	0/1625	0.66	4/2197 (0.2%)
63	Rg	0.27	0/1779	0.62	1/2379 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
63	Sg	0.29	0/1839	0.64	3/2460 (0.1%)
64	Rh	0.28	0/1511	0.58	0/2036
64	Sh	0.34	0/1498	0.73	1/2019 (0.0%)
65	Ri	0.28	0/1514	0.57	0/2021
65	Si	0.37	0/1501	0.68	0/2006
66	Rj	0.31	0/1519	0.64	2/2035 (0.1%)
66	Sj	0.31	0/1504	0.66	2/2016 (0.1%)
67	Rk	0.36	0/757	0.61	0/1022
67	Sk	0.44	0/769	0.95	5/1039 (0.5%)
68	Rl	0.32	0/1194	0.57	0/1610
68	Sl	0.39	0/1185	0.64	0/1598
69	Rm	0.30	0/898	0.75	2/1220 (0.2%)
69	Sm	0.32	0/883	0.85	4/1199 (0.3%)
70	Rn	0.35	0/1215	0.70	2/1638 (0.1%)
70	Sn	0.38	0/1215	0.68	1/1638 (0.1%)
71	So	0.34	0/937	0.83	4/1261 (0.3%)
72	Rp	0.32	0/959	0.71	1/1288 (0.1%)
72	Sp	0.37	0/936	0.82	1/1259 (0.1%)
73	Rq	0.30	0/1125	0.60	1/1510 (0.1%)
73	Sq	0.34	0/1125	0.63	0/1510
74	Sr	0.38	0/957	0.79	1/1283 (0.1%)
75	Rs	0.32	0/1211	0.71	1/1628 (0.1%)
75	Ss	0.34	0/1211	0.71	0/1628
76	Rt	0.32	0/1130	0.66	2/1517 (0.1%)
76	St	0.37	0/1130	0.79	5/1517 (0.3%)
77	Ru	0.33	0/815	0.72	2/1102 (0.2%)
77	Su	0.33	0/807	0.72	1/1091 (0.1%)
78	Rv	0.35	0/693	0.67	0/935
78	Sv	0.37	0/682	0.73	1/921 (0.1%)
79	Rw	0.33	0/1038	0.64	1/1395 (0.1%)
79	Sw	0.35	0/1038	0.58	0/1395
80	Rx	0.31	0/1139	0.60	0/1518
80	Sx	0.35	0/1139	0.64	0/1518
81	Ry	0.33	0/1087	0.69	3/1449 (0.2%)
81	Sy	0.33	0/1087	0.67	1/1449 (0.1%)
82	Rz	0.35	0/566	0.72	0/761
82	Sz	0.34	0/661	0.80	1/888 (0.1%)
83	RC	0.32	0/499	0.78	1/670 (0.1%)
84	Ro	0.36	0/960	0.82	3/1290 (0.2%)
85	Rr	0.32	0/1010	0.73	2/1355 (0.1%)
86	MA	0.34	0/1251	0.58	0/1682
87	M1	0.69	0/75384	0.94	153/117530 (0.1%)
88	DQ	0.43	1/1836 (0.1%)	0.89	3/2859 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
89	MQ	0.27	0/1558	0.60	2/2107 (0.1%)
90	MP	0.25	0/1210	0.52	0/1627
91	DP	0.29	0/1788	0.95	0/2786
All	All	0.54	4/435297 (0.0%)	0.85	833/639512 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	MB	0	1
10	LC	0	3
11	LD	0	1
13	LF	0	1
14	LG	0	2
15	LH	0	1
16	LI	0	1
17	LJ	0	1
20	LM	0	1
25	Mc	0	1
28	Mf	0	1
32	Lj	0	1
38	Lp	0	1
40	Mr	0	1
42	Lt	0	1
45	Lw	0	1
46	Lx	0	4
47	Ly	0	2
47	My	0	1
50	SA	0	1
55	SF	0	1
57	Ra	0	1
58	Sb	0	2
61	Re	0	1
61	Se	0	1
63	Sg	0	1
64	Rh	0	2
64	Sh	0	1
65	Si	0	1
67	Rk	0	1
69	Sm	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
72	Sp	0	1
73	Rq	0	1
73	Sq	0	1
75	Rs	0	1
75	Ss	0	1
77	Ru	0	1
80	Sx	0	2
82	Rz	0	1
All	All	0	54

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	DQ	1	C	OP3-P	-10.57	1.48	1.61
4	CP	34	I	C5-C6	6.44	1.52	1.39
4	CP	34	I	N3-C4	6.14	1.48	1.35
4	CP	34	I	C2-N3	5.17	1.46	1.35

