



Full wwPDB EM Validation Report ⓘ

Oct 11, 2022 – 08:21 pm BST

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

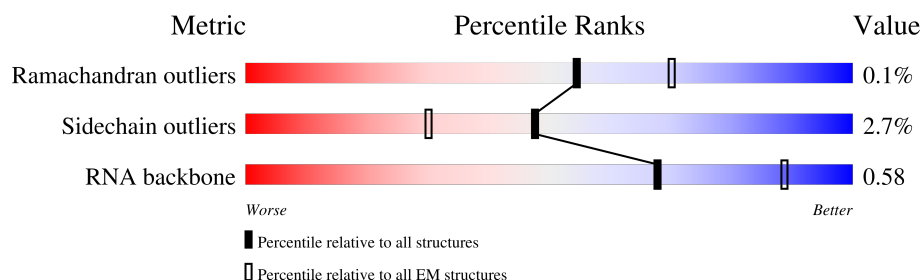
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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.



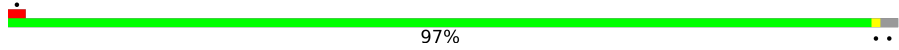
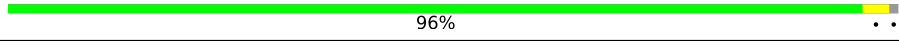
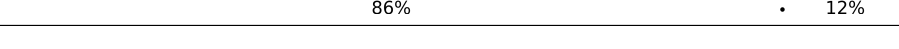
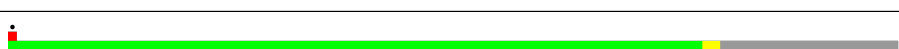


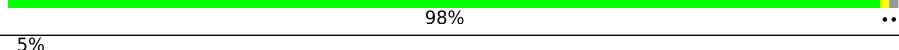
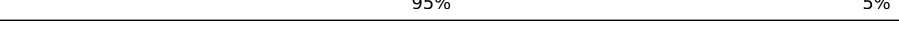


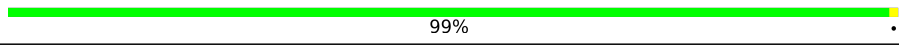
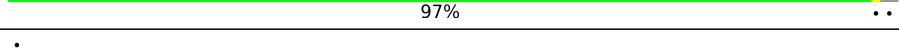

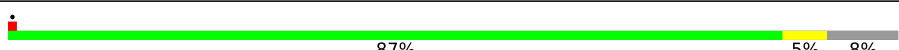
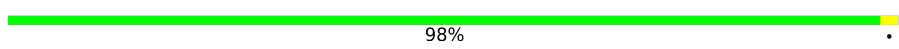
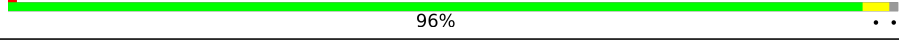
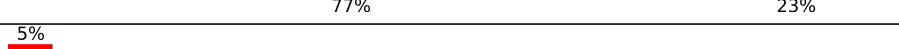


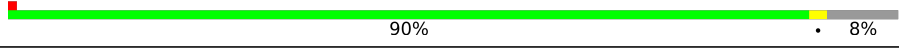
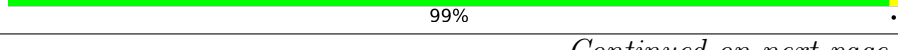



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	<div> <div>8%</div> <div>83%</div> <div>16%</div> </div>
2	F	90	<div> <div>10%</div> <div>69%</div> <div>31%</div> </div>
3	I	1072	<div> <div>7%</div> <div>10%</div> <div>83%</div> </div>
4	S	855	<div> <div>95%</div> </div>
5	B	854	<div> <div>23%</div> <div>76%</div> </div>
6	L5	4808	<div> <div>65%</div> <div>13%</div> <div>22%</div> </div>
7	L7	119	<div> <div>93%</div> <div>7%</div> </div>
8	L8	158	<div> <div>85%</div> <div>13%</div> </div>

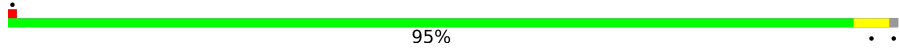

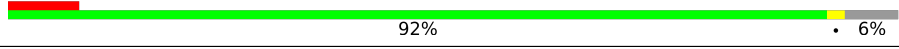

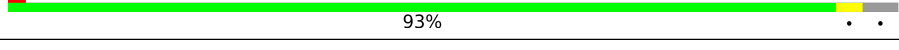
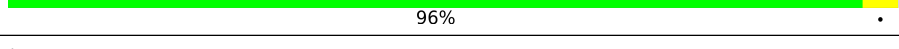
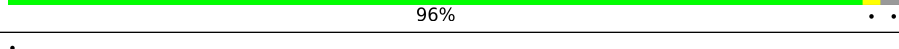
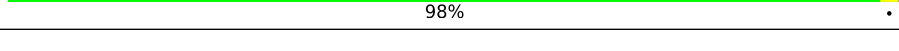
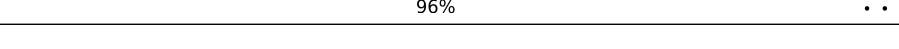
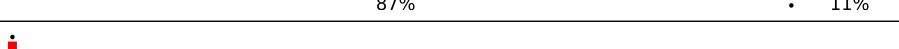
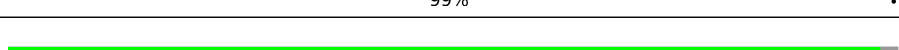
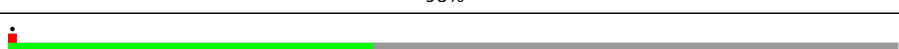
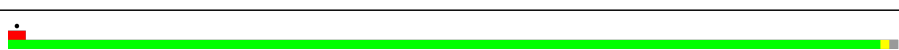
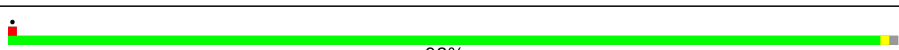
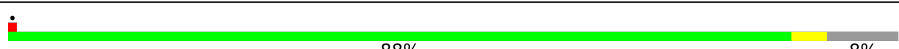

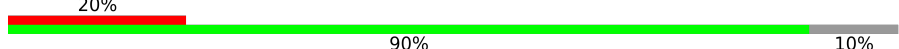

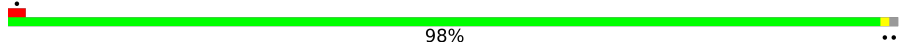




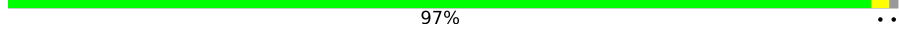

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Mol	Chain	Length	Quality of chain
9	LD	257	
10	LE	403	
11	LF	413	
12	LG	297	
13	LH	291	
14	LI	247	
15	LJ	266	
16	LK	192	
17	LL	214	
18	LM	178	
19	LO	211	
20	LP	218	
21	LQ	204	
22	LR	203	
23	LS	184	
24	LT	188	
25	LU	196	
26	LV	176	
27	LW	160	
28	LX	128	
29	LY	140	
30	LZ	157	
31	La	156	
32	Lb	145	
33	Lc	136	

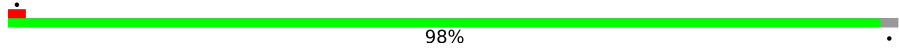




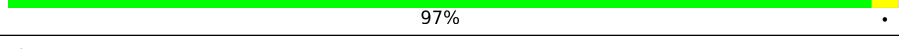
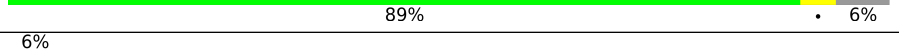
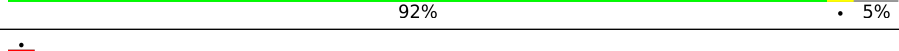
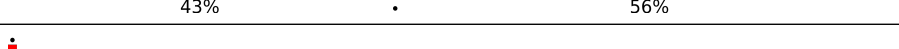
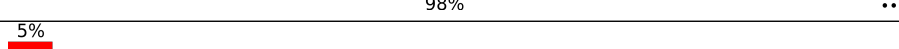
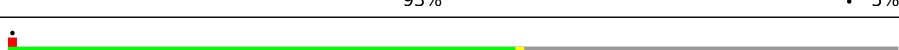

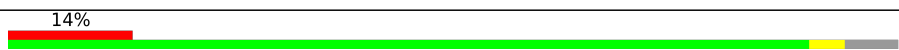
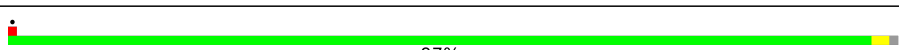
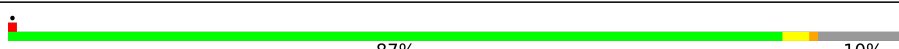


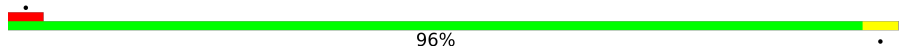
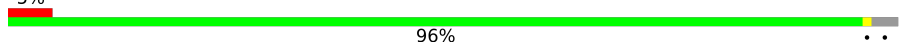
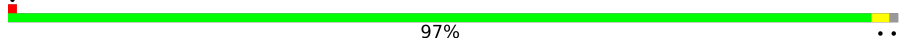
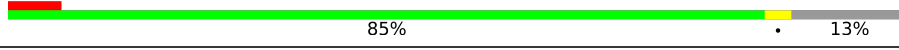
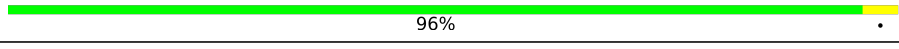
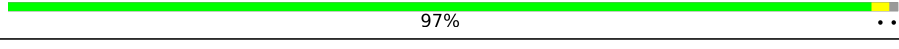
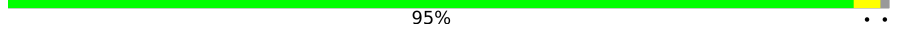

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Mol	Chain	Length	Quality of chain
34	Ld	148	
35	Le	245	
36	Lf	115	
37	Lg	125	
38	Lh	135	
39	Li	110	
40	Lj	117	
41	Lk	123	
42	Ll	105	
43	Lm	97	
44	Ln	70	
45	Lo	51	
46	Lp	128	
47	Lq	106	
48	Lr	92	
49	Ls	137	
50	Lt	318	
51	Lx	217	
52	S2	1870	
53	SB	84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

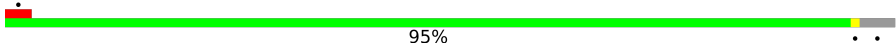

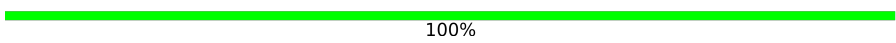
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Mol	Chain	Length	Quality of chain
59	SH	56	
60	SL	295	
61	SM	264	
62	SN	293	
63	SO	281	
64	SP	263	
65	SQ	204	
66	SR	249	
67	SS	432	
68	ST	208	
69	SU	194	
70	SV	165	
71	SW	158	
72	SX	132	
73	SY	151	
74	SZ	151	
75	Sa	145	
76	Sb	172	
77	Sc	135	
78	Sd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

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Mol	Chain	Length	Quality of chain
84	Sj	130	 95%
85	Sk	124	 58%40%
86	Sl	25	 100%

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	C	N	O	S	0	0
			3335	2110	616	599	10		

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	C	N	O	P	0	0
			1914	853	334	637	90		

- Molecule 3 is a RNA chain called CrPV IRES.

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

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

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

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
5	B	204	Total	C	N	O	S	0	0
			1379	881	257	238	3		

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
6	L5	3764	Total	C	N	O	P	0	0
			80771	36002	14762	26243	3764		

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

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

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

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

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

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

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

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

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

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

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

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

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
13	LH	232	Total	C	N	O	S	0	0
			1859	1197	354	305	3		

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

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

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
15	LJ	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

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
16	LK	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

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

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

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

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

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

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

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
20	LP	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

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

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

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

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

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
23	LS	159	Total	C	N	O	S	0	0
			1288	808	249	222	9		

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

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

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
25	LU	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

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

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

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
27	LW	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

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

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

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
29	LY	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

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

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

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

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

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

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

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

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

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

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

- 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
42	Ll	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
51	Lx	196	Total	C	N	O	0	0
			972	580	196	196		

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

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

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
53	SB	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

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

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

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

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

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

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

- Molecule 57 is a protein called Ribosomal protein eS26.

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

- Molecule 58 is a protein called RACK1.

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

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

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

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

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

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

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

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

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

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
63	SO	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

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

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

- Molecule 65 is a protein called Ribosomal protein S5.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

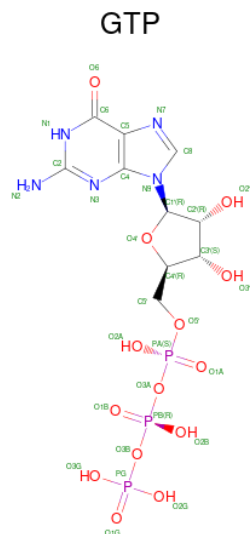
- Molecule 85 is a protein called 40S ribosomal protein S25.

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

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

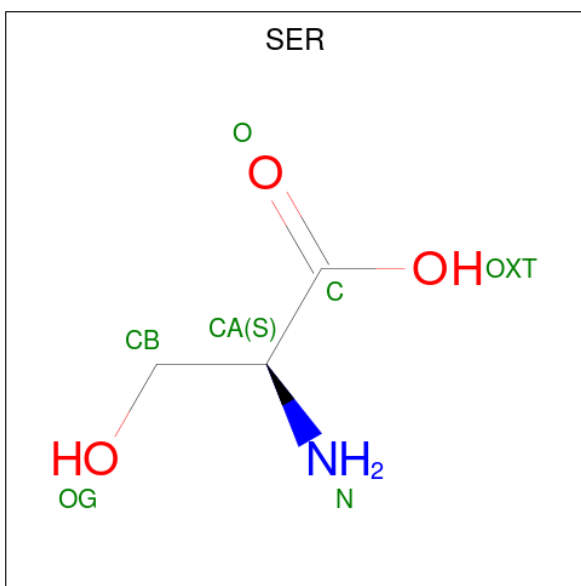
Mol	Chain	Residues	Atoms					AltConf	Trace
86	Sl	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 87 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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: $\text{C}_3\text{H}_7\text{NO}_3$).



