Full wwPDB EM Validation Report ⓘ

Nov 11, 2023 – 11:15 pm GMT

PDB ID	:	7ZJW
EMDB ID	:	EMD-14751
Title	:	Rabbit 80S ribosome as it decodes the Sec-UGA codon
Authors	:	Hilal, T.; Simonovic, M.; Spahn, C.M.T.
Deposited on	:	2022-04-12
Resolution	:	2.80 Å(reported)
Based on initial model	:	7O7Y

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

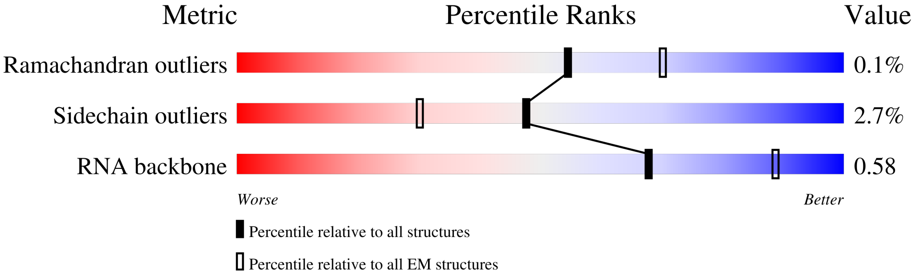
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

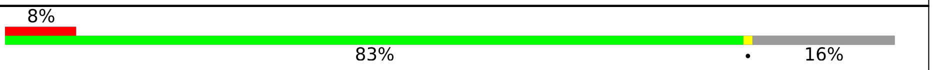
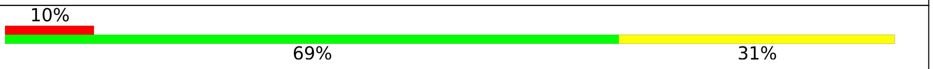
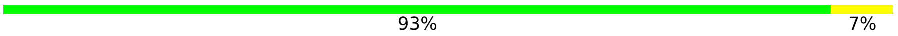
The reported resolution of this entry is 2.80 Å.

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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	E	616	
2	F	90	
3	I	1072	
4	S	855	
5	B	854	
6	L5	4808	
7	L7	119	
8	L8	158	

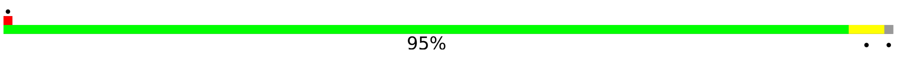
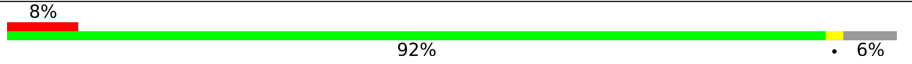
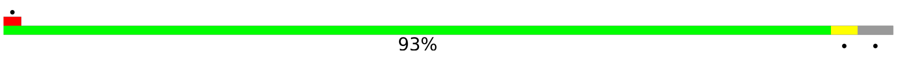
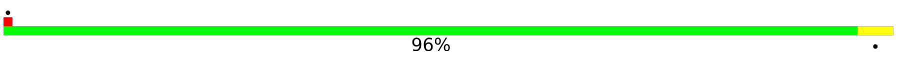
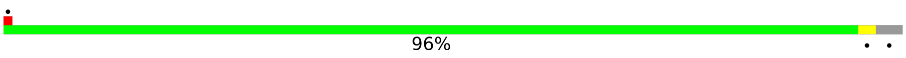
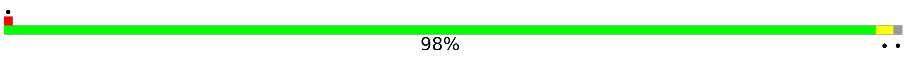
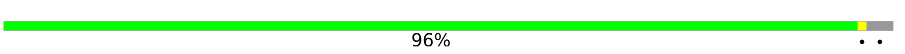
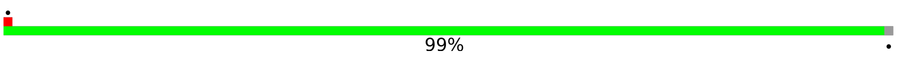
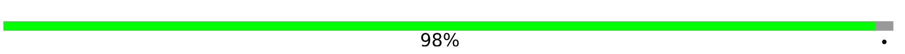
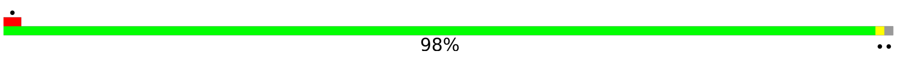
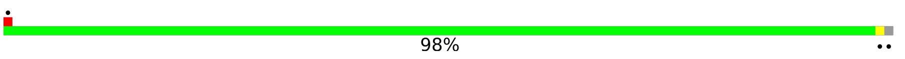
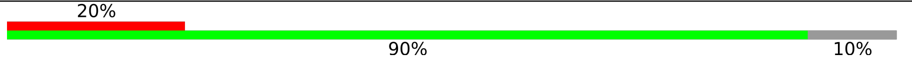
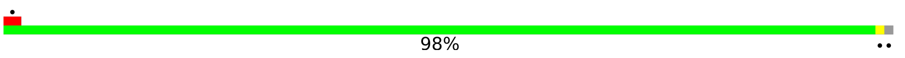
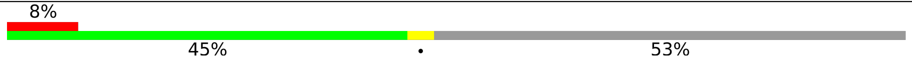
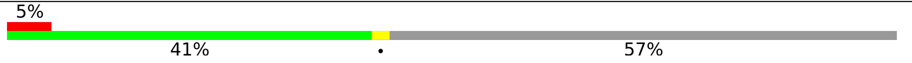
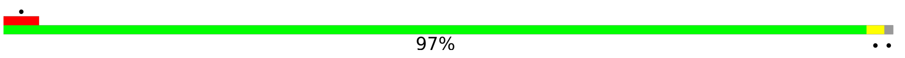
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	LD	257	• 97% • •
10	LE	403	96% • •
11	LF	413	86% • 12%
12	LG	297	97% • •
13	LH	291	• 78% • 20%
14	LI	247	89% • 9%
15	LJ	266	• 85% • 12%
16	LK	192	• 98% ••
17	LL	214	5% 95% 5%
18	LM	178	92% • •
19	LO	211	• 98% •
20	LP	218	• 62% • 37%
21	LQ	204	99% •
22	LR	203	97% • •
23	LS	184	• 85% • 14%
24	LT	188	98% ••
25	LU	196	• 87% 5% 8%
26	LV	176	98% •
27	LW	160	• 96% • •
28	LX	128	77% 23%
29	LY	140	5% 99% ••
30	LZ	157	• 58% • 41%
31	La	156	• 74% • 24%
32	Lb	145	• 90% • 8%
33	Lc	136	99% ••

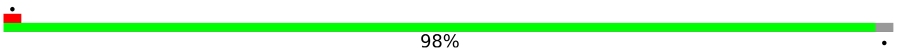
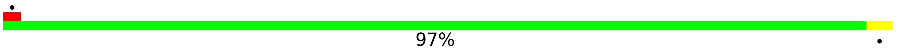
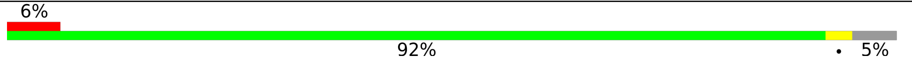
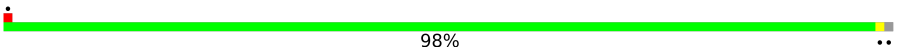
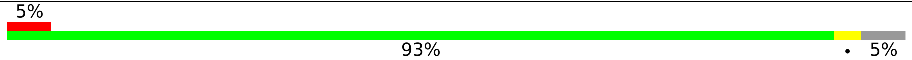
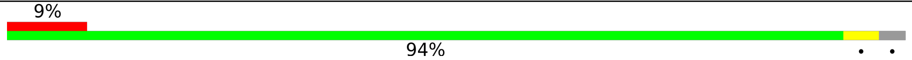
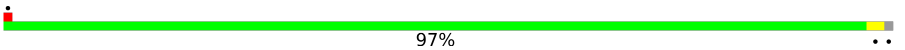
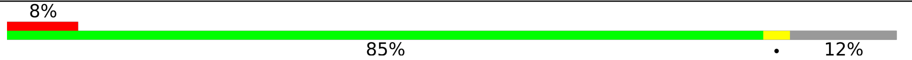
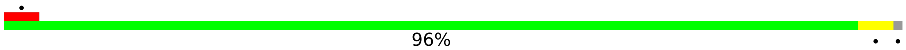
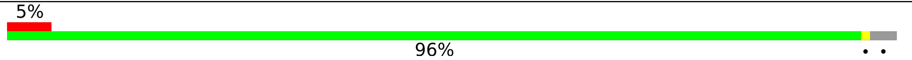
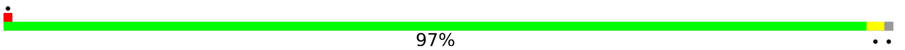
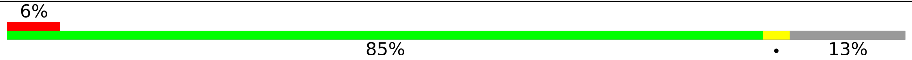
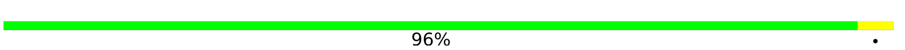
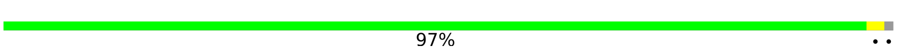
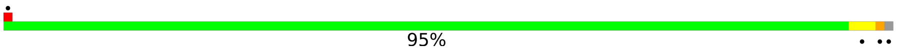
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	Ld	148	
35	Le	245	
36	Lf	115	
37	Lg	125	
38	Lh	135	
39	Li	110	
40	Lj	117	
41	Lk	123	
42	Ll	105	
43	Lm	97	
44	Ln	70	
45	Lo	51	
46	Lp	128	
47	Lq	106	
48	Lr	92	
49	Ls	137	
50	Lt	318	
51	Lx	217	
52	S2	1870	
53	SB	84	
54	SC	69	
55	SD	156	
56	SE	133	
57	SF	115	
58	SG	317	

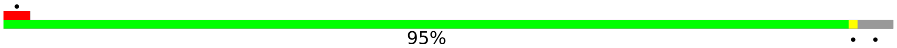
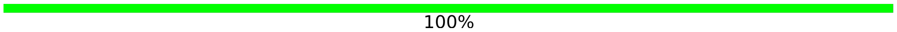
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	SH	56	
60	SL	295	
61	SM	264	
62	SN	293	
63	SO	281	
64	SP	263	
65	SQ	204	
66	SR	249	
67	SS	432	
68	ST	208	
69	SU	194	
70	SV	165	
71	SW	158	
72	SX	132	
73	SY	151	
74	SZ	151	
75	Sa	145	
76	Sb	172	
77	Sc	135	
78	Sd	152	
79	Se	145	
80	Sf	119	
81	Sg	83	
82	Sh	130	
83	Si	143	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
84	Sj	130	
85	Sk	124	
86	Sl	25	

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 230266 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 eEFSec.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	519	Total 3335	C 2110	N 616	O 599	S 10	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	initiating methionine	UNP P57772
E	-18	GLY	-	expression tag	UNP P57772
E	-17	SER	-	expression tag	UNP P57772
E	-16	SER	-	expression tag	UNP P57772
E	-15	HIS	-	expression tag	UNP P57772
E	-14	HIS	-	expression tag	UNP P57772
E	-13	HIS	-	expression tag	UNP P57772
E	-12	HIS	-	expression tag	UNP P57772
E	-11	HIS	-	expression tag	UNP P57772
E	-10	HIS	-	expression tag	UNP P57772
E	-9	SER	-	expression tag	UNP P57772
E	-8	SER	-	expression tag	UNP P57772
E	-7	GLY	-	expression tag	UNP P57772
E	-6	LEU	-	expression tag	UNP P57772
E	-5	VAL	-	expression tag	UNP P57772
E	-4	PRO	-	expression tag	UNP P57772
E	-3	ARG	-	expression tag	UNP P57772
E	-2	GLY	-	expression tag	UNP P57772
E	-1	SER	-	expression tag	UNP P57772
E	0	HIS	-	expression tag	UNP P57772
E	409	GLU	GLN	conflict	UNP P57772

- Molecule 2 is a RNA chain called human Ser-tRNA-Sec.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	90	Total 1914	C 853	N 334	O 637	P 90	0	0

- Molecule 3 is a RNA chain called CrPV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	I	183	3882	1739	675	1285	183	0	0

- Molecule 4 is a RNA chain called GPX4 SECIS element.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	S	46	983	438	179	320	46	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1118	U	C	conflict	GB 25123295
S	1126	A	C	conflict	GB 25123295
S	1132	A	U	conflict	GB 25123295
S	1133	G	-	insertion	GB 25123295
S	1134	C	-	insertion	GB 25123295
S	1135	C	-	insertion	GB 25123295
S	1136	C	-	insertion	GB 25123295
S	1150	U	A	conflict	GB 25123295

- Molecule 5 is a protein called SECIS Binding Protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	204	1379	881	257	238	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	687	ARG	LYS	conflict	UNP Q96T21
B	692	ILE	VAL	conflict	UNP Q96T21

- Molecule 6 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	L5	3764	80771	36002	14762	26243	3764	0	0

- Molecule 7 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	L7	119	2538	1131	451	837	119	0	0

- Molecule 8 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	L8	156	3319	1481	585	1097	156	0	0

- Molecule 9 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LD	253	1939	1214	396	323	6	0	0

- Molecule 10 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LE	398	3206	2042	605	546	13	0	0

- Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LF	362	2886	1814	577	481	14	0	0

- Molecule 12 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LG	294	2398	1516	439	429	14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LG	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 13 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LH	232	1859	1197	354	305	3	0	0

- Molecule 14 is a protein called 60S ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LI	226	1886	1211	362	304	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	182	ASN	GLY	conflict	UNP A0A7J8C453
LI	199	HIS	ARG	conflict	UNP A0A7J8C453

- Molecule 15 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LJ	233	1877	1197	361	315	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LJ	184	LEU	ILE	conflict	UNP P62424

- Molecule 16 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LK	190	1516	954	284	272	6	0	0

- Molecule 17 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LL	213	1717	1086	332	285	14	0	0

- Molecule 18 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LM	170	1362	861	254	241	6	0	0

- Molecule 19 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LO	210	1702	1065	354	279	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LO	74	ARG	HIS	conflict	UNP G1TKB3
LO	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 20 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LP	138	1137	727	221	182	7	0	0

- Molecule 21 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LQ	203	1701	1072	359	266	4	0	0

- Molecule 22 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	LR	199	1630	1051	319	255	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LR	174	LEU	ILE	conflict	UNP A0A0N8ETI8
LR	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 23 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LS	159	1288	808	249	222	9	0	0

- Molecule 24 is a protein called 60S ribosomal Protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LT	187	1515	946	315	250	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LT	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 25 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LU	180	1508	933	328	238	9	0	0

- Molecule 26 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LV	176	1457	924	288	234	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LV	36	ASN	ILE	conflict	UNP A0A1Z5LHJ5

- Molecule 27 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LW	159	1298	823	252	217	6	0	0

- Molecule 28 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LX	99	806	516	141	147	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LX	60	ALA	VAL	conflict	UNP Q4R5I3

- Molecule 29 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LY	139	1034	648	199	182	5	0	0

- Molecule 30 is a protein called 60S ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LZ	93	766	480	153	129	4	0	0

- Molecule 31 is a protein called 60S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	La	118	967	618	181	167	1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Lb	134	1115	700	226	186	3	0	0

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Lc	135	1107	714	208	182	3	0	0

- Molecule 34 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Ld	147	1162	734	239	185	4	0	0

- Molecule 35 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 36 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 37 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lg	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 38 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lh	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 39 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Li	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 40 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lj	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 41 is a protein called 60S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lk	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 42 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Ll	102	830	520	176	129	5	0	0

- Molecule 43 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Lm	86	705	434	155	111	5	0	0

- Molecule 44 is a protein called 60S ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Ln	69	569	366	103	99	1	0	0

- Molecule 45 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Lo	50	447	286	96	64	1	0	0

- Molecule 46 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Lp	52	431	269	90	66	6	0	0

- Molecule 47 is a protein called 60S ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Lq	105	863	543	175	139	6	0	0

- Molecule 48 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Lr	91	708	445	136	120	7	0	0

- Molecule 49 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Ls	126	1014	629	209	170	6	0	0

- Molecule 50 is a protein called 60S ribosomal protein P0.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	Lt	115	567	337	115	115	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lt	106	LEU	LYS	conflict	UNP G1SPK4

- Molecule 51 is a protein called 60S ribosomal protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	Lx	196	972	580	196	196	0	0

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	S2	1770	37825	16906	6780	12369	1770	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	251	C	U	conflict	GB 37956930
S2	583	U	C	conflict	GB 37956930
S2	584	A	C	conflict	GB 37956930
S2	585	A	G	conflict	GB 37956930
S2	1338	4AC	C	conflict	GB 37956930
S2	1843	4AC	C	conflict	GB 37956930

- Molecule 53 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	SB	83	651	408	121	115	7	0	0

- Molecule 54 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	SC	63	495	302	98	93	2	0	0

- Molecule 55 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	SD	74	610	385	117	101	7	0	0

- Molecule 56 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	SE	57	457	282	101	73	1	0	0

- Molecule 57 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	SF	101	814	507	170	132	5	0	0

- Molecule 58 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	SG	313	2436	1535	424	465	12	0	0

- Molecule 59 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	SH	55	459	286	94	74	5	0	0

- Molecule 60 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	SL	221	1743	1107	305	323	8	0	0

- Molecule 61 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	SM	224	1815	1152	328	321	14	0	0

- Molecule 62 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	SN	220	1706	1105	292	300	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SN	33	ILE	VAL	conflict	UNP O18789
SN	101	ALA	SER	conflict	UNP O18789

- Molecule 63 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	SO	225	1751	1116	315	313	7	0	0

- Molecule 64 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	SP	262	2076	1324	386	358	8	0	0

- Molecule 65 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	SQ	191	1509	943	286	273	7	0	0

- Molecule 66 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	SR	237	1923	1200	387	329	7	0	0

- Molecule 67 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SS	190	Total 1529	C 975	N 281	O 272	S 1	0	0

- Molecule 68 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	ST	206	Total 1686	C 1058	N 332	O 291	S 5	0	0

- Molecule 69 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SU	185	Total 1525	C 969	N 306	O 248	S 2	0	0

- Molecule 70 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SV	96	Total 810	C 530	N 143	O 131	S 6	0	0

- Molecule 71 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SW	154	Total 1262	C 804	N 236	O 216	S 6	0	0

- Molecule 72 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SX	124	Total 958	C 600	N 170	O 179	S 9	0	0

- Molecule 73 is a protein called 40S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SY	150	Total 1208	C 773	N 229	O 205	S 1	0	0

- Molecule 74 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	SZ	136	1016	621	199	190	6	0	0

- Molecule 75 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	Sa	128	1048	665	197	179	7	0	0

- Molecule 76 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	Sb	141	1124	715	212	194	3	0	0

- Molecule 77 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Sc	134	1080	678	201	197	4	0	0

- Molecule 78 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	Sd	148	1217	763	245	208	1	0	0

- Molecule 79 is a protein called 40S Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Se	143	1113	698	214	198	3	0	0

- Molecule 80 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	Sf	104	821	514	155	148	4	0	0

- Molecule 81 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	Sg	83	640	394	117	124	5	0	0

- Molecule 82 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	Sh	129	1034	659	193	176	6	0	0

- Molecule 83 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	Si	141	1099	693	219	184	3	0	0

- Molecule 84 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Sj	125	1015	642	199	169	5	0	0

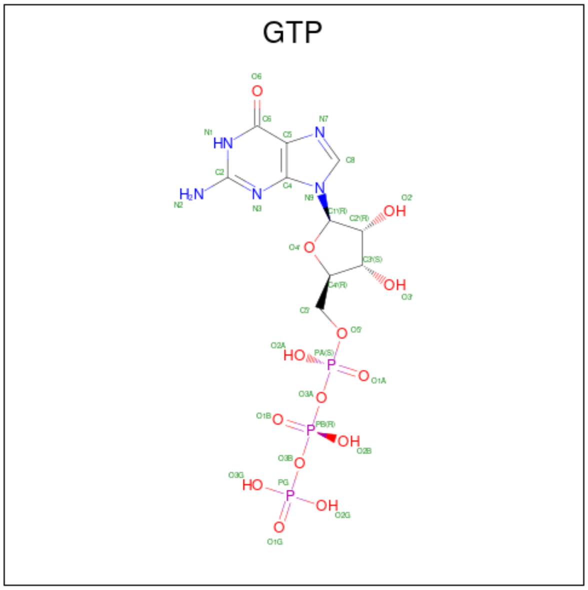
- Molecule 85 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Sk	75	598	382	111	104	1	0	0

- Molecule 86 is a protein called 60S ribosomal protein L41.

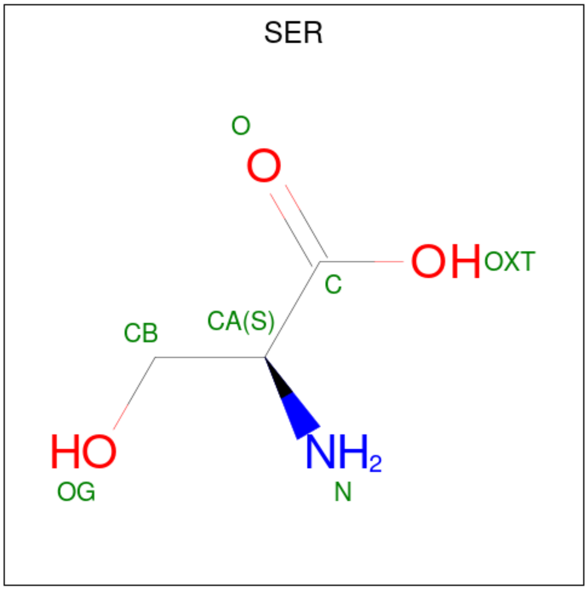
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Sl	25	239	145	64	27	3	0	0

- Molecule 87 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
87	E	1	Total 32	C 10	N 5	O 14	P 3	0
87	L7	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 88 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				AltConf
88	F	1	Total 6	C 3	N 1	O 2	0

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
89	I	2	Total Mg 2 2	0
89	L5	162	Total Mg 162 162	0
89	L7	2	Total Mg 2 2	0
89	L8	1	Total Mg 1 1	0
89	LD	1	Total Mg 1 1	0
89	LS	1	Total Mg 1 1	0
89	LY	1	Total Mg 1 1	0
89	S2	55	Total Mg 55 55	0

- Molecule 90 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
90	L5	17	Total K 17 17	0
90	S2	1	Total K 1 1	0

- Molecule 91 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
91	Lj	1	Total Zn 1 1	0
91	Lm	1	Total Zn 1 1	0
91	Lp	1	Total Zn 1 1	0
91	Lq	1	Total Zn 1 1	0
91	Lr	1	Total Zn 1 1	0
91	SD	1	Total Zn 1 1	0
91	SF	2	Total Zn 2 2	0
91	SH	1	Total Zn 1 1	0

- Molecule 92 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
92	SZ	1	Total Na 1 1	0

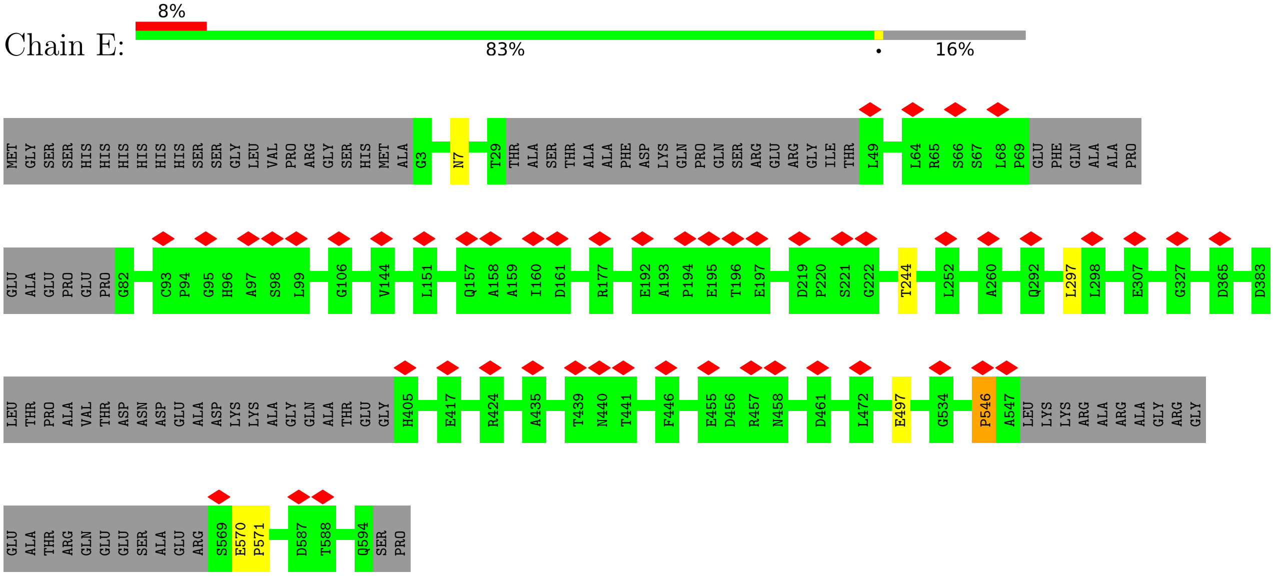
- Molecule 93 is water.

Mol	Chain	Residues	Atoms	AltConf
93	L5	56	Total O 56 56	0
93	L7	1	Total O 1 1	0
93	L8	1	Total O 1 1	0
93	LD	1	Total O 1 1	0
93	LE	1	Total O 1 1	0
93	LH	1	Total O 1 1	0
93	LK	1	Total O 1 1	0
93	LL	1	Total O 1 1	0
93	LQ	1	Total O 1 1	0
93	LV	1	Total O 1 1	0
93	Ld	1	Total O 1 1	0
93	S2	34	Total O 34 34	0
93	SF	1	Total O 1 1	0
93	SH	1	Total O 1 1	0
93	SW	1	Total O 1 1	0
93	Sd	1	Total O 1 1	0
93	Se	1	Total O 1 1	0
93	Si	2	Total O 2 2	0

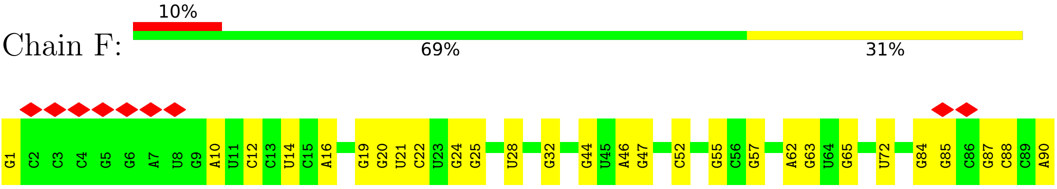
3 Residue-property plots

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.

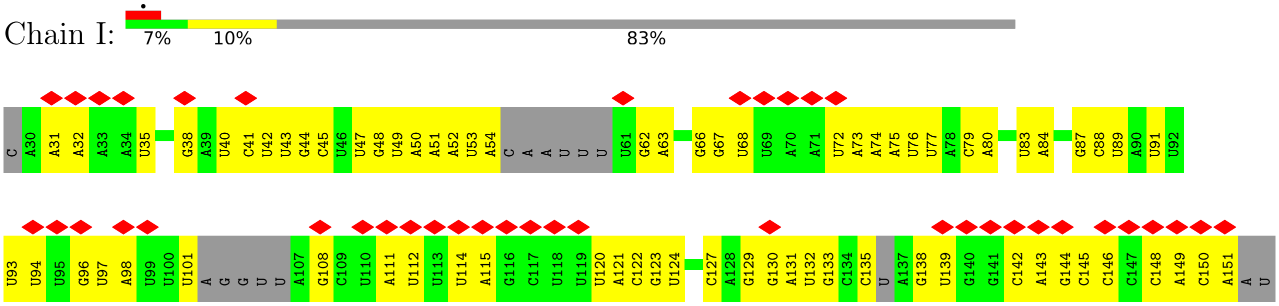
- Molecule 1: eEFSec

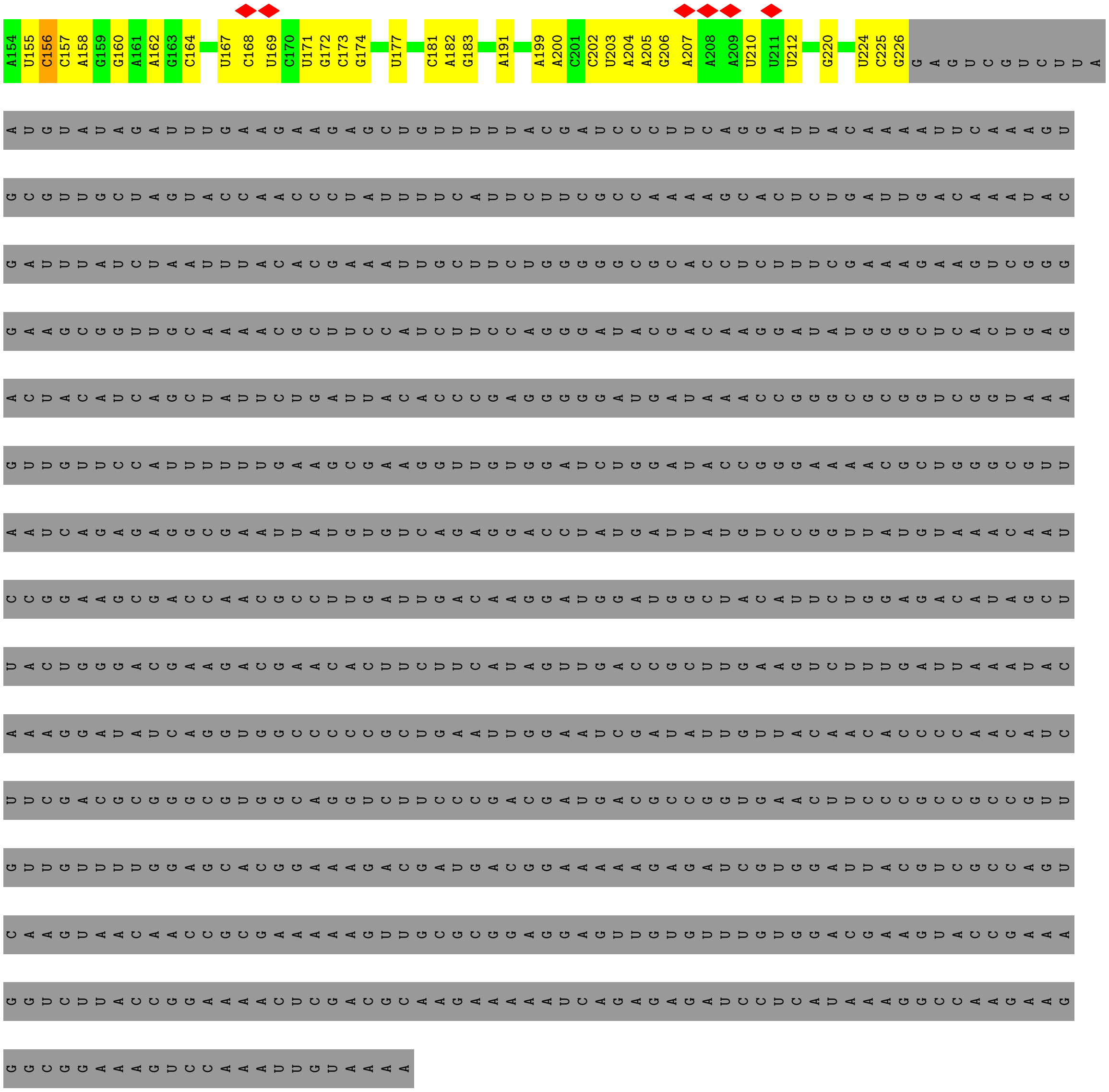


- Molecule 2: human Ser-tRNA-Sec

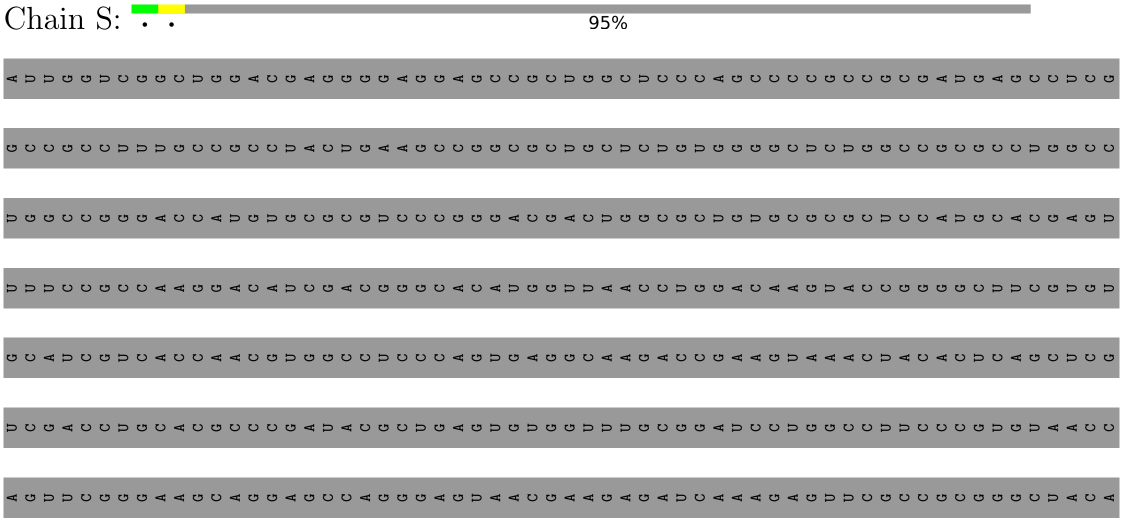


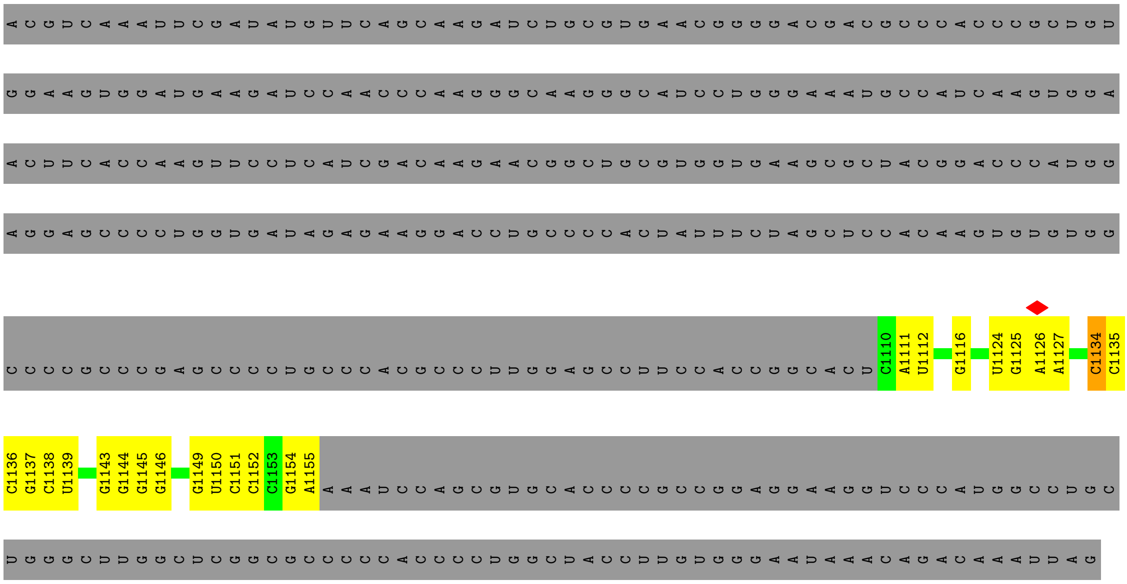
- Molecule 3: CrPV IRES





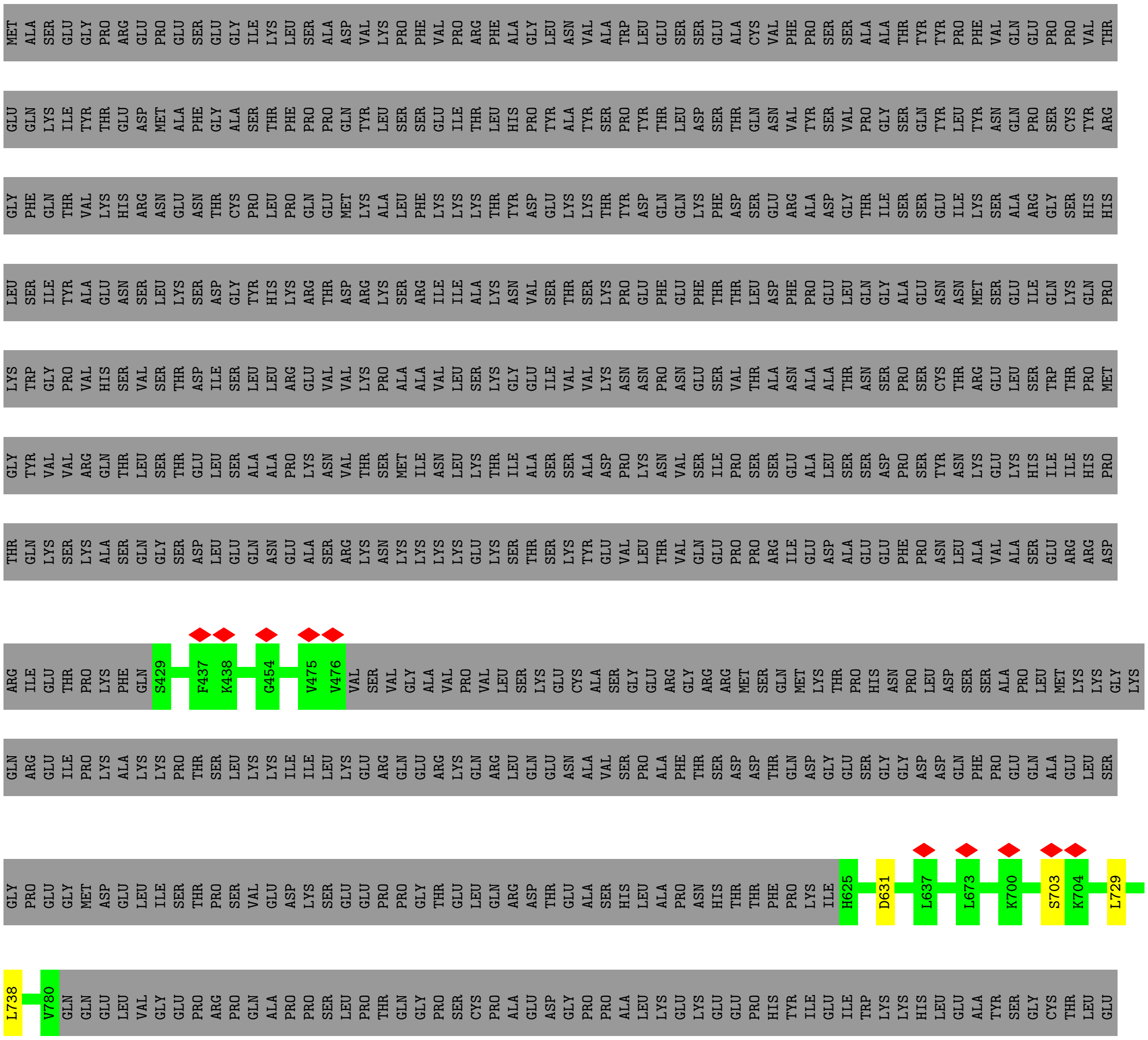
- Molecule 4: GPX4 SECIS element



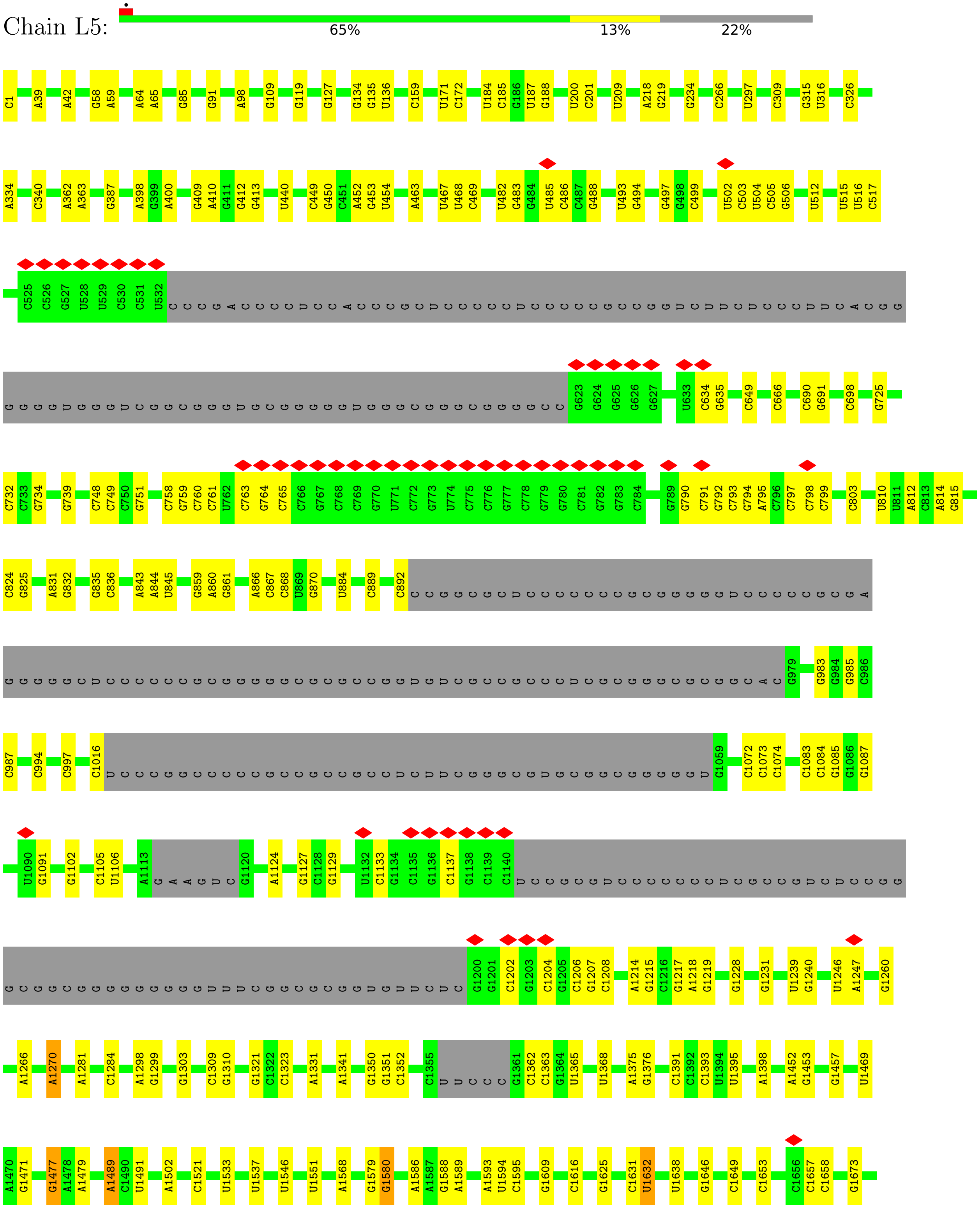


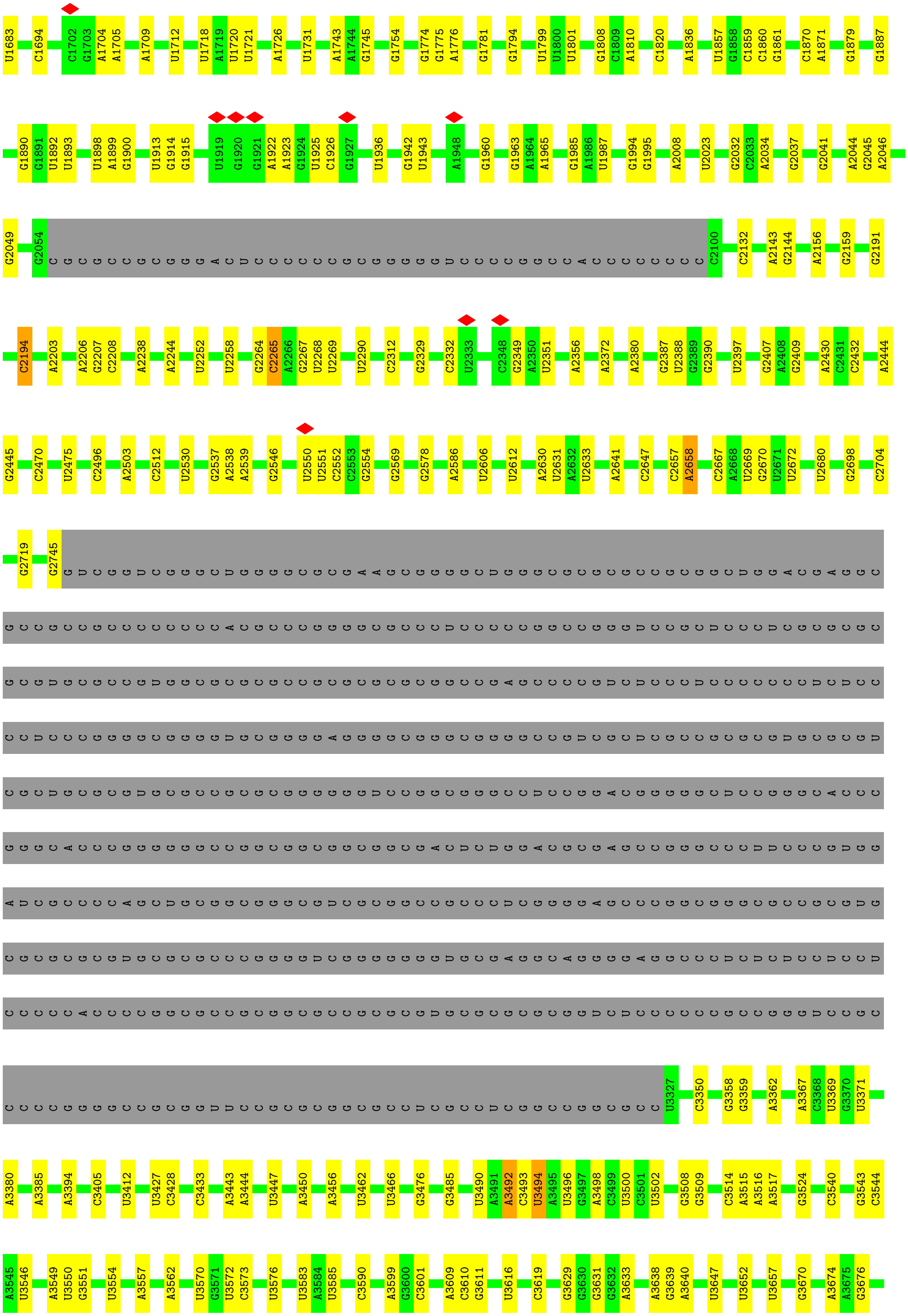
- Molecule 5: SECIS Binding Protein 2

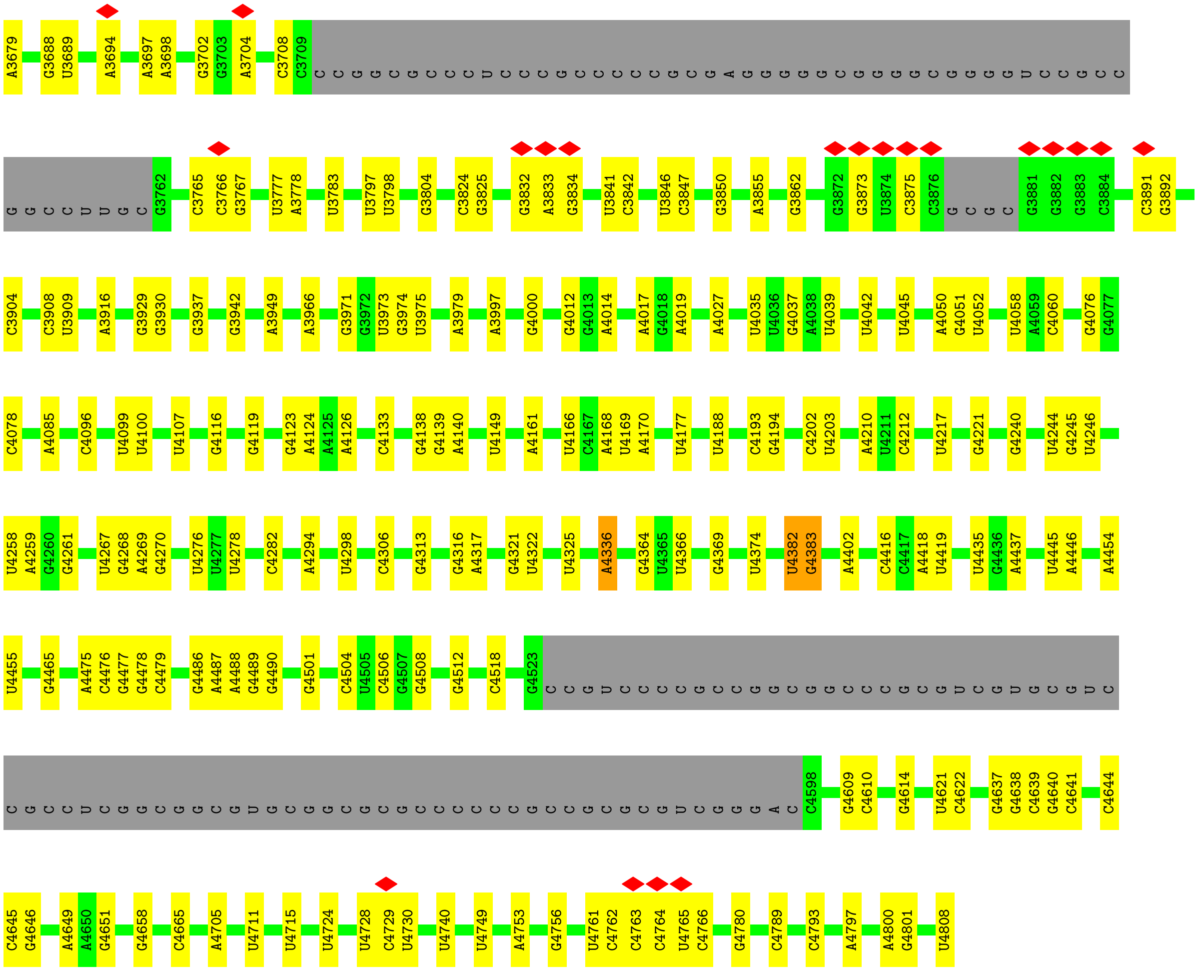
Chain B:



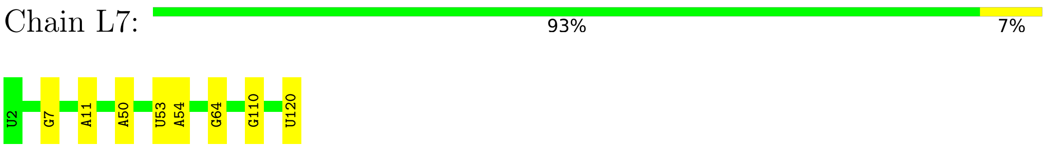
- Molecule 6: 28S rRNA



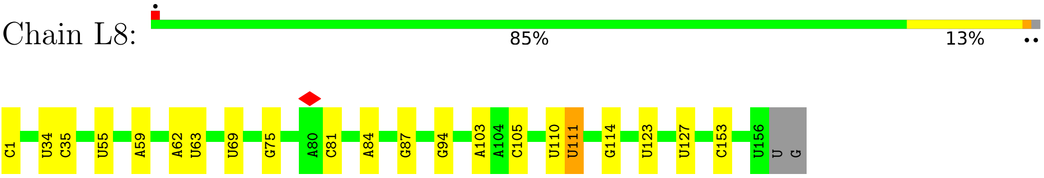

U1683 C1694 C1702 G1703 A1704 A1705 A1709 U1712 U1718 A1719 U1720 U1721 A1726 U1731 A1743 A1744 G1745 G1754 G1774 G1775 A1776 G1781 G1794 U1799 U1800 U1801 G1808 C1809 A1810 C1820 A1836 U1857 G1858 C1859 C1860 G1861 C1870 A1871 G1879 G1887
G1890 G1891 U1892 U1893 U1898 A1899 G1900 U1913 G1914 G1915 U1919 G1920 G1921 A1922 A1923 G1924 U1925 C1926 G1927 U1936 G1942 U1943 A1948 G1960 G1963 A1964 A1965 G1985 A1986 U1987 G1994 G1995 A2008 U2023 G2032 C2033 A2034 G2037 G2041 A2044 G2045 A2046
G2049 G2054 C G C G C C C G C G G G A C U C C C C C C G C G G G G G U C C C C G G G C C A C C C C C C C C C C2100 C2132 A2143 G2144 A2156 G2159 G2191
C2194 A2203 A2206 G2207 C2208 A2238 A2244 U2252 U2258 G2264 C2265 A2266 G2267 U2268 U2269 U2290 C2312 G2329 C2332 U2333 C2348 G2349 A2350 U2351 A2356 A2372 A2380 G2387 U2388 G2389 G2390 U2397 G2407 A2408 G2409 A2430 C2431 C2432 A2444
G2445 C2470 U2475 C2496 A2503 C2512 U2530 G2537 A2538 A2539 G2546 U2550 U2551 C2552 C2553 G2554 G2569 G2578 A2586 U2606 U2612 A2630 U2631 A2632 U2633 A2641 C2647 C2657 A2658 C2667 A2668 U2669 G2670 U2671 U2672 U2680 G2698 C2704
G2719 G2745 G U C G G U C G G G C U G G G G C G C G A A G C G G G G C U G G G C G C G C G C C G C G G C U G G A C G A G G C
G C C G C C G C C C C C C C A C G C C C C G G G G C G C C C U C C C C C G G C C G G G U C C G C U C C C U C G C G G C
G C G U G C G C C G U G G C G C G C G C C G C G C G C G C G C G G C C C G A G C C C C G U C U C C C U C C C C C C C U C U C C
C C U C C C G G G C G G G G U G C G G G G A G G G G C G G G G C G G G G C C G U C G G C U C G C C C G C C G C G G U C C G G U
C G C U G C G C G U G C G C C C G C C G C C G G G G G G U C C G G G C G G G C C U C C G G G A C G G G G C U C C G G G G C A C C C
G G G C A C C C G G G G G G C C G C C G C G G C G C C G G C C G G A C U C U G G A C G C G A G C C G G G G C C C U U C C C G U G G
A U C G C C C C A G C C U G G C G G C G C C G U C C G C G G C C C G C C C U C G G G G A G C C C G G G G G C C G C C G C G U G
C G C G C G C G U G C G C C G C C C G G G G G U C G G G G G G U G C C G A G G C A G G G G A G G C C C U C U C U C C U C C U
C C C C C A C C C G G C G C C C C G G C G C G G G U G C C G C C G C C G C C G G U C U C C C C C C G C C C G G G G U C C G G C
C C C G G G G G C C C G C C G G U U C C G G G C G G C G C C C U C G C C U C G G C C C G G C G C C C U3327 C3350 G3358 G3359 A3362 A3367 C3368 U3369 G3370 U3371
A3380 A3385 A3394 C3405 U3412 U3427 C3428 G3433 A3443 A3444 U3447 A3450 A3456 U3462 U3466 G3476 G3485 U3490 A3491 A3492 C3493 U3494 A3495 U3496 G3497 A3498 G3499 U3500 C3501 U3502 G3508 G3509 C3514 A3515 A3516 A3517 G3524 C3540 G3543 C3544
A3545 U3546 A3549 U3550 G3551 U3554 A3557 A3562 U3570 G3571 U3572 C3573 U3576 U3583 A3584 U3585 C3590 A3599 G3600 C3601 A3609 C3610 G3611 U3616 C3619 G3629 G3630 G3631 G3632 A3633 A3638 G3639 A3640 U3647 U3652 U3657 G3670 A3674 A3675 G3676



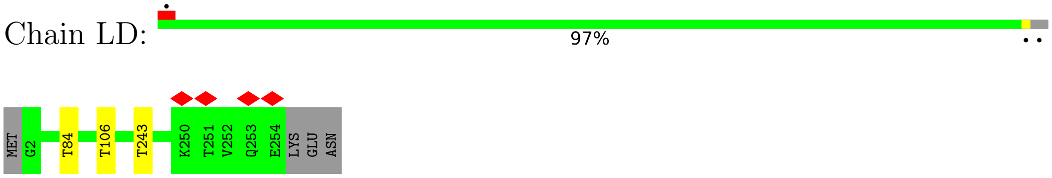
- Molecule 7: 5S rRNA



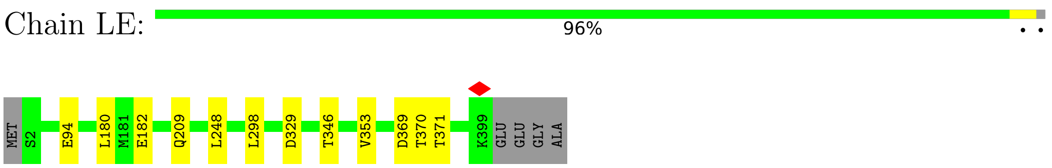
- Molecule 8: 5.8S rRNA



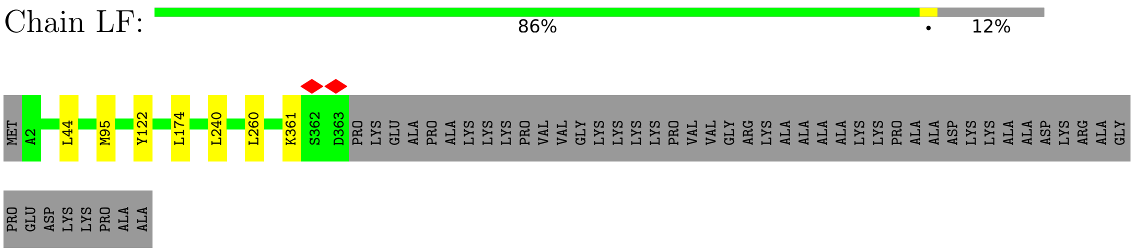
- Molecule 9: 60S ribosomal protein uL2



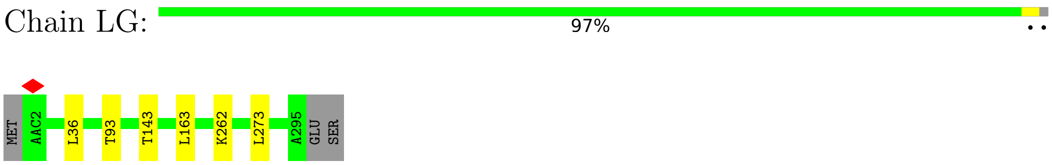
- Molecule 10: 60S ribosomal protein L3



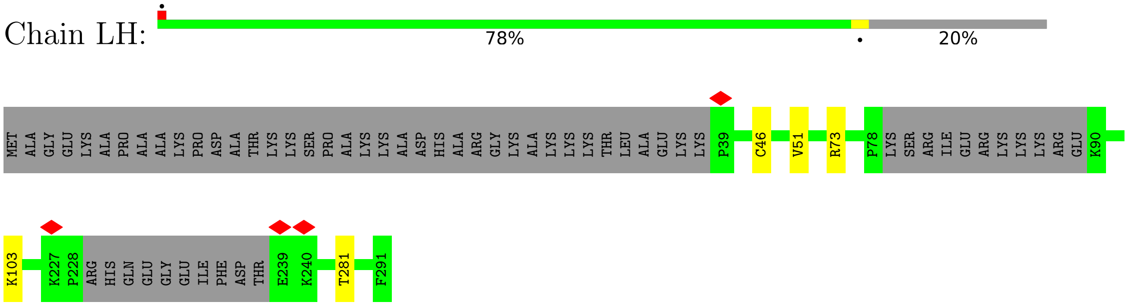
- Molecule 11: 60S ribosomal protein L4



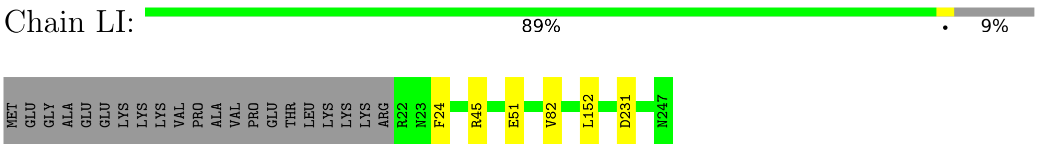
- Molecule 12: Ribosomal_L18_c domain-containing protein



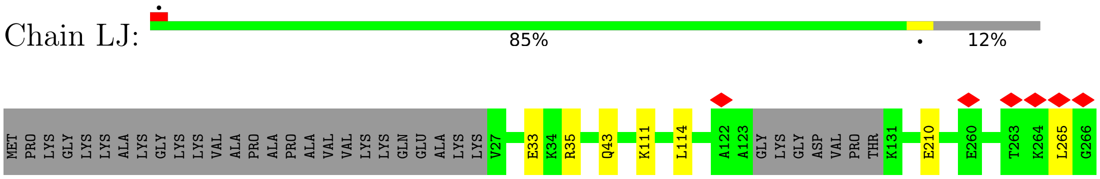
- Molecule 13: 60S ribosomal protein L6



- Molecule 14: 60S ribosomal Protein uL30

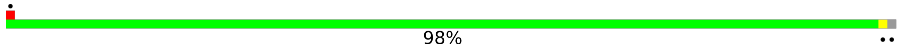


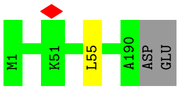
- Molecule 15: 60S ribosomal protein eL8



- Molecule 16: 60S ribosomal protein L9

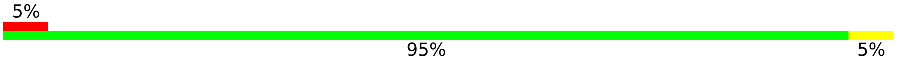
Chain LK:

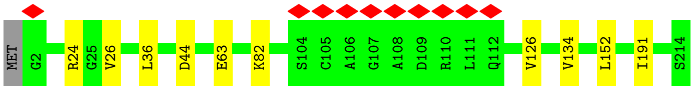




- Molecule 17: 60S ribosomal protein L10

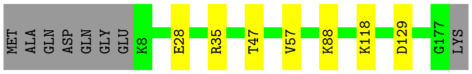
Chain LL:





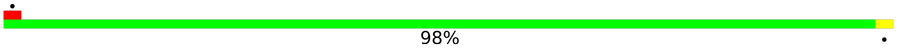
- Molecule 18: 60S ribosomal protein L11

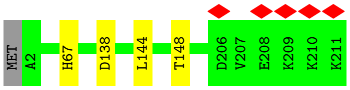
Chain LM:



- Molecule 19: 60S ribosomal protein eL13

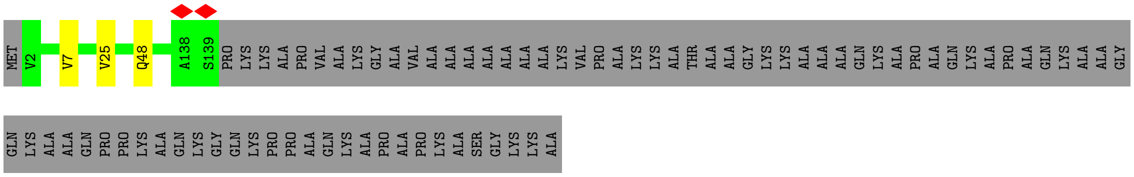
Chain LO:





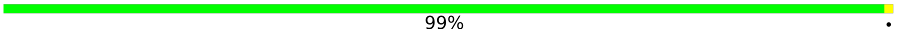
- Molecule 20: 60S ribosomal protein L14

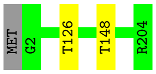
Chain LP:



- Molecule 21: 60S ribosomal protein L15

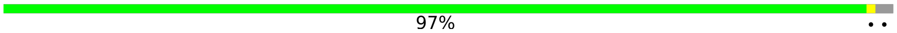
Chain LQ:

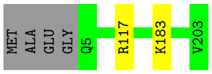




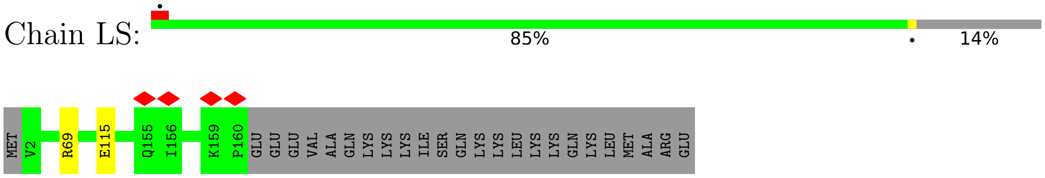
- Molecule 22: 60S ribosomal protein uL13

Chain LR:

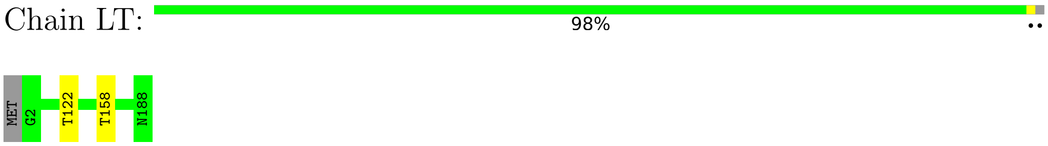




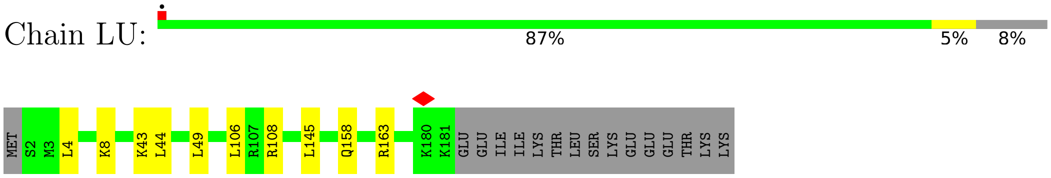
- Molecule 23: 60S ribosomal protein uL22



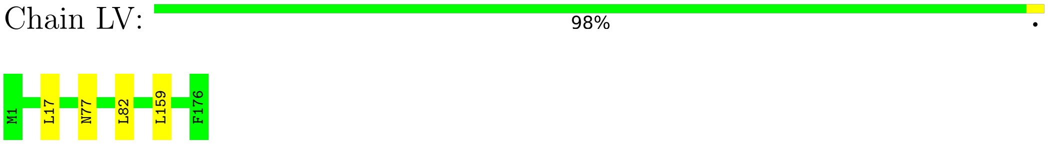
- Molecule 24: 60S ribosomal Protein eL18



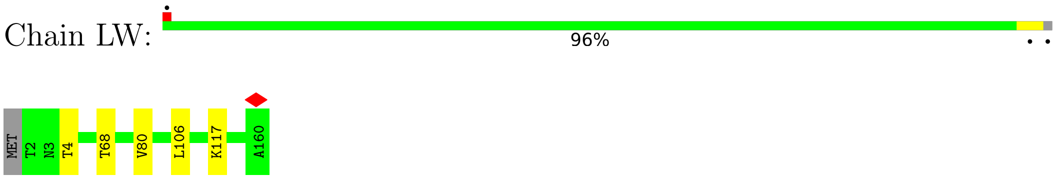
- Molecule 25: 60S ribosomal protein L19



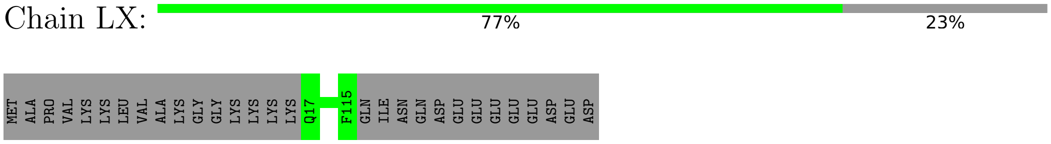
- Molecule 26: 60S ribosomal protein eL20



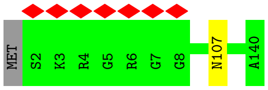
- Molecule 27: 60S ribosomal protein eL21



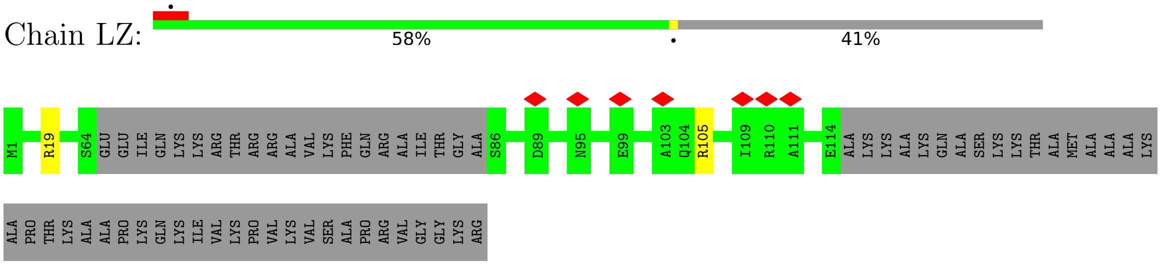
- Molecule 28: 60S ribosomal protein eL22



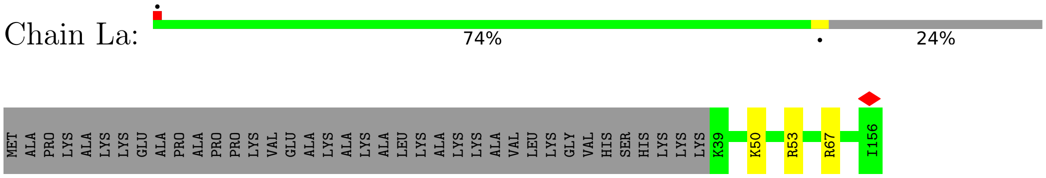
- Molecule 29: 60S ribosomal protein L23



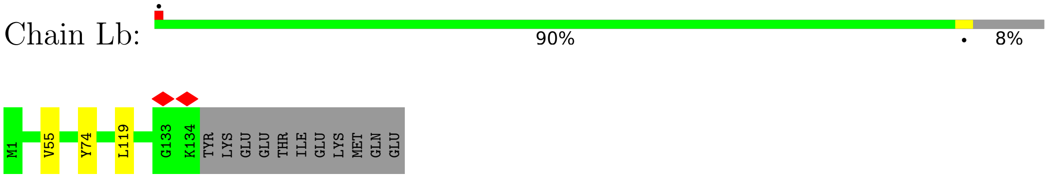
- Molecule 30: 60S ribosomal protein eL24



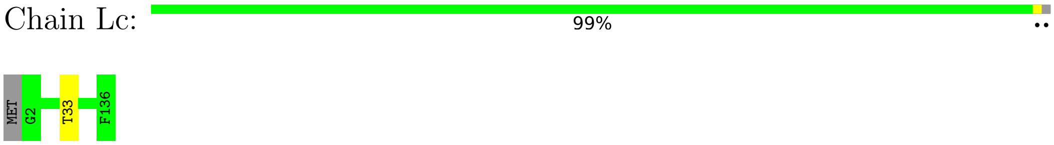
- Molecule 31: 60S ribosomal protein uL23



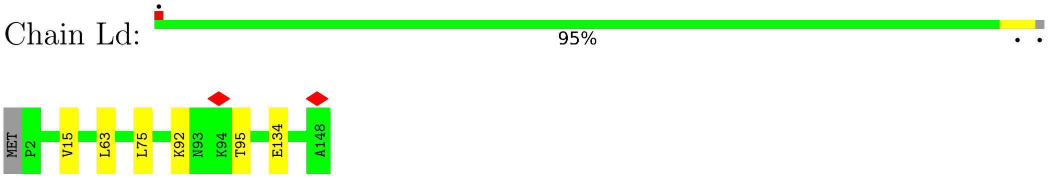
- Molecule 32: 60S ribosomal protein L26



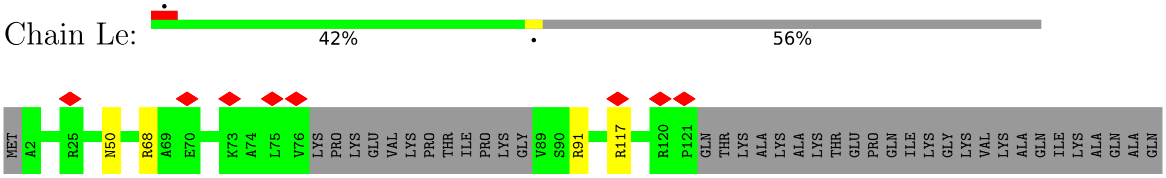
- Molecule 33: 60S ribosomal protein L27

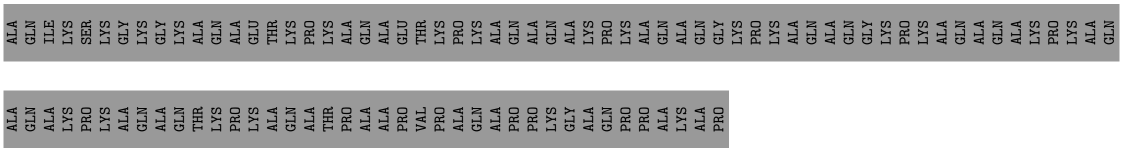


- Molecule 34: 60S ribosomal protein L27a



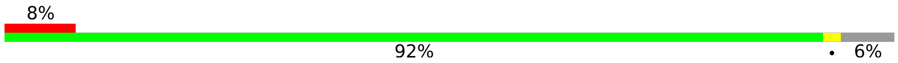
- Molecule 35: 60S ribosomal protein L29

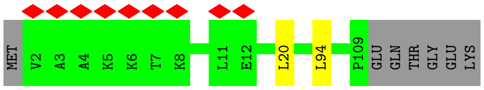




- Molecule 36: 60S ribosomal protein eL30

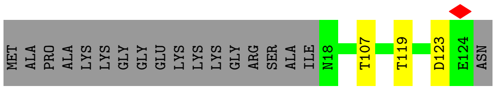
Chain Lf:





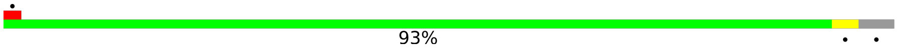
- Molecule 37: 60S ribosomal protein eL31

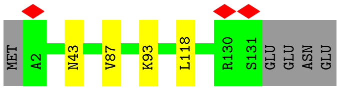
Chain Lg:



- Molecule 38: 60S ribosomal protein eL32

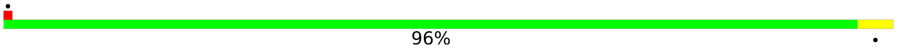
Chain Lh:

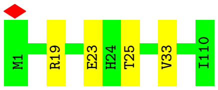




- Molecule 39: 60S ribosomal protein eL33

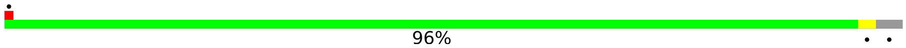
Chain Li:

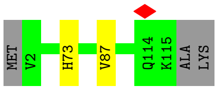




- Molecule 40: 60S ribosomal protein L34

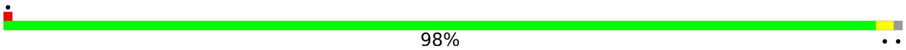
Chain Lj:

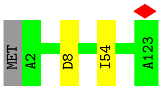




- Molecule 41: 60S ribosomal protein uL29

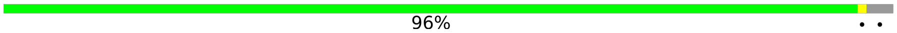
Chain Lk:

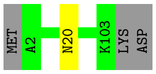




- Molecule 42: 60S ribosomal protein L36

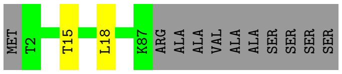
Chain Ll:





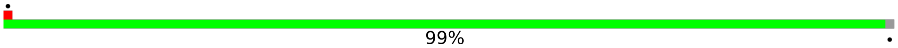
- Molecule 43: 60S ribosomal protein L37

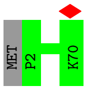
Chain Lm:



- Molecule 44: 60S ribosomal protein eL38

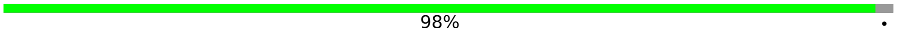
Chain Ln:

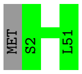




- Molecule 45: 60S ribosomal protein eL39

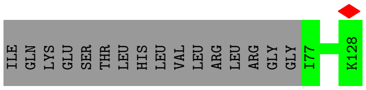
Chain Lo:





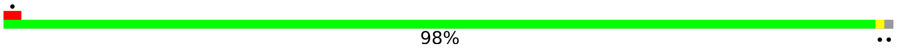
- Molecule 46: 60S ribosomal protein L40

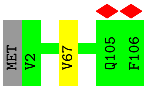
Chain Lp:



- Molecule 47: 60S ribosomal protein eL42

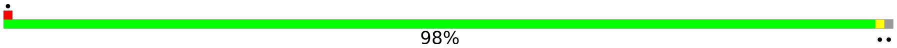
Chain Lq:

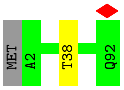




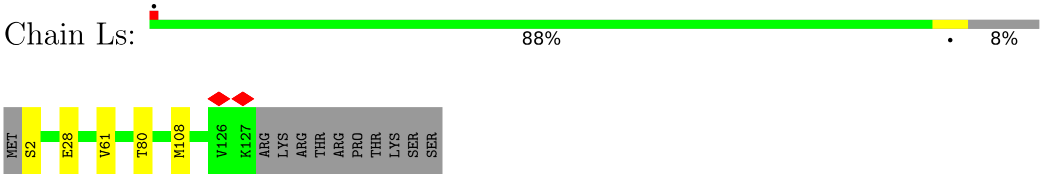
- Molecule 48: 60S ribosomal protein eL43

Chain Lr:

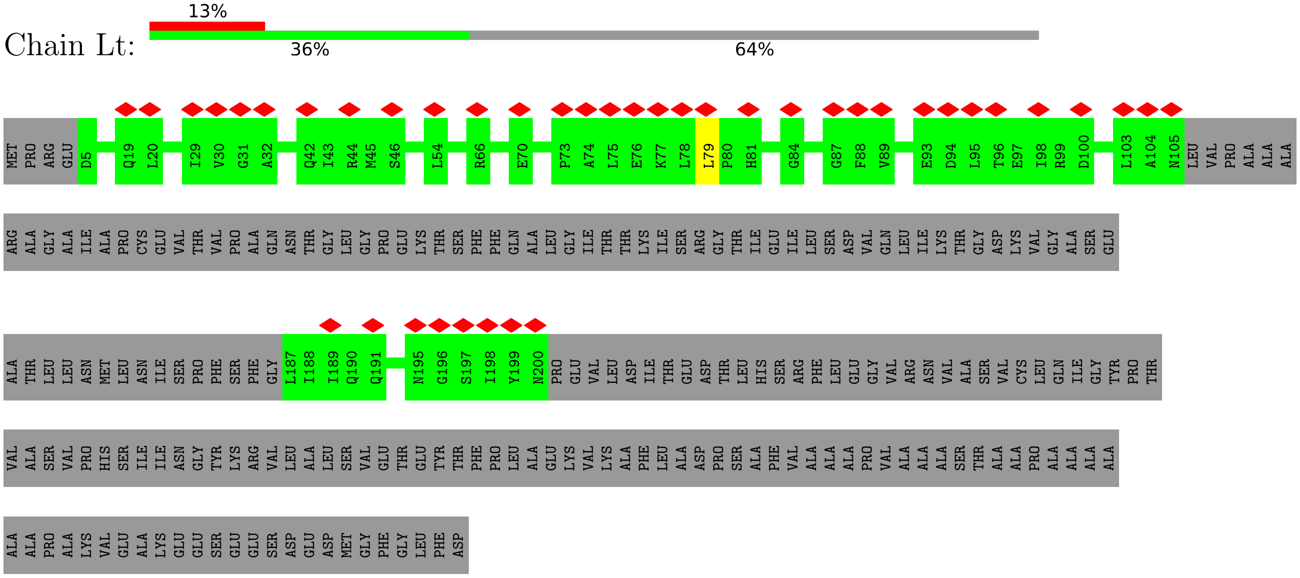




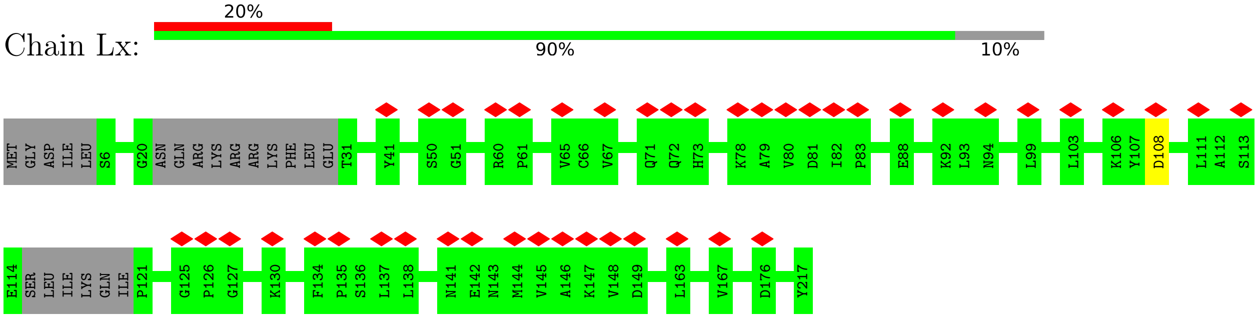
- Molecule 49: 60S ribosomal protein eL28



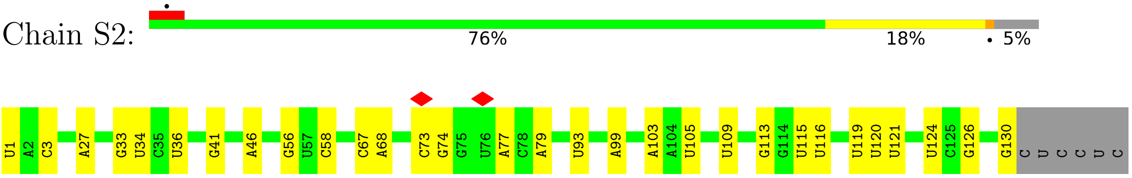
- Molecule 50: 60S ribosomal protein P0

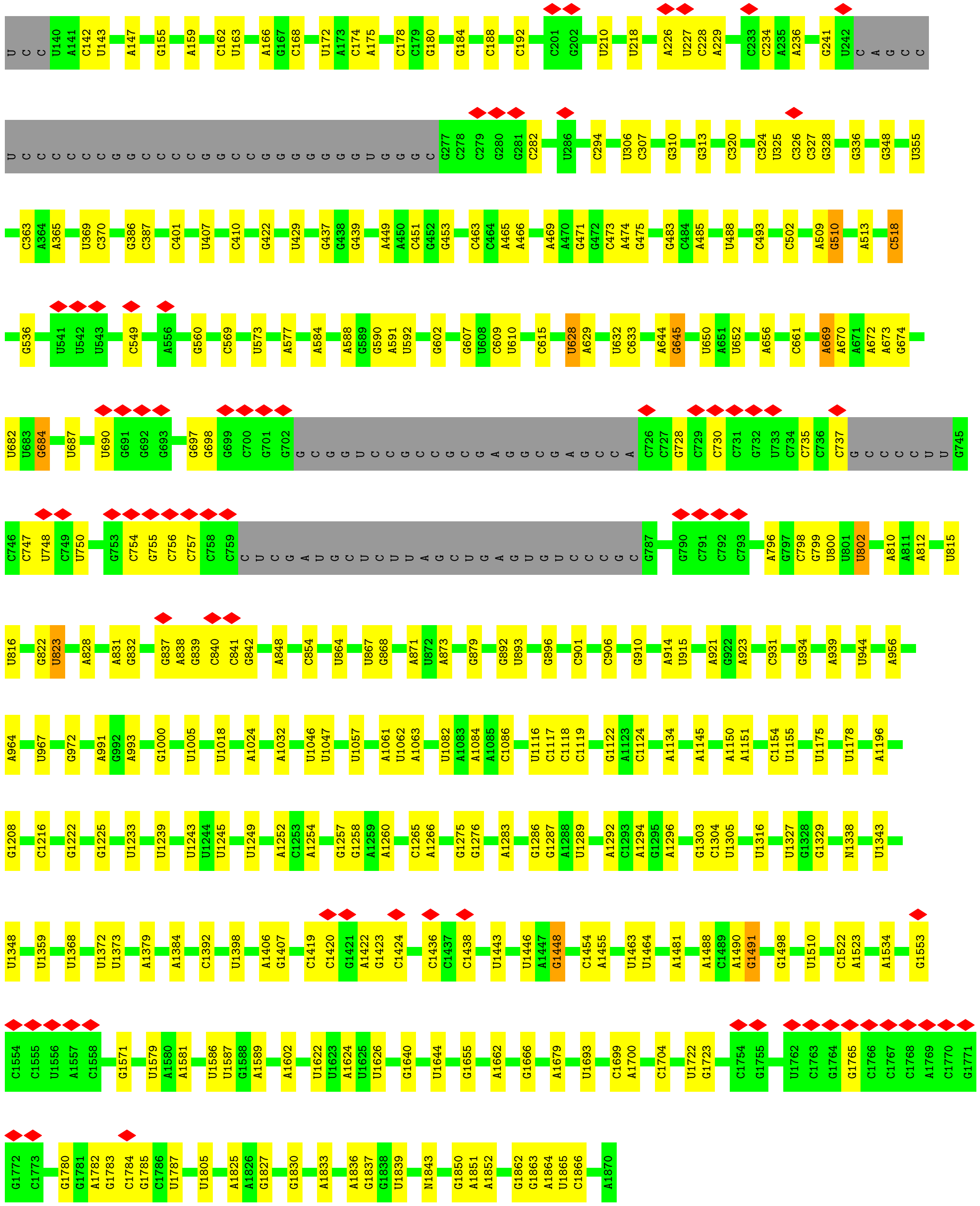


- Molecule 51: 60S ribosomal protein uL1



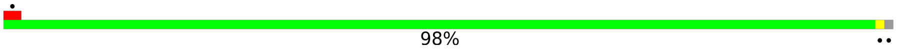
- Molecule 52: 18S rRNA

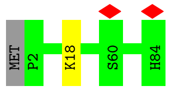




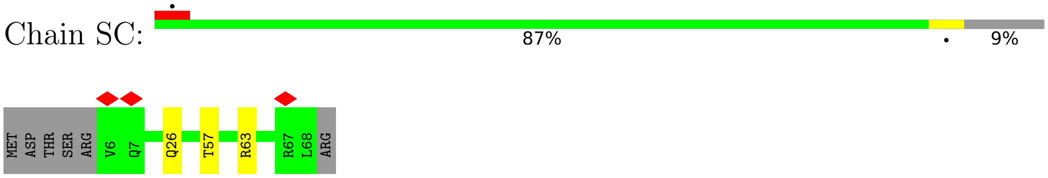
• Molecule 53: 40S ribosomal protein S27

Chain SB:

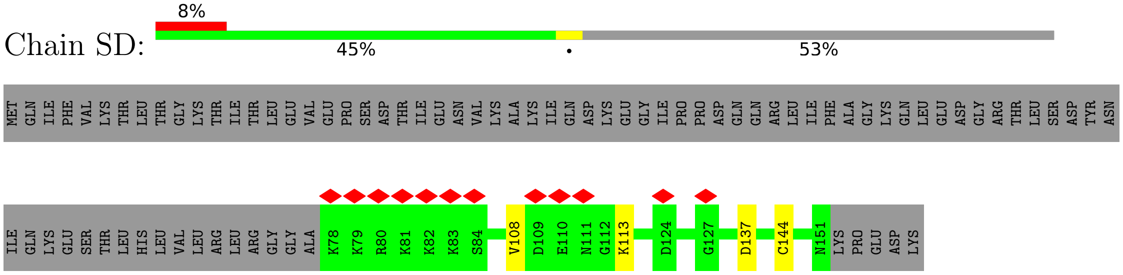




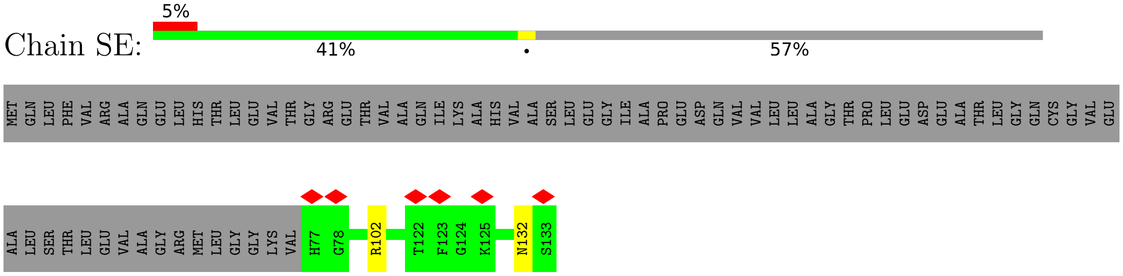
- Molecule 54: 40S ribosomal protein S28



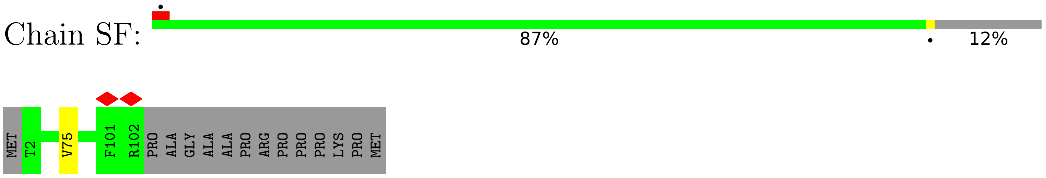
- Molecule 55: 40S ribosomal protein S27a



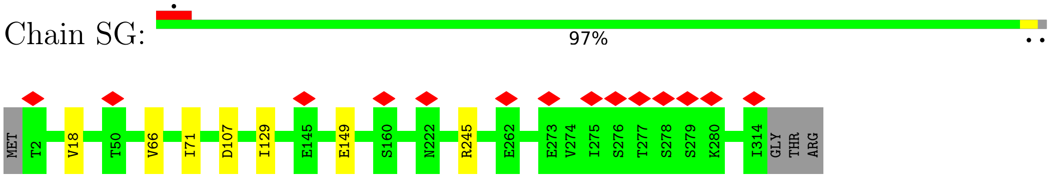
- Molecule 56: 40S ribosomal protein S30