All (833) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	3278	C	C2-N1-C1'	12.14	132.16	118.80
87	M1	3278	C	N1-C2-O2	11.78	125.97	118.90
49	R1	989	U	N1-C2-O2	11.08	130.56	122.80
63	Rg	69	LEU	CA-CB-CG	10.80	140.15	115.30
49	R1	989	U	N3-C2-O2	-10.47	114.87	122.20
5	L1	3217	C	N1-C2-O2	10.42	125.15	118.90
6	L2	125	U	N1-C2-O2	10.38	130.07	122.80
49	R1	75	U	C2-N1-C1'	10.32	130.08	117.70
49	S1	1527	C	C2-N1-C1'	10.30	130.13	118.80
49	R1	989	U	C2-N1-C1'	10.17	129.90	117.70
49	R1	75	U	N1-C2-O2	10.08	129.86	122.80
87	M1	2269	U	N1-C2-O2	10.08	129.86	122.80
87	M1	2269	U	C2-N1-C1'	10.05	129.76	117.70
6	L2	125	U	C2-N1-C1'	10.02	129.72	117.70
5	L1	1556	C	N1-C2-O2	9.98	124.89	118.90
87	M1	2269	U	N3-C2-O2	-9.87	115.29	122.20
87	M1	406	G	O4'-C1'-N9	9.82	116.06	108.20
6	L2	125	U	N3-C2-O2	-9.69	115.42	122.20
87	M1	620	U	C2-N1-C1'	9.65	129.28	117.70
71	So	117	ASP	CB-CG-OD2	9.57	126.92	118.30
87	M1	3278	C	N3-C2-O2	-9.57	115.20	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	Ru	113	ASP	CB-CG-OD2	9.53	126.88	118.30
49	R1	989	U	C5-C6-N1	9.51	127.45	122.70
5	L1	846	A	N7-C8-N9	9.49	118.54	113.80
36	Mn	97	LEU	CA-CB-CG	9.45	137.03	115.30
49	S1	1082	C	C2-N1-C1'	9.38	129.11	118.80
87	M1	620	U	N1-C2-O2	9.35	129.34	122.80
49	R1	75	U	N3-C2-O2	-9.23	115.74	122.20
5	L1	3217	C	C2-N1-C1'	9.17	128.88	118.80
21	LN	109	ASP	CB-CG-OD2	9.16	126.55	118.30
13	LF	28	ASP	CB-CG-OD2	9.08	126.47	118.30
87	M1	620	U	N3-C2-O2	-9.04	115.87	122.20
49	R1	491	C	N3-C2-O2	-9.03	115.58	121.90
69	Rm	62	LEU	CA-CB-CG	8.91	135.79	115.30
66	Sj	89	ASP	CB-CG-OD2	8.84	126.25	118.30
87	M1	2836	C	N3-C2-O2	-8.82	115.72	121.90
87	M1	1222	G	O4'-C1'-N9	8.73	115.19	108.20
5	L1	1269	U	C2-N1-C1'	8.73	128.18	117.70
87	M1	1283	C	N3-C2-O2	-8.71	115.81	121.90
85	Rr	92	ASP	CB-CG-OD2	8.71	126.14	118.30
84	Ro	117	ASP	CB-CG-OD1	8.68	126.11	118.30
5	L1	846	A	C8-N9-C4	-8.63	102.35	105.80
87	M1	3278	C	C6-N1-C1'	-8.62	110.46	120.80
58	Sb	31	ASP	CB-CG-OD2	8.62	126.06	118.30
44	Mv	39	ASP	CB-CG-OD2	8.57	126.02	118.30
87	M1	922	U	N1-C2-O2	8.57	128.80	122.80
41	Ms	126	LEU	CA-CB-CG	8.56	134.98	115.30
5	L1	1556	C	N3-C2-O2	-8.55	115.92	121.90
49	R1	978	A	C8-N9-C4	-8.55	102.38	105.80
5	L1	3181	C	N1-C2-O2	8.49	124.00	118.90
49	R1	1389	C	C2-N1-C1'	8.48	128.13	118.80
49	S1	1389	C	C2-N1-C1'	8.48	128.13	118.80
5	L1	3217	C	N3-C2-O2	-8.48	115.97	121.90
63	Sg	69	LEU	CA-CB-CG	8.47	134.79	115.30
19	ML	41	ASP	CB-CG-OD1	8.45	125.91	118.30
49	R1	990	C	N1-C2-O2	8.43	123.95	118.90
5	L1	406	G	O4'-C1'-N9	8.42	114.94	108.20
5	L1	922	U	C2-N1-C1'	8.40	127.78	117.70
87	M1	922	U	C2-N1-C1'	8.40	127.78	117.70
5	L1	2772	C	N1-C2-O2	8.39	123.94	118.90
10	LC	83	ASP	CB-CG-OD2	8.33	125.80	118.30
48	Mz	213	ASP	CB-CG-OD1	8.31	125.78	118.30
48	Lz	238	ASP	CB-CG-OD2	8.31	125.78	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	R1	408	C	N1-C2-O2	8.31	123.89	118.90
49	S1	934	C	C2-N1-C1'	8.30	127.93	118.80
5	L1	2836	C	N3-C2-O2	-8.29	116.09	121.90
5	L1	1269	U	N1-C2-O2	8.28	128.60	122.80
75	Rs	53	ASP	CB-CG-OD2	8.27	125.74	118.30
49	R1	408	C	N3-C2-O2	-8.26	116.12	121.90
50	RA	52	ASP	CB-CG-OD2	8.25	125.73	118.30
87	M1	3181	C	C2-N1-C1'	8.09	127.69	118.80
49	R1	581	U	C2-N1-C1'	8.08	127.40	117.70
5	L1	2836	C	C2-N1-C1'	8.07	127.68	118.80
5	L1	1556	C	C2-N1-C1'	8.05	127.66	118.80
49	S1	555	A	N7-C8-N9	8.04	117.82	113.80
49	R1	990	C	C5-C6-N1	8.02	125.01	121.00
15	LH	40	ASP	CB-CG-OD2	8.00	125.50	118.30
79	Rw	54	ASP	CB-CG-OD2	8.00	125.50	118.30
87	M1	3181	C	N1-C2-O2	8.00	123.70	118.90
5	L1	2846	U	C2-N1-C1'	7.99	127.29	117.70
49	R1	683	C	N3-C2-O2	-7.98	116.31	121.90
49	R1	1274	C	N1-C2-O2	7.98	123.69	118.90
5	L1	1208	U	N1-C2-O2	7.96	128.37	122.80
5	L1	3181	C	C2-N1-C1'	7.95	127.55	118.80
87	M1	2836	C	C6-N1-C2	-7.95	117.12	120.30
5	L1	2772	C	C2-N1-C1'	7.94	127.53	118.80
67	Sk	82	LEU	CA-CB-CG	7.94	133.56	115.30
56	SG	272	ASP	CB-CG-OD2	7.93	125.44	118.30
62	Sf	55	ASP	CB-CG-OD2	7.93	125.43	118.30
49	R1	980	G	C4-N9-C1'	7.87	136.73	126.50
49	R1	581	U	N1-C2-O2	7.86	128.30	122.80
49	S1	238	U	C2-N1-C1'	7.85	127.12	117.70
49	S1	1257	U	C2-N1-C1'	7.78	127.03	117.70
36	Mn	110	GLU	CA-CB-CG	7.78	130.51	113.40
5	L1	3057	U	N3-C2-O2	-7.77	116.76	122.20
5	L1	2836	C	N1-C2-O2	7.76	123.56	118.90
5	L1	3181	C	N3-C2-O2	-7.75	116.47	121.90
49	R1	991	G	C6-C5-N7	-7.75	125.75	130.40
49	R1	1058	U	N3-C2-O2	-7.74	116.78	122.20
49	R1	989	U	C6-N1-C2	-7.73	116.36	121.00
49	S1	1527	C	C6-N1-C1'	-7.72	111.53	120.80
49	S1	1182	U	N3-C2-O2	-7.72	116.80	122.20
49	R1	965	U	C2-N1-C1'	7.72	126.96	117.70
60	Rd	169	ASP	CB-CG-OD2	7.70	125.23	118.30
5	L1	1208	U	C2-N1-C1'	7.68	126.91	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Lg	7	ASP	CB-CG-OD2	7.68	125.21	118.30
49	R1	1058	U	N1-C2-O2	7.67	128.17	122.80
5	L1	1269	U	N3-C2-O2	-7.65	116.85	122.20
44	Mv	29	ASP	CB-CG-OD1	7.64	125.17	118.30
47	My	182	LEU	CA-CB-CG	7.64	132.87	115.30
49	S1	965	U	C2-N1-C1'	7.63	126.86	117.70
87	M1	3214	U	C2-N1-C1'	7.63	126.86	117.70
87	M1	2873	U	N3-C2-O2	-7.62	116.87	122.20
87	M1	2836	C	C2-N1-C1'	7.61	127.17	118.80
82	Sz	67	ASP	CB-CG-OD1	7.61	125.15	118.30
87	M1	1283	C	N1-C2-O2	7.59	123.45	118.90
49	S1	639	U	N3-C2-O2	-7.58	116.89	122.20
87	M1	922	U	N3-C2-O2	-7.56	116.91	122.20
49	S1	934	C	N1-C2-O2	7.51	123.41	118.90
5	L1	3058	U	C2-N1-C1'	7.48	126.67	117.70
2	CM	4	U	C2-N1-C1'	7.48	126.67	117.70
71	So	124	ASP	CB-CG-OD2	7.48	125.03	118.30
20	LM	116	ASP	CB-CG-OD2	7.47	125.03	118.30
49	R1	1274	C	C2-N1-C1'	7.46	127.01	118.80
49	R1	990	C	C6-N1-C2	-7.44	117.32	120.30
49	S1	1491	U	N1-C2-O2	7.43	128.00	122.80
49	R1	1560	U	C2-N1-C1'	7.43	126.62	117.70
49	S1	494	U	C2-N1-C1'	7.43	126.61	117.70
87	M1	2836	C	N1-C2-O2	7.43	123.36	118.90
49	R1	581	U	N3-C2-O2	-7.41	117.01	122.20
87	M1	2550	U	N3-C2-O2	-7.41	117.02	122.20
58	Sb	210	ILE	CG1-CB-CG2	-7.40	95.11	111.40
5	L1	1556	C	C6-N1-C2	-7.40	117.34	120.30
5	L1	3269	U	N1-C2-O2	7.39	127.97	122.80
5	L1	3317	U	N1-C2-O2	7.38	127.97	122.80
2	CM	16	U	N1-C2-O2	7.38	127.97	122.80
49	R1	1390	U	C2-N1-C1'	7.37	126.54	117.70
67	Sk	26	ASP	CB-CG-OD2	7.36	124.92	118.30
87	M1	2550	U	C2-N1-C1'	7.36	126.53	117.70
87	M1	2388	U	N3-C2-O2	-7.35	117.06	122.20
49	R1	184	C	C2-N1-C1'	7.33	126.86	118.80
2	CM	2	U	N3-C2-O2	-7.32	117.07	122.20
49	S1	639	U	N1-C2-O2	7.32	127.93	122.80
87	M1	3278	C	C6-N1-C2	-7.32	117.37	120.30
5	L1	979	U	N3-C2-O2	-7.30	117.09	122.20
49	R1	507	U	C2-N1-C1'	7.30	126.46	117.70
42	Mt	134	ASP	CB-CG-OD2	7.30	124.87	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	Sr	27	ASP	CB-CG-OD1	7.30	124.87	118.30
57	Sa	72	ASP	CB-CG-OD1	7.28	124.86	118.30
87	M1	2846	U	C2-N1-C1'	7.28	126.43	117.70
5	L1	979	U	C2-N1-C1'	7.27	126.42	117.70
49	R1	1014	G	N3-C4-N9	7.25	130.35	126.00
76	Rt	29	GLU	CA-CB-CG	7.23	129.31	113.40
5	L1	2846	U	N3-C2-O2	-7.23	117.14	122.20
5	L1	922	U	N1-C2-O2	7.22	127.85	122.80
49	S1	1347	U	N1-C2-O2	7.20	127.84	122.80
5	L1	2388	U	N3-C2-O2	-7.18	117.17	122.20
87	M1	3181	C	N3-C2-O2	-7.18	116.88	121.90
49	R1	990	C	C2-N1-C1'	7.18	126.69	118.80
49	S1	1491	U	C2-N1-C1'	7.17	126.31	117.70
2	CM	2	U	N1-C2-O2	7.17	127.82	122.80
5	L1	1208	U	N3-C2-O2	-7.16	117.19	122.20
81	Sy	38	ASP	CB-CG-OD2	7.16	124.74	118.30
49	S1	555	A	C8-N9-C4	-7.15	102.94	105.80
87	M1	2550	U	N1-C2-O2	7.15	127.81	122.80
49	R1	1739	C	C6-N1-C2	-7.15	117.44	120.30
5	L1	1496	C	C2-N1-C1'	7.13	126.65	118.80
49	S1	1799	U	N1-C2-O2	7.13	127.79	122.80
49	R1	507	U	N1-C2-O2	7.13	127.79	122.80
2	CM	16	U	C2-N1-C1'	7.13	126.25	117.70
49	S1	494	U	N1-C2-O2	7.12	127.78	122.80
5	L1	3317	U	N3-C2-O2	-7.11	117.22	122.20
49	S1	861	U	C2-N1-C1'	7.11	126.23	117.70
5	L1	2772	C	N3-C2-O2	-7.10	116.93	121.90
6	L2	64	U	N3-C2-O2	-7.10	117.23	122.20
49	R1	1473	U	C2-N1-C1'	7.08	126.20	117.70
5	L1	3269	U	N3-C2-O2	-7.07	117.25	122.20
5	L1	758	C	C2-N1-C1'	7.07	126.58	118.80
49	S1	1347	U	C2-N1-C1'	7.06	126.17	117.70
49	S1	1082	C	C6-N1-C1'	-7.06	112.33	120.80
5	L1	3317	U	C2-N1-C1'	7.05	126.17	117.70
49	S1	1347	U	N3-C2-O2	-7.04	117.27	122.20
49	R1	959	U	N1-C2-O2	7.04	127.73	122.80
49	S1	186	C	C2-N1-C1'	7.04	126.54	118.80
87	M1	3058	U	N1-C2-O2	7.04	127.73	122.80
49	S1	1389	C	N1-C2-O2	7.03	123.11	118.90
87	M1	3057	U	N3-C2-O2	-7.03	117.28	122.20
5	L1	922	U	N3-C2-O2	-7.02	117.28	122.20
5	L1	3057	U	N1-C2-O2	7.02	127.71	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	St	140	LEU	CA-CB-CG	7.02	131.44	115.30
48	Lz	213	ASP	CB-CG-OD2	7.02	124.61	118.30
49	R1	1458	G	C4-N9-C1'	7.00	135.61	126.50
5	L1	3269	U	C2-N1-C1'	6.99	126.09	117.70
5	L1	2237	C	N3-C2-O2	-6.98	117.01	121.90
60	Rd	4	LEU	CA-CB-CG	6.98	131.36	115.30
49	S1	121	U	C2-N1-C1'	6.97	126.06	117.70
49	R1	959	U	N3-C2-O2	-6.96	117.33	122.20
5	L1	2836	C	C6-N1-C2	-6.94	117.52	120.30
49	S1	1182	U	C2-N1-C1'	6.94	126.03	117.70
5	L1	2772	C	C6-N1-C2	-6.94	117.53	120.30
49	S1	1458	G	C4-N9-C1'	6.93	135.51	126.50
70	Rn	36	GLN	CA-CB-CG	6.93	128.66	113.40
49	R1	1458	G	N3-C4-N9	6.92	130.15	126.00
49	S1	322	G	P-O3'-C3'	6.91	128.00	119.70
49	S1	140	A	O5'-P-OP2	6.90	118.98	110.70
49	R1	317	C	C2-N1-C1'	6.88	126.37	118.80
16	LI	136	ASP	CB-CG-OD2	6.88	124.49	118.30
49	R1	648	G	C4-N9-C1'	6.87	135.43	126.50
49	S1	1182	U	N1-C2-O2	6.86	127.60	122.80
18	LK	108	ASP	CB-CG-OD2	6.86	124.47	118.30
49	R1	978	A	N7-C8-N9	6.85	117.22	113.80
87	M1	1767	C	C2-N1-C1'	6.85	126.33	118.80
49	R1	1390	U	N1-C2-O2	6.83	127.58	122.80
49	S1	121	U	N3-C2-O2	-6.83	117.42	122.20
49	R1	980	G	C8-N9-C1'	-6.82	118.13	127.00
77	Su	93	LEU	CA-CB-CG	6.81	130.96	115.30
87	M1	2773	C	C2-N1-C1'	6.81	126.29	118.80
49	S1	238	U	N1-C2-O2	6.80	127.56	122.80
58	Sb	22	ASP	CB-CG-OD2	6.80	124.42	118.30
5	L1	979	U	N1-C2-O2	6.79	127.55	122.80
49	S1	1216	C	N1-C2-O2	6.79	122.97	118.90
49	R1	980	G	N3-C4-C5	-6.79	125.21	128.60
87	M1	2270	A	N7-C8-N9	6.79	117.19	113.80
2	CM	16	U	N3-C2-O2	-6.77	117.46	122.20
49	S1	1491	U	N3-C2-O2	-6.77	117.46	122.20
49	R1	75	U	C6-N1-C1'	-6.75	111.74	121.20
49	R1	1560	U	N3-C2-O2	-6.75	117.47	122.20
58	Sb	203	ASP	CB-CG-OD1	6.75	124.37	118.30
49	R1	1060	U	C2-N1-C1'	6.75	125.80	117.70
49	R1	861	U	C2-N1-C1'	6.73	125.77	117.70
49	S1	639	U	C2-N1-C1'	6.71	125.75	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	835	G	O4'-C1'-N9	6.70	113.56	108.20
49	S1	494	U	N3-C2-O2	-6.70	117.51	122.20
76	St	108	LEU	CB-CG-CD2	6.70	122.39	111.00
49	R1	1058	U	C2-N1-C1'	6.69	125.73	117.70
87	M1	3058	U	C2-N1-C1'	6.68	125.72	117.70
49	S1	1332	C	C2-N1-C1'	6.67	126.13	118.80
87	M1	1604	G	C4-N9-C1'	6.66	135.16	126.50
49	R1	1514	U	N1-C2-O2	6.66	127.46	122.80
87	M1	873	C	P-O3'-C3'	6.64	127.67	119.70
49	R1	507	U	N3-C2-O2	-6.62	117.56	122.20
49	R1	980	G	N3-C4-N9	6.61	129.97	126.00
49	S1	1799	U	N3-C2-O2	-6.59	117.59	122.20
49	R1	976	G	N3-C2-N2	-6.59	115.29	119.90
49	S1	1527	C	N1-C2-O2	6.59	122.85	118.90
83	RC	35	ASP	CB-CG-OD1	6.58	124.23	118.30
49	S1	1560	U	C2-N1-C1'	6.58	125.60	117.70
87	M1	1496	C	C2-N1-C1'	6.58	126.04	118.80
49	R1	730	G	C4-N9-C1'	6.57	135.04	126.50
5	L1	2237	C	N1-C2-O2	6.55	122.83	118.90
49	S1	1560	U	N3-C2-O2	-6.54	117.62	122.20
49	S1	1082	C	N1-C2-O2	6.53	122.82	118.90
49	S1	1097	U	C2-N1-C1'	6.53	125.54	117.70
87	M1	3214	U	N1-C2-O2	6.51	127.36	122.80
49	S1	959	U	N1-C2-O2	6.51	127.35	122.80
49	R1	683	C	N1-C2-O2	6.49	122.80	118.90
87	M1	3057	U	N1-C2-O2	6.49	127.34	122.80
49	R1	991	G	N3-C4-N9	6.49	129.89	126.00
49	S1	1791	A	P-O3'-C3'	6.48	127.48	119.70
49	R1	1473	U	N1-C2-O2	6.48	127.33	122.80
5	L1	3217	C	C6-N1-C1'	-6.47	113.04	120.80
49	R1	648	G	C8-N9-C1'	-6.47	118.59	127.00
5	L1	3078	U	C2-N1-C1'	6.45	125.44	117.70
49	S1	238	U	N3-C2-O2	-6.45	117.69	122.20
49	S1	1527	C	C5-C6-N1	6.44	124.22	121.00
87	M1	620	U	C6-N1-C1'	-6.44	112.19	121.20
49	S1	1458	G	N3-C4-N9	6.43	129.86	126.00
49	S1	166	C	N1-C2-O2	6.43	122.76	118.90
87	M1	2846	U	N3-C2-O2	-6.43	117.70	122.20
49	S1	656	G	C4-N9-C1'	6.42	134.85	126.50
6	L2	125	U	C6-N1-C1'	-6.42	112.21	121.20
49	S1	934	C	C6-N1-C1'	-6.41	113.10	120.80
27	Le	92	ASP	CB-CG-OD2	6.41	124.06	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	Sf	60	ASP	CB-CG-OD2	6.39	124.05	118.30
5	L1	3034	C	N1-C2-O2	6.38	122.73	118.90
87	M1	2652	U	N3-C2-O2	-6.38	117.73	122.20
5	L1	3155	U	N1-C2-O2	6.38	127.27	122.80
2	CM	4	U	N1-C2-O2	6.37	127.26	122.80
71	So	124	ASP	CB-CG-OD1	-6.36	112.57	118.30
87	M1	3058	U	N3-C2-O2	-6.36	117.75	122.20
49	R1	1458	G	C8-N9-C1'	-6.36	118.73	127.00
49	S1	959	U	C2-N1-C1'	6.36	125.33	117.70
49	S1	1216	C	N3-C2-O2	-6.35	117.45	121.90
5	L1	3058	U	N1-C2-O2	6.35	127.24	122.80
49	S1	609	U	P-O3'-C3'	6.34	127.31	119.70
87	M1	2477	G	N3-C4-C5	-6.32	125.44	128.60
49	R1	1332	C	C2-N1-C1'	6.32	125.75	118.80
5	L1	1280	C	N3-C2-O2	-6.31	117.48	121.90
5	L1	2652	U	N3-C2-O2	-6.31	117.78	122.20
84	Ro	124	ASP	CB-CG-OD1	6.31	123.98	118.30
49	S1	1489	U	C2-N1-C1'	6.30	125.26	117.70
49	S1	77	U	P-O3'-C3'	6.29	127.25	119.70
49	S1	1012	U	C2-N1-C1'	6.29	125.25	117.70
49	R1	1060	U	N1-C2-O2	6.28	127.20	122.80
87	M1	2444	C	C2-N1-C1'	6.28	125.71	118.80
5	L1	1604	G	C4-N9-C1'	6.28	134.66	126.50
49	R1	1060	U	N3-C2-O2	-6.27	117.81	122.20
5	L1	3155	U	C2-N1-C1'	6.26	125.22	117.70
49	S1	555	A	C5-N7-C8	-6.26	100.77	103.90
5	L1	1349	G	C4-N9-C1'	6.26	134.63	126.50
49	S1	959	U	N3-C2-O2	-6.26	117.82	122.20
60	Rd	218	LEU	CA-CB-CG	6.26	129.69	115.30
49	S1	1560	U	N1-C2-O2	6.25	127.18	122.80
49	R1	1514	U	N3-C2-O2	-6.25	117.83	122.20
5	L1	2617	U	N3-C2-O2	-6.25	117.83	122.20
87	M1	1425	U	N3-C2-O2	-6.25	117.83	122.20
49	S1	1256	A	P-O3'-C3'	6.24	127.19	119.70
5	L1	1815	U	P-O3'-C3'	6.24	127.19	119.70
49	R1	638	U	N3-C2-O2	-6.24	117.83	122.20
49	R1	1796	C	C2-N1-C1'	6.23	125.66	118.80
49	R1	139	C	P-O3'-C3'	6.22	127.16	119.70
5	L1	2531	C	N1-C2-O2	6.21	122.63	118.90
87	M1	2269	U	C6-N1-C1'	-6.21	112.51	121.20
87	M1	2846	U	N1-C2-O2	6.20	127.14	122.80
49	R1	287	G	O4'-C1'-N9	6.20	113.16	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	R1	830	U	O4'-C1'-N1	6.20	113.16	108.20
49	R1	1014	G	N3-C2-N2	6.20	124.24	119.90
49	R1	993	A	C8-N9-C4	-6.19	103.32	105.80
87	M1	2270	A	C8-N9-C4	-6.19	103.32	105.80
49	R1	927	C	C2-N1-C1'	6.19	125.61	118.80
6	M2	100	U	C2-N1-C1'	6.19	125.13	117.70
87	M1	2477	G	C4-N9-C1'	6.19	134.54	126.50
49	R1	1560	U	N1-C2-O2	6.18	127.13	122.80
49	S1	1363	U	N1-C2-O2	6.18	127.13	122.80
49	S1	711	U	P-O3'-C3'	6.18	127.11	119.70
49	R1	829	A	P-O3'-C3'	6.17	127.10	119.70
87	M1	1872	C	N1-C2-O2	6.16	122.60	118.90
49	S1	121	U	N1-C2-O2	6.16	127.11	122.80
49	R1	959	U	C2-N1-C1'	6.16	125.09	117.70
5	L1	2189	U	N1-C2-O2	6.15	127.10	122.80
63	Sg	147	LEU	CA-CB-CG	6.15	129.44	115.30
87	M1	78	U	N3-C2-O2	-6.14	117.90	122.20
5	L1	2873	U	N3-C2-O2	-6.14	117.90	122.20
49	S1	1012	U	N1-C2-O2	6.13	127.09	122.80
64	Sh	18	LEU	CA-CB-CG	6.13	129.39	115.30
49	R1	419	G	N1-C2-N2	-6.12	110.69	116.20
49	S1	1145	U	N3-C2-O2	-6.12	117.92	122.20
49	S1	184	C	C2-N1-C1'	6.11	125.53	118.80
49	S1	1584	G	P-O3'-C3'	6.10	127.02	119.70
20	MM	116	ASP	CB-CG-OD2	6.10	123.79	118.30
87	M1	3131	U	C2-N1-C1'	6.10	125.02	117.70
70	Sn	53	LEU	CA-CB-CG	6.09	129.31	115.30
78	Sv	8	LEU	CA-CB-CG	6.09	129.31	115.30
5	L1	2112	U	OP2-P-O3'	6.08	118.59	105.20
49	R1	393	C	C2-N1-C1'	6.08	125.48	118.80
49	S1	185	U	C2-N1-C1'	6.06	124.98	117.70
87	M1	3269	U	C2-N1-C1'	6.06	124.97	117.70
87	M1	3214	U	N3-C2-O2	-6.06	117.96	122.20
49	S1	166	C	N3-C2-O2	-6.06	117.66	121.90
49	S1	1535	U	C2-N1-C1'	6.06	124.97	117.70
49	R1	949	C	N1-C2-O2	6.06	122.53	118.90
49	R1	1796	C	N1-C2-O2	6.06	122.53	118.90
49	R1	1225	U	N1-C2-O2	6.05	127.04	122.80
49	S1	1799	U	C2-N1-C1'	6.05	124.96	117.70
44	Lv	91	ASP	CB-CG-OD2	6.04	123.74	118.30
87	M1	2873	U	N1-C2-O2	6.04	127.03	122.80
19	LL	41	ASP	CB-CG-OD2	6.04	123.73	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	2274	U	N1-C2-O2	6.04	127.03	122.80
49	S1	120	U	N1-C2-O2	6.03	127.02	122.80
5	L1	3131	U	C2-N1-C1'	6.03	124.93	117.70
5	L1	2132	C	C6-N1-C2	-6.03	117.89	120.30
49	R1	1258	U	N3-C2-O2	-6.02	117.98	122.20
49	R1	991	G	N1-C6-O6	6.01	123.51	119.90
5	L1	2112	U	P-O3'-C3'	6.01	126.91	119.70
5	L1	2846	U	N1-C2-O2	6.01	127.01	122.80
10	MC	136	LEU	CA-CB-CG	6.01	129.11	115.30
49	R1	648	G	N3-C4-N9	6.00	129.60	126.00
49	R1	408	C	P-O3'-C3'	6.00	126.89	119.70
49	R1	1390	U	N3-C2-O2	-6.00	118.00	122.20
49	S1	1257	U	N3-C2-O2	-5.99	118.01	122.20
69	Sm	39	ASP	CB-CG-OD2	5.98	123.68	118.30
87	M1	1562	C	P-O3'-C3'	5.97	126.86	119.70
5	L1	1349	G	N3-C4-C5	-5.97	125.62	128.60
2	CM	2	U	C2-N1-C1'	5.96	124.86	117.70
5	L1	3235	C	C2-N1-C1'	5.96	125.36	118.80
42	Lt	78	ASP	CB-CG-OD2	5.96	123.67	118.30
49	S1	1257	U	N1-C2-O2	5.96	126.97	122.80
49	S1	819	G	P-O3'-C3'	5.95	126.84	119.70
49	R1	730	G	N3-C4-N9	5.95	129.57	126.00
39	Lq	133	LEU	CA-CB-CG	5.95	128.99	115.30
49	S1	1535	U	N3-C2-O2	-5.95	118.03	122.20
49	R1	280	U	N1-C2-O2	5.95	126.97	122.80
7	L3	26	C	N1-C2-O2	5.95	122.47	118.90
49	R1	1389	C	C6-N1-C1'	-5.95	113.66	120.80
49	S1	1458	G	C8-N9-C1'	-5.95	119.27	127.00
5	L1	637	C	P-O3'-C3'	5.93	126.82	119.70
49	R1	934	C	C2-N1-C1'	5.93	125.33	118.80
5	L1	2550	U	N3-C2-O2	-5.93	118.05	122.20
49	S1	116	U	N3-C2-O2	-5.93	118.05	122.20
49	S1	765	G	P-O3'-C3'	5.92	126.80	119.70
49	R1	1596	C	C2-N1-C1'	5.91	125.31	118.80
5	L1	2189	U	N3-C2-O2	-5.90	118.07	122.20
49	S1	1389	C	C6-N1-C1'	-5.90	113.72	120.80
49	R1	280	U	C2-N1-C1'	5.89	124.77	117.70
87	M1	2269	U	C5-C6-N1	5.89	125.65	122.70
87	M1	2983	C	C2-N1-C1'	5.89	125.28	118.80
49	S1	1274	C	P-O3'-C3'	5.89	126.77	119.70
5	L1	1437	C	C2-N1-C1'	5.89	125.28	118.80
81	Ry	51	GLU	CA-CB-CG	5.88	126.34	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	1014	U	N3-C2-O2	-5.88	118.08	122.20
49	R1	864	U	N3-C2-O2	-5.88	118.08	122.20
5	L1	270	U	N1-C2-O2	5.88	126.92	122.80
49	R1	685	A	P-O3'-C3'	5.88	126.75	119.70
49	R1	1013	A	O4'-C1'-N9	5.88	112.90	108.20
87	M1	2366	C	C2-N1-C1'	5.88	125.26	118.80
49	S1	656	G	N3-C4-N9	5.87	129.52	126.00
49	S1	1145	U	C2-N1-C1'	5.87	124.75	117.70
49	R1	730	G	N3-C4-C5	-5.87	125.67	128.60
88	DQ	35	C	N1-C2-O2	5.87	122.42	118.90
5	L1	1876	U	N3-C2-O2	-5.85	118.10	122.20
61	Se	193	GLY	N-CA-C	5.85	127.73	113.10
5	L1	1878	G	C4-N9-C1'	5.85	134.11	126.50
71	So	102	LEU	CA-CB-CG	5.85	128.76	115.30
49	R1	1274	C	N3-C2-O2	-5.85	117.80	121.90
49	S1	352	A	P-O3'-C3'	5.84	126.71	119.70
5	L1	3217	C	C6-N1-C2	-5.84	117.96	120.30
12	LE	185	ARG	CA-CB-CG	5.84	126.25	113.40
49	S1	1535	U	N1-C2-O2	5.83	126.88	122.80
87	M1	1496	C	C6-N1-C2	-5.83	117.97	120.30
5	L1	78	U	N3-C2-O2	-5.83	118.12	122.20
5	L1	3277	U	C2-N1-C1'	5.83	124.69	117.70
6	L2	64	U	N1-C2-O2	5.83	126.88	122.80
49	S1	1458	G	N3-C4-C5	-5.83	125.69	128.60
49	S1	1363	U	C2-N1-C1'	5.82	124.69	117.70
57	Sa	27	ARG	CA-CB-CG	5.82	126.20	113.40
5	L1	2101	C	P-O3'-C3'	5.82	126.68	119.70
87	M1	3269	U	N1-C2-O2	5.81	126.87	122.80
87	M1	2477	G	N3-C4-N9	5.80	129.48	126.00
5	L1	1064	A	P-O3'-C3'	5.80	126.66	119.70
85	Rr	119	LEU	CA-CB-CG	5.80	128.64	115.30
87	M1	2873	U	C2-N1-C1'	5.79	124.65	117.70
5	L1	3300	U	N3-C2-O2	-5.79	118.14	122.20
87	M1	1878	G	C4-N9-C1'	5.79	134.03	126.50
87	M1	3181	C	C6-N1-C1'	-5.79	113.85	120.80
5	L1	1097	G	P-O3'-C3'	5.79	126.65	119.70
5	L1	2366	C	C2-N1-C1'	5.79	125.17	118.80
49	R1	1566	U	N3-C2-O2	-5.79	118.15	122.20
49	R1	75	U	C5-C6-N1	5.79	125.59	122.70
87	M1	2794	G	O4'-C1'-N9	5.79	112.83	108.20
49	R1	990	C	C5-C4-N4	-5.78	116.16	120.20
5	L1	3306	U	C2-N1-C1'	5.77	124.62	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S1	1636	C	P-O3'-C3'	5.77	126.62	119.70
49	R1	1458	G	N3-C4-C5	-5.76	125.72	128.60
87	M1	2585	G	N3-C4-C5	-5.76	125.72	128.60
2	CM	4	U	N3-C2-O2	-5.75	118.17	122.20
67	Sk	80	LEU	CA-CB-CG	5.75	128.52	115.30
5	L1	524	U	N3-C2-O2	-5.75	118.18	122.20
12	ME	103	LEU	CA-CB-CG	5.74	128.51	115.30
49	R1	1796	C	N3-C2-O2	-5.74	117.89	121.90
5	L1	1716	U	P-O3'-C3'	5.73	126.57	119.70
5	L1	1872	C	N1-C2-O2	5.73	122.34	118.90
66	Sj	105	LEU	CA-CB-CG	5.73	128.47	115.30
87	M1	2405	C	N3-C2-O2	-5.72	117.89	121.90
69	Rm	88	LEU	CA-CB-CG	5.72	128.45	115.30
88	DQ	52	C	C2-N1-C1'	5.72	125.09	118.80
5	L1	2726	C	N3-C2-O2	-5.72	117.90	121.90
6	L2	125	U	C5-C6-N1	5.71	125.56	122.70
5	L1	315	C	C2-N1-C1'	5.71	125.08	118.80
5	L1	3306	U	N3-C2-O2	-5.71	118.20	122.20
87	M1	2773	C	C6-N1-C2	-5.71	118.02	120.30
87	M1	1872	C	N3-C2-O2	-5.71	117.91	121.90
49	R1	1082	C	C6-N1-C2	-5.70	118.02	120.30
87	M1	2444	C	C5-C6-N1	5.70	123.85	121.00
49	R1	1185	U	N1-C2-O2	5.70	126.79	122.80
49	R1	1674	C	N1-C2-O2	5.70	122.32	118.90
87	M1	2388	U	N1-C2-O2	5.70	126.79	122.80
5	L1	1115	G	C4-N9-C1'	5.69	133.90	126.50
5	L1	2336	U	N3-C2-O2	-5.69	118.22	122.20
49	R1	380	U	N1-C2-O2	5.69	126.78	122.80
49	S1	656	G	N3-C4-C5	-5.69	125.76	128.60
63	Sg	216	LEU	CA-CB-CG	5.68	128.37	115.30
5	L1	835	G	O4'-C1'-N9	5.68	112.75	108.20
49	R1	1274	C	C6-N1-C1'	-5.68	113.99	120.80
5	L1	1239	C	C2-N1-C1'	5.68	125.04	118.80
49	R1	491	C	C6-N1-C2	-5.67	118.03	120.30
49	S1	965	U	N1-C2-O2	5.67	126.77	122.80
49	R1	73	U	P-O3'-C3'	5.67	126.51	119.70
87	M1	3278	C	C5-C6-N1	5.67	123.83	121.00
5	L1	36	C	N1-C2-O2	5.67	122.30	118.90
49	R1	638	U	N1-C2-O2	5.66	126.76	122.80
5	L1	3155	U	N3-C2-O2	-5.66	118.24	122.20
5	L1	1349	G	N3-C4-N9	5.66	129.39	126.00
69	Sm	137	MET	CA-CB-CG	5.66	122.91	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	R1	1344	A	P-O3'-C3'	5.65	126.48	119.70
87	M1	922	U	C6-N1-C1'	-5.65	113.29	121.20
49	S1	1489	U	N3-C2-O2	-5.64	118.25	122.20
87	M1	969	C	C6-N1-C2	-5.64	118.04	120.30
5	L1	1269	U	C6-N1-C1'	-5.63	113.32	121.20
5	L1	663	C	C5-C6-N1	5.63	123.81	121.00
5	L1	3181	C	C6-N1-C2	-5.62	118.05	120.30
56	RG	270	LEU	CA-CB-CG	5.62	128.24	115.30
62	Sf	65	ARG	CA-CB-CG	5.62	125.77	113.40
49	R1	946	U	C2-N1-C1'	5.62	124.44	117.70
49	S1	1023	A	P-O3'-C3'	5.62	126.44	119.70
49	R1	1573	A	P-O3'-C3'	5.62	126.44	119.70
69	Sm	131	ASP	CB-CG-OD2	5.62	123.36	118.30
87	M1	2405	C	C6-N1-C2	-5.62	118.05	120.30
87	M1	2821	C	N1-C2-O2	5.61	122.27	118.90
5	L1	2996	U	C2-N1-C1'	5.61	124.43	117.70
87	M1	2638	C	N1-C2-O2	5.61	122.26	118.90
76	St	29	GLU	CA-CB-CG	5.60	125.72	113.40
87	M1	2269	U	C6-N1-C2	-5.60	117.64	121.00
87	M1	2272	G	O4'-C1'-N9	5.60	112.68	108.20
49	R1	1000	C	C2-N1-C1'	5.60	124.96	118.80
5	L1	846	A	C4-N9-C1'	5.59	136.35	126.30
49	S1	530	C	N1-C2-O2	5.58	122.25	118.90
5	L1	3181	C	C6-N1-C1'	-5.58	114.10	120.80
5	L1	65	A	P-O3'-C3'	5.58	126.40	119.70
49	S1	1389	C	N3-C2-O2	-5.58	118.00	121.90
49	S1	1389	C	C6-N1-C2	-5.57	118.07	120.30
49	R1	1185	U	C2-N1-C1'	5.57	124.39	117.70
87	M1	2983	C	N3-C2-O2	-5.57	118.00	121.90
5	L1	1355	A	P-O3'-C3'	5.57	126.38	119.70
57	Sa	206	ASP	C-N-CD	5.57	140.10	128.40
49	R1	1225	U	N3-C2-O2	-5.57	118.31	122.20
49	S1	1066	C	C2-N1-C1'	5.56	124.92	118.80
49	R1	1473	U	N3-C2-O2	-5.56	118.31	122.20
87	M1	1604	G	C8-N9-C1'	-5.56	119.77	127.00
87	M1	2843	U	C2-N1-C1'	5.56	124.37	117.70
36	Mn	42	LEU	CA-CB-CG	5.56	128.09	115.30
49	S1	90	C	C2-N1-C1'	5.55	124.91	118.80
87	M1	2274	U	N3-C2-O2	-5.55	118.31	122.20
5	L1	3153	U	C2-N1-C1'	5.55	124.36	117.70
69	Sm	68	GLU	CA-CB-CG	5.55	125.61	113.40
49	R1	491	C	N1-C2-O2	5.54	122.22	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S1	1573	A	P-O3'-C3'	5.54	126.35	119.70
5	L1	1608	C	C2-N1-C1'	5.54	124.89	118.80
6	L2	100	U	C2-N1-C1'	5.54	124.34	117.70
56	SG	111	MET	CB-CG-SD	5.53	129.00	112.40
5	L1	637	C	OP1-P-O3'	5.53	117.37	105.20
5	L1	3034	C	N3-C2-O2	-5.53	118.03	121.90
49	R1	1058	U	C5-C6-N1	5.53	125.47	122.70
5	L1	2974	U	N3-C2-O2	-5.53	118.33	122.20
5	L1	2388	U	N1-C2-O2	5.53	126.67	122.80
49	S1	1596	C	N3-C2-O2	-5.53	118.03	121.90
70	Rn	28	LEU	CA-CB-CG	5.53	128.01	115.30
49	R1	496	G	N3-C4-N9	5.52	129.31	126.00
49	R1	927	C	C6-N1-C2	-5.52	118.09	120.30
49	S1	120	U	N3-C2-O2	-5.52	118.34	122.20
49	R1	965	U	N1-C2-O2	5.52	126.66	122.80
49	S1	1528	U	C2-N1-C1'	5.51	124.32	117.70
49	S1	1596	C	C2-N1-C1'	5.51	124.87	118.80
5	L1	2407	C	C6-N1-C2	-5.51	118.10	120.30
5	L1	1230	G	N1-C2-N2	-5.50	111.25	116.20
5	L1	1496	C	C6-N1-C2	-5.50	118.10	120.30
76	St	67	MET	CB-CG-SD	5.50	128.90	112.40
62	Sf	25	LEU	CA-CB-CG	5.50	127.95	115.30
49	S1	1363	U	N3-C2-O2	-5.50	118.35	122.20
49	R1	991	G	N9-C4-C5	-5.50	103.20	105.40
5	L1	2772	C	C5-C6-N1	5.50	123.75	121.00
5	L1	922	U	C6-N1-C1'	-5.49	113.52	121.20
49	S1	1274	C	N1-C2-O2	5.49	122.19	118.90
49	S1	965	U	C6-N1-C1'	-5.48	113.52	121.20
87	M1	2488	A	C2-N3-C4	5.48	113.34	110.60
5	L1	2405	C	N3-C2-O2	-5.48	118.06	121.90
49	R1	1783	C	C2-N1-C1'	5.47	124.82	118.80
49	S1	313	U	P-O3'-C3'	5.47	126.26	119.70
87	M1	3214	U	C6-N1-C1'	-5.47	113.55	121.20
5	L1	2935	U	C2-N1-C1'	5.46	124.25	117.70
49	S1	1258	U	N3-C2-O2	-5.46	118.38	122.20
5	L1	524	U	N1-C2-O2	5.46	126.62	122.80
49	R1	1572	G	C4-N9-C1'	5.46	133.59	126.50
87	M1	2652	U	N1-C2-O2	5.45	126.62	122.80
89	MQ	15	LEU	CA-CB-CG	5.45	127.84	115.30
49	S1	639	U	P-O3'-C3'	5.45	126.24	119.70
87	M1	3306	U	N3-C2-O2	-5.45	118.39	122.20
5	L1	270	U	N3-C2-O2	-5.45	118.39	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	Sk	80	LEU	CB-CG-CD1	5.45	120.26	111.00
87	M1	2971	A	P-O3'-C3'	5.44	126.23	119.70
87	M1	142	C	N1-C2-O2	5.44	122.16	118.90
2	CM	2	U	C5-C6-N1	5.43	125.42	122.70
5	L1	3058	U	N3-C2-O2	-5.43	118.40	122.20
49	S1	1489	U	N1-C2-O2	5.43	126.60	122.80
5	L1	2726	C	C2-N1-C1'	5.43	124.77	118.80
5	L1	1604	G	N3-C4-C5	-5.43	125.89	128.60
49	R1	864	U	N1-C2-O2	5.43	126.60	122.80
49	S1	387	A	OP2-P-O3'	5.42	117.13	105.20
49	R1	184	C	C6-N1-C1'	-5.42	114.30	120.80
56	SG	234	LEU	CA-CB-CG	5.42	127.75	115.30
49	S1	278	U	P-O3'-C3'	5.41	126.19	119.70
49	R1	1596	C	N1-C2-O2	5.41	122.15	118.90
49	S1	1012	U	C5-C6-N1	5.41	125.41	122.70
49	R1	278	U	N3-C2-O2	-5.41	118.42	122.20
5	L1	1604	G	C8-N9-C1'	-5.41	119.97	127.00
87	M1	3306	U	C2-N1-C1'	5.40	124.18	117.70
5	L1	982	C	C2-N1-C1'	5.40	124.74	118.80
49	S1	864	U	N3-C2-O2	-5.40	118.42	122.20
49	R1	730	G	C8-N9-C1'	-5.40	119.98	127.00
5	L1	1508	C	N1-C2-O2	5.40	122.14	118.90
5	L1	2836	C	C6-N1-C1'	-5.40	114.32	120.80
5	L1	1604	G	N3-C4-N9	5.40	129.24	126.00
49	R1	479	C	C2-N1-C1'	5.40	124.73	118.80
5	L1	2983	C	C2-N1-C1'	5.39	124.73	118.80
5	L1	1368	U	C2-N1-C1'	5.39	124.17	117.70
49	R1	1529	C	C2-N1-C1'	5.39	124.73	118.80
5	L1	2873	U	C2-N1-C1'	5.38	124.16	117.70
49	R1	270	C	C2-N1-C1'	5.38	124.72	118.80
49	R1	536	C	C2-N1-C1'	5.38	124.72	118.80
49	R1	989	U	C6-N1-C1'	-5.38	113.66	121.20
49	S1	656	G	C8-N9-C1'	-5.38	120.01	127.00
67	Sk	3	MET	CA-CB-CG	5.38	122.44	113.30
42	Lt	38	LEU	CA-CB-CG	5.37	127.66	115.30
87	M1	3181	C	C6-N1-C2	-5.37	118.15	120.30
49	R1	116	U	N3-C2-O2	-5.37	118.44	122.20
87	M1	895	A	N9-C4-C5	-5.37	103.65	105.80
49	S1	1273	G	P-O3'-C3'	5.37	126.14	119.70
5	L1	1278	A	O4'-C1'-N9	5.37	112.50	108.20
5	L1	192	C	C2-N1-C1'	5.37	124.70	118.80
5	L1	1556	C	C5-C6-N1	5.37	123.68	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	1031	C	C2-N1-C1'	5.37	124.70	118.80
49	S1	387	A	P-O3'-C3'	5.36	126.14	119.70
49	S1	1258	U	N1-C2-O2	5.36	126.55	122.80
5	L1	2434	U	C2-N1-C1'	5.36	124.14	117.70
81	Ry	125	LEU	CA-CB-CG	5.36	127.63	115.30
87	M1	2726	C	N3-C2-O2	-5.36	118.15	121.90
56	SG	177	MET	CA-CB-CG	5.36	122.41	113.30
5	L1	3078	U	N1-C2-O2	5.35	126.55	122.80
49	R1	758	U	N1-C2-O2	5.35	126.54	122.80
66	Rj	65	LYS	CA-CB-CG	5.35	125.16	113.40
49	S1	1307	U	N1-C2-O2	5.35	126.54	122.80
49	R1	1389	C	C6-N1-C2	-5.34	118.16	120.30
66	Rj	118	LEU	CA-CB-CG	5.34	127.59	115.30
5	L1	1368	U	N1-C2-O2	5.34	126.54	122.80
60	Sd	78	LYS	CA-CB-CG	5.34	125.15	113.40
10	MC	109	LEU	CA-CB-CG	5.34	127.58	115.30
49	S1	1596	C	N1-C2-O2	5.34	122.10	118.90
76	St	45	MET	CB-CG-SD	5.34	128.41	112.40
87	M1	895	A	C6-C5-N7	-5.34	128.56	132.30
87	M1	1023	C	C2-N1-C1'	5.33	124.67	118.80
89	MQ	128	MET	CA-CB-CG	5.33	122.36	113.30
49	R1	1568	C	P-O3'-C3'	5.33	126.10	119.70
49	S1	1307	U	N3-C2-O2	-5.33	118.47	122.20
87	M1	916	G	P-O3'-C3'	5.33	126.09	119.70
56	RG	316	MET	CA-CB-CG	5.32	122.34	113.30
2	CM	2	U	C6-N1-C2	-5.32	117.81	121.00
5	L1	3228	C	P-O3'-C3'	5.32	126.08	119.70
49	R1	949	C	C2-N1-C1'	5.32	124.65	118.80
49	R1	1012	U	N1-C2-O2	5.32	126.52	122.80
87	M1	3269	U	N3-C2-O2	-5.32	118.48	122.20
5	L1	1724	U	O4'-C1'-N1	5.31	112.45	108.20
5	L1	3057	U	C2-N1-C1'	5.31	124.08	117.70
88	DQ	35	C	N3-C2-O2	-5.31	118.18	121.90
49	R1	1014	G	N9-C4-C5	-5.31	103.28	105.40
76	Rt	45	MET	CB-CG-SD	5.31	128.32	112.40
49	S1	617	U	C2-N1-C1'	5.30	124.06	117.70
49	R1	1389	C	N1-C2-O2	5.30	122.08	118.90
49	R1	1014	G	C5-C6-N1	5.30	114.15	111.50
49	R1	1063	U	N1-C2-O2	5.30	126.51	122.80
13	MF	168	ASP	CB-CG-OD1	5.30	123.07	118.30
49	R1	990	C	N3-C2-O2	-5.29	118.19	121.90
5	L1	3078	U	N3-C2-O2	-5.29	118.49	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	2843	U	N1-C2-O2	5.29	126.51	122.80
49	R1	417	A	P-O3'-C3'	5.29	126.05	119.70
5	L1	3058	U	C6-N1-C1'	-5.29	113.80	121.20
44	Lv	90	ARG	C-N-CA	5.29	134.92	121.70
87	M1	2407	C	C5-C6-N1	5.28	123.64	121.00
49	R1	581	U	C6-N1-C1'	-5.28	113.81	121.20
87	M1	1854	C	C6-N1-C2	-5.28	118.19	120.30
87	M1	1014	U	N1-C2-O2	5.28	126.50	122.80
49	R1	1058	U	C6-N1-C2	-5.28	117.83	121.00
49	R1	1595	U	C2-N1-C1'	5.28	124.03	117.70
49	S1	1257	U	C6-N1-C1'	-5.27	113.82	121.20
49	S1	185	U	N1-C2-O2	5.27	126.49	122.80
6	M2	64	U	N3-C2-O2	-5.27	118.51	122.20
5	L1	986	U	N3-C2-O2	-5.27	118.51	122.20
49	R1	1742	U	C2-N1-C1'	5.27	124.02	117.70
49	R1	1235	C	N1-C2-O2	5.27	122.06	118.90
58	Rb	224	ASP	CB-CG-OD1	5.27	123.04	118.30
49	S1	640	U	P-O3'-C3'	5.26	126.01	119.70
49	R1	409	C	C6-N1-C2	-5.26	118.20	120.30
87	M1	97	U	N3-C2-O2	-5.26	118.52	122.20
87	M1	524	U	N1-C2-O2	5.25	126.48	122.80
49	S1	1251	U	C2-N1-C1'	5.25	124.00	117.70
87	M1	2726	C	C2-N1-C1'	5.25	124.58	118.80
87	M1	915	A	N7-C8-N9	5.25	116.42	113.80
5	L1	2726	C	C6-N1-C2	-5.25	118.20	120.30
5	L1	3362	A	N7-C8-N9	5.25	116.42	113.80
87	M1	524	U	N3-C2-O2	-5.24	118.53	122.20
49	R1	132	U	P-O3'-C3'	5.24	125.99	119.70
49	R1	924	A	P-O3'-C3'	5.24	125.98	119.70
49	S1	280	U	P-O3'-C3'	5.24	125.98	119.70
5	L1	2585	G	N3-C4-C5	-5.24	125.98	128.60
49	R1	280	U	N3-C2-O2	-5.23	118.54	122.20
5	L1	270	U	C2-N1-C1'	5.23	123.98	117.70
59	Sc	38	VAL	CG1-CB-CG2	-5.23	102.53	110.90
49	R1	927	C	N1-C2-O2	5.23	122.04	118.90
49	R1	965	U	N3-C2-O2	-5.23	118.54	122.20
87	M1	1604	G	N3-C4-C5	-5.23	125.98	128.60
39	Mq	91	LEU	CA-CB-CG	5.23	127.33	115.30
49	R1	1246	C	N1-C2-O2	5.23	122.04	118.90
49	R1	1225	U	C2-N1-C1'	5.23	123.97	117.70
49	S1	400	A	P-O3'-C3'	5.22	125.97	119.70
5	L1	3218	A	P-O3'-C3'	5.22	125.96	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L1	3350	C	C6-N1-C2	-5.22	118.21	120.30
49	R1	1214	U	N1-C2-O2	5.22	126.45	122.80
87	M1	2137	U	C2-N1-C1'	5.22	123.96	117.70
5	L1	1115	G	C8-N9-C1'	-5.22	120.22	127.00
87	M1	2585	G	N3-C4-N9	5.22	129.13	126.00
44	Mv	18	ASP	CB-CG-OD1	5.22	123.00	118.30
49	S1	186	C	C6-N1-C1'	-5.21	114.54	120.80
49	S1	120	U	C2-N1-C1'	5.21	123.95	117.70
87	M1	1264	G	C4-N9-C1'	5.21	133.27	126.50
5	L1	1349	G	C8-N9-C1'	-5.20	120.24	127.00
5	L1	1280	C	C6-N1-C2	-5.20	118.22	120.30
49	R1	965	U	C6-N1-C1'	-5.20	113.92	121.20
49	R1	1258	U	N1-C2-O2	5.20	126.44	122.80
87	M1	2270	A	O4'-C1'-N9	5.19	112.35	108.20
87	M1	3057	U	C2-N1-C1'	5.19	123.92	117.70
5	L1	2263	C	C5-C6-N1	5.18	123.59	121.00
49	S1	1063	U	N1-C2-O2	5.18	126.43	122.80
87	M1	36	C	N1-C2-O2	5.18	122.01	118.90
49	S1	354	C	N1-C2-O2	5.18	122.01	118.90
49	R1	380	U	C2-N1-C1'	5.18	123.92	117.70
49	R1	498	G	N7-C8-N9	5.18	115.69	113.10
5	L1	2652	U	N1-C2-O2	5.18	126.42	122.80
49	R1	1535	U	P-O3'-C3'	5.17	125.91	119.70
49	S1	88	U	N3-C2-O2	-5.17	118.58	122.20
49	S1	1527	C	C6-N1-C2	-5.17	118.23	120.30
87	M1	1246	G	C4-N9-C1'	5.17	133.22	126.50
87	M1	2253	G	P-O3'-C3'	5.17	125.90	119.70
38	Lp	25	LYS	N-CA-CB	5.16	119.89	110.60
5	L1	916	G	P-O3'-C3'	5.16	125.89	119.70
49	R1	991	G	C4-C5-C6	5.16	121.90	118.80
87	M1	2274	U	C2-N1-C1'	5.16	123.89	117.70
87	M1	1767	C	N1-C2-O2	5.16	121.99	118.90
5	L1	2553	U	C2-N1-C1'	5.16	123.89	117.70
49	R1	1000	C	N3-C2-O2	-5.16	118.29	121.90
5	L1	42	C	C6-N1-C2	-5.15	118.24	120.30
5	L1	3350	C	N1-C2-O2	5.15	121.99	118.90
36	Ln	42	LEU	CA-CB-CG	5.15	127.14	115.30
87	M1	915	A	C8-N9-C4	-5.14	103.74	105.80
5	L1	2935	U	N1-C2-O2	5.14	126.40	122.80
49	S1	517	U	N3-C2-O2	-5.14	118.60	122.20
5	L1	846	A	C5-N7-C8	-5.14	101.33	103.90
5	L1	2281	A	O4'-C1'-N9	5.14	112.31	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	247	C	N3-C2-O2	-5.14	118.30	121.90
5	L1	1448	U	N3-C2-O2	-5.14	118.60	122.20
5	L1	2842	U	N1-C2-O2	5.14	126.39	122.80
49	S1	1633	A	P-O3'-C3'	5.14	125.86	119.70
13	LF	108	GLU	C-N-CA	5.13	134.53	121.70
49	S1	758	U	N1-C2-O2	5.13	126.39	122.80
87	M1	986	U	N3-C2-O2	-5.13	118.61	122.20
87	M1	2763	U	N3-C2-O2	-5.13	118.61	122.20
5	L1	2899	C	C2-N1-C1'	5.13	124.44	118.80
87	M1	985	U	N3-C2-O2	-5.13	118.61	122.20
58	Sb	147	ALA	C-N-CA	5.13	134.52	121.70
87	M1	865	U	N1-C2-O2	5.12	126.39	122.80
36	Ln	97	LEU	CA-CB-CG	5.12	127.08	115.30
49	R1	1016	C	N1-C2-O2	5.12	121.97	118.90
72	Rp	72	LYS	CA-CB-CG	5.12	124.67	113.40
49	S1	934	C	N3-C2-O2	-5.12	118.32	121.90
49	S1	1632	C	N3-C2-O2	-5.12	118.32	121.90
81	Ry	115	ASP	CB-CG-OD2	5.11	122.90	118.30
57	Ra	43	ASP	CB-CG-OD2	5.11	122.90	118.30
20	LM	164	LEU	CA-CB-CG	5.11	127.05	115.30
49	R1	380	U	N3-C2-O2	-5.11	118.62	122.20
87	M1	2496	C	C2-N1-C1'	5.11	124.42	118.80
5	L1	2984	C	N1-C2-O2	5.11	121.97	118.90
87	M1	2867	C	N1-C2-O2	5.11	121.96	118.90
5	L1	113	C	C2-N1-C1'	5.10	124.41	118.80
49	R1	767	U	C2-N1-C1'	5.10	123.82	117.70
5	L1	2836	C	O4'-C1'-N1	5.10	112.28	108.20
49	R1	830	U	C2-N1-C1'	5.10	123.82	117.70
5	L1	1208	U	C6-N1-C1'	-5.09	114.07	121.20
5	L1	1820	U	P-O3'-C3'	5.09	125.81	119.70
5	L1	2263	C	C6-N1-C2	-5.09	118.26	120.30
84	Ro	129	LYS	CA-CB-CG	5.09	124.60	113.40
87	M1	283	G	C4-N9-C1'	5.09	133.12	126.50
87	M1	2378	C	C6-N1-C2	-5.09	118.26	120.30
5	L1	1190	A	C4-N9-C1'	5.09	135.46	126.30
5	L1	2531	C	C2-N1-C1'	5.09	124.39	118.80
49	R1	758	U	N3-C2-O2	-5.09	118.64	122.20
87	M1	421	G	C4-N9-C1'	5.08	133.11	126.50
87	M1	1190	A	C4-N9-C1'	5.08	135.45	126.30
72	Sp	25	LEU	CA-CB-CG	5.08	126.99	115.30
5	L1	3269	U	P-O3'-C3'	5.08	125.80	119.70
49	S1	700	C	C5-C6-N1	5.08	123.54	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	R1	934	C	N1-C2-O2	5.08	121.95	118.90
49	S1	238	U	C6-N1-C1'	-5.08	114.09	121.20
49	R1	1674	C	C6-N1-C2	-5.08	118.27	120.30
5	L1	1495	U	C5-C6-N1	-5.08	120.16	122.70
7	L3	26	C	N3-C2-O2	-5.08	118.35	121.90
49	R1	1185	U	N3-C2-O2	-5.08	118.65	122.20
87	M1	1525	G	C4-N9-C1'	5.08	133.10	126.50
87	M1	2935	U	C2-N1-C1'	5.08	123.79	117.70
49	R1	184	C	N1-C2-O2	5.07	121.94	118.90
73	Rq	28	LEU	CA-CB-CG	5.07	126.97	115.30
49	R1	1739	C	C5-C6-N1	5.07	123.54	121.00
5	L1	1878	G	C8-N9-C1'	-5.07	120.41	127.00
5	L1	2873	U	N1-C2-O2	5.07	126.35	122.80
49	R1	691	C	N1-C2-O2	5.07	121.94	118.90
49	S1	1097	U	N1-C2-O2	5.07	126.35	122.80
77	Ru	50	LEU	CA-CB-CG	5.07	126.95	115.30
5	L1	1269	U	C5-C6-N1	5.06	125.23	122.70
5	L1	2553	U	N1-C2-O2	5.06	126.34	122.80
5	L1	1854	C	C6-N1-C2	-5.06	118.28	120.30
87	M1	2821	C	N3-C2-O2	-5.06	118.36	121.90
49	S1	1003	A	O4'-C1'-N9	5.06	112.25	108.20
87	M1	2436	U	N3-C2-O2	-5.06	118.66	122.20
5	L1	1554	U	P-O3'-C3'	5.05	125.77	119.70
5	L1	1876	U	N1-C2-O2	5.05	126.34	122.80
49	S1	928	U	P-O3'-C3'	5.05	125.77	119.70
49	R1	497	G	N1-C2-N2	-5.05	111.65	116.20
49	R1	1390	U	C6-N1-C1'	-5.05	114.12	121.20
87	M1	283	G	C8-N9-C1'	-5.05	120.43	127.00
87	M1	2189	U	N3-C2-O2	-5.05	118.66	122.20
5	L1	1279	C	N1-C2-O2	5.05	121.93	118.90
49	R1	1246	C	C2-N1-C1'	5.05	124.35	118.80
50	RA	52	ASP	CB-CG-OD1	-5.05	113.76	118.30
49	R1	1332	C	N1-C2-O2	5.05	121.93	118.90
87	M1	2477	G	C8-N9-C1'	-5.05	120.44	127.00
5	L1	3351	U	P-O3'-C3'	5.04	125.75	119.70
87	M1	1878	G	N3-C4-N9	5.04	129.03	126.00
5	L1	2204	C	C2-N1-C1'	5.04	124.34	118.80
49	S1	1389	C	C5-C6-N1	5.04	123.52	121.00
87	M1	1037	C	C2-N1-C1'	5.04	124.34	118.80
17	LJ	187	GLU	CA-CB-CG	5.04	124.48	113.40
51	SB	36	LYS	CB-CG-CD	5.04	124.70	111.60
49	S1	610	G	C4-N9-C1'	5.04	133.05	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Mj	41	LEU	CA-CB-CG	5.03	126.88	115.30
5	L1	2842	U	C2-N1-C1'	5.03	123.73	117.70
5	L1	2996	U	N1-C2-O2	5.03	126.32	122.80
49	S1	1497	U	N1-C2-O2	5.03	126.32	122.80
49	S1	517	U	N1-C2-O2	5.03	126.32	122.80
5	L1	969	C	N1-C2-O2	5.02	121.91	118.90
87	M1	271	C	N1-C2-O2	5.02	121.91	118.90
87	M1	2189	U	N1-C2-O2	5.02	126.31	122.80
87	M1	2359	C	C6-N1-C2	-5.01	118.29	120.30
87	M1	2550	U	C6-N1-C1'	-5.01	114.19	121.20
87	M1	1115	G	C4-N9-C1'	5.01	133.01	126.50
5	L1	3121	U	OP1-P-O3'	5.00	116.21	105.20
49	S1	608	U	N3-C2-O2	-5.00	118.70	122.20
5	L1	979	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	LC	158	ASP	Peptide
10	LC	30	THR	Peptide
10	LC	76	ALA	Peptide
11	LD	21	LYS	Peptide
13	LF	115	LYS	Peptide
14	LG	46	ILE	Peptide
14	LG	75	PHE	Peptide
15	LH	12	TRP	Peptide
16	LI	92	LEU	Peptide
17	LJ	110	PRO	Peptide
20	LM	52	LYS	Peptide
32	Lj	83	LYS	Peptide
38	Lp	19	ASN	Peptide
42	Lt	43	ALA	Peptide
45	Lw	70	ARG	Sidechain
46	Lx	127	LYS	Peptide
46	Lx	139	GLN	Peptide
46	Lx	141	GLY	Peptide
46	Lx	3	HIS	Peptide
47	Ly	13	GLY	Peptide
47	Ly	318	LEU	Peptide
9	MB	232	ARG	Peptide
25	Mc	7	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
28	Mf	32	ASN	Peptide
40	Mr	102	GLU	Peptide
47	My	318	LEU	Peptide
57	Ra	184	LEU	Peptide
61	Re	195	ILE	Peptide
64	Rh	130	VAL	Peptide
64	Rh	64	VAL	Peptide
67	Rk	23	ALA	Peptide
73	Rq	40	GLU	Peptide
75	Rs	90	ASN	Peptide
77	Ru	69	LYS	Peptide
82	Rz	68	ARG	Sidechain
50	SA	9	GLY	Peptide
55	SF	144	CYS	Peptide
58	Sb	211	HIS	Peptide
58	Sb	81	PHE	Peptide
61	Se	42	LEU	Peptide
63	Sg	68	LEU	Peptide
64	Sh	64	VAL	Peptide
65	Si	9	HIS	Peptide
69	Sm	108	ARG	Peptide
69	Sm	110	GLY	Peptide
69	Sm	130	THR	Peptide
69	Sm	137	MET	Peptide
69	Sm	84	ASN	Peptide
69	Sm	90	LYS	Peptide
72	Sp	27	GLU	Peptide
73	Sq	40	GLU	Peptide
75	Ss	90	ASN	Peptide
80	Sx	41	SER	Peptide
80	Sx	88	PRO	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CC	12/233 (5%)	11 (92%)	1 (8%)	0	100	100
3	CN	132/151 (87%)	130 (98%)	2 (2%)	0	100	100
8	LA	163/176 (93%)	153 (94%)	10 (6%)	0	100	100
9	LB	220/244 (90%)	208 (94%)	12 (6%)	0	100	100
9	MB	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
10	LC	231/256 (90%)	215 (93%)	16 (7%)	0	100	100
10	MC	231/256 (90%)	221 (96%)	10 (4%)	0	100	100
11	LD	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
11	MD	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
12	LE	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
12	ME	213/221 (96%)	202 (95%)	11 (5%)	0	100	100
13	LF	167/174 (96%)	151 (90%)	16 (10%)	0	100	100
13	MF	167/174 (96%)	153 (92%)	14 (8%)	0	100	100
14	LG	191/199 (96%)	173 (91%)	16 (8%)	2 (1%)	13	40
14	MG	191/199 (96%)	173 (91%)	17 (9%)	1 (0%)	25	56
15	LH	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
15	MH	134/138 (97%)	128 (96%)	6 (4%)	0	100	100
16	LI	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
16	MI	201/204 (98%)	187 (93%)	14 (7%)	0	100	100
17	LJ	195/199 (98%)	188 (96%)	5 (3%)	2 (1%)	13	40
17	MJ	195/199 (98%)	191 (98%)	4 (2%)	0	100	100
18	LK	181/184 (98%)	171 (94%)	10 (6%)	0	100	100
18	MK	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
19	LL	183/186 (98%)	171 (93%)	12 (7%)	0	100	100
19	ML	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
20	LM	186/189 (98%)	181 (97%)	4 (2%)	1 (0%)	25	56
20	MM	174/189 (92%)	169 (97%)	4 (2%)	1 (1%)	22	52
21	LN	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
21	MN	170/172 (99%)	159 (94%)	11 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	LO	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
22	MO	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
23	La	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
23	Ma	127/137 (93%)	123 (97%)	4 (3%)	0	100	100
24	Lb	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
24	Mb	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
25	Lc	101/106 (95%)	96 (95%)	5 (5%)	0	100	100
25	Mc	100/106 (94%)	93 (93%)	7 (7%)	0	100	100
26	Ld	23/25 (92%)	23 (100%)	0	0	100	100
26	Md	23/25 (92%)	23 (100%)	0	0	100	100
27	Le	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
27	Me	50/128 (39%)	50 (100%)	0	0	100	100
28	Lf	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
28	Mf	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
29	Lg	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
29	Mg	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
30	Lh	83/88 (94%)	80 (96%)	3 (4%)	0	100	100
30	Mh	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
31	Li	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
31	Mi	97/100 (97%)	86 (89%)	11 (11%)	0	100	100
32	Lj	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
32	Mj	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
33	Lk	104/121 (86%)	100 (96%)	4 (4%)	0	100	100
33	Mk	107/121 (88%)	105 (98%)	2 (2%)	0	100	100
34	Ll	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
34	Ml	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
35	Lm	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
35	Mm	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
36	Ln	107/113 (95%)	97 (91%)	10 (9%)	0	100	100
36	Mn	107/113 (95%)	98 (92%)	8 (8%)	1 (1%)	14	43
37	Lo	94/105 (90%)	94 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Mo	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
38	Lp	56/59 (95%)	46 (82%)	10 (18%)	0	100	100
38	Mp	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
39	Lq	146/149 (98%)	124 (85%)	21 (14%)	1 (1%)	19	49
39	Mq	146/149 (98%)	133 (91%)	12 (8%)	1 (1%)	19	49
40	Lr	133/136 (98%)	123 (92%)	10 (8%)	0	100	100
40	Mr	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
41	Ls	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
41	Ms	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
42	Lt	119/142 (84%)	112 (94%)	6 (5%)	1 (1%)	16	45
42	Mt	118/142 (83%)	112 (95%)	6 (5%)	0	100	100
43	Lu	124/155 (80%)	115 (93%)	9 (7%)	0	100	100
43	Mu	61/155 (39%)	61 (100%)	0	0	100	100
44	Lv	98/121 (81%)	91 (93%)	7 (7%)	0	100	100
44	Mv	95/121 (78%)	86 (90%)	9 (10%)	0	100	100
45	Lw	249/254 (98%)	227 (91%)	22 (9%)	0	100	100
45	Mw	250/254 (98%)	239 (96%)	11 (4%)	0	100	100
46	Lx	384/387 (99%)	356 (93%)	26 (7%)	2 (0%)	25	56
46	Mx	384/387 (99%)	365 (95%)	19 (5%)	0	100	100
47	Ly	359/362 (99%)	331 (92%)	26 (7%)	2 (1%)	22	52
47	My	359/362 (99%)	340 (95%)	19 (5%)	0	100	100
48	Lz	292/297 (98%)	277 (95%)	14 (5%)	1 (0%)	37	66
48	Mz	294/297 (99%)	278 (95%)	16 (5%)	0	100	100
50	RA	95/119 (80%)	82 (86%)	13 (14%)	0	100	100
50	SA	95/119 (80%)	83 (87%)	10 (10%)	2 (2%)	5	22
51	RB	79/82 (96%)	69 (87%)	10 (13%)	0	100	100
51	SB	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
52	SC	60/67 (90%)	58 (97%)	2 (3%)	0	100	100
53	RD	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
53	SD	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
54	RE	46/63 (73%)	45 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	SE	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
55	RF	68/152 (45%)	53 (78%)	15 (22%)	0	100	100
55	SF	71/152 (47%)	50 (70%)	21 (30%)	0	100	100
56	RG	311/319 (98%)	297 (96%)	14 (4%)	0	100	100
56	SG	310/319 (97%)	282 (91%)	28 (9%)	0	100	100
57	Ra	204/252 (81%)	173 (85%)	30 (15%)	1 (0%)	25	56
57	Sa	204/252 (81%)	181 (89%)	23 (11%)	0	100	100
58	Rb	214/255 (84%)	201 (94%)	13 (6%)	0	100	100
58	Sb	222/255 (87%)	194 (87%)	26 (12%)	2 (1%)	14	43
59	Rc	215/254 (85%)	208 (97%)	7 (3%)	0	100	100
59	Sc	214/254 (84%)	203 (95%)	11 (5%)	0	100	100
60	Rd	221/240 (92%)	207 (94%)	14 (6%)	0	100	100
60	Sd	220/240 (92%)	211 (96%)	9 (4%)	0	100	100
61	Re	258/261 (99%)	239 (93%)	18 (7%)	1 (0%)	30	60
61	Se	256/261 (98%)	230 (90%)	25 (10%)	1 (0%)	30	60
62	Rf	204/225 (91%)	186 (91%)	18 (9%)	0	100	100
62	Sf	204/225 (91%)	190 (93%)	14 (7%)	0	100	100
63	Rg	216/236 (92%)	204 (94%)	12 (6%)	0	100	100
63	Sg	226/236 (96%)	210 (93%)	14 (6%)	2 (1%)	14	43
64	Rh	183/190 (96%)	169 (92%)	14 (8%)	0	100	100
64	Sh	182/190 (96%)	169 (93%)	13 (7%)	0	100	100
65	Ri	184/200 (92%)	178 (97%)	6 (3%)	0	100	100
65	Si	183/200 (92%)	162 (88%)	19 (10%)	2 (1%)	12	37
66	Rj	183/197 (93%)	166 (91%)	17 (9%)	0	100	100
66	Sj	182/197 (92%)	164 (90%)	18 (10%)	0	100	100
67	Rk	90/105 (86%)	73 (81%)	17 (19%)	0	100	100
67	Sk	90/105 (86%)	79 (88%)	11 (12%)	0	100	100
68	Rl	144/156 (92%)	135 (94%)	9 (6%)	0	100	100
68	Sl	142/156 (91%)	129 (91%)	13 (9%)	0	100	100
69	Rm	122/143 (85%)	101 (83%)	21 (17%)	0	100	100
69	Sm	119/143 (83%)	90 (76%)	27 (23%)	2 (2%)	7	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	Rn	148/151 (98%)	137 (93%)	11 (7%)	0	100	100
70	Sn	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
71	So	125/137 (91%)	108 (86%)	16 (13%)	1 (1%)	16	45
72	Rp	117/142 (82%)	102 (87%)	14 (12%)	1 (1%)	14	43
72	Sp	115/142 (81%)	103 (90%)	12 (10%)	0	100	100
73	Rq	139/143 (97%)	129 (93%)	10 (7%)	0	100	100
73	Sq	139/143 (97%)	126 (91%)	12 (9%)	1 (1%)	19	49
74	Sr	117/136 (86%)	111 (95%)	6 (5%)	0	100	100
75	Rs	143/146 (98%)	125 (87%)	18 (13%)	0	100	100
75	Ss	143/146 (98%)	128 (90%)	13 (9%)	2 (1%)	9	31
76	Rt	141/144 (98%)	132 (94%)	9 (6%)	0	100	100
76	St	141/144 (98%)	126 (89%)	15 (11%)	0	100	100
77	Ru	99/121 (82%)	90 (91%)	8 (8%)	1 (1%)	13	40
77	Su	98/121 (81%)	91 (93%)	7 (7%)	0	100	100
78	Rv	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
78	Sv	85/87 (98%)	73 (86%)	12 (14%)	0	100	100
79	Rw	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
79	Sw	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
80	Rx	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
80	Sx	142/145 (98%)	123 (87%)	18 (13%)	1 (1%)	19	49
81	Ry	132/135 (98%)	122 (92%)	9 (7%)	1 (1%)	16	45
81	Sy	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
82	Rz	67/108 (62%)	63 (94%)	4 (6%)	0	100	100
82	Sz	80/108 (74%)	69 (86%)	11 (14%)	0	100	100
83	RC	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
84	Ro	126/138 (91%)	106 (84%)	20 (16%)	0	100	100
85	Rr	123/136 (90%)	116 (94%)	7 (6%)	0	100	100
86	MA	151/176 (86%)	140 (93%)	11 (7%)	0	100	100
89	MQ	195/312 (62%)	189 (97%)	6 (3%)	0	100	100
90	MP	156/165 (94%)	146 (94%)	10 (6%)	0	100	100
All	All	22304/24622 (91%)	20726 (93%)	1541 (7%)	37 (0%)	45	73