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

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

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

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

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

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

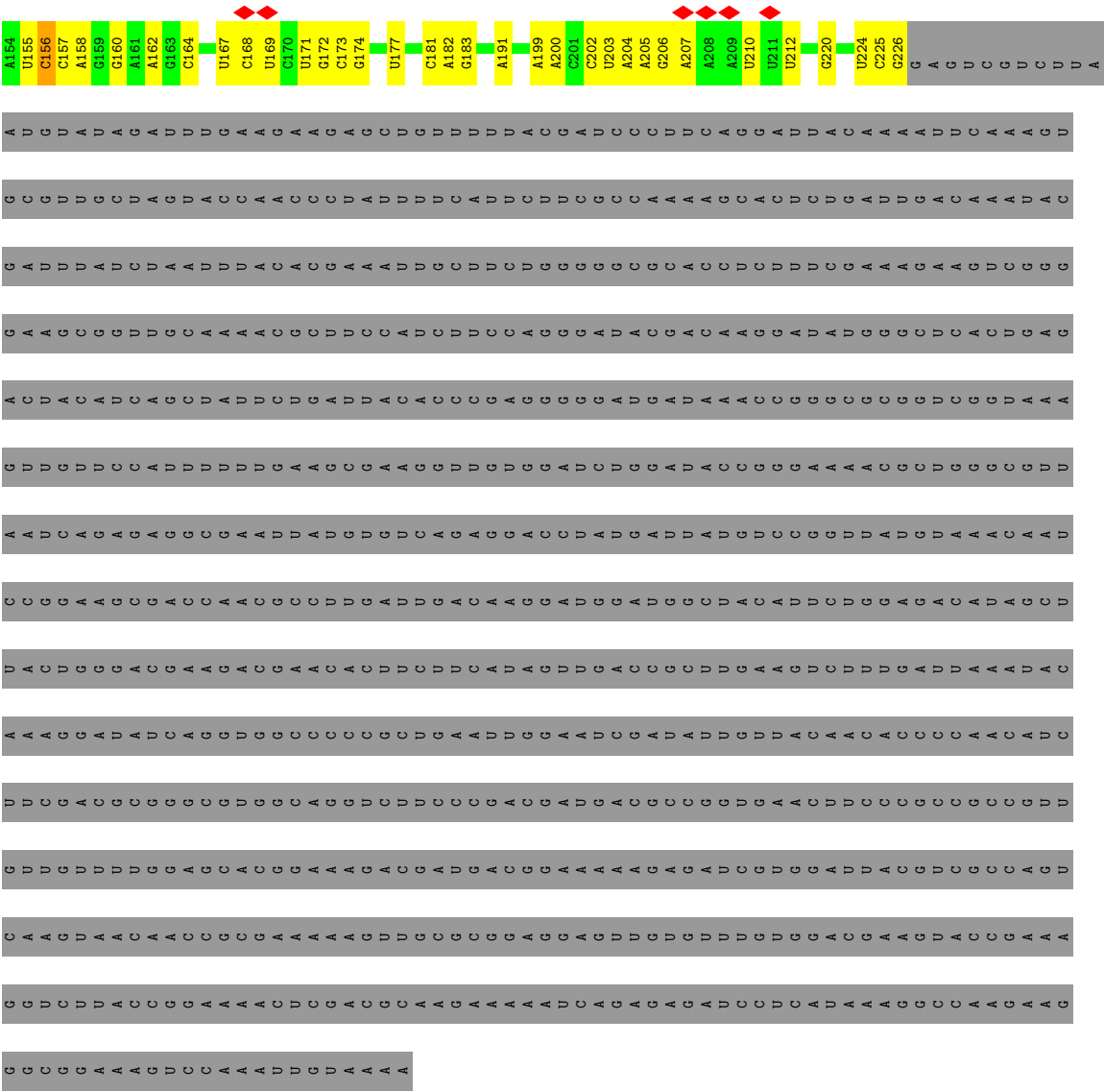
Mol	Chain	Residues	Atoms		AltConf
91	Lj	1	Total 1	Zn 1	0
91	Lm	1	Total 1	Zn 1	0
91	Lp	1	Total 1	Zn 1	0
91	Lq	1	Total 1	Zn 1	0
91	Lr	1	Total 1	Zn 1	0
91	SD	1	Total 1	Zn 1	0
91	SF	2	Total 2	Zn 2	0
91	SH	1	Total 1	Zn 1	0

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

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

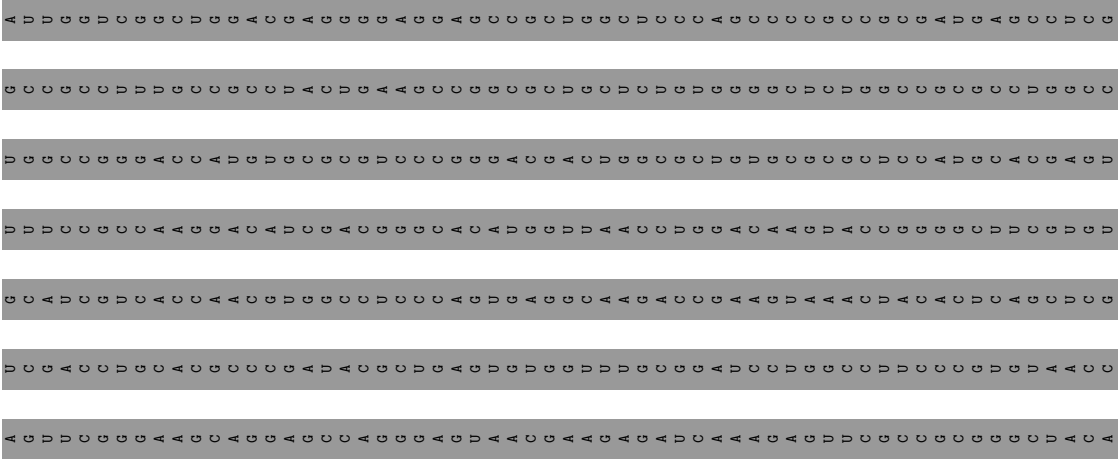
- Molecule 93 is water.

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



● Molecule 4: GPX4 SECIS element

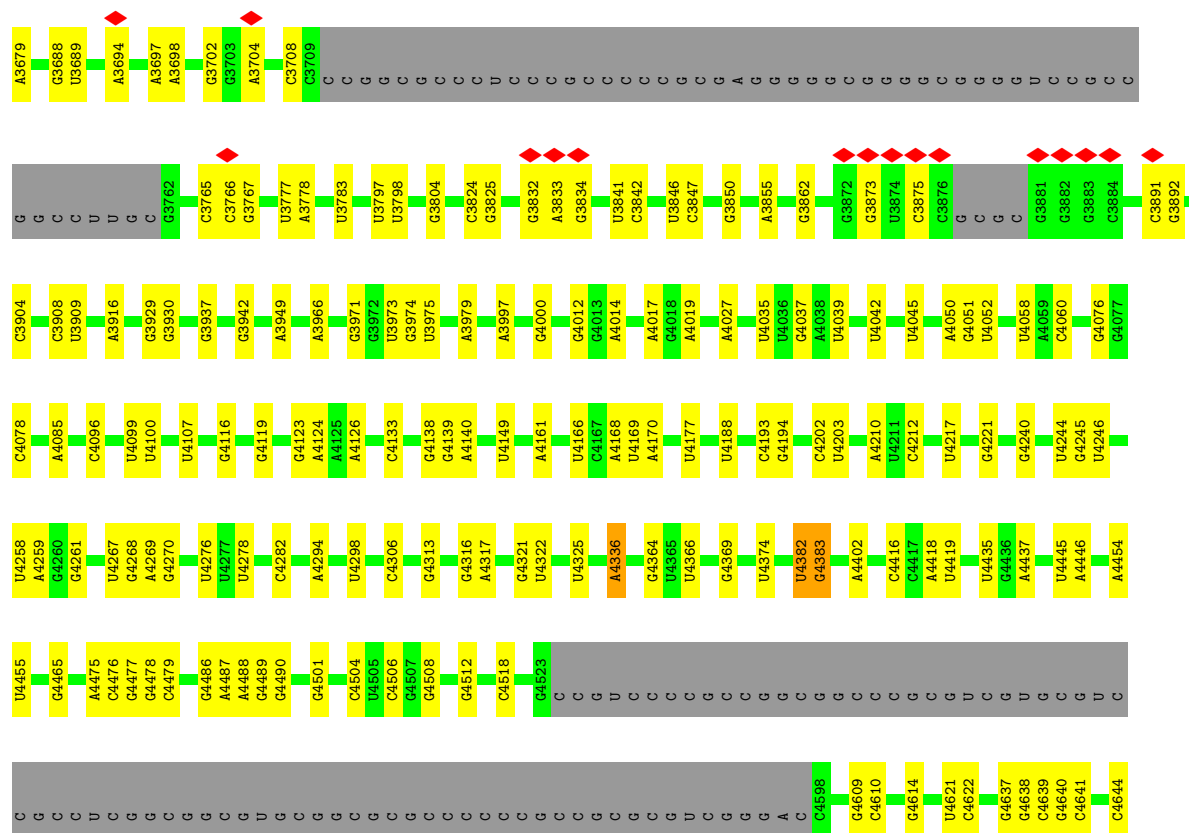
Chain S:  95%



- Molecule 6: 28S rRNA

Chromosome	Position (Mb)	Gene	Strand	Feature
1	100	U1090	+	UTR
1	100	G1091	+	UTR
1	100	G1102	+	UTR
1	100	C1105	+	UTR
1	100	U1106	+	UTR
1	100	A1113	+	UTR
1	100	G1120	+	UTR
1	100	A1124	+	UTR
1	100	G1127	+	UTR
1	100	C1128	+	UTR
1	100	G1129	+	UTR
1	100	U1132	+	UTR
1	100	C1133	+	UTR
1	100	G1134	+	UTR
1	100	C1135	+	UTR
1	100	G1136	+	UTR
1	100	C1137	+	UTR
1	100	G1138	+	UTR
1	100	C1139	+	UTR
1	100	G1140	+	UTR
1	100	U1141	+	UTR
1	100	C1142	+	UTR
1	100	G1143	+	UTR
1	100	C1144	+	UTR
1	100	G1145	+	UTR
1	100	C1146	+	UTR
1	100	G1147	+	UTR
1	100	C1148	+	UTR
1	100	G1149	+	UTR
1	100	C1150	+	UTR
1	100	G1151	+	UTR
1	100	C1152	+	UTR
1	100	G1153	+	UTR
1	100	C1154	+	UTR
1	100	G1155	+	UTR
1	100	C1156	+	UTR
1	100	G1157	+	UTR
1	100	C1158	+	UTR
1	100	G1159	+	UTR
1	100	C1160	+	UTR
1	100	G1161	+	UTR
1	100	C1162	+	UTR
1	100	G1163	+	UTR
1	100	C1164	+	UTR
1	100	G1165	+	UTR
1	100	C1166	+	UTR
1	100	G1167	+	UTR
1	100	C1168	+	UTR
1	100	G1169	+	UTR
1	100	C1170	+	UTR
1	100	G1171	+	UTR
1	100	C1172	+	UTR
1	100	G1173	+	UTR
1	100	C1174	+	UTR
1	100	G1175	+	UTR
1	100	C1176	+	UTR
1	100	G1177	+	UTR
1	100	C1178	+	UTR
1	100	G1179	+	UTR
1	100	C1180	+	UTR
1	100	G1181	+	UTR
1	100	C1182	+	UTR
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1	100	C1184	+	UTR
1	100	G1185	+	UTR
1	100	C1186	+	UTR
1	100	G1187	+	UTR
1	100	C1188	+	UTR
1	100	G1189	+	UTR
1	100	C1190	+	UTR
1	100	G1191	+	UTR
1	100	C1192	+	UTR
1	100	G1193	+	UTR
1	100	C1194	+	UTR
1	100	G1195	+	UTR
1	100	C1196	+	UTR
1	100	G1197	+	UTR
1	100	C1198	+	UTR
1	100	G1199	+	UTR
1	100	C1200	+	UTR
1	100	G1201	+	UTR
1	100	C1202	+	UTR
1	100	G1203	+	UTR
1	100	C1204	+	UTR
1	100	G1205	+	UTR
1	100	C1206	+	UTR
1	100	G1207	+	UTR
1	100	C1208	+	UTR
1	100	G1209	+	UTR
1	100	C1210	+	UTR
1	100	G1211	+	UTR
1	100	C1212	+	UTR
1	100	G1213	+	UTR
1	100	C1214	+	UTR
1	100	G1215	+	UTR
1	100	C1216	+	UTR
1	100	G1217	+	UTR
1	100	C1218	+	UTR
1	100	G1219	+	UTR
1	100	C1220	+	UTR
1	100	G1221	+	





- Molecule 7: 5S rRNA

Chain L7: 93% 7%



- Molecule 8: 5.8S rRNA

Chain L8: 85% 13% ..



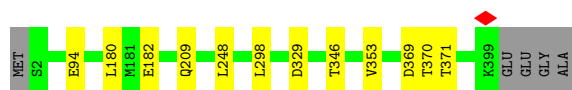
- Molecule 9: 60S ribosomal protein uL2

Chain LD: 97% ..



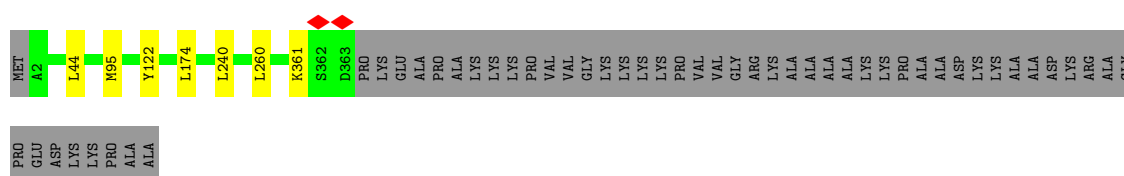
- Molecule 10: 60S ribosomal protein L3

Chain LE:  96%



- Molecule 11: 60S ribosomal protein L4

Chain LF:  86%




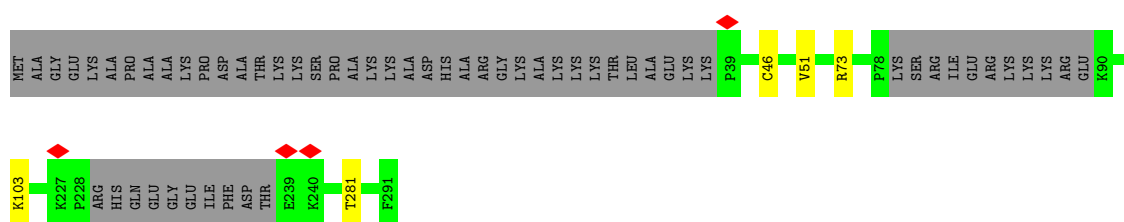
- Molecule 12: Ribosomal_L18_c domain-containing protein

Chain LG:  97%



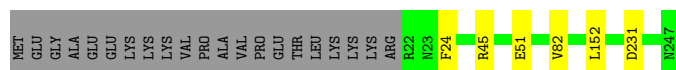
- Molecule 13: 60S ribosomal protein L6

Chain LH:  78%




- Molecule 14: 60S ribosomal Protein uL30

Chain LI:  89%

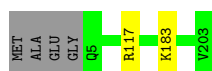


- Molecule 15: 60S ribosomal protein eL8

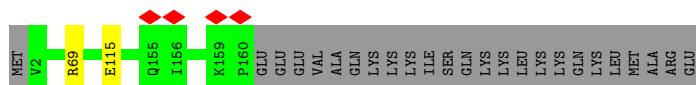
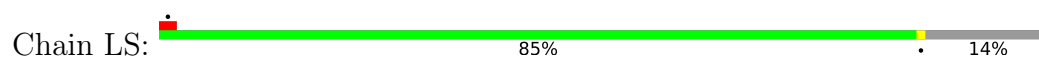
Chain LJ:  85%



- Chain LR: 97% ...



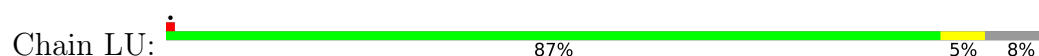
- Molecule 23: 60S ribosomal protein uL22



- Molecule 24: 60S ribosomal Protein eL18



- Molecule 25: 60S ribosomal protein L19



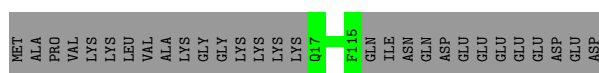
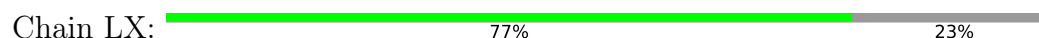
- Molecule 26: 60S ribosomal protein eL20



- Molecule 27: 60S ribosomal protein eL21

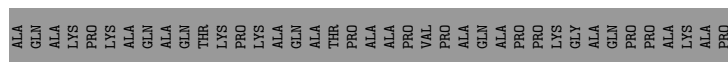


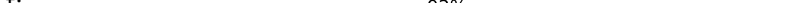
- Molecule 28: 60S ribosomal protein eL22

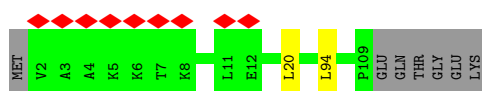


- Molecule 29: 60S ribosomal protein L23

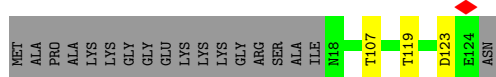




- Chain Lf:  8% 92% 6%



- Chain Lg: 83% 14%



- Chain Lh: 



- Chain Li:  96%



- Chain Lj: 



- Chain Lk:  98%



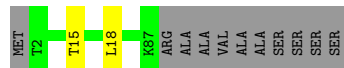
- Molecule 42: 60S ribosomal protein L36

Chain Ll:  96% ..



- Molecule 43: 60S ribosomal protein L37

Chain Lm:  87% . 11%



- Molecule 44: 60S ribosomal protein eL38

Chain Ln:  99% .




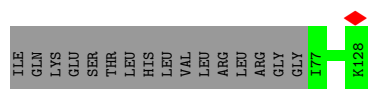
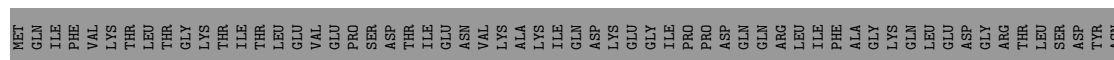
- Molecule 45: 60S ribosomal protein eL39

Chain Lo:  98% .