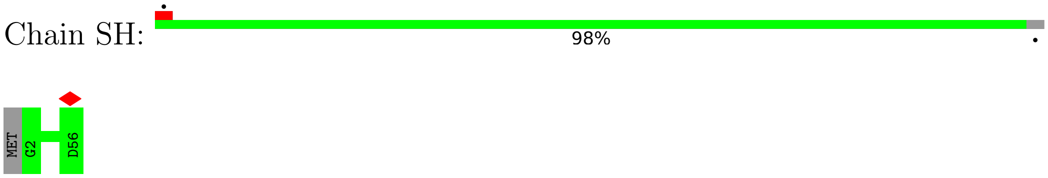
- Molecule 57: Ribosomal protein eS26



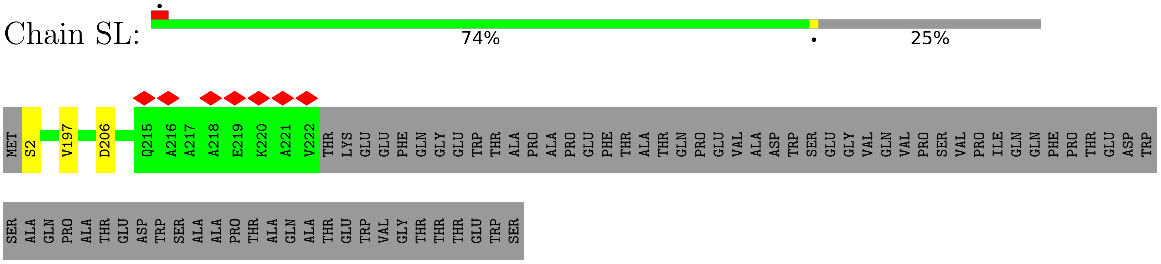
- Molecule 58: RACK1



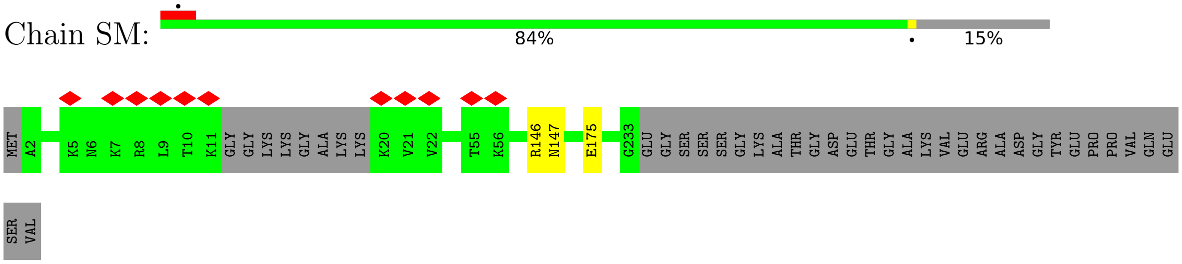
- Molecule 59: 40S ribosomal protein uS14



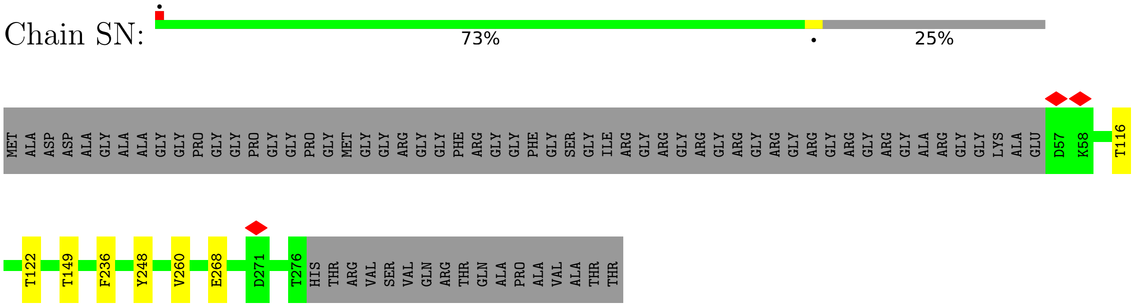
- Molecule 60: 40S ribosomal protein SA



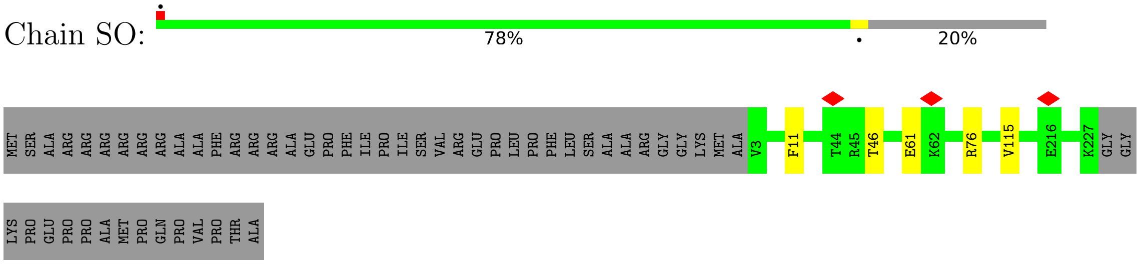
- Molecule 61: 40S ribosomal protein S3a



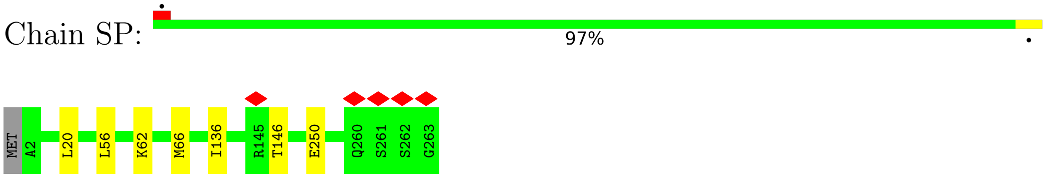
- Molecule 62: 40S ribosomal protein uS5



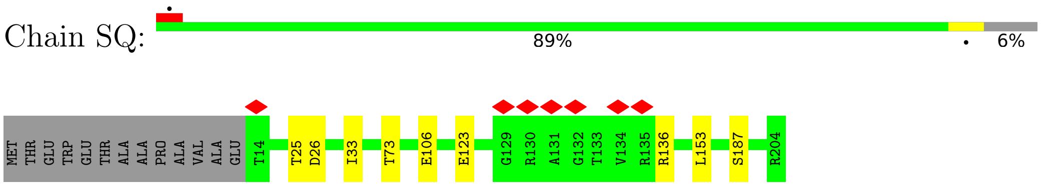
- Molecule 63: 40S ribosomal protein S3



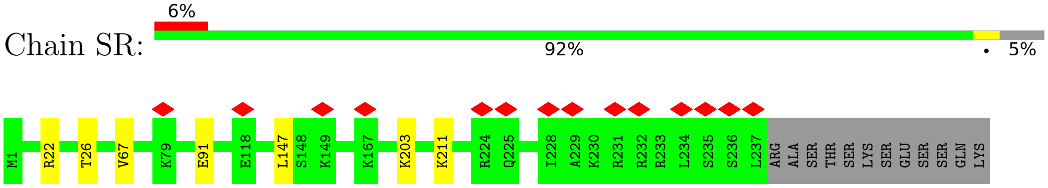
- Molecule 64: 40S ribosomal protein eS4



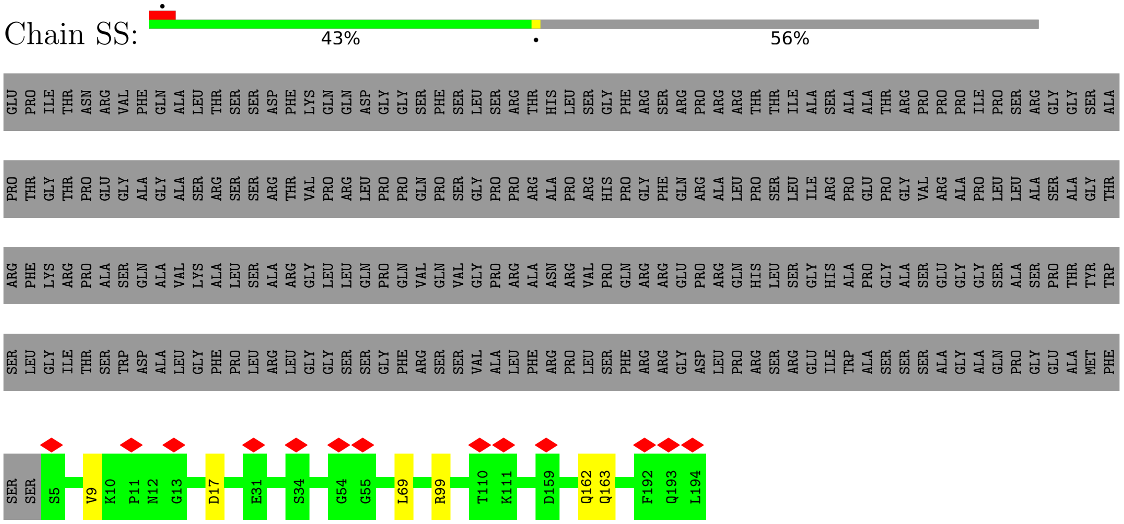
- Molecule 65: Ribosomal protein S5



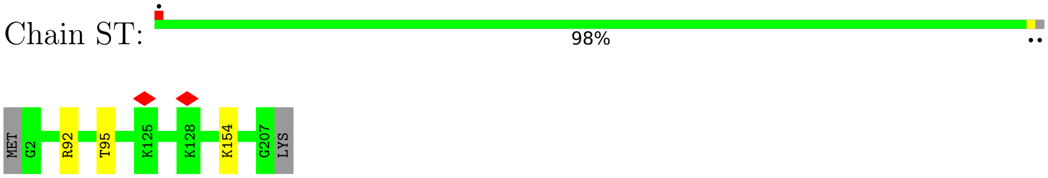
• Molecule 66: 40S ribosomal protein S6



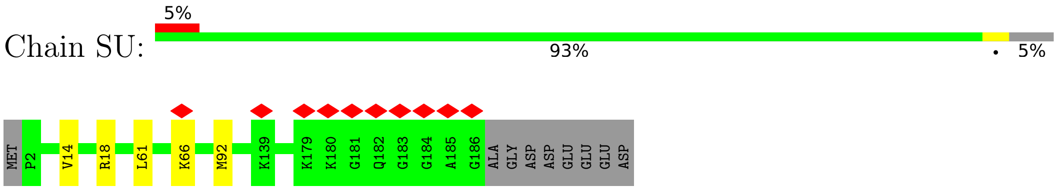
• Molecule 67: 40S ribosomal protein S7



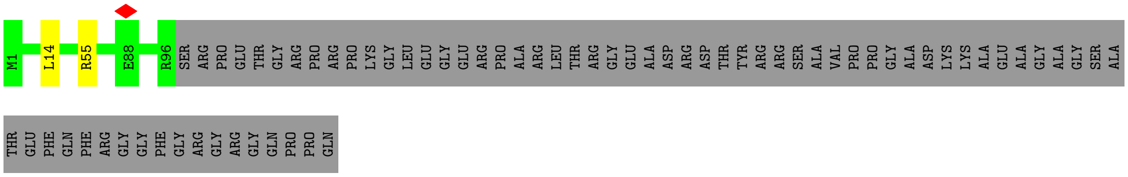
• Molecule 68: 40S ribosomal protein S8



• Molecule 69: 40S ribosomal protein S9

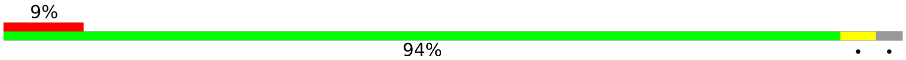


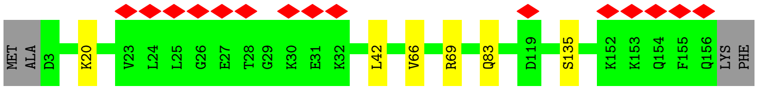
• Molecule 70: 40S ribosomal protein eS10



- Molecule 71: 40S ribosomal protein S11

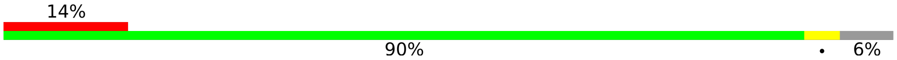
Chain SW:

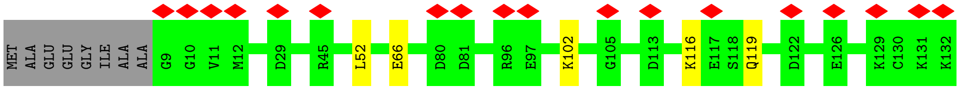




- Molecule 72: 40S ribosomal protein S12

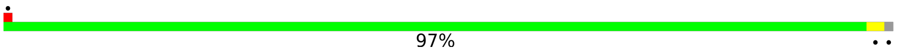
Chain SX:

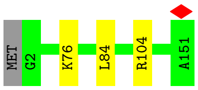




- Molecule 73: 40S ribosomal protein uS15

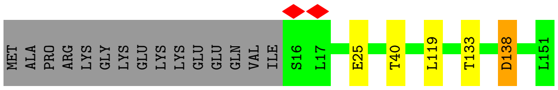
Chain SY:





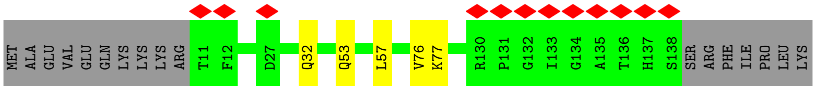
- Molecule 74: 40S ribosomal protein uS11

Chain SZ:



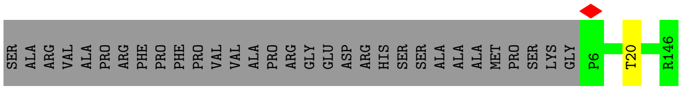
- Molecule 75: 40S ribosomal protein uS19

Chain Sa:

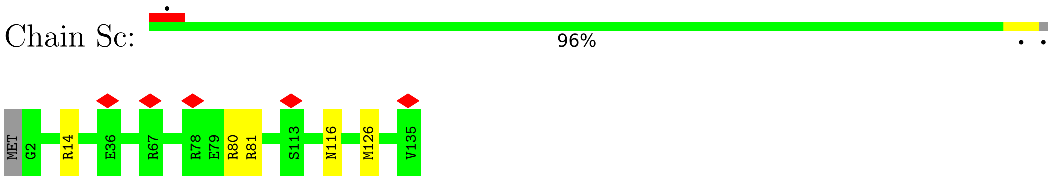


- Molecule 76: 40S ribosomal protein uS9

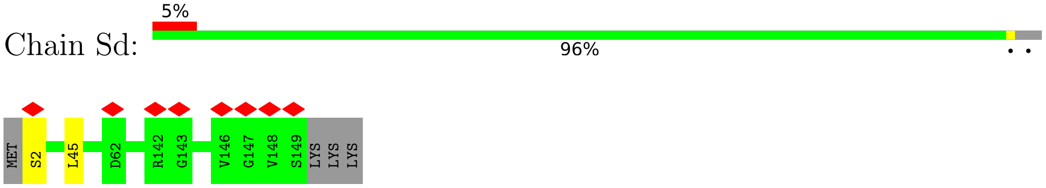
Chain Sb:



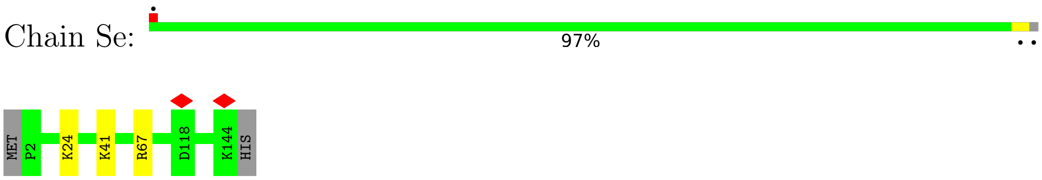
- Molecule 77: 40S ribosomal protein eS17



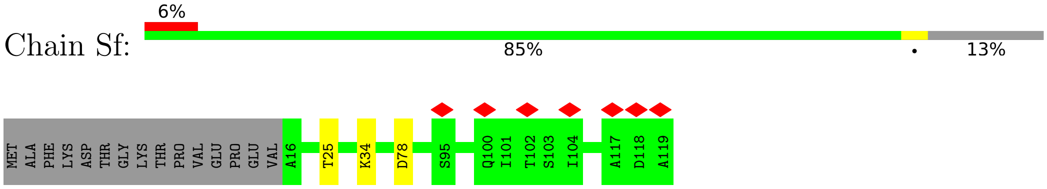
- Molecule 78: 40S ribosomal protein S18



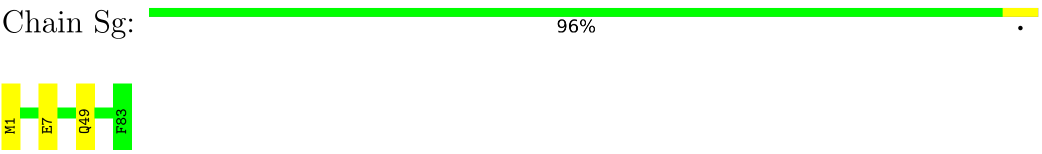
- Molecule 79: 40S Ribosomal protein eS19



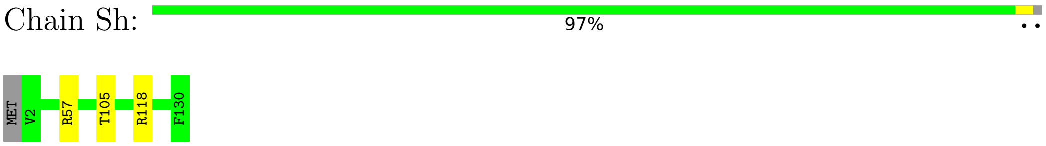
- Molecule 80: 40S ribosomal protein uS10



- Molecule 81: 40S ribosomal protein eS21

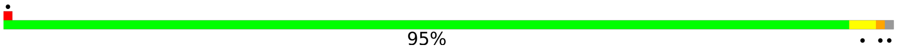


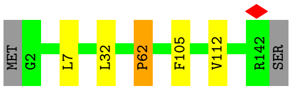
- Molecule 82: 40S ribosomal protein S15a



- Molecule 83: 40S ribosomal protein S23

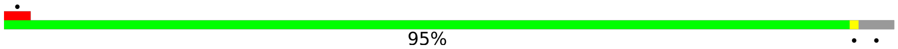
Chain Si:

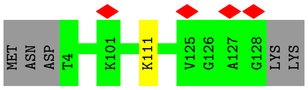




- Molecule 84: 40S ribosomal protein S24

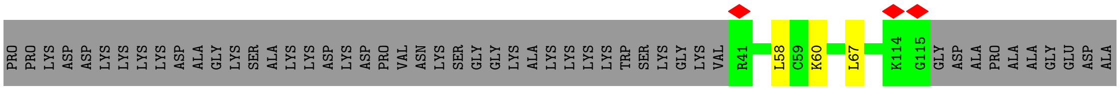
Chain Sj:





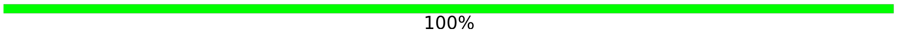
- Molecule 85: 40S ribosomal protein S25

Chain Sk:



- Molecule 86: 60S ribosomal protein L41

Chain Sl:



There are no outlier residues recorded for this chain.

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.629	Depositor
Minimum map value	0.000	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	520.704, 520.704, 520.704	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.017, 1.017, 1.017	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AAC, SAC, MG, 5MC, 6MZ, AYA, OMU, MA6, HIC, ZN, OMC, MLZ, 1MA, HY3, UR3, NA, M3L, AME, GTP, A2M, PSU, K, 4AC, 7MG, NMM, OMG

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	E	0.25	0/3403	0.49	2/4656 (0.0%)
2	F	0.41	3/2136 (0.1%)	0.84	5/3325 (0.2%)
3	I	0.19	0/4335	0.72	1/6738 (0.0%)
4	S	0.18	0/1098	0.77	2/1710 (0.1%)
5	B	0.27	0/1398	0.45	0/1905
6	L5	0.36	1/87426 (0.0%)	0.70	10/136397 (0.0%)
7	L7	0.36	0/2835	0.69	0/4418
8	L8	0.40	1/3635 (0.0%)	0.71	3/5661 (0.1%)
9	LD	0.29	0/1977	0.55	0/2651
10	LE	0.28	0/3261	0.51	0/4364
11	LF	0.27	0/2932	0.52	0/3939
12	LG	0.28	0/2437	0.49	0/3264
13	LH	0.27	0/1896	0.50	0/2541
14	LI	0.28	0/1922	0.50	0/2563
15	LJ	0.26	0/1908	0.49	0/2566
16	LK	0.27	0/1535	0.51	0/2063
17	LL	0.28	0/1756	0.51	0/2346
18	LM	0.26	0/1385	0.52	0/1852
19	LO	0.27	0/1733	0.54	0/2316
20	LP	0.28	0/1158	0.50	0/1547
21	LQ	0.29	0/1746	0.55	0/2338
22	LR	0.28	0/1662	0.51	0/2222
23	LS	0.27	0/1315	0.50	0/1763
24	LT	0.28	0/1539	0.56	0/2054
25	LU	0.25	0/1524	0.54	0/2013
26	LV	0.29	0/1497	0.53	0/2008
27	LW	0.28	0/1326	0.49	0/1770
28	LX	0.26	0/820	0.49	0/1100
29	LY	0.28	0/1048	0.52	0/1402
30	LZ	0.28	0/779	0.50	0/1034
31	La	0.27	0/984	0.50	0/1323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Lb	0.27	0/1132	0.53	0/1504
33	Lc	0.28	0/1130	0.50	0/1507
34	Ld	0.29	0/1191	0.52	0/1590
35	Le	0.25	0/884	0.53	0/1169
36	Lf	0.27	0/847	0.45	0/1134
37	Lg	0.27	0/903	0.53	0/1216
38	Lh	0.28	0/1088	0.52	0/1451
39	Li	0.30	0/903	0.54	0/1208
40	Lj	0.28	0/916	0.56	0/1220
41	Lk	0.25	0/1021	0.49	0/1348
42	Ll	0.25	0/841	0.52	0/1112
43	Lm	0.29	0/720	0.58	0/952
44	Ln	0.26	0/575	0.47	0/761
45	Lo	0.25	0/459	0.53	0/608
46	Lp	0.26	0/425	0.51	0/562
47	Lq	0.28	0/866	0.52	0/1141
48	Lr	0.27	0/718	0.50	0/953
49	Ls	0.27	0/1020	0.54	0/1366
50	Lt	0.24	0/565	0.38	0/783
51	Lx	0.24	0/969	0.43	0/1347
52	S2	0.27	1/40365 (0.0%)	0.70	12/62915 (0.0%)
53	SB	0.25	0/665	0.47	0/891
54	SC	0.24	0/497	0.57	0/666
55	SD	0.25	0/622	0.50	0/822
56	SE	0.24	0/462	0.55	0/607
57	SF	0.25	0/828	0.54	0/1109
58	SG	0.24	0/2493	0.48	0/3394
59	SH	0.27	0/470	0.51	0/623
60	SL	0.25	0/1771	0.47	0/2406
61	SM	0.25	0/1841	0.48	0/2459
62	SN	0.26	0/1742	0.46	0/2354
63	SO	0.26	0/1779	0.50	0/2395
64	SP	0.25	0/2118	0.51	0/2849
65	SQ	0.24	0/1531	0.49	0/2059
66	SR	0.24	0/1946	0.54	0/2590
67	SS	0.25	0/1552	0.48	0/2079
68	ST	0.25	0/1715	0.53	0/2287
69	SU	0.25	0/1550	0.53	0/2069
70	SV	0.25	0/834	0.45	0/1125
71	SW	0.26	0/1284	0.53	0/1717
72	SX	0.23	0/968	0.44	0/1296
73	SY	0.24	0/1232	0.48	0/1656
74	SZ	0.26	0/1029	0.54	0/1380

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	Sa	0.26	0/1069	0.50	0/1429
76	Sb	0.25	0/1142	0.51	0/1528
77	Sc	0.24	0/1094	0.50	0/1469
78	Sd	0.25	0/1226	0.55	0/1643
79	Se	0.24	0/1119	0.47	0/1498
80	Sf	0.24	0/831	0.53	0/1115
81	Sg	0.26	0/636	0.50	0/852
82	Sh	0.25	0/1051	0.50	0/1406
83	Si	0.25	0/1107	0.51	0/1475
84	Sj	0.24	0/1032	0.53	0/1371
85	Sk	0.23	0/604	0.50	0/810
86	Sl	0.23	0/240	0.65	0/305
All	All	0.31	6/242024 (0.0%)	0.64	35/355430 (0.0%)

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
83	Si	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	52	C	C4-N4	-11.56	1.23	1.33
52	S2	1	U	OP3-P	-10.65	1.48	1.61
6	L5	1	C	OP3-P	-10.65	1.48	1.61
8	L8	1	C	OP3-P	-10.63	1.48	1.61
2	F	1	G	OP3-P	-10.55	1.48	1.61
2	F	52	C	N3-C4	6.41	1.38	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	52	C	N3-C4-C5	-18.51	114.50	121.90
2	F	52	C	C2-N3-C4	14.32	127.06	119.90
2	F	52	C	C5-C4-N4	8.12	125.89	120.20
6	L5	2312	C	C2-N1-C1'	7.34	126.87	118.80
52	S2	1454	C	C2-N1-C1'	7.25	126.78	118.80
52	S2	939	A	C6-N1-C2	-7.12	114.33	118.60
52	S2	1454	C	N1-C2-O2	7.01	123.11	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L5	1594	U	C2-N1-C1'	6.80	125.86	117.70
6	L5	2312	C	N1-C2-O2	6.66	122.89	118.90
4	S	1134	C	C2-N1-C1'	6.46	125.90	118.80
1	E	546	PRO	N-CA-CB	6.38	110.95	103.30
52	S2	1	U	N1-C2-O2	6.30	127.21	122.80
2	F	52	C	N1-C2-O2	6.29	122.67	118.90
6	L5	2252	U	C2-N1-C1'	6.28	125.23	117.70
1	E	571	PRO	N-CA-CB	6.23	110.78	103.30
52	S2	1	U	C2-N1-C1'	6.09	125.01	117.70
8	L8	111	U	C2-N1-C1'	5.94	124.83	117.70
2	F	52	C	N1-C2-N3	-5.93	115.05	119.20
52	S2	294	C	N1-C2-O2	5.93	122.46	118.90
52	S2	294	C	C2-N1-C1'	5.76	125.14	118.80
4	S	1134	C	N1-C2-O2	5.72	122.33	118.90
52	S2	1	U	N3-C2-O2	-5.67	118.23	122.20
6	L5	1594	U	N1-C2-O2	5.66	126.77	122.80
52	S2	1454	C	N3-C2-O2	-5.50	118.05	121.90
6	L5	2252	U	N1-C2-O2	5.48	126.63	122.80
8	L8	111	U	N1-C2-O2	5.34	126.54	122.80
6	L5	2312	C	N3-C2-O2	-5.33	118.17	121.90
3	I	156	C	N1-C2-O2	5.20	122.02	118.90
52	S2	854	C	C2-N1-C1'	5.19	124.51	118.80
6	L5	3590	C	N1-C2-O2	5.12	121.97	118.90
6	L5	2312	C	C6-N1-C1'	-5.11	114.67	120.80
6	L5	1594	U	N3-C2-O2	-5.10	118.63	122.20
8	L8	111	U	N3-C2-O2	-5.03	118.68	122.20
52	S2	939	A	N1-C2-N3	5.02	131.81	129.30
52	S2	1454	C	C6-N1-C1'	-5.01	114.78	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	Si	62	HY3	Mainchain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	E	509/616 (83%)	460 (90%)	46 (9%)	3 (1%)	25	56
5	B	200/854 (23%)	171 (86%)	28 (14%)	1 (0%)	29	61
9	LD	251/257 (98%)	241 (96%)	10 (4%)	0	100	100
10	LE	395/403 (98%)	386 (98%)	9 (2%)	0	100	100
11	LF	360/413 (87%)	355 (99%)	5 (1%)	0	100	100
12	LG	291/297 (98%)	287 (99%)	4 (1%)	0	100	100
13	LH	226/291 (78%)	220 (97%)	6 (3%)	0	100	100
14	LI	224/247 (91%)	217 (97%)	7 (3%)	0	100	100
15	LJ	229/266 (86%)	227 (99%)	2 (1%)	0	100	100
16	LK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
17	LL	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
18	LM	168/178 (94%)	162 (96%)	6 (4%)	0	100	100
19	LO	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
20	LP	136/218 (62%)	135 (99%)	1 (1%)	0	100	100
21	LQ	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
22	LR	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
23	LS	157/184 (85%)	153 (98%)	4 (2%)	0	100	100
24	LT	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
25	LU	178/196 (91%)	178 (100%)	0	0	100	100
26	LV	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
27	LW	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
28	LX	97/128 (76%)	94 (97%)	3 (3%)	0	100	100
29	LY	137/140 (98%)	134 (98%)	3 (2%)	0	100	100
30	LZ	89/157 (57%)	89 (100%)	0	0	100	100
31	La	116/156 (74%)	115 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	Lb	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
33	Lc	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
34	Ld	145/148 (98%)	140 (97%)	4 (3%)	1 (1%)	22	53
35	Le	103/245 (42%)	102 (99%)	1 (1%)	0	100	100
36	Lf	106/115 (92%)	106 (100%)	0	0	100	100
37	Lg	105/125 (84%)	105 (100%)	0	0	100	100
38	Lh	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
39	Li	108/110 (98%)	108 (100%)	0	0	100	100
40	Lj	112/117 (96%)	112 (100%)	0	0	100	100
41	Lk	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
42	Ll	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
43	Lm	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
44	Ln	67/70 (96%)	67 (100%)	0	0	100	100
45	Lo	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
46	Lp	49/128 (38%)	49 (100%)	0	0	100	100
47	Lq	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
48	Lr	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
49	Ls	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
50	Lt	111/318 (35%)	105 (95%)	5 (4%)	1 (1%)	17	46
51	Lx	190/217 (88%)	172 (90%)	17 (9%)	1 (0%)	29	61
53	SB	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
54	SC	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
55	SD	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
56	SE	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
57	SF	99/115 (86%)	99 (100%)	0	0	100	100
58	SG	311/317 (98%)	297 (96%)	14 (4%)	0	100	100
59	SH	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
60	SL	219/295 (74%)	213 (97%)	6 (3%)	0	100	100
61	SM	220/264 (83%)	216 (98%)	4 (2%)	0	100	100
62	SN	218/293 (74%)	216 (99%)	2 (1%)	0	100	100
63	SO	223/281 (79%)	219 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	SP	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
65	SQ	189/204 (93%)	183 (97%)	6 (3%)	0	100	100
66	SR	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
67	SS	188/432 (44%)	183 (97%)	5 (3%)	0	100	100
68	ST	204/208 (98%)	197 (97%)	7 (3%)	0	100	100
69	SU	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
70	SV	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
71	SW	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
72	SX	122/132 (92%)	116 (95%)	6 (5%)	0	100	100
73	SY	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
74	SZ	134/151 (89%)	127 (95%)	6 (4%)	1 (1%)	22	53
75	Sa	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
76	Sb	139/172 (81%)	132 (95%)	7 (5%)	0	100	100
77	Sc	132/135 (98%)	132 (100%)	0	0	100	100
78	Sd	146/152 (96%)	144 (99%)	2 (1%)	0	100	100
79	Se	140/145 (97%)	138 (99%)	2 (1%)	0	100	100
80	Sf	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
81	Sg	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
82	Sh	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
83	Si	137/143 (96%)	136 (99%)	1 (1%)	0	100	100
84	Sj	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
85	Sk	73/124 (59%)	72 (99%)	1 (1%)	0	100	100
86	Sl	23/25 (92%)	23 (100%)	0	0	100	100
All	All	12310/15142 (81%)	11992 (97%)	310 (2%)	8 (0%)	54	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	546	PRO
51	Lx	108	ASP
50	Lt	79	LEU
1	E	297	LEU
5	B	703	SER
34	Ld	15	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
74	SZ	138	ASP
1	E	570	GLU

5.3.2 Protein sidechains ⓘ

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	E	227/524 (43%)	224 (99%)	3 (1%)	69	91
5	B	102/761 (13%)	99 (97%)	3 (3%)	42	76
9	LD	195/199 (98%)	192 (98%)	3 (2%)	65	89
10	LE	344/347 (99%)	332 (96%)	12 (4%)	36	70
11	LF	302/337 (90%)	295 (98%)	7 (2%)	50	82
12	LG	247/250 (99%)	241 (98%)	6 (2%)	49	81
13	LH	205/251 (82%)	200 (98%)	5 (2%)	49	81
14	LI	197/215 (92%)	191 (97%)	6 (3%)	41	75
15	LJ	199/223 (89%)	192 (96%)	7 (4%)	36	70
16	LK	169/171 (99%)	168 (99%)	1 (1%)	86	96
17	LL	180/181 (99%)	170 (94%)	10 (6%)	21	51
18	LM	143/149 (96%)	136 (95%)	7 (5%)	25	57
19	LO	175/176 (99%)	171 (98%)	4 (2%)	50	82
20	LP	117/161 (73%)	114 (97%)	3 (3%)	46	79
21	LQ	171/172 (99%)	169 (99%)	2 (1%)	71	92
22	LR	171/173 (99%)	169 (99%)	2 (1%)	71	92
23	LS	139/163 (85%)	137 (99%)	2 (1%)	67	90
24	LT	164/165 (99%)	162 (99%)	2 (1%)	71	92
25	LU	159/175 (91%)	149 (94%)	10 (6%)	18	46
26	LV	154/154 (100%)	150 (97%)	4 (3%)	46	79
27	LW	139/140 (99%)	134 (96%)	5 (4%)	35	69
28	LX	88/113 (78%)	88 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	LY	106/107 (99%)	105 (99%)	1 (1%)	78	94
30	LZ	79/126 (63%)	77 (98%)	2 (2%)	47	80
31	La	106/134 (79%)	103 (97%)	3 (3%)	43	77
32	Lb	124/135 (92%)	121 (98%)	3 (2%)	49	81
33	Lc	117/118 (99%)	116 (99%)	1 (1%)	78	94
34	Ld	119/120 (99%)	114 (96%)	5 (4%)	30	63
35	Le	87/183 (48%)	83 (95%)	4 (5%)	27	60
36	Lf	92/98 (94%)	90 (98%)	2 (2%)	52	83
37	Lg	98/110 (89%)	95 (97%)	3 (3%)	40	74
38	Lh	116/121 (96%)	112 (97%)	4 (3%)	37	71
39	Li	89/89 (100%)	85 (96%)	4 (4%)	27	60
40	Lj	98/100 (98%)	96 (98%)	2 (2%)	55	84
41	Lk	109/110 (99%)	107 (98%)	2 (2%)	59	86
42	Ll	86/89 (97%)	85 (99%)	1 (1%)	71	92
43	Lm	73/80 (91%)	71 (97%)	2 (3%)	44	78
44	Ln	64/65 (98%)	64 (100%)	0	100	100
45	Lo	47/48 (98%)	47 (100%)	0	100	100
46	Lp	47/115 (41%)	47 (100%)	0	100	100
47	Lq	92/93 (99%)	91 (99%)	1 (1%)	73	92
48	Lr	74/75 (99%)	73 (99%)	1 (1%)	67	90
49	Ls	109/120 (91%)	105 (96%)	4 (4%)	34	68
53	SB	75/76 (99%)	74 (99%)	1 (1%)	69	91
54	SC	56/62 (90%)	53 (95%)	3 (5%)	22	53
55	SD	67/140 (48%)	63 (94%)	4 (6%)	19	48
56	SE	47/106 (44%)	45 (96%)	2 (4%)	29	62
57	SF	88/98 (90%)	87 (99%)	1 (1%)	73	92
58	SG	272/275 (99%)	265 (97%)	7 (3%)	46	79
59	SH	48/49 (98%)	48 (100%)	0	100	100
60	SL	182/243 (75%)	180 (99%)	2 (1%)	73	92
61	SM	203/231 (88%)	200 (98%)	3 (2%)	65	89
62	SN	185/223 (83%)	178 (96%)	7 (4%)	33	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	SO	189/232 (82%)	184 (97%)	5 (3%)	46	79
64	SP	224/225 (100%)	217 (97%)	7 (3%)	40	74
65	SQ	161/170 (95%)	152 (94%)	9 (6%)	21	51
66	SR	207/218 (95%)	200 (97%)	7 (3%)	37	71
67	SS	170/360 (47%)	164 (96%)	6 (4%)	36	70
68	ST	178/180 (99%)	175 (98%)	3 (2%)	60	87
69	SU	161/168 (96%)	156 (97%)	5 (3%)	40	74
70	SV	87/136 (64%)	85 (98%)	2 (2%)	50	82
71	SW	139/142 (98%)	133 (96%)	6 (4%)	29	62
72	SX	104/108 (96%)	99 (95%)	5 (5%)	25	58
73	SY	130/131 (99%)	127 (98%)	3 (2%)	50	82
74	SZ	106/119 (89%)	101 (95%)	5 (5%)	26	59
75	Sa	114/130 (88%)	109 (96%)	5 (4%)	28	61
76	Sb	117/140 (84%)	116 (99%)	1 (1%)	78	94
77	Sc	120/121 (99%)	115 (96%)	5 (4%)	30	63
78	Sd	127/131 (97%)	126 (99%)	1 (1%)	81	94
79	Se	112/114 (98%)	110 (98%)	2 (2%)	59	86
80	Sf	94/107 (88%)	91 (97%)	3 (3%)	39	73
81	Sg	67/67 (100%)	65 (97%)	2 (3%)	41	75
82	Sh	112/113 (99%)	109 (97%)	3 (3%)	44	78
83	Si	112/114 (98%)	108 (96%)	4 (4%)	35	69
84	Sj	107/112 (96%)	106 (99%)	1 (1%)	78	94
85	Sk	66/102 (65%)	63 (96%)	3 (4%)	27	60
86	Sl	24/24 (100%)	24 (100%)	0	100	100
All	All	10170/12403 (82%)	9898 (97%)	272 (3%)	48	78

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	7	ASN
1	E	244	THR
1	E	497	GLU
5	B	631	ASP
5	B	729	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	738	LEU
9	LD	84	THR
9	LD	106	THR
9	LD	243	THR
10	LE	94	GLU
10	LE	180	LEU
10	LE	182	GLU
10	LE	209	GLN
10	LE	248	LEU
10	LE	298	LEU
10	LE	329	ASP
10	LE	346	THR
10	LE	353	VAL
10	LE	369	ASP
10	LE	370	THR
10	LE	371	THR
11	LF	44	LEU
11	LF	95	MET
11	LF	122	TYR
11	LF	174	LEU
11	LF	240	LEU
11	LF	260	LEU
11	LF	361	LYS
12	LG	36	LEU
12	LG	93	THR
12	LG	143	THR
12	LG	163	LEU
12	LG	262	LYS
12	LG	273	LEU
13	LH	46	CYS
13	LH	51	VAL
13	LH	73	ARG
13	LH	103	LYS
13	LH	281	THR
14	LI	24	PHE
14	LI	45	ARG
14	LI	51	GLU
14	LI	82	VAL
14	LI	152	LEU
14	LI	231	ASP
15	LJ	33	GLU
15	LJ	35	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	LJ	43	GLN
15	LJ	111	LYS
15	LJ	114	LEU
15	LJ	210	GLU
15	LJ	265	LEU
16	LK	55	LEU
17	LL	24	ARG
17	LL	26	VAL
17	LL	36	LEU
17	LL	44	ASP
17	LL	63	GLU
17	LL	82	LYS
17	LL	126	VAL
17	LL	134	VAL
17	LL	152	LEU
17	LL	191	ILE
18	LM	28	GLU
18	LM	35	ARG
18	LM	47	THR
18	LM	57	VAL
18	LM	88	LYS
18	LM	118	LYS
18	LM	129	ASP
19	LO	67	HIS
19	LO	138	ASP
19	LO	144	LEU
19	LO	148	THR
20	LP	7	VAL
20	LP	25	VAL
20	LP	48	GLN
21	LQ	126	THR
21	LQ	148	THR
22	LR	117	ARG
22	LR	183	LYS
23	LS	69	ARG
23	LS	115	GLU
24	LT	122	THR
24	LT	158	THR
25	LU	4	LEU
25	LU	8	LYS
25	LU	43	LYS
25	LU	44	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LU	49	LEU
25	LU	106	LEU
25	LU	108	ARG
25	LU	145	LEU
25	LU	158	GLN
25	LU	163	ARG
26	LV	17	LEU
26	LV	77	ASN
26	LV	82	LEU
26	LV	159	LEU
27	LW	4	THR
27	LW	68	THR
27	LW	80	VAL
27	LW	106	LEU
27	LW	117	LYS
29	LY	107	ASN
30	LZ	19	ARG
30	LZ	105	ARG
31	La	50	LYS
31	La	53	ARG
31	La	67	ARG
32	Lb	55	VAL
32	Lb	74	TYR
32	Lb	119	LEU
33	Lc	33	THR
34	Ld	63	LEU
34	Ld	75	LEU
34	Ld	92	LYS
34	Ld	95	THR
34	Ld	134	GLU
35	Le	50	ASN
35	Le	68	ARG
35	Le	91	ARG
35	Le	117	ARG
36	Lf	20	LEU
36	Lf	94	LEU
37	Lg	107	THR
37	Lg	119	THR
37	Lg	123	ASP
38	Lh	43	ASN
38	Lh	87	VAL
38	Lh	93	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	Lh	118	LEU
39	Li	19	ARG
39	Li	23	GLU
39	Li	25	THR
39	Li	33	VAL
40	Lj	73	HIS
40	Lj	87	VAL
41	Lk	8	ASP
41	Lk	54	ILE
42	Ll	20	ASN
43	Lm	15	THR
43	Lm	18	LEU
47	Lq	67	VAL
48	Lr	38	THR
49	Ls	28	GLU
49	Ls	61	VAL
49	Ls	80	THR
49	Ls	108	MET
53	SB	18	LYS
54	SC	26	GLN
54	SC	57	THR
54	SC	63	ARG
55	SD	108	VAL
55	SD	113	LYS
55	SD	137	ASP
55	SD	144	CYS
56	SE	102	ARG
56	SE	132	ASN
57	SF	75	VAL
58	SG	18	VAL
58	SG	66	VAL
58	SG	71	ILE
58	SG	107	ASP
58	SG	129	ILE
58	SG	149	GLU
58	SG	245	ARG
60	SL	197	VAL
60	SL	206	ASP
61	SM	146	ARG
61	SM	147	ASN
61	SM	175	GLU
62	SN	116	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	SN	122	THR
62	SN	149	THR
62	SN	236	PHE
62	SN	248	TYR
62	SN	260	VAL
62	SN	268	GLU
63	SO	11	PHE
63	SO	46	THR
63	SO	61	GLU
63	SO	76	ARG
63	SO	115	VAL
64	SP	20	LEU
64	SP	56	LEU
64	SP	62	LYS
64	SP	66	MET
64	SP	136	ILE
64	SP	146	THR
64	SP	250	GLU
65	SQ	25	THR
65	SQ	26	ASP
65	SQ	33	ILE
65	SQ	73	THR
65	SQ	106	GLU
65	SQ	123	GLU
65	SQ	136	ARG
65	SQ	153	LEU
65	SQ	187	SER
66	SR	22	ARG
66	SR	26	THR
66	SR	67	VAL
66	SR	91	GLU
66	SR	147	LEU
66	SR	203	LYS
66	SR	211	LYS
67	SS	9	VAL
67	SS	17	ASP
67	SS	69	LEU
67	SS	99	ARG
67	SS	162	GLN
67	SS	163	GLN
68	ST	92	ARG
68	ST	95	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
68	ST	154	LYS
69	SU	14	VAL
69	SU	18	ARG
69	SU	61	LEU
69	SU	66	LYS
69	SU	92	MET
70	SV	14	LEU
70	SV	55	ARG
71	SW	20	LYS
71	SW	42	LEU
71	SW	66	VAL
71	SW	69	ARG
71	SW	83	GLN
71	SW	135	SER
72	SX	52	LEU
72	SX	66	GLU
72	SX	102	LYS
72	SX	116	LYS
72	SX	119	GLN
73	SY	76	LYS
73	SY	84	LEU
73	SY	104	ARG
74	SZ	25	GLU
74	SZ	40	THR
74	SZ	119	LEU
74	SZ	133	THR
74	SZ	138	ASP
75	Sa	32	GLN
75	Sa	53	GLN
75	Sa	57	LEU
75	Sa	76	VAL
75	Sa	77	LYS
76	Sb	20	THR
77	Sc	14	ARG
77	Sc	80	ARG
77	Sc	81	ARG
77	Sc	116	ASN
77	Sc	126	MET
78	Sd	45	LEU
79	Se	24	LYS
79	Se	41	LYS
80	Sf	25	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	Sf	34	LYS
80	Sf	78	ASP
81	Sg	7	GLU
81	Sg	49	GLN
82	Sh	57	ARG
82	Sh	105	THR
82	Sh	118	ARG
83	Si	7	LEU
83	Si	32	LEU
83	Si	105	PHE
83	Si	112	VAL
84	Sj	111	LYS
85	Sk	58	LEU
85	Sk	60	LYS
85	Sk	67	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	378	GLN
5	B	683	HIS
12	LG	267	ASN
18	LM	168	GLN
21	LQ	8	GLN
21	LQ	158	HIS
54	SC	29	GLN
56	SE	89	GLN
57	SF	7	ASN
58	SG	117	ASN
60	SL	50	ASN
77	Sc	31	ASN
78	Sd	105	ASN
79	Se	11	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	89/90 (98%)	26 (29%)	0
3	I	178/1072 (16%)	103 (57%)	1 (0%)
4	S	45/855 (5%)	22 (48%)	1 (2%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	S2	1759/1870 (94%)	266 (15%)	1 (0%)
6	L5	3751/4808 (78%)	523 (13%)	3 (0%)
7	L7	118/119 (99%)	8 (6%)	0
8	L8	155/158 (98%)	17 (10%)	0
All	All	6095/8972 (67%)	965 (15%)	6 (0%)