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	LJ	111	PRO
50	SA	84	VAL
65	Si	10	LYS
14	MG	63	VAL
14	LG	63	VAL
39	Lq	78	LEU
42	Lt	44	PRO
46	Lx	4	ARG
69	Sm	131	ASP
75	Ss	91	ASP
81	Ry	37	LYS
46	Lx	128	LYS
48	Lz	20	PHE
63	Sg	173	PRO
39	Mq	78	LEU
61	Se	43	PRO
63	Sg	68	LEU
72	Rp	125	PRO
20	MM	131	ALA
14	LG	77	LEU
17	LJ	110	PRO
47	Ly	4	PRO
50	SA	9	GLY
69	Sm	109	GLU
71	So	124	ASP
77	Ru	71	PRO
20	LM	53	LYS
47	Ly	292	SER
58	Sb	213	ARG
65	Si	9	HIS
36	Mn	110	GLU
57	Ra	31	VAL
73	Sq	33	GLY
75	Ss	92	ILE
58	Sb	212	VAL
80	Sx	42	PRO
61	Re	196	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CC	13/215 (6%)	11 (85%)	2 (15%)	2 7
3	CN	112/123 (91%)	104 (93%)	8 (7%)	12 36
8	LA	138/155 (89%)	131 (95%)	7 (5%)	20 51
9	LB	186/205 (91%)	173 (93%)	13 (7%)	12 36
9	MB	186/205 (91%)	183 (98%)	3 (2%)	58 84
10	LC	187/208 (90%)	176 (94%)	11 (6%)	16 45
10	MC	187/208 (90%)	177 (95%)	10 (5%)	19 49
11	LD	168/171 (98%)	157 (94%)	11 (6%)	14 40
11	MD	171/171 (100%)	160 (94%)	11 (6%)	14 41
12	LE	185/187 (99%)	169 (91%)	16 (9%)	8 27
12	ME	184/187 (98%)	176 (96%)	8 (4%)	25 57
13	LF	146/150 (97%)	137 (94%)	9 (6%)	15 43
13	MF	147/150 (98%)	137 (93%)	10 (7%)	13 38
14	LG	154/159 (97%)	144 (94%)	10 (6%)	14 40
14	MG	154/159 (97%)	146 (95%)	8 (5%)	19 50
15	LH	107/109 (98%)	100 (94%)	7 (6%)	14 40
15	MH	107/109 (98%)	104 (97%)	3 (3%)	38 73
16	LI	175/176 (99%)	163 (93%)	12 (7%)	13 37
16	MI	175/176 (99%)	166 (95%)	9 (5%)	20 51
17	LJ	160/162 (99%)	154 (96%)	6 (4%)	28 63
17	MJ	160/162 (99%)	158 (99%)	2 (1%)	65 88
18	LK	138/146 (94%)	131 (95%)	7 (5%)	20 51
18	MK	125/146 (86%)	117 (94%)	8 (6%)	14 41
19	LL	150/151 (99%)	144 (96%)	6 (4%)	27 61
19	ML	150/151 (99%)	148 (99%)	2 (1%)	65 88
20	LM	152/154 (99%)	143 (94%)	9 (6%)	16 45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	MM	143/154 (93%)	136 (95%)	7 (5%)	21 53
21	LN	155/156 (99%)	146 (94%)	9 (6%)	17 46
21	MN	156/156 (100%)	148 (95%)	8 (5%)	20 51
22	LO	136/137 (99%)	126 (93%)	10 (7%)	11 34
22	MO	136/137 (99%)	128 (94%)	8 (6%)	16 45
23	La	104/105 (99%)	95 (91%)	9 (9%)	8 27
23	Ma	101/105 (96%)	98 (97%)	3 (3%)	36 71
24	Lb	71/72 (99%)	69 (97%)	2 (3%)	38 73
24	Mb	71/72 (99%)	69 (97%)	2 (3%)	38 73
25	Lc	87/91 (96%)	77 (88%)	10 (12%)	4 15
25	Mc	87/91 (96%)	82 (94%)	5 (6%)	17 47
26	Ld	22/23 (96%)	21 (96%)	1 (4%)	23 56
26	Md	23/23 (100%)	19 (83%)	4 (17%)	1 5
27	Le	47/116 (40%)	47 (100%)	0	100 100
27	Me	47/116 (40%)	46 (98%)	1 (2%)	48 78
28	Lf	45/46 (98%)	44 (98%)	1 (2%)	47 78
28	Mf	45/46 (98%)	45 (100%)	0	100 100
29	Lg	68/69 (99%)	64 (94%)	4 (6%)	16 45
29	Mg	68/69 (99%)	62 (91%)	6 (9%)	8 26
30	Lh	69/71 (97%)	66 (96%)	3 (4%)	25 57
30	Mh	69/71 (97%)	66 (96%)	3 (4%)	25 57
31	Li	80/82 (98%)	75 (94%)	5 (6%)	15 42
31	Mi	81/82 (99%)	77 (95%)	4 (5%)	21 53
32	Lj	104/105 (99%)	99 (95%)	5 (5%)	21 54
32	Mj	104/105 (99%)	100 (96%)	4 (4%)	28 63
33	Lk	91/103 (88%)	89 (98%)	2 (2%)	47 78
33	Mk	94/103 (91%)	92 (98%)	2 (2%)	48 78
34	Ll	90/91 (99%)	88 (98%)	2 (2%)	47 78
34	Ml	90/91 (99%)	88 (98%)	2 (2%)	47 78
35	Lm	108/111 (97%)	103 (95%)	5 (5%)	23 55
35	Mm	109/111 (98%)	106 (97%)	3 (3%)	38 73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	Ln	92/97 (95%)	85 (92%)	7 (8%)	11 32
36	Mn	94/97 (97%)	90 (96%)	4 (4%)	25 57
37	Lo	81/88 (92%)	75 (93%)	6 (7%)	11 34
37	Mo	81/88 (92%)	78 (96%)	3 (4%)	29 64
38	Lp	46/47 (98%)	44 (96%)	2 (4%)	25 57
38	Mp	46/47 (98%)	46 (100%)	0	100 100
39	Lq	118/119 (99%)	109 (92%)	9 (8%)	11 32
39	Mq	118/119 (99%)	108 (92%)	10 (8%)	8 27
40	Lr	115/116 (99%)	106 (92%)	9 (8%)	10 31
40	Mr	115/116 (99%)	111 (96%)	4 (4%)	31 66
41	Ls	108/110 (98%)	97 (90%)	11 (10%)	6 19
41	Ms	109/110 (99%)	104 (95%)	5 (5%)	23 55
42	Lt	104/118 (88%)	101 (97%)	3 (3%)	37 72
42	Mt	104/118 (88%)	99 (95%)	5 (5%)	21 54
43	Lu	56/129 (43%)	56 (100%)	0	100 100
43	Mu	55/129 (43%)	54 (98%)	1 (2%)	54 82
44	Lv	87/107 (81%)	84 (97%)	3 (3%)	32 67
44	Mv	84/107 (78%)	77 (92%)	7 (8%)	9 28
45	Lw	190/196 (97%)	183 (96%)	7 (4%)	29 64
45	Mw	193/196 (98%)	190 (98%)	3 (2%)	58 84
46	Lx	319/323 (99%)	302 (95%)	17 (5%)	19 49
46	Mx	320/323 (99%)	309 (97%)	11 (3%)	32 67
47	Ly	288/289 (100%)	273 (95%)	15 (5%)	19 50
47	My	288/289 (100%)	280 (97%)	8 (3%)	38 73
48	Lz	241/245 (98%)	232 (96%)	9 (4%)	29 64
48	Mz	244/245 (100%)	236 (97%)	8 (3%)	33 68
50	RA	83/101 (82%)	77 (93%)	6 (7%)	12 35
50	SA	83/101 (82%)	79 (95%)	4 (5%)	21 54
51	RB	70/71 (99%)	65 (93%)	5 (7%)	12 36
51	SB	70/71 (99%)	66 (94%)	4 (6%)	17 47
52	SC	55/60 (92%)	51 (93%)	4 (7%)	11 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	RD	47/49 (96%)	44 (94%)	3 (6%)	14 41
53	SD	47/49 (96%)	43 (92%)	4 (8%)	8 27
54	RE	41/54 (76%)	40 (98%)	1 (2%)	44 76
54	SE	50/54 (93%)	45 (90%)	5 (10%)	6 20
55	RF	55/135 (41%)	50 (91%)	5 (9%)	7 25
55	SF	56/135 (42%)	49 (88%)	7 (12%)	3 12
56	RG	255/262 (97%)	242 (95%)	13 (5%)	20 51
56	SG	250/262 (95%)	237 (95%)	13 (5%)	19 50
57	Ra	165/210 (79%)	156 (94%)	9 (6%)	18 48
57	Sa	170/210 (81%)	157 (92%)	13 (8%)	11 32
58	Rb	192/224 (86%)	184 (96%)	8 (4%)	25 59
58	Sb	200/224 (89%)	185 (92%)	15 (8%)	11 33
59	Rc	176/205 (86%)	172 (98%)	4 (2%)	45 77
59	Sc	175/205 (85%)	165 (94%)	10 (6%)	17 47
60	Rd	182/195 (93%)	164 (90%)	18 (10%)	6 21
60	Sd	182/195 (93%)	170 (93%)	12 (7%)	14 39
61	Re	221/222 (100%)	213 (96%)	8 (4%)	30 65
61	Se	220/222 (99%)	210 (96%)	10 (4%)	23 56
62	Rf	173/191 (91%)	167 (96%)	6 (4%)	31 66
62	Sf	172/191 (90%)	166 (96%)	6 (4%)	31 66
63	Rg	187/201 (93%)	180 (96%)	7 (4%)	29 64
63	Sg	189/201 (94%)	177 (94%)	12 (6%)	15 42
64	Rh	165/170 (97%)	157 (95%)	8 (5%)	21 54
64	Sh	163/170 (96%)	151 (93%)	12 (7%)	11 34
65	Ri	150/161 (93%)	145 (97%)	5 (3%)	33 68
65	Si	148/161 (92%)	139 (94%)	9 (6%)	15 43
66	Rj	158/166 (95%)	150 (95%)	8 (5%)	20 51
66	Sj	156/166 (94%)	145 (93%)	11 (7%)	12 36
67	Rk	73/98 (74%)	68 (93%)	5 (7%)	13 38
67	Sk	77/98 (79%)	65 (84%)	12 (16%)	2 7
68	Rl	129/137 (94%)	120 (93%)	9 (7%)	12 36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
68	Sl	129/137 (94%)	120 (93%)	9 (7%)	12 36
69	Rm	88/119 (74%)	80 (91%)	8 (9%)	7 25
69	Sm	88/119 (74%)	78 (89%)	10 (11%)	4 15
70	Rn	127/128 (99%)	119 (94%)	8 (6%)	15 42
70	Sn	127/128 (99%)	118 (93%)	9 (7%)	12 36
71	So	91/105 (87%)	86 (94%)	5 (6%)	18 48
72	Rp	98/118 (83%)	88 (90%)	10 (10%)	6 19
72	Sp	95/118 (80%)	85 (90%)	10 (10%)	5 18
73	Rq	117/119 (98%)	113 (97%)	4 (3%)	32 67
73	Sq	117/119 (98%)	110 (94%)	7 (6%)	16 44
74	Sr	101/124 (82%)	94 (93%)	7 (7%)	13 37
75	Rs	128/129 (99%)	119 (93%)	9 (7%)	12 36
75	Ss	128/129 (99%)	121 (94%)	7 (6%)	18 48
76	Rt	115/116 (99%)	110 (96%)	5 (4%)	25 57
76	St	115/116 (99%)	107 (93%)	8 (7%)	12 36
77	Ru	94/114 (82%)	88 (94%)	6 (6%)	14 41
77	Su	93/114 (82%)	87 (94%)	6 (6%)	14 40
78	Rv	74/74 (100%)	69 (93%)	5 (7%)	13 38
78	Sv	71/74 (96%)	64 (90%)	7 (10%)	6 21
79	Rw	110/111 (99%)	104 (94%)	6 (6%)	18 48
79	Sw	110/111 (99%)	103 (94%)	7 (6%)	14 41
80	Rx	119/120 (99%)	115 (97%)	4 (3%)	32 67
80	Sx	119/120 (99%)	113 (95%)	6 (5%)	20 52
81	Ry	112/113 (99%)	109 (97%)	3 (3%)	40 73
81	Sy	112/113 (99%)	106 (95%)	6 (5%)	18 49
82	Rz	61/89 (68%)	55 (90%)	6 (10%)	6 21
82	Sz	67/89 (75%)	63 (94%)	4 (6%)	16 44
83	RC	56/60 (93%)	55 (98%)	1 (2%)	54 82
84	Ro	97/105 (92%)	87 (90%)	10 (10%)	6 19
85	Rr	113/124 (91%)	107 (95%)	6 (5%)	19 49
86	MA	133/153 (87%)	126 (95%)	7 (5%)	19 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
89	MQ	167/254 (66%)	154 (92%)	13 (8%)	10 31
90	MP	129/136 (95%)	125 (97%)	4 (3%)	35 70
All	All	18800/20698 (91%)	17781 (95%)	1019 (5%)	21 49