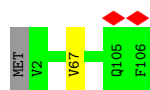
- Molecule 46: 60S ribosomal protein L40

Chain Lp:  41% 59%



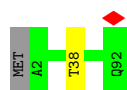
- Molecule 47: 60S ribosomal protein eL42

Chain Lq:  98% ..

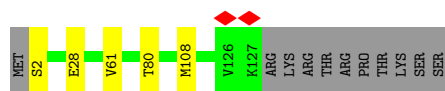


- Molecule 48: 60S ribosomal protein eL43

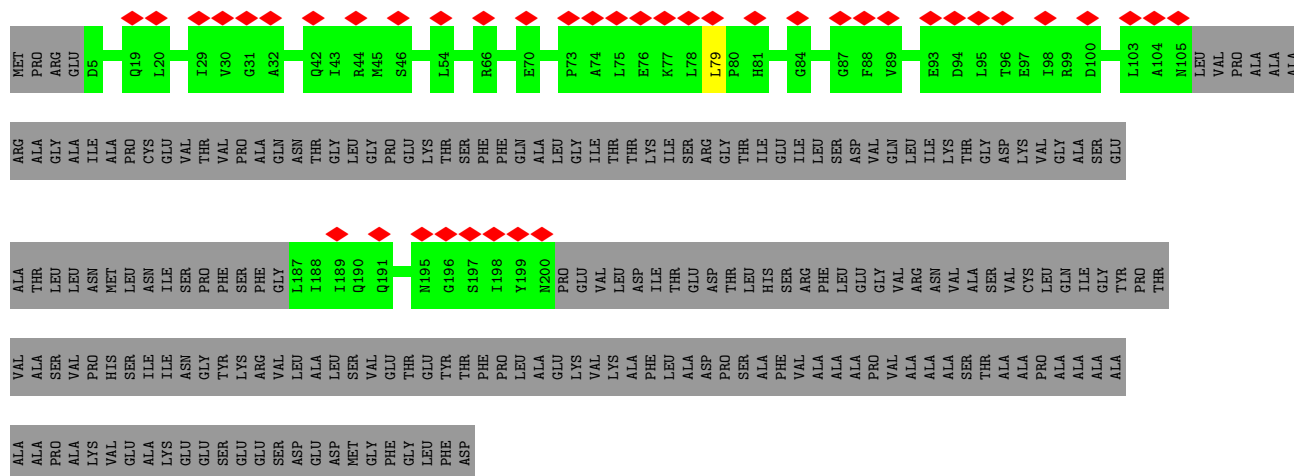
Chain Lr:  98% ..



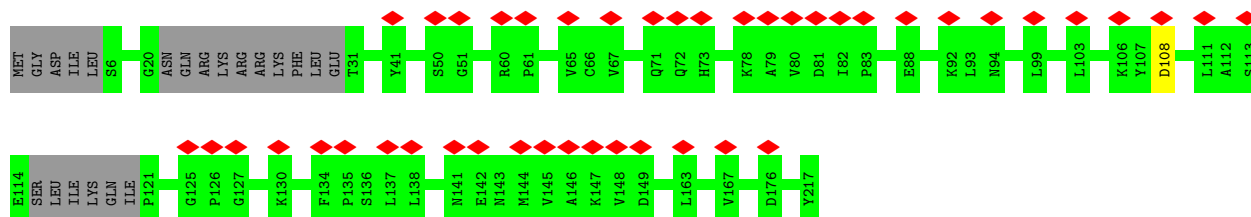
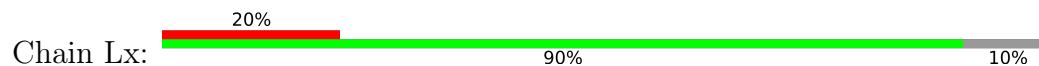
- Molecule 49: 60S ribosomal protein eL28



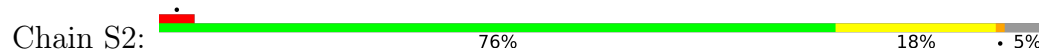
- Molecule 50: 60S ribosomal protein P0




- Molecule 51: 60S ribosomal protein uL1

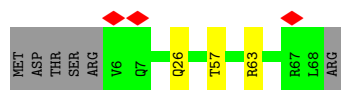


- Molecule 52: 18S rRNA



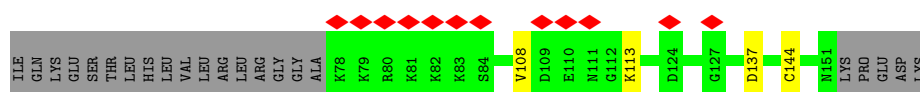
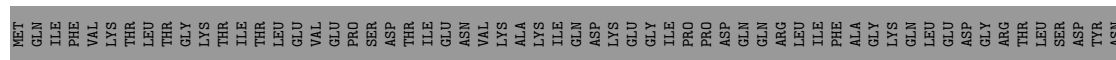
- Molecule 54: 40S ribosomal protein S28

Chain SC:  87% 9%



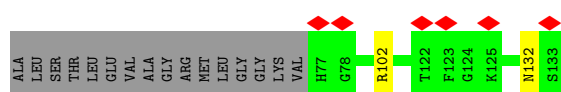
- Molecule 55: 40S ribosomal protein S27a

Chain SD:  8% 45% 53%




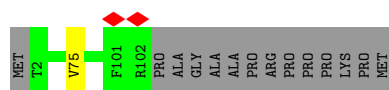
- Molecule 56: 40S ribosomal protein S30

Chain SE:  5% 41% 57%



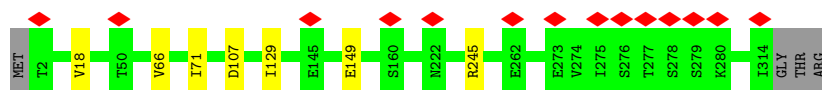
- Molecule 57: Ribosomal protein eS26

Chain SF:  87% 12%



- Molecule 58: RACK1

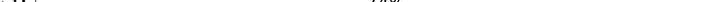
Chain SG:  97% 2%



- Molecule 59: 40S ribosomal protein uS14

Chain SH:  98% 2%



- Chain SL: 

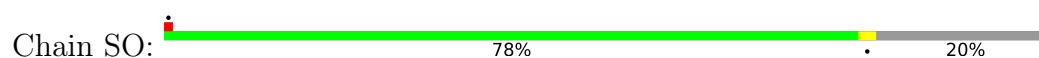
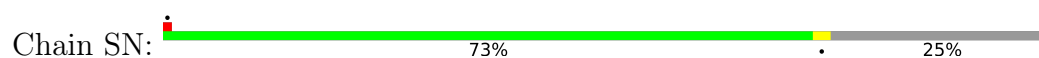
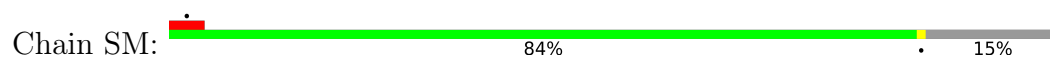
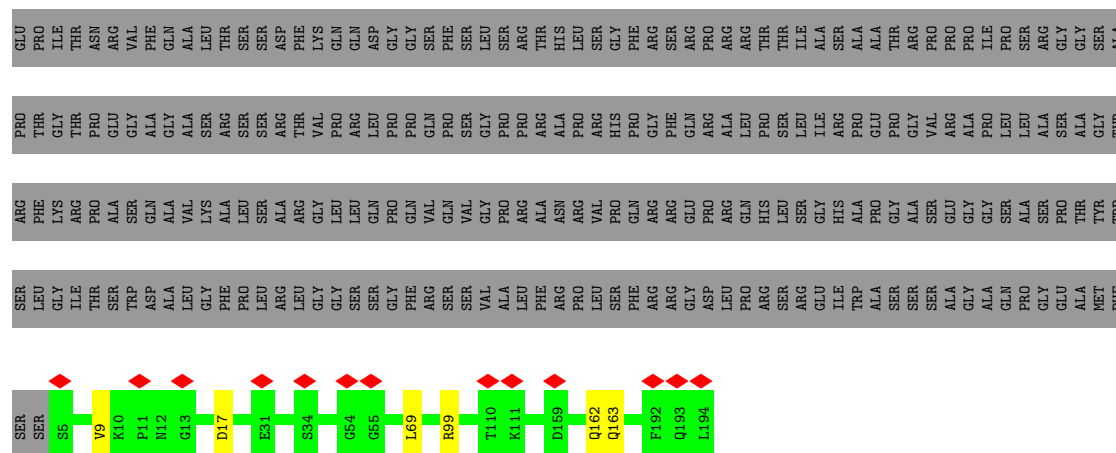


Figure 1: Schematic representation of the 20 amino acids. The amino acids are arranged in a horizontal bar, color-coded by their chemical properties: MET (grey), THR (grey), GLU (grey), TRP (grey), GLU (grey), THR (grey), ALA (grey), ALA (grey), PRO (grey), ALA (grey), VAL (grey), ALA (grey), ALA (grey), GLU (grey), T14 (red), T25 (yellow), D26 (yellow), I33 (yellow), T73 (yellow), E106 (yellow), E123 (yellow), G129 (green), R130 (green), A131 (green), G132 (green), T133 (green), V134 (green), R135 (green), R136 (green), L153 (green), S187 (green), and R204 (green). Red diamonds are placed above the T14, G129, R130, A131, G132, T133, V134, and R135 labels.

- Chain SR: 



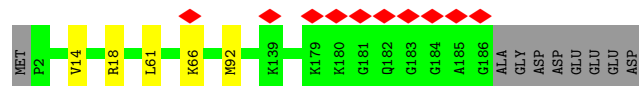
- Chain SS: 



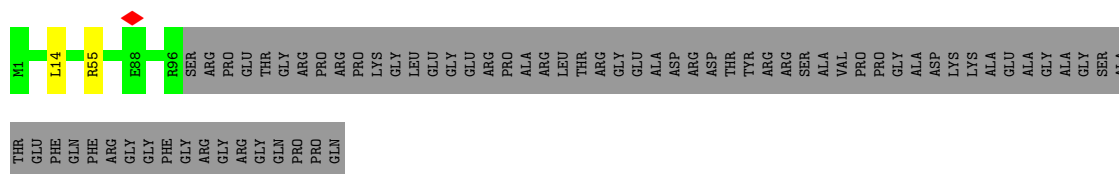
- Chain ST:  98%



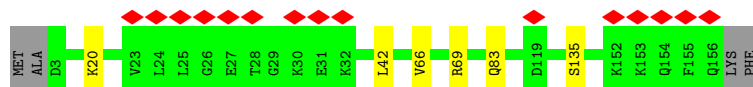
- Chain SU:  5% 93% 5%



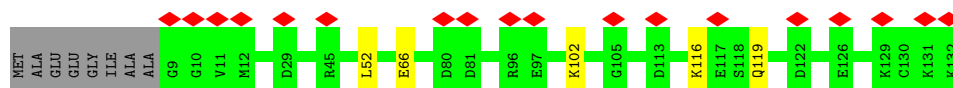
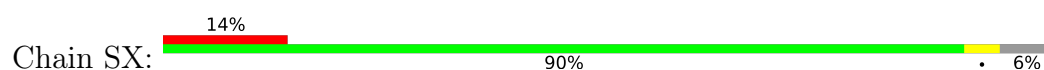
- Chain SV:



- Molecule 71: 40S ribosomal protein S11



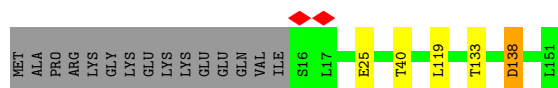
- Molecule 72: 40S ribosomal protein S12



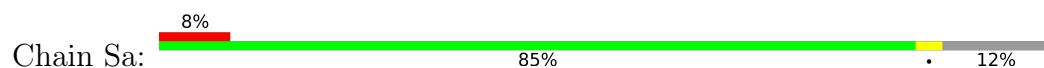
- Molecule 73: 40S ribosomal protein uS15



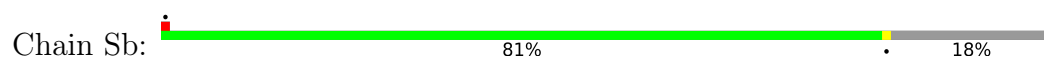
- Molecule 74: 40S ribosomal protein uS11

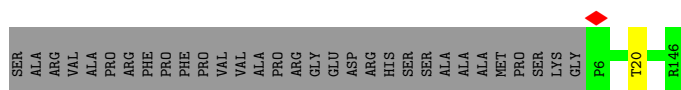


- Molecule 75: 40S ribosomal protein uS19



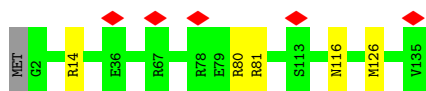
- Molecule 76: 40S ribosomal protein uS9





- Molecule 77: 40S ribosomal protein eS17

Chain Sc: 96%



- Molecule 78: 40S ribosomal protein S18

Chain Sd: 5% 96%



- Molecule 79: 40S Ribosomal protein eS19

Chain Se: 97%



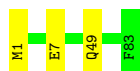
- Molecule 80: 40S ribosomal protein uS10

Chain Sf: 6% 85% 13%



- Molecule 81: 40S ribosomal protein eS21

Chain Sg: 96%



- Molecule 82: 40S ribosomal protein S15a

Chain Sh: 97%



- Molecule 83: 40S ribosomal protein S23

- Chain Sj:  95% . .

- Chain Sk:  58% 40%

PRO PRO LYS ASP ASP LYS LYS LYS LYS ASP ALA GLY SER LYS ALA LYS LYS ASP LYS VAL ASN LYS SER GLY GLY LYS LYS LYS TRP SER GLY LYS LYS VAL R41 L58 C59 K60 L67 K114 G115 ASP ALA ALA ALA GLU ASP

- Chain Sl:  100%

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 ($e^-/\text{\AA}^2$)	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 ⓘ

5.1 Standard geometry ⓘ

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

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%)

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(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	509/616 (83%)	460 (90%)	46 (9%)	3 (1%)	25 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	136/143 (95%)	135 (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	12309/15142 (81%)	11991 (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
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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:

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Mol	Chain	Res	Type
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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 [i](#)

