



Full wwPDB EM Validation Report ⓘ

Feb 3, 2025 – 08:04 pm GMT

PDB ID : 8QHU
EMDB ID : EMD-18419
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
LM32Cs1C1 snoRNA overexpression
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2023-09-10
Resolution : 2.72 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

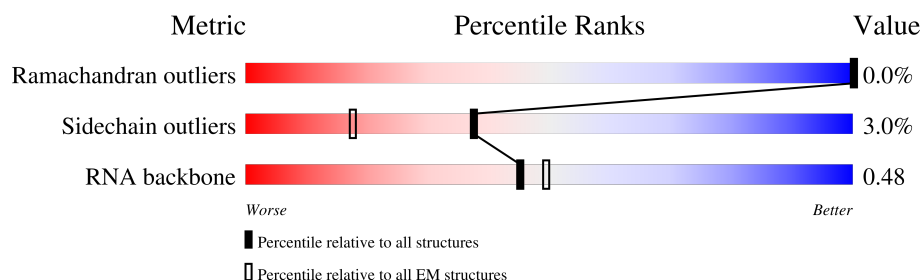
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.72 Å.

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



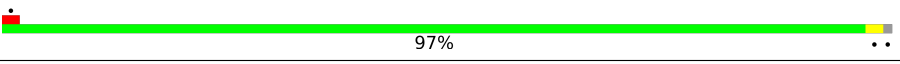

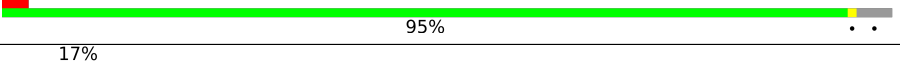


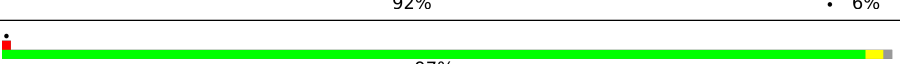
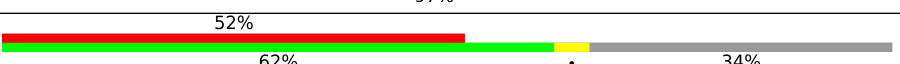
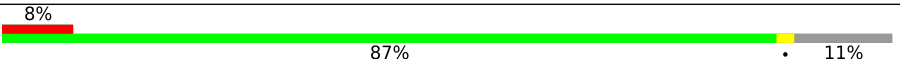
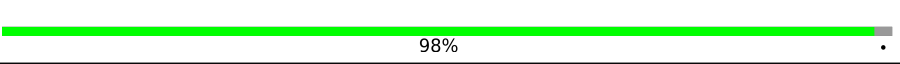
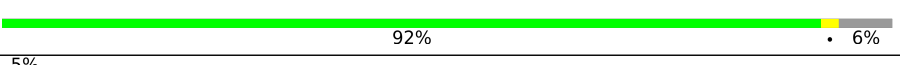
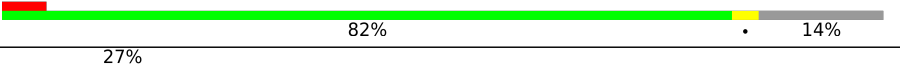
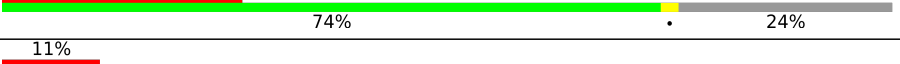

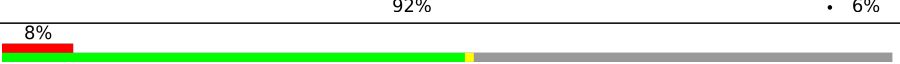
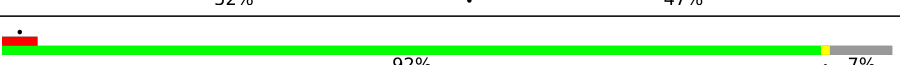


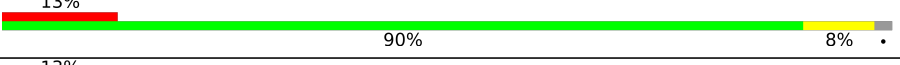


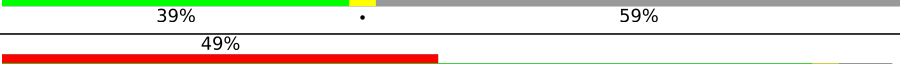
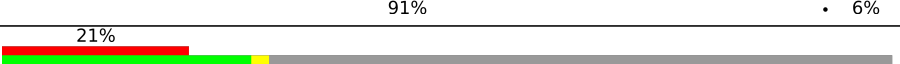



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	SB	246	<div> <div>8%</div> <div>81%</div> <div>15%</div> </div>
2	SC	219	<div> <div>11%</div> <div>94%</div> <div>•</div> </div>
3	SD	190	<div> <div>6%</div> <div>94%</div> <div>•</div> </div>
4	SE	273	<div> <div>6%</div> <div>94%</div> <div>• 5%</div> </div>
5	SF	265	<div> <div>6%</div> <div>81%</div> <div>• 17%</div> </div>
6	SG	249	<div> <div>12%</div> <div>89%</div> <div>• 7%</div> </div>
7	SH	190	<div> <div>•</div> <div>93%</div> <div>•</div> </div>
8	SI	200	<div> <div>13%</div> <div>98%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	SJ	130	
10	SK	220	
11	SL	149	
12	SM	116	
13	SN	168	
14	SO	144	
15	SP	143	
16	SQ	141	
17	SR	153	
18	SS	57	
19	ST	151	
20	SU	173	
21	SV	143	
22	SW	152	
23	SX	161	
24	SY	164	
25	SZ	137	
26	Sa	120	
27	Sb	112	
28	Sc	86	
29	Sd	87	
30	Se	66	
31	Sf	152	
32	Sg	312	
33	Sh	235	


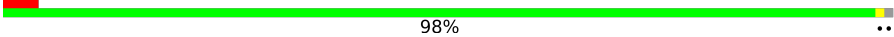
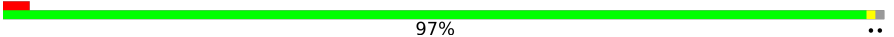
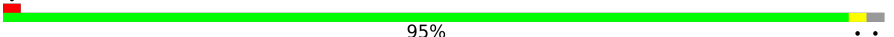






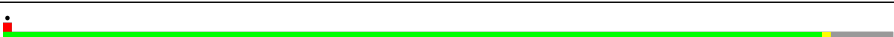


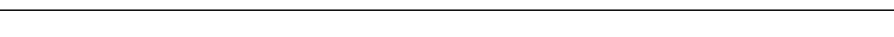
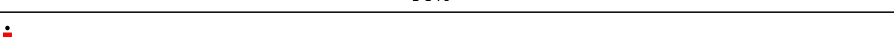
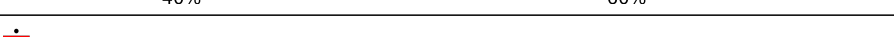
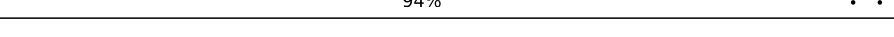
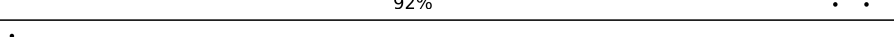

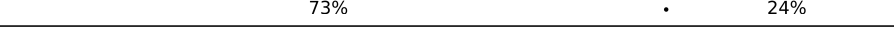



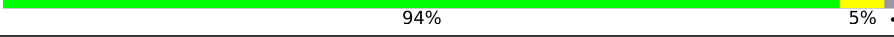

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Mol	Chain	Length	Quality of chain
34	S4	76	
35	S1	2204	
36	SA	264	
37	4	184	
38	6	73	
39	8	123	
40	A	260	
41	B	419	
42	C	373	
43	D	188	
44	E	190	
45	H	222	
46	I	220	
47	J	139	
48	K	175	
49	L	145	
50	M	204	
51	P	198	
52	Q	254	
53	R	179	
54	S	159	
55	T	166	
56	U	129	
57	V	145	
58	W	143	