All (1019) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CC	13	CYS
1	CC	14	ARG
3	CN	13	ARG
3	CN	38	GLN
3	CN	40	LEU
3	CN	61	ARG
3	CN	73	LYS
3	CN	87	ARG
3	CN	93	LYS
3	CN	94	MET
8	LA	12	SER
8	LA	65	VAL
8	LA	90	LYS
8	LA	98	VAL
8	LA	137	ASP
8	LA	146	LEU
8	LA	152	THR
9	LB	30	ARG
9	LB	37	ASN
9	LB	40	LYS
9	LB	52	GLN
9	LB	82	LYS
9	LB	83	LEU
9	LB	98	LYS
9	LB	113	SER
9	LB	146	GLN
9	LB	164	SER
9	LB	172	ASN
9	LB	211	SER
9	LB	228	SER
10	LC	70	LYS
10	LC	81	THR
10	LC	83	ASP
10	LC	89	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	LC	108	ARG
10	LC	118	GLU
10	LC	189	LEU
10	LC	197	VAL
10	LC	204	ARG
10	LC	216	SER
10	LC	246	MET
11	LD	2	LYS
11	LD	14	GLU
11	LD	16	VAL
11	LD	42	ASP
11	LD	62	ARG
11	LD	84	LYS
11	LD	92	TYR
11	LD	94	TYR
11	LD	107	ASP
11	LD	130	ASP
11	LD	157	ASN
12	LE	7	ARG
12	LE	28	ASP
12	LE	44	ASP
12	LE	74	LYS
12	LE	87	LEU
12	LE	91	VAL
12	LE	109	ASP
12	LE	111	LEU
12	LE	113	GLN
12	LE	123	HIS
12	LE	169	LYS
12	LE	180	GLU
12	LE	183	LYS
12	LE	185	ARG
12	LE	192	ASP
12	LE	200	LEU
13	LF	11	ASP
13	LF	34	SER
13	LF	38	GLU
13	LF	52	TYR
13	LF	77	GLU
13	LF	81	GLU
13	LF	107	ASP
13	LF	111	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	LF	161	SER
14	LG	4	SER
14	LG	5	LYS
14	LG	58	VAL
14	LG	67	ARG
14	LG	75	PHE
14	LG	104	ARG
14	LG	120	GLN
14	LG	122	LYS
14	LG	164	GLU
14	LG	165	SER
15	LH	37	GLU
15	LH	40	ASP
15	LH	47	ASP
15	LH	69	THR
15	LH	105	GLN
15	LH	116	GLU
15	LH	133	LYS
16	LI	5	LYS
16	LI	17	ASP
16	LI	18	VAL
16	LI	20	ARG
16	LI	29	GLU
16	LI	62	TYR
16	LI	83	LYS
16	LI	99	ARG
16	LI	109	ARG
16	LI	122	ASN
16	LI	147	ARG
16	LI	167	THR
17	LJ	59	ARG
17	LJ	84	LEU
17	LJ	136	THR
17	LJ	174	PHE
17	LJ	187	GLU
17	LJ	193	GLN
18	LK	9	THR
18	LK	13	LYS
18	LK	29	THR
18	LK	30	ARG
18	LK	54	HIS
18	LK	126	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	LK	171	ARG
19	LL	12	ARG
19	LL	21	SER
19	LL	72	LYS
19	LL	74	GLU
19	LL	100	THR
19	LL	125	ASP
20	LM	6	THR
20	LM	110	ARG
20	LM	133	LYS
20	LM	151	ARG
20	LM	156	ASN
20	LM	157	GLU
20	LM	160	GLU
20	LM	165	LYS
20	LM	173	ARG
21	LN	23	LYS
21	LN	27	MET
21	LN	45	LEU
21	LN	59	VAL
21	LN	65	ASN
21	LN	82	ASP
21	LN	128	GLU
21	LN	158	LYS
21	LN	172	TYR
22	LO	18	ASP
22	LO	52	MET
22	LO	79	MET
22	LO	82	ASN
22	LO	86	GLU
22	LO	107	GLU
22	LO	118	GLU
22	LO	131	GLN
22	LO	139	ARG
22	LO	144	GLU
23	La	11	PHE
23	La	32	ARG
23	La	72	LYS
23	La	73	VAL
23	La	74	MET
23	La	89	ASP
23	La	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	La	106	LYS
23	La	135	VAL
24	Lb	60	CYS
24	Lb	61	LYS
25	Lc	10	THR
25	Lc	12	CYS
25	Lc	29	LYS
25	Lc	32	LYS
25	Lc	35	LEU
25	Lc	47	GLN
25	Lc	57	VAL
25	Lc	68	VAL
25	Lc	80	ARG
25	Lc	98	LYS
26	Ld	6	ARG
28	Lf	47	THR
29	Lg	30	LYS
29	Lg	33	LYS
29	Lg	72	THR
29	Lg	78	LEU
30	Lh	46	SER
30	Lh	71	SER
30	Lh	82	SER
31	Li	3	VAL
31	Li	18	THR
31	Li	55	ARG
31	Li	59	ASP
31	Li	76	ARG
32	Lj	36	LEU
32	Lj	71	LYS
32	Lj	79	ASP
32	Lj	81	ARG
32	Lj	119	LYS
33	Lk	17	SER
33	Lk	87	GLU
34	Ll	56	SER
34	Ll	59	VAL
35	Lm	31	ASN
35	Lm	36	LYS
35	Lm	41	VAL
35	Lm	92	TYR
35	Lm	95	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	Ln	9	THR
36	Ln	31	ARG
36	Ln	41	LYS
36	Ln	79	ARG
36	Ln	84	ASP
36	Ln	87	ASN
36	Ln	100	SER
37	Lo	22	LYS
37	Lo	23	TYR
37	Lo	24	THR
37	Lo	63	SER
37	Lo	90	VAL
37	Lo	98	SER
38	Lp	19	ASN
38	Lp	59	LYS
39	Lq	26	ARG
39	Lq	45	MET
39	Lq	60	TYR
39	Lq	75	LEU
39	Lq	87	ARG
39	Lq	92	LYS
39	Lq	120	ASN
39	Lq	130	VAL
39	Lq	144	VAL
40	Lr	30	ASP
40	Lr	88	ASP
40	Lr	94	SER
40	Lr	98	THR
40	Lr	105	SER
40	Lr	108	GLU
40	Lr	120	GLU
40	Lr	123	GLN
40	Lr	128	GLN
41	Ls	3	LYS
41	Ls	7	ASP
41	Ls	11	ASP
41	Ls	42	GLN
41	Ls	56	VAL
41	Ls	57	LEU
41	Ls	74	TYR
41	Ls	76	LEU
41	Ls	86	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	Ls	108	LYS
41	Ls	125	LYS
42	Lt	25	LYS
42	Lt	27	ARG
42	Lt	56	ARG
44	Lv	21	SER
44	Lv	56	VAL
44	Lv	102	GLU
45	Lw	21	ARG
45	Lw	47	GLN
45	Lw	60	LYS
45	Lw	126	LEU
45	Lw	130	SER
45	Lw	191	LEU
45	Lw	247	ARG
46	Lx	10	ARG
46	Lx	34	LYS
46	Lx	66	LYS
46	Lx	84	VAL
46	Lx	90	VAL
46	Lx	102	LEU
46	Lx	104	THR
46	Lx	146	ARG
46	Lx	196	ARG
46	Lx	197	GLU
46	Lx	289	ASP
46	Lx	302	LYS
46	Lx	320	ASP
46	Lx	332	ARG
46	Lx	335	ILE
46	Lx	348	ARG
46	Lx	380	MET
47	Ly	5	GLN
47	Ly	55	LYS
47	Ly	60	THR
47	Ly	93	MET
47	Ly	105	THR
47	Ly	112	LYS
47	Ly	120	TYR
47	Ly	144	LYS
47	Ly	177	ASP
47	Ly	194	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	Ly	209	TYR
47	Ly	259	ASP
47	Ly	300	ARG
47	Ly	304	GLN
47	Ly	342	LYS
48	Lz	95	TRP
48	Lz	136	GLU
48	Lz	167	SER
48	Lz	197	SER
48	Lz	218	ARG
48	Lz	221	GLU
48	Lz	258	LYS
48	Lz	279	LYS
48	Lz	293	LEU
50	SA	15	ARG
50	SA	68	TYR
50	SA	85	ARG
50	SA	95	ARG
51	SB	72	LYS
51	SB	74	SER
51	SB	77	THR
51	SB	78	SER
52	SC	29	ARG
52	SC	38	ARG
52	SC	61	ARG
52	SC	64	ARG
53	SD	8	PHE
53	SD	13	ARG
53	SD	14	TYR
53	SD	53	ASN
54	SE	3	LYS
54	SE	4	VAL
54	SE	22	GLU
54	SE	23	LYS
54	SE	55	ARG
55	SF	85	TYR
55	SF	107	LYS
55	SF	116	LYS
55	SF	117	LEU
55	SF	136	LYS
55	SF	138	ARG
55	SF	148	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	SG	54	PHE
56	SG	58	VAL
56	SG	62	LYS
56	SG	121	MET
56	SG	183	LEU
56	SG	198	ASN
56	SG	202	LEU
56	SG	231	MET
56	SG	232	TYR
56	SG	234	LEU
56	SG	265	LEU
56	SG	272	ASP
56	SG	316	MET
57	Sa	8	ASP
57	Sa	21	ASN
57	Sa	24	LEU
57	Sa	27	ARG
57	Sa	32	HIS
57	Sa	53	THR
57	Sa	57	LEU
57	Sa	140	ASN
57	Sa	148	ASP
57	Sa	157	ASP
57	Sa	164	ASN
57	Sa	200	ASP
57	Sa	204	TYR
58	Sb	31	ASP
58	Sb	55	LYS
58	Sb	81	PHE
58	Sb	92	GLN
58	Sb	95	ASN
58	Sb	132	ASP
58	Sb	148	ASN
58	Sb	170	GLU
58	Sb	181	LEU
58	Sb	205	PHE
58	Sb	211	HIS
58	Sb	215	VAL
58	Sb	222	LYS
58	Sb	223	PHE
58	Sb	229	MET
59	Sc	78	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	Sc	111	VAL
59	Sc	120	GLU
59	Sc	126	ARG
59	Sc	150	GLN
59	Sc	189	GLN
59	Sc	228	ASN
59	Sc	235	LEU
59	Sc	238	SER
59	Sc	241	ASP
60	Sd	14	ASP
60	Sd	35	SER
60	Sd	76	ARG
60	Sd	91	VAL
60	Sd	101	GLN
60	Sd	107	PHE
60	Sd	120	TYR
60	Sd	150	MET
60	Sd	178	ARG
60	Sd	189	MET
60	Sd	224	ASP
60	Sd	225	TYR
61	Se	9	LEU
61	Se	76	VAL
61	Se	146	THR
61	Se	182	TYR
61	Se	211	LYS
61	Se	221	ARG
61	Se	238	LEU
61	Se	242	LYS
61	Se	255	ARG
61	Se	256	ARG
62	Sf	53	VAL
62	Sf	54	LYS
62	Sf	65	ARG
62	Sf	102	ARG
62	Sf	127	GLN
62	Sf	161	ASP
63	Sg	1	MET
63	Sg	22	HIS
63	Sg	51	LYS
63	Sg	58	LYS
63	Sg	63	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	Sg	65	GLN
63	Sg	68	LEU
63	Sg	69	LEU
63	Sg	127	THR
63	Sg	128	THR
63	Sg	149	LYS
63	Sg	190	GLN
64	Sh	22	GLN
64	Sh	26	GLU
64	Sh	38	LEU
64	Sh	39	ARG
64	Sh	55	LYS
64	Sh	83	LYS
64	Sh	95	GLU
64	Sh	118	LEU
64	Sh	141	ARG
64	Sh	147	ASN
64	Sh	154	LEU
64	Sh	163	ASP
65	Si	10	LYS
65	Si	17	LYS
65	Si	18	ARG
65	Si	21	PHE
65	Si	47	ARG
65	Si	76	THR
65	Si	110	ARG
65	Si	140	GLU
65	Si	151	LYS
66	Sj	12	TYR
66	Sj	38	ASN
66	Sj	114	TYR
66	Sj	120	LYS
66	Sj	122	VAL
66	Sj	136	VAL
66	Sj	149	ARG
66	Sj	154	LYS
66	Sj	168	ARG
66	Sj	175	ARG
66	Sj	180	LYS
67	Sk	1	MET
67	Sk	8	ARG
67	Sk	15	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	Sk	16	PHE
67	Sk	31	LYS
67	Sk	34	GLU
67	Sk	41	TYR
67	Sk	56	LYS
67	Sk	63	TYR
67	Sk	64	TYR
67	Sk	75	TYR
67	Sk	80	LEU
68	Sl	11	ARG
68	Sl	46	LYS
68	Sl	50	GLU
68	Sl	67	ARG
68	Sl	77	SER
68	Sl	116	ARG
68	Sl	124	THR
68	Sl	138	ASN
68	Sl	143	SER
69	Sm	29	LYS
69	Sm	66	VAL
69	Sm	68	GLU
69	Sm	73	LYS
69	Sm	81	ASP
69	Sm	83	GLU
69	Sm	86	VAL
69	Sm	103	LEU
69	Sm	131	ASP
69	Sm	137	MET
70	Sn	28	LEU
70	Sn	29	SER
70	Sn	30	SER
70	Sn	35	GLU
70	Sn	55	ARG
70	Sn	64	ARG
70	Sn	80	LEU
70	Sn	99	ARG
70	Sn	134	VAL
71	So	20	TYR
71	So	42	VAL
71	So	117	ASP
71	So	136	ARG
71	So	137	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
72	Sp	17	TYR
72	Sp	21	ASP
72	Sp	28	MET
72	Sp	31	GLU
72	Sp	49	MET
72	Sp	52	LYS
72	Sp	64	LYS
72	Sp	77	ARG
72	Sp	89	MET
72	Sp	112	LEU
73	Sq	17	THR
73	Sq	28	LEU
73	Sq	46	PHE
73	Sq	59	LYS
73	Sq	64	ASP
73	Sq	66	ARG
73	Sq	107	LYS
74	Sr	14	LYS
74	Sr	24	LEU
74	Sr	35	CYS
74	Sr	79	GLU
74	Sr	82	ASP
74	Sr	84	TYR
74	Sr	105	GLN
75	Ss	4	VAL
75	Ss	6	GLN
75	Ss	85	PHE
75	Ss	109	LEU
75	Ss	110	ARG
75	Ss	144	ARG
75	Ss	145	ARG
76	St	33	TYR
76	St	45	MET
76	St	71	VAL
76	St	95	ASP
76	St	129	GLN
76	St	133	ASP
76	St	140	LEU
76	St	142	GLU
77	Su	21	LYS
77	Su	27	THR
77	Su	28	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
77	Su	36	ASN
77	Su	53	LYS
77	Su	70	THR
78	Sv	4	ASP
78	Sv	5	LYS
78	Sv	12	TYR
78	Sv	22	ARG
78	Sv	31	SER
78	Sv	76	ASP
78	Sv	85	TYR
79	Sw	2	THR
79	Sw	26	LEU
79	Sw	30	SER
79	Sw	31	SER
79	Sw	51	GLU
79	Sw	66	ASN
79	Sw	93	LEU
80	Sx	87	VAL
80	Sx	93	LEU
80	Sx	97	ASP
80	Sx	107	PHE
80	Sx	121	ARG
80	Sx	128	SER
81	Sy	22	GLN
81	Sy	24	VAL
81	Sy	53	ASP
81	Sy	90	ARG
81	Sy	125	LEU
81	Sy	132	ARG
82	Sz	46	LYS
82	Sz	52	LYS
82	Sz	69	LEU
82	Sz	75	LEU
75	Rs	7	GLU
75	Rs	8	GLN
75	Rs	57	ARG
75	Rs	62	THR
75	Rs	78	HIS
75	Rs	85	PHE
75	Rs	91	ASP
75	Rs	103	ASN
75	Rs	136	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	Rt	27	LYS
76	Rt	119	LYS
76	Rt	132	LEU
76	Rt	134	ARG
76	Rt	138	GLN
77	Ru	33	GLN
77	Ru	52	LYS
77	Ru	102	ARG
77	Ru	104	THR
77	Ru	109	GLU
77	Ru	113	ASP
78	Rv	2	GLU
78	Rv	10	GLU
78	Rv	11	LEU
78	Rv	69	LEU
78	Rv	87	ARG
79	Rw	23	ARG
79	Rw	25	VAL
79	Rw	93	LEU
79	Rw	98	GLN
79	Rw	104	LEU
79	Rw	118	ARG
80	Rx	3	LYS
80	Rx	40	SER
80	Rx	89	ASN
80	Rx	107	PHE
81	Ry	31	ASN
81	Ry	100	VAL
81	Ry	123	LYS
82	Rz	47	TYR
82	Rz	48	ASP
82	Rz	52	LYS
82	Rz	65	LEU
82	Rz	68	ARG
82	Rz	75	LEU
50	RA	10	ARG
50	RA	44	ILE
50	RA	58	VAL
50	RA	83	ILE
50	RA	87	ARG
50	RA	91	ASP
51	RB	37	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	RB	40	CYS
51	RB	41	LEU
51	RB	59	CYS
51	RB	82	LYS
83	RC	67	ARG
53	RD	8	PHE
53	RD	22	ARG
53	RD	39	CYS
54	RE	13	LYS
55	RF	92	LYS
55	RF	100	LEU
55	RF	119	ARG
55	RF	147	VAL
55	RF	150	VAL
56	RG	10	ARG
56	RG	38	ARG
56	RG	118	LYS
56	RG	206	PRO
56	RG	219	GLU
56	RG	221	MET
56	RG	225	LEU
56	RG	231	MET
56	RG	232	TYR
56	RG	245	PHE
56	RG	283	LYS
56	RG	297	ASP
56	RG	316	MET
57	Ra	8	ASP
57	Ra	21	ASN
57	Ra	30	GLN
57	Ra	38	PHE
57	Ra	72	ASP
57	Ra	101	ARG
57	Ra	119	ARG
57	Ra	185	ARG
57	Ra	188	LEU
58	Rb	24	PHE
58	Rb	31	ASP
58	Rb	59	ASP
58	Rb	96	LEU
58	Rb	105	PHE
58	Rb	108	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	Rb	195	LYS
58	Rb	205	PHE
59	Rc	78	ASP
59	Rc	111	VAL
59	Rc	208	GLU
59	Rc	245	ASP
60	Rd	14	ASP
60	Rd	18	TYR
60	Rd	27	ARG
60	Rd	42	THR
60	Rd	45	LYS
60	Rd	46	THR
60	Rd	56	GLN
60	Rd	76	ARG
60	Rd	90	ARG
60	Rd	93	ASP
60	Rd	124	ARG
60	Rd	169	ASP
60	Rd	194	LYS
60	Rd	206	VAL
60	Rd	218	LEU
60	Rd	223	LYS
60	Rd	224	ASP
60	Rd	225	TYR
61	Re	66	MET
61	Re	104	ASP
61	Re	118	GLU
61	Re	133	LYS
61	Re	206	ASP
61	Re	212	ASP
61	Re	250	GLU
61	Re	252	ARG
62	Rf	23	VAL
62	Rf	50	GLU
62	Rf	51	VAL
62	Rf	63	GLN
62	Rf	99	MET
62	Rf	135	ASP
63	Rg	15	THR
63	Rg	29	ASP
63	Rg	49	VAL
63	Rg	127	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	Rg	131	LYS
63	Rg	197	ASN
63	Rg	210	GLN
64	Rh	7	LYS
64	Rh	14	THR
64	Rh	39	ARG
64	Rh	78	THR
64	Rh	79	ARG
64	Rh	83	LYS
64	Rh	107	ARG
64	Rh	139	ARG
65	Ri	46	VAL
65	Ri	59	ARG
65	Ri	137	LYS
65	Ri	141	ARG
65	Ri	164	ARG
66	Rj	25	ASP
66	Rj	33	GLU
66	Rj	65	LYS
66	Rj	78	ARG
66	Rj	90	LYS
66	Rj	140	ILE
66	Rj	149	ARG
66	Rj	151	ASP
67	Rk	10	LYS
67	Rk	16	PHE
67	Rk	17	GLN
67	Rk	56	LYS
67	Rk	70	GLU
68	Rl	6	THR
68	Rl	11	ARG
68	Rl	35	TYR
68	Rl	43	LYS
68	Rl	60	PHE
68	Rl	67	ARG
68	Rl	116	ARG
68	Rl	132	SER
68	Rl	140	VAL
69	Rm	26	ASP
69	Rm	28	LEU
69	Rm	39	ASP
69	Rm	61	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
69	Rm	85	LYS
69	Rm	90	LYS
69	Rm	135	MET
69	Rm	137	MET
70	Rn	20	ARG
70	Rn	27	LYS
70	Rn	29	SER
70	Rn	36	GLN
70	Rn	46	THR
70	Rn	52	VAL
70	Rn	105	ASN
70	Rn	106	ARG
84	Ro	14	PHE
84	Ro	33	LEU
84	Ro	42	VAL
84	Ro	51	ASP
84	Ro	79	VAL
84	Ro	81	VAL
84	Ro	99	GLN
84	Ro	107	ARG
84	Ro	124	ASP
84	Ro	132	ARG
72	Rp	21	ASP
72	Rp	31	GLU
72	Rp	49	MET
72	Rp	52	LYS
72	Rp	58	LYS
72	Rp	64	LYS
72	Rp	83	MET
72	Rp	88	GLU
72	Rp	126	VAL
72	Rp	128	HIS
73	Rq	26	LYS
73	Rq	61	SER
73	Rq	83	GLN
73	Rq	114	ARG
85	Rr	60	ARG
85	Rr	67	ARG
85	Rr	72	LYS
85	Rr	81	LYS
85	Rr	84	TYR
85	Rr	91	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
86	MA	5	LYS
86	MA	29	LYS
86	MA	31	ARG
86	MA	59	GLU
86	MA	92	SER
86	MA	167	ASN
86	MA	173	MET
17	MJ	126	VAL
17	MJ	180	SER
18	MK	13	LYS
18	MK	53	ASP
18	MK	87	SER
18	MK	112	LEU
18	MK	120	ASN
18	MK	126	ARG
18	MK	149	VAL
18	MK	153	LYS
19	ML	4	ASP
19	ML	130	ARG
20	MM	68	GLN
20	MM	86	GLU
20	MM	116	ASP
20	MM	134	HIS
20	MM	163	ARG
20	MM	172	ARG
20	MM	176	ARG
89	MQ	16	ARG
89	MQ	23	LYS
89	MQ	38	MET
89	MQ	48	ARG
89	MQ	52	LEU
89	MQ	53	MET
89	MQ	60	ARG
89	MQ	88	PHE
89	MQ	114	VAL
89	MQ	135	PHE
89	MQ	144	LYS
89	MQ	158	VAL
89	MQ	164	LYS
21	MN	1	MET
21	MN	32	SER
21	MN	45	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	MN	50	LYS
21	MN	79	VAL
21	MN	96	ASP
21	MN	147	ASP
21	MN	172	TYR
45	Mw	72	ARG
45	Mw	137	ILE
45	Mw	155	LYS
90	MP	68	GLN
90	MP	90	ARG
90	MP	116	MET
90	MP	118	ASP
22	MO	79	MET
22	MO	83	ARG
22	MO	99	SER
22	MO	103	GLN
22	MO	118	GLU
22	MO	144	GLU
22	MO	149	GLN
22	MO	159	PHE
46	Mx	67	PHE
46	Mx	121	ASN
46	Mx	136	LYS
46	Mx	145	GLU
46	Mx	246	LEU
46	Mx	282	ILE
46	Mx	291	GLU
46	Mx	332	ARG
46	Mx	335	ILE
46	Mx	349	LYS
46	Mx	385	LYS
44	Mv	20	SER
44	Mv	24	GLU
44	Mv	25	ASN
44	Mv	33	TYR
44	Mv	47	VAL
44	Mv	50	LEU
44	Mv	107	PHE
47	My	6	VAL
47	My	93	MET
47	My	120	TYR
47	My	186	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	My	211	GLU
47	My	327	LEU
47	My	350	LYS
47	My	362	ASP
23	Ma	57	MET
23	Ma	88	ARG
23	Ma	124	ASP
48	Mz	85	ARG
48	Mz	95	TRP
48	Mz	125	VAL
48	Mz	140	ARG
48	Mz	206	GLN
48	Mz	232	ASP
48	Mz	250	ASP
48	Mz	273	ARG
43	Mu	47	ARG
42	Mt	74	LYS
42	Mt	101	GLU
42	Mt	108	LEU
42	Mt	131	ASP
42	Mt	137	ASN
9	MB	30	ARG
9	MB	165	ASP
9	MB	211	SER
41	Ms	3	LYS
41	Ms	55	GLU
41	Ms	74	TYR
41	Ms	115	ARG
41	Ms	125	LYS
10	MC	40	VAL
10	MC	83	ASP
10	MC	84	ARG
10	MC	98	ARG
10	MC	106	LYS
10	MC	108	ARG
10	MC	163	VAL
10	MC	180	VAL
10	MC	224	ASP
10	MC	248	LYS
40	Mr	3	LYS
40	Mr	34	LYS
40	Mr	88	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	Mr	100	THR
11	MD	3	TYR
11	MD	12	VAL
11	MD	23	ARG
11	MD	73	SER
11	MD	82	VAL
11	MD	101	VAL
11	MD	107	ASP
11	MD	113	GLU
11	MD	137	SER
11	MD	157	ASN
11	MD	177	ASP
39	Mq	60	TYR
39	Mq	76	ASP
39	Mq	78	LEU
39	Mq	85	ASP
39	Mq	86	LYS
39	Mq	89	GLN
39	Mq	95	SER
39	Mq	123	VAL
39	Mq	135	GLU
39	Mq	145	VAL
12	ME	28	ASP
12	ME	36	LEU
12	ME	82	ARG
12	ME	103	LEU
12	ME	130	ASP
12	ME	144	ASN
12	ME	150	GLU
12	ME	180	GLU
13	MF	11	ASP
13	MF	25	GLU
13	MF	55	ARG
13	MF	57	PHE
13	MF	62	ASN
13	MF	88	GLU
13	MF	107	ASP
13	MF	112	LEU
13	MF	117	ASP
13	MF	168	ASP
37	Mo	9	SER
37	Mo	22	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	Mo	54	SER
14	MG	5	LYS
14	MG	45	LYS
14	MG	104	ARG
14	MG	121	SER
14	MG	128	ARG
14	MG	140	SER
14	MG	153	ASP
14	MG	184	GLU
36	Mn	28	ARG
36	Mn	35	GLU
36	Mn	47	ASP
36	Mn	97	LEU
15	MH	4	ASP
15	MH	8	LYS
15	MH	27	GLN
35	Mm	23	ASP
35	Mm	31	ASN
35	Mm	67	SER
16	MI	17	ASP
16	MI	73	ARG
16	MI	96	ARG
16	MI	99	ARG
16	MI	104	GLU
16	MI	118	SER
16	MI	128	LYS
16	MI	155	VAL
16	MI	159	ARG
34	Ml	21	ARG
34	Ml	49	ILE
33	Mk	64	THR
33	Mk	65	VAL
32	Mj	37	SER
32	Mj	41	LEU
32	Mj	102	GLU
32	Mj	119	LYS
31	Mi	36	ARG
31	Mi	45	ARG
31	Mi	55	ARG
31	Mi	99	ARG
30	Mh	67	LEU
30	Mh	75	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	Mh	82	SER
29	Mg	3	ARG
29	Mg	4	GLU
29	Mg	24	THR
29	Mg	29	LYS
29	Mg	33	LYS
29	Mg	65	LEU
27	Me	92	ASP
26	Md	13	LEU
26	Md	19	LYS
26	Md	23	ARG
26	Md	24	SER
25	Mc	2	VAL
25	Mc	8	ARG
25	Mc	24	LYS
25	Mc	26	THR
25	Mc	73	GLU
24	Mb	60	CYS
24	Mb	85	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
13	LF	95	ASN
15	LH	41	GLN
61	Se	57	ASN
62	Sf	63	GLN
65	Si	159	GLN
66	Sj	38	ASN
67	Sk	9	ASN
69	Sm	139	HIS
74	Sr	105	GLN
77	Su	47	GLN
81	Sy	34	ASN
62	Rf	37	GLN
70	Rn	36	GLN
70	Rn	58	HIS
28	Mf	33	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	CM	40/41 (97%)	17 (42%)	1 (2%)
4	CP	75/76 (98%)	11 (14%)	0
49	R1	1755/1800 (97%)	474 (27%)	26 (1%)
49	S1	1768/1800 (98%)	461 (26%)	37 (2%)
5	L1	3111/3396 (91%)	583 (18%)	33 (1%)
6	L2	157/158 (99%)	26 (16%)	1 (0%)
6	M2	157/158 (99%)	24 (15%)	0
7	L3	120/121 (99%)	13 (10%)	1 (0%)
7	M3	120/121 (99%)	11 (9%)	1 (0%)
87	M1	3185/3396 (93%)	505 (15%)	14 (0%)
88	DQ	76/77 (98%)	13 (17%)	0
91	DP	75/76 (98%)	26 (34%)	1 (1%)
All	All	10639/11220 (94%)	2164 (20%)	115 (1%)