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	$\# Z > 2$
6	A2M	L5	4269	6,89	18,25,26	1.96	5 (27%)	18,36,39	2.21	5 (27%)
52	PSU	S2	652	52	18,21,22	1.39	3 (16%)	22,30,33	1.84	4 (18%)
6	OMC	L5	1284	6	19,22,23	1.16	2 (10%)	26,31,34	0.86	0
6	OMU	L5	2258	6	19,22,23	0.99	2 (10%)	26,31,34	1.77	5 (19%)
6	OMU	L5	4366	6,29	19,22,23	1.00	2 (10%)	26,31,34	1.81	6 (23%)
6	A2M	L5	3456	6	18,25,26	1.96	5 (27%)	18,36,39	2.10	4 (22%)
52	6MZ	S2	1833	52,89	18,25,26	0.87	1 (5%)	16,36,39	1.81	4 (25%)
52	PSU	S2	1348	52	18,21,22	1.38	3 (16%)	22,30,33	1.81	3 (13%)
6	A2M	L5	1810	6,89	18,25,26	1.95	5 (27%)	18,36,39	2.26	6 (33%)
6	PSU	L5	4325	6	18,21,22	1.35	3 (16%)	22,30,33	1.85	5 (22%)
6	OMC	L5	2667	6	19,22,23	1.14	2 (10%)	26,31,34	0.87	0
52	OMC	S2	1392	52	19,22,23	1.16	2 (10%)	26,31,34	0.94	1 (3%)
52	PSU	S2	93	52	18,21,22	1.42	3 (16%)	22,30,33	1.76	3 (13%)
52	A2M	S2	1679	52	18,25,26	1.97	5 (27%)	18,36,39	2.13	4 (22%)
6	PSU	L5	4039	6	18,21,22	1.35	3 (16%)	22,30,33	1.87	5 (22%)
52	PSU	S2	1239	52	18,21,22	1.37	3 (16%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	SAC	Ls	2	49	7,8,9	0.53	0	8,9,11	0.84	1 (12%)
6	5MC	L5	4193	6	18,22,23	1.24	3 (16%)	26,32,35	1.53	3 (11%)
52	A2M	S2	166	52	18,25,26	2.00	5 (27%)	18,36,39	2.21	6 (33%)
52	OMG	S2	645	52	18,26,27	1.96	2 (11%)	19,38,41	1.73	5 (26%)
6	PSU	L5	3427	6	18,21,22	1.36	3 (16%)	22,30,33	1.81	5 (22%)
6	A2M	L5	2206	6,89	18,25,26	1.95	5 (27%)	18,36,39	2.15	5 (27%)
6	OMG	L5	3942	6	18,26,27	1.96	2 (11%)	19,38,41	1.66	4 (21%)
52	PSU	S2	650	52	18,21,22	1.38	3 (16%)	22,30,33	1.83	4 (18%)
6	PSU	L5	4419	6	18,21,22	1.34	3 (16%)	22,30,33	1.84	5 (22%)
52	MA6	S2	1852	52	19,26,27	0.96	1 (5%)	18,38,41	1.66	5 (27%)
81	AME	Sg	1	81	9,10,11	0.47	0	9,11,13	0.88	1 (11%)
52	PSU	S2	864	82,52	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
52	A2M	S2	513	52	18,25,26	1.97	5 (27%)	18,36,39	2.15	4 (22%)
52	OMG	S2	1448	52	18,26,27	1.96	2 (11%)	19,38,41	1.65	4 (21%)
6	PSU	L5	4058	6	18,21,22	1.37	3 (16%)	22,30,33	1.80	5 (22%)
52	PSU	S2	1005	52	18,21,22	1.63	5 (27%)	22,30,33	2.85	6 (27%)
6	A2M	L5	2658	6,89	18,25,26	1.95	5 (27%)	18,36,39	2.11	5 (27%)
10	HIC	LE	245	10	8,11,12	0.86	0	6,14,16	0.81	0
6	PSU	L5	4188	6	18,21,22	1.33	3 (16%)	22,30,33	1.93	4 (18%)
52	PSU	S2	1368	52	18,21,22	1.41	3 (16%)	22,30,33	1.85	5 (22%)
52	PSU	S2	802	52	18,21,22	1.40	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	PSU	S2	34	52	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
6	OMG	L5	4245	6	18,26,27	1.98	2 (11%)	19,38,41	1.67	5 (26%)
6	PSU	L5	4246	6	18,21,22	1.39	3 (16%)	22,30,33	1.88	5 (22%)
52	OMC	S2	1704	52,89	19,22,23	1.13	2 (10%)	26,31,34	0.89	1 (3%)
6	OMG	L5	4383	6,90	18,26,27	1.97	2 (11%)	19,38,41	1.68	5 (26%)
52	PSU	S2	573	52,84	18,21,22	1.43	3 (16%)	22,30,33	1.84	4 (18%)
52	PSU	S2	1082	52	18,21,22	1.33	3 (16%)	22,30,33	1.82	4 (18%)
6	PSU	L5	4042	6	18,21,22	1.36	3 (16%)	22,30,33	1.87	4 (18%)
6	OMG	L5	4364	6	18,26,27	1.97	2 (11%)	19,38,41	1.68	5 (26%)
6	PSU	L5	4203	6	18,21,22	1.33	3 (16%)	22,30,33	1.81	4 (18%)
6	PSU	L5	1537	6	18,21,22	1.38	3 (16%)	22,30,33	1.81	4 (18%)
6	PSU	L5	3616	6	18,21,22	1.34	3 (16%)	22,30,33	1.86	5 (22%)
52	A2M	S2	669	52,89	18,25,26	1.86	5 (27%)	18,36,39	2.21	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A2M	L5	3562	6	18,25,26	1.92	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%)
6	PSU	L5	3371	6	18,21,22	1.33	3 (16%)	22,30,33	1.82	5 (22%)
52	A2M	S2	469	52	18,25,26	1.96	5 (27%)	18,36,39	2.18	5 (27%)
52	OMC	S2	174	52	19,22,23	1.20	3 (15%)	26,31,34	0.88	0
6	OMC	L5	2194	6	19,22,23	1.11	2 (10%)	26,31,34	0.95	1 (3%)
52	OMG	S2	1491	52,89	18,26,27	1.97	2 (11%)	19,38,41	1.66	4 (21%)
6	OMC	L5	2647	6	19,22,23	1.14	2 (10%)	26,31,34	0.88	1 (3%)
47	MLZ	Lq	53	47	8,9,10	0.46	0	4,9,11	0.08	0
6	PSU	L5	3583	6	18,21,22	1.33	3 (16%)	22,30,33	1.90	5 (22%)
79	NMM	Se	67	79	9,11,12	1.56	1 (11%)	6,12,14	3.48	2 (33%)
6	A2M	L5	400	6	18,25,26	1.98	5 (27%)	18,36,39	2.15	4 (22%)
6	OMG	L5	3676	6	18,26,27	1.94	2 (11%)	19,38,41	1.68	4 (21%)
6	UR3	L5	4276	6	19,22,23	1.30	3 (15%)	26,32,35	1.20	2 (7%)
52	OMG	S2	437	52	18,26,27	1.96	2 (11%)	19,38,41	1.66	4 (21%)
11	AYA	LF	2	11	6,7,8	0.75	0	5,8,10	0.25	0
6	PSU	L5	4169	6	18,21,22	1.37	3 (16%)	22,30,33	1.85	5 (22%)
8	OMG	L8	75	8	18,26,27	1.98	2 (11%)	19,38,41	1.65	4 (21%)
6	PSU	L5	4177	6	18,21,22	1.33	3 (16%)	22,30,33	1.86	5 (22%)
52	OMC	S2	518	52	19,22,23	1.15	2 (10%)	26,31,34	0.91	1 (3%)
6	PSU	L5	3585	6,89	18,21,22	1.32	3 (16%)	22,30,33	1.83	4 (18%)
52	4AC	S2	1843	52,86	21,24,25	1.15	2 (9%)	29,34,37	1.10	2 (6%)
6	PSU	L5	3576	6	18,21,22	1.36	3 (16%)	22,30,33	1.77	4 (18%)
52	OMU	S2	1805	52	19,22,23	0.98	2 (10%)	26,31,34	1.80	5 (19%)
52	PSU	S2	1644	52,89	18,21,22	1.36	3 (16%)	22,30,33	1.83	4 (18%)
52	OMU	S2	116	52	19,22,23	1.01	2 (10%)	26,31,34	1.80	6 (23%)
52	OMU	S2	121	52	19,22,23	0.99	2 (10%)	26,31,34	1.75	5 (19%)
6	PSU	L5	4217	6,16	18,21,22	1.34	3 (16%)	22,30,33	1.81	5 (22%)
52	A2M	S2	27	52	18,25,26	1.97	5 (27%)	18,36,39	2.12	4 (22%)
6	OMC	L5	4202	6	19,22,23	1.14	2 (10%)	26,31,34	0.93	1 (3%)
8	PSU	L8	69	8	18,21,22	1.36	3 (16%)	22,30,33	1.90	5 (22%)
52	A2M	S2	591	52	18,25,26	2.00	5 (27%)	18,36,39	2.31	5 (27%)
52	A2M	S2	1032	52	18,25,26	1.92	5 (27%)	18,36,39	2.14	4 (22%)
6	PSU	L5	1718	6,12	18,21,22	1.35	3 (16%)	22,30,33	1.82	4 (18%)
6	OMG	L5	3476	6	18,26,27	1.98	2 (11%)	19,38,41	1.68	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	OMU	S2	1289	52,55	19,22,23	0.97	1 (5%)	26,31,34	1.76	5 (19%)
6	6MZ	L5	3966	6,27	18,25,26	0.82	1 (5%)	16,36,39	2.03	4 (25%)
6	A2M	L5	3557	6	18,25,26	1.93	5 (27%)	18,36,39	2.13	4 (22%)
52	PSU	S2	816	52	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
52	PSU	S2	682	52	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
6	PSU	L5	4435	6	18,21,22	1.35	3 (16%)	22,30,33	1.84	4 (18%)
52	A2M	S2	159	52	18,25,26	1.96	5 (27%)	18,36,39	2.09	5 (27%)
6	PSU	L5	4749	6	18,21,22	1.39	3 (16%)	22,30,33	1.84	4 (18%)
52	OMG	S2	602	52	18,26,27	1.96	2 (11%)	19,38,41	1.66	5 (26%)
6	PSU	L5	1721	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	5 (22%)
52	OMU	S2	1443	52,89	19,22,23	0.99	2 (10%)	26,31,34	1.74	4 (15%)
6	OMU	L5	3973	6	19,22,23	1.00	2 (10%)	26,31,34	1.83	6 (23%)
52	OMU	S2	429	52	19,22,23	1.02	2 (10%)	26,31,34	1.79	5 (19%)
6	OMG	L5	1580	6	18,26,27	1.98	2 (11%)	19,38,41	1.67	4 (21%)
52	PSU	S2	823	52	18,21,22	1.40	3 (16%)	22,30,33	1.80	4 (18%)
6	OMC	L5	3573	6	19,22,23	1.13	2 (10%)	26,31,34	0.89	2 (7%)
6	OMC	L5	3619	6,22	19,22,23	1.14	2 (10%)	26,31,34	0.93	1 (3%)
83	HY3	Si	62	83	6,8,9	1.32	1 (16%)	5,10,12	1.43	1 (20%)
6	A2M	L5	2244	6	18,25,26	1.95	5 (27%)	18,36,39	2.20	5 (27%)
6	OMG	L5	3524	6	18,26,27	1.97	2 (11%)	19,38,41	1.67	5 (26%)
52	PSU	S2	218	52	18,21,22	1.38	3 (16%)	22,30,33	1.81	4 (18%)
52	OMU	S2	355	71,52	19,22,23	0.98	2 (10%)	26,31,34	1.83	5 (19%)
52	PSU	S2	1175	52	18,21,22	1.36	3 (16%)	22,30,33	1.84	5 (22%)
52	A2M	S2	1384	52	18,25,26	2.01	5 (27%)	18,36,39	2.18	5 (27%)
52	PSU	S2	1046	52	18,21,22	1.35	3 (16%)	22,30,33	1.88	4 (18%)
6	PSU	L5	1801	6,17	18,21,22	1.35	3 (16%)	22,30,33	1.83	3 (13%)
52	PSU	S2	867	52	18,21,22	1.44	3 (16%)	22,30,33	1.81	4 (18%)
52	OMG	S2	510	52,89	18,26,27	1.96	2 (11%)	19,38,41	1.69	5 (26%)
6	OMG	L5	1477	6,11	18,26,27	1.97	2 (11%)	19,38,41	1.69	4 (21%)
6	PSU	L5	4099	6	18,21,22	1.35	3 (16%)	22,30,33	1.90	5 (22%)
6	PSU	L5	4267	6,89	18,21,22	1.33	3 (16%)	22,30,33	1.93	4 (18%)
8	PSU	L8	55	8	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
6	A2M	L5	2630	6	18,25,26	1.97	5 (27%)	18,36,39	2.34	5 (27%)
6	OMC	L5	3540	6	19,22,23	1.10	2 (10%)	26,31,34	0.89	2 (7%)
6	PSU	L5	4374	6	18,21,22	1.36	3 (16%)	22,30,33	1.82	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	L5	1638	6,90,34	18,21,22	1.34	3 (16%)	22,30,33	1.87	5 (22%)
6	OMG	L5	1260	6,38	18,26,27	2.00	2 (11%)	19,38,41	1.73	5 (26%)
52	OMU	S2	628	52	19,22,23	1.01	2 (10%)	26,31,34	1.82	6 (23%)
6	PSU	L5	4298	6	18,21,22	1.34	3 (16%)	22,30,33	1.83	4 (18%)
6	PSU	L5	4045	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	4 (18%)
6	PSU	L5	3466	6	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
6	PSU	L5	4166	6	18,21,22	1.38	3 (16%)	22,30,33	1.79	4 (18%)
6	PSU	L5	1731	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	4 (18%)
6	PSU	L5	3502	6	18,21,22	1.39	3 (16%)	22,30,33	1.83	4 (18%)
52	MA6	S2	1851	52	19,26,27	0.94	1 (5%)	18,38,41	1.71	6 (33%)
6	PSU	L5	1491	6	18,21,22	1.34	3 (16%)	22,30,33	1.85	4 (18%)
52	PSU	S2	119	52	18,21,22	1.41	3 (16%)	22,30,33	1.78	4 (18%)
6	5MC	L5	3514	6,89	18,22,23	1.27	3 (16%)	26,32,35	1.26	4 (15%)
6	PSU	L5	4711	6	18,21,22	1.35	3 (16%)	22,30,33	1.82	5 (22%)
6	PSU	L5	4107	6	18,21,22	1.33	3 (16%)	22,30,33	1.79	3 (13%)
52	PSU	S2	610	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	4 (18%)
6	A2M	L5	398	6	18,25,26	1.95	5 (27%)	18,36,39	2.15	5 (27%)
6	1MA	L5	1266	6,89	16,25,26	2.54	3 (18%)	18,37,40	2.27	3 (16%)
6	OMG	L5	3359	6	18,26,27	1.97	2 (11%)	19,38,41	1.69	5 (26%)
6	A2M	L5	1479	6	18,25,26	1.89	5 (27%)	18,36,39	2.22	4 (22%)
6	A2M	L5	3517	6	18,25,26	1.79	4 (22%)	18,36,39	2.28	5 (27%)
6	OMG	L5	3631	6	18,26,27	2.01	2 (11%)	19,38,41	1.70	5 (26%)
52	OMG	S2	684	52	18,26,27	1.96	2 (11%)	19,38,41	1.74	5 (26%)
52	PSU	S2	109	52	18,21,22	1.42	3 (16%)	22,30,33	1.80	5 (22%)
52	PSU	S2	1693	52	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
52	PSU	S2	210	52	18,21,22	1.45	3 (16%)	22,30,33	1.84	4 (18%)
52	7MG	S2	1640	52	22,26,27	1.22	2 (9%)	29,39,42	2.14	9 (31%)
6	OMU	L5	4244	6	19,22,23	1.00	2 (10%)	26,31,34	1.83	5 (19%)
6	PSU	L5	3500	6	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
46	M3L	Lp	98	46	10,11,12	0.51	0	9,14,16	0.47	0
6	OMG	L5	2267	6	18,26,27	1.98	2 (11%)	19,38,41	1.66	4 (21%)
6	OMU	L5	3657	6	19,22,23	1.01	2 (10%)	26,31,34	1.82	5 (19%)
52	A2M	S2	99	52,89	18,25,26	1.98	5 (27%)	18,36,39	2.12	5 (27%)
6	OMG	L5	4116	6	18,26,27	1.97	2 (11%)	19,38,41	1.68	5 (26%)
52	PSU	S2	687	67,52	18,21,22	1.41	3 (16%)	22,30,33	1.84	5 (22%)