All (965) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	10	A
2	F	12	C
2	F	14	U
2	F	16	A
2	F	19	G
2	F	20	G
2	F	21	U
2	F	22	C
2	F	24	G
2	F	25	G
2	F	28	U
2	F	32	G
2	F	44	G
2	F	46	A
2	F	47	G
2	F	55	G
2	F	57	G
2	F	62	A
2	F	63	G
2	F	65	G
2	F	72	U
2	F	84	G
2	F	85	G
2	F	87	G
2	F	88	C
2	F	90	A
3	I	31	A
3	I	32	A
3	I	35	U
3	I	38	G
3	I	40	U
3	I	41	C
3	I	42	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	43	U
3	I	44	G
3	I	45	C
3	I	47	U
3	I	48	G
3	I	49	U
3	I	50	A
3	I	51	A
3	I	52	A
3	I	53	U
3	I	54	A
3	I	62	G
3	I	63	A
3	I	67	G
3	I	68	U
3	I	72	U
3	I	73	A
3	I	74	A
3	I	75	A
3	I	76	U
3	I	77	U
3	I	79	C
3	I	80	A
3	I	83	U
3	I	84	A
3	I	87	G
3	I	88	C
3	I	89	U
3	I	91	U
3	I	93	U
3	I	94	U
3	I	96	G
3	I	97	U
3	I	98	A
3	I	101	U
3	I	108	G
3	I	111	A
3	I	112	U
3	I	114	U
3	I	115	A
3	I	120	U
3	I	121	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	122	C
3	I	123	G
3	I	124	U
3	I	127	C
3	I	129	G
3	I	130	G
3	I	131	A
3	I	132	U
3	I	133	G
3	I	135	C
3	I	138	G
3	I	139	U
3	I	142	C
3	I	143	A
3	I	144	G
3	I	145	C
3	I	146	C
3	I	148	C
3	I	149	A
3	I	150	C
3	I	151	A
3	I	155	U
3	I	156	C
3	I	157	C
3	I	158	A
3	I	160	G
3	I	162	A
3	I	164	C
3	I	167	U
3	I	168	C
3	I	169	U
3	I	171	U
3	I	172	G
3	I	173	C
3	I	174	G
3	I	177	U
3	I	181	C
3	I	182	A
3	I	183	G
3	I	191	A
3	I	199	A
3	I	200	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	202	C
3	I	203	U
3	I	204	A
3	I	205	A
3	I	206	G
3	I	207	A
3	I	210	U
3	I	212	U
3	I	220	G
3	I	224	U
3	I	225	C
3	I	226	G
4	S	1112	U
4	S	1116	G
4	S	1124	U
4	S	1125	G
4	S	1126	A
4	S	1127	A
4	S	1134	C
4	S	1135	C
4	S	1136	C
4	S	1137	G
4	S	1138	C
4	S	1139	U
4	S	1143	G
4	S	1144	G
4	S	1145	G
4	S	1146	G
4	S	1149	G
4	S	1150	U
4	S	1151	C
4	S	1152	C
4	S	1154	G
4	S	1155	A
6	L5	39	A
6	L5	42	A
6	L5	58	G
6	L5	59	A
6	L5	64	A
6	L5	65	A
6	L5	85	G
6	L5	91	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	98	A
6	L5	109	G
6	L5	119	G
6	L5	127	G
6	L5	134	G
6	L5	135	G
6	L5	136	U
6	L5	159	C
6	L5	171	U
6	L5	172	C
6	L5	184	U
6	L5	185	C
6	L5	187	U
6	L5	188	G
6	L5	200	U
6	L5	201	C
6	L5	209	U
6	L5	218	A
6	L5	219	G
6	L5	234	G
6	L5	266	C
6	L5	297	U
6	L5	309	C
6	L5	315	G
6	L5	316	U
6	L5	326	C
6	L5	334	A
6	L5	340	C
6	L5	362	A
6	L5	363	A
6	L5	387	G
6	L5	409	G
6	L5	410	A
6	L5	412	G
6	L5	413	G
6	L5	440	U
6	L5	449	C
6	L5	450	G
6	L5	452	A
6	L5	453	G
6	L5	454	U
6	L5	463	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	467	U
6	L5	468	U
6	L5	469	C
6	L5	482	U
6	L5	483	G
6	L5	485	U
6	L5	486	C
6	L5	488	G
6	L5	493	U
6	L5	494	G
6	L5	497	G
6	L5	499	C
6	L5	502	U
6	L5	503	C
6	L5	504	U
6	L5	505	C
6	L5	506	G
6	L5	512	U
6	L5	515	U
6	L5	516	U
6	L5	517	C
6	L5	634	C
6	L5	635	G
6	L5	649	C
6	L5	666	C
6	L5	690	C
6	L5	691	G
6	L5	698	C
6	L5	725	G
6	L5	732	C
6	L5	734	G
6	L5	739	G
6	L5	748	C
6	L5	749	C
6	L5	751	G
6	L5	758	C
6	L5	759	G
6	L5	760	C
6	L5	761	C
6	L5	763	C
6	L5	764	G
6	L5	765	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	790	G
6	L5	791	C
6	L5	792	G
6	L5	793	C
6	L5	794	G
6	L5	795	A
6	L5	797	C
6	L5	798	C
6	L5	799	C
6	L5	803	C
6	L5	810	U
6	L5	812	A
6	L5	814	A
6	L5	815	G
6	L5	824	C
6	L5	825	G
6	L5	831	A
6	L5	832	G
6	L5	835	G
6	L5	836	C
6	L5	843	A
6	L5	844	A
6	L5	845	U
6	L5	859	G
6	L5	860	A
6	L5	861	G
6	L5	866	A
6	L5	867	C
6	L5	868	C
6	L5	870	G
6	L5	884	U
6	L5	889	C
6	L5	892	C
6	L5	983	G
6	L5	985	G
6	L5	987	C
6	L5	994	C
6	L5	997	C
6	L5	1016	C
6	L5	1072	C
6	L5	1073	C
6	L5	1074	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	1083	C
6	L5	1084	C
6	L5	1085	G
6	L5	1087	G
6	L5	1091	G
6	L5	1102	G
6	L5	1105	C
6	L5	1106	U
6	L5	1124	A
6	L5	1127	G
6	L5	1129	G
6	L5	1133	C
6	L5	1137	C
6	L5	1202	C
6	L5	1204	C
6	L5	1206	C
6	L5	1207	G
6	L5	1208	C
6	L5	1214	A
6	L5	1215	G
6	L5	1217	G
6	L5	1218	A
6	L5	1219	G
6	L5	1228	G
6	L5	1231	G
6	L5	1239	U
6	L5	1240	G
6	L5	1246	U
6	L5	1247	A
6	L5	1270	A2M
6	L5	1281	A
6	L5	1298	A
6	L5	1299	G
6	L5	1303	G
6	L5	1309	C
6	L5	1310	G
6	L5	1321	G
6	L5	1323	C
6	L5	1331	A
6	L5	1341	A
6	L5	1350	G
6	L5	1351	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	1352	C
6	L5	1362	C
6	L5	1363	C
6	L5	1365	U
6	L5	1368	U
6	L5	1375	A
6	L5	1376	G
6	L5	1391	C
6	L5	1393	C
6	L5	1395	U
6	L5	1398	A
6	L5	1452	A
6	L5	1453	G
6	L5	1457	G
6	L5	1469	U
6	L5	1471	G
6	L5	1477	OMG
6	L5	1489	A2M
6	L5	1502	A
6	L5	1521	C
6	L5	1533	U
6	L5	1546	U
6	L5	1551	U
6	L5	1568	A
6	L5	1579	G
6	L5	1580	OMG
6	L5	1586	A
6	L5	1588	G
6	L5	1589	A
6	L5	1593	A
6	L5	1595	C
6	L5	1609	G
6	L5	1616	C
6	L5	1625	G
6	L5	1631	C
6	L5	1632	PSU
6	L5	1646	G
6	L5	1649	C
6	L5	1653	C
6	L5	1657	C
6	L5	1658	C
6	L5	1673	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	1694	C
6	L5	1704	A
6	L5	1705	A
6	L5	1709	A
6	L5	1712	U
6	L5	1726	A
6	L5	1743	A
6	L5	1745	G
6	L5	1754	G
6	L5	1774	G
6	L5	1775	G
6	L5	1776	A
6	L5	1781	G
6	L5	1794	G
6	L5	1808	G
6	L5	1836	A
6	L5	1857	U
6	L5	1859	C
6	L5	1860	C
6	L5	1861	G
6	L5	1870	C
6	L5	1871	A
6	L5	1879	G
6	L5	1887	G
6	L5	1890	G
6	L5	1893	U
6	L5	1898	U
6	L5	1899	A
6	L5	1900	G
6	L5	1913	U
6	L5	1914	G
6	L5	1915	G
6	L5	1922	A
6	L5	1923	A
6	L5	1925	U
6	L5	1926	C
6	L5	1936	U
6	L5	1942	G
6	L5	1943	U
6	L5	1960	G
6	L5	1963	G
6	L5	1965	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	1985	G
6	L5	1987	U
6	L5	1994	G
6	L5	1995	G
6	L5	2008	A
6	L5	2023	U
6	L5	2032	G
6	L5	2034	A
6	L5	2037	G
6	L5	2041	G
6	L5	2044	A
6	L5	2045	G
6	L5	2046	A
6	L5	2049	G
6	L5	2132	C
6	L5	2143	A
6	L5	2144	G
6	L5	2156	A
6	L5	2159	G
6	L5	2191	G
6	L5	2194	OMC
6	L5	2203	A
6	L5	2238	A
6	L5	2264	G
6	L5	2265	OMC
6	L5	2268	U
6	L5	2269	U
6	L5	2290	U
6	L5	2329	G
6	L5	2332	C
6	L5	2349	G
6	L5	2356	A
6	L5	2372	A
6	L5	2380	A
6	L5	2387	G
6	L5	2388	U
6	L5	2390	G
6	L5	2397	U
6	L5	2407	G
6	L5	2409	G
6	L5	2430	A
6	L5	2432	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	2444	A
6	L5	2445	G
6	L5	2470	C
6	L5	2496	C
6	L5	2503	A
6	L5	2512	C
6	L5	2530	U
6	L5	2537	G
6	L5	2538	A
6	L5	2539	A
6	L5	2546	G
6	L5	2550	U
6	L5	2551	U
6	L5	2552	C
6	L5	2554	G
6	L5	2569	G
6	L5	2578	G
6	L5	2586	A
6	L5	2606	U
6	L5	2612	U
6	L5	2631	U
6	L5	2633	U
6	L5	2641	A
6	L5	2657	C
6	L5	2658	A2M
6	L5	2669	U
6	L5	2670	G
6	L5	2672	U
6	L5	2698	G
6	L5	2745	G
6	L5	3350	C
6	L5	3358	G
6	L5	3362	A
6	L5	3367	A
6	L5	3380	A
6	L5	3385	A
6	L5	3394	A
6	L5	3405	C
6	L5	3412	U
6	L5	3428	C
6	L5	3443	A
6	L5	3444	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	3485	G
6	L5	3492	A2M
6	L5	3493	C
6	L5	3494	PSU
6	L5	3498	A
6	L5	3508	G
6	L5	3509	G
6	L5	3515	A
6	L5	3516	A
6	L5	3543	G
6	L5	3544	C
6	L5	3546	U
6	L5	3549	A
6	L5	3550	U
6	L5	3551	G
6	L5	3570	U
6	L5	3572	U
6	L5	3609	A
6	L5	3610	C
6	L5	3611	G
6	L5	3629	G
6	L5	3633	A
6	L5	3638	A
6	L5	3639	G
6	L5	3640	A
6	L5	3647	U
6	L5	3670	G
6	L5	3674	A
6	L5	3679	A
6	L5	3688	G
6	L5	3689	U
6	L5	3694	A
6	L5	3697	A
6	L5	3698	A
6	L5	3702	G
6	L5	3704	A
6	L5	3708	C
6	L5	3765	C
6	L5	3766	C
6	L5	3767	G
6	L5	3777	U
6	L5	3778	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	3783	U
6	L5	3797	U
6	L5	3798	U
6	L5	3804	G
6	L5	3824	C
6	L5	3825	G
6	L5	3832	G
6	L5	3833	A
6	L5	3834	G
6	L5	3841	U
6	L5	3842	C
6	L5	3846	U
6	L5	3847	C
6	L5	3850	G
6	L5	3855	A
6	L5	3862	G
6	L5	3873	G
6	L5	3875	C
6	L5	3891	C
6	L5	3892	G
6	L5	3904	C
6	L5	3908	C
6	L5	3909	U
6	L5	3916	A
6	L5	3929	G
6	L5	3930	G
6	L5	3937	G
6	L5	3949	A
6	L5	3971	G
6	L5	3975	U
6	L5	3979	A
6	L5	3997	A
6	L5	4000	G
6	L5	4012	G
6	L5	4014	A
6	L5	4017	A
6	L5	4019	A
6	L5	4027	A
6	L5	4035	U
6	L5	4037	G
6	L5	4050	A
6	L5	4051	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	4060	C
6	L5	4076	G
6	L5	4078	C
6	L5	4085	A
6	L5	4096	C
6	L5	4100	U
6	L5	4119	G
6	L5	4123	G
6	L5	4124	A
6	L5	4126	A
6	L5	4133	C
6	L5	4139	G
6	L5	4140	A
6	L5	4161	A
6	L5	4168	A
6	L5	4170	A
6	L5	4194	G
6	L5	4210	A
6	L5	4212	C
6	L5	4221	G
6	L5	4258	U
6	L5	4259	A
6	L5	4261	G
6	L5	4268	G
6	L5	4270	G
6	L5	4294	A
6	L5	4306	C
6	L5	4313	G
6	L5	4316	G
6	L5	4321	G
6	L5	4336	A2M
6	L5	4382	PSU
6	L5	4383	OMG
6	L5	4402	A
6	L5	4416	C
6	L5	4418	A
6	L5	4437	A
6	L5	4446	A
6	L5	4454	A
6	L5	4455	U
6	L5	4465	G
6	L5	4475	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	4476	C
6	L5	4477	G
6	L5	4478	G
6	L5	4479	C
6	L5	4486	G
6	L5	4487	A
6	L5	4488	A
6	L5	4489	G
6	L5	4490	G
6	L5	4501	G
6	L5	4504	C
6	L5	4506	C
6	L5	4508	G
6	L5	4512	G
6	L5	4518	C
6	L5	4609	G
6	L5	4610	C
6	L5	4614	G
6	L5	4621	U
6	L5	4622	C
6	L5	4637	G
6	L5	4638	G
6	L5	4639	C
6	L5	4640	G
6	L5	4641	C
6	L5	4644	C
6	L5	4645	C
6	L5	4646	G
6	L5	4649	A
6	L5	4651	G
6	L5	4658	G
6	L5	4665	C
6	L5	4705	A
6	L5	4715	U
6	L5	4724	U
6	L5	4728	U
6	L5	4729	C
6	L5	4730	U
6	L5	4753	A
6	L5	4756	G
6	L5	4761	U
6	L5	4762	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L5	4763	C
6	L5	4764	C
6	L5	4765	U
6	L5	4766	C
6	L5	4780	G
6	L5	4789	C
6	L5	4793	C
6	L5	4797	A
6	L5	4800	A
6	L5	4801	G
6	L5	4808	U
7	L7	7	G
7	L7	11	A
7	L7	50	A
7	L7	53	U
7	L7	54	A
7	L7	64	G
7	L7	110	G
7	L7	120	U
8	L8	34	U
8	L8	35	C
8	L8	59	A
8	L8	62	A
8	L8	63	U
8	L8	81	C
8	L8	84	A
8	L8	87	G
8	L8	94	G
8	L8	103	A
8	L8	105	C
8	L8	110	U
8	L8	111	U
8	L8	114	G
8	L8	123	U
8	L8	127	U
8	L8	153	C
52	S2	3	C
52	S2	33	G
52	S2	41	G
52	S2	46	A
52	S2	56	G
52	S2	58	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	S2	67	C
52	S2	68	A
52	S2	73	C
52	S2	74	G
52	S2	77	A
52	S2	79	A
52	S2	103	A
52	S2	113	G
52	S2	115	U
52	S2	120	U
52	S2	124	U
52	S2	126	G
52	S2	130	G
52	S2	142	C
52	S2	143	U
52	S2	147	A
52	S2	155	G
52	S2	162	C
52	S2	163	U
52	S2	168	C
52	S2	175	A
52	S2	178	C
52	S2	180	G
52	S2	184	G
52	S2	188	C
52	S2	192	C
52	S2	226	A
52	S2	227	U
52	S2	228	C
52	S2	229	A
52	S2	234	C
52	S2	236	A
52	S2	241	G
52	S2	282	C
52	S2	306	U
52	S2	307	C
52	S2	310	G
52	S2	313	G
52	S2	320	C
52	S2	324	C
52	S2	325	U
52	S2	326	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	S2	327	C
52	S2	328	G
52	S2	336	G
52	S2	348	G
52	S2	363	C
52	S2	365	A
52	S2	369	U
52	S2	370	C
52	S2	386	G
52	S2	387	C
52	S2	401	C
52	S2	410	C
52	S2	422	G
52	S2	439	G
52	S2	449	A
52	S2	451	C
52	S2	453	G
52	S2	465	A
52	S2	466	A
52	S2	471	G
52	S2	473	C
52	S2	474	A
52	S2	475	G
52	S2	483	G
52	S2	488	U
52	S2	493	C
52	S2	502	C
52	S2	509	A
52	S2	510	OMG
52	S2	518	OMC
52	S2	536	G
52	S2	549	C
52	S2	560	G
52	S2	569	C
52	S2	584	A
52	S2	588	A
52	S2	590	G
52	S2	592	U
52	S2	607	G
52	S2	609	C
52	S2	615	C
52	S2	628	OMU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	S2	629	A
52	S2	632	U
52	S2	633	C
52	S2	644	A
52	S2	645	OMG
52	S2	656	A
52	S2	661	C
52	S2	669	A2M
52	S2	670	A
52	S2	672	A
52	S2	673	A
52	S2	674	G
52	S2	684	OMG
52	S2	690	U
52	S2	697	G
52	S2	698	G
52	S2	728	G
52	S2	730	C
52	S2	735	C
52	S2	737	C
52	S2	747	C
52	S2	748	U
52	S2	750	U
52	S2	754	C
52	S2	755	G
52	S2	756	C
52	S2	757	C
52	S2	796	A
52	S2	798	C
52	S2	799	G
52	S2	800	U
52	S2	802	PSU
52	S2	810	A
52	S2	812	A
52	S2	822	G
52	S2	823	PSU
52	S2	828	A
52	S2	831	A
52	S2	832	G
52	S2	837	G
52	S2	838	A
52	S2	839	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	S2	840	C
52	S2	841	C
52	S2	842	G
52	S2	848	A
52	S2	871	A
52	S2	873	A
52	S2	879	G
52	S2	892	G
52	S2	893	U
52	S2	896	G
52	S2	901	C
52	S2	906	C
52	S2	910	G
52	S2	914	A
52	S2	915	U
52	S2	921	A
52	S2	923	A
52	S2	931	C
52	S2	934	G
52	S2	944	U
52	S2	956	A
52	S2	964	A
52	S2	972	G
52	S2	991	A
52	S2	993	A
52	S2	1000	G
52	S2	1018	U
52	S2	1024	A
52	S2	1061	A
52	S2	1062	U
52	S2	1063	A
52	S2	1084	A
52	S2	1086	C
52	S2	1116	U
52	S2	1117	C
52	S2	1118	C
52	S2	1119	C
52	S2	1122	G
52	S2	1124	C
52	S2	1134	A
52	S2	1145	A
52	S2	1150	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	S2	1151	A
52	S2	1154	C
52	S2	1155	U
52	S2	1196	A
52	S2	1208	G
52	S2	1216	C
52	S2	1222	G
52	S2	1225	G
52	S2	1243	U
52	S2	1249	U
52	S2	1252	A
52	S2	1254	A
52	S2	1257	G
52	S2	1258	G
52	S2	1260	A
52	S2	1266	A
52	S2	1275	G
52	S2	1276	G
52	S2	1283	A
52	S2	1286	G
52	S2	1287	G
52	S2	1292	A
52	S2	1294	A
52	S2	1296	A
52	S2	1303	G
52	S2	1304	C
52	S2	1305	U
52	S2	1316	U
52	S2	1343	U
52	S2	1359	U
52	S2	1372	U
52	S2	1373	U
52	S2	1379	A
52	S2	1398	U
52	S2	1406	A
52	S2	1407	G
52	S2	1419	C
52	S2	1420	C
52	S2	1422	A
52	S2	1423	G
52	S2	1424	C
52	S2	1436	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	S2	1438	C
52	S2	1448	OMG
52	S2	1455	A
52	S2	1463	U
52	S2	1464	U
52	S2	1481	A
52	S2	1488	A
52	S2	1490	A
52	S2	1491	OMG
52	S2	1498	G
52	S2	1510	U
52	S2	1522	C
52	S2	1523	A
52	S2	1534	A
52	S2	1553	G
52	S2	1571	G
52	S2	1579	U
52	S2	1581	A
52	S2	1586	U
52	S2	1587	U
52	S2	1589	A
52	S2	1602	A
52	S2	1622	U
52	S2	1624	A
52	S2	1655	G
52	S2	1662	A
52	S2	1666	G
52	S2	1699	C
52	S2	1700	A
52	S2	1722	U
52	S2	1723	G
52	S2	1765	G
52	S2	1780	G
52	S2	1782	A
52	S2	1783	G
52	S2	1784	C
52	S2	1785	G
52	S2	1787	U
52	S2	1825	A
52	S2	1827	G
52	S2	1830	G
52	S2	1836	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	S2	1837	G
52	S2	1839	U
52	S2	1850	G
52	S2	1862	G
52	S2	1863	G
52	S2	1864	A
52	S2	1865	U
52	S2	1866	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	I	66	G
4	S	1111	A
6	L5	1588	G
6	L5	1892	U
6	L5	4445	U
52	S2	1265	C

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

218 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	$\#\|Z\| > 2$
52	PSU	S2	1348	52	18,21,22	1.38	3 (16%)	22,30,33	1.81	3 (13%)
6	PSU	L5	4058	6	18,21,22	1.37	3 (16%)	22,30,33	1.80	5 (22%)
52	OMG	S2	868	52	18,26,27	1.95	2 (11%)	19,38,41	1.67	4 (21%)
6	OMC	L5	1284	6	19,22,23	1.16	2 (10%)	26,31,34	0.86	0
6	PSU	L5	3496	6	18,21,22	1.37	3 (16%)	22,30,33	1.84	5 (22%)
52	PSU	S2	864	52,82	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
47	MLZ	Lq	53	47	8,9,10	0.46	0	4,9,11	0.08	0
6	OMU	L5	3973	6	19,22,23	1.00	2 (10%)	26,31,34	1.83	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	A2M	L5	3450	6	18,25,26	1.90	5 (27%)	18,36,39	2.15	4 (22%)
6	PSU	L5	3369	6,90,89	18,21,22	1.29	3 (16%)	22,30,33	1.87	4 (18%)
6	PSU	L5	4322	6	18,21,22	1.39	3 (16%)	22,30,33	1.79	5 (22%)
52	PSU	S2	610	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	4 (18%)
52	7MG	S2	1640	52	22,26,27	1.22	2 (9%)	29,39,42	2.14	9 (31%)
6	OMC	L5	2647	6	19,22,23	1.14	2 (10%)	26,31,34	0.88	1 (3%)
52	4AC	S2	1338	52	21,24,25	1.12	2 (9%)	29,34,37	1.21	3 (10%)
6	OMG	L5	4245	6	18,26,27	1.98	2 (11%)	19,38,41	1.67	5 (26%)
52	PSU	S2	967	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	4 (18%)
49	SAC	Ls	2	49	7,8,9	0.53	0	8,9,11	0.84	1 (12%)
6	OMG	L5	4383	6,90	18,26,27	1.97	2 (11%)	19,38,41	1.68	5 (26%)
52	PSU	S2	682	52	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
6	PSU	L5	4217	6,16	18,21,22	1.34	3 (16%)	22,30,33	1.81	5 (22%)
52	OMG	S2	1329	52	18,26,27	1.95	2 (11%)	19,38,41	1.68	5 (26%)
6	PSU	L5	4169	6	18,21,22	1.37	3 (16%)	22,30,33	1.85	5 (22%)
6	OMG	L5	2267	6	18,26,27	1.98	2 (11%)	19,38,41	1.66	4 (21%)
52	OMC	S2	518	52	19,22,23	1.15	2 (10%)	26,31,34	0.91	1 (3%)
52	OMU	S2	172	52	19,22,23	0.99	2 (10%)	26,31,34	1.85	7 (26%)
6	PSU	L5	4099	6	18,21,22	1.35	3 (16%)	22,30,33	1.90	5 (22%)
6	PSU	L5	1683	6,90	18,21,22	1.36	3 (16%)	22,30,33	1.82	4 (18%)
6	PSU	L5	3490	6	18,21,22	1.35	3 (16%)	22,30,33	1.81	4 (18%)
6	PSU	L5	1801	6,17	18,21,22	1.35	3 (16%)	22,30,33	1.83	3 (13%)
6	PSU	L5	1491	6	18,21,22	1.34	3 (16%)	22,30,33	1.85	4 (18%)
6	PSU	L5	1718	6,12	18,21,22	1.35	3 (16%)	22,30,33	1.82	4 (18%)
52	PSU	S2	1368	52	18,21,22	1.41	3 (16%)	22,30,33	1.85	5 (22%)
79	NMM	Se	67	79	9,11,12	1.56	1 (11%)	6,12,14	3.48	2 (33%)
6	OMC	L5	1820	6,89	19,22,23	1.15	2 (10%)	26,31,34	0.89	0
52	PSU	S2	93	52	18,21,22	1.42	3 (16%)	22,30,33	1.76	3 (13%)
52	OMU	S2	116	52	19,22,23	1.01	2 (10%)	26,31,34	1.80	6 (23%)
6	A2M	L5	1810	6,89	18,25,26	1.95	5 (27%)	18,36,39	2.26	6 (33%)
6	PSU	L5	4278	6	18,21,22	1.38	3 (16%)	22,30,33	1.79	4 (18%)
52	OMU	S2	429	52	19,22,23	1.02	2 (10%)	26,31,34	1.79	5 (19%)
10	HIC	LE	245	10	8,11,12	0.86	0	6,14,16	0.81	0
6	OMC	L5	2667	6	19,22,23	1.14	2 (10%)	26,31,34	0.87	0
52	PSU	S2	1046	52	18,21,22	1.35	3 (16%)	22,30,33	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
52	OMU	S2	628	52	19,22,23	1.01	2 (10%)	26,31,34	1.82	6 (23%)
6	PSU	L5	1632	6	18,21,22	1.41	3 (16%)	22,30,33	1.74	4 (18%)
6	PSU	L5	3585	6,89	18,21,22	1.32	3 (16%)	22,30,33	1.83	4 (18%)
52	PSU	S2	1233	52	18,21,22	1.37	3 (16%)	22,30,33	1.81	5 (22%)
6	OMG	L5	1260	6,38	18,26,27	2.00	2 (11%)	19,38,41	1.73	5 (26%)
52	A2M	S2	1679	52	18,25,26	1.97	5 (27%)	18,36,39	2.13	4 (22%)
52	PSU	S2	34	52	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
6	A2M	L5	1270	6	18,25,26	1.89	5 (27%)	18,36,39	2.16	5 (27%)
6	A2M	L5	2658	6,89	18,25,26	1.95	5 (27%)	18,36,39	2.11	5 (27%)
52	OMC	S2	1704	52,89	19,22,23	1.13	2 (10%)	26,31,34	0.89	1 (3%)
6	A2M	L5	4269	6,89	18,25,26	1.96	5 (27%)	18,36,39	2.21	5 (27%)
6	PSU	L5	3576	6	18,21,22	1.36	3 (16%)	22,30,33	1.77	4 (18%)
6	PSU	L5	1799	6	18,21,22	1.38	3 (16%)	22,30,33	1.86	5 (22%)
52	MA6	S2	1851	52	19,26,27	0.94	1 (5%)	18,38,41	1.71	6 (33%)
52	PSU	S2	823	52	18,21,22	1.40	3 (16%)	22,30,33	1.80	4 (18%)
6	PSU	L5	4203	6	18,21,22	1.33	3 (16%)	22,30,33	1.81	4 (18%)
52	PSU	S2	1239	52	18,21,22	1.37	3 (16%)	22,30,33	1.83	5 (22%)
52	PSU	S2	1626	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	5 (22%)
52	PSU	S2	1245	52	18,21,22	1.36	3 (16%)	22,30,33	1.85	4 (18%)
6	A2M	L5	3599	6	18,25,26	1.92	5 (27%)	18,36,39	2.13	5 (27%)
6	OMG	L5	3942	6	18,26,27	1.96	2 (11%)	19,38,41	1.66	4 (21%)
52	PSU	S2	1693	52	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
11	AYA	LF	2	11	6,7,8	0.75	0	5,8,10	0.25	0
6	PSU	L5	4042	6	18,21,22	1.36	3 (16%)	22,30,33	1.87	4 (18%)
52	PSU	S2	867	52	18,21,22	1.44	3 (16%)	22,30,33	1.81	4 (18%)
6	PSU	L5	1720	6	18,21,22	1.36	3 (16%)	22,30,33	1.82	5 (22%)
6	OMG	L5	4116	6	18,26,27	1.97	2 (11%)	19,38,41	1.68	5 (26%)
6	PSU	L5	4188	6	18,21,22	1.33	3 (16%)	22,30,33	1.93	4 (18%)
6	PSU	L5	2475	6	18,21,22	1.37	3 (16%)	22,30,33	1.82	5 (22%)
52	PSU	S2	815	52	18,21,22	1.38	3 (16%)	22,30,33	1.83	4 (18%)
6	OMG	L5	4240	6	18,26,27	1.99	2 (11%)	19,38,41	1.69	5 (26%)
6	PSU	L5	4374	6	18,21,22	1.36	3 (16%)	22,30,33	1.82	5 (22%)
52	PSU	S2	1644	52,89	18,21,22	1.36	3 (16%)	22,30,33	1.83	4 (18%)
52	PSU	S2	105	52	18,21,22	1.39	3 (16%)	22,30,33	1.81	4 (18%)
52	PSU	S2	802	52	18,21,22	1.40	3 (16%)	22,30,33	1.77	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	6MZ	L5	3966	6,27	18,25,26	0.82	1 (5%)	16,36,39	2.03	4 (25%)
6	PSU	L5	3466	6	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
52	OMU	S2	1805	52	19,22,23	0.98	2 (10%)	26,31,34	1.80	5 (19%)
52	MA6	S2	1852	52	19,26,27	0.96	1 (5%)	18,38,41	1.66	5 (27%)
6	OMU	L5	4052	6,24	19,22,23	1.00	2 (10%)	26,31,34	1.74	4 (15%)
6	PSU	L5	3500	6	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
6	OMG	L5	2207	6	18,26,27	2.00	2 (11%)	19,38,41	1.67	4 (21%)
52	PSU	S2	407	52	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
6	PSU	L5	1731	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	4 (18%)
52	OMG	S2	437	52	18,26,27	1.96	2 (11%)	19,38,41	1.66	4 (21%)
6	A2M	L5	3557	6	18,25,26	1.93	5 (27%)	18,36,39	2.13	4 (22%)
6	PSU	L5	1537	6	18,21,22	1.38	3 (16%)	22,30,33	1.81	4 (18%)
6	A2M	L5	4317	6	18,25,26	1.96	5 (27%)	18,36,39	2.11	4 (22%)
6	OMC	L5	3601	6	19,22,23	1.16	2 (10%)	26,31,34	0.89	0
6	OMC	L5	4282	6	19,22,23	1.15	2 (10%)	26,31,34	0.91	1 (3%)
6	A2M	L5	3492	6,89	18,25,26	2.00	5 (27%)	18,36,39	2.17	5 (27%)
52	A2M	S2	99	52,89	18,25,26	1.98	5 (27%)	18,36,39	2.12	5 (27%)
52	A2M	S2	27	52	18,25,26	1.97	5 (27%)	18,36,39	2.12	4 (22%)
52	A2M	S2	159	52	18,25,26	1.96	5 (27%)	18,36,39	2.09	5 (27%)
8	OMG	L8	75	8	18,26,27	1.98	2 (11%)	19,38,41	1.65	4 (21%)
52	OMU	S2	1443	52,89	19,22,23	0.99	2 (10%)	26,31,34	1.74	4 (15%)
6	PSU	L5	4039	6	18,21,22	1.35	3 (16%)	22,30,33	1.87	5 (22%)
6	PSU	L5	4419	6	18,21,22	1.34	3 (16%)	22,30,33	1.84	5 (22%)
52	OMU	S2	121	52	19,22,23	0.99	2 (10%)	26,31,34	1.75	5 (19%)
52	A2M	S2	513	52	18,25,26	1.97	5 (27%)	18,36,39	2.15	4 (22%)
52	OMG	S2	645	52	18,26,27	1.96	2 (11%)	19,38,41	1.73	5 (26%)
6	PSU	L5	3371	6	18,21,22	1.33	3 (16%)	22,30,33	1.82	5 (22%)
6	PSU	L5	4166	6	18,21,22	1.38	3 (16%)	22,30,33	1.79	4 (18%)
6	OMG	L5	4364	6	18,26,27	1.97	2 (11%)	19,38,41	1.68	5 (26%)
6	A2M	L5	400	6	18,25,26	1.98	5 (27%)	18,36,39	2.15	4 (22%)
6	OMU	L5	4244	6	19,22,23	1.00	2 (10%)	26,31,34	1.83	5 (19%)
6	A2M	L5	3456	6	18,25,26	1.96	5 (27%)	18,36,39	2.10	4 (22%)
6	PSU	L5	2351	6	18,21,22	1.34	3 (16%)	22,30,33	1.86	4 (18%)
6	PSU	L5	3616	6	18,21,22	1.34	3 (16%)	22,30,33	1.86	5 (22%)
52	A2M	S2	577	52	18,25,26	1.98	5 (27%)	18,36,39	2.25	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	A2M	L5	4336	6	18,25,26	1.99	5 (27%)	18,36,39	2.26	5 (27%)
52	PSU	S2	650	52	18,21,22	1.38	3 (16%)	22,30,33	1.83	4 (18%)
52	PSU	S2	1057	52	18,21,22	1.37	3 (16%)	22,30,33	1.84	5 (22%)
6	A2M	L5	1479	6	18,25,26	1.89	5 (27%)	18,36,39	2.22	4 (22%)
6	PSU	L5	3652	6,89	18,21,22	1.31	3 (16%)	22,30,33	1.86	4 (18%)
6	PSU	L5	3427	6	18,21,22	1.36	3 (16%)	22,30,33	1.81	5 (22%)
35	MLZ	Le	5	35	8,9,10	0.47	0	4,9,11	0.13	0
6	A2M	L5	2244	6	18,25,26	1.95	5 (27%)	18,36,39	2.20	5 (27%)
6	A2M	L5	398	6	18,25,26	1.95	5 (27%)	18,36,39	2.15	5 (27%)
6	OMG	L5	3476	6	18,26,27	1.98	2 (11%)	19,38,41	1.68	4 (21%)
6	OMC	L5	4202	6	19,22,23	1.14	2 (10%)	26,31,34	0.93	1 (3%)
52	4AC	S2	1843	86,52	21,24,25	1.15	2 (9%)	29,34,37	1.10	2 (6%)
52	OMC	S2	1392	52	19,22,23	1.16	2 (10%)	26,31,34	0.94	1 (3%)
6	A2M	L5	2206	6,89	18,25,26	1.95	5 (27%)	18,36,39	2.15	5 (27%)
81	AME	Sg	1	81	9,10,11	0.47	0	9,11,13	0.88	1 (11%)
52	PSU	S2	109	52	18,21,22	1.42	3 (16%)	22,30,33	1.80	5 (22%)
52	A2M	S2	166	52	18,25,26	2.00	5 (27%)	18,36,39	2.21	6 (33%)
6	PSU	L5	3583	6	18,21,22	1.33	3 (16%)	22,30,33	1.90	5 (22%)
52	6MZ	S2	1833	52,89	18,25,26	0.87	1 (5%)	16,36,39	1.81	4 (25%)
78	SAC	Sd	2	78	7,8,9	0.52	0	8,9,11	0.90	1 (12%)
6	OMC	L5	2194	6	19,22,23	1.11	2 (10%)	26,31,34	0.95	1 (3%)
6	OMC	L5	3619	6,22	19,22,23	1.14	2 (10%)	26,31,34	0.93	1 (3%)
6	PSU	L5	4246	6	18,21,22	1.39	3 (16%)	22,30,33	1.88	5 (22%)
6	PSU	L5	4740	6,10	18,21,22	1.38	3 (16%)	22,30,33	1.78	3 (13%)
52	PSU	S2	1082	52	18,21,22	1.33	3 (16%)	22,30,33	1.82	4 (18%)
6	OMG	L5	3359	6	18,26,27	1.97	2 (11%)	19,38,41	1.69	5 (26%)
52	PSU	S2	119	52	18,21,22	1.41	3 (16%)	22,30,33	1.78	4 (18%)
52	OMU	S2	355	52,71	19,22,23	0.98	2 (10%)	26,31,34	1.83	5 (19%)
52	PSU	S2	652	52	18,21,22	1.39	3 (16%)	22,30,33	1.84	4 (18%)
52	PSU	S2	1047	52	18,21,22	1.39	3 (16%)	22,30,33	1.79	4 (18%)
6	5MC	L5	3514	6,89	18,22,23	1.27	3 (16%)	26,32,35	1.26	4 (15%)
52	A2M	S2	1384	52	18,25,26	2.01	5 (27%)	18,36,39	2.18	5 (27%)
6	PSU	L5	3554	6	18,21,22	1.36	3 (16%)	22,30,33	1.81	5 (22%)
52	OMG	S2	1448	52	18,26,27	1.96	2 (11%)	19,38,41	1.65	4 (21%)
46	M3L	Lp	98	46	10,11,12	0.51	0	9,14,16	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
52	A2M	S2	485	52	18,25,26	1.91	5 (27%)	18,36,39	2.22	4 (22%)
6	PSU	L5	3447	6	18,21,22	1.36	3 (16%)	22,30,33	1.81	4 (18%)
52	PSU	S2	1446	52	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
6	UR3	L5	4276	6	19,22,23	1.30	3 (15%)	26,32,35	1.20	2 (7%)
52	A2M	S2	669	52,89	18,25,26	1.86	5 (27%)	18,36,39	2.21	4 (22%)
52	PSU	S2	816	52	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
6	PSU	L5	1638	6,90,34	18,21,22	1.34	3 (16%)	22,30,33	1.87	5 (22%)
8	PSU	L8	69	8	18,21,22	1.36	3 (16%)	22,30,33	1.90	5 (22%)
6	A2M	L5	3562	6	18,25,26	1.92	5 (27%)	18,36,39	2.18	5 (27%)
6	5MC	L5	4193	6	18,22,23	1.24	3 (16%)	26,32,35	1.53	3 (11%)
52	PSU	S2	1005	52	18,21,22	1.63	5 (27%)	22,30,33	2.85	6 (27%)
6	PSU	L5	4435	6	18,21,22	1.35	3 (16%)	22,30,33	1.84	4 (18%)
6	OMG	L5	1477	6,11	18,26,27	1.97	2 (11%)	19,38,41	1.69	4 (21%)
52	A2M	S2	469	52	18,25,26	1.96	5 (27%)	18,36,39	2.18	5 (27%)
6	PSU	L5	4149	6	18,21,22	1.33	3 (16%)	22,30,33	1.93	5 (22%)
52	PSU	S2	1178	52	18,21,22	1.39	3 (16%)	22,30,33	1.80	4 (18%)
6	OMG	L5	3631	6	18,26,27	2.01	2 (11%)	19,38,41	1.70	5 (26%)
6	PSU	L5	3494	6	18,21,22	1.39	3 (16%)	22,30,33	1.78	5 (22%)
6	PSU	L5	4325	6	18,21,22	1.35	3 (16%)	22,30,33	1.85	5 (22%)
52	OMG	S2	1491	52,89	18,26,27	1.97	2 (11%)	19,38,41	1.66	4 (21%)
6	OMG	L5	1580	6	18,26,27	1.98	2 (11%)	19,38,41	1.67	4 (21%)
52	PSU	S2	218	52	18,21,22	1.38	3 (16%)	22,30,33	1.81	4 (18%)
6	PSU	L5	3502	6	18,21,22	1.39	3 (16%)	22,30,33	1.83	4 (18%)
6	PSU	L5	4177	6	18,21,22	1.33	3 (16%)	22,30,33	1.86	5 (22%)
52	PSU	S2	573	84,52	18,21,22	1.43	3 (16%)	22,30,33	1.84	4 (18%)
6	PSU	L5	4045	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	4 (18%)
6	1MA	L5	1266	6,89	16,25,26	2.54	3 (18%)	18,37,40	2.27	3 (16%)
6	OMC	L5	3433	6,90	19,22,23	1.16	2 (10%)	26,31,34	0.92	1 (3%)
6	PSU	L5	4298	6	18,21,22	1.34	3 (16%)	22,30,33	1.83	4 (18%)
6	OMC	L5	3573	6	19,22,23	1.13	2 (10%)	26,31,34	0.89	2 (7%)
6	PSU	L5	4711	6	18,21,22	1.35	3 (16%)	22,30,33	1.82	5 (22%)
6	OMG	L5	3974	6	18,26,27	1.98	2 (11%)	19,38,41	1.70	4 (21%)
83	HY3	Si	62	83	6,8,9	1.32	1 (16%)	5,10,12	1.43	1 (20%)
6	OMG	L5	4138	6	18,26,27	1.98	2 (11%)	19,38,41	1.70	5 (26%)
52	OMU	S2	1289	55,52	19,22,23	0.97	1 (5%)	26,31,34	1.76	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PSU	L5	3462	6	18,21,22	1.38	3 (16%)	22,30,33	1.80	5 (22%)
6	A2M	L5	3517	6	18,25,26	1.79	4 (22%)	18,36,39	2.28	5 (27%)
6	OMC	L5	3540	6	19,22,23	1.10	2 (10%)	26,31,34	0.89	2 (7%)
6	OMC	L5	2704	6	19,22,23	1.14	2 (10%)	26,31,34	0.86	0
52	PSU	S2	687	67,52	18,21,22	1.41	3 (16%)	22,30,33	1.84	5 (22%)
6	OMG	L5	2719	6	18,26,27	1.97	2 (11%)	19,38,41	1.68	5 (26%)
52	OMC	S2	463	52	19,22,23	1.16	2 (10%)	26,31,34	0.90	0
52	OMG	S2	602	52	18,26,27	1.96	2 (11%)	19,38,41	1.66	5 (26%)
6	A2M	L5	1489	6,89	18,25,26	1.91	5 (27%)	18,36,39	2.10	3 (16%)
6	PSU	L5	4382	6,37	18,21,22	1.42	4 (22%)	22,30,33	2.01	3 (13%)
8	PSU	L8	55	8	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
6	OMG	L5	3676	6	18,26,27	1.94	2 (11%)	19,38,41	1.68	4 (21%)
52	PSU	S2	210	52	18,21,22	1.45	3 (16%)	22,30,33	1.84	4 (18%)
6	OMU	L5	2680	6	19,22,23	0.99	2 (10%)	26,31,34	1.82	6 (23%)
52	OMC	S2	174	52	19,22,23	1.20	3 (15%)	26,31,34	0.88	0
6	PSU	L5	1721	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	5 (22%)
6	OMG	L5	4369	6	18,26,27	1.98	2 (11%)	19,38,41	1.68	4 (21%)
52	OMU	S2	1327	52,89	19,22,23	1.00	2 (10%)	26,31,34	1.79	5 (19%)
6	OMC	L5	2208	6,89	19,22,23	1.13	2 (10%)	26,31,34	0.91	1 (3%)
6	A2M	L5	2630	6	18,25,26	1.97	5 (27%)	18,36,39	2.34	5 (27%)
52	OMG	S2	510	52,89	18,26,27	1.96	2 (11%)	19,38,41	1.69	5 (26%)
6	PSU	L5	4107	6	18,21,22	1.33	3 (16%)	22,30,33	1.79	3 (13%)
6	PSU	L5	4749	6	18,21,22	1.39	3 (16%)	22,30,33	1.84	4 (18%)
6	PSU	L5	4267	6,89	18,21,22	1.33	3 (16%)	22,30,33	1.93	4 (18%)
6	OMC	L5	2265	6,89	19,22,23	1.12	2 (10%)	26,31,34	0.90	2 (7%)
6	OMG	L5	3524	6	18,26,27	1.97	2 (11%)	19,38,41	1.67	5 (26%)
52	A2M	S2	591	52	18,25,26	2.00	5 (27%)	18,36,39	2.31	5 (27%)
52	OMG	S2	684	52	18,26,27	1.96	2 (11%)	19,38,41	1.74	5 (26%)
60	SAC	SL	2	60	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
6	OMU	L5	2258	6	19,22,23	0.99	2 (10%)	26,31,34	1.77	5 (19%)
6	OMU	L5	3657	6	19,22,23	1.01	2 (10%)	26,31,34	1.82	5 (19%)
52	A2M	S2	1032	52	18,25,26	1.92	5 (27%)	18,36,39	2.14	4 (22%)
6	OMU	L5	4366	6,29	19,22,23	1.00	2 (10%)	26,31,34	1.81	6 (23%)
52	PSU	S2	1175	52	18,21,22	1.36	3 (16%)	22,30,33	1.84	5 (22%)
52	PSU	S2	36	52	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)