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Mol	Chain	Length	Quality of chain
59	X	124	
60	Y	134	
61	Z	147	
62	a	127	
63	b	70	
64	c	252	
65	d	104	
66	f	133	
67	g	144	
68	h	168	
69	i	105	
70	j	83	
71	k	83	
72	l	51	
73	m	128	
74	n	34	
75	o	92	
76	p	106	
77	F	195	
78	G	264	
79	N	213	
80	O	305	
81	e	188	
82	1	1782	
83	3	216	

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Mol	Chain	Length	Quality of chain
84	5	135	
85	7	171	
86	2	1526	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 209021 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 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SB	208	Total	C	N	O	S	0	0
			1627	1034	297	284	12		

- Molecule 2 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SC	212	Total	C	N	O	S	1	0
			1630	1032	299	286	13		

- Molecule 3 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SD	182	Total	C	N	O	S	0	0
			1482	933	300	241	8		

- Molecule 4 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SE	260	Total	C	N	O	S	0	0
			2050	1299	393	349	9		

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SF	219	Total	C	N	O	S	0	0
			1670	1068	298	294	10		

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SG	231	Total	C	N	O	S	0	0
			1831	1144	374	310	3		

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SH	182	Total	C	N	O	S	0	0
			1436	892	278	259	7		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SI	199	Total	C	N	O	S	0	0
			1619	1032	313	267	7		

- Molecule 9 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SJ	129	Total	C	N	O	S	0	0
			1021	646	188	179	8		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	182	Total	C	N	O	S	0	0
			1443	906	305	230	2		

- Molecule 11 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SL	143	Total	C	N	O	S	0	0
			1124	724	206	191	3		

- Molecule 12 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SM	102	Total	C	N	O	S	0	0
			796	498	145	151	2		

- Molecule 13 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SN	100	Total	C	N	O	S	0	0
			813	521	142	143	7		

- Molecule 14 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SO	136	Total	C	N	O	S	0	0
			1015	627	198	182	8		

- Molecule 15 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SP	141	Total	C	N	O	S	0	0
			1100	694	217	186	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SQ	93	Total	C	N	O	S	0	0
			656	406	121	124	5		

- Molecule 17 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SR	136	Total	C	N	O	S	0	0
			1080	682	213	181	4		

- Molecule 18 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SS	56	Total	C	N	O	S	0	0
			452	279	94	73	6		

- Molecule 19 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	ST	142	Total	C	N	O	S	0	0
			1155	728	229	190	8		

- Molecule 20 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SU	148	Total	C	N	O	S	0	0
			1184	749	236	194	5		

- Molecule 21 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SV	109	Total	C	N	O	S	0	0
			850	538	164	144	4		

- Molecule 22 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SW	115	Total	C	N	O	S	0	0
			925	590	176	155	4		

- Molecule 23 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SX	152	Total	C	N	O	S	0	0
			1202	764	237	197	4		

- Molecule 24 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SY	87	Total	C	N	O	S	0	0
			640	397	120	119	4		

- Molecule 25 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SZ	127	Total	C	N	O	S	0	0
			1031	662	200	166	3		

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sa	71	Total	C	N	O	S	0	0
			558	356	99	100	3		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Sb	103	Total	C	N	O	S	0	0
			820	508	176	129	7		

- Molecule 28 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sc	84	Total	C	N	O	S	0	0
			647	400	125	114	8		

- Molecule 29 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Sd	65	Total	C	N	O	S	0	0
			474	290	95	85	4		

- Molecule 30 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Se	51	Total	C	N	O	S	0	0
			405	255	87	62	1		

- Molecule 31 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Sf	63	Total	C	N	O	S	0	0
			530	337	103	84	6		

- Molecule 32 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sg	294	Total	C	N	O	S	0	0
			2219	1396	393	419	11		

- Molecule 33 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sh	71	Total	C	N	O	S	0	0
			522	334	96	90	2		

- Molecule 34 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S4	68	Total	C	N	O	P	0	0
			1447	646	258	476	67		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S4	3	G	C	conflict	GB 1851743410
S4	70	C	G	conflict	GB 1851743410

- Molecule 35 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S1	1847	Total	C	N	O	P	1	0
			39517	17680	7108	12881	1848		

- Molecule 36 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SA	225	Total	C	N	O	S	1	0
			1820	1141	346	321	12		

- Molecule 37 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	184	Total	C	N	O	P	1	0
			3956	1765	714	1292	185		

- Molecule 38 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6	71	Total	C	N	O	P	0	0
			1506	675	271	489	71		

- Molecule 39 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 40 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A	255	Total	C	N	O	S	1	0
			1927	1200	395	321	11		

- Molecule 41 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B	401	Total	C	N	O	S	0	0
			3145	1985	625	522	13		

- Molecule 42 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	C	366	Total	C	N	O	S	0	0
			2799	1752	558	474	15		

- Molecule 43 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	D	173	Total	C	N	O	S	0	0
			1290	819	245	218	8		

- Molecule 44 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	E	186	Total	C	N	O	S	0	0
			1472	934	273	259	6		

- Molecule 45 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	H	221	Total	C	N	O	S	0	0
			1765	1123	353	282	7		

- Molecule 46 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	I	209	Total	C	N	O	S	0	0
			1645	1026	334	277	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	203	ARG	ASN	conflict	UNP E9AEA8

- Molecule 47 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	J	134	Total	C	N	O	S	0	0
			996	630	189	171	6		

- Molecule 48 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	K	170	Total	C	N	O	S	0	0
			1313	823	263	219	8		

- Molecule 49 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L	144	Total	C	N	O	S	0	0
			1110	700	225	179	6		

- Molecule 50 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	M	203	Total	C	N	O	S	0	0
			1704	1076	362	258	8		

- Molecule 51 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	P	197	Total	C	N	O	S	0	0
			1532	964	306	256	6		

- Molecule 52 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Q	185	Total	C	N	O	S	0	0
			1527	947	336	238	6		

- Molecule 53 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	R	178	Total	C	N	O	S	0	0
			1452	925	279	243	5		

- Molecule 54 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S	158	Total	C	N	O	S	0	0
			1253	797	243	209	4		

- Molecule 55 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	T	151	Total	C	N	O	S	0	0
			1215	760	241	203	11		

- Molecule 56 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	U	12	Total	C	N	O	0	0
			81	48	19	14		

- Molecule 57 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	V	118	Total	C	N	O	S	0	0
			934	593	180	159	2		

- Molecule 58 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	W	120	Total	C	N	O	S	0	0
			955	597	199	155	4		

- Molecule 59 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	X	64	Total	C	N	O	S	0	0
			548	359	105	80	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Y	133	Total	C	N	O	S	0	0
			1048	674	212	159	3		

- Molecule 61 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Z	145	Total	C	N	O	S	0	0
			1121	687	238	191	5		

- Molecule 62 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	a	124	Total	C	N	O	S	0	0
			1028	644	216	164	4		

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	b	68	Total	C	N	O	S	0	0
			546	335	125	86			

- Molecule 64 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	c	229	Total	C	N	O	S	0	0
			1866	1188	359	308	11		

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	d	92	Total	C	N	O	S	0	0
			705	438	129	133	5		

- Molecule 66 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f	126	Total	C	N	O	S	0	0
			1023	645	203	171	4		

- Molecule 67 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	g	143	Total	C	N	O	S	0	0
			1149	714	240	190	5		

- Molecule 68 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	h	125	Total	C	N	O	S	0	0
			1011	621	220	164	6		