All (2164) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	CM	2	U
2	CM	7	U
2	CM	14	U
2	CM	15	U
2	CM	16	U
2	CM	17	U
2	CM	19	U
2	CM	21	U
2	CM	22	U
2	CM	23	U
2	CM	24	U
2	CM	25	U
2	CM	26	U
2	CM	30	U
2	CM	31	U
2	CM	35	C
2	CM	38	C
4	CP	16	U
4	CP	17	G
4	CP	19	U
4	CP	24	G
4	CP	34	I
4	CP	42	G
4	CP	47	U
4	CP	48	U
4	CP	58	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	CP	73	G
4	CP	76	A
5	L1	6	A
5	L1	12	A
5	L1	13	A
5	L1	14	U
5	L1	18	G
5	L1	26	A
5	L1	40	A
5	L1	43	A
5	L1	49	A
5	L1	58	G
5	L1	59	G
5	L1	60	A
5	L1	65	A
5	L1	66	A
5	L1	67	A
5	L1	75	G
5	L1	92	G
5	L1	109	A
5	L1	110	G
5	L1	111	C
5	L1	116	A
5	L1	120	G
5	L1	121	A
5	L1	122	A
5	L1	133	U
5	L1	135	C
5	L1	136	G
5	L1	148	G
5	L1	156	G
5	L1	157	A
5	L1	165	A
5	L1	166	C
5	L1	172	G
5	L1	173	G
5	L1	187	A
5	L1	190	U
5	L1	191	U
5	L1	200	C
5	L1	206	G
5	L1	210	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	211	A
5	L1	213	A
5	L1	218	G
5	L1	219	A
5	L1	220	G
5	L1	234	G
5	L1	240	U
5	L1	241	G
5	L1	243	G
5	L1	245	U
5	L1	249	U
5	L1	252	U
5	L1	269	G
5	L1	283	G
5	L1	286	U
5	L1	290	G
5	L1	291	C
5	L1	295	A
5	L1	298	U
5	L1	305	U
5	L1	323	A
5	L1	329	U
5	L1	338	A
5	L1	339	C
5	L1	350	C
5	L1	376	G
5	L1	390	G
5	L1	398	A
5	L1	401	U
5	L1	402	A
5	L1	403	C
5	L1	407	A
5	L1	421	G
5	L1	422	A
5	L1	429	U
5	L1	498	A
5	L1	510	G
5	L1	518	G
5	L1	521	A
5	L1	523	A
5	L1	535	G
5	L1	546	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	547	G
5	L1	552	G
5	L1	555	U
5	L1	557	A
5	L1	558	U
5	L1	559	A
5	L1	578	A
5	L1	579	G
5	L1	597	G
5	L1	600	G
5	L1	604	G
5	L1	609	G
5	L1	610	G
5	L1	611	A
5	L1	620	U
5	L1	621	A
5	L1	622	A
5	L1	637	C
5	L1	638	C
5	L1	649	A
5	L1	660	A
5	L1	677	A
5	L1	681	U
5	L1	683	U
5	L1	689	U
5	L1	705	A
5	L1	712	G
5	L1	715	A
5	L1	716	A
5	L1	719	U
5	L1	720	A
5	L1	727	G
5	L1	764	U
5	L1	765	C
5	L1	767	U
5	L1	776	U
5	L1	777	U
5	L1	780	A
5	L1	781	G
5	L1	785	G
5	L1	786	A
5	L1	799	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	802	C
5	L1	806	A
5	L1	817	A
5	L1	830	A
5	L1	846	A
5	L1	847	A
5	L1	849	C
5	L1	861	C
5	L1	869	G
5	L1	874	U
5	L1	879	U
5	L1	890	C
5	L1	896	A
5	L1	897	U
5	L1	907	G
5	L1	908	G
5	L1	909	G
5	L1	914	A
5	L1	916	G
5	L1	917	A
5	L1	920	A
5	L1	921	A
5	L1	923	C
5	L1	924	G
5	L1	925	A
5	L1	932	U
5	L1	937	G
5	L1	944	C
5	L1	959	C
5	L1	960	U
5	L1	962	A
5	L1	981	U
5	L1	982	C
5	L1	984	G
5	L1	991	G
5	L1	994	G
5	L1	1000	C
5	L1	1001	G
5	L1	1002	A
5	L1	1010	G
5	L1	1015	U
5	L1	1017	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	1018	G
5	L1	1020	G
5	L1	1024	G
5	L1	1036	A
5	L1	1037	C
5	L1	1047	A
5	L1	1049	C
5	L1	1064	A
5	L1	1065	A
5	L1	1072	G
5	L1	1081	U
5	L1	1087	G
5	L1	1093	A
5	L1	1094	U
5	L1	1095	U
5	L1	1097	G
5	L1	1098	A
5	L1	1103	A
5	L1	1104	G
5	L1	1117	G
5	L1	1129	A
5	L1	1131	G
5	L1	1135	A
5	L1	1144	U
5	L1	1150	A
5	L1	1153	A
5	L1	1155	C
5	L1	1159	A
5	L1	1178	G
5	L1	1179	A
5	L1	1180	A
5	L1	1181	U
5	L1	1186	G
5	L1	1192	C
5	L1	1193	A
5	L1	1196	C
5	L1	1201	C
5	L1	1202	A
5	L1	1206	G
5	L1	1208	U
5	L1	1217	A
5	L1	1222	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	1225	A
5	L1	1227	C
5	L1	1230	G
5	L1	1232	C
5	L1	1233	G
5	L1	1235	U
5	L1	1236	G
5	L1	1240	A
5	L1	1241	U
5	L1	1243	G
5	L1	1245	A
5	L1	1246	G
5	L1	1248	C
5	L1	1251	A
5	L1	1253	U
5	L1	1254	C
5	L1	1258	U
5	L1	1262	G
5	L1	1263	A
5	L1	1264	G
5	L1	1265	U
5	L1	1269	U
5	L1	1270	A
5	L1	1271	A
5	L1	1272	C
5	L1	1274	A
5	L1	1278	A
5	L1	1279	C
5	L1	1285	G
5	L1	1286	A
5	L1	1287	A
5	L1	1295	G
5	L1	1305	U
5	L1	1309	U
5	L1	1313	G
5	L1	1331	U
5	L1	1348	U
5	L1	1349	G
5	L1	1351	U
5	L1	1352	A
5	L1	1354	G
5	L1	1355	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	1356	U
5	L1	1357	G
5	L1	1386	A
5	L1	1391	C
5	L1	1392	G
5	L1	1399	A
5	L1	1400	G
5	L1	1419	A
5	L1	1431	G
5	L1	1434	G
5	L1	1437	C
5	L1	1443	G
5	L1	1446	A
5	L1	1450	G
5	L1	1469	C
5	L1	1477	A
5	L1	1481	A
5	L1	1482	A
5	L1	1483	G
5	L1	1484	U
5	L1	1488	G
5	L1	1508	C
5	L1	1536	G
5	L1	1555	U
5	L1	1556	C
5	L1	1557	A
5	L1	1560	G
5	L1	1562	C
5	L1	1563	C
5	L1	1566	A
5	L1	1567	U
5	L1	1568	U
5	L1	1569	U
5	L1	1572	U
5	L1	1575	A
5	L1	1576	G
5	L1	1580	A
5	L1	1582	C
5	L1	1583	A
5	L1	1587	A
5	L1	1588	A
5	L1	1589	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	1590	G
5	L1	1593	A
5	L1	1605	A
5	L1	1607	U
5	L1	1608	C
5	L1	1619	A
5	L1	1629	U
5	L1	1639	C
5	L1	1642	A
5	L1	1643	A
5	L1	1645	U
5	L1	1677	G
5	L1	1683	A
5	L1	1716	U
5	L1	1717	U
5	L1	1724	U
5	L1	1725	C
5	L1	1736	G
5	L1	1741	A
5	L1	1750	A
5	L1	1751	G
5	L1	1760	A
5	L1	1764	U
5	L1	1765	U
5	L1	1766	G
5	L1	1770	G
5	L1	1775	G
5	L1	1780	G
5	L1	1797	A
5	L1	1814	A
5	L1	1816	A
5	L1	1820	U
5	L1	1821	U
5	L1	1834	U
5	L1	1835	A
5	L1	1839	A
5	L1	1840	U
5	L1	1842	A
5	L1	1846	C
5	L1	1849	C
5	L1	1850	A
5	L1	1858	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	1866	C
5	L1	1867	A
5	L1	1880	U
5	L1	1881	A
5	L1	1886	A
5	L1	1893	A
5	L1	1899	G
5	L1	1906	G
5	L1	1914	G
5	L1	1952	G
5	L1	1953	G
5	L1	1954	G
5	L1	2094	C
5	L1	2101	C
5	L1	2102	U
5	L1	2110	G
5	L1	2111	G
5	L1	2112	U
5	L1	2113	A
5	L1	2121	G
5	L1	2122	G
5	L1	2126	A
5	L1	2131	A
5	L1	2140	U
5	L1	2144	A
5	L1	2158	A
5	L1	2160	G
5	L1	2169	G
5	L1	2171	G
5	L1	2176	U
5	L1	2184	U
5	L1	2188	A
5	L1	2192	C
5	L1	2201	G
5	L1	2205	U
5	L1	2206	G
5	L1	2207	A
5	L1	2209	U
5	L1	2210	G
5	L1	2223	A
5	L1	2225	U
5	L1	2249	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	2250	G
5	L1	2256	A
5	L1	2257	C
5	L1	2272	G
5	L1	2273	G
5	L1	2280	A
5	L1	2281	A
5	L1	2282	U
5	L1	2288	G
5	L1	2307	G
5	L1	2308	C
5	L1	2310	U
5	L1	2313	A
5	L1	2314	U
5	L1	2315	G
5	L1	2318	U
5	L1	2334	U
5	L1	2335	G
5	L1	2364	G
5	L1	2372	A
5	L1	2373	A
5	L1	2374	C
5	L1	2375	G
5	L1	2385	G
5	L1	2388	U
5	L1	2393	G
5	L1	2394	G
5	L1	2397	A
5	L1	2402	A
5	L1	2403	G
5	L1	2404	A
5	L1	2411	U
5	L1	2419	A
5	L1	2435	G
5	L1	2514	U
5	L1	2515	A
5	L1	2522	G
5	L1	2526	C
5	L1	2531	C
5	L1	2532	U
5	L1	2548	C
5	L1	2549	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	2550	U
5	L1	2552	C
5	L1	2555	G
5	L1	2561	A
5	L1	2569	A
5	L1	2570	U
5	L1	2571	U
5	L1	2572	C
5	L1	2573	G
5	L1	2585	G
5	L1	2593	A
5	L1	2594	C
5	L1	2595	A
5	L1	2606	G
5	L1	2607	G
5	L1	2614	G
5	L1	2626	A
5	L1	2629	U
5	L1	2651	G
5	L1	2652	U
5	L1	2656	A
5	L1	2666	C
5	L1	2672	G
5	L1	2674	A
5	L1	2677	G
5	L1	2689	A
5	L1	2691	A
5	L1	2694	A
5	L1	2696	A
5	L1	2704	A
5	L1	2714	G
5	L1	2719	U
5	L1	2728	G
5	L1	2729	U
5	L1	2752	U
5	L1	2753	G
5	L1	2761	G
5	L1	2772	C
5	L1	2777	G
5	L1	2778	G
5	L1	2788	C
5	L1	2796	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	2799	A
5	L1	2800	G
5	L1	2801	A
5	L1	2803	A
5	L1	2809	C
5	L1	2810	C
5	L1	2814	G
5	L1	2815	G
5	L1	2817	A
5	L1	2818	U
5	L1	2821	C
5	L1	2842	U
5	L1	2844	C
5	L1	2845	A
5	L1	2849	C
5	L1	2867	C
5	L1	2871	G
5	L1	2872	A
5	L1	2875	U
5	L1	2876	C
5	L1	2887	A
5	L1	2894	C
5	L1	2898	G
5	L1	2899	C
5	L1	2911	A
5	L1	2923	U
5	L1	2935	U
5	L1	2936	A
5	L1	2938	G
5	L1	2941	A
5	L1	2942	C
5	L1	2947	G
5	L1	2948	C
5	L1	2971	A
5	L1	2983	C
5	L1	2990	G
5	L1	2992	U
5	L1	2996	U
5	L1	2997	G
5	L1	3012	A
5	L1	3039	C
5	L1	3049	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	3056	U
5	L1	3078	U
5	L1	3086	A
5	L1	3092	C
5	L1	3101	G
5	L1	3104	U
5	L1	3122	A
5	L1	3129	A
5	L1	3130	A
5	L1	3131	U
5	L1	3139	A
5	L1	3140	G
5	L1	3142	A
5	L1	3143	C
5	L1	3151	U
5	L1	3154	C
5	L1	3155	U
5	L1	3156	U
5	L1	3157	U
5	L1	3158	G
5	L1	3165	A
5	L1	3170	A
5	L1	3172	A
5	L1	3173	G
5	L1	3174	A
5	L1	3175	U
5	L1	3176	G
5	L1	3179	U
5	L1	3181	C
5	L1	3187	A
5	L1	3195	U
5	L1	3196	U
5	L1	3207	U
5	L1	3210	A
5	L1	3217	C
5	L1	3218	A
5	L1	3219	G
5	L1	3224	G
5	L1	3229	G
5	L1	3235	C
5	L1	3242	G
5	L1	3243	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L1	3245	A
5	L1	3247	G
5	L1	3259	U
5	L1	3263	G
5	L1	3270	U
5	L1	3276	G
5	L1	3278	C
5	L1	3281	U
5	L1	3287	U
5	L1	3289	G
5	L1	3294	A
5	L1	3295	A
5	L1	3304	U
5	L1	3307	A
5	L1	3313	U
5	L1	3316	A
5	L1	3318	G
5	L1	3319	U
5	L1	3320	A
5	L1	3341	U
5	L1	3342	A
5	L1	3345	G
5	L1	3351	U
5	L1	3352	U
5	L1	3353	G
5	L1	3354	U
5	L1	3355	U
5	L1	3356	G
5	L1	3363	U
5	L1	3368	U
5	L1	3369	G
5	L1	3375	A
5	L1	3378	C
5	L1	3382	U
5	L1	3383	G
5	L1	3386	G
5	L1	3389	U
5	L1	3390	G
5	L1	3396	U
6	L2	34	U
6	L2	35	C
6	L2	48	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L2	52	A
6	L2	59	A
6	L2	62	C
6	L2	63	G
6	L2	80	A
6	L2	81	U
6	L2	82	U
6	L2	83	C
6	L2	84	C
6	L2	86	U
6	L2	87	G
6	L2	90	U
6	L2	95	G
6	L2	104	A
6	L2	105	A
6	L2	106	C
6	L2	111	A
6	L2	113	U
6	L2	125	U
6	L2	126	A
6	L2	138	A
6	L2	152	G
6	L2	158	U
7	L3	7	G
7	L3	11	A
7	L3	33	U
7	L3	53	U
7	L3	54	U
7	L3	55	A
7	L3	65	G
7	L3	77	G
7	L3	91	G
7	L3	99	G
7	L3	102	A
7	L3	112	G
7	L3	121	U
49	S1	2	A
49	S1	4	C
49	S1	25	C
49	S1	26	A
49	S1	34	G
49	S1	42	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	43	A
49	S1	45	U
49	S1	46	A
49	S1	47	A
49	S1	51	A
49	S1	56	U
49	S1	57	G
49	S1	62	A
49	S1	63	G
49	S1	65	A
49	S1	68	A
49	S1	69	G
49	S1	71	A
49	S1	73	U
49	S1	74	U
49	S1	75	U
49	S1	76	A
49	S1	78	A
49	S1	79	C
49	S1	81	G
49	S1	104	A
49	S1	114	C
49	S1	116	U
49	S1	121	U
49	S1	126	A
49	S1	129	U
49	S1	130	C
49	S1	131	C
49	S1	132	U
49	S1	134	U
49	S1	135	A
49	S1	138	A
49	S1	140	A
49	S1	141	U
49	S1	142	G
49	S1	145	A
49	S1	153	G
49	S1	155	U
49	S1	168	A
49	S1	171	A
49	S1	174	U
49	S1	176	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	178	U
49	S1	179	A
49	S1	180	A
49	S1	185	U
49	S1	186	C
49	S1	187	G
49	S1	188	A
49	S1	191	C
49	S1	193	U
49	S1	195	G
49	S1	216	U
49	S1	218	A
49	S1	224	C
49	S1	225	A
49	S1	227	U
49	S1	228	G
49	S1	229	U
49	S1	230	C
49	S1	232	U
49	S1	233	C
49	S1	234	G
49	S1	235	G
49	S1	240	U
49	S1	241	U
49	S1	250	C
49	S1	257	A
49	S1	260	U
49	S1	261	U
49	S1	265	A
49	S1	272	U
49	S1	274	G
49	S1	276	C
49	S1	277	U
49	S1	278	U
49	S1	279	G
49	S1	280	U
49	S1	281	G
49	S1	287	G
49	S1	299	A
49	S1	314	C
49	S1	316	A
49	S1	320	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	322	G
49	S1	323	A
49	S1	330	G
49	S1	334	G
49	S1	337	G
49	S1	338	C
49	S1	352	A
49	S1	353	A
49	S1	359	A
49	S1	361	C
49	S1	373	G
49	S1	388	G
49	S1	390	G
49	S1	399	A
49	S1	400	A
49	S1	401	A
49	S1	402	C
49	S1	404	G
49	S1	416	A
49	S1	417	A
49	S1	418	G
49	S1	419	G
49	S1	423	G
49	S1	424	C
49	S1	425	A
49	S1	426	G
49	S1	428	A
49	S1	434	G
49	S1	437	A
49	S1	439	U
49	S1	444	C
49	S1	445	A
49	S1	446	A
49	S1	448	C
49	S1	455	C
49	S1	459	G
49	S1	460	A
49	S1	468	A
49	S1	471	A
49	S1	477	A
49	S1	483	A
49	S1	485	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	487	G
49	S1	489	C
49	S1	491	C
49	S1	492	A
49	S1	493	U
49	S1	494	U
49	S1	496	G
49	S1	498	G
49	S1	499	U
49	S1	500	C
49	S1	502	U
49	S1	505	A
49	S1	506	A
49	S1	507	U
49	S1	510	G
49	S1	511	A
49	S1	527	A
49	S1	534	A
49	S1	538	A
49	S1	539	G
49	S1	540	G
49	S1	541	A
49	S1	542	A
49	S1	543	C
49	S1	544	A
49	S1	546	U
49	S1	555	A
49	S1	556	A
49	S1	557	G
49	S1	558	U
49	S1	559	C
49	S1	565	C
49	S1	568	G
49	S1	579	A
49	S1	580	A
49	S1	582	U
49	S1	583	C
49	S1	594	A
49	S1	595	G
49	S1	606	A
49	S1	610	G
49	S1	611	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	619	A
49	S1	620	A
49	S1	621	A
49	S1	622	A
49	S1	623	A
49	S1	624	G
49	S1	629	U
49	S1	630	A
49	S1	639	U
49	S1	640	U
49	S1	641	G
49	S1	643	G
49	S1	645	C
49	S1	650	U
49	S1	651	G
49	S1	653	C
49	S1	654	C
49	S1	655	G
49	S1	656	G
49	S1	657	U
49	S1	677	G
49	S1	680	U
49	S1	681	U
49	S1	687	G
49	S1	694	U
49	S1	696	C
49	S1	697	C
49	S1	698	U
49	S1	699	U
49	S1	700	C
49	S1	702	G
49	S1	703	G
49	S1	704	C
49	S1	705	U
49	S1	706	A
49	S1	707	A
49	S1	708	C
49	S1	709	C
49	S1	710	U
49	S1	711	U
49	S1	712	G
49	S1	713	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	714	G
49	S1	728	U
49	S1	729	G
49	S1	730	G
49	S1	732	G
49	S1	733	A
49	S1	734	A
49	S1	738	G
49	S1	741	C
49	S1	742	U
49	S1	743	U
49	S1	745	U
49	S1	753	A
49	S1	765	G
49	S1	766	U
49	S1	767	U
49	S1	771	A
49	S1	774	A
49	S1	775	G
49	S1	778	G
49	S1	779	U
49	S1	780	A
49	S1	781	U
49	S1	782	U
49	S1	783	G
49	S1	787	G
49	S1	789	A
49	S1	812	A
49	S1	813	U
49	S1	814	A
49	S1	815	G
49	S1	816	G
49	S1	819	G
49	S1	820	U
49	S1	821	U
49	S1	823	G
49	S1	824	G
49	S1	832	U
49	S1	833	U
49	S1	835	U
49	S1	838	G
49	S1	840	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	841	U
49	S1	846	G
49	S1	852	C
49	S1	855	A
49	S1	856	A
49	S1	857	U
49	S1	863	A
49	S1	899	G
49	S1	901	G
49	S1	902	G
49	S1	912	U
49	S1	913	G
49	S1	914	G
49	S1	921	U
49	S1	929	A
49	S1	933	A
49	S1	934	C
49	S1	935	U
49	S1	942	G
49	S1	945	U
49	S1	960	U
49	S1	966	A
49	S1	970	A
49	S1	988	A
49	S1	992	A
49	S1	993	A
49	S1	1004	U
49	S1	1005	A
49	S1	1012	U
49	S1	1023	A
49	S1	1024	U
49	S1	1026	A
49	S1	1028	C
49	S1	1032	G
49	S1	1039	A
49	S1	1053	G
49	S1	1058	U
49	S1	1060	U
49	S1	1061	A
49	S1	1076	A
49	S1	1082	C
49	S1	1092	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	1093	A
49	S1	1096	C
49	S1	1098	U
49	S1	1100	G
49	S1	1101	G
49	S1	1109	G
49	S1	1138	A
49	S1	1150	G
49	S1	1158	C
49	S1	1159	C
49	S1	1160	A
49	S1	1164	G
49	S1	1167	G
49	S1	1170	G
49	S1	1182	U
49	S1	1185	U
49	S1	1194	A
49	S1	1196	A
49	S1	1199	G
49	S1	1200	G
49	S1	1202	A
49	S1	1207	C
49	S1	1216	C
49	S1	1217	A
49	S1	1218	G
49	S1	1227	A
49	S1	1229	G
49	S1	1241	G
49	S1	1243	G
49	S1	1244	A
49	S1	1245	G
49	S1	1246	C
49	S1	1252	C
49	S1	1256	A
49	S1	1257	U
49	S1	1274	C
49	S1	1275	A
49	S1	1285	U
49	S1	1286	U
49	S1	1291	G
49	S1	1301	U
49	S1	1307	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	1314	U
49	S1	1316	G
49	S1	1318	G
49	S1	1321	A
49	S1	1322	A
49	S1	1325	A
49	S1	1337	A
49	S1	1344	A
49	S1	1345	A
49	S1	1346	A
49	S1	1348	A
49	S1	1349	G
49	S1	1361	U
49	S1	1363	U
49	S1	1364	G
49	S1	1367	G
49	S1	1370	U
49	S1	1371	A
49	S1	1373	C
49	S1	1381	U
49	S1	1382	A
49	S1	1383	G
49	S1	1389	C
49	S1	1390	U
49	S1	1398	U
49	S1	1399	C
49	S1	1400	A
49	S1	1402	G
49	S1	1410	A
49	S1	1414	U
49	S1	1425	A
49	S1	1427	A
49	S1	1431	C
49	S1	1432	U
49	S1	1433	G
49	S1	1436	A
49	S1	1444	A
49	S1	1445	G
49	S1	1446	A
49	S1	1447	C
49	S1	1459	C
49	S1	1466	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	1468	U
49	S1	1469	A
49	S1	1471	A
49	S1	1472	C
49	S1	1479	A
49	S1	1486	G
49	S1	1490	C
49	S1	1491	U
49	S1	1492	A
49	S1	1493	A
49	S1	1496	U
49	S1	1503	A
49	S1	1506	G
49	S1	1514	U
49	S1	1516	A
49	S1	1517	U
49	S1	1518	C
49	S1	1521	G
49	S1	1523	G
49	S1	1524	A
49	S1	1528	U
49	S1	1535	U
49	S1	1536	G
49	S1	1537	C
49	S1	1540	G
49	S1	1543	A
49	S1	1554	U
49	S1	1556	A
49	S1	1558	U
49	S1	1559	A
49	S1	1570	A
49	S1	1572	G
49	S1	1573	A
49	S1	1574	G
49	S1	1575	G
49	S1	1576	A
49	S1	1577	A
49	S1	1583	A
49	S1	1584	G
49	S1	1585	U
49	S1	1590	G
49	S1	1601	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	1607	G
49	S1	1611	A
49	S1	1616	G
49	S1	1622	G
49	S1	1631	A
49	S1	1634	C
49	S1	1635	A
49	S1	1636	C
49	S1	1637	C
49	S1	1657	U
49	S1	1658	G
49	S1	1682	U
49	S1	1688	U
49	S1	1697	G
49	S1	1701	A
49	S1	1703	C
49	S1	1709	C
49	S1	1715	G
49	S1	1716	C
49	S1	1717	G
49	S1	1760	G
49	S1	1762	A
49	S1	1766	A
49	S1	1767	G
49	S1	1769	U
49	S1	1780	G
49	S1	1782	A
49	S1	1783	C
49	S1	1791	A
49	S1	1792	G
49	S1	1793	G
49	S1	1794	A
49	S1	1795	U
49	S1	1796	C
49	S1	1799	U
49	R1	2	A
49	R1	4	C
49	R1	25	C
49	R1	26	A
49	R1	27	U
49	R1	34	G
49	R1	42	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	43	A
49	R1	45	U
49	R1	47	A
49	R1	57	G
49	R1	63	G
49	R1	68	A
49	R1	69	G
49	R1	72	A
49	R1	73	U
49	R1	74	U
49	R1	75	U
49	R1	77	U
49	R1	100	A
49	R1	104	A
49	R1	114	C
49	R1	115	G
49	R1	116	U
49	R1	127	G
49	R1	128	U
49	R1	131	C
49	R1	132	U
49	R1	133	U
49	R1	134	U
49	R1	135	A
49	R1	136	C
49	R1	137	U
49	R1	138	A
49	R1	140	A
49	R1	141	U
49	R1	145	A
49	R1	146	U
49	R1	157	A
49	R1	158	U
49	R1	160	C
49	R1	165	G
49	R1	176	C
49	R1	178	U
49	R1	179	A
49	R1	184	C
49	R1	185	U
49	R1	190	C
49	R1	191	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	192	U
49	R1	193	U
49	R1	195	G
49	R1	196	G
49	R1	197	A
49	R1	200	A
49	R1	215	A
49	R1	218	A
49	R1	219	A
49	R1	220	A
49	R1	226	A
49	R1	227	U
49	R1	228	G
49	R1	231	U
49	R1	232	U
49	R1	233	C
49	R1	234	G
49	R1	236	A
49	R1	237	C
49	R1	238	U
49	R1	240	U
49	R1	241	U
49	R1	249	U
49	R1	261	U
49	R1	265	A
49	R1	272	U
49	R1	275	C
49	R1	277	U
49	R1	278	U
49	R1	279	G
49	R1	280	U
49	R1	281	G
49	R1	288	A
49	R1	299	A
49	R1	313	U
49	R1	314	C
49	R1	316	A
49	R1	320	U
49	R1	321	C
49	R1	333	A
49	R1	337	G
49	R1	338	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	352	A
49	R1	359	A
49	R1	360	A
49	R1	361	C
49	R1	399	A
49	R1	400	A
49	R1	402	C
49	R1	404	G
49	R1	407	A
49	R1	409	C
49	R1	411	C
49	R1	415	C
49	R1	416	A
49	R1	417	A
49	R1	418	G
49	R1	423	G
49	R1	424	C
49	R1	425	A
49	R1	426	G
49	R1	434	G
49	R1	435	C
49	R1	439	U
49	R1	444	C
49	R1	446	A
49	R1	448	C
49	R1	452	A
49	R1	475	A
49	R1	477	A
49	R1	480	G
49	R1	493	U
49	R1	496	G
49	R1	497	G
49	R1	498	G
49	R1	499	U
49	R1	500	C
49	R1	502	U
49	R1	503	G
49	R1	504	U
49	R1	505	A
49	R1	506	A
49	R1	510	G
49	R1	514	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	515	A
49	R1	519	C
49	R1	527	A
49	R1	534	A
49	R1	539	G
49	R1	541	A
49	R1	543	C
49	R1	548	G
49	R1	555	A
49	R1	556	A
49	R1	558	U
49	R1	559	C
49	R1	565	C
49	R1	568	G
49	R1	578	U
49	R1	579	A
49	R1	585	A
49	R1	594	A
49	R1	595	G
49	R1	611	U
49	R1	619	A
49	R1	620	A
49	R1	622	A
49	R1	623	A
49	R1	639	U
49	R1	640	U
49	R1	642	G
49	R1	648	G
49	R1	649	U
49	R1	650	U
49	R1	651	G
49	R1	654	C
49	R1	655	G
49	R1	656	G
49	R1	658	C
49	R1	677	G
49	R1	684	A
49	R1	685	A
49	R1	686	C
49	R1	693	U
49	R1	694	U
49	R1	695	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	696	C
49	R1	697	C
49	R1	698	U
49	R1	702	G
49	R1	703	G
49	R1	704	C
49	R1	706	A
49	R1	707	A
49	R1	708	C
49	R1	709	C
49	R1	710	U
49	R1	711	U
49	R1	718	U
49	R1	719	U
49	R1	721	U
49	R1	722	G
49	R1	723	G
49	R1	725	U
49	R1	727	U
49	R1	728	U
49	R1	731	C
49	R1	732	G
49	R1	733	A
49	R1	734	A
49	R1	736	C
49	R1	737	A
49	R1	738	G
49	R1	740	A
49	R1	743	U
49	R1	755	A
49	R1	756	A
49	R1	765	G
49	R1	766	U
49	R1	774	A
49	R1	775	G
49	R1	778	G
49	R1	781	U
49	R1	782	U
49	R1	783	G
49	R1	784	C
49	R1	787	G
49	R1	789	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	794	U
49	R1	803	A
49	R1	813	U
49	R1	814	A
49	R1	815	G
49	R1	819	G
49	R1	820	U
49	R1	821	U
49	R1	823	G
49	R1	829	A
49	R1	830	U
49	R1	831	U
49	R1	833	U
49	R1	841	U
49	R1	846	G
49	R1	863	A
49	R1	876	G
49	R1	880	C
49	R1	881	A
49	R1	884	A
49	R1	887	A
49	R1	898	A
49	R1	900	A
49	R1	901	G
49	R1	905	A
49	R1	906	A
49	R1	912	U
49	R1	913	G
49	R1	914	G
49	R1	922	G
49	R1	923	A
49	R1	924	A
49	R1	925	G
49	R1	926	A
49	R1	927	C
49	R1	928	U
49	R1	929	A
49	R1	933	A
49	R1	935	U
49	R1	942	G
49	R1	945	U
49	R1	946	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	951	A
49	R1	960	U
49	R1	966	A
49	R1	970	A
49	R1	973	A
49	R1	976	G
49	R1	980	G
49	R1	981	U
49	R1	982	U
49	R1	983	A
49	R1	985	G
49	R1	986	G
49	R1	990	C
49	R1	991	G
49	R1	992	A
49	R1	993	A
49	R1	996	U
49	R1	997	G
49	R1	1004	U
49	R1	1005	A
49	R1	1011	G
49	R1	1016	C
49	R1	1017	U
49	R1	1018	U
49	R1	1019	A
49	R1	1020	A
49	R1	1021	C
49	R1	1022	C
49	R1	1023	A
49	R1	1024	U
49	R1	1025	A
49	R1	1026	A
49	R1	1028	C
49	R1	1031	U
49	R1	1032	G
49	R1	1039	A
49	R1	1040	G
49	R1	1052	U
49	R1	1053	G
49	R1	1058	U
49	R1	1060	U
49	R1	1061	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	1075	C
49	R1	1076	A
49	R1	1080	U
49	R1	1082	C
49	R1	1086	A
49	R1	1092	A
49	R1	1096	C
49	R1	1097	U
49	R1	1100	G
49	R1	1113	A
49	R1	1123	C
49	R1	1124	A
49	R1	1125	A
49	R1	1126	G
49	R1	1128	C
49	R1	1138	A
49	R1	1150	G
49	R1	1155	G
49	R1	1158	C
49	R1	1160	A
49	R1	1163	A
49	R1	1167	G
49	R1	1174	C
49	R1	1175	U
49	R1	1185	U
49	R1	1194	A
49	R1	1196	A
49	R1	1199	G
49	R1	1200	G
49	R1	1201	G
49	R1	1202	A
49	R1	1207	C
49	R1	1217	A
49	R1	1218	G
49	R1	1220	C
49	R1	1225	U
49	R1	1228	G
49	R1	1229	G
49	R1	1230	A
49	R1	1241	G
49	R1	1242	A
49	R1	1243	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	1244	A
49	R1	1245	G
49	R1	1252	C
49	R1	1255	G
49	R1	1256	A
49	R1	1257	U
49	R1	1258	U
49	R1	1284	C
49	R1	1286	U
49	R1	1314	U
49	R1	1315	U
49	R1	1321	A
49	R1	1338	C
49	R1	1341	A
49	R1	1344	A
49	R1	1345	A
49	R1	1354	G
49	R1	1359	C
49	R1	1360	A
49	R1	1361	U
49	R1	1362	U
49	R1	1363	U
49	R1	1367	G
49	R1	1370	U
49	R1	1371	A
49	R1	1372	U
49	R1	1390	U
49	R1	1396	U
49	R1	1398	U
49	R1	1399	C
49	R1	1400	A
49	R1	1413	U
49	R1	1415	U
49	R1	1422	A
49	R1	1427	A
49	R1	1428	G
49	R1	1432	U
49	R1	1436	A
49	R1	1445	G
49	R1	1446	A
49	R1	1448	G
49	R1	1452	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	1458	G
49	R1	1459	C
49	R1	1460	A
49	R1	1466	G
49	R1	1471	A
49	R1	1474	G
49	R1	1481	C
49	R1	1482	C
49	R1	1486	G
49	R1	1490	C
49	R1	1491	U
49	R1	1492	A
49	R1	1493	A
49	R1	1496	U
49	R1	1506	G
49	R1	1514	U
49	R1	1516	A
49	R1	1521	G
49	R1	1523	G
49	R1	1524	A
49	R1	1529	C
49	R1	1534	G
49	R1	1536	G
49	R1	1537	C
49	R1	1538	U
49	R1	1542	G
49	R1	1557	U
49	R1	1559	A
49	R1	1569	A
49	R1	1574	G
49	R1	1575	G
49	R1	1584	G
49	R1	1596	C
49	R1	1598	U
49	R1	1601	G
49	R1	1607	G
49	R1	1616	G
49	R1	1619	C
49	R1	1634	C
49	R1	1635	A
49	R1	1643	U
49	R1	1657	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	1658	G
49	R1	1665	U
49	R1	1666	U
49	R1	1667	A
49	R1	1668	G
49	R1	1669	U
49	R1	1670	G
49	R1	1671	A
49	R1	1672	G
49	R1	1678	A
49	R1	1680	G
49	R1	1681	A
49	R1	1682	U
49	R1	1715	G
49	R1	1716	C
49	R1	1717	G
49	R1	1728	A
49	R1	1729	C
49	R1	1730	A
49	R1	1731	A
49	R1	1732	A
49	R1	1733	C
49	R1	1734	U
49	R1	1736	G
49	R1	1737	G
49	R1	1738	U
49	R1	1741	U
49	R1	1743	U
49	R1	1750	A
49	R1	1755	A
49	R1	1757	G
49	R1	1760	G
49	R1	1766	A
49	R1	1767	G
49	R1	1769	U
49	R1	1780	G
49	R1	1781	A
49	R1	1782	A
49	R1	1786	G
49	R1	1792	G
49	R1	1793	G
49	R1	1794	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	1795	U
49	R1	1796	C
49	R1	1797	A
49	R1	1799	U
49	R1	1800	A
87	M1	4	U
87	M1	6	A
87	M1	21	G
87	M1	26	A
87	M1	40	A
87	M1	43	A
87	M1	49	A
87	M1	59	G
87	M1	60	A
87	M1	65	A
87	M1	66	A
87	M1	86	G
87	M1	92	G
87	M1	99	A
87	M1	110	G
87	M1	111	C
87	M1	116	A
87	M1	117	U
87	M1	122	A
87	M1	135	C
87	M1	136	G
87	M1	147	U
87	M1	156	G
87	M1	157	A
87	M1	174	C
87	M1	190	U
87	M1	200	C
87	M1	211	A
87	M1	219	A
87	M1	220	G
87	M1	241	G
87	M1	243	G
87	M1	249	U
87	M1	251	G
87	M1	252	U
87	M1	269	G
87	M1	286	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	295	A
87	M1	305	U
87	M1	329	U
87	M1	337	G
87	M1	349	A
87	M1	374	A
87	M1	376	G
87	M1	398	A
87	M1	401	U
87	M1	402	A
87	M1	403	C
87	M1	420	G
87	M1	421	G
87	M1	422	A
87	M1	521	A
87	M1	532	A
87	M1	533	A
87	M1	534	U
87	M1	545	U
87	M1	548	G
87	M1	555	U
87	M1	557	A
87	M1	558	U
87	M1	559	A
87	M1	560	G
87	M1	592	A
87	M1	602	A
87	M1	607	A
87	M1	611	A
87	M1	620	U
87	M1	621	A
87	M1	636	C
87	M1	649	A2M
87	M1	660	A
87	M1	677	A
87	M1	678	G
87	M1	680	G
87	M1	681	U
87	M1	691	A
87	M1	705	A
87	M1	712	G
87	M1	715	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	719	U
87	M1	758	C
87	M1	763	G
87	M1	766	U
87	M1	767	U
87	M1	776	U
87	M1	781	G
87	M1	785	G
87	M1	786	A
87	M1	817	A2M
87	M1	830	A
87	M1	849	C
87	M1	861	C
87	M1	869	G
87	M1	874	U
87	M1	879	U
87	M1	880	G
87	M1	896	A
87	M1	907	G
87	M1	908	OMG
87	M1	914	A
87	M1	916	G
87	M1	917	A
87	M1	921	A
87	M1	923	C
87	M1	924	G
87	M1	925	A
87	M1	937	G
87	M1	938	C
87	M1	944	C
87	M1	953	G
87	M1	959	C
87	M1	960	U
87	M1	961	C
87	M1	964	G
87	M1	980	A
87	M1	982	C
87	M1	993	G
87	M1	995	U
87	M1	1000	C
87	M1	1015	U
87	M1	1017	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	1018	G
87	M1	1023	C
87	M1	1026	A
87	M1	1027	A
87	M1	1028	U
87	M1	1029	G
87	M1	1032	C
87	M1	1034	U
87	M1	1036	A
87	M1	1037	C
87	M1	1047	A
87	M1	1064	A
87	M1	1066	G
87	M1	1072	G
87	M1	1081	U
87	M1	1083	G
87	M1	1087	G
87	M1	1096	U
87	M1	1097	G
87	M1	1098	A
87	M1	1103	A
87	M1	1104	G
87	M1	1117	G
87	M1	1131	G
87	M1	1143	A
87	M1	1144	U
87	M1	1153	A
87	M1	1159	A
87	M1	1178	G
87	M1	1179	A
87	M1	1180	A
87	M1	1181	U
87	M1	1182	A
87	M1	1191	U
87	M1	1193	A
87	M1	1196	C
87	M1	1201	C
87	M1	1208	U
87	M1	1209	G
87	M1	1222	G
87	M1	1231	A
87	M1	1235	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	1236	G
87	M1	1237	G
87	M1	1244	A
87	M1	1245	A
87	M1	1246	G
87	M1	1249	G
87	M1	1253	U
87	M1	1254	C
87	M1	1257	C
87	M1	1258	U
87	M1	1262	G
87	M1	1263	A
87	M1	1264	G
87	M1	1265	U
87	M1	1272	C
87	M1	1275	C
87	M1	1281	G
87	M1	1284	C
87	M1	1285	G
87	M1	1286	A
87	M1	1287	A
87	M1	1302	A
87	M1	1307	G
87	M1	1308	A
87	M1	1309	U
87	M1	1313	G
87	M1	1330	A
87	M1	1345	G
87	M1	1348	U
87	M1	1349	G
87	M1	1351	U
87	M1	1352	A
87	M1	1353	U
87	M1	1355	A
87	M1	1356	U
87	M1	1357	G
87	M1	1386	A
87	M1	1391	C
87	M1	1392	G
87	M1	1399	A
87	M1	1400	G
87	M1	1418	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	1421	G
87	M1	1425	U
87	M1	1434	G
87	M1	1437	OMC
87	M1	1446	A
87	M1	1450	OMG
87	M1	1469	C
87	M1	1481	A
87	M1	1483	G
87	M1	1484	U
87	M1	1487	G
87	M1	1496	C
87	M1	1502	C
87	M1	1508	C
87	M1	1525	G
87	M1	1536	G
87	M1	1539	A
87	M1	1555	U
87	M1	1556	C
87	M1	1560	G
87	M1	1561	G
87	M1	1562	C
87	M1	1563	C
87	M1	1566	A
87	M1	1568	U
87	M1	1569	U
87	M1	1571	A
87	M1	1572	U
87	M1	1573	G
87	M1	1575	A
87	M1	1580	A
87	M1	1581	C
87	M1	1583	A
87	M1	1587	A
87	M1	1589	A
87	M1	1590	G
87	M1	1593	A
87	M1	1605	A
87	M1	1629	U
87	M1	1630	U
87	M1	1642	A
87	M1	1643	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	1645	U
87	M1	1657	C
87	M1	1683	A
87	M1	1688	U
87	M1	1716	U
87	M1	1724	U
87	M1	1730	G
87	M1	1741	A
87	M1	1742	U
87	M1	1750	A
87	M1	1751	G
87	M1	1759	C
87	M1	1762	C
87	M1	1763	U
87	M1	1765	U
87	M1	1769	G
87	M1	1775	G
87	M1	1780	G
87	M1	1797	A
87	M1	1808	G
87	M1	1812	G
87	M1	1813	A
87	M1	1815	U
87	M1	1816	A
87	M1	1817	G
87	M1	1821	U
87	M1	1842	A
87	M1	1858	A
87	M1	1866	C
87	M1	1867	A
87	M1	1878	G
87	M1	1879	A
87	M1	1880	U
87	M1	1893	A
87	M1	1899	G
87	M1	1906	G
87	M1	2102	U
87	M1	2110	G
87	M1	2111	G
87	M1	2112	U
87	M1	2114	C
87	M1	2122	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	2131	A
87	M1	2140	U
87	M1	2144	A
87	M1	2146	C
87	M1	2158	A
87	M1	2168	A
87	M1	2169	G
87	M1	2170	U
87	M1	2171	G
87	M1	2176	U
87	M1	2188	A
87	M1	2207	A
87	M1	2209	U
87	M1	2223	A
87	M1	2225	U
87	M1	2244	A
87	M1	2254	U
87	M1	2267	C
87	M1	2268	U
87	M1	2269	U
87	M1	2271	A
87	M1	2273	G
87	M1	2281	A2M
87	M1	2304	C
87	M1	2307	G
87	M1	2310	U
87	M1	2313	A
87	M1	2315	G
87	M1	2334	U
87	M1	2335	G
87	M1	2336	U
87	M1	2363	A
87	M1	2373	A
87	M1	2374	C
87	M1	2375	G
87	M1	2388	U
87	M1	2393	G
87	M1	2394	G
87	M1	2397	A
87	M1	2401	A
87	M1	2402	A
87	M1	2403	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	2404	A
87	M1	2411	U
87	M1	2412	G
87	M1	2418	G
87	M1	2419	A
87	M1	2435	G
87	M1	2438	A
87	M1	2444	C
87	M1	2447	A
87	M1	2450	G
87	M1	2453	U
87	M1	2454	G
87	M1	2459	A
87	M1	2460	U
87	M1	2461	A
87	M1	2462	A
87	M1	2464	U
87	M1	2465	G
87	M1	2466	G
87	M1	2467	G
87	M1	2468	A
87	M1	2470	C
87	M1	2471	U
87	M1	2472	U
87	M1	2474	G
87	M1	2475	G
87	M1	2476	C
87	M1	2477	G
87	M1	2478	C
87	M1	2479	C
87	M1	2480	A
87	M1	2488	A
87	M1	2489	C
87	M1	2490	C
87	M1	2492	C
87	M1	2493	U
87	M1	2494	A
87	M1	2495	C
87	M1	2496	C
87	M1	2499	U
87	M1	2501	U
87	M1	2511	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	2514	U
87	M1	2515	A
87	M1	2522	G
87	M1	2523	A
87	M1	2552	C
87	M1	2554	A
87	M1	2555	G
87	M1	2560	C
87	M1	2561	A
87	M1	2569	A
87	M1	2570	U
87	M1	2571	U
87	M1	2572	C
87	M1	2573	G
87	M1	2585	G
87	M1	2593	A
87	M1	2606	G
87	M1	2607	G
87	M1	2614	G
87	M1	2651	G
87	M1	2652	U
87	M1	2656	A
87	M1	2672	G
87	M1	2674	A
87	M1	2677	G
87	M1	2678	A
87	M1	2689	A
87	M1	2691	A
87	M1	2696	A
87	M1	2704	A
87	M1	2705	A
87	M1	2714	G
87	M1	2728	G
87	M1	2753	G
87	M1	2755	C
87	M1	2772	C
87	M1	2777	G
87	M1	2778	G
87	M1	2793	OMG
87	M1	2795	U
87	M1	2796	G
87	M1	2799	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	2800	G
87	M1	2801	A
87	M1	2802	A
87	M1	2808	A
87	M1	2809	C
87	M1	2810	C
87	M1	2814	G
87	M1	2817	A
87	M1	2844	C
87	M1	2845	A
87	M1	2860	U
87	M1	2861	U
87	M1	2871	G
87	M1	2872	A
87	M1	2875	U
87	M1	2876	C
87	M1	2887	A
87	M1	2889	C
87	M1	2899	C
87	M1	2914	G
87	M1	2922	OMG
87	M1	2935	U
87	M1	2936	A
87	M1	2942	C
87	M1	2943	G
87	M1	2947	G
87	M1	2951	G
87	M1	2971	A
87	M1	2972	G
87	M1	2977	G
87	M1	2983	C
87	M1	2990	G
87	M1	2996	U
87	M1	2997	G
87	M1	3012	A
87	M1	3049	A
87	M1	3056	U
87	M1	3059	G
87	M1	3078	U
87	M1	3080	G
87	M1	3092	C
87	M1	3122	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	3130	A
87	M1	3131	U
87	M1	3142	A
87	M1	3143	C
87	M1	3153	U
87	M1	3154	C
87	M1	3155	U
87	M1	3156	U
87	M1	3157	U
87	M1	3168	A
87	M1	3170	A
87	M1	3172	A
87	M1	3173	G
87	M1	3176	G
87	M1	3179	U
87	M1	3181	C
87	M1	3187	A
87	M1	3199	G
87	M1	3207	U
87	M1	3210	A
87	M1	3216	G
87	M1	3217	C
87	M1	3218	A
87	M1	3219	G
87	M1	3243	A
87	M1	3247	G
87	M1	3273	A
87	M1	3276	G
87	M1	3277	U
87	M1	3278	C
87	M1	3281	U
87	M1	3294	A
87	M1	3303	G
87	M1	3304	U
87	M1	3313	U
87	M1	3316	A
87	M1	3320	A
87	M1	3341	U
87	M1	3345	G
87	M1	3351	U
87	M1	3352	U
87	M1	3353	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	M1	3369	G
87	M1	3378	C
87	M1	3382	U
87	M1	3386	G
87	M1	3389	U
87	M1	3390	G
7	M3	7	G
7	M3	11	A
7	M3	54	U
7	M3	55	A
7	M3	65	G
7	M3	73	C
7	M3	74	C
7	M3	76	A
7	M3	91	G
7	M3	99	G
7	M3	112	G
6	M2	23	U
6	M2	34	U
6	M2	35	C
6	M2	38	U
6	M2	39	G
6	M2	52	A
6	M2	59	A
6	M2	62	C
6	M2	63	G
6	M2	75	G
6	M2	82	U
6	M2	83	C
6	M2	84	C
6	M2	86	U
6	M2	87	G
6	M2	91	C
6	M2	95	G
6	M2	104	A
6	M2	106	C
6	M2	113	U
6	M2	125	U
6	M2	126	A
6	M2	152	G
6	M2	155	A
88	DQ	8	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
88	DQ	10	G
88	DQ	18	C
88	DQ	19	G
88	DQ	20	G
88	DQ	21	U
88	DQ	22	A
88	DQ	48	U
88	DQ	49	C
88	DQ	56	U
88	DQ	62	C
88	DQ	63	C
88	DQ	77	A
91	DP	6	U
91	DP	8	U
91	DP	9	A
91	DP	10	G
91	DP	15	G
91	DP	16	U
91	DP	17	U
91	DP	18	G
91	DP	19	G
91	DP	21	A
91	DP	22	G
91	DP	24	G
91	DP	30	G
91	DP	34	G
91	DP	36	A
91	DP	41	U
91	DP	46	G
91	DP	47	U
91	DP	48	C
91	DP	59	U
91	DP	62	A
91	DP	63	C
91	DP	65	G
91	DP	70	C
91	DP	74	C
91	DP	75	C