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
52	PSU	S2	1348	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4058	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	868	52	-	0/5/27/28	0/3/3/3
6	OMC	L5	1284	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	3496	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	864	52,82	-	0/7/25/26	0/2/2/2
47	MLZ	Lq	53	47	-	0/7/8/10	-
6	OMU	L5	3973	6	-	0/9/27/28	0/2/2/2
6	A2M	L5	3450	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	3369	6,90,89	-	0/7/25/26	0/2/2/2
6	PSU	L5	4322	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	610	52	-	0/7/25/26	0/2/2/2
52	7MG	S2	1640	52	-	0/7/37/38	0/3/3/3
6	OMC	L5	2647	6	-	0/9/27/28	0/2/2/2
52	4AC	S2	1338	52	-	4/11/29/30	0/2/2/2
6	OMG	L5	4245	6	-	0/5/27/28	0/3/3/3
52	PSU	S2	967	52	-	0/7/25/26	0/2/2/2
49	SAC	Ls	2	49	-	0/7/8/10	-
6	OMG	L5	4383	6,90	-	0/5/27/28	0/3/3/3
52	PSU	S2	682	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4217	6,16	-	0/7/25/26	0/2/2/2
52	OMG	S2	1329	52	-	0/5/27/28	0/3/3/3
6	PSU	L5	4169	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	2267	6	-	0/5/27/28	0/3/3/3
52	OMC	S2	518	52	-	2/9/27/28	0/2/2/2
52	OMU	S2	172	52	-	0/9/27/28	0/2/2/2
6	PSU	L5	4099	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1683	6,90	-	0/7/25/26	0/2/2/2
6	PSU	L5	3490	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1801	6,17	-	0/7/25/26	0/2/2/2
6	PSU	L5	1491	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1718	6,12	-	0/7/25/26	0/2/2/2
52	PSU	S2	1368	52	-	0/7/25/26	0/2/2/2
79	NMM	Se	67	79	-	3/9/11/13	-
6	OMC	L5	1820	6,89	-	0/9/27/28	0/2/2/2
52	PSU	S2	93	52	-	0/7/25/26	0/2/2/2
52	OMU	S2	116	52	-	0/9/27/28	0/2/2/2
6	A2M	L5	1810	6,89	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	L5	4278	6	-	0/7/25/26	0/2/2/2
52	OMU	S2	429	52	-	4/9/27/28	0/2/2/2
10	HIC	LE	245	10	-	1/5/6/8	0/1/1/1
6	OMC	L5	2667	6	-	0/9/27/28	0/2/2/2
52	PSU	S2	1046	52	-	0/7/25/26	0/2/2/2
52	OMU	S2	628	52	-	6/9/27/28	0/2/2/2
6	PSU	L5	1632	6	-	1/7/25/26	0/2/2/2
6	PSU	L5	3585	6,89	-	0/7/25/26	0/2/2/2
52	PSU	S2	1233	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	1260	6,38	-	0/5/27/28	0/3/3/3
52	A2M	S2	1679	52	-	0/5/27/28	0/3/3/3
52	PSU	S2	34	52	-	0/7/25/26	0/2/2/2
6	A2M	L5	1270	6	-	1/5/27/28	0/3/3/3
6	A2M	L5	2658	6,89	-	1/5/27/28	0/3/3/3
52	OMC	S2	1704	52,89	-	0/9/27/28	0/2/2/2
6	A2M	L5	4269	6,89	-	0/5/27/28	0/3/3/3
6	PSU	L5	3576	6	-	1/7/25/26	0/2/2/2
6	PSU	L5	1799	6	-	0/7/25/26	0/2/2/2
52	MA6	S2	1851	52	-	2/7/29/30	0/3/3/3
52	PSU	S2	823	52	-	2/7/25/26	0/2/2/2
6	PSU	L5	4203	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1239	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1626	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1245	52	-	0/7/25/26	0/2/2/2
6	A2M	L5	3599	6	-	0/5/27/28	0/3/3/3
6	OMG	L5	3942	6	-	0/5/27/28	0/3/3/3
52	PSU	S2	1693	52	-	0/7/25/26	0/2/2/2
11	AYA	LF	2	11	-	2/4/6/8	-
6	PSU	L5	4042	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	867	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	1720	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	4116	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	4188	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	2475	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	815	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	4240	6	-	1/5/27/28	0/3/3/3
6	PSU	L5	4374	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1644	52,89	-	0/7/25/26	0/2/2/2
52	PSU	S2	105	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	802	52	-	3/7/25/26	0/2/2/2
6	6MZ	L5	3966	6,27	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	L5	3466	6	-	0/7/25/26	0/2/2/2
52	OMU	S2	1805	52	-	0/9/27/28	0/2/2/2
52	MA6	S2	1852	52	-	2/7/29/30	0/3/3/3
6	OMU	L5	4052	6,24	-	0/9/27/28	0/2/2/2
6	PSU	L5	3500	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	2207	6	-	0/5/27/28	0/3/3/3
52	PSU	S2	407	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	1731	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	437	52	-	0/5/27/28	0/3/3/3
6	A2M	L5	3557	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	1537	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	4317	6	-	0/5/27/28	0/3/3/3
6	OMC	L5	3601	6	-	0/9/27/28	0/2/2/2
6	OMC	L5	4282	6	-	0/9/27/28	0/2/2/2
6	A2M	L5	3492	6,89	-	3/5/27/28	0/3/3/3
52	A2M	S2	99	52,89	-	1/5/27/28	0/3/3/3
52	A2M	S2	27	52	-	0/5/27/28	0/3/3/3
52	A2M	S2	159	52	-	0/5/27/28	0/3/3/3
8	OMG	L8	75	8	-	0/5/27/28	0/3/3/3
52	OMU	S2	1443	52,89	-	0/9/27/28	0/2/2/2
6	PSU	L5	4039	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4419	6	-	0/7/25/26	0/2/2/2
52	OMU	S2	121	52	-	0/9/27/28	0/2/2/2
52	A2M	S2	513	52	-	0/5/27/28	0/3/3/3
52	OMG	S2	645	52	-	3/5/27/28	0/3/3/3
6	PSU	L5	3371	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4166	6	-	2/7/25/26	0/2/2/2
6	OMG	L5	4364	6	-	0/5/27/28	0/3/3/3
6	A2M	L5	400	6	-	0/5/27/28	0/3/3/3
6	OMU	L5	4244	6	-	0/9/27/28	0/2/2/2
6	A2M	L5	3456	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	2351	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3616	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	577	52	-	1/5/27/28	0/3/3/3
6	A2M	L5	4336	6	-	2/5/27/28	0/3/3/3
52	PSU	S2	650	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1057	52	-	0/7/25/26	0/2/2/2
6	A2M	L5	1479	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	3652	6,89	-	0/7/25/26	0/2/2/2
6	PSU	L5	3427	6	-	0/7/25/26	0/2/2/2
35	MLZ	Le	5	35	-	2/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A2M	L5	2244	6	-	1/5/27/28	0/3/3/3
6	A2M	L5	398	6	-	0/5/27/28	0/3/3/3
6	OMG	L5	3476	6	-	0/5/27/28	0/3/3/3
6	OMC	L5	4202	6	-	0/9/27/28	0/2/2/2
52	4AC	S2	1843	86,52	-	2/11/29/30	0/2/2/2
52	OMC	S2	1392	52	-	2/9/27/28	0/2/2/2
6	A2M	L5	2206	6,89	-	0/5/27/28	0/3/3/3
81	AME	Sg	1	81	-	2/9/10/12	-
52	PSU	S2	109	52	-	0/7/25/26	0/2/2/2
52	A2M	S2	166	52	-	0/5/27/28	0/3/3/3
6	PSU	L5	3583	6	-	0/7/25/26	0/2/2/2
52	6MZ	S2	1833	52,89	-	1/5/27/28	0/3/3/3
78	SAC	Sd	2	78	-	0/7/8/10	-
6	OMC	L5	2194	6	-	1/9/27/28	0/2/2/2
6	OMC	L5	3619	6,22	-	2/9/27/28	0/2/2/2
6	PSU	L5	4246	6	-	1/7/25/26	0/2/2/2
6	PSU	L5	4740	6,10	-	0/7/25/26	0/2/2/2
52	PSU	S2	1082	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	3359	6	-	0/5/27/28	0/3/3/3
52	PSU	S2	119	52	-	0/7/25/26	0/2/2/2
52	OMU	S2	355	52,71	-	0/9/27/28	0/2/2/2
52	PSU	S2	652	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1047	52	-	0/7/25/26	0/2/2/2
6	5MC	L5	3514	6,89	-	0/7/25/26	0/2/2/2
52	A2M	S2	1384	52	-	0/5/27/28	0/3/3/3
6	PSU	L5	3554	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	1448	52	-	3/5/27/28	0/3/3/3
46	M3L	Lp	98	46	-	0/9/10/12	-
52	A2M	S2	485	52	-	1/5/27/28	0/3/3/3
6	PSU	L5	3447	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1446	52	-	0/7/25/26	0/2/2/2
6	UR3	L5	4276	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	669	52,89	-	2/5/27/28	0/3/3/3
52	PSU	S2	816	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	1638	6,90,34	-	0/7/25/26	0/2/2/2
8	PSU	L8	69	8	-	0/7/25/26	0/2/2/2
6	A2M	L5	3562	6	-	0/5/27/28	0/3/3/3
6	5MC	L5	4193	6	-	3/7/25/26	0/2/2/2
52	PSU	S2	1005	52	-	1/7/25/26	0/2/2/2
6	PSU	L5	4435	6	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMG	L5	1477	6,11	-	3/5/27/28	0/3/3/3
52	A2M	S2	469	52	-	0/5/27/28	0/3/3/3
6	PSU	L5	4149	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1178	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	3631	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	3494	6	-	2/7/25/26	0/2/2/2
6	PSU	L5	4325	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	1491	52,89	-	1/5/27/28	0/3/3/3
6	OMG	L5	1580	6	-	1/5/27/28	0/3/3/3
52	PSU	S2	218	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	3502	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4177	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	573	84,52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4045	6	-	0/7/25/26	0/2/2/2
6	1MA	L5	1266	6,89	-	0/3/25/26	0/3/3/3
6	OMC	L5	3433	6,90	-	4/9/27/28	0/2/2/2
6	PSU	L5	4298	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	3573	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	4711	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	3974	6	-	0/5/27/28	0/3/3/3
83	HY3	Si	62	83	-	1/1/12/14	0/1/1/1
6	OMG	L5	4138	6	-	0/5/27/28	0/3/3/3
52	OMU	S2	1289	55,52	-	0/9/27/28	0/2/2/2
6	PSU	L5	3462	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	3517	6	-	2/5/27/28	0/3/3/3
6	OMC	L5	3540	6	-	0/9/27/28	0/2/2/2
6	OMC	L5	2704	6	-	0/9/27/28	0/2/2/2
52	PSU	S2	687	67,52	-	0/7/25/26	0/2/2/2
6	OMG	L5	2719	6	-	1/5/27/28	0/3/3/3
52	OMC	S2	463	52	-	0/9/27/28	0/2/2/2
52	OMG	S2	602	52	-	0/5/27/28	0/3/3/3
6	A2M	L5	1489	6,89	-	2/5/27/28	0/3/3/3
6	PSU	L5	4382	6,37	-	2/7/25/26	0/2/2/2
8	PSU	L8	55	8	-	0/7/25/26	0/2/2/2
6	OMG	L5	3676	6	-	1/5/27/28	0/3/3/3
52	PSU	S2	210	52	-	0/7/25/26	0/2/2/2
6	OMU	L5	2680	6	-	0/9/27/28	0/2/2/2
52	OMC	S2	174	52	-	0/9/27/28	0/2/2/2
6	PSU	L5	1721	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	4369	6	-	2/5/27/28	0/3/3/3
52	OMU	S2	1327	52,89	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMC	L5	2208	6,89	-	0/9/27/28	0/2/2/2
6	A2M	L5	2630	6	-	0/5/27/28	0/3/3/3
52	OMG	S2	510	52,89	-	2/5/27/28	0/3/3/3
6	PSU	L5	4107	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4749	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4267	6,89	-	0/7/25/26	0/2/2/2
6	OMC	L5	2265	6,89	-	2/9/27/28	0/2/2/2
6	OMG	L5	3524	6	-	0/5/27/28	0/3/3/3
52	A2M	S2	591	52	-	0/5/27/28	0/3/3/3
52	OMG	S2	684	52	-	2/5/27/28	0/3/3/3
60	SAC	SL	2	60	-	1/7/8/10	-
6	OMU	L5	2258	6	-	0/9/27/28	0/2/2/2
6	OMU	L5	3657	6	-	0/9/27/28	0/2/2/2
52	A2M	S2	1032	52	-	0/5/27/28	0/3/3/3
6	OMU	L5	4366	6,29	-	0/9/27/28	0/2/2/2
52	PSU	S2	1175	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	36	52	-	0/7/25/26	0/2/2/2

All (613) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	1266	1MA	C2-N3	8.67	1.39	1.29
6	L5	2207	OMG	C5-C6	-7.25	1.32	1.47
6	L5	3631	OMG	C5-C6	-7.11	1.33	1.47
6	L5	4138	OMG	C5-C6	-7.09	1.33	1.47
6	L5	2267	OMG	C5-C6	-7.07	1.33	1.47
8	L8	75	OMG	C5-C6	-7.06	1.33	1.47
6	L5	4240	OMG	C5-C6	-7.06	1.33	1.47
6	L5	3974	OMG	C5-C6	-7.06	1.33	1.47
6	L5	1260	OMG	C5-C6	-7.05	1.33	1.47
6	L5	3476	OMG	C5-C6	-7.05	1.33	1.47
52	S2	1491	OMG	C5-C6	-7.05	1.33	1.47
6	L5	2719	OMG	C5-C6	-7.05	1.33	1.47
6	L5	3524	OMG	C5-C6	-7.05	1.33	1.47
6	L5	1580	OMG	C5-C6	-7.04	1.33	1.47
6	L5	4245	OMG	C5-C6	-7.03	1.33	1.47
52	S2	602	OMG	C5-C6	-7.02	1.33	1.47
52	S2	510	OMG	C5-C6	-7.00	1.33	1.47
6	L5	4116	OMG	C5-C6	-6.99	1.33	1.47
6	L5	4364	OMG	C5-C6	-6.98	1.33	1.47
6	L5	4369	OMG	C5-C6	-6.98	1.33	1.47
52	S2	437	OMG	C5-C6	-6.97	1.33	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	1477	OMG	C5-C6	-6.97	1.33	1.47
6	L5	3359	OMG	C5-C6	-6.97	1.33	1.47
6	L5	4383	OMG	C5-C6	-6.96	1.33	1.47
52	S2	1448	OMG	C5-C6	-6.96	1.33	1.47
6	L5	3942	OMG	C5-C6	-6.96	1.33	1.47
52	S2	684	OMG	C5-C6	-6.95	1.33	1.47
52	S2	1329	OMG	C5-C6	-6.93	1.33	1.47
52	S2	645	OMG	C5-C6	-6.93	1.33	1.47
52	S2	868	OMG	C5-C6	-6.91	1.33	1.47
6	L5	3676	OMG	C5-C6	-6.88	1.33	1.47
52	S2	166	A2M	C2-N3	4.94	1.40	1.32
52	S2	1384	A2M	C2-N3	4.90	1.40	1.32
52	S2	27	A2M	C2-N3	4.89	1.40	1.32
52	S2	469	A2M	C2-N3	4.88	1.40	1.32
52	S2	159	A2M	C2-N3	4.87	1.40	1.32
52	S2	591	A2M	C2-N3	4.86	1.39	1.32
6	L5	4317	A2M	C2-N3	4.85	1.39	1.32
52	S2	513	A2M	C2-N3	4.85	1.39	1.32
52	S2	1679	A2M	C2-N3	4.85	1.39	1.32
6	L5	3456	A2M	C2-N3	4.84	1.39	1.32
52	S2	99	A2M	C2-N3	4.84	1.39	1.32
6	L5	400	A2M	C2-N3	4.81	1.39	1.32
52	S2	577	A2M	C2-N3	4.81	1.39	1.32
6	L5	3492	A2M	C2-N3	4.81	1.39	1.32
52	S2	485	A2M	C2-N3	4.79	1.39	1.32
6	L5	4336	A2M	C2-N3	4.77	1.39	1.32
6	L5	1489	A2M	C2-N3	4.77	1.39	1.32
6	L5	3517	A2M	C2-N3	4.75	1.39	1.32
6	L5	398	A2M	C2-N3	4.74	1.39	1.32
6	L5	2658	A2M	C2-N3	4.73	1.39	1.32
6	L5	2630	A2M	C2-N3	4.71	1.39	1.32
6	L5	4269	A2M	C2-N3	4.70	1.39	1.32
6	L5	3599	A2M	C2-N3	4.69	1.39	1.32
52	S2	669	A2M	C2-N3	4.69	1.39	1.32
6	L5	2244	A2M	C2-N3	4.67	1.39	1.32
52	S2	1032	A2M	C2-N3	4.66	1.39	1.32
6	L5	3557	A2M	C2-N3	4.65	1.39	1.32
6	L5	1479	A2M	C2-N3	4.65	1.39	1.32
6	L5	2206	A2M	C2-N3	4.65	1.39	1.32
6	L5	3450	A2M	C2-N3	4.62	1.39	1.32
6	L5	1270	A2M	C2-N3	4.59	1.39	1.32
6	L5	3562	A2M	C2-N3	4.58	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	1810	A2M	C2-N3	4.56	1.39	1.32
79	Se	67	NMM	CZ-NH2	4.23	1.44	1.34
6	L5	1260	OMG	C5-C4	-3.92	1.33	1.43
6	L5	3631	OMG	C5-C4	-3.90	1.33	1.43
6	L5	1477	OMG	C5-C4	-3.89	1.33	1.43
6	L5	1266	1MA	C5-C4	-3.88	1.33	1.43
6	L5	4116	OMG	C5-C4	-3.85	1.33	1.43
6	L5	3359	OMG	C5-C4	-3.84	1.33	1.43
52	S2	591	A2M	O4'-C1'	3.84	1.46	1.41
6	L5	3974	OMG	C5-C4	-3.81	1.33	1.43
6	L5	4240	OMG	C5-C4	-3.81	1.33	1.43
6	L5	4138	OMG	C5-C4	-3.81	1.33	1.43
6	L5	4383	OMG	C5-C4	-3.81	1.33	1.43
6	L5	2267	OMG	C5-C4	-3.81	1.33	1.43
6	L5	3476	OMG	C5-C4	-3.80	1.33	1.43
6	L5	4245	OMG	C5-C4	-3.80	1.33	1.43
6	L5	1580	OMG	C5-C4	-3.80	1.33	1.43
6	L5	4369	OMG	C5-C4	-3.78	1.33	1.43
6	L5	3524	OMG	C5-C4	-3.78	1.33	1.43
6	L5	4364	OMG	C5-C4	-3.77	1.33	1.43
6	L5	3492	A2M	O4'-C1'	3.76	1.46	1.41
6	L5	3942	OMG	C5-C4	-3.76	1.33	1.43
52	S2	867	PSU	C6-C5	3.76	1.39	1.35
52	S2	602	OMG	C5-C4	-3.75	1.33	1.43
8	L8	75	OMG	C5-C4	-3.74	1.33	1.43
52	S2	645	OMG	C5-C4	-3.73	1.33	1.43
52	S2	1491	OMG	C5-C4	-3.73	1.33	1.43
52	S2	684	OMG	C5-C4	-3.72	1.33	1.43
52	S2	573	PSU	C6-C5	3.71	1.39	1.35
52	S2	816	PSU	C6-C5	3.71	1.39	1.35
52	S2	864	PSU	C6-C5	3.71	1.39	1.35
52	S2	868	OMG	C5-C4	-3.71	1.33	1.43
52	S2	166	A2M	O4'-C1'	3.71	1.46	1.41
52	S2	687	PSU	C6-C5	3.70	1.39	1.35
52	S2	109	PSU	C6-C5	3.69	1.39	1.35
52	S2	1329	OMG	C5-C4	-3.69	1.33	1.43
52	S2	437	OMG	C5-C4	-3.69	1.33	1.43
52	S2	1368	PSU	C6-C5	3.68	1.39	1.35
6	L5	2719	OMG	C5-C4	-3.68	1.33	1.43
6	L5	2207	OMG	C5-C4	-3.68	1.33	1.43
52	S2	1626	PSU	C6-C5	3.67	1.39	1.35
52	S2	93	PSU	C6-C5	3.67	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3676	OMG	C5-C4	-3.66	1.33	1.43
52	S2	210	PSU	C6-C5	3.66	1.39	1.35
52	S2	510	OMG	C5-C4	-3.66	1.33	1.43
52	S2	577	A2M	O4'-C1'	3.66	1.46	1.41
52	S2	1448	OMG	C5-C4	-3.66	1.33	1.43
52	S2	1640	7MG	C5-C6	-3.64	1.34	1.43
52	S2	1640	7MG	C4-N9	-3.63	1.33	1.37
52	S2	610	PSU	C6-C5	3.63	1.39	1.35
52	S2	802	PSU	C6-C5	3.63	1.39	1.35
52	S2	99	A2M	O4'-C1'	3.63	1.46	1.41
52	S2	119	PSU	C6-C5	3.59	1.39	1.35
52	S2	36	PSU	C6-C5	3.58	1.39	1.35
6	L5	3502	PSU	C6-C5	3.58	1.39	1.35
52	S2	105	PSU	C6-C5	3.58	1.39	1.35
52	S2	1348	PSU	C6-C5	3.57	1.39	1.35
6	L5	1632	PSU	C6-C5	3.57	1.39	1.35
6	L5	4336	A2M	O4'-C1'	3.56	1.46	1.41
52	S2	967	PSU	C6-C5	3.56	1.39	1.35
52	S2	823	PSU	C6-C5	3.55	1.39	1.35
52	S2	1446	PSU	C6-C5	3.55	1.39	1.35
52	S2	34	PSU	C6-C5	3.54	1.39	1.35
52	S2	1384	A2M	O4'-C1'	3.53	1.46	1.41
6	L5	3466	PSU	C6-C5	3.53	1.39	1.35
6	L5	3494	PSU	C6-C5	3.53	1.39	1.35
6	L5	4749	PSU	C6-C5	3.52	1.39	1.35
52	S2	1233	PSU	C6-C5	3.52	1.39	1.35
6	L5	4278	PSU	C6-C5	3.52	1.39	1.35
52	S2	407	PSU	C6-C5	3.51	1.39	1.35
6	L5	4322	PSU	C6-C5	3.51	1.39	1.35
6	L5	1683	PSU	C6-C5	3.51	1.39	1.35
6	L5	3462	PSU	C6-C5	3.51	1.39	1.35
52	S2	650	PSU	C6-C5	3.50	1.39	1.35
52	S2	1047	PSU	C6-C5	3.50	1.39	1.35
52	S2	652	PSU	C6-C5	3.50	1.39	1.35
6	L5	4740	PSU	C6-C5	3.49	1.39	1.35
6	L5	4246	PSU	C6-C5	3.49	1.39	1.35
52	S2	218	PSU	C6-C5	3.48	1.39	1.35
52	S2	1178	PSU	C6-C5	3.48	1.39	1.35
6	L5	1799	PSU	C6-C5	3.47	1.39	1.35
52	S2	1239	PSU	C6-C5	3.47	1.39	1.35
8	L8	55	PSU	C6-C5	3.47	1.39	1.35
52	S2	815	PSU	C6-C5	3.46	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	1175	PSU	C6-C5	3.46	1.39	1.35
52	S2	1245	PSU	C6-C5	3.45	1.39	1.35
6	L5	3496	PSU	C6-C5	3.44	1.39	1.35
6	L5	3490	PSU	C6-C5	3.44	1.39	1.35
6	L5	3576	PSU	C6-C5	3.44	1.39	1.35
6	L5	1718	PSU	C6-C5	3.44	1.39	1.35
6	L5	3500	PSU	C6-C5	3.44	1.39	1.35
52	S2	1057	PSU	C6-C5	3.42	1.39	1.35
6	L5	4169	PSU	C6-C5	3.42	1.39	1.35
52	S2	1644	PSU	C6-C5	3.41	1.39	1.35
6	L5	3447	PSU	C6-C5	3.41	1.39	1.35
6	L5	2475	PSU	C6-C5	3.41	1.39	1.35
6	L5	4374	PSU	C6-C5	3.41	1.39	1.35
6	L5	3554	PSU	C6-C5	3.41	1.39	1.35
52	S2	1693	PSU	C6-C5	3.41	1.39	1.35
6	L5	1801	PSU	C6-C5	3.40	1.39	1.35
52	S2	1046	PSU	C6-C5	3.40	1.39	1.35
6	L5	3427	PSU	C6-C5	3.39	1.39	1.35
6	L5	1720	PSU	C6-C5	3.39	1.39	1.35
6	L5	4039	PSU	C6-C5	3.39	1.39	1.35
8	L8	69	PSU	C6-C5	3.39	1.39	1.35
52	S2	682	PSU	C6-C5	3.39	1.39	1.35
6	L5	4711	PSU	C6-C5	3.38	1.39	1.35
6	L5	4166	PSU	C6-C5	3.38	1.39	1.35
52	S2	513	A2M	O4'-C1'	3.38	1.45	1.41
6	L5	4435	PSU	C6-C5	3.38	1.39	1.35
52	S2	159	A2M	O4'-C1'	3.38	1.45	1.41
6	L5	1721	PSU	C6-C5	3.37	1.39	1.35
6	L5	4058	PSU	C6-C5	3.37	1.39	1.35
6	L5	4042	PSU	C6-C5	3.37	1.39	1.35
6	L5	2630	A2M	O4'-C1'	3.37	1.45	1.41
6	L5	4298	PSU	C6-C5	3.36	1.39	1.35
52	S2	1679	A2M	O4'-C1'	3.36	1.45	1.41
6	L5	1537	PSU	C6-C5	3.36	1.39	1.35
6	L5	4045	PSU	C6-C5	3.36	1.39	1.35
6	L5	1731	PSU	C6-C5	3.35	1.39	1.35
6	L5	4217	PSU	C6-C5	3.34	1.39	1.35
6	L5	398	A2M	O4'-C1'	3.34	1.45	1.41
6	L5	4099	PSU	C6-C5	3.33	1.39	1.35
6	L5	4325	PSU	C6-C5	3.32	1.39	1.35
6	L5	4107	PSU	C6-C5	3.32	1.39	1.35
6	L5	3616	PSU	C6-C5	3.32	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	1843	4AC	C4-N4	-3.31	1.34	1.39
6	L5	3456	A2M	O4'-C1'	3.31	1.45	1.41
6	L5	1638	PSU	C6-C5	3.30	1.39	1.35
6	L5	4419	PSU	C6-C5	3.29	1.39	1.35
6	L5	1491	PSU	C6-C5	3.28	1.39	1.35
52	S2	1082	PSU	C6-C5	3.27	1.39	1.35
6	L5	4177	PSU	C6-C5	3.27	1.39	1.35
6	L5	4382	PSU	C6-C5	3.27	1.39	1.35
6	L5	2351	PSU	C6-C5	3.26	1.39	1.35
6	L5	3583	PSU	C6-C5	3.26	1.39	1.35
52	S2	577	A2M	C2-N1	3.24	1.39	1.33
6	L5	4188	PSU	C6-C5	3.23	1.39	1.35
6	L5	4149	PSU	C6-C5	3.22	1.39	1.35
52	S2	469	A2M	C2-N1	3.22	1.39	1.33
6	L5	4203	PSU	C6-C5	3.22	1.39	1.35
52	S2	513	A2M	C2-N1	3.20	1.39	1.33
6	L5	3371	PSU	C6-C5	3.20	1.39	1.35
52	S2	27	A2M	C2-N1	3.19	1.39	1.33
52	S2	159	A2M	C2-N1	3.19	1.39	1.33
52	S2	485	A2M	C2-N1	3.18	1.39	1.33
6	L5	4269	A2M	O4'-C1'	3.17	1.45	1.41
6	L5	4267	PSU	C6-C5	3.17	1.39	1.35
6	L5	3585	PSU	C6-C5	3.17	1.39	1.35
6	L5	4317	A2M	C2-N1	3.17	1.39	1.33
6	L5	3492	A2M	C2-N1	3.16	1.39	1.33
52	S2	166	A2M	C2-N1	3.16	1.39	1.33
52	S2	1384	A2M	C2-N1	3.16	1.39	1.33
52	S2	591	A2M	C2-N1	3.16	1.39	1.33
6	L5	3652	PSU	C6-C5	3.14	1.39	1.35
52	S2	469	A2M	O4'-C1'	3.14	1.45	1.41
6	L5	1810	A2M	O4'-C1'	3.13	1.45	1.41
6	L5	2244	A2M	O4'-C1'	3.13	1.45	1.41
6	L5	3369	PSU	C6-C5	3.11	1.39	1.35
6	L5	3456	A2M	C2-N1	3.11	1.39	1.33
6	L5	400	A2M	O4'-C1'	3.08	1.45	1.41
6	L5	398	A2M	C2-N1	3.07	1.39	1.33
52	S2	1032	A2M	O4'-C1'	3.07	1.45	1.41
52	S2	1338	4AC	C4-N4	-3.07	1.35	1.39
52	S2	1679	A2M	C2-N1	3.07	1.39	1.33
6	L5	1489	A2M	C2-N1	3.07	1.39	1.33
6	L5	4336	A2M	C2-N1	3.06	1.39	1.33
6	L5	3450	A2M	C2-N1	3.06	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	2630	A2M	C5-C4	-3.05	1.32	1.40
6	L5	400	A2M	C2-N1	3.04	1.39	1.33
52	S2	99	A2M	C2-N1	3.03	1.39	1.33
6	L5	3562	A2M	C2-N1	3.03	1.39	1.33
6	L5	2658	A2M	C2-N1	3.02	1.39	1.33
52	S2	669	A2M	C2-N1	3.02	1.39	1.33
6	L5	3557	A2M	O4'-C1'	3.01	1.45	1.41
6	L5	3562	A2M	O4'-C1'	3.01	1.45	1.41
6	L5	1810	A2M	C2-N1	3.00	1.39	1.33
52	S2	1005	PSU	C2-N3	3.00	1.42	1.37
52	S2	27	A2M	O4'-C1'	2.98	1.45	1.41
52	S2	1032	A2M	C2-N1	2.97	1.39	1.33
6	L5	3557	A2M	C2-N1	2.97	1.39	1.33
6	L5	1810	A2M	C5-C4	-2.97	1.33	1.40
6	L5	4269	A2M	C2-N1	2.96	1.39	1.33
6	L5	4276	UR3	C2-N1	-2.96	1.34	1.38
6	L5	2206	A2M	C2-N1	2.96	1.39	1.33
6	L5	2658	A2M	O4'-C1'	2.95	1.45	1.41
6	L5	3599	A2M	C2-N1	2.94	1.39	1.33
6	L5	1479	A2M	C2-N1	2.94	1.39	1.33
6	L5	4269	A2M	C5-C4	-2.94	1.33	1.40
6	L5	1270	A2M	C2-N1	2.94	1.39	1.33
6	L5	1270	A2M	C5-C4	-2.94	1.33	1.40
6	L5	4276	UR3	C4-N3	-2.93	1.34	1.40
6	L5	3517	A2M	C2-N1	2.92	1.39	1.33
6	L5	4193	5MC	C6-C5	2.92	1.39	1.34
6	L5	2206	A2M	C5-C4	-2.92	1.33	1.40
6	L5	2244	A2M	C2-N1	2.92	1.39	1.33
6	L5	3514	5MC	C4-N3	2.92	1.39	1.34
52	S2	1005	PSU	C6-C5	2.91	1.38	1.35
52	S2	669	A2M	C5-C4	-2.91	1.33	1.40
6	L5	3562	A2M	C5-C4	-2.91	1.33	1.40
6	L5	2658	A2M	C5-C4	-2.90	1.33	1.40
6	L5	2206	A2M	O4'-C1'	2.90	1.45	1.41
6	L5	1489	A2M	C5-C4	-2.89	1.33	1.40
6	L5	3517	A2M	C5-C4	-2.89	1.33	1.40
6	L5	3599	A2M	C5-C4	-2.89	1.33	1.40
52	S2	1032	A2M	C5-C4	-2.88	1.33	1.40
6	L5	2630	A2M	C2-N1	2.88	1.39	1.33
6	L5	2244	A2M	C5-C4	-2.88	1.33	1.40
6	L5	4317	A2M	O4'-C1'	2.88	1.45	1.41
6	L5	1479	A2M	C5-C4	-2.87	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3557	A2M	C5-C4	-2.87	1.33	1.40
6	L5	3450	A2M	C5-C4	-2.87	1.33	1.40
52	S2	27	A2M	C5-C4	-2.86	1.33	1.40
6	L5	4336	A2M	C5-C4	-2.85	1.33	1.40
6	L5	400	A2M	C5-C4	-2.85	1.33	1.40
6	L5	4317	A2M	C5-C4	-2.85	1.33	1.40
6	L5	1489	A2M	O4'-C1'	2.84	1.45	1.41
52	S2	210	PSU	C2-N1	2.84	1.40	1.36
6	L5	3456	A2M	C5-C4	-2.83	1.33	1.40
52	S2	1679	A2M	C5-C4	-2.83	1.33	1.40
6	L5	398	A2M	C5-C4	-2.82	1.33	1.40
52	S2	485	A2M	C5-C4	-2.82	1.33	1.40
52	S2	1384	A2M	C5-C4	-2.82	1.33	1.40
6	L5	1270	A2M	C6-C5	-2.81	1.32	1.43
52	S2	99	A2M	C5-C4	-2.81	1.33	1.40
6	L5	1810	A2M	C6-C5	-2.79	1.32	1.43
52	S2	513	A2M	C5-C4	-2.79	1.33	1.40
6	L5	3492	A2M	C5-C4	-2.79	1.33	1.40
52	S2	1005	PSU	C4-N3	2.79	1.44	1.38
6	L5	1284	OMC	C2-N1	-2.79	1.33	1.40
6	L5	3517	A2M	C6-C5	-2.78	1.33	1.43
6	L5	3562	A2M	C6-C5	-2.78	1.33	1.43
6	L5	3557	A2M	C6-C5	-2.78	1.33	1.43
52	S2	469	A2M	C5-C4	-2.77	1.33	1.40
52	S2	166	A2M	C5-C4	-2.77	1.33	1.40
52	S2	1032	A2M	C6-C5	-2.76	1.33	1.43
6	L5	3657	OMU	C2-N1	-2.76	1.34	1.38
6	L5	3433	OMC	C2-N1	-2.76	1.34	1.40
52	S2	159	A2M	C5-C4	-2.76	1.33	1.40
6	L5	2244	A2M	C6-C5	-2.76	1.33	1.43
6	L5	3514	5MC	C6-C5	2.75	1.39	1.34
6	L5	4336	A2M	C6-C5	-2.75	1.33	1.43
52	S2	577	A2M	C5-C4	-2.75	1.33	1.40
6	L5	4282	OMC	C2-N1	-2.75	1.34	1.40
6	L5	1489	A2M	C6-C5	-2.75	1.33	1.43
6	L5	400	A2M	C6-C5	-2.74	1.33	1.43
6	L5	4269	A2M	C6-C5	-2.74	1.33	1.43
6	L5	2206	A2M	C6-C5	-2.74	1.33	1.43
6	L5	1820	OMC	C2-N1	-2.74	1.34	1.40
6	L5	3450	A2M	C6-C5	-2.74	1.33	1.43
52	S2	591	A2M	C5-C4	-2.74	1.33	1.40
6	L5	4244	OMU	C2-N1	-2.74	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3599	A2M	C6-C5	-2.73	1.33	1.43
6	L5	2630	A2M	C6-C5	-2.73	1.33	1.43
52	S2	1005	PSU	C6-N1	-2.73	1.31	1.36
6	L5	2647	OMC	C2-N1	-2.72	1.34	1.40
6	L5	3492	A2M	C6-C5	-2.72	1.33	1.43
6	L5	4317	A2M	C6-C5	-2.72	1.33	1.43
6	L5	1479	A2M	C6-C5	-2.72	1.33	1.43
52	S2	27	A2M	C6-C5	-2.72	1.33	1.43
52	S2	669	A2M	C6-C5	-2.72	1.33	1.43
6	L5	2658	A2M	C6-C5	-2.71	1.33	1.43
52	S2	34	PSU	C2-N1	2.71	1.40	1.36
52	S2	1679	A2M	C6-C5	-2.71	1.33	1.43
52	S2	1384	A2M	C6-C5	-2.71	1.33	1.43
83	Si	62	HY3	C3-CA	-2.71	1.52	1.55
6	L5	2208	OMC	C2-N1	-2.71	1.34	1.40
52	S2	1704	OMC	C2-N1	-2.70	1.34	1.40
52	S2	159	A2M	C6-C5	-2.70	1.33	1.43
6	L5	3619	OMC	C2-N1	-2.70	1.34	1.40
6	L5	398	A2M	C6-C5	-2.70	1.33	1.43
52	S2	99	A2M	C6-C5	-2.70	1.33	1.43
52	S2	485	A2M	C6-C5	-2.69	1.33	1.43
52	S2	174	OMC	C4-N3	2.69	1.40	1.34
6	L5	3456	A2M	C6-C5	-2.69	1.33	1.43
52	S2	1446	PSU	C2-N1	2.68	1.40	1.36
6	L5	3450	A2M	O4'-C1'	2.67	1.44	1.41
6	L5	3466	PSU	C2-N1	2.67	1.40	1.36
52	S2	1327	OMU	C2-N1	-2.67	1.34	1.38
52	S2	513	A2M	C6-C5	-2.66	1.33	1.43
52	S2	573	PSU	C2-N1	2.66	1.40	1.36
52	S2	591	A2M	C6-C5	-2.66	1.33	1.43
6	L5	3973	OMU	C2-N1	-2.66	1.34	1.38
6	L5	4366	OMU	C2-N1	-2.66	1.34	1.38
52	S2	577	A2M	C6-C5	-2.66	1.33	1.43
6	L5	4202	OMC	C2-N1	-2.65	1.34	1.40
6	L5	4193	5MC	C2-N1	-2.65	1.34	1.40
6	L5	4166	PSU	C2-N1	2.64	1.40	1.36
52	S2	628	OMU	C2-N1	-2.64	1.34	1.38
6	L5	3573	OMC	C2-N1	-2.63	1.34	1.40
6	L5	3601	OMC	C2-N1	-2.63	1.34	1.40
52	S2	469	A2M	C6-C5	-2.62	1.33	1.43
52	S2	815	PSU	C2-N1	2.62	1.40	1.36
52	S2	218	PSU	C2-N1	2.62	1.40	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	166	A2M	C6-C5	-2.61	1.33	1.43
6	L5	2194	OMC	C2-N1	-2.60	1.34	1.40
6	L5	2704	OMC	C2-N1	-2.60	1.34	1.40
52	S2	36	PSU	C2-N1	2.60	1.40	1.36
6	L5	2680	OMU	C2-N1	-2.59	1.34	1.38
6	L5	2667	OMC	C2-N1	-2.59	1.34	1.40
52	S2	816	PSU	C2-N1	2.59	1.40	1.36
52	S2	518	OMC	C4-N3	2.59	1.39	1.34
52	S2	463	OMC	C4-N3	2.58	1.39	1.34
52	S2	1005	PSU	C2-N1	2.58	1.40	1.36
52	S2	429	OMU	C2-N1	-2.58	1.34	1.38
52	S2	652	PSU	C2-N1	2.57	1.40	1.36
6	L5	4042	PSU	C2-N1	2.57	1.40	1.36
6	L5	4382	PSU	C6-N1	-2.57	1.32	1.36
52	S2	867	PSU	C2-N1	2.56	1.40	1.36
6	L5	2258	OMU	C2-N1	-2.55	1.34	1.38
6	L5	4749	PSU	C2-N1	2.54	1.40	1.36
6	L5	3540	OMC	C2-N1	-2.54	1.34	1.40
6	L5	4052	OMU	C2-N1	-2.54	1.34	1.38
6	L5	4435	PSU	C6-N1	-2.54	1.32	1.36
52	S2	1392	OMC	C4-N3	2.53	1.39	1.34
52	S2	967	PSU	C2-N1	2.53	1.40	1.36
6	L5	1537	PSU	C2-N1	2.53	1.40	1.36
52	S2	174	OMC	C2-N1	-2.53	1.34	1.40
52	S2	1047	PSU	C2-N1	2.53	1.40	1.36
52	S2	109	PSU	C2-N1	2.53	1.40	1.36
6	L5	2265	OMC	C2-N1	-2.52	1.34	1.40
6	L5	4322	PSU	C2-N1	2.52	1.40	1.36
52	S2	650	PSU	C2-N1	2.52	1.40	1.36
6	L5	4267	PSU	C2-N1	2.52	1.40	1.36
52	S2	463	OMC	C2-N1	-2.52	1.34	1.40
6	L5	1731	PSU	C2-N1	2.51	1.40	1.36
52	S2	355	OMU	C2-N1	-2.51	1.34	1.38
6	L5	3433	OMC	C4-N3	2.51	1.39	1.34
52	S2	119	PSU	C2-N1	2.51	1.40	1.36
52	S2	1368	PSU	C2-N1	2.51	1.40	1.36
52	S2	518	OMC	C2-N1	-2.51	1.34	1.40
52	S2	407	PSU	C2-N1	2.50	1.40	1.36
52	S2	864	PSU	C2-N1	2.50	1.40	1.36
52	S2	93	PSU	C2-N1	2.49	1.40	1.36
6	L5	3619	OMC	C4-N3	2.49	1.39	1.34
6	L5	1632	PSU	C6-N1	-2.49	1.32	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3599	A2M	O4'-C1'	2.49	1.44	1.41
6	L5	4193	5MC	C4-N3	2.49	1.38	1.34
6	L5	4149	PSU	C6-N1	-2.48	1.32	1.36
52	S2	116	OMU	C2-N1	-2.48	1.34	1.38
6	L5	1479	A2M	O4'-C1'	2.48	1.44	1.41
52	S2	1626	PSU	C2-N1	2.48	1.40	1.36
52	S2	1644	PSU	C2-N1	2.48	1.40	1.36
6	L5	3601	OMC	C4-N3	2.48	1.39	1.34
6	L5	4058	PSU	C2-N1	2.47	1.40	1.36
6	L5	3494	PSU	C2-N1	2.47	1.40	1.36
6	L5	1820	OMC	C4-N3	2.47	1.39	1.34
52	S2	1851	MA6	C5-C4	2.47	1.47	1.40
6	L5	4099	PSU	C2-N1	2.47	1.40	1.36
6	L5	4188	PSU	C2-N1	2.47	1.40	1.36
6	L5	4740	PSU	C2-N1	2.47	1.40	1.36
52	S2	1392	OMC	C2-N1	-2.46	1.34	1.40
6	L5	2475	PSU	C2-N1	2.46	1.40	1.36
6	L5	2667	OMC	C4-N3	2.46	1.39	1.34
6	L5	4276	UR3	C2-N3	-2.45	1.34	1.39
6	L5	2704	OMC	C4-N3	2.45	1.39	1.34
52	S2	1245	PSU	C2-N1	2.45	1.40	1.36
52	S2	172	OMU	C2-N1	-2.45	1.34	1.38
52	S2	105	PSU	C2-N1	2.45	1.40	1.36
8	L8	69	PSU	C2-N1	2.44	1.40	1.36
52	S2	1805	OMU	C2-N1	-2.44	1.34	1.38
52	S2	687	PSU	C2-N1	2.44	1.40	1.36
52	S2	1057	PSU	C2-N1	2.44	1.40	1.36
6	L5	3462	PSU	C2-N1	2.44	1.40	1.36
6	L5	1801	PSU	C2-N1	2.44	1.40	1.36
6	L5	3502	PSU	C2-N1	2.44	1.40	1.36
52	S2	610	PSU	C2-N1	2.44	1.40	1.36
52	S2	1046	PSU	C2-N1	2.44	1.40	1.36
6	L5	3496	PSU	C2-N1	2.44	1.40	1.36
6	L5	3514	5MC	C2-N1	-2.43	1.34	1.40
6	L5	3447	PSU	C2-N1	2.43	1.40	1.36
52	S2	1082	PSU	C2-N1	2.43	1.40	1.36
6	L5	2351	PSU	C2-N1	2.42	1.40	1.36
6	L5	4325	PSU	C6-N1	-2.42	1.32	1.36
6	L5	1537	PSU	C6-N1	-2.42	1.32	1.36
6	L5	4169	PSU	C2-N1	2.42	1.40	1.36
52	S2	1178	PSU	C2-N1	2.41	1.40	1.36
6	L5	3490	PSU	C2-N1	2.41	1.40	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3616	PSU	C6-N1	-2.41	1.32	1.36
52	S2	1852	MA6	C5-C4	2.41	1.47	1.40
6	L5	2265	OMC	C4-N3	2.41	1.39	1.34
52	S2	1239	PSU	C2-N1	2.40	1.40	1.36
52	S2	802	PSU	C6-N1	-2.40	1.32	1.36
6	L5	4177	PSU	C6-N1	-2.40	1.32	1.36
6	L5	1718	PSU	C6-N1	-2.39	1.32	1.36
52	S2	682	PSU	C6-N1	-2.39	1.32	1.36
6	L5	1799	PSU	C6-N1	-2.39	1.32	1.36
6	L5	3652	PSU	C6-N1	-2.39	1.32	1.36
52	S2	1178	PSU	C6-N1	-2.39	1.32	1.36
6	L5	1720	PSU	C2-N1	2.39	1.40	1.36
6	L5	4298	PSU	C6-N1	-2.39	1.32	1.36
6	L5	3371	PSU	C6-N1	-2.38	1.32	1.36
6	L5	4374	PSU	C6-N1	-2.38	1.32	1.36
6	L5	3369	PSU	C6-N1	-2.38	1.32	1.36
6	L5	4267	PSU	C6-N1	-2.38	1.32	1.36
6	L5	1270	A2M	O4'-C1'	2.38	1.44	1.41
6	L5	4107	PSU	C6-N1	-2.38	1.32	1.36
52	S2	1348	PSU	C2-N1	2.38	1.39	1.36
6	L5	4045	PSU	C6-N1	-2.37	1.32	1.36
6	L5	4246	PSU	C6-N1	-2.37	1.32	1.36
6	L5	4169	PSU	C6-N1	-2.37	1.32	1.36
52	S2	1693	PSU	C2-N1	2.37	1.39	1.36
6	L5	3500	PSU	C2-N1	2.37	1.39	1.36
6	L5	4039	PSU	C6-N1	-2.37	1.32	1.36
8	L8	69	PSU	C6-N1	-2.37	1.32	1.36
6	L5	1284	OMC	C4-N3	2.37	1.39	1.34
6	L5	4282	OMC	C4-N3	2.36	1.39	1.34
52	S2	1443	OMU	C2-N1	-2.36	1.34	1.38
6	L5	3576	PSU	C6-N1	-2.36	1.32	1.36
6	L5	3583	PSU	C6-N1	-2.36	1.32	1.36
6	L5	4099	PSU	C6-N1	-2.36	1.32	1.36
6	L5	1491	PSU	C6-N1	-2.36	1.32	1.36
6	L5	4419	PSU	C6-N1	-2.36	1.32	1.36
52	S2	1704	OMC	C4-N3	2.36	1.39	1.34
6	L5	4246	PSU	C2-N1	2.36	1.39	1.36
6	L5	1683	PSU	C6-N1	-2.36	1.32	1.36
6	L5	1799	PSU	C2-N1	2.36	1.39	1.36
6	L5	1638	PSU	C6-N1	-2.36	1.32	1.36
6	L5	2351	PSU	C6-N1	-2.36	1.32	1.36
6	L5	4278	PSU	C2-N1	2.35	1.39	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	1721	PSU	C6-N1	-2.35	1.32	1.36
52	S2	1175	PSU	C6-N1	-2.35	1.32	1.36
6	L5	1720	PSU	C6-N1	-2.35	1.32	1.36
6	L5	1718	PSU	C2-N1	2.35	1.39	1.36
6	L5	3369	PSU	C2-N1	2.35	1.39	1.36
6	L5	3371	PSU	C2-N1	2.35	1.39	1.36
6	L5	1632	PSU	C2-N1	2.35	1.39	1.36
6	L5	4711	PSU	C2-N1	2.34	1.39	1.36
6	L5	3427	PSU	C2-N1	2.34	1.39	1.36
6	L5	3427	PSU	C6-N1	-2.34	1.32	1.36
6	L5	4322	PSU	C6-N1	-2.34	1.32	1.36
6	L5	3583	PSU	C2-N1	2.34	1.39	1.36
6	L5	3462	PSU	C6-N1	-2.34	1.32	1.36
6	L5	2208	OMC	C4-N3	2.34	1.39	1.34
52	S2	121	OMU	C2-N1	-2.34	1.34	1.38
6	L5	3573	OMC	C4-N3	2.34	1.39	1.34
6	L5	3496	PSU	C6-N1	-2.34	1.32	1.36
6	L5	4217	PSU	C6-N1	-2.34	1.32	1.36
52	S2	1245	PSU	C6-N1	-2.34	1.32	1.36
52	S2	1693	PSU	C6-N1	-2.33	1.32	1.36
52	S2	407	PSU	C6-N1	-2.33	1.32	1.36
6	L5	4202	OMC	C4-N3	2.33	1.39	1.34
52	S2	1057	PSU	C6-N1	-2.33	1.32	1.36
52	S2	1843	4AC	C7-N4	-2.33	1.32	1.37
6	L5	4740	PSU	C6-N1	-2.33	1.32	1.36
6	L5	4278	PSU	C6-N1	-2.33	1.32	1.36
52	S2	1233	PSU	C2-N1	2.33	1.39	1.36
8	L8	55	PSU	C2-N1	2.32	1.39	1.36
8	L8	55	PSU	C6-N1	-2.32	1.32	1.36
6	L5	4045	PSU	C2-N1	2.32	1.39	1.36
6	L5	4042	PSU	C6-N1	-2.32	1.32	1.36
6	L5	4711	PSU	C6-N1	-2.32	1.32	1.36
6	L5	1638	PSU	C2-N1	2.32	1.39	1.36
6	L5	3540	OMC	C4-N3	2.32	1.39	1.34
52	S2	864	PSU	C6-N1	-2.32	1.32	1.36
52	S2	93	PSU	C6-N1	-2.32	1.32	1.36
52	S2	1833	6MZ	C5-C4	2.31	1.47	1.40
52	S2	823	PSU	C6-N1	-2.31	1.32	1.36
52	S2	1644	PSU	C6-N1	-2.31	1.32	1.36
6	L5	2647	OMC	C4-N3	2.31	1.39	1.34
6	L5	4058	PSU	C6-N1	-2.31	1.32	1.36
52	S2	687	PSU	C6-N1	-2.31	1.32	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	1239	PSU	C6-N1	-2.31	1.32	1.36
6	L5	3554	PSU	C6-N1	-2.31	1.32	1.36
6	L5	3554	PSU	C2-N1	2.31	1.39	1.36
6	L5	3585	PSU	C6-N1	-2.31	1.32	1.36
6	L5	4039	PSU	C2-N1	2.31	1.39	1.36
52	S2	1233	PSU	C6-N1	-2.30	1.32	1.36
6	L5	4166	PSU	C6-N1	-2.30	1.32	1.36
6	L5	3494	PSU	C6-N1	-2.30	1.32	1.36
6	L5	4325	PSU	C2-N1	2.30	1.39	1.36
6	L5	4419	PSU	C2-N1	2.30	1.39	1.36
6	L5	4188	PSU	C6-N1	-2.30	1.32	1.36
6	L5	1731	PSU	C6-N1	-2.29	1.32	1.36
6	L5	2475	PSU	C6-N1	-2.29	1.32	1.36
6	L5	4749	PSU	C6-N1	-2.29	1.32	1.36
6	L5	1721	PSU	C2-N1	2.29	1.39	1.36
52	S2	1348	PSU	C6-N1	-2.29	1.32	1.36
52	S2	967	PSU	C6-N1	-2.29	1.32	1.36
6	L5	3500	PSU	C6-N1	-2.29	1.32	1.36
52	S2	1175	PSU	C2-N1	2.28	1.39	1.36
52	S2	610	PSU	C6-N1	-2.28	1.32	1.36
52	S2	652	PSU	C6-N1	-2.28	1.32	1.36
6	L5	4203	PSU	C6-N1	-2.28	1.32	1.36
52	S2	1082	PSU	C6-N1	-2.28	1.32	1.36
52	S2	802	PSU	C2-N1	2.28	1.39	1.36
6	L5	4382	PSU	C2-N1	2.27	1.39	1.36
52	S2	105	PSU	C6-N1	-2.27	1.32	1.36
52	S2	1047	PSU	C6-N1	-2.27	1.32	1.36
6	L5	4217	PSU	C2-N1	2.27	1.39	1.36
6	L5	3447	PSU	C6-N1	-2.27	1.32	1.36
6	L5	4374	PSU	C2-N1	2.27	1.39	1.36
52	S2	682	PSU	C2-N1	2.27	1.39	1.36
6	L5	4203	PSU	C2-N1	2.27	1.39	1.36
52	S2	823	PSU	C2-N1	2.27	1.39	1.36
52	S2	867	PSU	C6-N1	-2.27	1.32	1.36
6	L5	3466	PSU	C6-N1	-2.26	1.32	1.36
6	L5	1683	PSU	C2-N1	2.26	1.39	1.36
6	L5	1801	PSU	C6-N1	-2.26	1.32	1.36
6	L5	4298	PSU	C2-N1	2.26	1.39	1.36
52	S2	1626	PSU	C6-N1	-2.26	1.32	1.36
52	S2	650	PSU	C6-N1	-2.26	1.32	1.36
52	S2	1368	PSU	C6-N1	-2.25	1.32	1.36
52	S2	119	PSU	C6-N1	-2.25	1.32	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	815	PSU	C6-N1	-2.25	1.32	1.36
6	L5	3490	PSU	C6-N1	-2.25	1.32	1.36
6	L5	3502	PSU	C6-N1	-2.25	1.32	1.36
6	L5	3966	6MZ	C5-C4	2.25	1.46	1.40
6	L5	3585	PSU	C2-N1	2.25	1.39	1.36
52	S2	1046	PSU	C6-N1	-2.24	1.32	1.36
6	L5	3652	PSU	C2-N1	2.24	1.39	1.36
52	S2	1289	OMU	C2-N1	-2.24	1.34	1.38
52	S2	485	A2M	O4'-C1'	2.23	1.44	1.41
6	L5	1266	1MA	C6-N6	2.23	1.33	1.27
52	S2	573	PSU	C6-N1	-2.23	1.32	1.36
52	S2	36	PSU	C6-N1	-2.23	1.32	1.36
52	S2	218	PSU	C6-N1	-2.22	1.32	1.36
52	S2	1446	PSU	C6-N1	-2.22	1.32	1.36
52	S2	109	PSU	C6-N1	-2.22	1.32	1.36
6	L5	2194	OMC	C4-N3	2.22	1.39	1.34
6	L5	4177	PSU	C2-N1	2.22	1.39	1.36
52	S2	210	PSU	C6-N1	-2.22	1.32	1.36
6	L5	4366	OMU	C5-C4	-2.22	1.38	1.43
52	S2	816	PSU	C6-N1	-2.21	1.32	1.36
52	S2	34	PSU	C6-N1	-2.21	1.32	1.36
6	L5	4107	PSU	C2-N1	2.20	1.39	1.36
52	S2	1338	4AC	C7-N4	-2.19	1.33	1.37
6	L5	1491	PSU	C2-N1	2.19	1.39	1.36
6	L5	4052	OMU	C5-C4	-2.19	1.38	1.43
6	L5	3657	OMU	C5-C4	-2.17	1.38	1.43
6	L5	4435	PSU	C2-N1	2.17	1.39	1.36
6	L5	4149	PSU	C2-N1	2.16	1.39	1.36
6	L5	2258	OMU	C5-C4	-2.16	1.38	1.43
52	S2	669	A2M	O4'-C4'	-2.15	1.40	1.45
6	L5	2680	OMU	C5-C4	-2.14	1.38	1.43
52	S2	1327	OMU	C5-C4	-2.11	1.39	1.43
6	L5	3616	PSU	C2-N1	2.10	1.39	1.36
52	S2	116	OMU	C5-C4	-2.10	1.39	1.43
6	L5	3576	PSU	C2-N1	2.09	1.39	1.36
52	S2	1443	OMU	C5-C4	-2.08	1.39	1.43
6	L5	3973	OMU	C5-C4	-2.07	1.39	1.43
6	L5	4244	OMU	C5-C4	-2.06	1.39	1.43
52	S2	429	OMU	C5-C4	-2.04	1.39	1.43
52	S2	1805	OMU	C5-C4	-2.04	1.39	1.43
52	S2	121	OMU	C5-C4	-2.04	1.39	1.43
6	L5	4382	PSU	C1'-C5	2.03	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	628	OMU	C5-C4	-2.03	1.39	1.43
52	S2	172	OMU	C5-C4	-2.02	1.39	1.43
52	S2	174	OMC	C2-N3	2.02	1.40	1.36
52	S2	355	OMU	C5-C4	-2.01	1.39	1.43