- Molecule 69 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	i	98	Total	C	N	O	S	0	0
			777	492	159	124	2		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j	81	Total	C	N	O	S	0	0
			672	409	154	103	6		

- Molecule 71 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k	77	Total	C	N	O	S	0	0
			614	388	120	103	3		

- Molecule 72 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	l	50	Total	C	N	O	S	0	0
			450	291	95	63	1		

- Molecule 73 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	m	51	Total	C	N	O	S	0	0
			410	258	84	61	7		

- Molecule 74 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n	33	Total	C	N	O	S	0	0
			292	178	75	37	2		

- Molecule 75 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o	88	Total	C	N	O	S	0	0
			689	428	142	113	6		

- Molecule 76 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p	98	Total	C	N	O	S	0	0
			787	498	159	125	5		

- Molecule 77 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	F	148	Total	C	N	O	S	0	0
			1118	714	212	190	2		

- Molecule 78 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	G	228	Total	C	N	O	S	0	0
			1792	1130	354	301	7		

- Molecule 79 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	N	199	Total	C	N	O	S	0	0
			1615	1018	321	262	14		

- Molecule 80 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	O	282	Total	C	N	O	S	0	0
			2125	1359	409	351	6		

- Molecule 81 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	e	185	Total	C	N	O	S	0	0
			1456	915	295	242	4		

- Molecule 82 is a RNA chain called RNA (1646-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
82	1	1646	Total	C	N	O	P	0	0
			35315	15785	6473	11411	1646		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	164	G	U	conflict	GB 321438308
1	165	U	C	conflict	GB 321438308
1	198	A	C	conflict	GB 321438308
1	523	A	G	conflict	GB 321438308
1	593	C	U	conflict	GB 321438308
1	1428	A	C	conflict	GB 321438308

- Molecule 83 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	3	178	Total	C	N	O	P	0	0
			3776	1689	656	1253	178		

- Molecule 84 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	5	117	Total	C	N	O	P	0	0
			2496	1113	447	819	117		

- Molecule 85 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	7	163	Total	C	N	O	P	0	0
			3472	1556	616	1138	162		

- Molecule 86 is a RNA chain called LSUb_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	2	1190	Total	C	N	O	P	0	0
			25463	11395	4598	8280	1190		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	SG	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
87	SK	1	Total 1	Mg 1	0
87	SS	1	Total 1	Mg 1	0
87	SX	2	Total 2	Mg 2	0
87	Sb	1	Total 1	Mg 1	0
87	S1	79	Total 79	Mg 79	0
87	4	7	Total 7	Mg 7	0
87	6	1	Total 1	Mg 1	0
87	8	6	Total 6	Mg 6	0
87	B	2	Total 2	Mg 2	0
87	I	1	Total 1	Mg 1	0
87	J	1	Total 1	Mg 1	0
87	S	1	Total 1	Mg 1	0
87	T	1	Total 1	Mg 1	0
87	f	1	Total 1	Mg 1	0
87	N	1	Total 1	Mg 1	0
87	1	119	Total 119	Mg 119	0
87	3	4	Total 4	Mg 4	0
87	5	1	Total 1	Mg 1	0
87	7	7	Total 7	Mg 7	0
87	2	97	Total 97	Mg 97	0

- Molecule 88 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
88	S1	11	Total 11	K 11	0
88	4	4	Total 4	K 4	0
88	A	1	Total 1	K 1	0
88	B	1	Total 1	K 1	0
88	M	1	Total 1	K 1	0
88	N	1	Total 1	K 1	0
88	1	11	Total 11	K 11	0
88	3	1	Total 1	K 1	0
88	5	2	Total 2	K 2	0
88	2	13	Total 13	K 13	0

- Molecule 89 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
89	S1	2	Total 2	Na 2	0
89	1	2	Total 2	Na 2	0
89	3	1	Total 1	Na 1	0
89	5	1	Total 1	Na 1	0
89	7	1	Total 1	Na 1	0
89	2	3	Total 3	Na 3	0

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	S1	44	Total 44	O 44	0
90	4	9	Total 9	O 9	0

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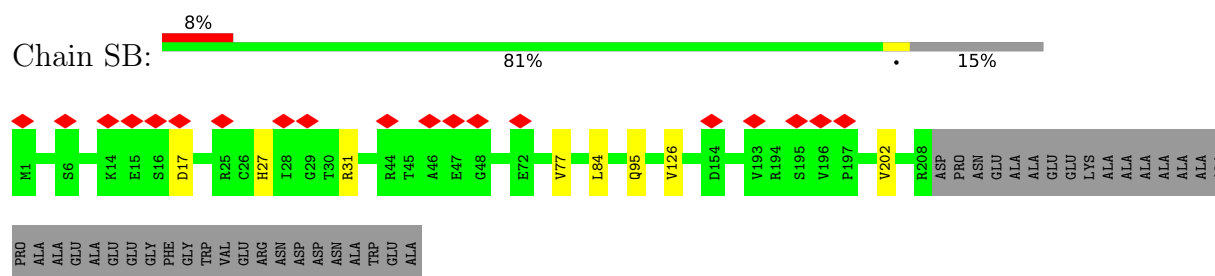
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Mol	Chain	Residues	Atoms		AltConf
90	8	4	Total 4	O 4	0
90	A	4	Total 4	O 4	0
90	B	4	Total 4	O 4	0
90	E	1	Total 1	O 1	0
90	H	1	Total 1	O 1	0
90	J	1	Total 1	O 1	0
90	T	2	Total 2	O 2	0
90	W	1	Total 1	O 1	0
90	b	1	Total 1	O 1	0
90	h	2	Total 2	O 2	0
90	j	3	Total 3	O 3	0
90	1	135	Total 135	O 135	0
90	3	4	Total 4	O 4	0
90	5	4	Total 4	O 4	0
90	7	6	Total 6	O 6	0
90	2	141	Total 141	O 141	0

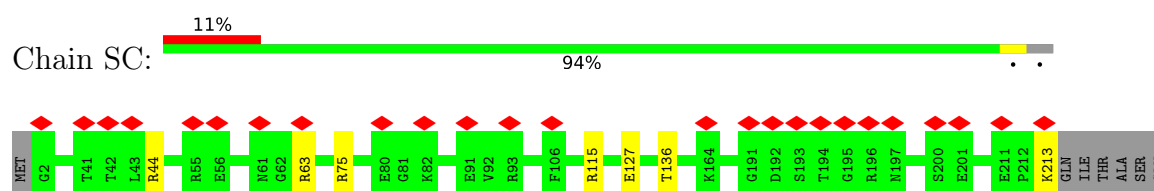
3 Residue-property plots [i](#)

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

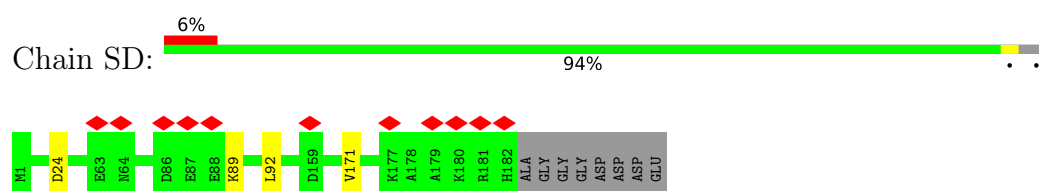
- Molecule 1: 40S ribosomal protein SA



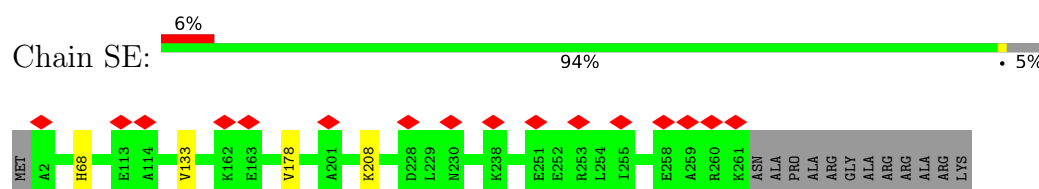
- Molecule 2: Putative 40S ribosomal protein S3