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	815	52	18,21,22	1.38	3 (16%)	22,30,33	1.83	4 (18%)
6	PSU	L5	3652	6,89	18,21,22	1.31	3 (16%)	22,30,33	1.86	4 (18%)
52	PSU	S2	407	52	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
6	OMG	L5	3974	6	18,26,27	1.98	2 (11%)	19,38,41	1.70	4 (21%)
6	OMG	L5	4138	6	18,26,27	1.98	2 (11%)	19,38,41	1.70	5 (26%)
6	PSU	L5	1720	6	18,21,22	1.36	3 (16%)	22,30,33	1.82	5 (22%)
52	PSU	S2	1178	52	18,21,22	1.39	3 (16%)	22,30,33	1.80	4 (18%)
6	A2M	L5	4317	6	18,25,26	1.96	5 (27%)	18,36,39	2.11	4 (22%)
6	OMC	L5	2704	6	19,22,23	1.14	2 (10%)	26,31,34	0.86	0
52	OMU	S2	1327	52,89	19,22,23	1.00	2 (10%)	26,31,34	1.79	5 (19%)
6	OMG	L5	4369	6	18,26,27	1.98	2 (11%)	19,38,41	1.68	4 (21%)
6	PSU	L5	4740	6,10	18,21,22	1.38	3 (16%)	22,30,33	1.78	3 (13%)
6	PSU	L5	3494	6	18,21,22	1.39	3 (16%)	22,30,33	1.78	5 (22%)
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%)
6	A2M	L5	1270	6	18,25,26	1.89	5 (27%)	18,36,39	2.16	5 (27%)
52	PSU	S2	1446	52	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
52	PSU	S2	36	52	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
52	PSU	S2	1245	52	18,21,22	1.36	3 (16%)	22,30,33	1.85	4 (18%)
6	OMG	L5	4240	6	18,26,27	1.99	2 (11%)	19,38,41	1.69	5 (26%)
52	PSU	S2	967	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	4 (18%)
52	4AC	S2	1338	52	21,24,25	1.12	2 (9%)	29,34,37	1.21	3 (10%)
6	OMC	L5	3433	6,90	19,22,23	1.16	2 (10%)	26,31,34	0.92	1 (3%)
6	PSU	L5	4278	6	18,21,22	1.38	3 (16%)	22,30,33	1.79	4 (18%)
6	OMC	L5	2265	6,89	19,22,23	1.12	2 (10%)	26,31,34	0.90	2 (7%)
52	A2M	S2	577	52	18,25,26	1.98	5 (27%)	18,36,39	2.25	6 (33%)
52	PSU	S2	1626	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	5 (22%)
6	OMC	L5	1820	6,89	19,22,23	1.15	2 (10%)	26,31,34	0.89	0
52	OMU	S2	172	52	19,22,23	0.99	2 (10%)	26,31,34	1.85	7 (26%)
52	PSU	S2	105	52	18,21,22	1.39	3 (16%)	22,30,33	1.81	4 (18%)
6	OMG	L5	2207	6	18,26,27	2.00	2 (11%)	19,38,41	1.67	4 (21%)
6	PSU	L5	3369	6,89,90	18,21,22	1.29	3 (16%)	22,30,33	1.87	4 (18%)
6	OMU	L5	4052	6,24	19,22,23	1.00	2 (10%)	26,31,34	1.74	4 (15%)
6	PSU	L5	4382	6,37	18,21,22	1.42	4 (22%)	22,30,33	2.01	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMC	L5	3601	6	19,22,23	1.16	2 (10%)	26,31,34	0.89	0
6	PSU	L5	1632	6	18,21,22	1.41	3 (16%)	22,30,33	1.74	4 (18%)
6	PSU	L5	1683	6,90	18,21,22	1.36	3 (16%)	22,30,33	1.82	4 (18%)
6	PSU	L5	3462	6	18,21,22	1.38	3 (16%)	22,30,33	1.80	5 (22%)
52	PSU	S2	1057	52	18,21,22	1.37	3 (16%)	22,30,33	1.84	5 (22%)
6	A2M	L5	1489	6,89	18,25,26	1.91	5 (27%)	18,36,39	2.10	3 (16%)
52	PSU	S2	1047	52	18,21,22	1.39	3 (16%)	22,30,33	1.79	4 (18%)
6	PSU	L5	2475	6	18,21,22	1.37	3 (16%)	22,30,33	1.82	5 (22%)
6	PSU	L5	3447	6	18,21,22	1.36	3 (16%)	22,30,33	1.81	4 (18%)
6	OMU	L5	2680	6	19,22,23	0.99	2 (10%)	26,31,34	1.82	6 (23%)
6	PSU	L5	2351	6	18,21,22	1.34	3 (16%)	22,30,33	1.86	4 (18%)
6	A2M	L5	3450	6	18,25,26	1.90	5 (27%)	18,36,39	2.15	4 (22%)
78	SAC	Sd	2	78	7,8,9	0.52	0	8,9,11	0.90	1 (12%)
60	SAC	SL	2	60	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
6	PSU	L5	3496	6	18,21,22	1.37	3 (16%)	22,30,33	1.84	5 (22%)
6	PSU	L5	4149	6	18,21,22	1.33	3 (16%)	22,30,33	1.93	5 (22%)
6	A2M	L5	3599	6	18,25,26	1.92	5 (27%)	18,36,39	2.13	5 (27%)
52	OMG	S2	1329	52	18,26,27	1.95	2 (11%)	19,38,41	1.68	5 (26%)
52	A2M	S2	485	52	18,25,26	1.91	5 (27%)	18,36,39	2.22	4 (22%)
35	MLZ	Le	5	35	8,9,10	0.47	0	4,9,11	0.13	0
52	OMC	S2	463	52	19,22,23	1.16	2 (10%)	26,31,34	0.90	0
6	PSU	L5	3490	6	18,21,22	1.35	3 (16%)	22,30,33	1.81	4 (18%)
6	OMG	L5	2719	6	18,26,27	1.97	2 (11%)	19,38,41	1.68	5 (26%)
6	OMC	L5	2208	6,89	19,22,23	1.13	2 (10%)	26,31,34	0.91	1 (3%)
6	PSU	L5	4322	6	18,21,22	1.39	3 (16%)	22,30,33	1.79	5 (22%)
52	OMG	S2	868	52	18,26,27	1.95	2 (11%)	19,38,41	1.67	4 (21%)
52	PSU	S2	1233	52	18,21,22	1.37	3 (16%)	22,30,33	1.81	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
6	A2M	L5	4269	6,89	-	0/5/27/28	0/3/3/3
52	PSU	S2	652	52	-	0/7/25/26	0/2/2/2
6	OMC	L5	1284	6	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMU	L5	2258	6	-	0/9/27/28	0/2/2/2
6	OMU	L5	4366	6,29	-	0/9/27/28	0/2/2/2
6	A2M	L5	3456	6	-	0/5/27/28	0/3/3/3
52	6MZ	S2	1833	52,89	-	1/5/27/28	0/3/3/3
52	PSU	S2	1348	52	-	0/7/25/26	0/2/2/2
6	A2M	L5	1810	6,89	-	0/5/27/28	0/3/3/3
6	PSU	L5	4325	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	2667	6	-	0/9/27/28	0/2/2/2
52	OMC	S2	1392	52	-	2/9/27/28	0/2/2/2
52	PSU	S2	93	52	-	0/7/25/26	0/2/2/2
52	A2M	S2	1679	52	-	0/5/27/28	0/3/3/3
6	PSU	L5	4039	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1239	52	-	0/7/25/26	0/2/2/2
49	SAC	Ls	2	49	-	0/7/8/10	-
6	5MC	L5	4193	6	-	3/7/25/26	0/2/2/2
52	A2M	S2	166	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	3427	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	2206	6,89	-	0/5/27/28	0/3/3/3
6	OMG	L5	3942	6	-	0/5/27/28	0/3/3/3
52	PSU	S2	650	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4419	6	-	0/7/25/26	0/2/2/2
52	MA6	S2	1852	52	-	2/7/29/30	0/3/3/3
81	AME	Sg	1	81	-	2/9/10/12	-
52	PSU	S2	864	82,52	-	0/7/25/26	0/2/2/2
52	A2M	S2	513	52	-	0/5/27/28	0/3/3/3
52	OMG	S2	1448	52	-	3/5/27/28	0/3/3/3
6	PSU	L5	4058	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1005	52	-	1/7/25/26	0/2/2/2
6	A2M	L5	2658	6,89	-	1/5/27/28	0/3/3/3
10	HIC	LE	245	10	-	1/5/6/8	0/1/1/1
6	PSU	L5	4188	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1368	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	802	52	-	3/7/25/26	0/2/2/2
6	PSU	L5	1799	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	34	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	4245	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	4246	6	-	1/7/25/26	0/2/2/2
52	OMC	S2	1704	52,89	-	0/9/27/28	0/2/2/2
6	OMG	L5	4383	6,90	-	0/5/27/28	0/3/3/3
52	PSU	S2	573	52,84	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	S2	1082	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4042	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	4364	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	4203	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1537	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	669	52,89	-	2/5/27/28	0/3/3/3
6	A2M	L5	3562	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	3554	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3371	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	469	52	-	0/5/27/28	0/3/3/3
52	OMC	S2	174	52	-	0/9/27/28	0/2/2/2
6	OMC	L5	2194	6	-	1/9/27/28	0/2/2/2
52	OMG	S2	1491	52,89	-	1/5/27/28	0/3/3/3
6	OMC	L5	2647	6	-	0/9/27/28	0/2/2/2
47	MLZ	Lq	53	47	-	0/7/8/10	-
6	PSU	L5	3583	6	-	0/7/25/26	0/2/2/2
79	NMM	Se	67	79	-	3/9/11/13	-
6	A2M	L5	400	6	-	0/5/27/28	0/3/3/3
6	OMG	L5	3676	6	-	1/5/27/28	0/3/3/3
6	UR3	L5	4276	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	437	52	-	0/5/27/28	0/3/3/3
11	AYA	LF	2	11	-	2/4/6/8	-
6	PSU	L5	4169	6	-	0/7/25/26	0/2/2/2
8	OMG	L8	75	8	-	0/5/27/28	0/3/3/3
6	PSU	L5	4177	6	-	0/7/25/26	0/2/2/2
52	OMC	S2	518	52	-	2/9/27/28	0/2/2/2
6	PSU	L5	3585	6,89	-	0/7/25/26	0/2/2/2
52	4AC	S2	1843	52,86	-	2/11/29/30	0/2/2/2
6	PSU	L5	3576	6	-	1/7/25/26	0/2/2/2
52	OMU	S2	1805	52	-	0/9/27/28	0/2/2/2
52	PSU	S2	1644	52,89	-	0/7/25/26	0/2/2/2
52	OMU	S2	116	52	-	0/9/27/28	0/2/2/2
52	OMU	S2	121	52	-	0/9/27/28	0/2/2/2
6	PSU	L5	4217	6,16	-	0/7/25/26	0/2/2/2
52	A2M	S2	27	52	-	0/5/27/28	0/3/3/3
6	OMC	L5	4202	6	-	0/9/27/28	0/2/2/2
8	PSU	L8	69	8	-	0/7/25/26	0/2/2/2
52	A2M	S2	591	52	-	0/5/27/28	0/3/3/3
52	A2M	S2	1032	52	-	0/5/27/28	0/3/3/3
6	PSU	L5	1718	6,12	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMG	L5	3476	6	-	0/5/27/28	0/3/3/3
52	OMU	S2	1289	52,55	-	0/9/27/28	0/2/2/2
6	6MZ	L5	3966	6,27	-	0/5/27/28	0/3/3/3
6	A2M	L5	3557	6	-	0/5/27/28	0/3/3/3
52	PSU	S2	816	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	682	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4435	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	159	52	-	0/5/27/28	0/3/3/3
6	PSU	L5	4749	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	602	52	-	0/5/27/28	0/3/3/3
6	PSU	L5	1721	6	-	0/7/25/26	0/2/2/2
52	OMU	S2	1443	52,89	-	0/9/27/28	0/2/2/2
6	OMU	L5	3973	6	-	0/9/27/28	0/2/2/2
52	OMU	S2	429	52	-	4/9/27/28	0/2/2/2
6	OMG	L5	1580	6	-	1/5/27/28	0/3/3/3
52	PSU	S2	823	52	-	2/7/25/26	0/2/2/2
6	OMC	L5	3573	6	-	0/9/27/28	0/2/2/2
6	OMC	L5	3619	6,22	-	2/9/27/28	0/2/2/2
83	HY3	Si	62	83	-	1/1/12/14	0/1/1/1
6	A2M	L5	2244	6	-	1/5/27/28	0/3/3/3
6	OMG	L5	3524	6	-	0/5/27/28	0/3/3/3
52	PSU	S2	218	52	-	0/7/25/26	0/2/2/2
52	OMU	S2	355	71,52	-	0/9/27/28	0/2/2/2
52	PSU	S2	1175	52	-	0/7/25/26	0/2/2/2
52	A2M	S2	1384	52	-	0/5/27/28	0/3/3/3
52	PSU	S2	1046	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	1801	6,17	-	0/7/25/26	0/2/2/2
52	PSU	S2	867	52	-	0/7/25/26	0/2/2/2
52	OMG	S2	510	52,89	-	2/5/27/28	0/3/3/3
6	OMG	L5	1477	6,11	-	3/5/27/28	0/3/3/3
6	PSU	L5	4099	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4267	6,89	-	0/7/25/26	0/2/2/2
8	PSU	L8	55	8	-	0/7/25/26	0/2/2/2
6	A2M	L5	2630	6	-	0/5/27/28	0/3/3/3
6	OMC	L5	3540	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	4374	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1638	6,90,34	-	0/7/25/26	0/2/2/2
6	OMG	L5	1260	6,38	-	0/5/27/28	0/3/3/3
52	OMU	S2	628	52	-	6/9/27/28	0/2/2/2
6	PSU	L5	4298	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4045	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	L5	3466	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4166	6	-	2/7/25/26	0/2/2/2
6	PSU	L5	1731	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3502	6	-	0/7/25/26	0/2/2/2
52	MA6	S2	1851	52	-	2/7/29/30	0/3/3/3
6	PSU	L5	1491	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	119	52	-	0/7/25/26	0/2/2/2
6	5MC	L5	3514	6,89	-	0/7/25/26	0/2/2/2
6	PSU	L5	4711	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4107	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	610	52	-	0/7/25/26	0/2/2/2
6	A2M	L5	398	6	-	0/5/27/28	0/3/3/3
6	1MA	L5	1266	6,89	-	0/3/25/26	0/3/3/3
6	OMG	L5	3359	6	-	0/5/27/28	0/3/3/3
6	A2M	L5	1479	6	-	0/5/27/28	0/3/3/3
6	A2M	L5	3517	6	-	2/5/27/28	0/3/3/3
6	OMG	L5	3631	6	-	0/5/27/28	0/3/3/3
52	OMG	S2	684	52	-	2/5/27/28	0/3/3/3
52	PSU	S2	109	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1693	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	210	52	-	0/7/25/26	0/2/2/2
52	7MG	S2	1640	52	-	0/7/37/38	0/3/3/3
6	OMU	L5	4244	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	3500	6	-	0/7/25/26	0/2/2/2
46	M3L	Lp	98	46	-	0/9/10/12	-
6	OMG	L5	2267	6	-	0/5/27/28	0/3/3/3
6	OMU	L5	3657	6	-	0/9/27/28	0/2/2/2
52	A2M	S2	99	52,89	-	1/5/27/28	0/3/3/3
6	OMG	L5	4116	6	-	0/5/27/28	0/3/3/3
52	PSU	S2	687	67,52	-	0/7/25/26	0/2/2/2
6	A2M	L5	4336	6	-	2/5/27/28	0/3/3/3
52	PSU	S2	815	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	3652	6,89	-	0/7/25/26	0/2/2/2
52	PSU	S2	407	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	3974	6	-	0/5/27/28	0/3/3/3
6	OMG	L5	4138	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	1720	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1178	52	-	0/7/25/26	0/2/2/2
6	A2M	L5	4317	6	-	0/5/27/28	0/3/3/3
6	OMC	L5	2704	6	-	0/9/27/28	0/2/2/2
52	OMU	S2	1327	52,89	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMG	L5	4369	6	-	2/5/27/28	0/3/3/3
6	PSU	L5	4740	6,10	-	0/7/25/26	0/2/2/2
6	PSU	L5	3494	6	-	2/7/25/26	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
6	A2M	L5	1270	6	-	1/5/27/28	0/3/3/3
52	PSU	S2	1446	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	36	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1245	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	4240	6	-	1/5/27/28	0/3/3/3
52	PSU	S2	967	52	-	0/7/25/26	0/2/2/2
52	4AC	S2	1338	52	-	4/11/29/30	0/2/2/2
6	OMC	L5	3433	6,90	-	4/9/27/28	0/2/2/2
6	PSU	L5	4278	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	2265	6,89	-	2/9/27/28	0/2/2/2
52	A2M	S2	577	52	-	1/5/27/28	0/3/3/3
52	PSU	S2	1626	52	-	0/7/25/26	0/2/2/2
6	OMC	L5	1820	6,89	-	0/9/27/28	0/2/2/2
52	OMU	S2	172	52	-	0/9/27/28	0/2/2/2
52	PSU	S2	105	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	2207	6	-	0/5/27/28	0/3/3/3
6	PSU	L5	3369	6,89,90	-	0/7/25/26	0/2/2/2
6	OMU	L5	4052	6,24	-	0/9/27/28	0/2/2/2
6	PSU	L5	4382	6,37	-	2/7/25/26	0/2/2/2
6	OMC	L5	3601	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	1632	6	-	1/7/25/26	0/2/2/2
6	PSU	L5	1683	6,90	-	0/7/25/26	0/2/2/2
6	PSU	L5	3462	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1057	52	-	0/7/25/26	0/2/2/2
6	A2M	L5	1489	6,89	-	2/5/27/28	0/3/3/3
52	PSU	S2	1047	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	2475	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3447	6	-	0/7/25/26	0/2/2/2
6	OMU	L5	2680	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	2351	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	3450	6	-	0/5/27/28	0/3/3/3
78	SAC	Sd	2	78	-	0/7/8/10	-
60	SAC	SL	2	60	-	1/7/8/10	-
6	PSU	L5	3496	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4149	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A2M	L5	3599	6	-	0/5/27/28	0/3/3/3
52	OMG	S2	1329	52	-	0/5/27/28	0/3/3/3
52	A2M	S2	485	52	-	1/5/27/28	0/3/3/3
35	MLZ	Le	5	35	-	2/7/8/10	-
52	OMC	S2	463	52	-	0/9/27/28	0/2/2/2
6	PSU	L5	3490	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	2719	6	-	1/5/27/28	0/3/3/3
6	OMC	L5	2208	6,89	-	0/9/27/28	0/2/2/2
6	PSU	L5	4322	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	868	52	-	0/5/27/28	0/3/3/3
52	PSU	S2	1233	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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-C2	-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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	O1-C1-C2	-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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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'