All (115) RNA pucker outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	CM	21	U
5	L1	13	A
5	L1	65	A
5	L1	239	G
5	L1	282	G
5	L1	406	G
5	L1	588	G
5	L1	637	C
5	L1	715	A
5	L1	763	G
5	L1	846	A
5	L1	916	G
5	L1	1064	A
5	L1	1097	G
5	L1	1355	A
5	L1	1554	U
5	L1	1562	C
5	L1	1607	U
5	L1	1716	U
5	L1	1815	U
5	L1	1820	U
5	L1	2101	C
5	L1	2112	U
5	L1	2525	G
5	L1	2875	U
5	L1	3121	U
5	L1	3140	G
5	L1	3218	A
5	L1	3228	C
5	L1	3269	U
5	L1	3319	U
5	L1	3350	C
5	L1	3351	U
5	L1	3375	A
6	L2	85	G
7	L3	52	G
49	S1	68	A
49	S1	77	U
49	S1	139	C
49	S1	141	U
49	S1	278	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	S1	280	U
49	S1	313	U
49	S1	322	G
49	S1	352	A
49	S1	387	A
49	S1	400	A
49	S1	539	G
49	S1	541	A
49	S1	555	A
49	S1	609	U
49	S1	639	U
49	S1	640	U
49	S1	705	U
49	S1	711	U
49	S1	765	G
49	S1	819	G
49	S1	928	U
49	S1	1023	A
49	S1	1226	A
49	S1	1256	A
49	S1	1273	G
49	S1	1274	C
49	S1	1344	A
49	S1	1382	A
49	S1	1430	U
49	S1	1471	A
49	S1	1573	A
49	S1	1584	G
49	S1	1615	C
49	S1	1633	A
49	S1	1636	C
49	S1	1791	A
49	R1	73	U
49	R1	130	C
49	R1	132	U
49	R1	139	C
49	R1	218	A
49	R1	240	U
49	R1	278	U
49	R1	408	C
49	R1	417	A
49	R1	501	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	R1	503	G
49	R1	555	A
49	R1	641	G
49	R1	685	A
49	R1	720	G
49	R1	721	U
49	R1	829	A
49	R1	924	A
49	R1	1244	A
49	R1	1255	G
49	R1	1344	A
49	R1	1451	C
49	R1	1481	C
49	R1	1535	U
49	R1	1568	C
49	R1	1573	A
87	M1	601	U
87	M1	619	A
87	M1	873	C
87	M1	916	G
87	M1	1033	U
87	M1	1562	C
87	M1	2101	C
87	M1	2253	G
87	M1	2372	A
87	M1	2487	U
87	M1	2500	A
87	M1	2792	A
87	M1	2971	A
87	M1	3121	U
7	M3	72	A
91	DP	69	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

43 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection.

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	UR3	M1	2634	87	19,22,23	2.99	8 (42%)	26,32,35	1.42	3 (11%)
87	A2M	M1	2640	87	18,25,26	4.21	8 (44%)	18,36,39	4.26	4 (22%)
87	OMU	M1	2921	87	19,22,23	2.95	8 (42%)	26,31,34	1.75	4 (15%)
87	OMG	M1	867	94,87	18,26,27	1.29	2 (11%)	19,38,41	0.93	1 (5%)
87	OMU	M1	2421	87	19,22,23	2.81	7 (36%)	26,31,34	1.85	5 (19%)
87	OMC	M1	2337	87	19,22,23	0.72	0	26,31,34	0.73	0
87	OMG	M1	1450	87	18,26,27	1.26	3 (16%)	19,38,41	0.88	1 (5%)
87	OMU	M1	2729	87	19,22,23	2.87	7 (36%)	26,31,34	1.81	5 (19%)
87	OMG	M1	2793	87	18,26,27	1.36	3 (16%)	19,38,41	0.86	1 (5%)
87	OMG	M1	908	87	18,26,27	1.26	2 (11%)	19,38,41	0.89	1 (5%)
87	OMG	M1	2922	91,87	18,26,27	1.25	3 (16%)	19,38,41	0.83	1 (5%)
87	OMU	M1	1888	87	19,22,23	2.94	8 (42%)	26,31,34	1.80	5 (19%)
87	OMG	M1	2791	87	18,26,27	1.24	2 (11%)	19,38,41	0.81	1 (5%)
87	5MC	M1	2870	94,87	18,22,23	0.85	1 (5%)	26,32,35	0.78	0
87	OMC	M1	663	87	19,22,23	0.69	0	26,31,34	0.93	1 (3%)
87	OMU	M1	898	87	19,22,23	2.88	8 (42%)	26,31,34	1.70	5 (19%)
87	OMC	M1	650	92,87	19,22,23	0.73	1 (5%)	26,31,34	0.73	0
87	OMG	M1	2288	87	18,26,27	1.32	3 (16%)	19,38,41	0.77	1 (5%)
87	A2M	M1	2281	87	18,25,26	4.00	7 (38%)	18,36,39	4.09	4 (22%)
87	OMC	M1	1437	92,87	19,22,23	0.71	0	26,31,34	0.99	1 (3%)
87	A2M	M1	1133	92,87	18,25,26	4.25	7 (38%)	18,36,39	4.05	4 (22%)
87	OMU	M1	2347	87	19,22,23	2.97	7 (36%)	26,31,34	1.78	5 (19%)
87	A2M	M1	817	92,87	18,25,26	4.16	8 (44%)	18,36,39	4.33	4 (22%)
87	OMG	M1	2619	87	18,26,27	1.25	3 (16%)	19,38,41	0.86	1 (5%)
87	A2M	M1	807	87	18,25,26	4.16	7 (38%)	18,36,39	4.33	4 (22%)
87	A2M	M1	2220	87	18,25,26	4.25	7 (38%)	18,36,39	4.26	4 (22%)
87	5MC	M1	2278	92,87	18,22,23	0.75	1 (5%)	26,32,35	1.05	2 (7%)
87	OMG	M1	2815	87	18,26,27	1.25	3 (16%)	19,38,41	0.95	1 (5%)
87	A2M	M1	1449	92,87	18,25,26	4.25	8 (44%)	18,36,39	4.35	4 (22%)
87	A2M	M1	2256	87	18,25,26	4.16	7 (38%)	18,36,39	4.36	7 (38%)
87	A2M	M1	2946	92,87	18,25,26	4.19	8 (44%)	18,36,39	4.26	5 (27%)
87	1MA	M1	2142	92,87	16,25,26	1.12	2 (12%)	18,37,40	1.12	1 (5%)
87	A2M	M1	649	87	18,25,26	4.10	7 (38%)	18,36,39	4.39	5 (27%)
87	A2M	M1	2280	87	18,25,26	4.27	8 (44%)	18,36,39	4.24	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	OMC	M1	2197	94,87	19,22,23	0.71	1 (5%)	26,31,34	0.67	0
91	YYG	DP	37	91	31,42,43	1.20	4 (12%)	33,62,65	1.90	3 (9%)
87	A2M	M1	876	87	18,25,26	4.23	8 (44%)	18,36,39	4.41	4 (22%)
87	OMU	M1	2417	87	19,22,23	2.79	7 (36%)	26,31,34	1.79	5 (19%)
87	OMU	M1	2724	87	19,22,23	2.88	8 (42%)	26,31,34	1.71	5 (19%)
87	OMC	M1	2948	87	19,22,23	0.68	0	26,31,34	0.93	2 (7%)
87	1MA	M1	645	92,87	16,25,26	1.07	2 (12%)	18,37,40	1.06	1 (5%)
87	OMG	M1	805	87	18,26,27	1.27	3 (16%)	19,38,41	0.93	1 (5%)
87	OMC	M1	2959	87	19,22,23	0.68	0	26,31,34	0.82	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	UR3	M1	2634	87	-	0/7/25/26	0/2/2/2
87	A2M	M1	2640	87	-	0/5/27/28	0/3/3/3
87	OMU	M1	2921	87	-	0/9/27/28	0/2/2/2
87	OMG	M1	867	94,87	-	0/5/27/28	0/3/3/3
87	OMU	M1	2421	87	-	0/9/27/28	0/2/2/2
87	OMC	M1	2337	87	-	0/9/27/28	0/2/2/2
87	OMG	M1	1450	87	-	2/5/27/28	0/3/3/3
87	OMU	M1	2729	87	-	0/9/27/28	0/2/2/2
87	OMG	M1	2793	87	-	0/5/27/28	0/3/3/3
87	OMG	M1	908	87	-	0/5/27/28	0/3/3/3
87	OMG	M1	2922	91,87	-	4/5/27/28	0/3/3/3
87	OMU	M1	1888	87	-	0/9/27/28	0/2/2/2
87	OMG	M1	2791	87	-	0/5/27/28	0/3/3/3
87	5MC	M1	2870	94,87	-	4/7/25/26	0/2/2/2
87	OMC	M1	663	87	-	0/9/27/28	0/2/2/2
87	OMU	M1	898	87	-	0/9/27/28	0/2/2/2
87	OMC	M1	650	92,87	-	0/9/27/28	0/2/2/2
87	OMG	M1	2288	87	-	0/5/27/28	0/3/3/3
87	A2M	M1	2281	87	-	2/5/27/28	0/3/3/3
87	OMC	M1	1437	92,87	-	2/9/27/28	0/2/2/2
87	A2M	M1	1133	92,87	-	0/5/27/28	0/3/3/3
87	OMU	M1	2347	87	-	1/9/27/28	0/2/2/2
87	A2M	M1	817	92,87	-	2/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OMG	M1	2619	87	-	3/5/27/28	0/3/3/3
87	A2M	M1	807	87	-	0/5/27/28	0/3/3/3
87	A2M	M1	2220	87	-	1/5/27/28	0/3/3/3
87	5MC	M1	2278	92,87	-	2/7/25/26	0/2/2/2
87	OMG	M1	2815	87	-	0/5/27/28	0/3/3/3
87	A2M	M1	1449	92,87	-	0/5/27/28	0/3/3/3
87	A2M	M1	2256	87	-	2/5/27/28	0/3/3/3
87	A2M	M1	2946	92,87	-	1/5/27/28	0/3/3/3
87	1MA	M1	2142	92,87	-	0/3/25/26	0/3/3/3
87	A2M	M1	649	87	-	2/5/27/28	0/3/3/3
87	A2M	M1	2280	87	-	2/5/27/28	0/3/3/3
87	OMC	M1	2197	94,87	-	4/9/27/28	0/2/2/2
91	YYG	DP	37	91	-	6/20/42/43	0/3/4/4
87	A2M	M1	876	87	-	0/5/27/28	0/3/3/3
87	OMU	M1	2417	87	-	1/9/27/28	0/2/2/2
87	OMU	M1	2724	87	-	1/9/27/28	0/2/2/2
87	OMC	M1	2948	87	-	0/9/27/28	0/2/2/2
87	1MA	M1	645	92,87	-	0/3/25/26	0/3/3/3
87	OMG	M1	805	87	-	0/5/27/28	0/3/3/3
87	OMC	M1	2959	87	-	0/9/27/28	0/2/2/2