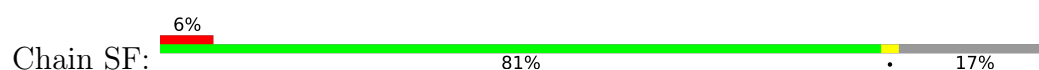
- Molecule 3: Putative 40S ribosomal protein S9

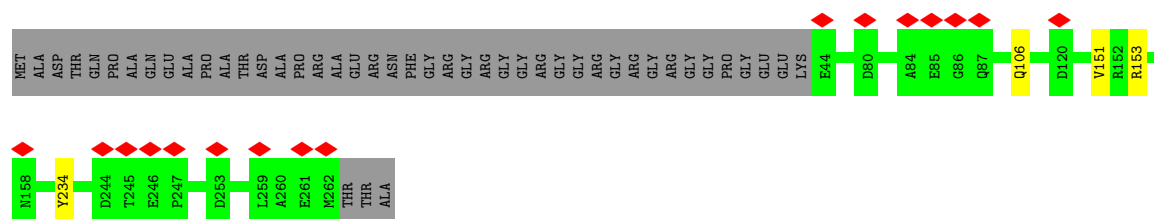


- Molecule 4: 40S ribosomal protein S4

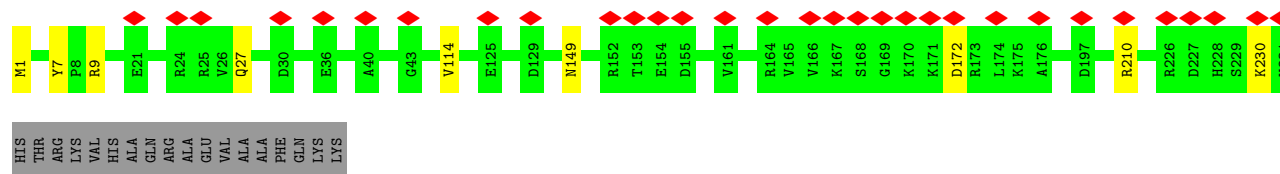
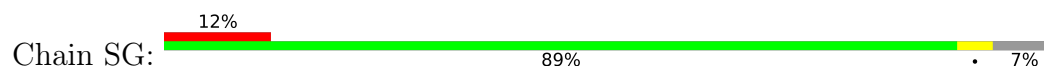


- Molecule 5: 40S ribosomal protein S2





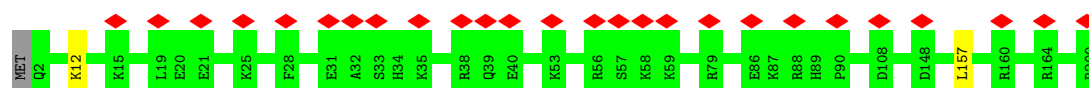
- Molecule 6: 40S ribosomal protein S6



- Molecule 7: 40S ribosomal protein S5



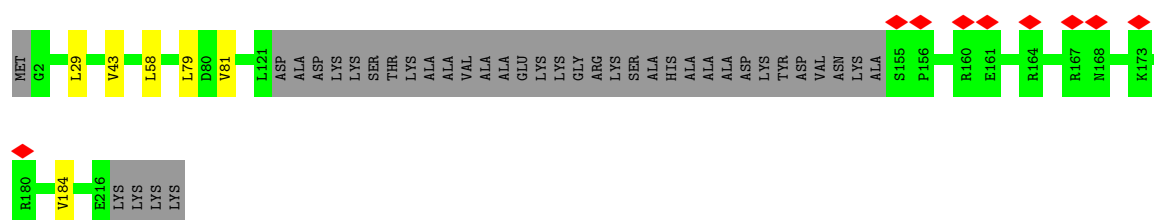
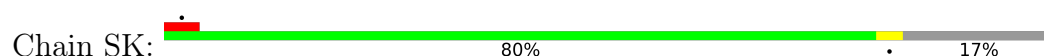
- Molecule 8: 40S ribosomal protein S7



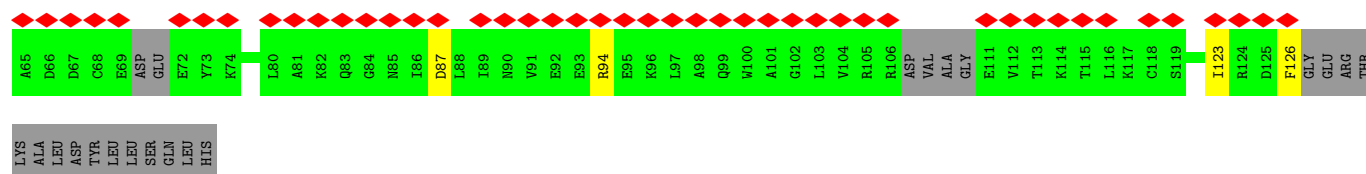
- Molecule 9: Putative 40S ribosomal protein S15A