All (867) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	S2	1005	PSU	C4-N3-C2	-8.37	114.28	126.34
79	Se	67	NMM	NE-CZ-NH2	-7.51	112.59	119.48
6	L5	1266	1MA	N1-C2-N3	-7.11	117.73	126.02
52	S2	485	A2M	N3-C2-N1	-6.85	117.97	128.68
6	L5	2630	A2M	N3-C2-N1	-6.84	117.99	128.68
52	S2	27	A2M	N3-C2-N1	-6.84	117.99	128.68
52	S2	1032	A2M	N3-C2-N1	-6.84	117.99	128.68
6	L5	4336	A2M	N3-C2-N1	-6.83	118.00	128.68
52	S2	513	A2M	N3-C2-N1	-6.79	118.07	128.68
52	S2	591	A2M	N3-C2-N1	-6.78	118.07	128.68
6	L5	3492	A2M	N3-C2-N1	-6.78	118.08	128.68
6	L5	1270	A2M	N3-C2-N1	-6.78	118.08	128.68
52	S2	577	A2M	N3-C2-N1	-6.77	118.10	128.68
52	S2	469	A2M	N3-C2-N1	-6.76	118.11	128.68
6	L5	2244	A2M	N3-C2-N1	-6.76	118.11	128.68
52	S2	1679	A2M	N3-C2-N1	-6.76	118.12	128.68
6	L5	400	A2M	N3-C2-N1	-6.75	118.12	128.68
52	S2	1384	A2M	N3-C2-N1	-6.75	118.12	128.68
52	S2	159	A2M	N3-C2-N1	-6.74	118.14	128.68
52	S2	669	A2M	N3-C2-N1	-6.74	118.15	128.68
6	L5	1810	A2M	N3-C2-N1	-6.73	118.15	128.68
6	L5	2206	A2M	N3-C2-N1	-6.73	118.16	128.68
6	L5	398	A2M	N3-C2-N1	-6.73	118.17	128.68
52	S2	166	A2M	N3-C2-N1	-6.72	118.17	128.68
6	L5	3562	A2M	N3-C2-N1	-6.72	118.18	128.68
6	L5	3456	A2M	N3-C2-N1	-6.71	118.19	128.68
6	L5	3557	A2M	N3-C2-N1	-6.70	118.21	128.68
6	L5	4269	A2M	N3-C2-N1	-6.70	118.21	128.68
6	L5	1489	A2M	N3-C2-N1	-6.69	118.23	128.68
6	L5	2658	A2M	N3-C2-N1	-6.68	118.23	128.68
6	L5	4317	A2M	N3-C2-N1	-6.68	118.24	128.68
52	S2	99	A2M	N3-C2-N1	-6.67	118.25	128.68
6	L5	3450	A2M	N3-C2-N1	-6.67	118.26	128.68
6	L5	1479	A2M	N3-C2-N1	-6.62	118.34	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3599	A2M	N3-C2-N1	-6.60	118.36	128.68
6	L5	3517	A2M	N3-C2-N1	-6.49	118.54	128.68
6	L5	3966	6MZ	C2-N1-C6	5.98	121.72	116.59
52	S2	1005	PSU	O2-C2-N1	-5.90	116.30	122.79
52	S2	1005	PSU	N1-C2-N3	5.89	121.80	115.13
6	L5	4382	PSU	C4-N3-C2	-5.83	117.93	126.34
52	S2	1833	6MZ	C2-N1-C6	5.48	121.29	116.59
52	S2	1640	7MG	C5-C6-N1	5.44	120.57	110.99
6	L5	4267	PSU	C4-N3-C2	-5.42	118.53	126.34
6	L5	4188	PSU	C4-N3-C2	-5.37	118.60	126.34
6	L5	4149	PSU	C4-N3-C2	-5.35	118.63	126.34
6	L5	1266	1MA	C5-C6-N1	5.33	121.85	113.90
8	L8	69	PSU	C4-N3-C2	-5.31	118.69	126.34
6	L5	2351	PSU	C4-N3-C2	-5.29	118.71	126.34
6	L5	3369	PSU	C4-N3-C2	-5.29	118.72	126.34
52	S2	1046	PSU	C4-N3-C2	-5.28	118.73	126.34
6	L5	4042	PSU	C4-N3-C2	-5.28	118.74	126.34
52	S2	1693	PSU	C4-N3-C2	-5.26	118.75	126.34
6	L5	4099	PSU	C4-N3-C2	-5.26	118.76	126.34
52	S2	34	PSU	C4-N3-C2	-5.25	118.77	126.34
6	L5	4244	OMU	C4-N3-C2	-5.24	119.66	126.58
6	L5	4039	PSU	C4-N3-C2	-5.24	118.78	126.34
52	S2	210	PSU	C4-N3-C2	-5.24	118.79	126.34
6	L5	3466	PSU	C4-N3-C2	-5.24	118.79	126.34
6	L5	3652	PSU	C4-N3-C2	-5.24	118.79	126.34
52	S2	1446	PSU	C4-N3-C2	-5.24	118.79	126.34
6	L5	3585	PSU	C4-N3-C2	-5.23	118.80	126.34
6	L5	3583	PSU	C4-N3-C2	-5.23	118.80	126.34
52	S2	815	PSU	C4-N3-C2	-5.23	118.81	126.34
52	S2	407	PSU	C4-N3-C2	-5.22	118.81	126.34
52	S2	1245	PSU	C4-N3-C2	-5.22	118.81	126.34
52	S2	1368	PSU	C4-N3-C2	-5.22	118.82	126.34
6	L5	4203	PSU	C4-N3-C2	-5.22	118.82	126.34
52	S2	1644	PSU	C4-N3-C2	-5.22	118.82	126.34
6	L5	3500	PSU	C4-N3-C2	-5.21	118.83	126.34
52	S2	573	PSU	C4-N3-C2	-5.21	118.84	126.34
6	L5	1801	PSU	C4-N3-C2	-5.21	118.84	126.34
6	L5	4749	PSU	C4-N3-C2	-5.21	118.84	126.34
6	L5	1731	PSU	C4-N3-C2	-5.21	118.84	126.34
6	L5	1638	PSU	C4-N3-C2	-5.20	118.84	126.34
52	S2	1082	PSU	C4-N3-C2	-5.20	118.85	126.34
52	S2	355	OMU	C4-N3-C2	-5.19	119.73	126.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4246	PSU	C4-N3-C2	-5.19	118.86	126.34
6	L5	1491	PSU	C4-N3-C2	-5.19	118.86	126.34
6	L5	3502	PSU	C4-N3-C2	-5.19	118.86	126.34
6	L5	3616	PSU	C4-N3-C2	-5.19	118.87	126.34
8	L8	55	PSU	C4-N3-C2	-5.18	118.87	126.34
6	L5	4419	PSU	C4-N3-C2	-5.18	118.88	126.34
6	L5	4325	PSU	C4-N3-C2	-5.18	118.88	126.34
52	S2	1057	PSU	C4-N3-C2	-5.17	118.89	126.34
52	S2	682	PSU	C4-N3-C2	-5.17	118.89	126.34
6	L5	3973	OMU	C4-N3-C2	-5.17	119.76	126.58
6	L5	4045	PSU	C4-N3-C2	-5.17	118.89	126.34
6	L5	3490	PSU	C4-N3-C2	-5.17	118.90	126.34
52	S2	652	PSU	C4-N3-C2	-5.16	118.90	126.34
52	S2	628	OMU	C4-N3-C2	-5.16	119.78	126.58
52	S2	650	PSU	C4-N3-C2	-5.16	118.91	126.34
6	L5	1799	PSU	C4-N3-C2	-5.16	118.91	126.34
6	L5	1537	PSU	C4-N3-C2	-5.15	118.91	126.34
52	S2	1175	PSU	C4-N3-C2	-5.15	118.91	126.34
6	L5	4169	PSU	C4-N3-C2	-5.15	118.92	126.34
6	L5	4298	PSU	C4-N3-C2	-5.15	118.92	126.34
52	S2	1348	PSU	C4-N3-C2	-5.15	118.92	126.34
52	S2	1239	PSU	C4-N3-C2	-5.15	118.93	126.34
6	L5	3496	PSU	C4-N3-C2	-5.14	118.93	126.34
52	S2	816	PSU	C4-N3-C2	-5.14	118.93	126.34
52	S2	429	OMU	C4-N3-C2	-5.14	119.80	126.58
52	S2	1640	7MG	C2-N3-C4	5.14	121.45	112.30
6	L5	4177	PSU	C4-N3-C2	-5.14	118.94	126.34
52	S2	218	PSU	C4-N3-C2	-5.13	118.94	126.34
6	L5	4166	PSU	C4-N3-C2	-5.13	118.95	126.34
52	S2	1178	PSU	C4-N3-C2	-5.13	118.95	126.34
6	L5	4711	PSU	C4-N3-C2	-5.13	118.95	126.34
6	L5	1721	PSU	C4-N3-C2	-5.13	118.95	126.34
6	L5	3371	PSU	C4-N3-C2	-5.12	118.96	126.34
6	L5	4435	PSU	C4-N3-C2	-5.12	118.97	126.34
6	L5	3427	PSU	C4-N3-C2	-5.11	118.97	126.34
52	S2	1233	PSU	C4-N3-C2	-5.11	118.97	126.34
52	S2	864	PSU	C4-N3-C2	-5.11	118.97	126.34
52	S2	967	PSU	C4-N3-C2	-5.11	118.97	126.34
6	L5	2475	PSU	C4-N3-C2	-5.11	118.98	126.34
6	L5	1720	PSU	C4-N3-C2	-5.11	118.98	126.34
6	L5	1683	PSU	C4-N3-C2	-5.10	118.98	126.34
6	L5	1718	PSU	C4-N3-C2	-5.10	118.99	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4107	PSU	C4-N3-C2	-5.10	118.99	126.34
6	L5	4322	PSU	C4-N3-C2	-5.10	118.99	126.34
52	S2	1805	OMU	C4-N3-C2	-5.10	119.85	126.58
6	L5	3447	PSU	C4-N3-C2	-5.10	118.99	126.34
52	S2	1327	OMU	C4-N3-C2	-5.10	119.86	126.58
52	S2	109	PSU	C4-N3-C2	-5.09	119.01	126.34
52	S2	1047	PSU	C4-N3-C2	-5.09	119.01	126.34
52	S2	36	PSU	C4-N3-C2	-5.08	119.01	126.34
6	L5	4374	PSU	C4-N3-C2	-5.08	119.02	126.34
6	L5	4740	PSU	C4-N3-C2	-5.08	119.02	126.34
6	L5	4058	PSU	C4-N3-C2	-5.08	119.02	126.34
6	L5	3462	PSU	C4-N3-C2	-5.08	119.02	126.34
52	S2	105	PSU	C4-N3-C2	-5.07	119.03	126.34
6	L5	4217	PSU	C4-N3-C2	-5.07	119.03	126.34
52	S2	116	OMU	C4-N3-C2	-5.07	119.89	126.58
6	L5	3657	OMU	C4-N3-C2	-5.06	119.90	126.58
52	S2	1626	PSU	C4-N3-C2	-5.06	119.05	126.34
52	S2	867	PSU	C4-N3-C2	-5.06	119.05	126.34
52	S2	119	PSU	C4-N3-C2	-5.05	119.07	126.34
6	L5	3554	PSU	C4-N3-C2	-5.04	119.08	126.34
6	L5	2680	OMU	C4-N3-C2	-5.04	119.94	126.58
52	S2	823	PSU	C4-N3-C2	-5.03	119.09	126.34
52	S2	172	OMU	C4-N3-C2	-5.03	119.94	126.58
52	S2	687	PSU	C4-N3-C2	-5.01	119.11	126.34
6	L5	2258	OMU	C4-N3-C2	-5.01	119.97	126.58
6	L5	4278	PSU	C4-N3-C2	-5.01	119.13	126.34
52	S2	610	PSU	C4-N3-C2	-5.00	119.13	126.34
52	S2	93	PSU	C4-N3-C2	-5.00	119.13	126.34
6	L5	3494	PSU	C4-N3-C2	-4.99	119.14	126.34
52	S2	1289	OMU	C4-N3-C2	-4.96	120.04	126.58
6	L5	4366	OMU	C4-N3-C2	-4.93	120.08	126.58
6	L5	3576	PSU	C4-N3-C2	-4.90	119.28	126.34
52	S2	121	OMU	C4-N3-C2	-4.90	120.12	126.58
52	S2	802	PSU	C4-N3-C2	-4.88	119.31	126.34
6	L5	4052	OMU	C4-N3-C2	-4.84	120.20	126.58
52	S2	1443	OMU	C4-N3-C2	-4.83	120.20	126.58
6	L5	4193	5MC	C5-C6-N1	-4.79	118.41	123.34
6	L5	1632	PSU	C4-N3-C2	-4.71	119.55	126.34
6	L5	4244	OMU	N3-C2-N1	4.69	121.12	114.89
6	L5	3657	OMU	N3-C2-N1	4.68	121.10	114.89
6	L5	4382	PSU	N1-C2-N3	4.64	120.39	115.13
52	S2	355	OMU	N3-C2-N1	4.64	121.05	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L5	3973	OMU	N3-C2-N1	4.60	120.99	114.89
6	L5	2680	OMU	N3-C2-N1	4.59	120.98	114.89
6	L5	4366	OMU	N3-C2-N1	4.55	120.93	114.89
6	L5	4149	PSU	N1-C2-N3	4.55	120.29	115.13
6	L5	3583	PSU	N1-C2-N3	4.54	120.28	115.13
6	L5	2258	OMU	N3-C2-N1	4.53	120.91	114.89
52	S2	1805	OMU	N3-C2-N1	4.52	120.89	114.89
8	L8	69	PSU	N1-C2-N3	4.51	120.25	115.13
6	L5	4188	PSU	N1-C2-N3	4.51	120.24	115.13
6	L5	2630	A2M	C1'-N9-C4	-4.50	118.73	126.64
6	L5	4267	PSU	N1-C2-N3	4.49	120.22	115.13
52	S2	1338	4AC	N4-C4-N3	4.48	121.37	113.85
52	S2	116	OMU	N3-C2-N1	4.46	120.81	114.89
6	L5	4039	PSU	N1-C2-N3	4.44	120.16	115.13
6	L5	3517	A2M	O4'-C1'-C2'	-4.44	98.89	106.59
6	L5	4246	PSU	N1-C2-N3	4.42	120.14	115.13
6	L5	4099	PSU	N1-C2-N3	4.42	120.14	115.13
6	L5	3369	PSU	N1-C2-N3	4.41	120.13	115.13
6	L5	3616	PSU	N1-C2-N3	4.41	120.12	115.13
6	L5	3652	PSU	N1-C2-N3	4.39	120.10	115.13
52	S2	1443	OMU	N3-C2-N1	4.39	120.71	114.89
52	S2	1693	PSU	N1-C2-N3	4.39	120.10	115.13
6	L5	1638	PSU	N1-C2-N3	4.38	120.09	115.13
6	L5	1799	PSU	N1-C2-N3	4.37	120.08	115.13
6	L5	4177	PSU	N1-C2-N3	4.37	120.08	115.13
6	L5	1491	PSU	N1-C2-N3	4.37	120.08	115.13
52	S2	121	OMU	N3-C2-N1	4.36	120.68	114.89
6	L5	4052	OMU	N3-C2-N1	4.36	120.68	114.89
52	S2	1046	PSU	N1-C2-N3	4.36	120.07	115.13
6	L5	4325	PSU	N1-C2-N3	4.36	120.07	115.13
6	L5	4435	PSU	N1-C2-N3	4.35	120.05	115.13
6	L5	4419	PSU	N1-C2-N3	4.35	120.05	115.13
52	S2	34	PSU	N1-C2-N3	4.34	120.04	115.13
52	S2	682	PSU	N1-C2-N3	4.33	120.04	115.13
6	L5	4045	PSU	N1-C2-N3	4.33	120.04	115.13
6	L5	3496	PSU	N1-C2-N3	4.33	120.03	115.13
52	S2	1368	PSU	N1-C2-N3	4.33	120.03	115.13
6	L5	3585	PSU	N1-C2-N3	4.32	120.02	115.13
6	L5	4169	PSU	N1-C2-N3	4.32	120.02	115.13
52	S2	1175	PSU	N1-C2-N3	4.32	120.02	115.13
6	L5	4217	PSU	N1-C2-N3	4.32	120.02	115.13
6	L5	3371	PSU	N1-C2-N3	4.31	120.02	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	S2	1644	PSU	N1-C2-N3	4.31	120.02	115.13
6	L5	3466	PSU	N1-C2-N3	4.31	120.01	115.13
52	S2	407	PSU	N1-C2-N3	4.30	120.00	115.13
6	L5	4374	PSU	N1-C2-N3	4.29	119.99	115.13
52	S2	1082	PSU	N1-C2-N3	4.29	119.99	115.13
6	L5	4203	PSU	N1-C2-N3	4.28	119.98	115.13
52	S2	1245	PSU	N1-C2-N3	4.28	119.98	115.13
6	L5	1721	PSU	N1-C2-N3	4.28	119.98	115.13
52	S2	687	PSU	N1-C2-N3	4.28	119.98	115.13
52	S2	1446	PSU	N1-C2-N3	4.28	119.98	115.13
6	L5	4298	PSU	N1-C2-N3	4.28	119.98	115.13
6	L5	4278	PSU	N1-C2-N3	4.28	119.98	115.13
52	S2	1057	PSU	N1-C2-N3	4.27	119.97	115.13
8	L8	55	PSU	N1-C2-N3	4.27	119.97	115.13
6	L5	3554	PSU	N1-C2-N3	4.27	119.97	115.13
6	L5	4042	PSU	N1-C2-N3	4.27	119.96	115.13
52	S2	172	OMU	N3-C2-N1	4.26	120.55	114.89
52	S2	652	PSU	N1-C2-N3	4.26	119.95	115.13
6	L5	4711	PSU	N1-C2-N3	4.26	119.95	115.13
52	S2	823	PSU	N1-C2-N3	4.26	119.95	115.13
6	L5	2351	PSU	N1-C2-N3	4.26	119.95	115.13
52	S2	1289	OMU	N3-C2-N1	4.25	120.54	114.89
6	L5	3427	PSU	N1-C2-N3	4.25	119.95	115.13
6	L5	3500	PSU	N1-C2-N3	4.25	119.95	115.13
6	L5	2475	PSU	N1-C2-N3	4.25	119.94	115.13
52	S2	1239	PSU	N1-C2-N3	4.25	119.94	115.13
6	L5	1683	PSU	N1-C2-N3	4.24	119.94	115.13
6	L5	4749	PSU	N1-C2-N3	4.24	119.94	115.13
6	L5	3502	PSU	N1-C2-N3	4.24	119.94	115.13
6	L5	1731	PSU	N1-C2-N3	4.24	119.93	115.13
52	S2	1233	PSU	N1-C2-N3	4.24	119.93	115.13
52	S2	573	PSU	N1-C2-N3	4.23	119.93	115.13
6	L5	1537	PSU	N1-C2-N3	4.23	119.92	115.13
6	L5	1479	A2M	O4'-C4'-C3'	-4.23	96.75	105.11
6	L5	1720	PSU	N1-C2-N3	4.23	119.92	115.13
52	S2	816	PSU	N1-C2-N3	4.23	119.92	115.13
52	S2	1178	PSU	N1-C2-N3	4.22	119.92	115.13
6	L5	1801	PSU	N1-C2-N3	4.22	119.91	115.13
52	S2	802	PSU	N1-C2-N3	4.22	119.91	115.13
6	L5	4107	PSU	N1-C2-N3	4.21	119.91	115.13
6	L5	4740	PSU	N1-C2-N3	4.21	119.90	115.13
6	L5	1632	PSU	N1-C2-N3	4.20	119.89	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	815	PSU	N1-C2-N3	4.20	119.89	115.13
52	S2	218	PSU	N1-C2-N3	4.20	119.89	115.13
6	L5	3447	PSU	N1-C2-N3	4.20	119.89	115.13
52	S2	628	OMU	N3-C2-N1	4.20	120.46	114.89
6	L5	3494	PSU	N1-C2-N3	4.20	119.88	115.13
6	L5	1718	PSU	N1-C2-N3	4.19	119.88	115.13
6	L5	3490	PSU	N1-C2-N3	4.19	119.88	115.13
52	S2	1348	PSU	N1-C2-N3	4.19	119.88	115.13
52	S2	105	PSU	N1-C2-N3	4.19	119.88	115.13
52	S2	36	PSU	N1-C2-N3	4.19	119.88	115.13
52	S2	864	PSU	N1-C2-N3	4.19	119.87	115.13
52	S2	1047	PSU	N1-C2-N3	4.18	119.87	115.13
6	L5	4322	PSU	N1-C2-N3	4.18	119.87	115.13
52	S2	650	PSU	N1-C2-N3	4.18	119.86	115.13
52	S2	610	PSU	N1-C2-N3	4.18	119.86	115.13
52	S2	210	PSU	N1-C2-N3	4.18	119.86	115.13
52	S2	867	PSU	N1-C2-N3	4.17	119.85	115.13
52	S2	109	PSU	N1-C2-N3	4.17	119.85	115.13
6	L5	4058	PSU	N1-C2-N3	4.16	119.85	115.13
52	S2	1626	PSU	N1-C2-N3	4.16	119.84	115.13
6	L5	3462	PSU	N1-C2-N3	4.16	119.84	115.13
52	S2	429	OMU	N3-C2-N1	4.16	120.41	114.89
6	L5	4166	PSU	N1-C2-N3	4.16	119.84	115.13
6	L5	3576	PSU	N1-C2-N3	4.16	119.84	115.13
52	S2	967	PSU	N1-C2-N3	4.14	119.82	115.13
52	S2	119	PSU	N1-C2-N3	4.11	119.79	115.13
52	S2	1327	OMU	N3-C2-N1	4.08	120.31	114.89
52	S2	93	PSU	N1-C2-N3	4.08	119.75	115.13
79	Se	67	NMM	NE-CZ-NH1	3.84	127.46	120.26
6	L5	2719	OMG	C2-N1-C6	-3.82	118.06	125.10
6	L5	1580	OMG	C2-N1-C6	-3.82	118.07	125.10
52	S2	1843	4AC	N4-C4-N3	3.81	120.25	113.85
52	S2	1329	OMG	C2-N1-C6	-3.79	118.13	125.10
52	S2	437	OMG	C2-N1-C6	-3.78	118.13	125.10
52	S2	1640	7MG	C5-C4-N3	-3.78	120.93	128.13
6	L5	3676	OMG	C2-N1-C6	-3.77	118.16	125.10
6	L5	4138	OMG	C2-N1-C6	-3.76	118.17	125.10
52	S2	510	OMG	C2-N1-C6	-3.75	118.20	125.10
52	S2	1491	OMG	C2-N1-C6	-3.74	118.21	125.10
52	S2	645	OMG	C2-N1-C6	-3.74	118.21	125.10
6	L5	2267	OMG	C2-N1-C6	-3.74	118.22	125.10
52	S2	1448	OMG	C2-N1-C6	-3.73	118.22	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4116	OMG	C2-N1-C6	-3.73	118.23	125.10
6	L5	4364	OMG	C2-N1-C6	-3.72	118.24	125.10
52	S2	1005	PSU	C6-C5-C4	3.72	120.80	118.20
52	S2	684	OMG	C2-N1-C6	-3.72	118.25	125.10
6	L5	3942	OMG	C2-N1-C6	-3.72	118.25	125.10
6	L5	4383	OMG	C2-N1-C6	-3.72	118.25	125.10
52	S2	1640	7MG	C2-N1-C6	-3.72	118.32	125.10
6	L5	3476	OMG	C2-N1-C6	-3.71	118.27	125.10
6	L5	4369	OMG	C2-N1-C6	-3.70	118.28	125.10
8	L8	75	OMG	C2-N1-C6	-3.67	118.35	125.10
52	S2	602	OMG	C2-N1-C6	-3.66	118.35	125.10
6	L5	1477	OMG	C2-N1-C6	-3.66	118.35	125.10
6	L5	4245	OMG	C2-N1-C6	-3.65	118.38	125.10
52	S2	669	A2M	O4'-C4'-C3'	-3.63	97.92	105.11
6	L5	1260	OMG	C2-N1-C6	-3.63	118.41	125.10
6	L5	3974	OMG	C2-N1-C6	-3.63	118.41	125.10
6	L5	3631	OMG	C2-N1-C6	-3.61	118.44	125.10
6	L5	3359	OMG	C2-N1-C6	-3.61	118.44	125.10
52	S2	868	OMG	C2-N1-C6	-3.61	118.45	125.10
6	L5	4240	OMG	C2-N1-C6	-3.60	118.46	125.10
6	L5	3524	OMG	C2-N1-C6	-3.60	118.47	125.10
6	L5	4276	UR3	C4-N3-C2	-3.55	121.22	124.56
6	L5	4382	PSU	O2-C2-N1	-3.52	118.92	122.79
6	L5	2207	OMG	C2-N1-C6	-3.51	118.63	125.10
52	S2	1851	MA6	C4-C5-N7	-3.42	105.84	109.40
52	S2	1852	MA6	C9-N6-C6	-3.41	109.18	119.51
6	L5	4138	OMG	C5-C6-N1	3.37	119.90	113.95
6	L5	2207	OMG	C5-C6-N1	3.35	119.86	113.95
52	S2	1851	MA6	C9-N6-C6	-3.34	109.39	119.51
52	S2	1491	OMG	C5-C6-N1	3.33	119.82	113.95
6	L5	2719	OMG	C5-C6-N1	3.32	119.82	113.95
52	S2	591	A2M	C2'-C3'-C4'	-3.32	94.78	101.99
52	S2	1851	MA6	N3-C2-N1	-3.32	123.49	128.68
6	L5	2267	OMG	C5-C6-N1	3.32	119.81	113.95
52	S2	684	OMG	C5-C6-N1	3.31	119.79	113.95
6	L5	3524	OMG	C5-C6-N1	3.30	119.79	113.95
52	S2	469	A2M	C2'-C3'-C4'	-3.30	94.83	101.99
6	L5	3942	OMG	C5-C6-N1	3.29	119.77	113.95
6	L5	1260	OMG	C5-C6-N1	3.29	119.76	113.95
6	L5	4383	OMG	C5-C6-N1	3.28	119.74	113.95
6	L5	3476	OMG	C5-C6-N1	3.27	119.73	113.95
52	S2	1327	OMU	C5-C4-N3	3.27	119.73	114.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	1477	OMG	C5-C6-N1	3.27	119.73	113.95
52	S2	645	OMG	C5-C6-N1	3.26	119.71	113.95
6	L5	4336	A2M	C2'-C3'-C4'	-3.26	94.92	101.99
6	L5	4245	OMG	C5-C6-N1	3.26	119.70	113.95
52	S2	1329	OMG	C5-C6-N1	3.26	119.70	113.95
52	S2	577	A2M	C2'-C3'-C4'	-3.26	94.92	101.99
52	S2	437	OMG	C5-C6-N1	3.25	119.69	113.95
6	L5	4364	OMG	C5-C6-N1	3.25	119.69	113.95
6	L5	4369	OMG	C5-C6-N1	3.25	119.69	113.95
6	L5	4116	OMG	C5-C6-N1	3.25	119.68	113.95
6	L5	3676	OMG	C5-C6-N1	3.24	119.68	113.95
52	S2	591	A2M	O4'-C4'-C3'	-3.23	98.71	105.11
6	L5	3966	6MZ	C9-N6-C6	-3.23	120.09	122.87
6	L5	1580	OMG	C5-C6-N1	3.23	119.66	113.95
52	S2	510	OMG	C5-C6-N1	3.23	119.66	113.95
8	L8	75	OMG	C5-C6-N1	3.23	119.65	113.95
6	L5	3631	OMG	C5-C6-N1	3.23	119.65	113.95
6	L5	3514	5MC	C5-C6-N1	-3.22	120.02	123.34
52	S2	429	OMU	C5-C4-N3	3.22	119.66	114.84
52	S2	602	OMG	C5-C6-N1	3.22	119.63	113.95
6	L5	3359	OMG	C5-C6-N1	3.21	119.62	113.95
52	S2	1289	OMU	C5-C4-N3	3.21	119.64	114.84
6	L5	3966	6MZ	N3-C2-N1	-3.20	123.67	128.68
6	L5	4193	5MC	C5-C4-N4	-3.20	116.69	121.48
52	S2	628	OMU	C5-C4-N3	3.19	119.62	114.84
6	L5	4240	OMG	C5-C6-N1	3.19	119.59	113.95
52	S2	116	OMU	C5-C4-N3	3.19	119.61	114.84
6	L5	3974	OMG	C5-C6-N1	3.18	119.57	113.95
52	S2	1852	MA6	N3-C2-N1	-3.18	123.70	128.68
52	S2	355	OMU	C5-C4-N3	3.18	119.60	114.84
52	S2	1805	OMU	C5-C4-N3	3.18	119.60	114.84
52	S2	1852	MA6	C4-C5-N7	-3.17	106.09	109.40
52	S2	868	OMG	C5-C6-N1	3.17	119.55	113.95
6	L5	2258	OMU	C5-C4-N3	3.17	119.58	114.84
6	L5	4244	OMU	C5-C4-N3	3.17	119.58	114.84
52	S2	513	A2M	C2'-C3'-C4'	-3.14	95.17	101.99
52	S2	1640	7MG	C5-C4-N9	3.14	110.42	106.35
6	L5	4366	OMU	C5-C4-N3	3.14	119.53	114.84
52	S2	1448	OMG	C5-C6-N1	3.13	119.48	113.95
6	L5	4052	OMU	C5-C4-N3	3.13	119.52	114.84
52	S2	172	OMU	C5-C4-N3	3.12	119.51	114.84
6	L5	2680	OMU	C5-C4-N3	3.12	119.50	114.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3973	OMU	C5-C4-N3	3.11	119.49	114.84
52	S2	121	OMU	C5-C4-N3	3.09	119.47	114.84
52	S2	1443	OMU	C5-C4-N3	3.08	119.44	114.84
6	L5	3657	OMU	C5-C4-N3	3.07	119.44	114.84
52	S2	485	A2M	O4'-C4'-C3'	-3.07	99.03	105.11
52	S2	1833	6MZ	N3-C2-N1	-3.04	123.93	128.68
6	L5	4188	PSU	C6-C5-C4	3.02	120.31	118.20
6	L5	2244	A2M	C2'-C3'-C4'	-3.01	95.47	101.99
6	L5	3514	5MC	C5-C4-N4	-2.97	117.04	121.48
6	L5	3599	A2M	C2'-C3'-C4'	-2.97	95.54	101.99
6	L5	3562	A2M	C2'-C3'-C4'	-2.95	95.58	101.99
6	L5	1810	A2M	C2'-C3'-C4'	-2.94	95.61	101.99
6	L5	3517	A2M	C5-C6-N6	-2.92	115.91	120.35
52	S2	166	A2M	C2'-C3'-C4'	-2.92	95.66	101.99
52	S2	1327	OMU	O4-C4-C5	-2.92	120.03	125.16
6	L5	4267	PSU	C6-C5-C4	2.91	120.23	118.20
6	L5	4336	A2M	O4'-C4'-C3'	-2.89	99.39	105.11
6	L5	3557	A2M	C5-C6-N6	-2.88	115.97	120.35
52	S2	1384	A2M	C2'-C3'-C4'	-2.87	95.76	101.99
6	L5	4269	A2M	C2'-C3'-C4'	-2.87	95.76	101.99
52	S2	823	PSU	O2-C2-N1	-2.87	119.63	122.79
6	L5	400	A2M	C5-C6-N6	-2.86	116.00	120.35
52	S2	645	OMG	C8-N7-C5	2.86	108.43	102.99
6	L5	3456	A2M	C2'-C3'-C4'	-2.85	95.81	101.99
6	L5	4099	PSU	C6-C5-C4	2.84	120.18	118.20
52	S2	429	OMU	O4-C4-C5	-2.83	120.18	125.16
52	S2	172	OMU	O4-C4-C5	-2.82	120.20	125.16
52	S2	116	OMU	O4-C4-C5	-2.82	120.21	125.16
6	L5	1260	OMG	C8-N7-C5	2.81	108.34	102.99
52	S2	1679	A2M	C5-C6-N6	-2.81	116.09	120.35
52	S2	628	OMU	O4-C4-C5	-2.80	120.23	125.16
52	S2	485	A2M	CM'-O2'-C2'	-2.80	107.19	114.52
6	L5	2680	OMU	O4-C4-C5	-2.80	120.24	125.16
52	S2	1032	A2M	C2'-C3'-C4'	-2.80	95.92	101.99
6	L5	3492	A2M	C2'-C3'-C4'	-2.79	95.93	101.99
6	L5	1489	A2M	C3'-C2'-C1'	-2.79	97.65	102.89
52	S2	27	A2M	C5-C6-N6	-2.79	116.12	120.35
6	L5	4336	A2M	C5-C6-N6	-2.78	116.12	120.35
6	L5	1477	OMG	C8-N7-C5	2.78	108.29	102.99
52	S2	1805	OMU	O4-C4-C5	-2.78	120.27	125.16
6	L5	3583	PSU	C6-C5-C4	2.78	120.14	118.20
6	L5	4269	A2M	C5-C6-N6	-2.77	116.14	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L5	4245	OMG	C8-N7-C5	2.77	108.26	102.99
52	S2	1679	A2M	C2'-C3'-C4'	-2.77	95.99	101.99
6	L5	1266	1MA	C8-N7-C5	2.76	108.26	102.99
6	L5	3973	OMU	O4-C4-C5	-2.76	120.30	125.16
6	L5	4138	OMG	C8-N7-C5	2.76	108.25	102.99
52	S2	1443	OMU	O4-C4-C5	-2.76	120.31	125.16
52	S2	868	OMG	C8-N7-C5	2.76	108.24	102.99
6	L5	4317	A2M	C5-C6-N6	-2.76	116.17	120.35
52	S2	99	A2M	C5-C6-N6	-2.75	116.17	120.35
6	L5	4116	OMG	C8-N7-C5	2.75	108.22	102.99
6	L5	1810	A2M	CM'-O2'-C2'	-2.74	107.33	114.52
52	S2	602	OMG	C8-N7-C5	2.74	108.21	102.99
6	L5	2244	A2M	C5-C6-N6	-2.74	116.19	120.35
6	L5	2206	A2M	C5-C6-N6	-2.73	116.20	120.35
6	L5	3657	OMU	O4-C4-C5	-2.73	120.35	125.16
6	L5	4383	OMG	C8-N7-C5	2.73	108.19	102.99
6	L5	3562	A2M	C5-C6-N6	-2.73	116.20	120.35
52	S2	684	OMG	C8-N7-C5	2.73	108.19	102.99
6	L5	4149	PSU	O2-C2-N1	-2.73	119.79	122.79
6	L5	4240	OMG	C8-N7-C5	2.73	108.18	102.99
6	L5	4244	OMU	O4-C4-C5	-2.72	120.37	125.16
6	L5	398	A2M	C5-C6-N6	-2.72	116.22	120.35
6	L5	1810	A2M	C5-C6-N6	-2.72	116.22	120.35
52	S2	1329	OMG	C8-N7-C5	2.72	108.18	102.99
6	L5	3557	A2M	C2'-C3'-C4'	-2.72	96.08	101.99
6	L5	4364	OMG	C8-N7-C5	2.72	108.17	102.99
6	L5	3599	A2M	C5-C6-N6	-2.72	116.22	120.35
6	L5	1489	A2M	C5-C6-N6	-2.72	116.22	120.35
52	S2	1384	A2M	C5-C6-N6	-2.71	116.23	120.35
6	L5	3359	OMG	C8-N7-C5	2.71	108.16	102.99
8	L8	69	PSU	C6-C5-C4	2.71	120.09	118.20
6	L5	3450	A2M	C5-C6-N6	-2.71	116.24	120.35
6	L5	2258	OMU	O4-C4-C5	-2.70	120.40	125.16
52	S2	513	A2M	C5-C6-N6	-2.70	116.24	120.35
6	L5	1479	A2M	C5-C6-N6	-2.70	116.25	120.35
6	L5	3974	OMG	C8-N7-C5	2.70	108.13	102.99
52	S2	159	A2M	C5-C6-N6	-2.70	116.25	120.35
6	L5	1270	A2M	C5-C6-N6	-2.69	116.26	120.35
6	L5	4369	OMG	C8-N7-C5	2.69	108.11	102.99
6	L5	3676	OMG	C8-N7-C5	2.69	108.11	102.99
52	S2	510	OMG	C8-N7-C5	2.69	108.11	102.99
52	S2	591	A2M	C1'-N9-C4	2.69	131.36	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	S2	669	A2M	C5-C6-N6	-2.69	116.27	120.35
52	S2	34	PSU	C6-C5-C4	2.69	120.08	118.20
52	S2	485	A2M	C5-C6-N6	-2.69	116.27	120.35
6	L5	3631	OMG	C8-N7-C5	2.69	108.11	102.99
6	L5	2206	A2M	C2'-C3'-C4'	-2.68	96.16	101.99
6	L5	2207	OMG	C8-N7-C5	2.68	108.10	102.99
6	L5	3942	OMG	C8-N7-C5	2.68	108.10	102.99
52	S2	166	A2M	C5-C6-N6	-2.68	116.28	120.35
52	S2	591	A2M	C5-C6-N6	-2.68	116.28	120.35
6	L5	2267	OMG	C8-N7-C5	2.68	108.09	102.99
6	L5	1270	A2M	C2'-C3'-C4'	-2.68	96.18	101.99
6	L5	4052	OMU	O4-C4-C5	-2.68	120.45	125.16
52	S2	1491	OMG	C8-N7-C5	2.68	108.09	102.99
6	L5	3476	OMG	C8-N7-C5	2.68	108.09	102.99
52	S2	121	OMU	O4-C4-C5	-2.67	120.47	125.16
52	S2	99	A2M	C2'-C3'-C4'	-2.66	96.21	101.99
6	L5	3456	A2M	C5-C6-N6	-2.66	116.31	120.35
52	S2	1640	7MG	C4-C5-N7	2.66	109.22	105.53
52	S2	1289	OMU	O4-C4-C5	-2.66	120.49	125.16
6	L5	4202	OMC	CM2-O2'-C2'	-2.66	107.55	114.52
52	S2	1032	A2M	C5-C6-N6	-2.66	116.31	120.35
6	L5	3524	OMG	C8-N7-C5	2.66	108.05	102.99
6	L5	4366	OMU	O4-C4-C5	-2.65	120.49	125.16
8	L8	75	OMG	C8-N7-C5	2.65	108.05	102.99
52	S2	1005	PSU	O4-C4-C5	-2.65	117.12	124.05
52	S2	577	A2M	C5-C6-N6	-2.65	116.33	120.35
6	L5	1270	A2M	O4'-C4'-C3'	-2.65	99.88	105.11
6	L5	3492	A2M	C5-C6-N6	-2.64	116.33	120.35
6	L5	1580	OMG	C8-N7-C5	2.64	108.03	102.99
6	L5	2630	A2M	C5-C6-N6	-2.64	116.34	120.35
6	L5	2658	A2M	C5-C6-N6	-2.64	116.34	120.35
52	S2	469	A2M	C5-C6-N6	-2.64	116.34	120.35
6	L5	4246	PSU	O2-C2-N1	-2.64	119.89	122.79
6	L5	2719	OMG	C8-N7-C5	2.64	108.01	102.99
52	S2	27	A2M	CM'-O2'-C2'	-2.63	107.61	114.52
52	S2	355	OMU	O4-C4-C5	-2.63	120.53	125.16
6	L5	4317	A2M	CM'-O2'-C2'	-2.63	107.62	114.52
52	S2	687	PSU	O2-C2-N1	-2.63	119.89	122.79
6	L5	3619	OMC	CM2-O2'-C2'	-2.63	107.62	114.52
52	S2	437	OMG	C8-N7-C5	2.63	108.00	102.99
52	S2	1446	PSU	C6-C5-C4	2.63	120.03	118.20
52	S2	1448	OMG	C8-N7-C5	2.62	107.99	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L5	4149	PSU	C6-C5-C4	2.62	120.03	118.20
52	S2	210	PSU	C6-C5-C4	2.62	120.03	118.20
6	L5	2244	A2M	O4'-C4'-C3'	-2.61	99.94	105.11
6	L5	3450	A2M	C2'-C3'-C4'	-2.61	96.33	101.99
6	L5	3557	A2M	CM'-O2'-C2'	-2.60	107.70	114.52
6	L5	4269	A2M	CM'-O2'-C2'	-2.60	107.71	114.52
52	S2	1032	A2M	CM'-O2'-C2'	-2.59	107.73	114.52
52	S2	573	PSU	O2-C2-N1	-2.58	119.94	122.79
6	L5	4374	PSU	O2-C2-N1	-2.57	119.96	122.79
6	L5	398	A2M	C2'-C3'-C4'	-2.57	96.41	101.99
52	S2	1852	MA6	N1-C6-N6	2.55	119.74	117.06
6	L5	4246	PSU	C6-C5-C4	2.55	119.98	118.20
6	L5	4244	OMU	O2-C2-N1	-2.54	119.41	122.79
52	S2	684	OMG	CM2-O2'-C2'	-2.54	107.87	114.52
52	S2	1245	PSU	O2-C2-N1	-2.53	120.00	122.79
52	S2	802	PSU	O2-C2-N1	-2.53	120.00	122.79
81	Sg	1	AME	O-C-CA	-2.53	118.14	124.78
6	L5	3554	PSU	O2-C2-N1	-2.53	120.01	122.79
52	S2	27	A2M	C2'-C3'-C4'	-2.52	96.51	101.99
52	S2	119	PSU	O2-C2-N1	-2.52	120.02	122.79
6	L5	3652	PSU	C6-C5-C4	2.52	119.96	118.20
52	S2	1368	PSU	O2-C2-N1	-2.51	120.03	122.79
6	L5	3966	6MZ	C4-C5-N7	-2.51	106.78	109.40
52	S2	1693	PSU	O2-C2-N1	-2.51	120.03	122.79
6	L5	4169	PSU	C6-C5-C4	2.51	119.95	118.20
6	L5	2658	A2M	C2'-C3'-C4'	-2.50	96.55	101.99
6	L5	1270	A2M	CM'-O2'-C2'	-2.50	107.95	114.52
6	L5	1799	PSU	O2-C2-N1	-2.50	120.03	122.79
6	L5	4177	PSU	O2-C2-N1	-2.50	120.03	122.79
6	L5	2206	A2M	CM'-O2'-C2'	-2.50	107.96	114.52
52	S2	1046	PSU	C6-C5-C4	2.50	119.95	118.20
52	S2	159	A2M	C2'-C3'-C4'	-2.50	96.56	101.99
52	S2	816	PSU	O2-C2-N1	-2.50	120.04	122.79
52	S2	1851	MA6	C10-N6-C9	-2.50	108.07	116.12
6	L5	3466	PSU	C6-C5-C4	2.50	119.94	118.20
6	L5	3576	PSU	O2-C2-N1	-2.49	120.04	122.79
6	L5	400	A2M	CM'-O2'-C2'	-2.49	107.99	114.52
52	S2	1239	PSU	O2-C2-N1	-2.49	120.05	122.79
6	L5	1491	PSU	O2-C2-N1	-2.49	120.05	122.79
6	L5	1683	PSU	O2-C2-N1	-2.49	120.05	122.79
6	L5	4099	PSU	O2-C2-N1	-2.49	120.05	122.79
6	L5	4166	PSU	C6-C5-C4	2.48	119.93	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	S2	867	PSU	O2-C2-N1	-2.48	120.06	122.79
52	S2	610	PSU	O2-C2-N1	-2.48	120.06	122.79
6	L5	3500	PSU	O2-C2-N1	-2.47	120.07	122.79
6	L5	4419	PSU	O2-C2-N1	-2.47	120.07	122.79
6	L5	4325	PSU	O2-C2-N1	-2.47	120.07	122.79
52	S2	105	PSU	O2-C2-N1	-2.47	120.08	122.79
6	L5	4435	PSU	O2-C2-N1	-2.47	120.08	122.79
6	L5	1632	PSU	C6-N1-C2	-2.47	120.16	122.68
52	S2	1833	6MZ	C9-N6-C6	-2.46	120.75	122.87
6	L5	3496	PSU	O2-C2-N1	-2.46	120.08	122.79
52	S2	682	PSU	O2-C2-N1	-2.46	120.09	122.79
6	L5	1721	PSU	O2-C2-N1	-2.45	120.09	122.79
52	S2	210	PSU	O2-C2-N1	-2.45	120.10	122.79
52	S2	864	PSU	O2-C2-N1	-2.45	120.10	122.79
6	L5	4240	OMG	CM2-O2'-C2'	-2.45	108.10	114.52
83	Si	62	HY3	O-C-CA	-2.45	118.01	124.83
6	L5	3494	PSU	O2-C2-N1	-2.45	120.10	122.79
6	L5	1720	PSU	O2-C2-N1	-2.44	120.10	122.79
6	L5	4267	PSU	O2-C2-N1	-2.44	120.10	122.79
8	L8	69	PSU	O2-C2-N1	-2.44	120.10	122.79
6	L5	2658	A2M	CM'-O2'-C2'	-2.44	108.12	114.52
6	L5	4269	A2M	O4'-C4'-C3'	-2.44	100.29	105.11
52	S2	36	PSU	O2-C2-N1	-2.44	120.11	122.79
6	L5	3450	A2M	CM'-O2'-C2'	-2.43	108.14	114.52
52	S2	652	PSU	C6-C5-C4	2.43	119.90	118.20
6	L5	3583	PSU	O2-C2-N1	-2.43	120.11	122.79
52	S2	99	A2M	C3'-C2'-C1'	-2.43	98.32	102.89
52	S2	1175	PSU	O2-C2-N1	-2.43	120.11	122.79
6	L5	3599	A2M	CM'-O2'-C2'	-2.43	108.14	114.52
6	L5	1718	PSU	O2-C2-N1	-2.43	120.12	122.79
52	S2	815	PSU	C6-C5-C4	2.43	119.90	118.20
6	L5	3562	A2M	CM'-O2'-C2'	-2.43	108.16	114.52
6	L5	4169	PSU	O2-C2-N1	-2.43	120.12	122.79
6	L5	4042	PSU	C6-C5-C4	2.42	119.89	118.20
52	S2	172	OMU	CM2-O2'-C2'	-2.42	108.17	114.52
6	L5	3447	PSU	O2-C2-N1	-2.42	120.13	122.79
6	L5	4711	PSU	O2-C2-N1	-2.42	120.13	122.79
52	S2	407	PSU	O2-C2-N1	-2.42	120.13	122.79
52	S2	166	A2M	CM'-O2'-C2'	-2.41	108.19	114.52
78	Sd	2	SAC	O-C-CA	-2.41	118.45	124.78
8	L8	55	PSU	O2-C2-N1	-2.41	120.14	122.79
6	L5	3616	PSU	O2-C2-N1	-2.41	120.14	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	116	OMU	O2-C2-N1	-2.41	119.59	122.79
52	S2	218	PSU	O2-C2-N1	-2.41	120.14	122.79
6	L5	3657	OMU	O2-C2-N1	-2.40	119.59	122.79
52	S2	1392	OMC	CM2-O2'-C2'	-2.40	108.22	114.52
6	L5	4138	OMG	CM2-O2'-C2'	-2.40	108.22	114.52
6	L5	2475	PSU	O2-C2-N1	-2.40	120.15	122.79
52	S2	1047	PSU	O2-C2-N1	-2.40	120.15	122.79
6	L5	3973	OMU	O2-C2-N1	-2.40	119.60	122.79
6	L5	3599	A2M	O4'-C4'-C3'	-2.40	100.37	105.11
52	S2	469	A2M	O4'-C4'-C3'	-2.39	100.38	105.11
52	S2	1046	PSU	O2-C2-N1	-2.39	120.16	122.79
6	L5	1479	A2M	CM'-O2'-C2'	-2.39	108.25	114.52
52	S2	1289	OMU	CM2-O2'-C2'	-2.39	108.25	114.52
52	S2	1640	7MG	O6-C6-C5	-2.39	121.68	127.54
52	S2	1338	4AC	C5-C4-N4	-2.39	118.77	122.92
6	L5	2351	PSU	O2-C2-N1	-2.38	120.17	122.79
52	S2	109	PSU	O2-C2-N1	-2.38	120.17	122.79
52	S2	1644	PSU	O2-C2-N1	-2.38	120.17	122.79
6	L5	4039	PSU	C6-C5-C4	2.38	119.86	118.20
52	S2	650	PSU	O2-C2-N1	-2.38	120.18	122.79
6	L5	3371	PSU	O2-C2-N1	-2.38	120.18	122.79
52	S2	1338	4AC	C6-C5-C4	2.37	119.86	116.96
52	S2	628	OMU	O2-C2-N1	-2.37	119.64	122.79
52	S2	650	PSU	C6-C5-C4	2.37	119.86	118.20
52	S2	687	PSU	C6-C5-C4	2.37	119.85	118.20
52	S2	1245	PSU	C6-C5-C4	2.37	119.85	118.20
52	S2	1057	PSU	O2-C2-N1	-2.37	120.19	122.79
6	L5	1638	PSU	O2-C2-N1	-2.37	120.19	122.79
52	S2	407	PSU	C6-C5-C4	2.36	119.85	118.20
6	L5	3585	PSU	O2-C2-N1	-2.36	120.19	122.79
52	S2	1233	PSU	O2-C2-N1	-2.36	120.20	122.79
6	L5	3496	PSU	C6-C5-C4	2.35	119.84	118.20
52	S2	577	A2M	O4'-C4'-C3'	-2.35	100.46	105.11
6	L5	3462	PSU	O2-C2-N1	-2.35	120.20	122.79
6	L5	4276	UR3	C6-N1-C2	-2.35	119.68	121.79
6	L5	3631	OMG	CM2-O2'-C2'	-2.35	108.36	114.52
52	S2	652	PSU	O2-C2-N1	-2.35	120.20	122.79
6	L5	2244	A2M	CM'-O2'-C2'	-2.35	108.36	114.52
6	L5	398	A2M	C3'-C2'-C1'	-2.35	98.47	102.89
52	S2	645	OMG	CM2-O2'-C2'	-2.35	108.37	114.52
6	L5	3517	A2M	C1'-N9-C4	2.34	130.75	126.64
6	L5	3369	PSU	C6-C5-C4	2.34	119.83	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	355	OMU	O2-C2-N1	-2.34	119.68	122.79
52	S2	1446	PSU	O2-C2-N1	-2.34	120.22	122.79
6	L5	1801	PSU	O2-C2-N1	-2.33	120.22	122.79
6	L5	4740	PSU	O2-C2-N1	-2.33	120.22	122.79
6	L5	2351	PSU	C6-C5-C4	2.33	119.83	118.20
6	L5	4039	PSU	O2-C2-N1	-2.33	120.23	122.79
52	S2	218	PSU	C6-C5-C4	2.33	119.83	118.20
6	L5	3502	PSU	O2-C2-N1	-2.33	120.23	122.79
52	S2	1626	PSU	O2-C2-N1	-2.32	120.23	122.79
52	S2	1239	PSU	C6-C5-C4	2.32	119.82	118.20
6	L5	1810	A2M	O4'-C4'-C3'	-2.32	100.53	105.11
6	L5	3652	PSU	O2-C2-N1	-2.31	120.24	122.79
6	L5	2208	OMC	CM2-O2'-C2'	-2.31	108.45	114.52
52	S2	816	PSU	C6-C5-C4	2.31	119.81	118.20
52	S2	1644	PSU	C6-C5-C4	2.31	119.81	118.20
6	L5	2475	PSU	C6-C5-C4	2.31	119.81	118.20
6	L5	4217	PSU	O2-C2-N1	-2.31	120.25	122.79
6	L5	1731	PSU	C6-C5-C4	2.31	119.81	118.20
6	L5	4193	5MC	N4-C4-N3	2.30	122.67	118.48
52	S2	682	PSU	C6-C5-C4	2.30	119.81	118.20
52	S2	1057	PSU	C6-C5-C4	2.30	119.81	118.20
6	L5	4203	PSU	O2-C2-N1	-2.30	120.26	122.79
6	L5	4749	PSU	C6-C5-C4	2.30	119.80	118.20
6	L5	2194	OMC	O2-C2-N3	-2.29	118.60	122.33
52	S2	1047	PSU	C6-C5-C4	2.29	119.80	118.20
6	L5	2206	A2M	O4'-C4'-C3'	-2.29	100.58	105.11
6	L5	3490	PSU	O2-C2-N1	-2.29	120.27	122.79
6	L5	3492	A2M	C3'-C2'-C1'	-2.28	98.60	102.89
52	S2	429	OMU	O2-C2-N1	-2.28	119.75	122.79
52	S2	802	PSU	C6-N1-C2	-2.28	120.35	122.68
8	L8	55	PSU	C6-C5-C4	2.28	119.79	118.20
52	S2	1327	OMU	O2-C2-N1	-2.28	119.75	122.79
6	L5	4188	PSU	O2-C2-N1	-2.28	120.28	122.79
60	SL	2	SAC	O-C-CA	-2.28	118.81	124.78
52	S2	1348	PSU	O2-C2-N1	-2.28	120.28	122.79
6	L5	4298	PSU	O2-C2-N1	-2.28	120.28	122.79
52	S2	577	A2M	C3'-C2'-C1'	-2.28	98.61	102.89
6	L5	2207	OMG	N1-C2-N3	-2.27	119.07	123.32
6	L5	400	A2M	O4'-C4'-C3'	-2.27	100.62	105.11
6	L5	2719	OMG	CM2-O2'-C2'	-2.27	108.56	114.52
52	S2	34	PSU	O2-C2-N1	-2.27	120.29	122.79
6	L5	1632	PSU	O2-C2-N1	-2.27	120.29	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3427	PSU	O2-C2-N1	-2.27	120.29	122.79
52	S2	1640	7MG	N1-C2-N3	-2.27	119.09	123.32
52	S2	1178	PSU	O2-C2-N1	-2.27	120.30	122.79
6	L5	1537	PSU	C6-C5-C4	2.26	119.78	118.20
6	L5	2647	OMC	CM2-O2'-C2'	-2.26	108.59	114.52
52	S2	815	PSU	O2-C2-N1	-2.26	120.31	122.79
6	L5	4366	OMU	CM2-O2'-C2'	-2.26	108.60	114.52
6	L5	3585	PSU	C6-C5-C4	2.26	119.78	118.20
6	L5	4322	PSU	O2-C2-N1	-2.25	120.31	122.79
6	L5	2630	A2M	C2'-C3'-C4'	-2.25	97.10	101.99
6	L5	3576	PSU	C6-N1-C2	-2.25	120.38	122.68
52	S2	513	A2M	C3'-C2'-C1'	-2.25	98.66	102.89
6	L5	3492	A2M	O2'-C2'-C1'	2.25	113.55	109.09
49	Ls	2	SAC	O-C-CA	-2.25	118.89	124.78
6	L5	4298	PSU	C6-C5-C4	2.25	119.77	118.20
52	S2	1082	PSU	O2-C2-N1	-2.24	120.32	122.79
6	L5	4045	PSU	O2-C2-N1	-2.24	120.32	122.79
6	L5	2680	OMU	O2-C2-N1	-2.24	119.81	122.79
6	L5	1638	PSU	C6-C5-C4	2.24	119.77	118.20
6	L5	1491	PSU	C6-N1-C2	-2.23	120.40	122.68
6	L5	3524	OMG	N1-C2-N3	-2.23	119.14	123.32
6	L5	4246	PSU	C6-N1-C2	-2.23	120.40	122.68
6	L5	4107	PSU	O2-C2-N1	-2.23	120.33	122.79
6	L5	1537	PSU	O2-C2-N1	-2.23	120.34	122.79
6	L5	4317	A2M	C2'-C3'-C4'	-2.23	97.15	101.99
6	L5	3524	OMG	CM2-O2'-C2'	-2.23	108.68	114.52
6	L5	1260	OMG	N1-C2-N3	-2.23	119.16	123.32
52	S2	1833	6MZ	C4-C5-N7	-2.23	107.08	109.40
6	L5	3466	PSU	O2-C2-N1	-2.22	120.34	122.79
6	L5	1799	PSU	C6-N1-C2	-2.22	120.41	122.68
52	S2	1704	OMC	CM2-O2'-C2'	-2.22	108.69	114.52
6	L5	3973	OMU	CM2-O2'-C2'	-2.22	108.71	114.52
6	L5	4278	PSU	C6-N1-C2	-2.22	120.42	122.68
6	L5	3631	OMG	N1-C2-N3	-2.22	119.18	123.32
52	S2	36	PSU	C6-C5-C4	2.21	119.75	118.20
6	L5	4058	PSU	O2-C2-N1	-2.21	120.36	122.79
6	L5	4278	PSU	O2-C2-N1	-2.21	120.36	122.79
6	L5	4325	PSU	C6-C5-C4	2.21	119.74	118.20
6	L5	3359	OMG	N1-C2-N3	-2.21	119.19	123.32
6	L5	4435	PSU	C6-N1-C2	-2.21	120.42	122.68
6	L5	4177	PSU	C6-N1-C2	-2.21	120.43	122.68
6	L5	2258	OMU	O2-C2-N1	-2.20	119.86	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L5	4749	PSU	O2-C2-N1	-2.20	120.37	122.79
52	S2	518	OMC	CM2-O2'-C2'	-2.20	108.75	114.52
6	L5	4366	OMU	O2-C2-N1	-2.20	119.86	122.79
52	S2	967	PSU	O2-C2-N1	-2.20	120.37	122.79
52	S2	1852	MA6	C10-N6-C6	-2.20	112.86	119.51
52	S2	823	PSU	C6-N1-C2	-2.20	120.44	122.68
6	L5	4166	PSU	O2-C2-N1	-2.20	120.37	122.79
52	S2	868	OMG	N1-C2-N3	-2.20	119.22	123.32
6	L5	4282	OMC	CM2-O2'-C2'	-2.19	108.77	114.52
6	L5	4042	PSU	O2-C2-N1	-2.19	120.38	122.79
52	S2	573	PSU	C6-C5-C4	2.19	119.73	118.20
6	L5	1731	PSU	O2-C2-N1	-2.19	120.38	122.79
6	L5	3616	PSU	C6-N1-C2	-2.19	120.44	122.68
6	L5	4245	OMG	N1-C2-N3	-2.19	119.23	123.32
6	L5	2658	A2M	O4'-C4'-C3'	-2.19	100.79	105.11
6	L5	1477	OMG	N1-C2-N3	-2.18	119.24	123.32
52	S2	1851	MA6	C10-N6-C6	-2.18	112.91	119.51
52	S2	864	PSU	C6-C5-C4	2.18	119.72	118.20
6	L5	4177	PSU	C6-C5-C4	2.18	119.72	118.20
6	L5	3554	PSU	C6-N1-C2	-2.17	120.46	122.68
52	S2	159	A2M	CM'-O2'-C2'	-2.17	108.82	114.52
6	L5	3562	A2M	C3'-C2'-C1'	-2.17	98.81	102.89
52	S2	687	PSU	C6-N1-C2	-2.17	120.46	122.68
52	S2	669	A2M	CM'-O2'-C2'	-2.17	108.83	114.52
6	L5	2267	OMG	N1-C2-N3	-2.17	119.27	123.32
6	L5	4325	PSU	C6-N1-C2	-2.17	120.47	122.68
6	L5	4045	PSU	C6-C5-C4	2.17	119.71	118.20
6	L5	3942	OMG	N1-C2-N3	-2.16	119.28	123.32
6	L5	4374	PSU	C6-N1-C2	-2.16	120.47	122.68
6	L5	3427	PSU	C6-C5-C4	2.16	119.71	118.20
6	L5	3514	5MC	N4-C4-N3	2.16	122.42	118.48
6	L5	3554	PSU	C6-C5-C4	2.16	119.71	118.20
52	S2	510	OMG	CM2-O2'-C2'	-2.16	108.86	114.52
52	S2	159	A2M	C3'-C2'-C1'	-2.16	98.84	102.89
52	S2	1693	PSU	C6-C5-C4	2.16	119.70	118.20
6	L5	4149	PSU	C6-N1-C2	-2.15	120.48	122.68
6	L5	3494	PSU	C6-N1-C2	-2.15	120.48	122.68
52	S2	684	OMG	N1-C2-N3	-2.15	119.30	123.32
6	L5	4240	OMG	N1-C2-N3	-2.15	119.30	123.32
52	S2	93	PSU	O2-C2-N1	-2.15	120.42	122.79
6	L5	1810	A2M	C3'-C2'-C1'	-2.15	98.85	102.89
52	S2	109	PSU	C6-C5-C4	2.15	119.70	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L5	3514	5MC	O2-C2-N3	-2.15	118.84	122.33
52	S2	166	A2M	C3'-C2'-C1'	-2.15	98.86	102.89
6	L5	3583	PSU	C6-N1-C2	-2.14	120.49	122.68
6	L5	3447	PSU	C6-C5-C4	2.14	119.70	118.20
6	L5	1260	OMG	CM2-O2'-C2'	-2.14	108.90	114.52
6	L5	1721	PSU	C6-C5-C4	2.14	119.70	118.20
6	L5	1799	PSU	C6-C5-C4	2.14	119.69	118.20
52	S2	116	OMU	CM2-O2'-C2'	-2.14	108.91	114.52
6	L5	3517	A2M	C3'-C2'-C1'	-2.14	98.87	102.89
6	L5	3371	PSU	C6-C5-C4	2.14	119.69	118.20
6	L5	4711	PSU	C6-C5-C4	2.14	119.69	118.20
6	L5	4419	PSU	C6-N1-C2	-2.13	120.50	122.68
6	L5	4336	A2M	CM'-O2'-C2'	-2.13	108.92	114.52
8	L8	75	OMG	N1-C2-N3	-2.13	119.33	123.32
52	S2	1843	4AC	C6-C5-C4	2.13	119.57	116.96
6	L5	3500	PSU	C6-C5-C4	2.13	119.69	118.20
52	S2	1491	OMG	N1-C2-N3	-2.13	119.34	123.32
6	L5	4374	PSU	C6-C5-C4	2.13	119.68	118.20
6	L5	4058	PSU	C6-C5-C4	2.12	119.68	118.20
52	S2	602	OMG	N1-C2-N3	-2.12	119.35	123.32
52	S2	36	PSU	C6-N1-C2	-2.12	120.51	122.68
6	L5	1638	PSU	C6-N1-C2	-2.12	120.51	122.68
6	L5	3502	PSU	C6-C5-C4	2.12	119.68	118.20
52	S2	1175	PSU	C6-N1-C2	-2.12	120.52	122.68
6	L5	4383	OMG	N1-C2-N3	-2.12	119.36	123.32
52	S2	628	OMU	CM2-O2'-C2'	-2.12	108.97	114.52
52	S2	1640	7MG	N9-C4-N3	2.12	128.63	125.47
6	L5	4217	PSU	C6-N1-C2	-2.12	120.52	122.68
6	L5	3476	OMG	N1-C2-N3	-2.12	119.37	123.32
6	L5	1718	PSU	C6-C5-C4	2.11	119.67	118.20
52	S2	867	PSU	C6-N1-C2	-2.11	120.52	122.68
6	L5	1720	PSU	C6-C5-C4	2.11	119.67	118.20
6	L5	3494	PSU	C6-C5-C4	2.11	119.67	118.20
6	L5	4039	PSU	C6-N1-C2	-2.11	120.53	122.68
6	L5	1721	PSU	C6-N1-C2	-2.11	120.53	122.68
52	S2	1178	PSU	C6-N1-C2	-2.11	120.53	122.68
6	L5	3371	PSU	C6-N1-C2	-2.10	120.53	122.68
52	S2	121	OMU	CM2-O2'-C2'	-2.10	109.00	114.52
6	L5	2265	OMC	O2-C2-N3	-2.10	118.91	122.33
6	L5	4217	PSU	C6-C5-C4	2.10	119.67	118.20
52	S2	172	OMU	O2'-C2'-C1'	2.10	113.17	109.08
6	L5	2475	PSU	C6-N1-C2	-2.10	120.54	122.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L5	4383	OMG	CM2-O2'-C2'	-2.10	109.02	114.52
6	L5	3974	OMG	N1-C2-N3	-2.10	119.40	123.32
6	L5	4245	OMG	CM2-O2'-C2'	-2.10	109.02	114.52
52	S2	166	A2M	O4'-C4'-C3'	-2.10	100.97	105.11
52	S2	577	A2M	CM'-O2'-C2'	-2.09	109.03	114.52
52	S2	1384	A2M	C3'-C2'-C1'	-2.09	98.95	102.89
52	S2	510	OMG	N1-C2-N3	-2.09	119.41	123.32
6	L5	4419	PSU	C6-C5-C4	2.09	119.66	118.20
6	L5	1720	PSU	C6-N1-C2	-2.09	120.55	122.68
52	S2	1384	A2M	O4'-C4'-C3'	-2.09	100.98	105.11
6	L5	3490	PSU	C6-C5-C4	2.09	119.66	118.20
6	L5	4169	PSU	C6-N1-C2	-2.09	120.55	122.68
6	L5	4369	OMG	N1-C2-N3	-2.09	119.42	123.32
6	L5	4711	PSU	C6-N1-C2	-2.09	120.55	122.68
52	S2	645	OMG	N1-C2-N3	-2.09	119.42	123.32
6	L5	4116	OMG	N1-C2-N3	-2.09	119.42	123.32
52	S2	610	PSU	C6-N1-C2	-2.09	120.55	122.68
6	L5	2265	OMC	CM2-O2'-C2'	-2.09	109.05	114.52
8	L8	69	PSU	C6-N1-C2	-2.08	120.56	122.68
52	S2	172	OMU	O2-C2-N1	-2.08	120.02	122.79
6	L5	2719	OMG	N1-C2-N3	-2.08	119.44	123.32
6	L5	4138	OMG	N1-C2-N3	-2.08	119.44	123.32
52	S2	1679	A2M	CM'-O2'-C2'	-2.08	109.07	114.52
52	S2	1368	PSU	C6-C5-C4	2.08	119.65	118.20
52	S2	1805	OMU	O2-C2-N1	-2.08	120.03	122.79
6	L5	3369	PSU	O2-C2-N1	-2.07	120.51	122.79
6	L5	4364	OMG	N1-C2-N3	-2.07	119.45	123.32
6	L5	3427	PSU	C6-N1-C2	-2.07	120.57	122.68
52	S2	1851	MA6	N1-C6-N6	2.07	119.23	117.06
52	S2	1233	PSU	C6-C5-C4	2.07	119.64	118.20
6	L5	3676	OMG	N1-C2-N3	-2.07	119.46	123.32
52	S2	1175	PSU	C6-C5-C4	2.06	119.64	118.20
52	S2	1626	PSU	C6-C5-C4	2.06	119.64	118.20
6	L5	4322	PSU	C6-C5-C4	2.06	119.64	118.20
6	L5	3496	PSU	C6-N1-C2	-2.06	120.58	122.68
6	L5	1683	PSU	C6-N1-C2	-2.06	120.58	122.68
52	S2	119	PSU	C6-N1-C2	-2.05	120.58	122.68
52	S2	1082	PSU	C6-C5-C4	2.05	119.63	118.20
52	S2	1329	OMG	CM2-O2'-C2'	-2.05	109.14	114.52
52	S2	967	PSU	C6-N1-C2	-2.05	120.59	122.68
6	L5	3462	PSU	C6-C5-C4	2.05	119.63	118.20
52	S2	682	PSU	C6-N1-C2	-2.05	120.59	122.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L5	398	A2M	CM'-O2'-C2'	-2.05	109.15	114.52
52	S2	1693	PSU	C6-N1-C2	-2.05	120.59	122.68
52	S2	1329	OMG	N1-C2-N3	-2.05	119.50	123.32
6	L5	3540	OMC	CM2-O2'-C2'	-2.04	109.16	114.52
52	S2	1368	PSU	C6-N1-C2	-2.04	120.59	122.68
6	L5	4116	OMG	CM2-O2'-C2'	-2.04	109.16	114.52
52	S2	99	A2M	CM'-O2'-C2'	-2.04	109.17	114.52
6	L5	4203	PSU	C6-N1-C2	-2.04	120.60	122.68
6	L5	3616	PSU	C6-C5-C4	2.04	119.62	118.20
6	L5	3540	OMC	O2-C2-N3	-2.03	119.02	122.33
52	S2	1233	PSU	C6-N1-C2	-2.03	120.60	122.68
6	L5	4322	PSU	C6-N1-C2	-2.03	120.60	122.68
6	L5	3433	OMC	CM2-O2'-C2'	-2.03	109.19	114.52
52	S2	437	OMG	N1-C2-N3	-2.03	119.52	123.32
52	S2	469	A2M	CM'-O2'-C2'	-2.03	109.19	114.52
6	L5	1580	OMG	N1-C2-N3	-2.03	119.53	123.32
6	L5	3456	A2M	CM'-O2'-C2'	-2.03	109.20	114.52
52	S2	105	PSU	C6-N1-C2	-2.03	120.61	122.68
52	S2	1005	PSU	C5-C4-N3	2.02	121.16	116.58
6	L5	4099	PSU	C6-N1-C2	-2.02	120.61	122.68
6	L5	3573	OMC	O2-C2-N3	-2.02	119.04	122.33
52	S2	602	OMG	CM2-O2'-C2'	-2.02	109.23	114.52
6	L5	2630	A2M	CM'-O2'-C2'	-2.01	109.24	114.52
52	S2	816	PSU	C6-N1-C2	-2.01	120.63	122.68
6	L5	3359	OMG	CM2-O2'-C2'	-2.01	109.25	114.52
6	L5	4058	PSU	C6-N1-C2	-2.01	120.63	122.68
6	L5	2680	OMU	CM2-O2'-C2'	-2.01	109.25	114.52
52	S2	1239	PSU	C6-N1-C2	-2.01	120.63	122.68
52	S2	1626	PSU	C6-N1-C2	-2.01	120.63	122.68
52	S2	1057	PSU	C6-N1-C2	-2.01	120.63	122.68
6	L5	3462	PSU	C6-N1-C2	-2.00	120.63	122.68
52	S2	1448	OMG	N1-C2-N3	-2.00	119.58	123.32
52	S2	109	PSU	C6-N1-C2	-2.00	120.64	122.68
6	L5	3573	OMC	CM2-O2'-C2'	-2.00	109.27	114.52
6	L5	4364	OMG	CM2-O2'-C2'	-2.00	109.28	114.52