All (197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	M1	2280	A2M	O4'-C1'	15.14	1.62	1.41
87	M1	2220	A2M	O4'-C1'	15.11	1.62	1.41
87	M1	1449	A2M	O4'-C1'	15.06	1.62	1.41
87	M1	1133	A2M	O4'-C1'	15.03	1.62	1.41
87	M1	876	A2M	O4'-C1'	15.01	1.62	1.41
87	M1	2640	A2M	O4'-C1'	14.93	1.61	1.41
87	M1	2946	A2M	O4'-C1'	14.92	1.61	1.41
87	M1	817	A2M	O4'-C1'	14.68	1.61	1.41
87	M1	2256	A2M	O4'-C1'	14.58	1.61	1.41
87	M1	807	A2M	O4'-C1'	14.50	1.61	1.41
87	M1	649	A2M	O4'-C1'	14.46	1.61	1.41
87	M1	2281	A2M	O4'-C1'	13.89	1.60	1.41
87	M1	2347	OMU	C2-N1	7.21	1.50	1.38
87	M1	2634	UR3	C2-N1	7.10	1.48	1.38
87	M1	807	A2M	O4'-C4'	-6.84	1.29	1.45
87	M1	2921	OMU	C2-N1	6.80	1.49	1.38
87	M1	817	A2M	O4'-C4'	-6.76	1.29	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	M1	1888	OMU	C2-N1	6.74	1.49	1.38
87	M1	2280	A2M	O4'-C4'	-6.60	1.30	1.45
87	M1	1449	A2M	O4'-C4'	-6.56	1.30	1.45
87	M1	2634	UR3	C6-C5	6.55	1.50	1.35
87	M1	2921	OMU	C2-N3	6.54	1.49	1.38
87	M1	1133	A2M	O4'-C4'	-6.54	1.30	1.45
87	M1	1888	OMU	C2-N3	6.52	1.49	1.38
87	M1	2347	OMU	C2-N3	6.51	1.49	1.38
87	M1	876	A2M	O4'-C4'	-6.51	1.30	1.45
87	M1	2281	A2M	O4'-C4'	-6.48	1.30	1.45
87	M1	898	OMU	C2-N1	6.46	1.48	1.38
87	M1	2724	OMU	C2-N3	6.45	1.49	1.38
87	M1	2729	OMU	C2-N1	6.45	1.48	1.38
87	M1	2724	OMU	C2-N1	6.44	1.48	1.38
87	M1	2220	A2M	O4'-C4'	-6.44	1.30	1.45
87	M1	649	A2M	O4'-C4'	-6.42	1.30	1.45
87	M1	2256	A2M	O4'-C4'	-6.41	1.30	1.45
87	M1	2640	A2M	O4'-C4'	-6.41	1.30	1.45
87	M1	2421	OMU	C2-N3	6.40	1.49	1.38
87	M1	898	OMU	C2-N3	6.35	1.49	1.38
87	M1	2946	A2M	O4'-C4'	-6.34	1.30	1.45
87	M1	2729	OMU	C2-N3	6.33	1.49	1.38
87	M1	2417	OMU	C2-N3	6.32	1.49	1.38
87	M1	2421	OMU	C2-N1	6.27	1.48	1.38
87	M1	2417	OMU	C2-N1	6.12	1.48	1.38
87	M1	2724	OMU	C6-C5	5.56	1.48	1.35
87	M1	898	OMU	C6-C5	5.54	1.47	1.35
87	M1	2921	OMU	C6-C5	5.45	1.47	1.35
87	M1	1888	OMU	C6-C5	5.41	1.47	1.35
87	M1	2634	UR3	C2-N3	5.38	1.49	1.39
87	M1	2421	OMU	C6-C5	5.34	1.47	1.35
87	M1	2729	OMU	C6-C5	5.32	1.47	1.35
87	M1	2347	OMU	C6-C5	5.30	1.47	1.35
87	M1	2417	OMU	C6-C5	5.27	1.47	1.35
87	M1	2921	OMU	C4-N3	3.93	1.45	1.38
87	M1	2634	UR3	O2-C2	-3.80	1.15	1.22
87	M1	2724	OMU	C4-N3	3.68	1.45	1.38
87	M1	2347	OMU	C4-N3	3.65	1.45	1.38
87	M1	1888	OMU	C4-N3	3.64	1.45	1.38
87	M1	2729	OMU	C4-N3	3.61	1.45	1.38
87	M1	2288	OMG	C8-N7	-3.57	1.28	1.35
87	M1	2729	OMU	O4-C4	-3.54	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	M1	2634	UR3	C6-N1	3.48	1.46	1.38
87	M1	2256	A2M	O2'-C2'	3.43	1.51	1.42
87	M1	2347	OMU	O4-C4	-3.42	1.17	1.24
87	M1	867	OMG	C8-N7	-3.42	1.29	1.35
91	DP	37	YYG	C8-N7	-3.40	1.29	1.35
87	M1	2281	A2M	C5-C4	-3.38	1.32	1.40
87	M1	898	OMU	C4-N3	3.37	1.44	1.38
87	M1	2417	OMU	C4-N3	3.37	1.44	1.38
87	M1	898	OMU	O4-C4	-3.37	1.18	1.24
87	M1	2417	OMU	O4-C4	-3.37	1.18	1.24
87	M1	2421	OMU	C4-N3	3.35	1.44	1.38
87	M1	1133	A2M	O3'-C3'	-3.29	1.35	1.43
87	M1	2220	A2M	O3'-C3'	-3.27	1.35	1.43
87	M1	1450	OMG	C8-N7	-3.27	1.29	1.35
87	M1	2421	OMU	O4-C4	-3.26	1.18	1.24
87	M1	1888	OMU	O4-C4	-3.26	1.18	1.24
87	M1	2793	OMG	C8-N7	-3.26	1.29	1.35
87	M1	876	A2M	O3'-C3'	-3.24	1.35	1.43
91	DP	37	YYG	C12-N1	3.22	1.42	1.36
91	DP	37	YYG	C2-N2	-3.22	1.29	1.35
87	M1	2921	OMU	O4-C4	-3.21	1.18	1.24
87	M1	2791	OMG	C8-N7	-3.18	1.29	1.35
87	M1	2619	OMG	C8-N7	-3.18	1.29	1.35
87	M1	2815	OMG	C8-N7	-3.18	1.29	1.35
87	M1	805	OMG	C8-N7	-3.17	1.29	1.35
87	M1	2724	OMU	O4-C4	-3.17	1.18	1.24
87	M1	2640	A2M	O3'-C3'	-3.16	1.35	1.43
87	M1	908	OMG	C8-N7	-3.16	1.29	1.35
87	M1	1449	A2M	O3'-C3'	-3.13	1.35	1.43
87	M1	2220	A2M	C6-N6	3.11	1.45	1.34
87	M1	2256	A2M	O3'-C3'	-3.11	1.35	1.43
87	M1	2256	A2M	C6-N6	3.11	1.45	1.34
87	M1	649	A2M	O3'-C3'	-3.10	1.35	1.43
87	M1	2280	A2M	O3'-C3'	-3.07	1.35	1.43
87	M1	2142	1MA	C8-N7	-3.07	1.29	1.35
87	M1	876	A2M	C6-N6	3.06	1.45	1.34
87	M1	2280	A2M	C6-N6	3.06	1.45	1.34
87	M1	807	A2M	C5-C4	-3.04	1.32	1.40
87	M1	807	A2M	C6-N6	3.03	1.45	1.34
87	M1	2280	A2M	C5-C4	-3.02	1.32	1.40
87	M1	817	A2M	C5-C4	-3.01	1.33	1.40
87	M1	807	A2M	O3'-C3'	-3.00	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	M1	2640	A2M	C5-C4	-2.98	1.33	1.40
87	M1	1449	A2M	C6-N6	2.97	1.44	1.34
87	M1	2256	A2M	C5-C4	-2.97	1.33	1.40
87	M1	2220	A2M	O2'-C2'	2.96	1.50	1.42
87	M1	2640	A2M	C6-N6	2.96	1.44	1.34
87	M1	2946	A2M	C5-C4	-2.96	1.33	1.40
87	M1	1133	A2M	C5-C4	-2.95	1.33	1.40
87	M1	649	A2M	C6-N6	2.95	1.44	1.34
87	M1	1133	A2M	C6-N6	2.94	1.44	1.34
87	M1	817	A2M	C6-N6	2.93	1.44	1.34
87	M1	2793	OMG	C5-C6	-2.93	1.41	1.47
87	M1	2281	A2M	O3'-C3'	-2.91	1.36	1.43
87	M1	2220	A2M	C5-C4	-2.90	1.33	1.40
87	M1	1888	OMU	O2-C2	-2.90	1.17	1.23
87	M1	2946	A2M	C6-N6	2.90	1.44	1.34
87	M1	1449	A2M	C5-C4	-2.90	1.33	1.40
87	M1	876	A2M	C5-C4	-2.89	1.33	1.40
87	M1	2922	OMG	C8-N7	-2.86	1.30	1.35
87	M1	807	A2M	O2'-C2'	2.85	1.49	1.42
87	M1	2640	A2M	O2'-C2'	2.85	1.49	1.42
87	M1	2946	A2M	O3'-C3'	-2.84	1.36	1.43
87	M1	649	A2M	C5-C4	-2.84	1.33	1.40
87	M1	649	A2M	O2'-C2'	2.84	1.49	1.42
87	M1	1133	A2M	O2'-C2'	2.84	1.49	1.42
87	M1	2946	A2M	O2'-C2'	2.84	1.49	1.42
87	M1	2417	OMU	O2-C2	-2.83	1.17	1.23
87	M1	645	1MA	C8-N7	-2.81	1.30	1.35
87	M1	2729	OMU	O2-C2	-2.80	1.17	1.23
87	M1	2280	A2M	O2'-C2'	2.77	1.49	1.42
87	M1	1449	A2M	O2'-C2'	2.76	1.49	1.42
87	M1	908	OMG	C5-C6	-2.76	1.41	1.47
87	M1	2921	OMU	C6-N1	2.75	1.44	1.38
87	M1	817	A2M	O3'-C3'	-2.74	1.36	1.43
87	M1	898	OMU	O2-C2	-2.74	1.18	1.23
87	M1	2421	OMU	O2-C2	-2.72	1.18	1.23
87	M1	898	OMU	C6-N1	2.71	1.44	1.38
87	M1	2347	OMU	C6-N1	2.71	1.44	1.38
87	M1	2724	OMU	O2-C2	-2.70	1.18	1.23
87	M1	2281	A2M	C6-N6	2.69	1.43	1.34
87	M1	2619	OMG	C5-C6	-2.68	1.42	1.47
87	M1	1888	OMU	C6-N1	2.68	1.44	1.38
87	M1	2921	OMU	O2-C2	-2.67	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	M1	867	OMG	C5-C6	-2.67	1.42	1.47
87	M1	2922	OMG	C5-C6	-2.66	1.42	1.47
87	M1	2634	UR3	O4-C4	-2.63	1.17	1.23
87	M1	2142	1MA	C5-C4	-2.62	1.36	1.43
87	M1	2347	OMU	O2-C2	-2.61	1.18	1.23
87	M1	876	A2M	O2'-C2'	2.61	1.49	1.42
87	M1	2791	OMG	C5-C6	-2.60	1.42	1.47
87	M1	2724	OMU	C6-N1	2.57	1.44	1.38
87	M1	645	1MA	C5-C4	-2.57	1.36	1.43
87	M1	2288	OMG	C5-C6	-2.57	1.42	1.47
87	M1	817	A2M	O2'-C2'	2.57	1.49	1.42
87	M1	1450	OMG	C5-C6	-2.52	1.42	1.47
87	M1	2729	OMU	C6-N1	2.51	1.44	1.38
87	M1	2417	OMU	C6-N1	2.51	1.44	1.38
87	M1	2281	A2M	O2'-C2'	2.50	1.49	1.42
87	M1	2634	UR3	C4-N3	2.50	1.46	1.40
87	M1	2815	OMG	C5-C6	-2.39	1.42	1.47
87	M1	2421	OMU	C6-N1	2.39	1.43	1.38
87	M1	805	OMG	C5-C6	-2.38	1.42	1.47
87	M1	2281	A2M	O5'-C5'	-2.33	1.39	1.44
87	M1	1449	A2M	C2-N3	2.28	1.35	1.32
87	M1	807	A2M	O5'-C5'	-2.28	1.39	1.44
87	M1	2634	UR3	C5-C4	2.28	1.49	1.43
87	M1	2280	A2M	C2-N3	2.24	1.35	1.32
87	M1	817	A2M	O5'-C5'	-2.23	1.39	1.44
87	M1	2220	A2M	C2-N3	2.21	1.35	1.32
87	M1	898	OMU	C5-C4	2.20	1.48	1.43
87	M1	2793	OMG	C5-C4	-2.20	1.37	1.43
87	M1	805	OMG	C5-C4	-2.20	1.37	1.43
87	M1	2815	OMG	C5-C4	-2.20	1.37	1.43
87	M1	1133	A2M	O5'-C5'	-2.19	1.39	1.44
87	M1	650	OMC	C4-N3	-2.17	1.30	1.34
87	M1	2278	5MC	C4-N3	-2.17	1.30	1.34
87	M1	2870	5MC	C4-N3	-2.16	1.30	1.34
87	M1	876	A2M	O5'-C5'	-2.15	1.39	1.44
87	M1	2640	A2M	C2-N3	2.15	1.35	1.32
87	M1	2288	OMG	C5-C4	-2.14	1.37	1.43
87	M1	2640	A2M	O5'-C5'	-2.14	1.39	1.44
91	DP	37	YYG	C4-N3	-2.13	1.36	1.40
87	M1	1450	OMG	C5-C4	-2.12	1.37	1.43
87	M1	1888	OMU	C5-C4	2.11	1.48	1.43
87	M1	2619	OMG	C5-C4	-2.11	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	M1	876	A2M	C2-N3	2.10	1.35	1.32
87	M1	817	A2M	C2-N3	2.09	1.35	1.32
87	M1	2946	A2M	O5'-C5'	-2.08	1.39	1.44
87	M1	2946	A2M	C2-N3	2.07	1.35	1.32
87	M1	2280	A2M	O5'-C5'	-2.07	1.39	1.44
87	M1	2197	OMC	C4-N3	-2.06	1.30	1.34
87	M1	2922	OMG	C5-C4	-2.06	1.37	1.43
87	M1	1449	A2M	O5'-C5'	-2.06	1.39	1.44
87	M1	2256	A2M	C2-N3	2.05	1.35	1.32
87	M1	2724	OMU	C5-C4	2.02	1.48	1.43
87	M1	2921	OMU	C5-C4	2.01	1.48	1.43
87	M1	649	A2M	C2-N3	2.00	1.35	1.32

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	649	A2M	C5-C6-N6	12.00	138.59	120.35
87	M1	817	A2M	C5-C6-N6	11.99	138.57	120.35
87	M1	876	A2M	C5-C6-N6	11.91	138.45	120.35
87	M1	807	A2M	C5-C6-N6	11.60	137.98	120.35
87	M1	1449	A2M	C5-C6-N6	11.48	137.80	120.35
87	M1	2220	A2M	C5-C6-N6	11.38	137.64	120.35
87	M1	2256	A2M	C5-C6-N6	11.36	137.61	120.35
87	M1	2640	A2M	C5-C6-N6	11.32	137.55	120.35
87	M1	2280	A2M	C5-C6-N6	11.29	137.51	120.35
87	M1	2946	A2M	C5-C6-N6	11.28	137.49	120.35
87	M1	2281	A2M	C5-C6-N6	11.06	137.16	120.35
87	M1	1133	A2M	C5-C6-N6	10.73	136.65	120.35
87	M1	817	A2M	N6-C6-N1	-9.95	97.91	118.57
87	M1	876	A2M	N6-C6-N1	-9.81	98.22	118.57
87	M1	649	A2M	N6-C6-N1	-9.76	98.31	118.57
87	M1	2281	A2M	N6-C6-N1	-9.74	98.35	118.57
87	M1	807	A2M	N6-C6-N1	-9.67	98.50	118.57
87	M1	1449	A2M	N6-C6-N1	-9.52	98.81	118.57
87	M1	2280	A2M	N6-C6-N1	-9.48	98.89	118.57
87	M1	2640	A2M	N6-C6-N1	-9.46	98.93	118.57
87	M1	2256	A2M	N6-C6-N1	-9.42	99.03	118.57
87	M1	2220	A2M	N6-C6-N1	-9.40	99.06	118.57
87	M1	2946	A2M	N6-C6-N1	-9.38	99.11	118.57
87	M1	1133	A2M	N6-C6-N1	-8.90	100.09	118.57
87	M1	1449	A2M	C1'-N9-C4	8.80	142.10	126.64
87	M1	876	A2M	C1'-N9-C4	8.36	141.33	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	2640	A2M	C1'-N9-C4	8.34	141.29	126.64
87	M1	807	A2M	C1'-N9-C4	8.03	140.75	126.64
87	M1	2946	A2M	C1'-N9-C4	8.03	140.75	126.64
87	M1	2280	A2M	C1'-N9-C4	8.02	140.74	126.64
87	M1	649	A2M	C1'-N9-C4	8.02	140.73	126.64
87	M1	2220	A2M	C1'-N9-C4	8.01	140.72	126.64
87	M1	2256	A2M	C1'-N9-C4	7.76	140.27	126.64
87	M1	1133	A2M	C1'-N9-C4	7.51	139.84	126.64
87	M1	817	A2M	C1'-N9-C4	7.28	139.42	126.64
91	DP	37	YYG	C3-N3-C4	7.22	129.53	116.71
91	DP	37	YYG	C3-N3-C2	-6.20	114.33	120.13
87	M1	2281	A2M	C1'-N9-C4	6.07	137.31	126.64
87	M1	2421	OMU	C4-N3-C2	-5.74	119.01	126.58
87	M1	817	A2M	N3-C2-N1	-5.72	119.73	128.68
87	M1	1133	A2M	N3-C2-N1	-5.71	119.76	128.68
87	M1	2220	A2M	N3-C2-N1	-5.70	119.77	128.68
87	M1	649	A2M	N3-C2-N1	-5.69	119.78	128.68
87	M1	2729	OMU	C4-N3-C2	-5.67	119.10	126.58
87	M1	807	A2M	N3-C2-N1	-5.67	119.81	128.68
87	M1	2281	A2M	N3-C2-N1	-5.59	119.94	128.68
87	M1	2256	A2M	N3-C2-N1	-5.58	119.96	128.68
87	M1	1449	A2M	N3-C2-N1	-5.56	119.98	128.68
87	M1	2417	OMU	C4-N3-C2	-5.53	119.28	126.58
87	M1	2640	A2M	N3-C2-N1	-5.50	120.08	128.68
87	M1	1888	OMU	C4-N3-C2	-5.48	119.35	126.58
87	M1	876	A2M	N3-C2-N1	-5.47	120.13	128.68
87	M1	2280	A2M	N3-C2-N1	-5.46	120.15	128.68
87	M1	2921	OMU	C4-N3-C2	-5.33	119.55	126.58
87	M1	2347	OMU	C4-N3-C2	-5.32	119.56	126.58
87	M1	2946	A2M	N3-C2-N1	-5.28	120.42	128.68
87	M1	898	OMU	C4-N3-C2	-5.18	119.74	126.58
87	M1	2634	UR3	C4-N3-C2	-5.11	119.75	124.56
87	M1	2724	OMU	C4-N3-C2	-5.05	119.92	126.58
87	M1	2421	OMU	N3-C2-N1	4.08	120.31	114.89
87	M1	1888	OMU	N3-C2-N1	4.08	120.30	114.89
87	M1	898	OMU	N3-C2-N1	4.03	120.24	114.89
87	M1	2417	OMU	N3-C2-N1	3.96	120.15	114.89
87	M1	2724	OMU	N3-C2-N1	3.92	120.10	114.89
87	M1	2729	OMU	N3-C2-N1	3.90	120.07	114.89
87	M1	2921	OMU	N3-C2-N1	3.79	119.93	114.89
87	M1	2347	OMU	C5-C4-N3	3.73	120.42	114.84
87	M1	2729	OMU	C5-C4-N3	3.68	120.34	114.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	2417	OMU	C5-C4-N3	3.66	120.31	114.84
87	M1	2256	A2M	O2'-C2'-C1'	3.64	116.31	109.09
87	M1	2921	OMU	C5-C4-N3	3.59	120.22	114.84
87	M1	2347	OMU	N3-C2-N1	3.58	119.64	114.89
87	M1	2421	OMU	C5-C4-N3	3.54	120.14	114.84
87	M1	898	OMU	C5-C4-N3	3.51	120.09	114.84
87	M1	1888	OMU	C5-C4-N3	3.49	120.06	114.84
87	M1	2724	OMU	C5-C4-N3	3.28	119.75	114.84
87	M1	2347	OMU	O4-C4-C5	-3.25	119.44	125.16
87	M1	2921	OMU	O4-C4-C5	-3.13	119.66	125.16
87	M1	2417	OMU	O4-C4-C5	-2.95	119.97	125.16
87	M1	2729	OMU	O4-C4-C5	-2.89	120.07	125.16
87	M1	2142	1MA	N1-C6-N6	2.89	127.11	119.77
87	M1	2421	OMU	O4-C4-C5	-2.88	120.09	125.16
87	M1	2948	OMC	C1'-N1-C2	2.86	124.81	118.42
91	DP	37	YYG	C11-C12-N1	-2.85	104.92	106.53
87	M1	2815	OMG	O6-C6-C5	2.77	129.79	124.37
87	M1	2347	OMU	C1'-N1-C2	2.73	122.50	117.57
87	M1	1437	OMC	C1'-N1-C2	2.68	124.40	118.42
87	M1	2724	OMU	O4-C4-C5	-2.67	120.46	125.16
87	M1	1888	OMU	O4-C4-C5	-2.66	120.47	125.16
87	M1	867	OMG	O6-C6-C5	2.63	129.51	124.37
87	M1	898	OMU	O4-C4-C5	-2.58	120.62	125.16
87	M1	2417	OMU	O2-C2-N1	-2.55	119.40	122.79
87	M1	1450	OMG	O6-C6-C5	2.53	129.31	124.37
87	M1	805	OMG	O6-C6-C5	2.51	129.28	124.37
87	M1	2256	A2M	CM'-O2'-C2'	2.51	121.11	114.52
87	M1	2256	A2M	O4'-C1'-C2'	-2.46	102.31	106.59
87	M1	2421	OMU	O2-C2-N1	-2.42	119.56	122.79
87	M1	2619	OMG	O6-C6-C5	2.40	129.06	124.37
87	M1	2278	5MC	C1'-N1-C6	-2.39	117.14	121.12
87	M1	2634	UR3	C6-N1-C2	-2.35	119.68	121.79
87	M1	2724	OMU	O2-C2-N1	-2.33	119.69	122.79
87	M1	645	1MA	N1-C6-N6	2.28	125.56	119.77
87	M1	2278	5MC	C1'-N1-C2	2.25	123.44	118.42
87	M1	2922	OMG	O6-C6-C5	2.23	128.73	124.37
87	M1	2634	UR3	C1'-N1-C2	2.23	120.75	116.99
87	M1	2791	OMG	O6-C6-C5	2.18	128.63	124.37
87	M1	2948	OMC	C1'-N1-C6	-2.16	116.13	120.84
87	M1	908	OMG	O6-C6-C5	2.15	128.58	124.37
87	M1	2729	OMU	O2-C2-N1	-2.14	119.94	122.79
87	M1	2793	OMG	O6-C6-C5	2.13	128.54	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	M1	663	OMC	C1'-N1-C2	2.10	123.11	118.42
87	M1	649	A2M	C3'-C2'-C1'	2.08	106.80	102.89
87	M1	2946	A2M	O4'-C4'-C3'	-2.05	101.05	105.11
87	M1	2288	OMG	O6-C6-C5	2.05	128.38	124.37
87	M1	1888	OMU	O2-C2-N1	-2.04	120.07	122.79
87	M1	2959	OMC	C1'-N1-C2	2.03	122.94	118.42
87	M1	898	OMU	O2-C2-N1	-2.00	120.12	122.79

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	M1	1437	OMC	C1'-C2'-O2'-CM2
87	M1	1450	OMG	O4'-C4'-C5'-O5'
87	M1	2220	A2M	C1'-C2'-O2'-CM'
87	M1	2256	A2M	C1'-C2'-O2'-CM'
87	M1	2417	OMU	C1'-C2'-O2'-CM2
87	M1	2619	OMG	C1'-C2'-O2'-CM2
87	M1	2724	OMU	C1'-C2'-O2'-CM2
87	M1	2946	A2M	C1'-C2'-O2'-CM'
91	DP	37	YYG	N20-C21-O23-C24
91	DP	37	YYG	O22-C21-O23-C24
91	DP	37	YYG	C15-C16-O18-C19
87	M1	2197	OMC	C2'-C1'-N1-C6
87	M1	1450	OMG	C3'-C4'-C5'-O5'
87	M1	2280	A2M	O4'-C4'-C5'-O5'
87	M1	2281	A2M	O4'-C4'-C5'-O5'
87	M1	2281	A2M	C3'-C4'-C5'-O5'
87	M1	2922	OMG	O4'-C4'-C5'-O5'
91	DP	37	YYG	O17-C16-O18-C19
87	M1	2278	5MC	O4'-C4'-C5'-O5'
87	M1	2280	A2M	C3'-C4'-C5'-O5'
87	M1	2922	OMG	C3'-C4'-C5'-O5'
91	DP	37	YYG	O23-C21-N20-C15
87	M1	2197	OMC	C2'-C1'-N1-C2
91	DP	37	YYG	O22-C21-N20-C15
87	M1	2278	5MC	C3'-C4'-C5'-O5'
87	M1	2197	OMC	O4'-C1'-N1-C6
87	M1	649	A2M	C4'-C5'-O5'-P
87	M1	817	A2M	C4'-C5'-O5'-P
87	M1	2870	5MC	C2'-C1'-N1-C6
87	M1	2197	OMC	O4'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
87	M1	2870	5MC	O4'-C1'-N1-C6
87	M1	2922	OMG	C3'-C2'-O2'-CM2
87	M1	2870	5MC	O4'-C1'-N1-C2
87	M1	2256	A2M	C4'-C5'-O5'-P
87	M1	1437	OMC	O4'-C4'-C5'-O5'
87	M1	2619	OMG	C3'-C4'-C5'-O5'
87	M1	649	A2M	C1'-C2'-O2'-CM'
87	M1	2922	OMG	C1'-C2'-O2'-CM2
87	M1	817	A2M	O4'-C4'-C5'-O5'
87	M1	2619	OMG	O4'-C4'-C5'-O5'
87	M1	2870	5MC	C2'-C1'-N1-C2
87	M1	2347	OMU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 327 ligands modelled in this entry, 324 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
95	SPD	M1	3604	-	9,9,9	0.28	0	8,8,8	0.41	0
95	SPD	M1	3603	-	9,9,9	0.31	0	8,8,8	0.32	0
95	SPD	M1	3602	-	9,9,9	0.28	0	8,8,8	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
95	SPD	M1	3604	-	-	3/7/7/7	-
95	SPD	M1	3603	-	-	3/7/7/7	-
95	SPD	M1	3602	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
95	M1	3604	SPD	C8-C7-N6-C5
95	M1	3603	SPD	C7-C8-C9-N10
95	M1	3603	SPD	N1-C2-C3-C4
95	M1	3603	SPD	C2-C3-C4-C5
95	M1	3604	SPD	C2-C3-C4-C5
95	M1	3604	SPD	C4-C5-N6-C7
95	M1	3602	SPD	C8-C7-N6-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

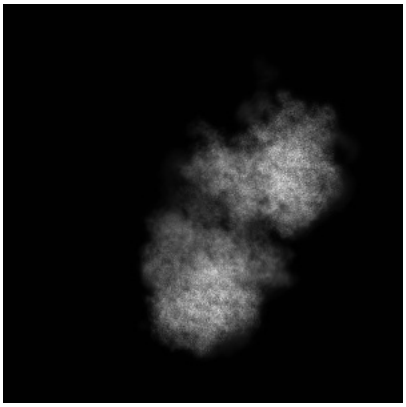
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50259. These allow visual inspection of the internal detail of the map and identification of artifacts.

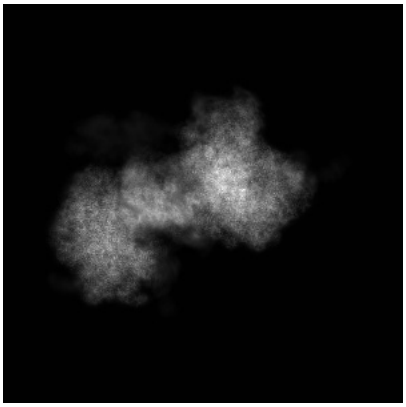
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

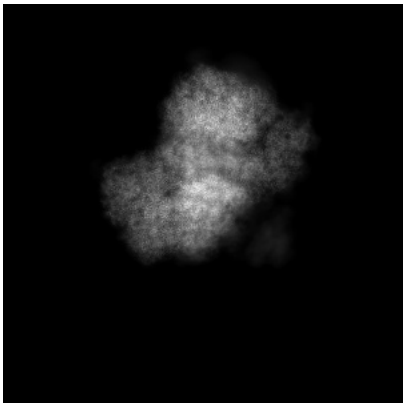
6.1.1 Primary map



X



Y

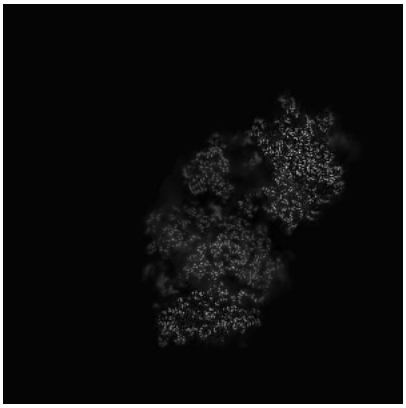


Z

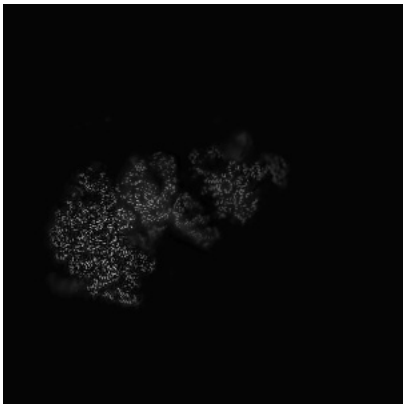
The images above show the map projected in three orthogonal directions.