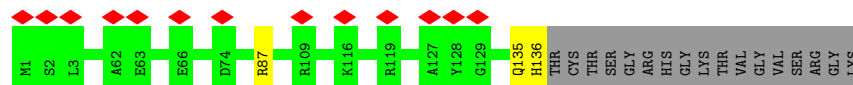
- Molecule 10: 40S ribosomal protein S8



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| MET | ALA | GLU | THR | VAL | ARG | VAL | VAL | PRO | ALA | VAL | GLU | GLU | ASN | VAL | VAL | VAL | ASP | VAL | ALA | ALA | PRO | GLU | SER | LEU | GLU | D28 | A29 | V30 | R31 | I32 | V33 | I34 | Q35 | K36 | S37 | L38 | E39 | A40 | N41 | G42 | L43 | V44 | R45 | E49 | R52 | T53 | L54 | D55 | C56 | K57 | T58 | A59 | H60 | I63 | L64 | D65 | C66 | K67 | T68 | A69 | H70 | I73 | L74 | D75 | C76 | K77 | T78 | A79 | H80 | I83 | L84 | D85 | C86 | K87 | T88 | A89 | H90 | I93 | L94 | D95 | C96 | K97 | T98 | A99 | H100 | I103 | L104 | D105 | C106 | K107 | T108 | A109 | H110 | I113 | L114 | D115 | C116 | K117 | T118 | A119 | H120 | I123 | L124 | D125 | C126 | K127 | T128 | A129 | H130 | I133 | L134 | D135 | C136 | K137 | T138 | A139 | H140 | I143 | L144 | D145 | C146 | K147 | T148 | A149 | H150 | I153 | L154 | D155 | C156 | K157 | T158 | A159 | H160 | I163 | L164 | D165 | C166 | K167 | T168 | A169 | H170 | I173 | L174 | D175 | C176 | K177 | T178 | A179 | H180 | I183 | L184 | D185 | C186 | K187 | T188 | A189 | H190 | I193 | L194 | D195 | C196 | K197 | T198 | A199 | H200 | I203 | L204 | D205 | C206 | K207 | T208 | A209 | H210 | I213 | L214 | D215 | C216 | K217 | T218 | A219 | H220 | I223 | L224 | D225 | C226 | K227 | T228 | A229 | H230 | I233 | L234 | D235 | C236 | K237 | T238 | A239 | H240 | I243 | L244 | D245 | C246 | K247 | T248 | A249 | H250 | I253 | L254 | D255 | C256 | K257 | T258 | A259 | H260 | I263 | L264 | D265 | C266 | K267 | T268 | A269 | H270 | I273 | L274 | D275 | C276 | K277 | T278 | A279 | H280 | I283 | L284 | D285 | C286 | K287 | T288 | A289 | H290 | I293 | L294 | D295 | C296 | K297 | T298 | A299 | H300 | I303 | L304 | D305 | C306 | K307 | T308 | A309 | H310 | I313 | L314 | D315 | C316 | K317 | T318 | A319 | H320 | I323 | L324 | D325 | C326 | K327 | T328 | A329 | H330 | I333 | L334 | D335 | C336 | K337 | T338 | A339 | H340 | I343 | L344 | D345 | C346 | K347 | T348 | A349 | H350 | I353 | L354 | D355 | C356 | K357 | T358 | A359 | H360 | I363 | L364 | D365 | C366 | K367 | T368 | A369 | H370 | I373 | L374 | D375 | C376 | K377 | T378 | A379 | H380 | I383 | L384 | D385 | C386 | K387 | T388 | A389 | H390 | I393 | L394 | D395 | C396 | K397 | T398 | A399 | H400 | I403 | L404 | D405 | C406 | K407 | T408 | A409 | H410 | I413 | L414 | D415 | C416 | K417 | T418 | A419 | H420 | I423 | L424 | D425 | C426 | K427 | T428 | A429 | H430 | I433 | L434 | D435 | C436 | K437 | T438 | A439 | H440 | I443 | L444 | D445 | C446 | K447 | T448 | A449 | H450 | I453 | L454 | D455 | C456 | K457 | T458 | A459 | H460 | I463 | L464 | D465 | C466 | K467 | T468 | A469 | H470 | I473 | L474 | D475 | C476 | K477 | T478 | A479 | H480 | I483 | L484 | D485 | C486 | K487 | T488 | A489 | H490 | I493 | L494 | D495 | C496 | K497 | T498 | A499 | H500 | I503 | L504 | D505 | C506 | K507 | T508 | A509 | H510 | I513 | L514 | D515 | C516 | K517 | T518 | A519 | H520 | I523 | L524 | D525 | C526 | K527 | T528 | A529 | H530 | I533 | L534 | D535 | C536 | K537 | T538 | A539 | H540 | I543 | L544 | D545 | C546 | K547 | T548 | A549 | H550 | I553 | L554 | D555 | C556 | K557 | T558 | A559 | H560 | I563 | L564 | D565 | C566 | K567 | T568 | A569 | H570 | I573 | L574 | D575 | C576 | K577 | T578 | A579 | H580 | I583 | L584 | D585 | C586 | K587 | T588 | A589 | H590 | I593 | L594 | D595 | C596 | K597 | T598 | A599 | H600 | I603 | L604 | D605 | C606 | K607 | T608 | A609 | H610 | I613 | L614 | D615 | C616 | K617 | T618 | A619 | H620 | I623 | L624 | D625 | C626 | K627 | T628 | A629 | H630 | I633 | L634 | D635 | C636 | K637 | T638 | A639 | H640 | I643 | L644 | D645 | C646 | K647 | T648 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|



- Molecule 17: Putative 40S ribosomal protein S18



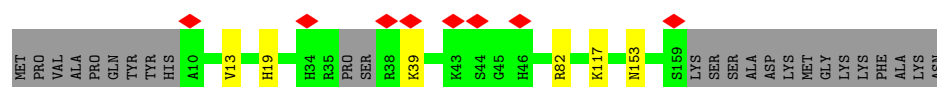
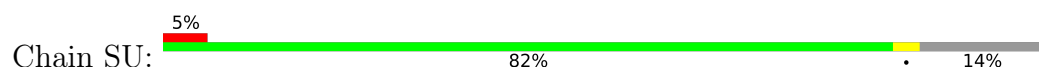
- Molecule 18: Putative ribosomal protein S29



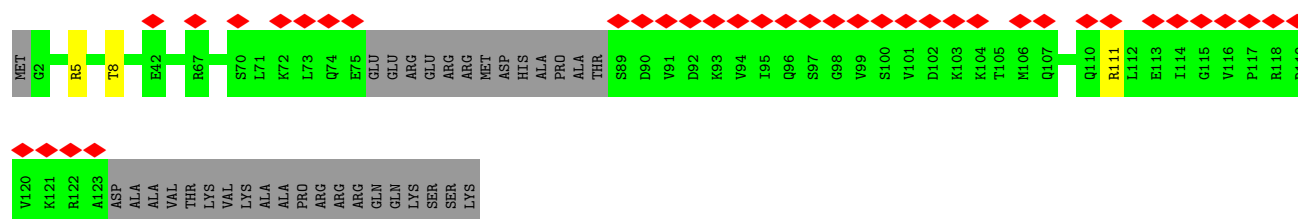
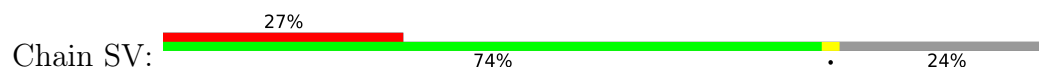
- Molecule 19: Putative 40S ribosomal protein S13



- Molecule 20: Putative 40S ribosomal protein S11

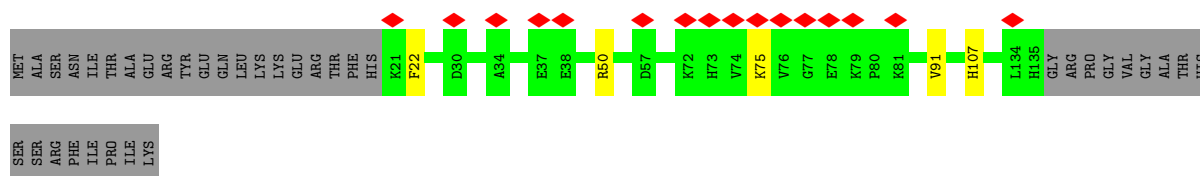


- Molecule 21: Putative 40S ribosomal protein S17



- Molecule 22: Putative 40S ribosomal protein S15

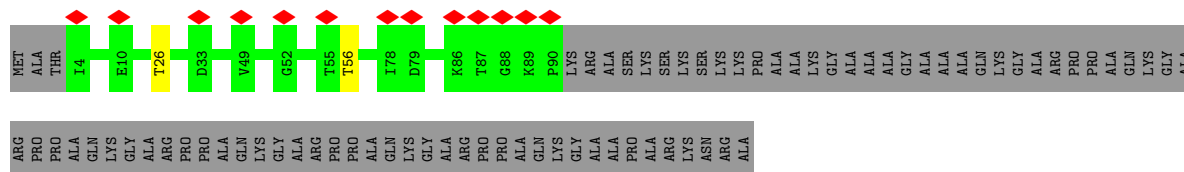




- Molecule 23: 40S ribosomal protein S19-like protein



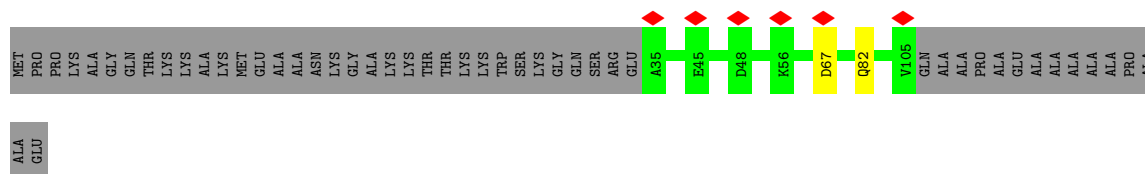
- Molecule 24: Putative 40S ribosomal protein S21



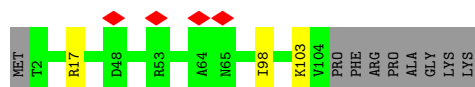
- Molecule 25: 40S ribosomal protein S24



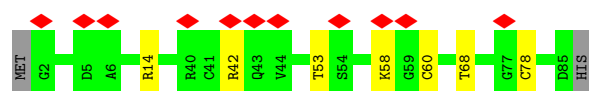
- Molecule 26: 40S ribosomal protein S25