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	LE	245	HIC	CA-CB-CG-ND1
11	LF	2	AYA	OT-CT-N-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	LF	2	AYA	CM-CT-N-CA
35	Le	5	MLZ	N-CA-CB-CG
35	Le	5	MLZ	C-CA-CB-CG
52	S2	429	OMU	C2'-C1'-N1-C2
52	S2	429	OMU	C2'-C1'-N1-C6
52	S2	645	OMG	O4'-C4'-C5'-O5'
52	S2	684	OMG	O4'-C4'-C5'-O5'
52	S2	684	OMG	C3'-C4'-C5'-O5'
52	S2	802	PSU	C3'-C4'-C5'-O5'
52	S2	1448	OMG	C3'-C4'-C5'-O5'
52	S2	1833	6MZ	N1-C6-N6-C9
52	S2	1851	MA6	C5-C6-N6-C10
79	Se	67	NMM	N-CA-CB-CG
83	Si	62	HY3	O-C-CA-C3
6	L5	1632	PSU	C2'-C1'-C5-C4
6	L5	3433	OMC	C2'-C1'-N1-C6
6	L5	3492	A2M	C1'-C2'-O2'-CM'
6	L5	3494	PSU	C3'-C4'-C5'-O5'
6	L5	3494	PSU	O4'-C4'-C5'-O5'
6	L5	3517	A2M	O4'-C4'-C5'-O5'
6	L5	4382	PSU	C3'-C4'-C5'-O5'
6	L5	4382	PSU	O4'-C4'-C5'-O5'
52	S2	1338	4AC	N3-C4-N4-C7
52	S2	1338	4AC	C5-C4-N4-C7
52	S2	1338	4AC	O7-C7-N4-C4
52	S2	1338	4AC	CM7-C7-N4-C4
52	S2	1843	4AC	N3-C4-N4-C7
52	S2	1843	4AC	C5-C4-N4-C7
6	L5	3433	OMC	C2'-C1'-N1-C2
52	S2	518	OMC	C3'-C4'-C5'-O5'
52	S2	645	OMG	C3'-C4'-C5'-O5'
6	L5	1477	OMG	O4'-C4'-C5'-O5'
6	L5	1477	OMG	C3'-C4'-C5'-O5'
6	L5	3517	A2M	C3'-C4'-C5'-O5'
6	L5	4166	PSU	C3'-C4'-C5'-O5'
81	Sg	1	AME	CT2-CT1-N-CA
81	Sg	1	AME	OT-CT1-N-CA
79	Se	67	NMM	NE-CD-CG-CB
6	L5	4336	A2M	C4'-C5'-O5'-P
52	S2	518	OMC	O4'-C4'-C5'-O5'
52	S2	669	A2M	C3'-C4'-C5'-O5'
52	S2	1448	OMG	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L5	2265	OMC	C3'-C4'-C5'-O5'
6	L5	2265	OMC	O4'-C4'-C5'-O5'
6	L5	4166	PSU	O4'-C4'-C5'-O5'
6	L5	1580	OMG	C3'-C2'-O2'-CM2
52	S2	628	OMU	C2'-C1'-N1-C6
52	S2	802	PSU	O4'-C4'-C5'-O5'
52	S2	823	PSU	C3'-C4'-C5'-O5'
52	S2	1392	OMC	C3'-C4'-C5'-O5'
52	S2	99	A2M	O4'-C4'-C5'-O5'
52	S2	628	OMU	O4'-C4'-C5'-O5'
52	S2	1851	MA6	C5-C6-N6-C9
52	S2	1852	MA6	C5-C6-N6-C10
52	S2	823	PSU	O4'-C4'-C5'-O5'
6	L5	1489	A2M	C4'-C5'-O5'-P
52	S2	1392	OMC	O4'-C4'-C5'-O5'
6	L5	4246	PSU	C4'-C5'-O5'-P
52	S2	510	OMG	O4'-C4'-C5'-O5'
52	S2	628	OMU	C3'-C4'-C5'-O5'
52	S2	628	OMU	C2'-C1'-N1-C2
52	S2	628	OMU	O4'-C1'-N1-C6
6	L5	1270	A2M	C4'-C5'-O5'-P
6	L5	1477	OMG	C4'-C5'-O5'-P
6	L5	3576	PSU	C4'-C5'-O5'-P
6	L5	3433	OMC	O4'-C1'-N1-C2
6	L5	3433	OMC	O4'-C1'-N1-C6
52	S2	577	A2M	C3'-C4'-C5'-O5'
6	L5	3619	OMC	C3'-C4'-C5'-O5'
79	Se	67	NMM	C-CA-CB-CG
52	S2	628	OMU	O4'-C1'-N1-C2
52	S2	645	OMG	C4'-C5'-O5'-P
6	L5	4336	A2M	C3'-C4'-C5'-O5'
52	S2	1852	MA6	C4'-C5'-O5'-P
52	S2	429	OMU	O4'-C1'-N1-C6
6	L5	4193	5MC	O4'-C1'-N1-C6
52	S2	1491	OMG	C4'-C5'-O5'-P
6	L5	4240	OMG	C3'-C2'-O2'-CM2
52	S2	1448	OMG	C4'-C5'-O5'-P
6	L5	2658	A2M	C4'-C5'-O5'-P
6	L5	3676	OMG	C3'-C4'-C5'-O5'
52	S2	429	OMU	O4'-C1'-N1-C2
52	S2	1005	PSU	O4'-C1'-C5-C4
6	L5	2719	OMG	C3'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L5	4193	5MC	C2'-C1'-N1-C6
6	L5	3492	A2M	O4'-C4'-C5'-O5'
6	L5	4193	5MC	O4'-C1'-N1-C2
6	L5	2194	OMC	O4'-C4'-C5'-O5'
52	S2	510	OMG	C3'-C4'-C5'-O5'
52	S2	669	A2M	O4'-C4'-C5'-O5'
6	L5	2244	A2M	C3'-C4'-C5'-O5'
6	L5	3492	A2M	C3'-C4'-C5'-O5'
52	S2	485	A2M	O4'-C4'-C5'-O5'
6	L5	4369	OMG	O4'-C4'-C5'-O5'
6	L5	4369	OMG	C3'-C4'-C5'-O5'
6	L5	1489	A2M	O4'-C4'-C5'-O5'
60	SL	2	SAC	C-CA-N-C1A
52	S2	802	PSU	C4'-C5'-O5'-P
6	L5	3619	OMC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 256 ligands modelled in this entry, 253 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	$\#\|Z\| > 2$
87	GTP	E	1001	1	26,34,34	1.14	2 (7%)	32,54,54	1.45	6 (18%)
88	SER	F	101	2	4,5,6	0.57	0	0,5,7	-	-
87	GTP	L7	203	7	26,34,34	0.90	1 (3%)	32,54,54	1.34	3 (9%)

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	GTP	E	1001	1	-	6/18/38/38	0/3/3/3
88	SER	F	101	2	-	0/2/4/6	-
87	GTP	L7	203	7	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	E	1001	GTP	C5-C6	-4.12	1.39	1.47
87	L7	203	GTP	C6-N1	-2.36	1.34	1.37
87	E	1001	GTP	C2-N3	2.12	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	L7	203	GTP	PB-O3B-PG	-3.61	120.43	132.83
87	L7	203	GTP	PA-O3A-PB	-3.61	120.44	132.83
87	E	1001	GTP	C5-C6-N1	3.04	119.32	113.95
87	E	1001	GTP	C3'-C2'-C1'	2.96	105.44	100.98
87	E	1001	GTP	PA-O3A-PB	-2.94	122.75	132.83
87	E	1001	GTP	C8-N7-C5	2.89	108.49	102.99
87	E	1001	GTP	C2-N1-C6	-2.79	119.96	125.10
87	L7	203	GTP	C5-C6-N1	2.54	118.43	113.95
87	E	1001	GTP	O6-C6-C5	-2.34	119.81	124.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

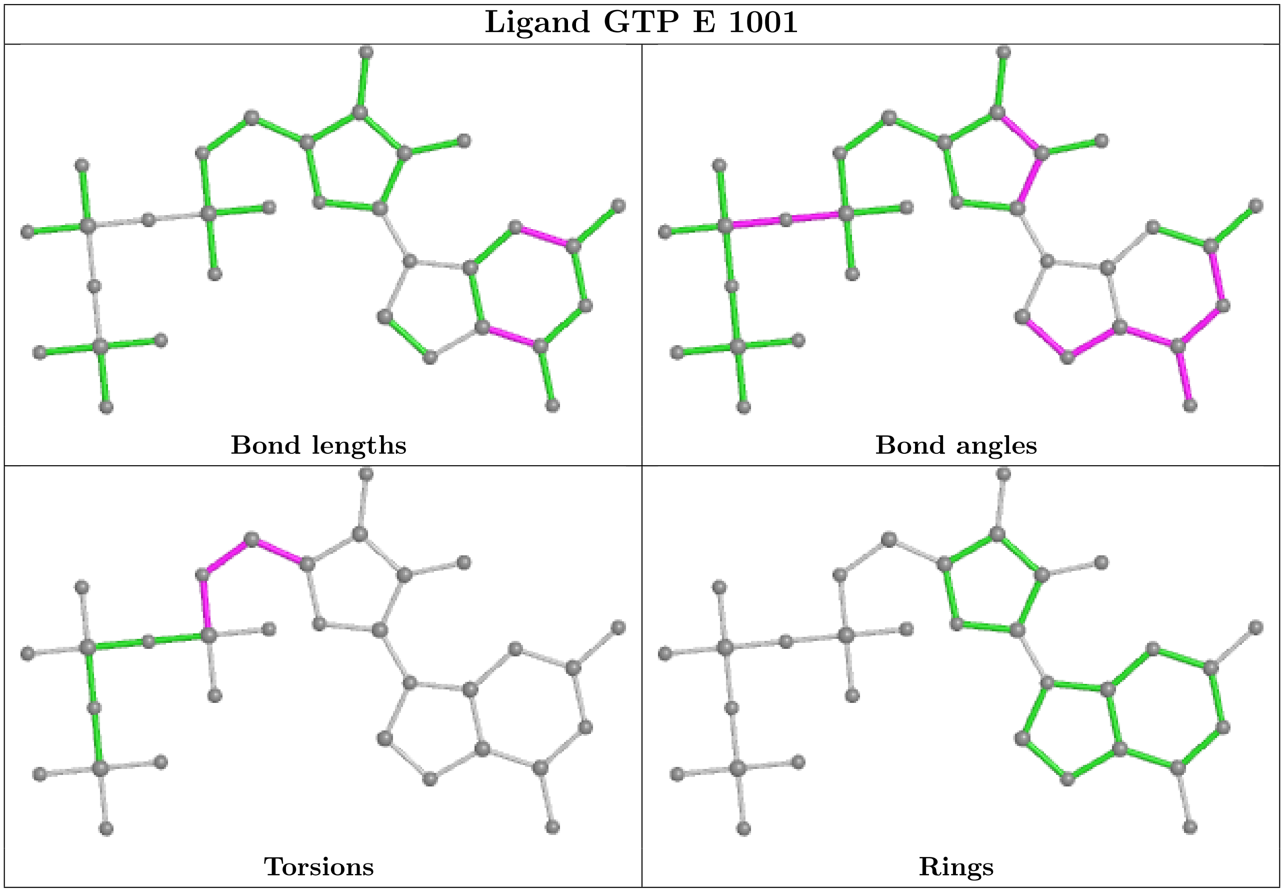
Mol	Chain	Res	Type	Atoms
87	E	1001	GTP	C5'-O5'-PA-O3A
87	E	1001	GTP	O4'-C4'-C5'-O5'
87	E	1001	GTP	C3'-C4'-C5'-O5'
87	E	1001	GTP	C5'-O5'-PA-O1A
87	E	1001	GTP	C5'-O5'-PA-O2A
87	E	1001	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP E 1001

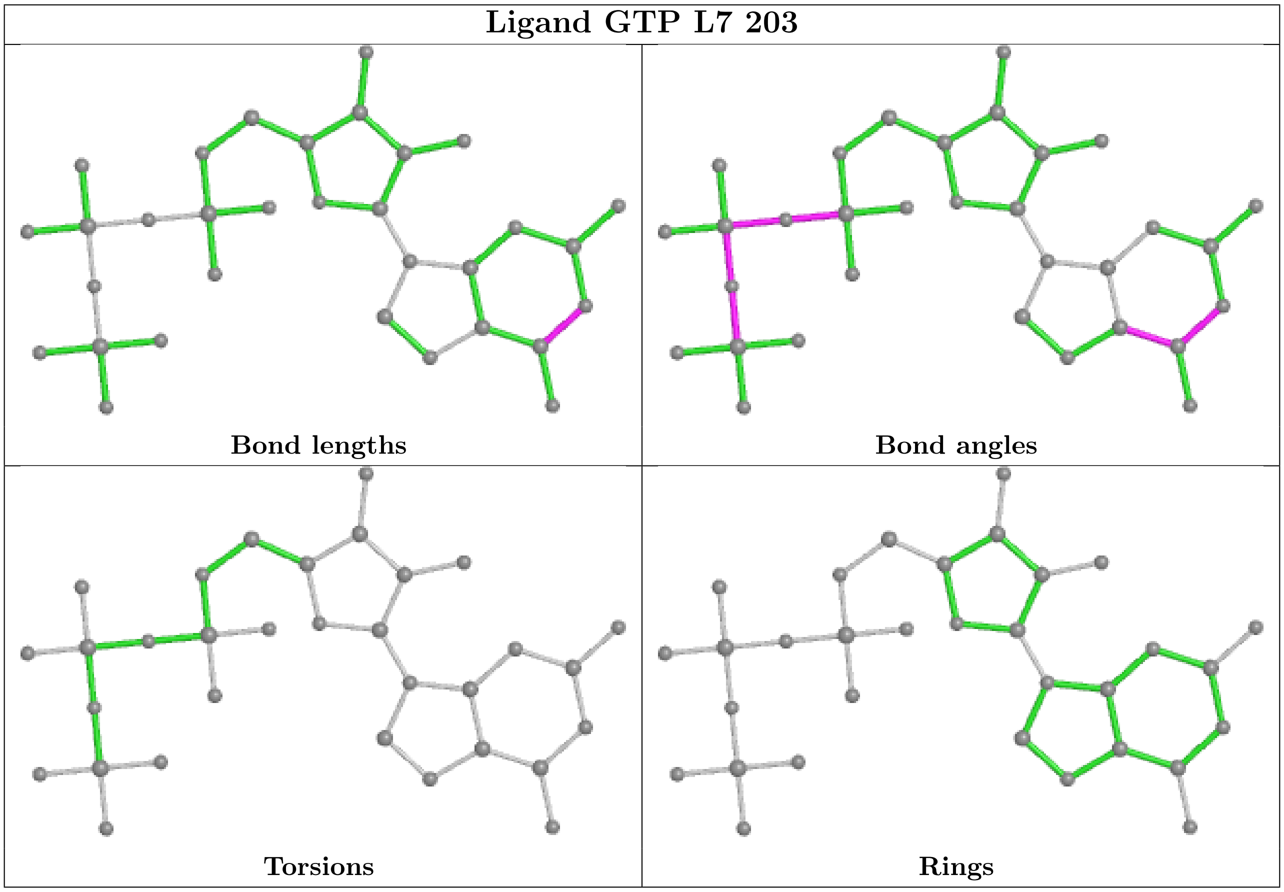


Bond lengths

Bond angles

Torsions

Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
83	Si	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Si	61:GLN	C	62:HY3	N	3.10

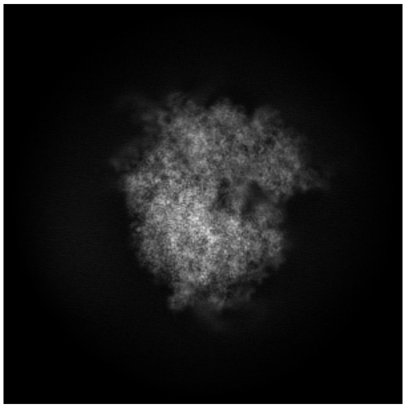
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-14751. These allow visual inspection of the internal detail of the map and identification of artifacts.