6.2 Central slices

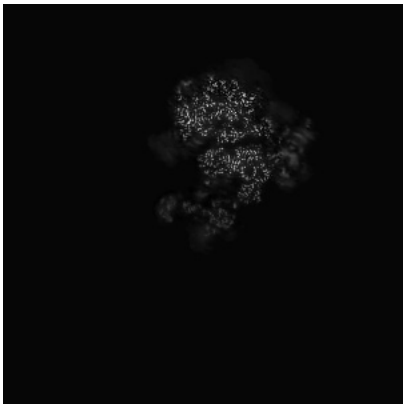
6.2.1 Primary map



X Index: 313



Y Index: 313

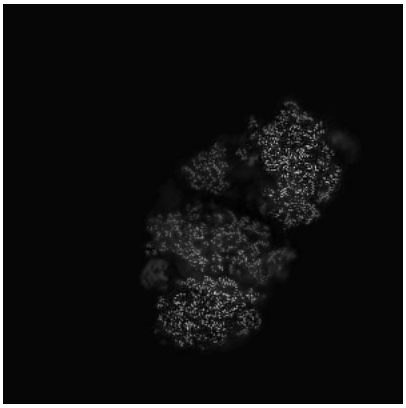


Z Index: 313

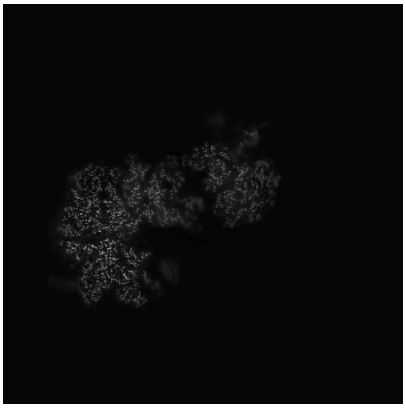
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

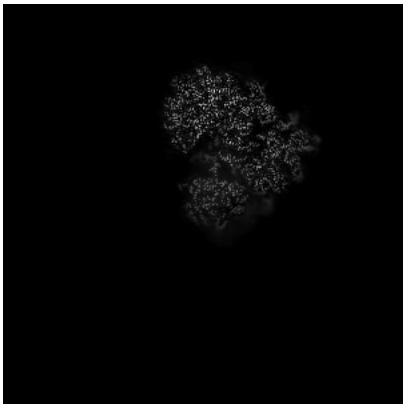
6.3.1 Primary map



X Index: 303



Y Index: 330

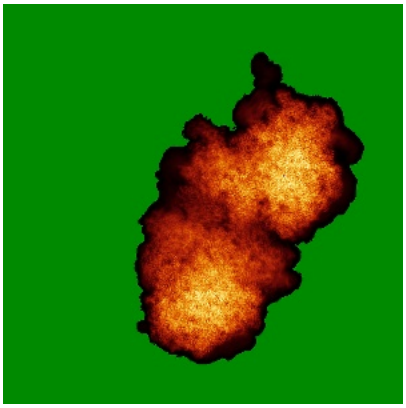


Z Index: 372

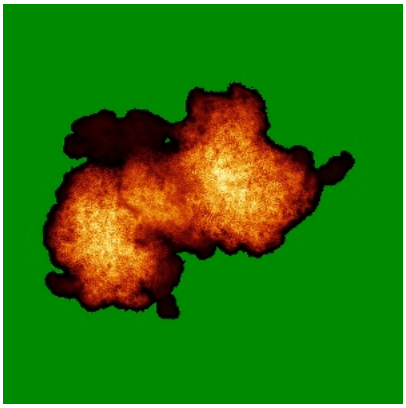
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

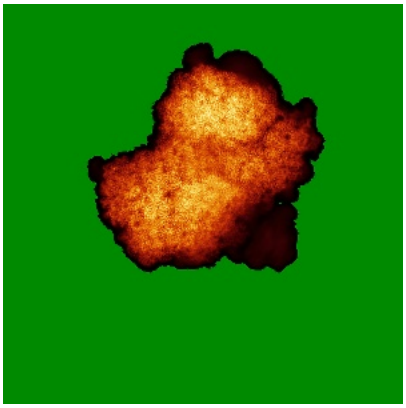
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

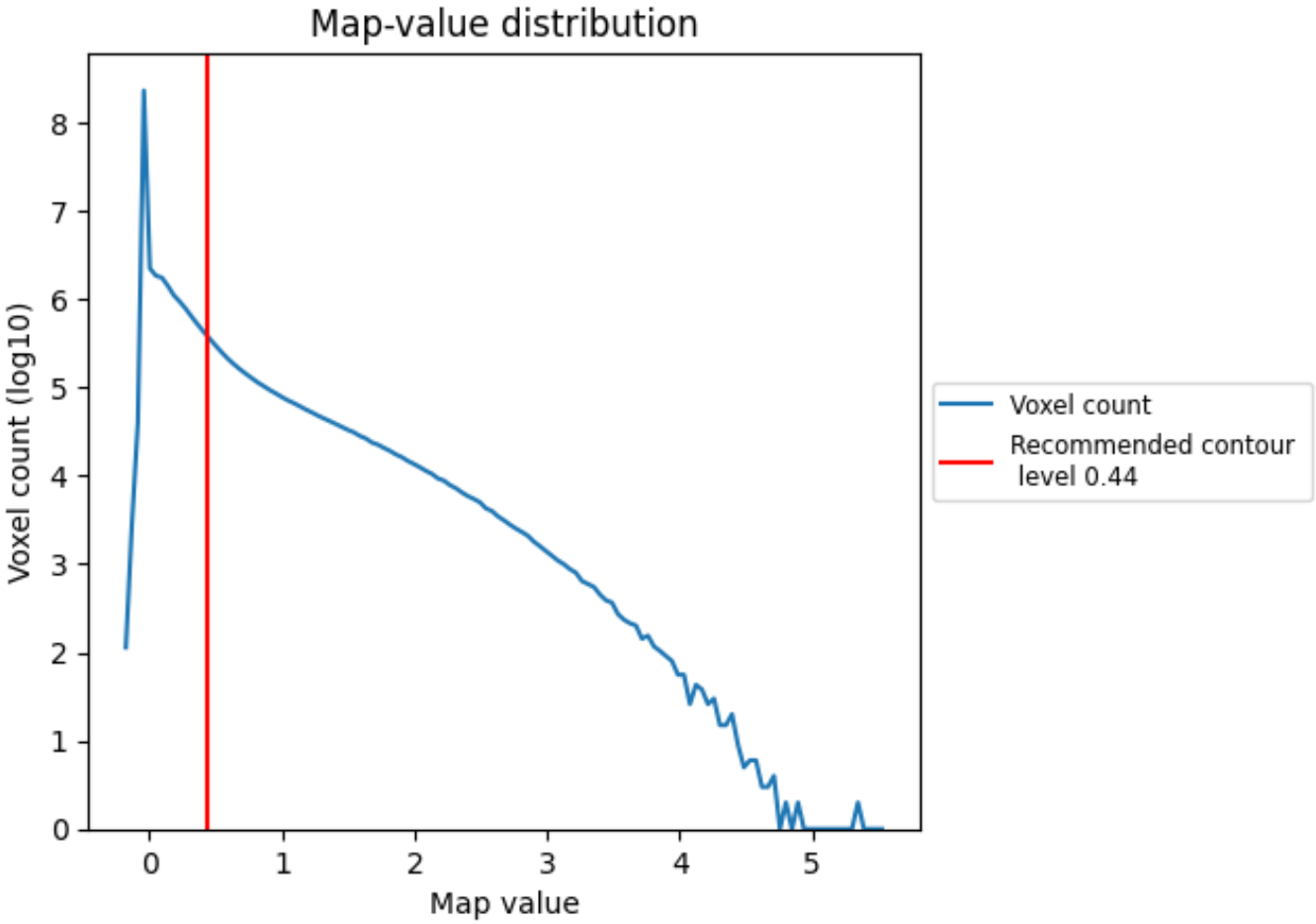
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

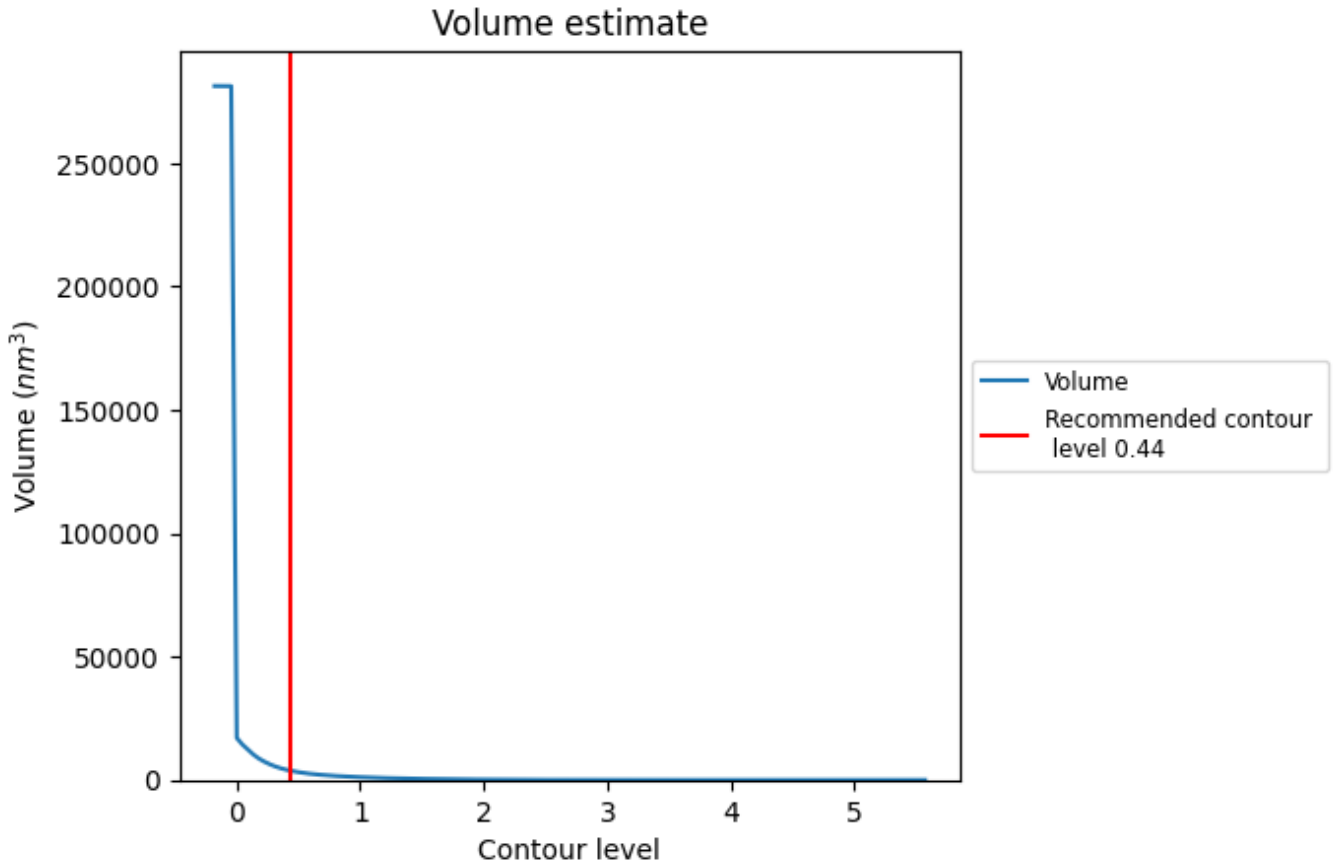
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

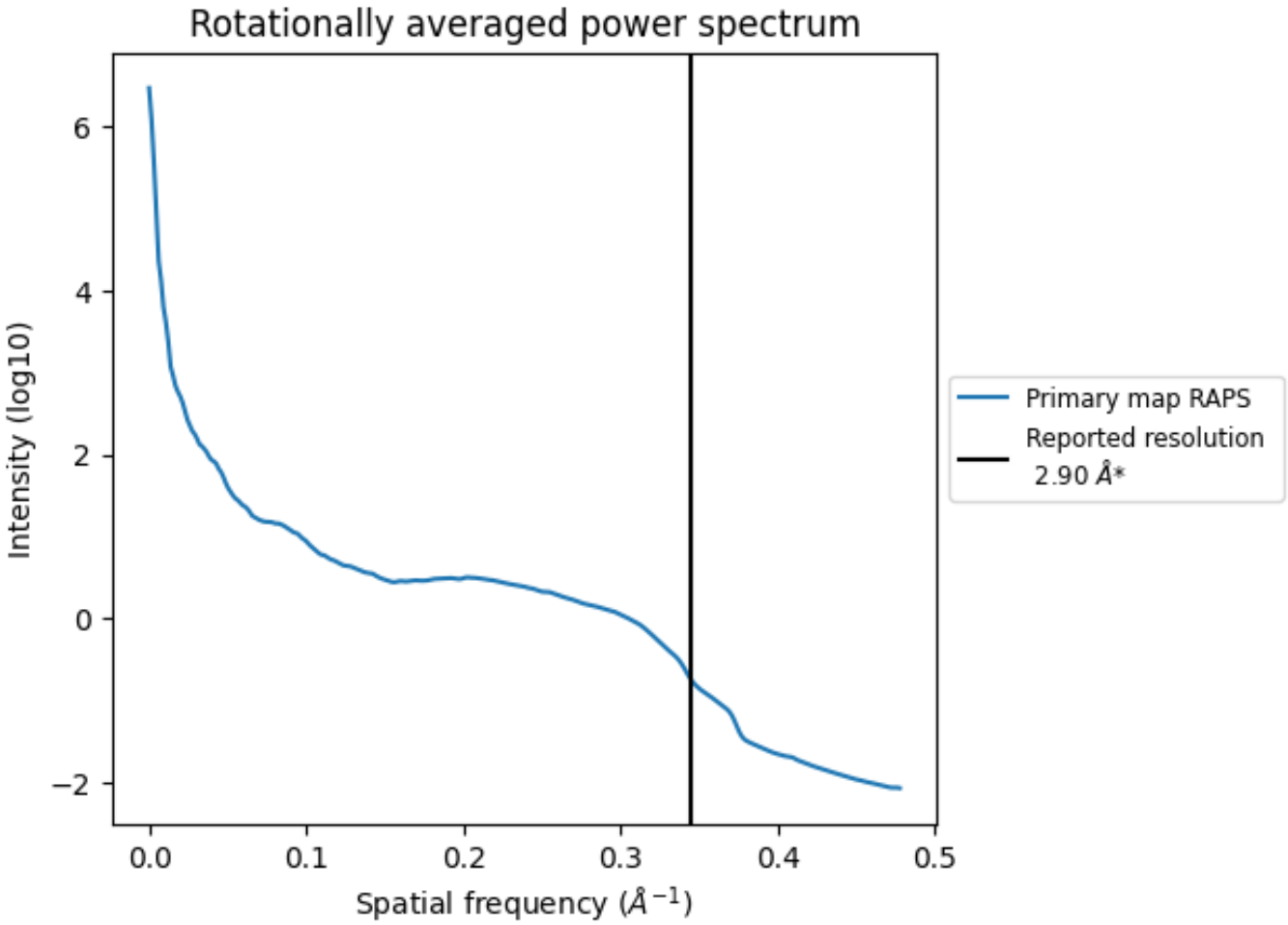
7.2 Volume estimate



The volume at the recommended contour level is 3730 nm^3; this corresponds to an approximate mass of 3369 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

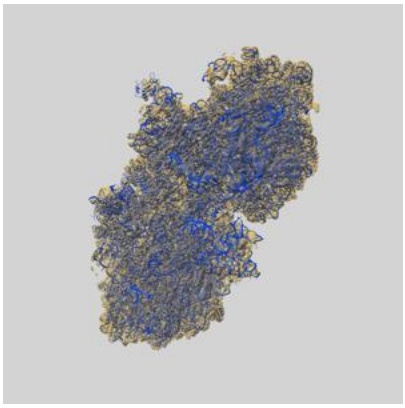
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

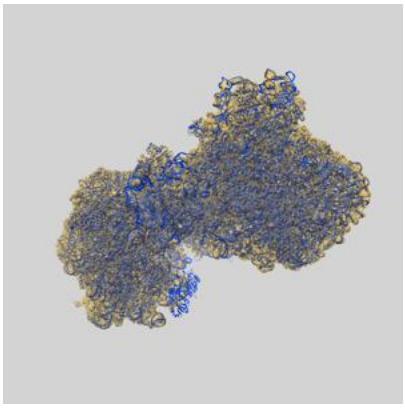
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50259 and PDB model 9F9S. Per-residue inclusion information can be found in section 3 on page 29.

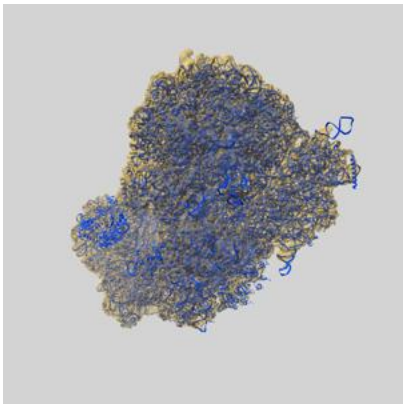
9.1 Map-model overlay



X



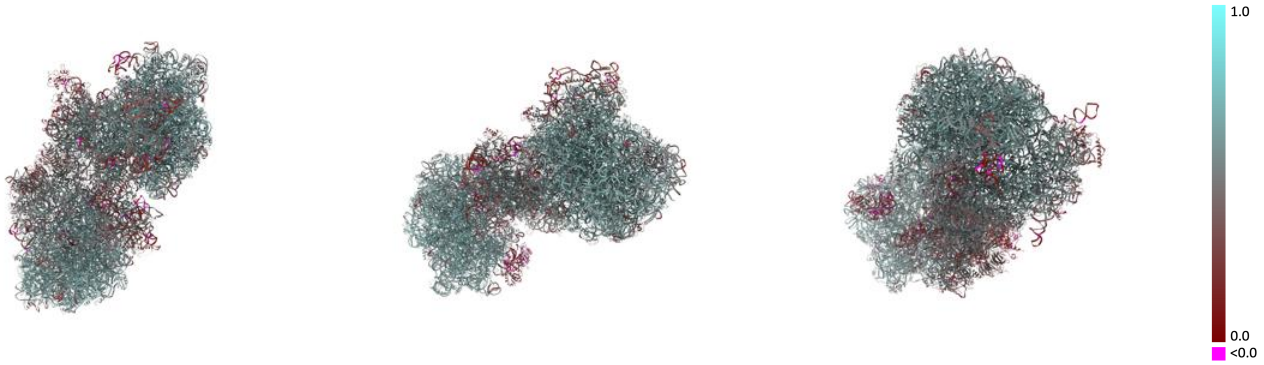
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

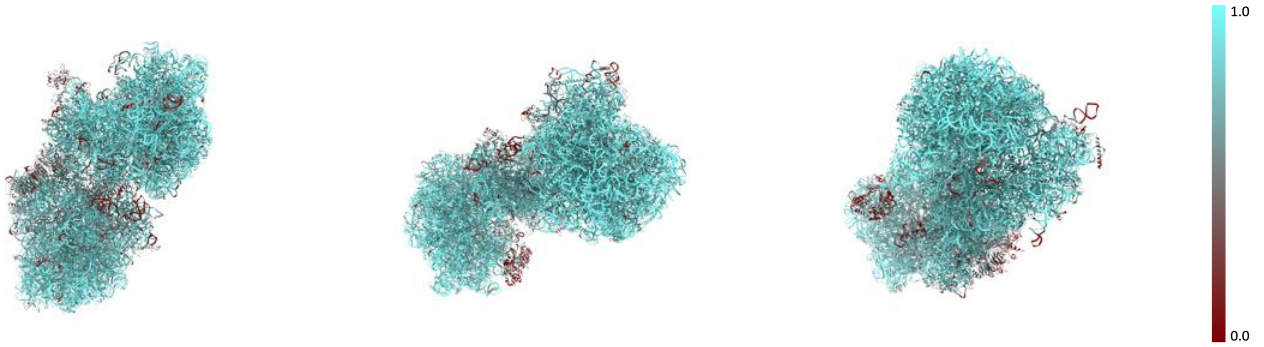
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

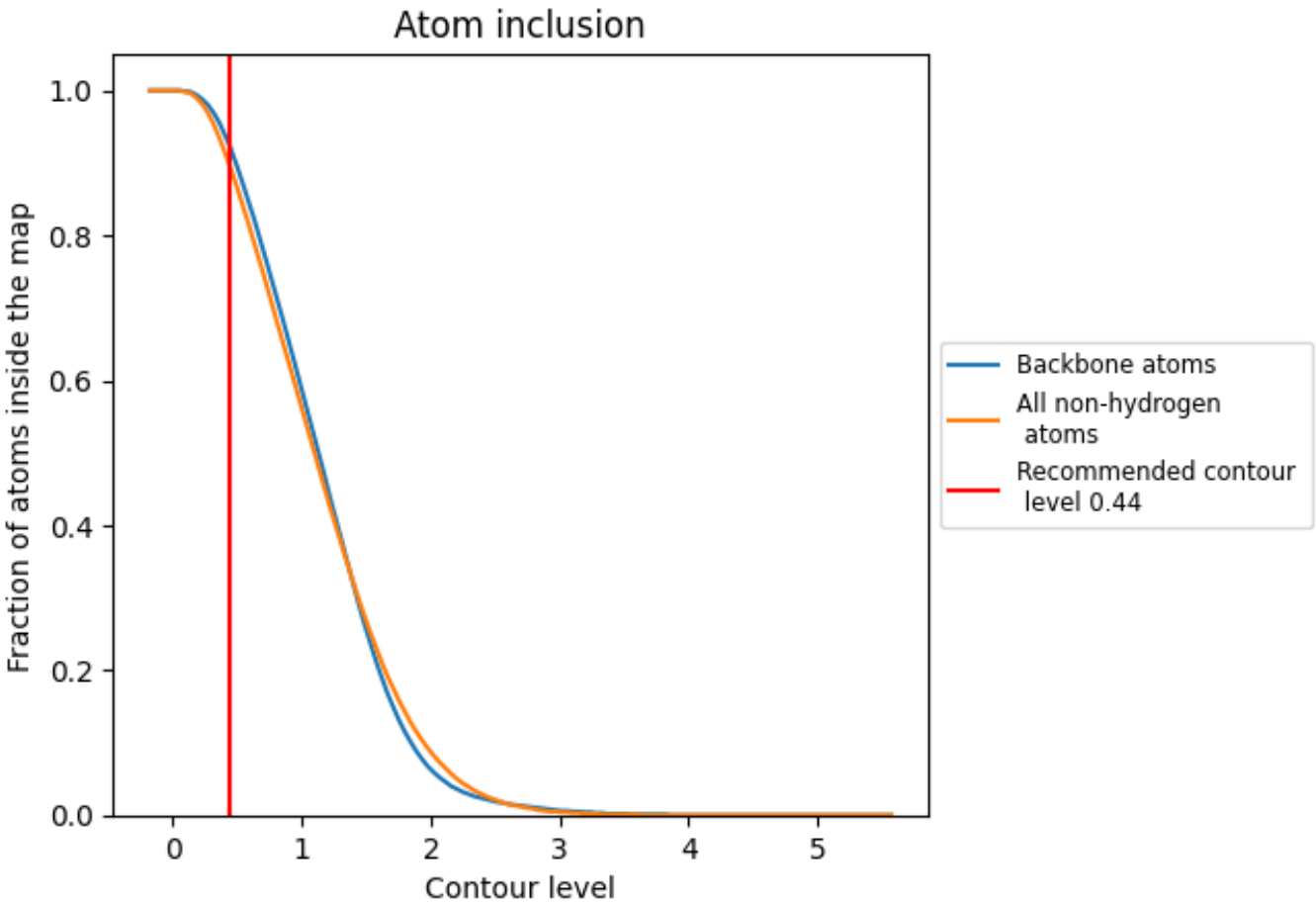
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.44).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.5400
CC	0.9590	0.5410
CM	0.7410	0.4200
CN	0.7350	0.4190
CP	0.9150	0.4080
DP	0.5840	0.3000
DQ	0.8320	0.3620
L1	0.9700	0.5780
L2	0.9780	0.6010
L3	0.9930	0.5740
LA	0.9190	0.5220
LB	0.9590	0.5860
LC	0.8560	0.5130
LD	0.9140	0.5420
LE	0.9100	0.5550
LF	0.8290	0.4730
LG	0.9210	0.5680
LH	0.9520	0.5560
LI	0.9930	0.6230
LJ	0.9680	0.5970
LK	0.9560	0.6060
LL	0.9770	0.5990
LM	0.8660	0.5520
LN	0.9530	0.5840
LO	0.9420	0.5750
La	0.9350	0.5950
Lb	0.9300	0.5960
Lc	0.9380	0.5810
Ld	0.9860	0.6140
Le	0.9280	0.5680
Lf	0.9810	0.6260
Lg	0.8830	0.5210
Lh	0.9940	0.6260
Li	0.8990	0.5420
Lj	0.9410	0.5710

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lk	0.9240	0.5810
Ll	0.9900	0.6200
Lm	0.9760	0.6100
Ln	0.9020	0.5650
Lo	0.8850	0.5570
Lp	0.9270	0.5400
Lq	0.9510	0.5940
Lr	0.9120	0.5500
Ls	0.9630	0.5870
Lt	0.9460	0.5670
Lu	0.7240	0.4730
Lv	0.8720	0.4970
Lw	0.9720	0.6150
Lx	0.9540	0.5890
Ly	0.9610	0.5870
Lz	0.8620	0.5020
M1	0.9580	0.5960
M2	0.9840	0.6280
M3	0.9940	0.6080
MA	0.9220	0.5750
MB	0.9640	0.6240
MC	0.8440	0.5670
MD	0.9230	0.5830
ME	0.9090	0.6030
MF	0.8270	0.5030
MG	0.9240	0.6000
MH	0.9540	0.5930
MI	0.9850	0.6600
MJ	0.9700	0.6290
MK	0.9760	0.6510
ML	0.9800	0.6360
MM	0.9040	0.5790
MN	0.9590	0.6190
MO	0.9550	0.6160
MP	0.0240	0.0980
MQ	0.1020	0.1700
Ma	0.9680	0.6250
Mb	0.9580	0.6300
Mc	0.9380	0.6180
Md	0.9430	0.5880
Me	0.9430	0.6070
Mf	0.9830	0.6400

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Mg	0.8660	0.5590
Mh	0.9980	0.6600
Mi	0.8950	0.5720
Mj	0.9420	0.5970
Mk	0.9050	0.6200
Ml	0.9850	0.6610
Mm	0.9710	0.6390
Mn	0.9110	0.5900
Mo	0.8510	0.5690
Mp	0.9430	0.5890
Mq	0.9690	0.6370
Mr	0.8870	0.5780
Ms	0.9710	0.6160
Mt	0.9530	0.6130
Mu	0.9430	0.6150
Mv	0.8810	0.5320
Mw	0.9590	0.6420
Mx	0.9650	0.6250
My	0.9650	0.6260
Mz	0.8580	0.5390
R1	0.8920	0.4830
RA	0.9260	0.5700
RB	0.7380	0.5050
RC	0.7070	0.4550
RD	0.9290	0.5460
RE	0.7990	0.4710
RF	0.3350	0.2440
RG	0.4030	0.3360
Ra	0.8030	0.4990
Rb	0.7870	0.5340
Rc	0.8760	0.5540
Rd	0.6730	0.4540
Re	0.7810	0.4810
Rf	0.6890	0.4390
Rg	0.7280	0.4120
Rh	0.6050	0.4160
Ri	0.8280	0.4570
Rj	0.7860	0.4660
Rk	0.6120	0.4190
Rl	0.8300	0.5010
Rm	0.1910	0.2300
Rn	0.8680	0.5280

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ro	0.8890	0.5600
Rp	0.6740	0.4390
Rq	0.7220	0.4430
Rr	0.6490	0.4220
Rs	0.7280	0.4570
Rt	0.7110	0.4360
Ru	0.6100	0.3840
Rv	0.8010	0.5210
Rw	0.9490	0.5810
Rx	0.9250	0.5650
Ry	0.7210	0.4250
Rz	0.5680	0.4300
S1	0.9150	0.5010
SA	0.9650	0.5730
SB	0.7570	0.4950
SC	0.8310	0.4860
SD	0.9240	0.5240
SE	0.7700	0.4520
SF	0.2870	0.2220
SG	0.5650	0.3430
Sa	0.8150	0.4860
Sb	0.7960	0.5110
Sc	0.9140	0.5480
Sd	0.7660	0.4560
Se	0.8940	0.5200
Sf	0.7810	0.4550
Sg	0.7910	0.4380
Sh	0.6500	0.4400
Si	0.9180	0.5520
Sj	0.8660	0.4920
Sk	0.6640	0.3720
Sl	0.9010	0.5640
Sm	0.2030	0.1860
Sn	0.8820	0.5440
So	0.9340	0.5440
Sp	0.6250	0.3830
Sq	0.8180	0.4670
Sr	0.7540	0.4590
Ss	0.7620	0.4140
St	0.7800	0.4090
Su	0.7060	0.4080
Sv	0.8320	0.5090

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sw	0.9560	0.5730
Sx	0.9320	0.5700
Sy	0.8290	0.4550
Sz	0.5950	0.3370