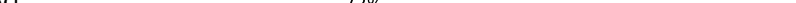


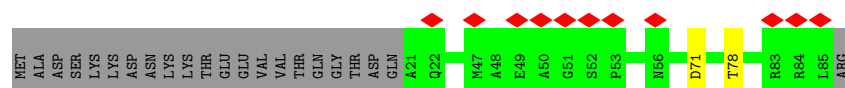
- Molecule 27: 40S ribosomal protein S26

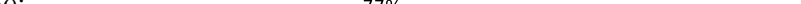


- Molecule 28: Putative 40S ribosomal protein S27-1



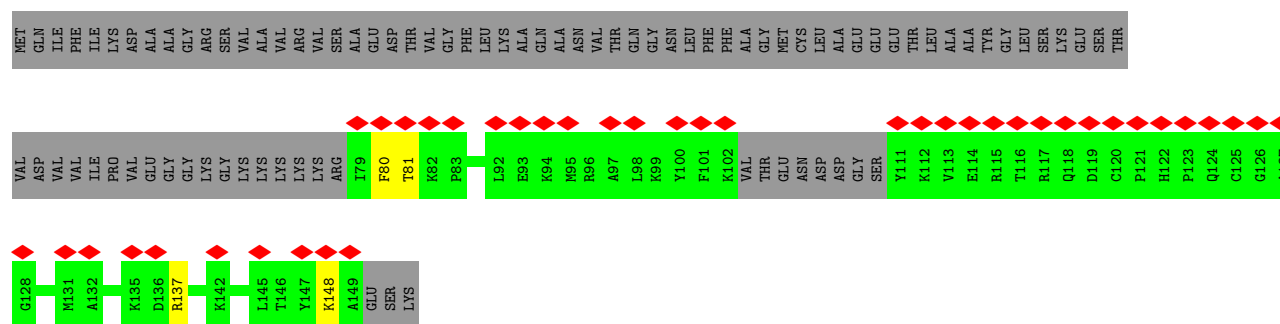
- Chain Sd: 

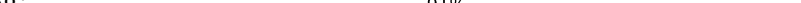


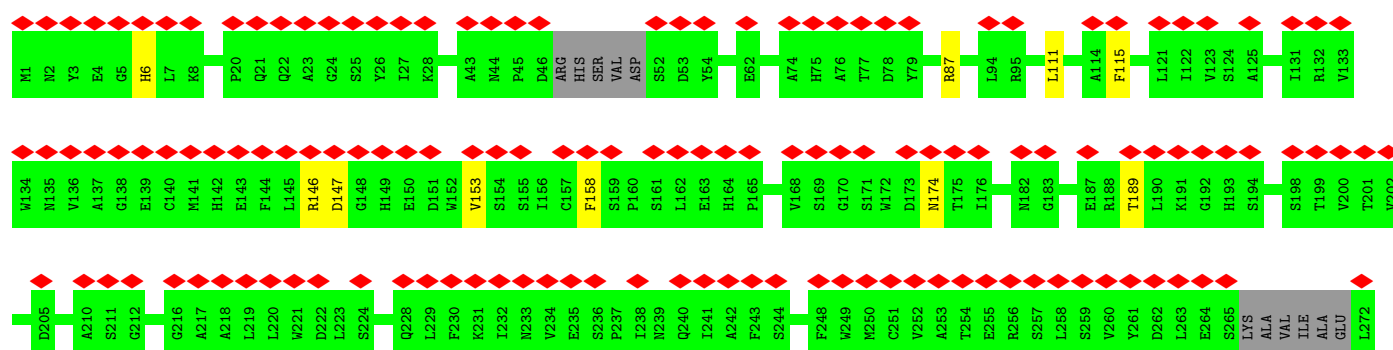
- Chain Se:  77% 23%



- Chain Sf: 

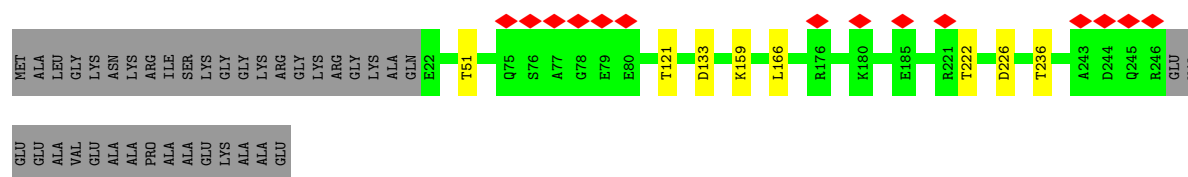
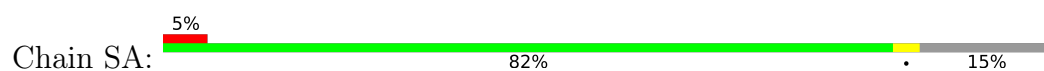


- Chain Sg:  49% 91% 6%

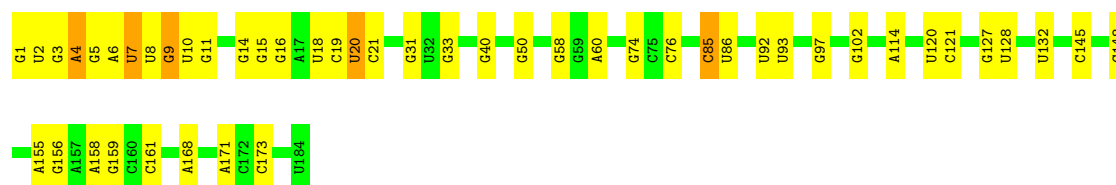




- Molecule 36: 40S ribosomal protein S3a



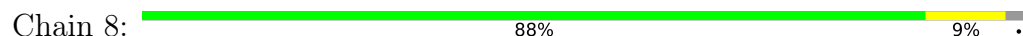
- Molecule 37: SR2 chain 4



- Molecule 38: SR6 chain 6

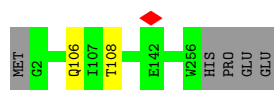


- Molecule 39: 5S rRNA chain 8



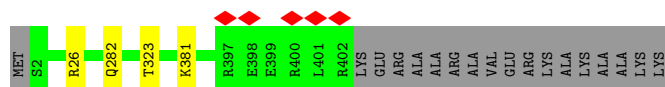
- Molecule 40: Putative 60S ribosomal protein L2

Chain A:  97%



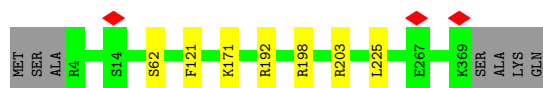
- Molecule 41: Putative ribosomal protein L3

Chain B:  95%

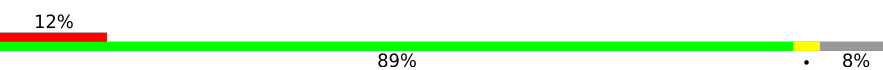


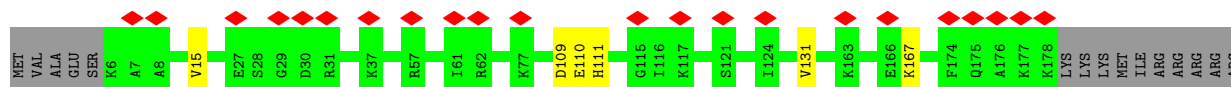
- Molecule 42: Putative ribosomal protein L1a

Chain C:  96%



- Molecule 43: 60S ribosomal protein L11

Chain D:  12% 89% 8%



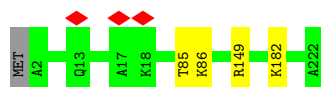
- Molecule 44: Putative 60S ribosomal protein L9

Chain E:  95%



- Molecule 45: Putative 60S ribosomal protein L13a

Chain H:  98%

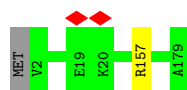


- Molecule 46: Putative 60S ribosomal protein L13

Chain I:  94% 5%

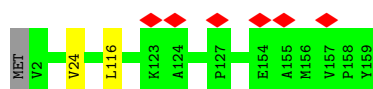
- Molecule 53: 60S ribosomal protein L18a