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Mol	Chain	Res	Type	Atoms
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	O1-C1-C2-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'
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'

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Mol	Chain	Res	Type	Atoms
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
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'

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Mol	Chain	Res	Type	Atoms
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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	L7	203	7	26,34,34	0.90	1 (3%)	32,54,54	1.34	3 (9%)
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	-	-

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	L7	203	7	-	0/18/38/38	0/3/3/3
87	GTP	E	1001	1	-	6/18/38/38	0/3/3/3

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Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SER	F	101	2	-	0/2/4/6	-

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(°)	Ideal(°)
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:

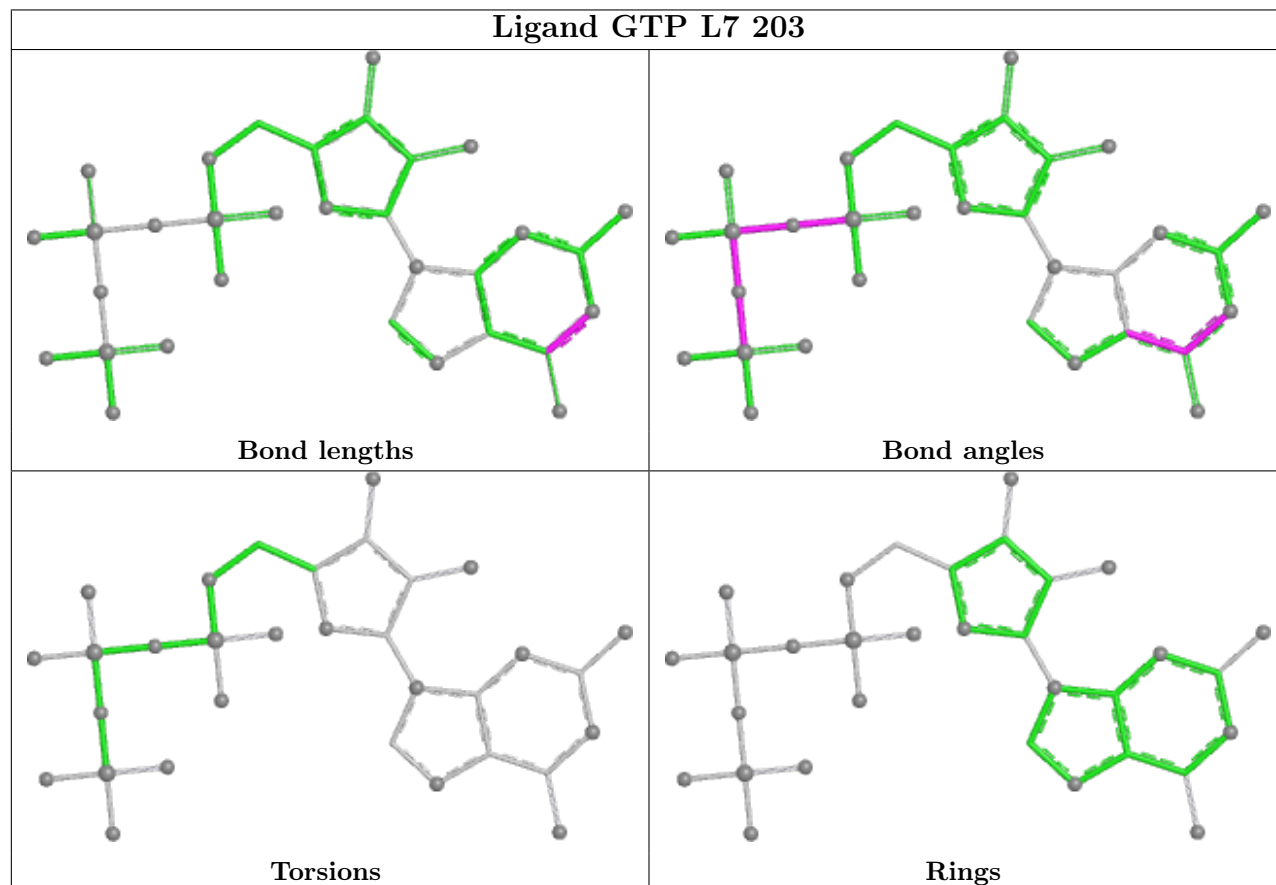
Mol	Chain	Res	Type	Atoms
87	E	1001	GTP	C5'-O5'-PA-O3A
87	E	1001	GTP	O4'-C4'-C5'-O5'
87	E	1001	GTP	C3'-C4'-C5'-O5'
87	E	1001	GTP	C5'-O5'-PA-O1A
87	E	1001	GTP	C5'-O5'-PA-O2A
87	E	1001	GTP	C4'-C5'-O5'-PA

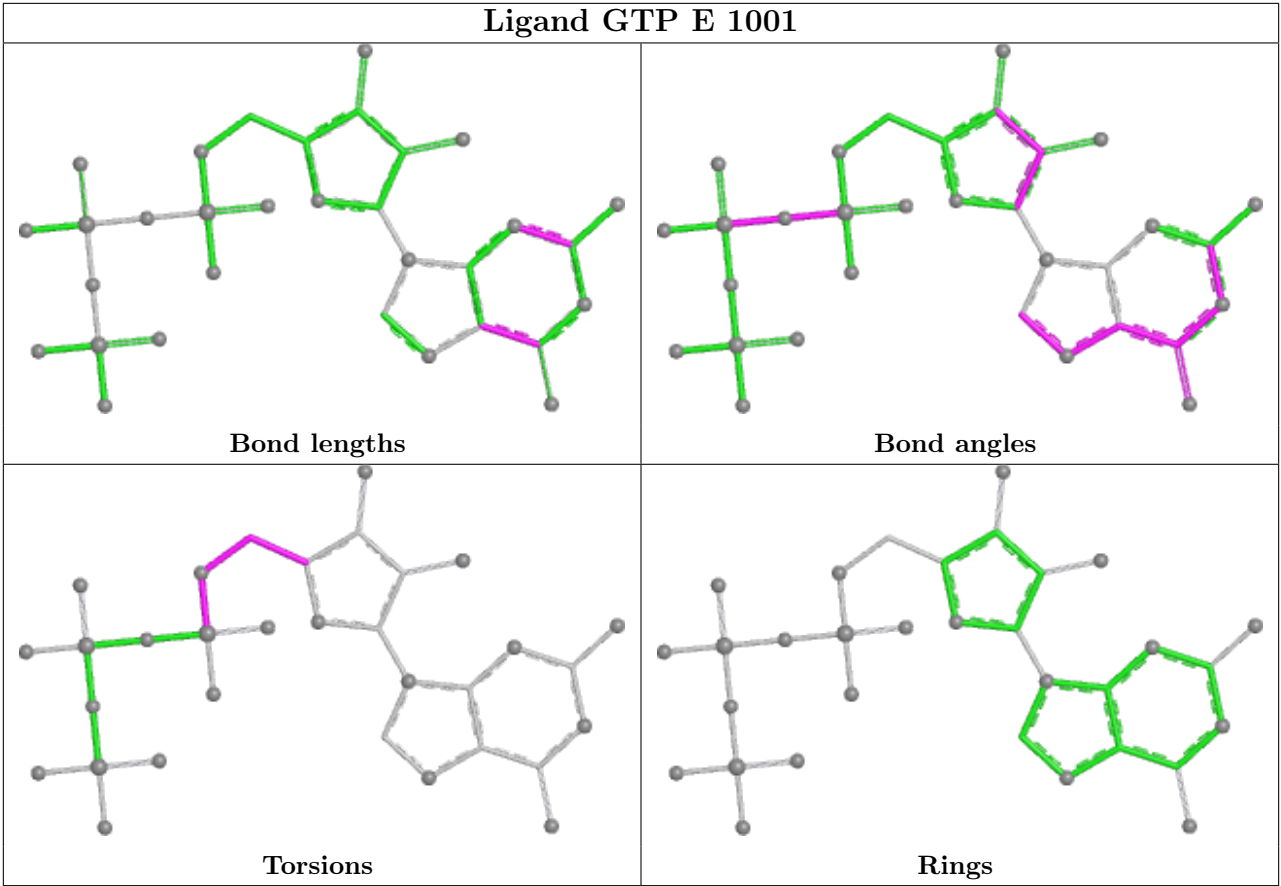
There are no ring outliers.

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 than 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.





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	N1	3.10

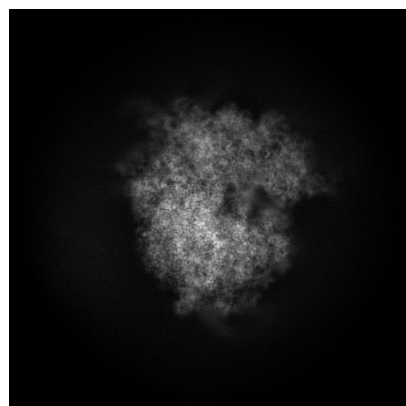
6 Map visualisation [i](#)

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.

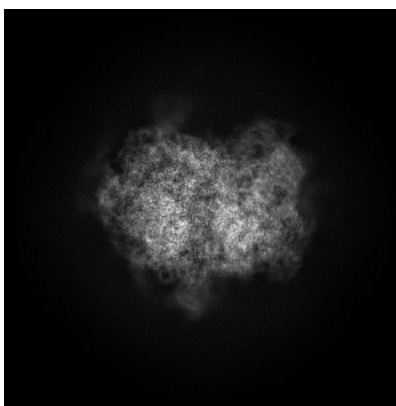
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

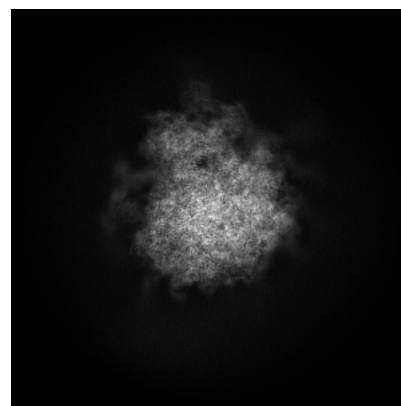
6.1.1 Primary map



X

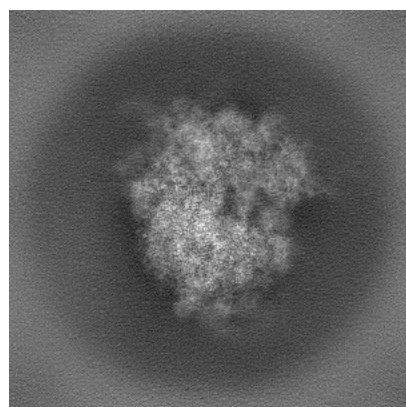


Y

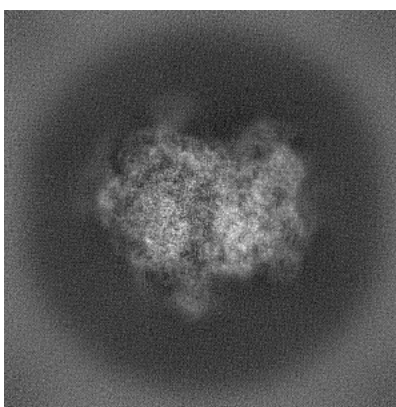


Z

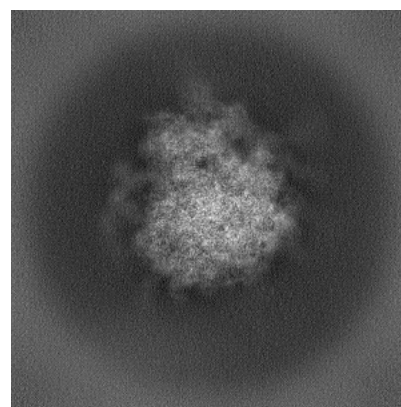
6.1.2 Raw map



X



Y

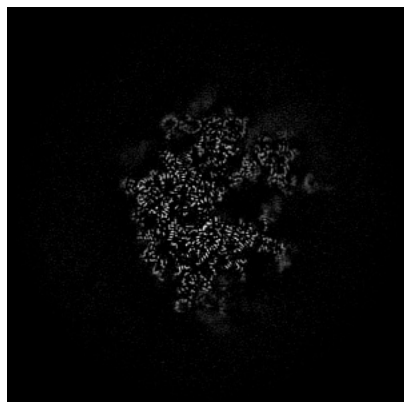


Z

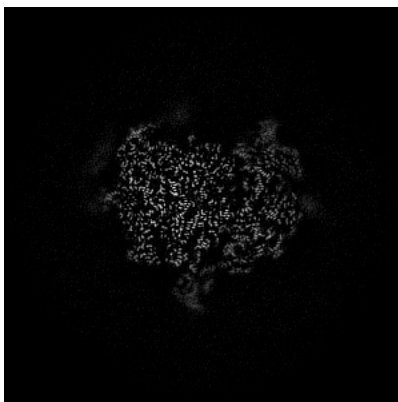
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

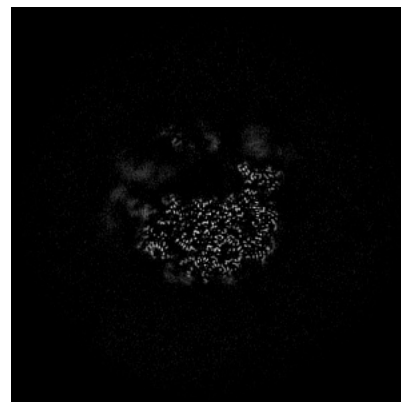
6.2.1 Primary map



X Index: 256

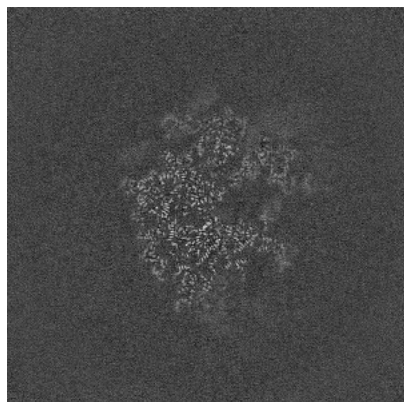


Y Index: 256

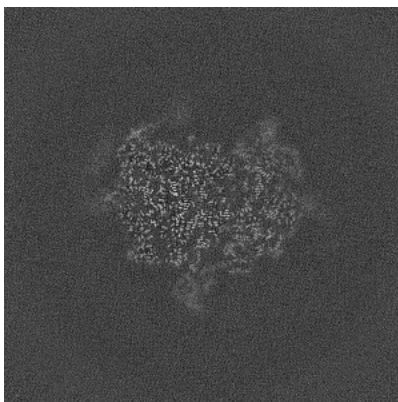


Z Index: 256

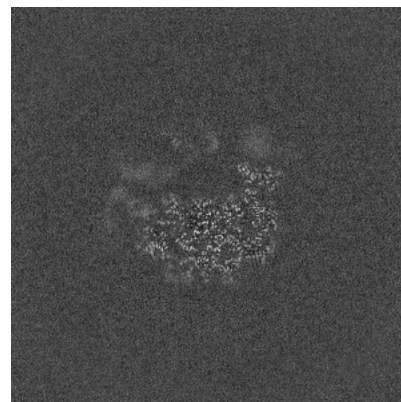
6.2.2 Raw map



X Index: 256



Y Index: 256

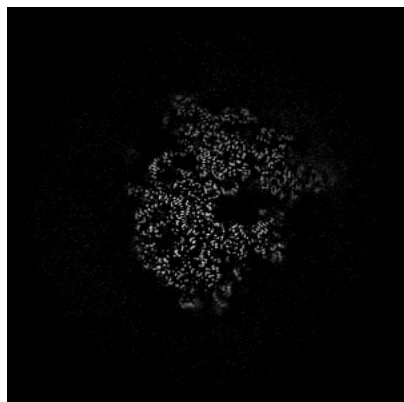


Z Index: 256

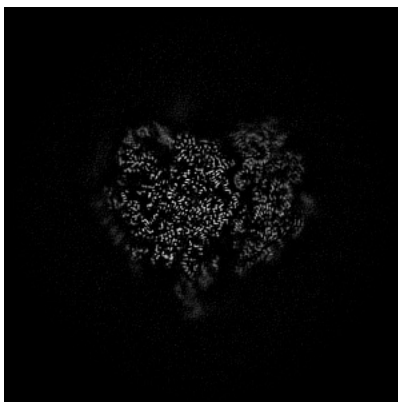
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