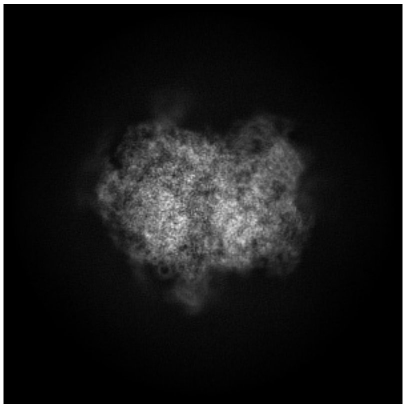
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

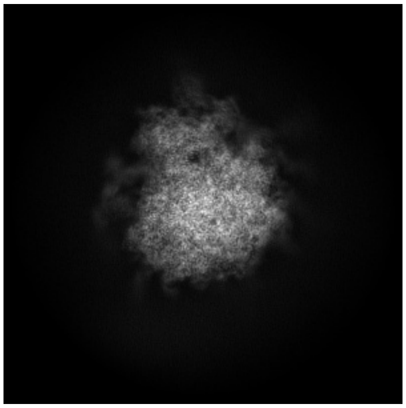
6.1.1 Primary map



X

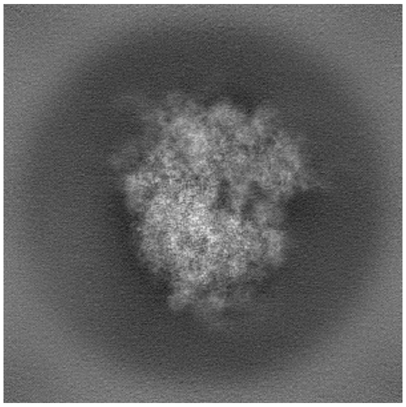


Y

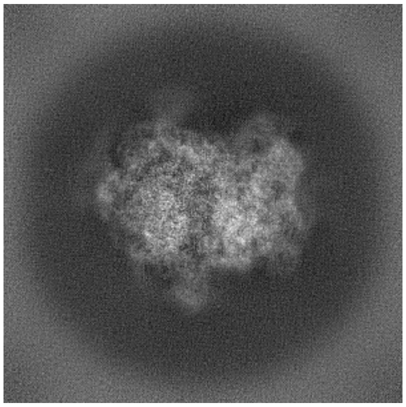


Z

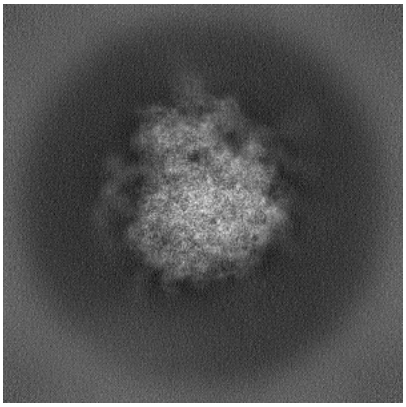
6.1.2 Raw map



X



Y

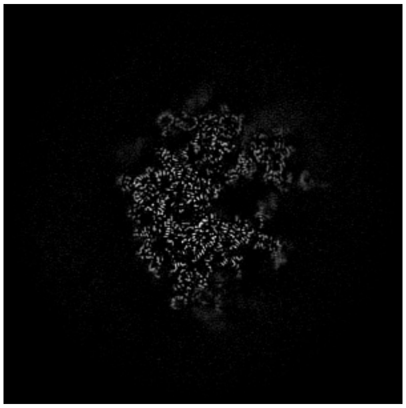


Z

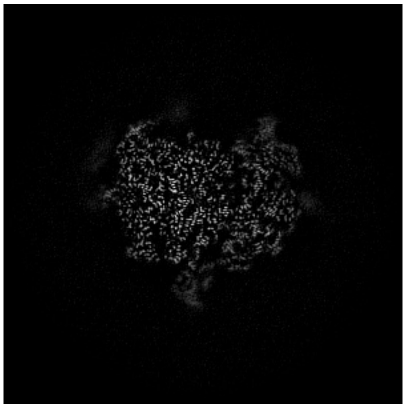
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

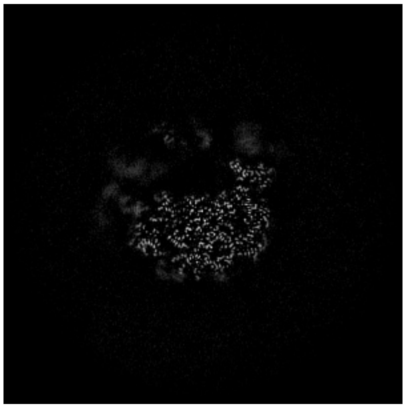
6.2.1 Primary map



X Index: 256

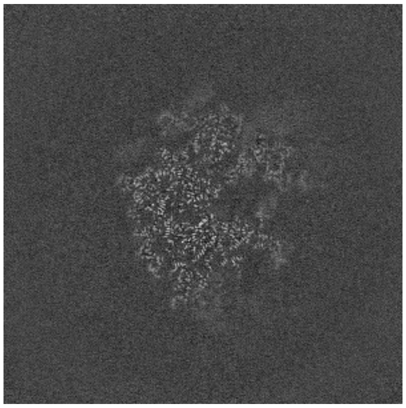


Y Index: 256

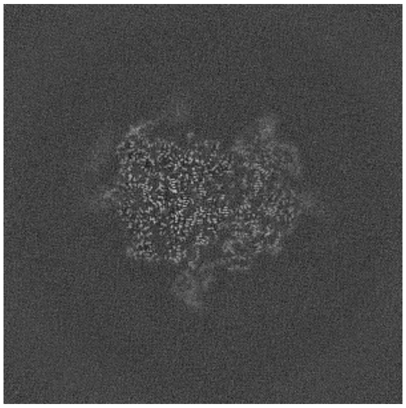


Z Index: 256

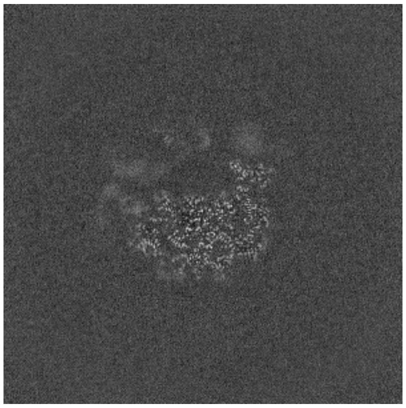
6.2.2 Raw map



X Index: 256



Y Index: 256

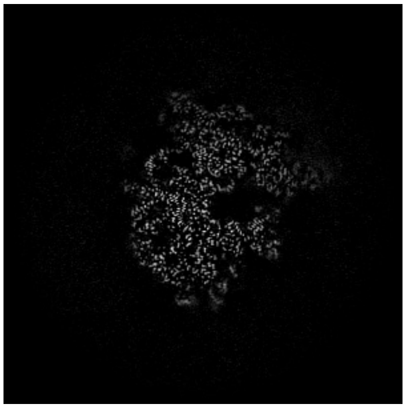


Z Index: 256

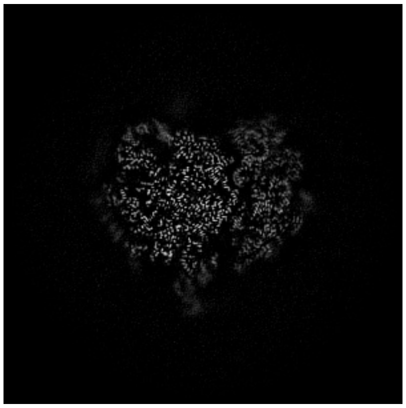
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

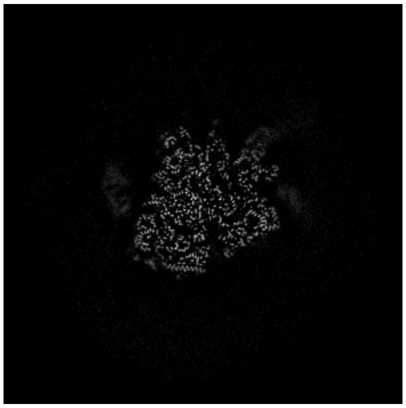
6.3.1 Primary map



X Index: 240

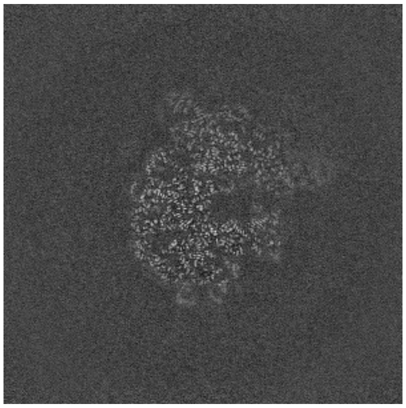


Y Index: 246

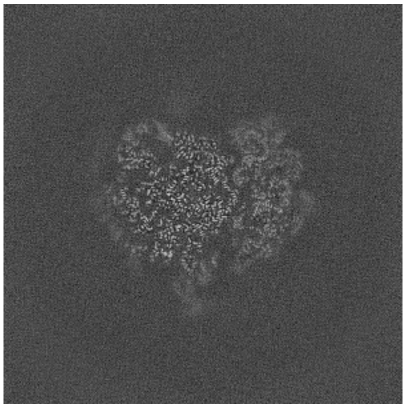


Z Index: 223

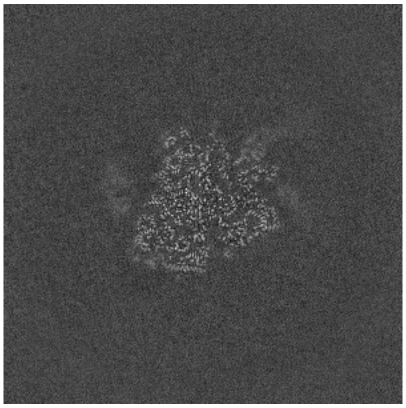
6.3.2 Raw map



X Index: 238



Y Index: 246

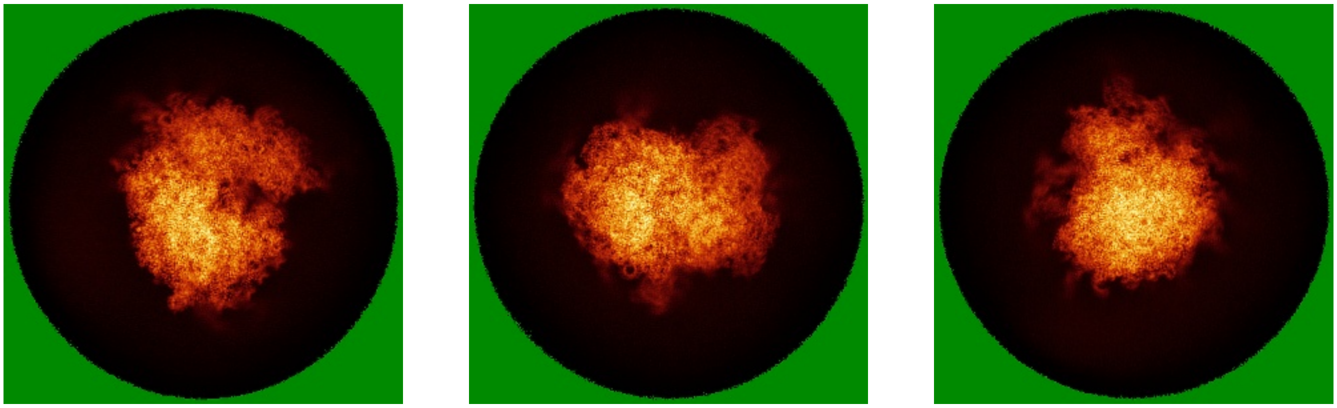


Z Index: 223

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

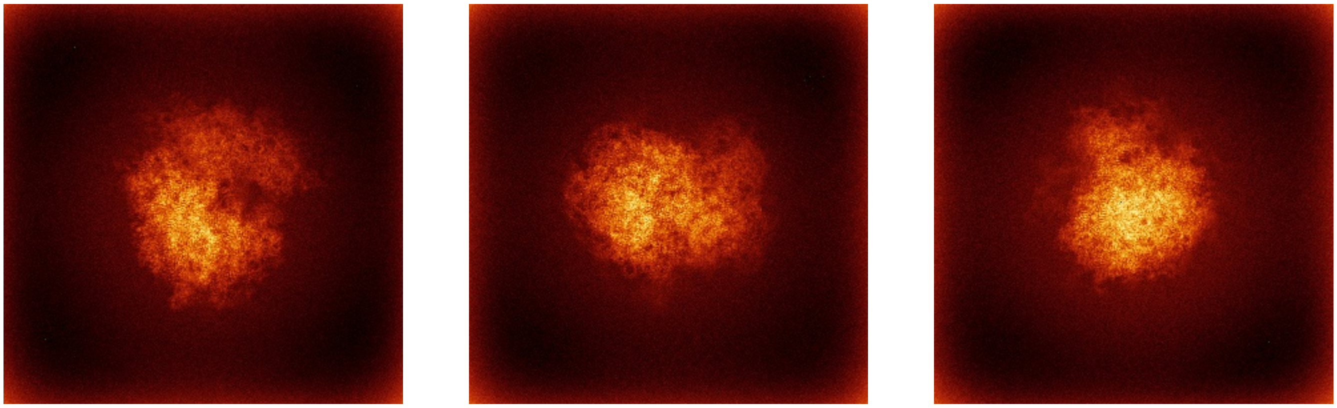
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



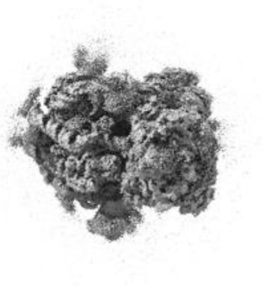
X Y Z

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

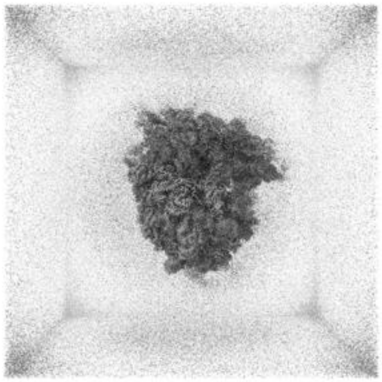

X

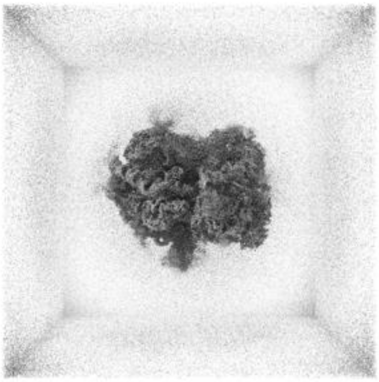

Y

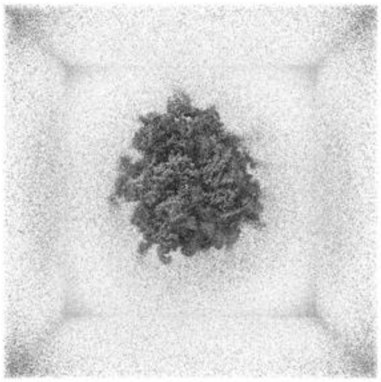

Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map


X


Y


Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

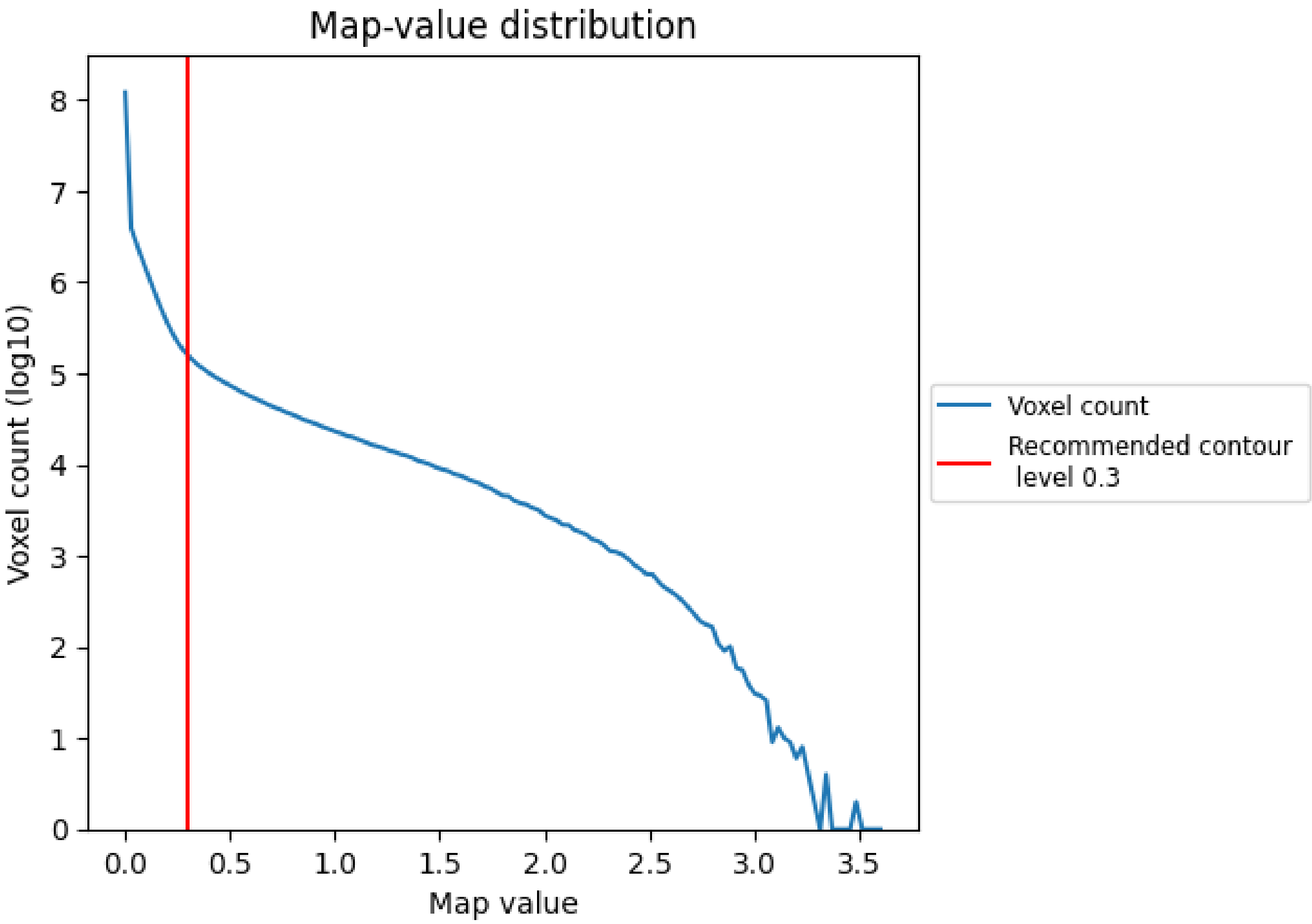
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

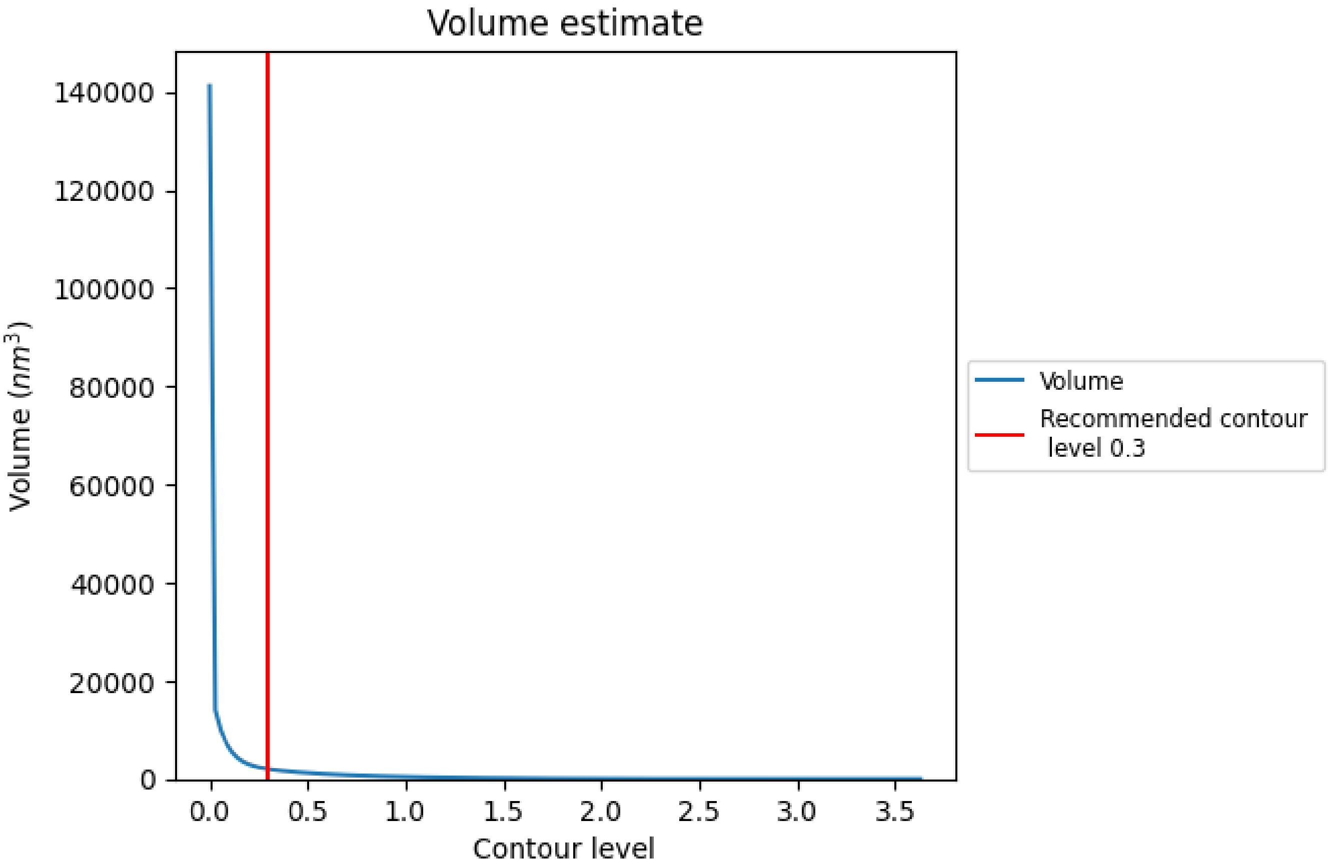
This section contains the results of statistical analysis of the map.

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.

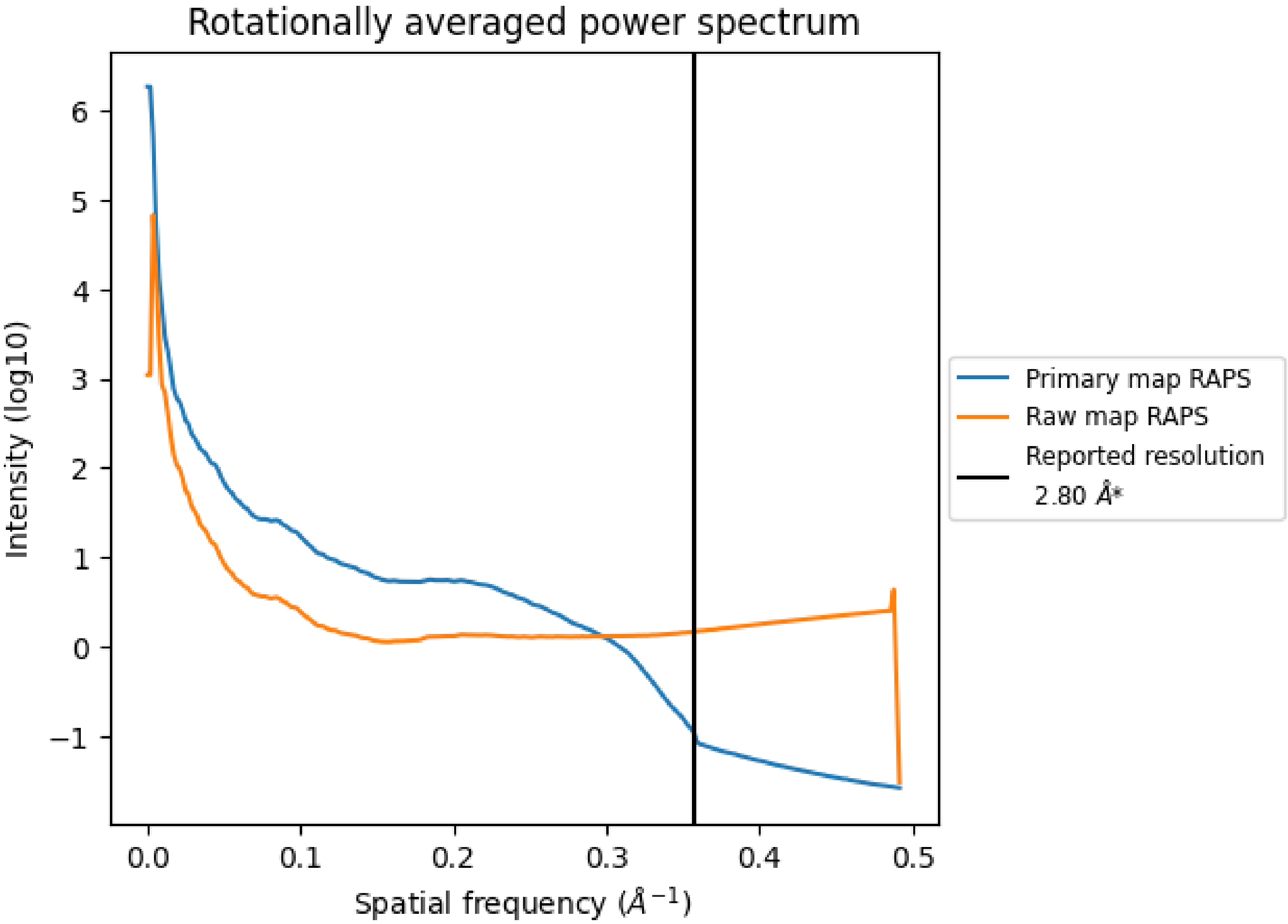
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2046 nm^3; this corresponds to an approximate mass of 1848 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 ⓘ

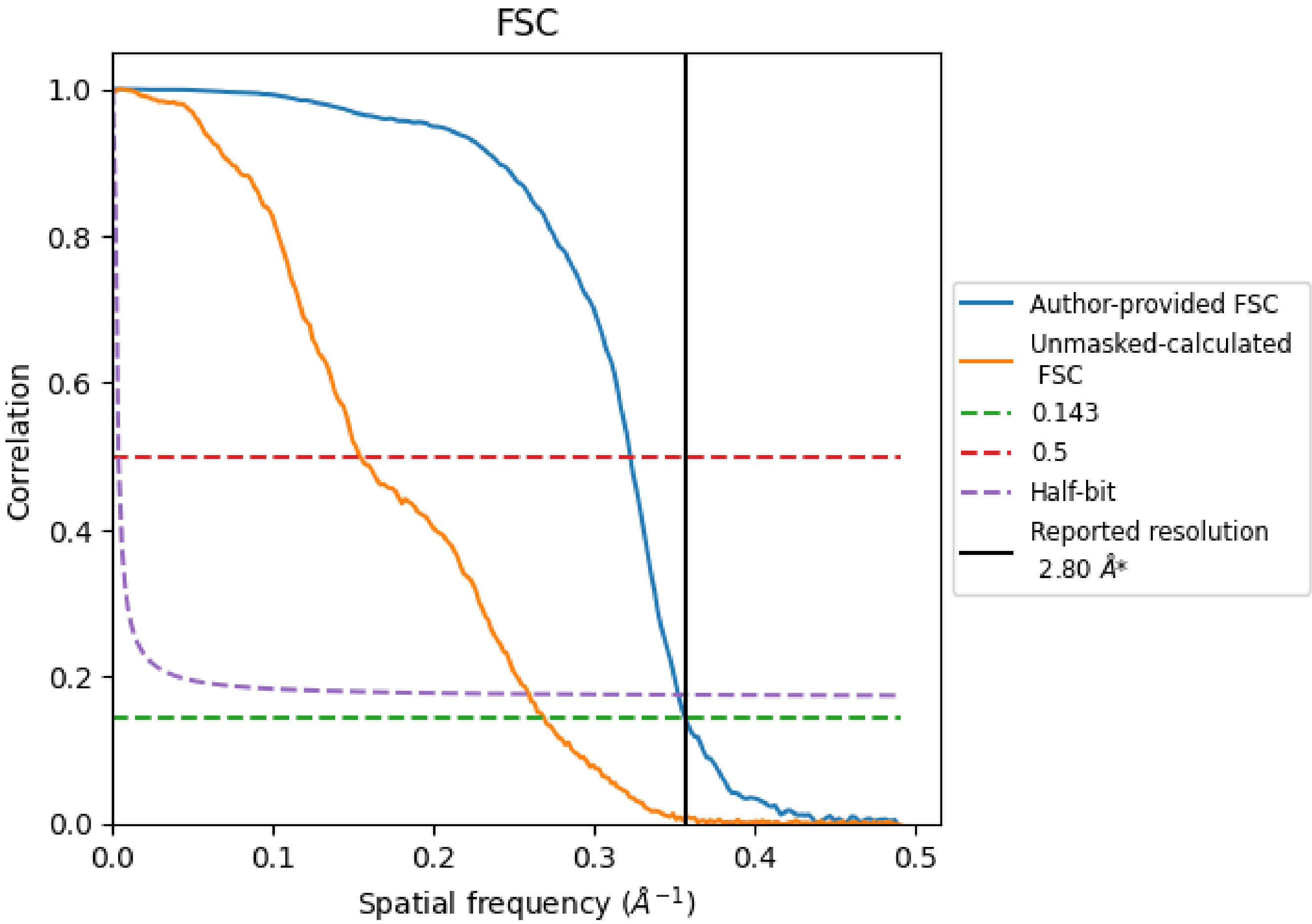


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

8.2 Resolution estimates ⓘ

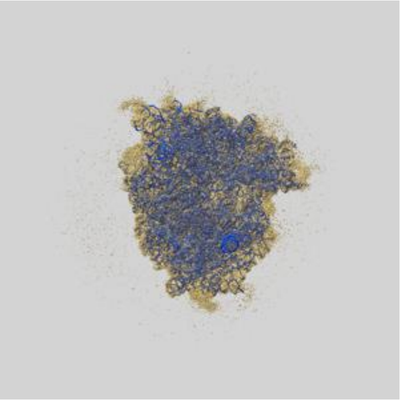
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.10	2.83
Unmasked-calculated*	3.72	6.49	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.72 differs from the reported value 2.8 by more than 10 %

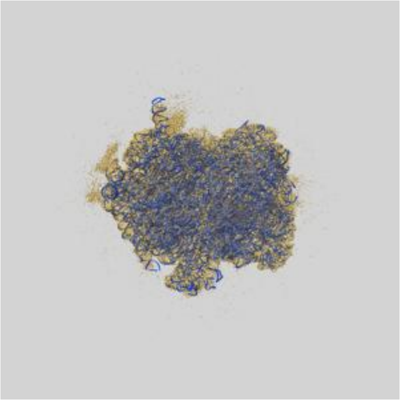
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-14751 and PDB model 7ZJW. Per-residue inclusion information can be found in section 3 on page 25.

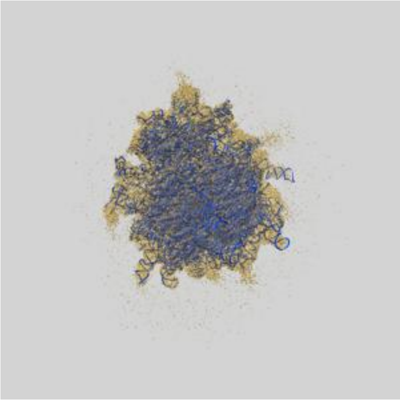
9.1 Map-model overlay ⓘ



X



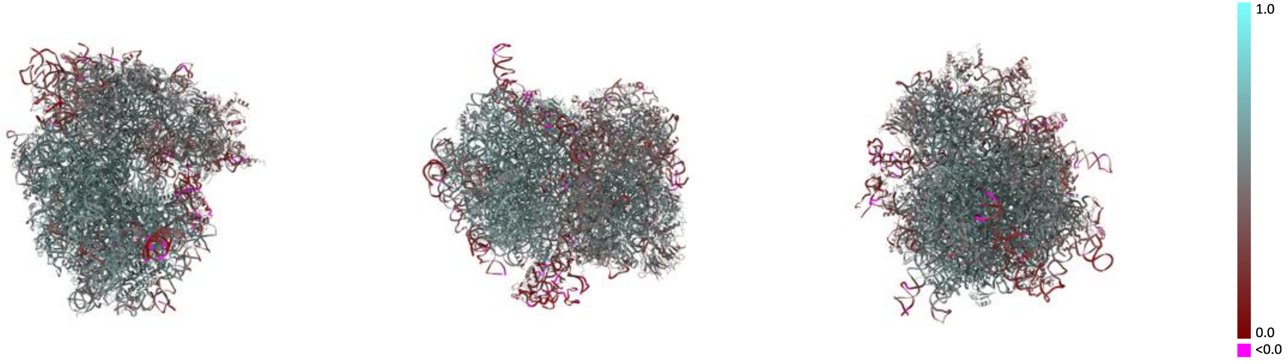
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

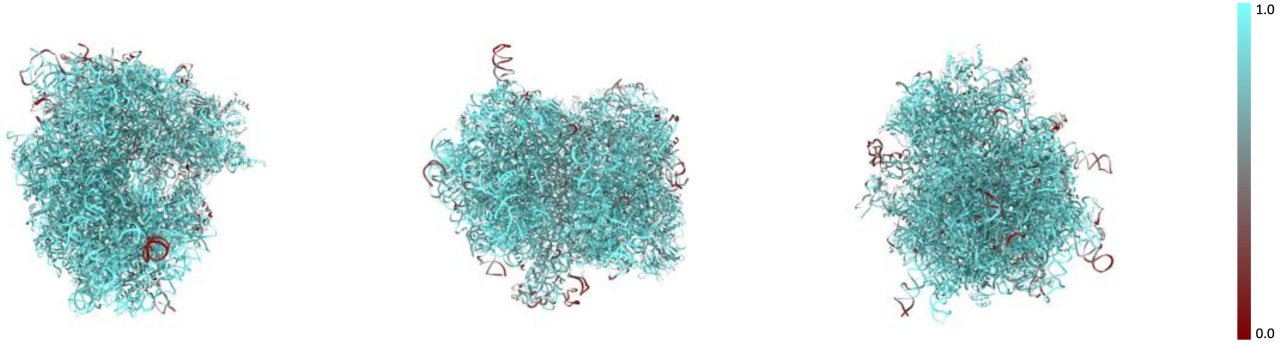
9.2 Q-score mapped to coordinate model ⓘ



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.

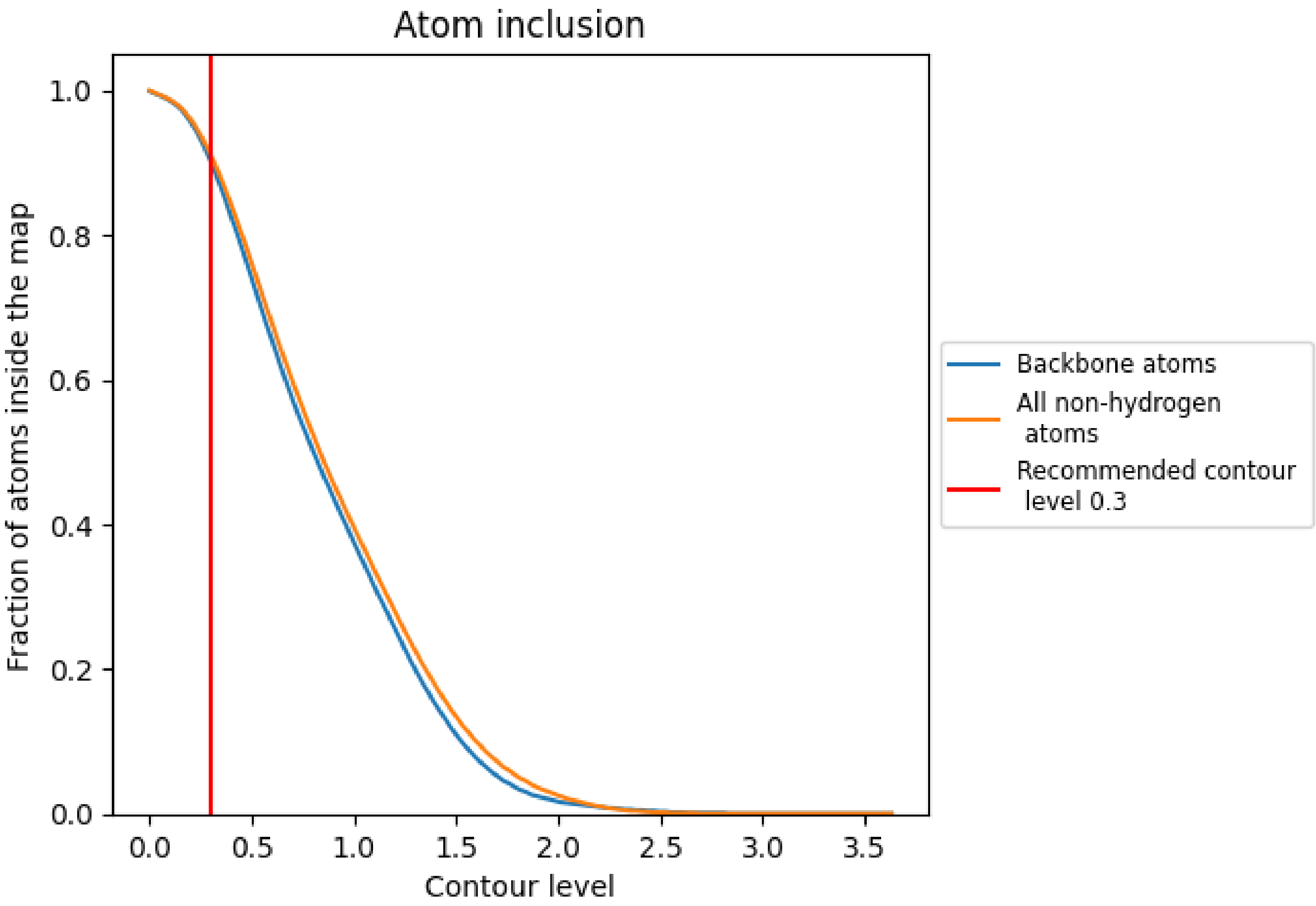
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.5140
B	0.8170	0.4050
E	0.7650	0.3700
F	0.7450	0.3280
I	0.6340	0.2040
L5	0.9540	0.5340
L7	0.9970	0.5910
L8	0.9790	0.5740
LD	0.9440	0.5950
LE	0.9460	0.5830
LF	0.9480	0.5850
LG	0.9410	0.5540
LH	0.9140	0.5460
LI	0.9430	0.5850
LJ	0.8990	0.5380
LK	0.9230	0.5660
LL	0.9030	0.5590
LM	0.9110	0.5300
LO	0.9160	0.5610
LP	0.9340	0.5650
LQ	0.9700	0.6080
LR	0.9490	0.5870
LS	0.9220	0.5770
LT	0.9480	0.5860
LU	0.9150	0.5480
LV	0.9610	0.5940
LW	0.9200	0.5650
LX	0.9210	0.5110
LY	0.9000	0.5750
LZ	0.8160	0.4910
La	0.9320	0.5610
Lb	0.9310	0.5730
Lc	0.9430	0.5590
Ld	0.9630	0.5940
Le	0.8330	0.4890

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lf	0.8520	0.5250
Lg	0.9360	0.5710
Lh	0.9430	0.5910
Li	0.9520	0.5940
Lj	0.9280	0.5670
Lk	0.9250	0.5620
Ll	0.9250	0.5570
Lm	0.9670	0.6070
Ln	0.8760	0.5360
Lo	0.9370	0.5810
Lp	0.9310	0.5710
Lq	0.9190	0.5790
Lr	0.9270	0.5760
Ls	0.9540	0.5850
Lt	0.6190	0.2220
Lx	0.6990	0.2950
S	0.8890	0.2700
S2	0.9330	0.4940
SB	0.8230	0.5070
SC	0.8070	0.4900
SD	0.6820	0.3590
SE	0.7160	0.4180
SF	0.8980	0.5410
SG	0.8230	0.4210
SH	0.9050	0.5370
SL	0.8620	0.5140
SM	0.8600	0.5110
SN	0.8820	0.5300
SO	0.8300	0.4860
SP	0.8270	0.4790
SQ	0.8430	0.4820
SR	0.8170	0.4060
SS	0.7670	0.4550
ST	0.8380	0.4760
SU	0.8260	0.4680
SV	0.8490	0.4690
SW	0.7760	0.4980
SX	0.6610	0.3040
SY	0.8800	0.5410
SZ	0.8760	0.5310
Sa	0.7780	0.4480
Sb	0.8620	0.5000

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sc	0.8050	0.4680
Sd	0.8620	0.4840
Se	0.8730	0.4940
Sf	0.8160	0.4630
Sg	0.8670	0.5210
Sh	0.9120	0.5560
Si	0.8980	0.5470
Sj	0.8500	0.4590
Sk	0.8080	0.4450
Sl	0.9270	0.5970