Chain R:  99%




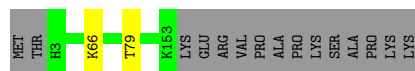
- Molecule 54: Putative 60S ribosomal protein L21

Chain S:  98%



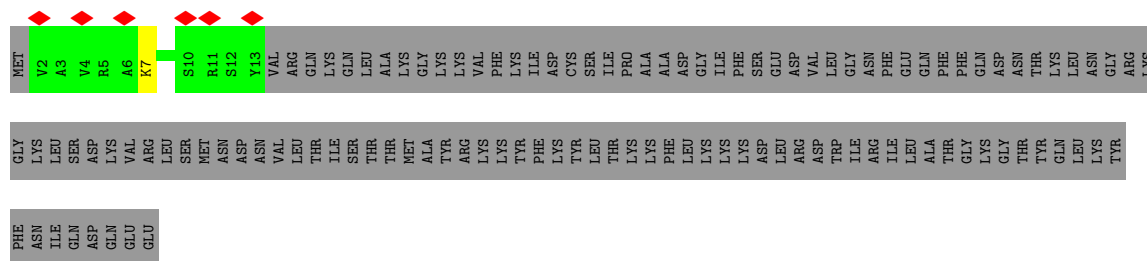
- Molecule 55: Putative 60S ribosomal protein L17

Chain T:  90%




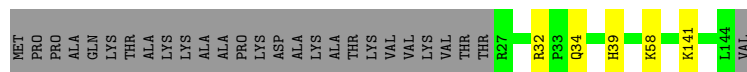
- Molecule 56: Putative 60S ribosomal protein L22

Chain U:  5%




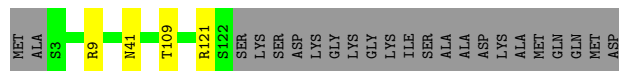
- Molecule 57: Putative 60S ribosomal protein L23a

Chain V:  78%



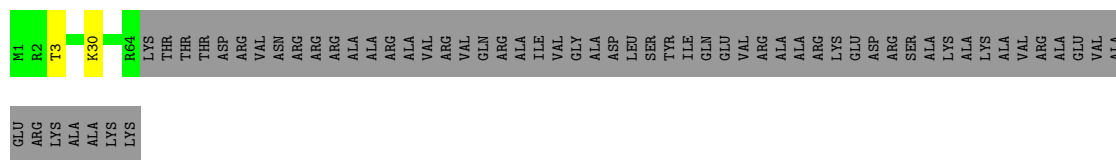
- Molecule 58: Putative 60S ribosomal protein L26

Chain W:  81%



- Molecule 59: Putative ribosomal protein L24

Chain X:  50% 48%



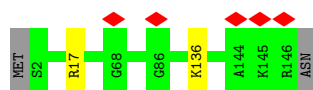
- Molecule 60: 60S ribosomal protein L27

Chain Y:  98%



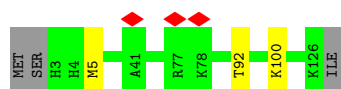
- Molecule 61: Putative 60S ribosomal protein L28

Chain Z:  97%



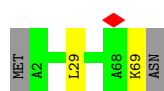
- Molecule 62: Putative 60S ribosomal protein L35

Chain a:  95%




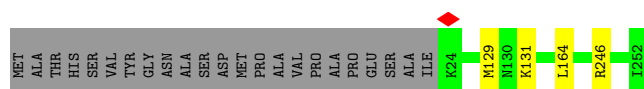
- Molecule 63: 60S ribosomal protein L29

Chain b:  94%




- Molecule 64: Putative 60S ribosomal protein L7

Chain c:  89% 9%

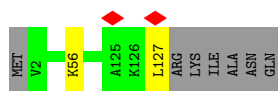
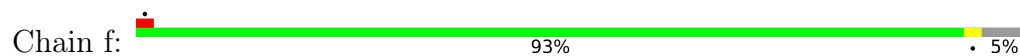


- Molecule 65: 60S ribosomal protein L30

Chain d:  5% 85% 12%



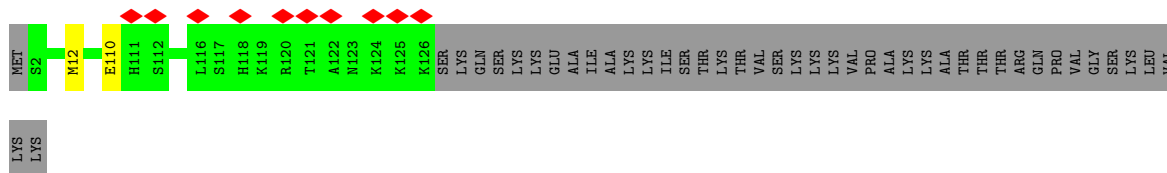
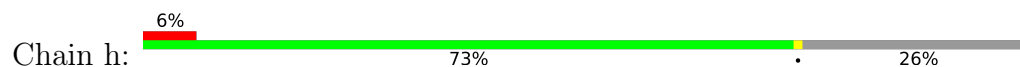
- Molecule 66: 60S ribosomal protein L32



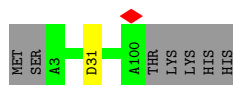
- Molecule 67: Putative ribosomal protein l35a



- Molecule 68: Putative 60S ribosomal protein L34



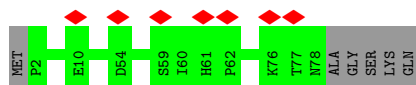
- Molecule 69: Putative 60S Ribosomal protein L36



- Molecule 70: Ribosomal protein L37



- Molecule 71: Putative ribosomal protein L38



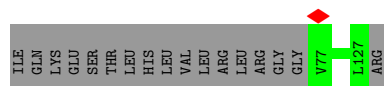
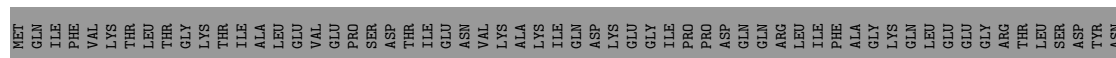
- Molecule 72: Putative 60S ribosomal protein L39

Chain l:  96%



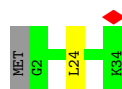
- Molecule 73: Ubiquitin-60S ribosomal protein L40

Chain m:  40%



- Molecule 74: 60S ribosomal protein L41

Chain n:  94%




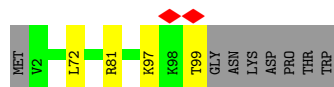
- Molecule 75: 60S ribosomal protein L37a

Chain o:  92%



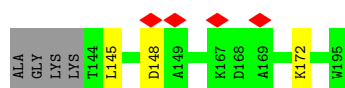
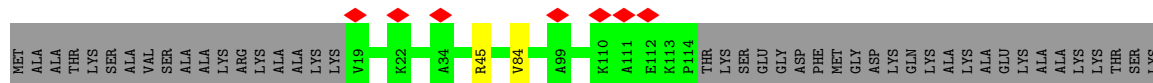
- Molecule 76: Putative 60S ribosomal protein L44

Chain p:  89%




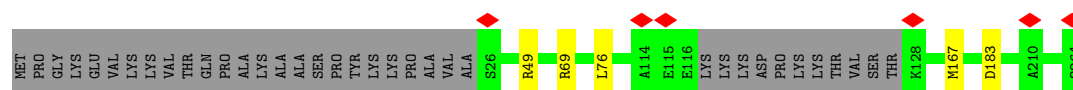
- Molecule 77: Putative 60S ribosomal protein L6