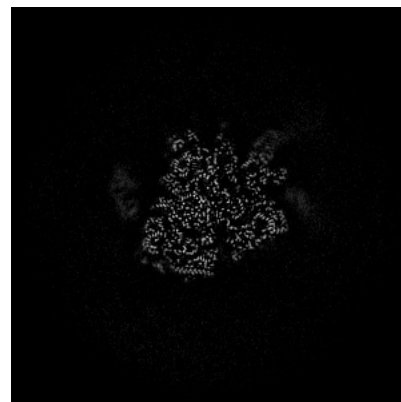
6.3.1 Primary map



X Index: 240

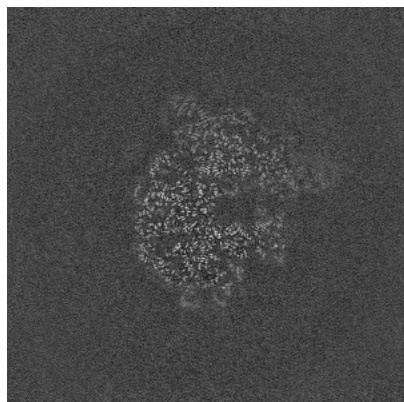


Y Index: 246

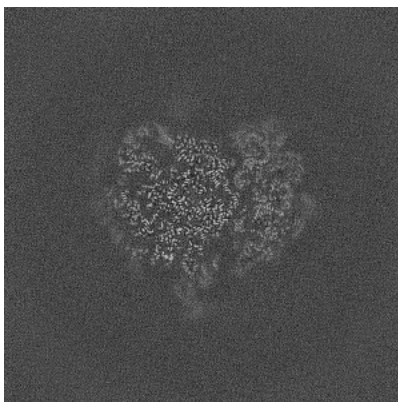


Z Index: 223

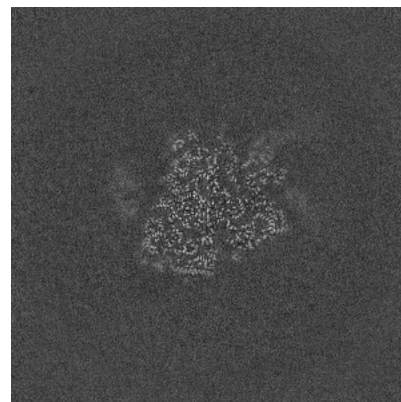
6.3.2 Raw map



X Index: 238



Y Index: 246



Z Index: 223

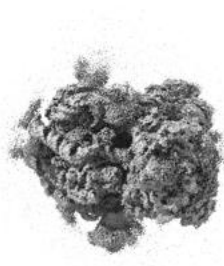
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



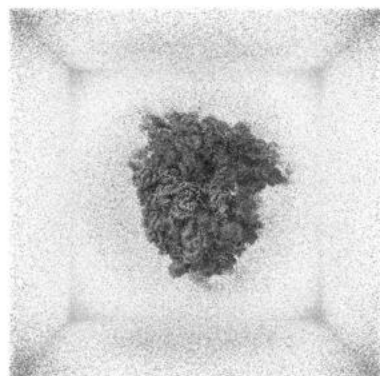
Y



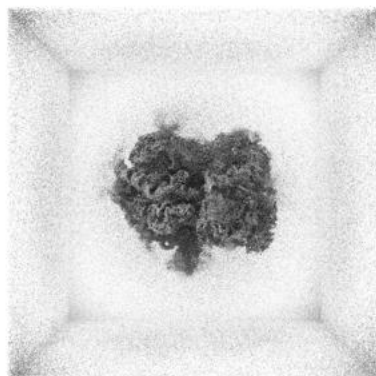
Z

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.

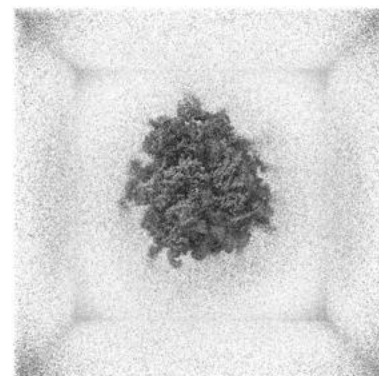
6.4.2 Raw map



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.

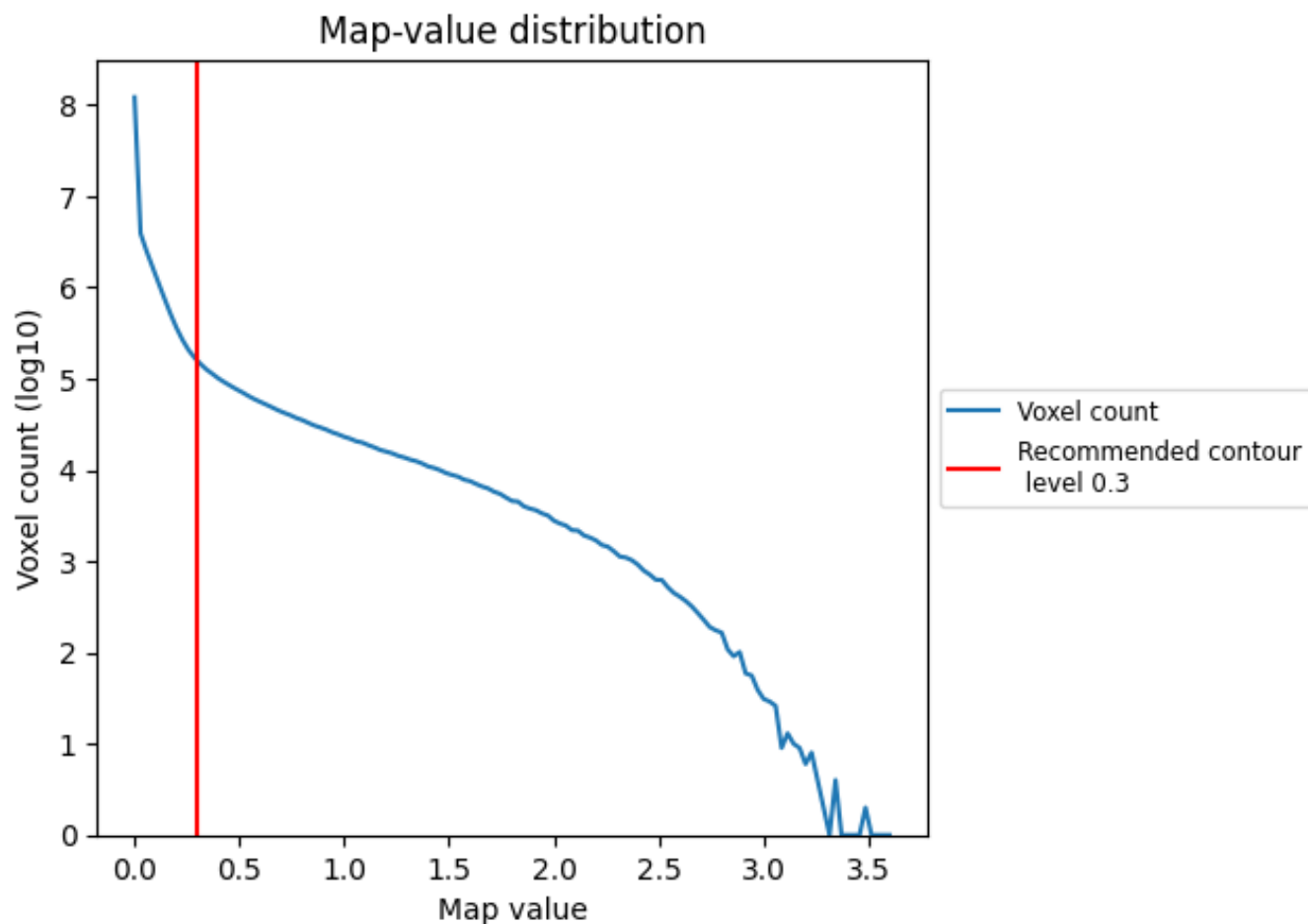
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

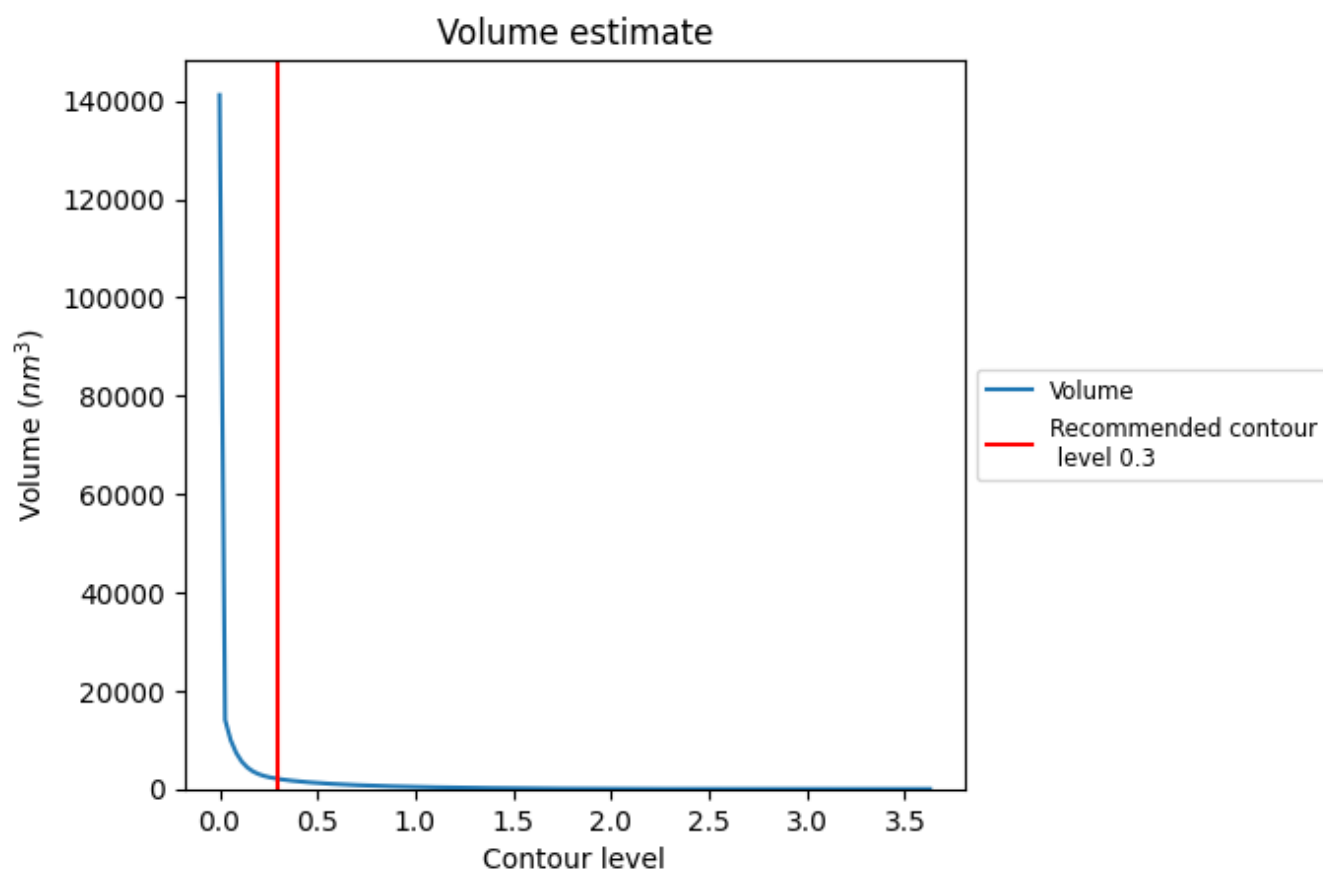
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

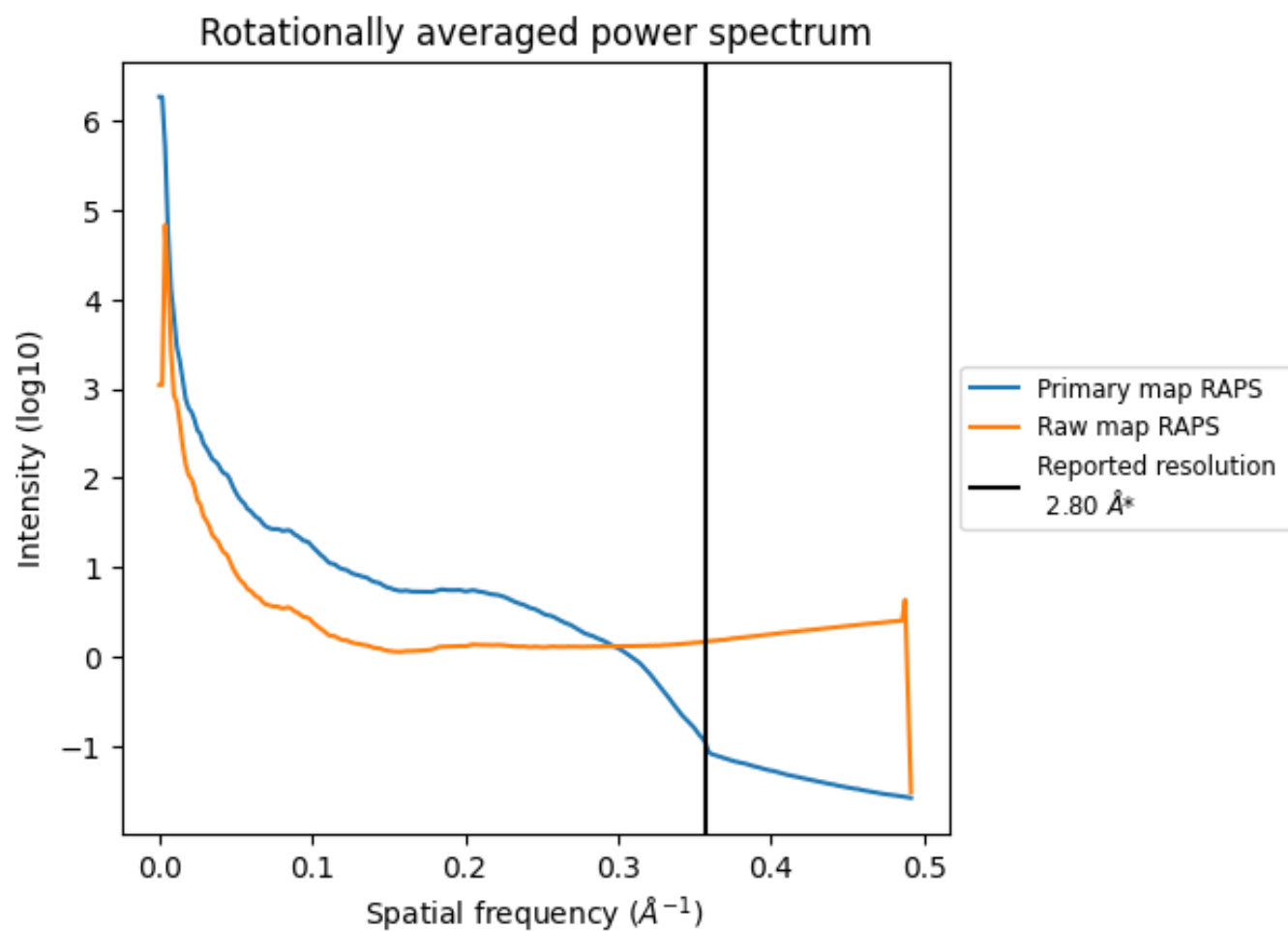
7.2 Volume estimate [i](#)



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 ⓘ

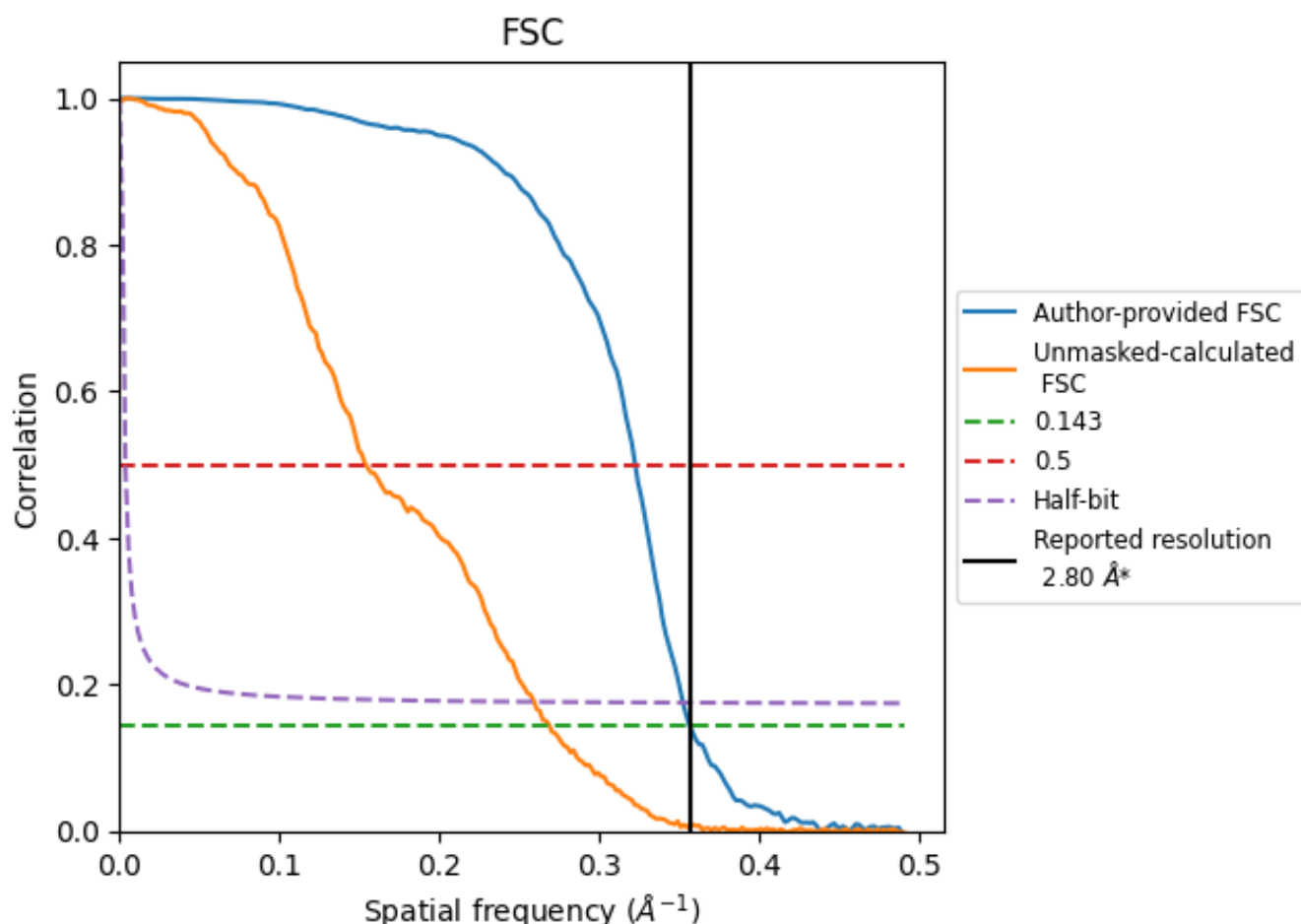


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

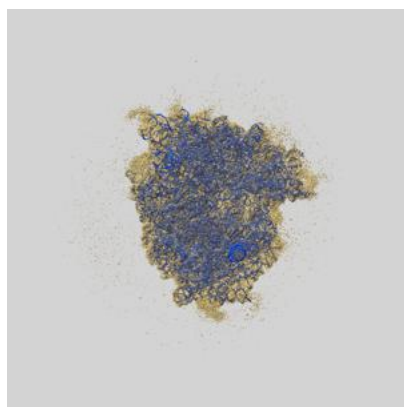
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.10	2.83
Unmasked-calculated*	3.72	6.49	3.85

*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 %

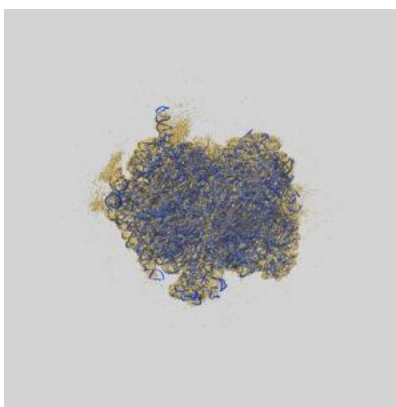
9 Map-model fit [i](#)

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.

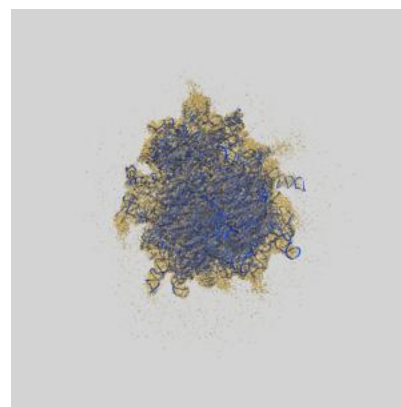
9.1 Map-model overlay [i](#)



X



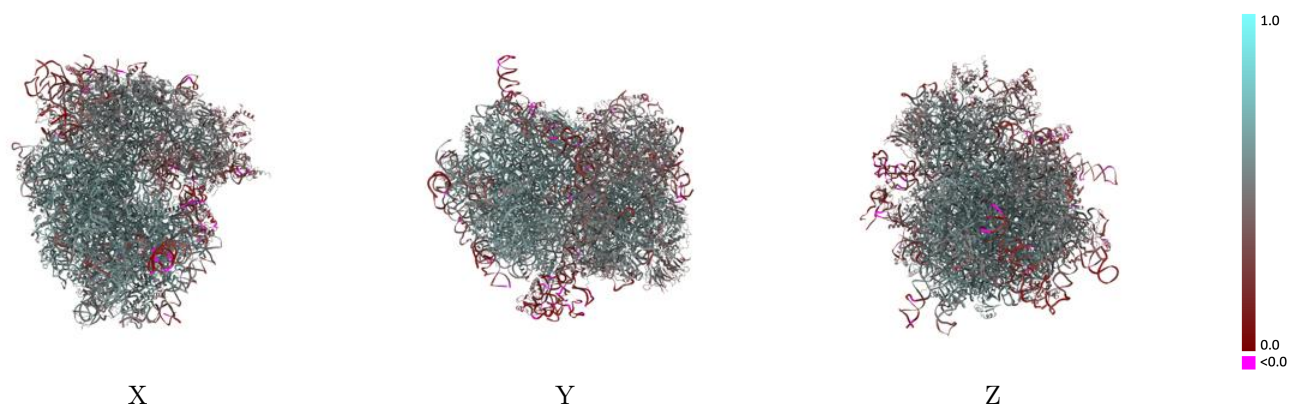
Y



Z

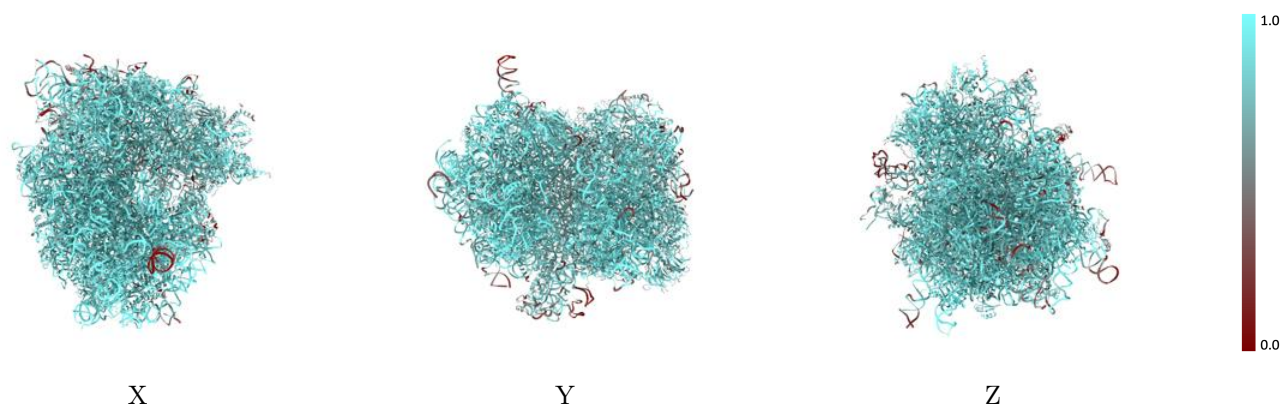
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



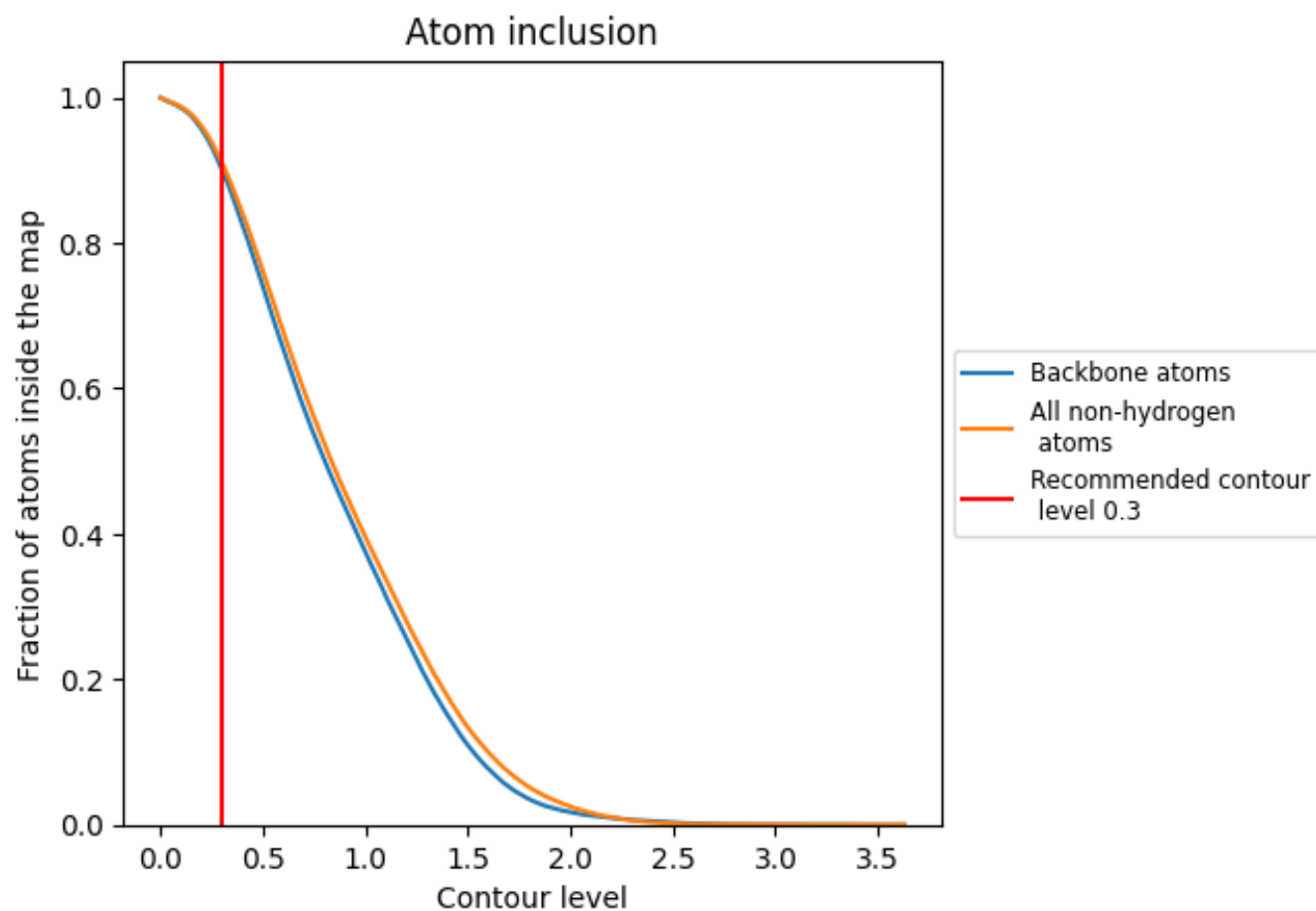
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 ⓘ





















































































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	 0.9103	 0.5140
B	 0.8174	 0.4050
E	 0.7651	 0.3700
F	 0.7453	 0.3280
I	 0.6336	 0.2040
L5	 0.9539	 0.5340
L7	 0.9965	 0.5910
L8	 0.9792	 0.5740
LD	 0.9435	 0.5950
LE	 0.9460	 0.5830
LF	 0.9483	 0.5850
LG	 0.9411	 0.5540
LH	 0.9137	 0.5460
LI	 0.9430	 0.5850
LJ	 0.8991	 0.5380
LK	 0.9235	 0.5660
LL	 0.9033	 0.5590
LM	 0.9107	 0.5300
LO	 0.9162	 0.5610
LP	 0.9345	 0.5650
LQ	 0.9698	 0.6080
LR	 0.9486	 0.5870
LS	 0.9218	 0.5770
LT	 0.9476	 0.5860
LU	 0.9153	 0.5480
LV	 0.9607	 0.5940
LW	 0.9200	 0.5650
LX	 0.9213	 0.5110
LY	 0.8999	 0.5750
LZ	 0.8160	 0.4910
La	 0.9319	 0.5610
Lb	 0.9314	 0.5730
Lc	 0.9432	 0.5590
Ld	 0.9628	 0.5940
Le	 0.8333	 0.4890























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Chain	Atom inclusion	Q-score
Lf	 0.8523	 0.5250
Lg	 0.9358	 0.5710
Lh	 0.9428	 0.5910
Li	 0.9518	 0.5940
Lj	 0.9276	 0.5670
Lk	 0.9254	 0.5620
Ll	 0.9246	 0.5570
Lm	 0.9673	 0.6070
Ln	 0.8761	 0.5360
Lo	 0.9368	 0.5810
Lp	 0.9306	 0.5710
Lq	 0.9189	 0.5790
Lr	 0.9274	 0.5760
Ls	 0.9538	 0.5850
Lt	 0.6190	 0.2220
Lx	 0.6986	 0.2950
S	 0.8891	 0.2700
S2	 0.9332	 0.4940
SB	 0.8232	 0.5070
SC	 0.8071	 0.4900
SD	 0.6818	 0.3590
SE	 0.7159	 0.4180
SF	 0.8978	 0.5410
SG	 0.8227	 0.4210
SH	 0.9050	 0.5370
SL	 0.8619	 0.5140
SM	 0.8598	 0.5110
SN	 0.8817	 0.5300
SO	 0.8302	 0.4860
SP	 0.8272	 0.4790
SQ	 0.8426	 0.4820
SR	 0.8173	 0.4060
SS	 0.7673	 0.4550
ST	 0.8377	 0.4760
SU	 0.8259	 0.4680
SV	 0.8494	 0.4690
SW	 0.7759	 0.4980
SX	 0.6610	 0.3040
SY	 0.8797	 0.5410
SZ	 0.8765	 0.5310
Sa	 0.7776	 0.4480
Sb	 0.8621	 0.5000

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Chain	Atom inclusion	Q-score
Sc	 0.8048	 0.4680
Sd	 0.8618	 0.4840
Se	 0.8726	 0.4940
Sf	 0.8163	 0.4630
Sg	 0.8674	 0.5210
Sh	 0.9119	 0.5560
Si	 0.8983	 0.5470
Sj	 0.8497	 0.4590
Sk	 0.8079	 0.4450
Sl	 0.9266	 0.5970