Chain F:  6%




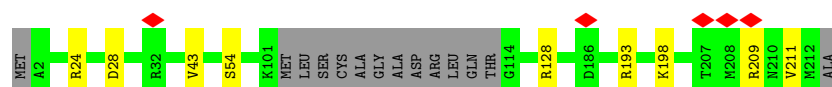
- Molecule 78: 60S ribosomal protein L7a

Chain G: 

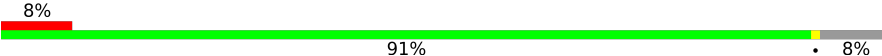


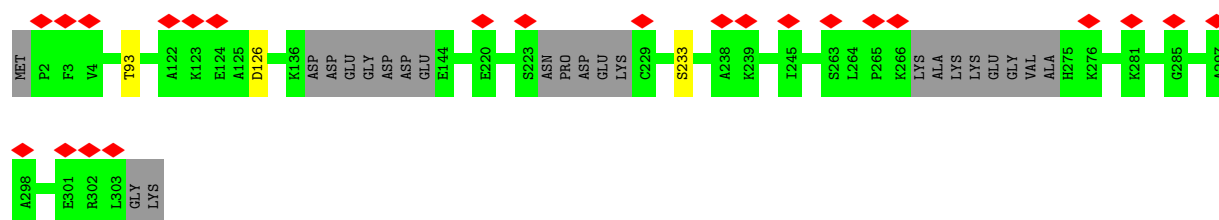
- Molecule 79: Putative 60S ribosomal protein L10

Chain N: 

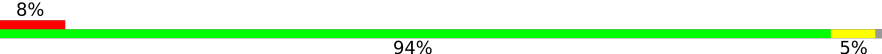


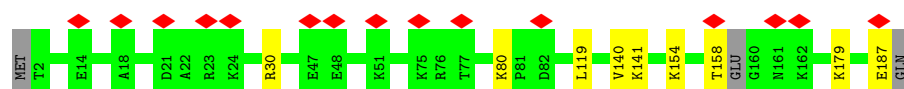
- Molecule 80: Putative 60S ribosomal protein L5

Chain O: 



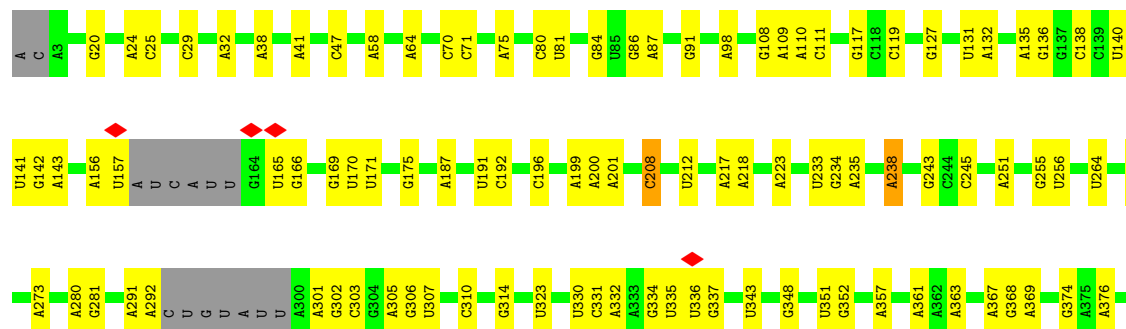
- Molecule 81: Putative 60S ribosomal subunit protein L31

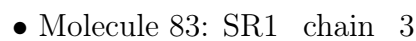
Chain e: 

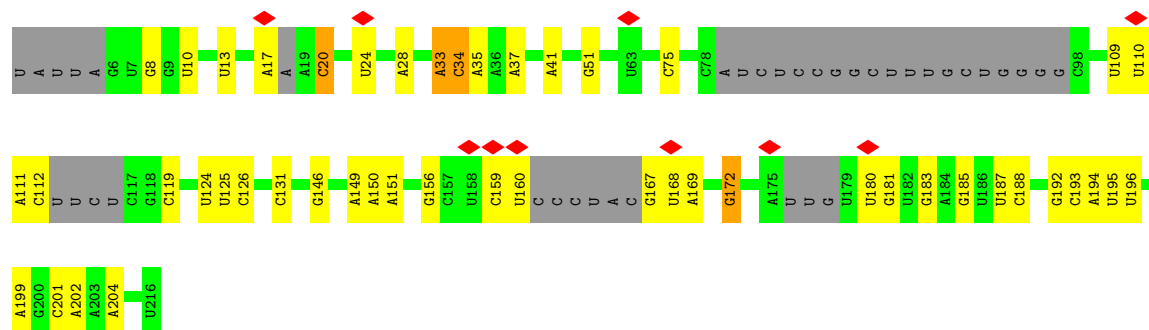


- Molecule 82: RNA (1646-MER)

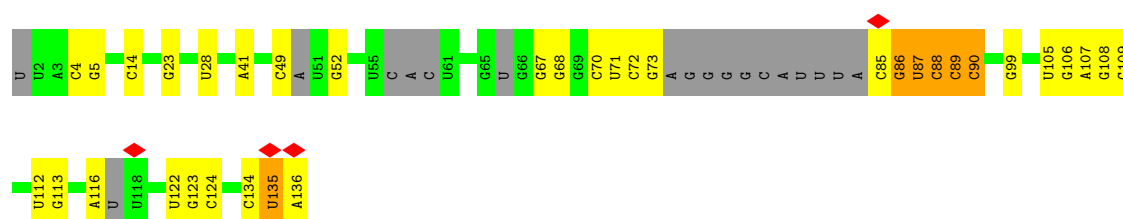
Chain 1: 



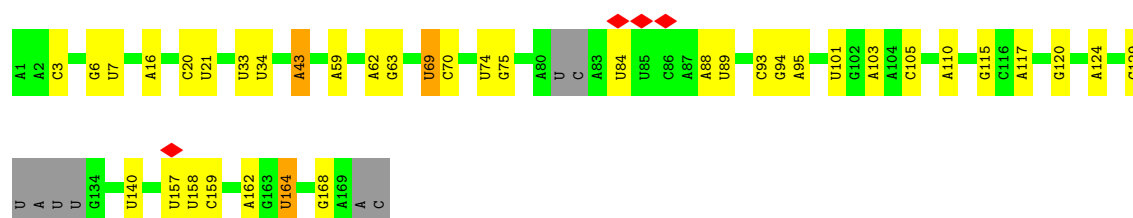




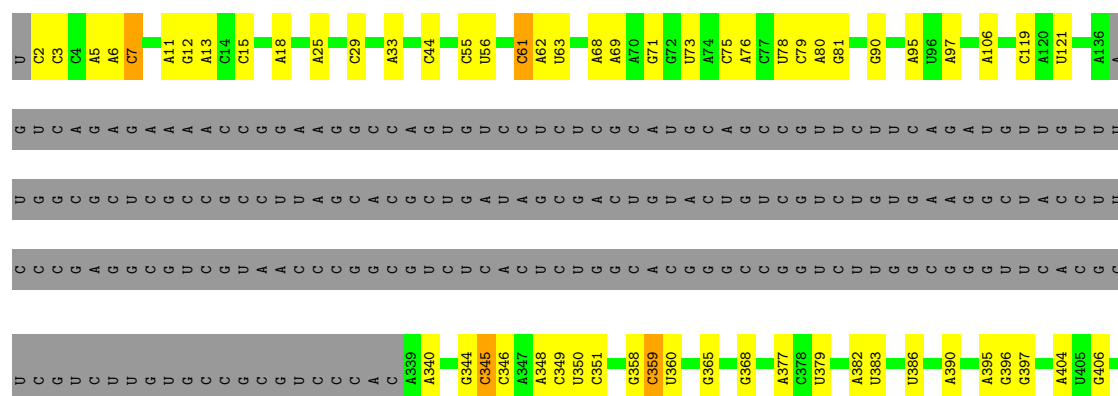
• Molecule 84: SR4_chain_5

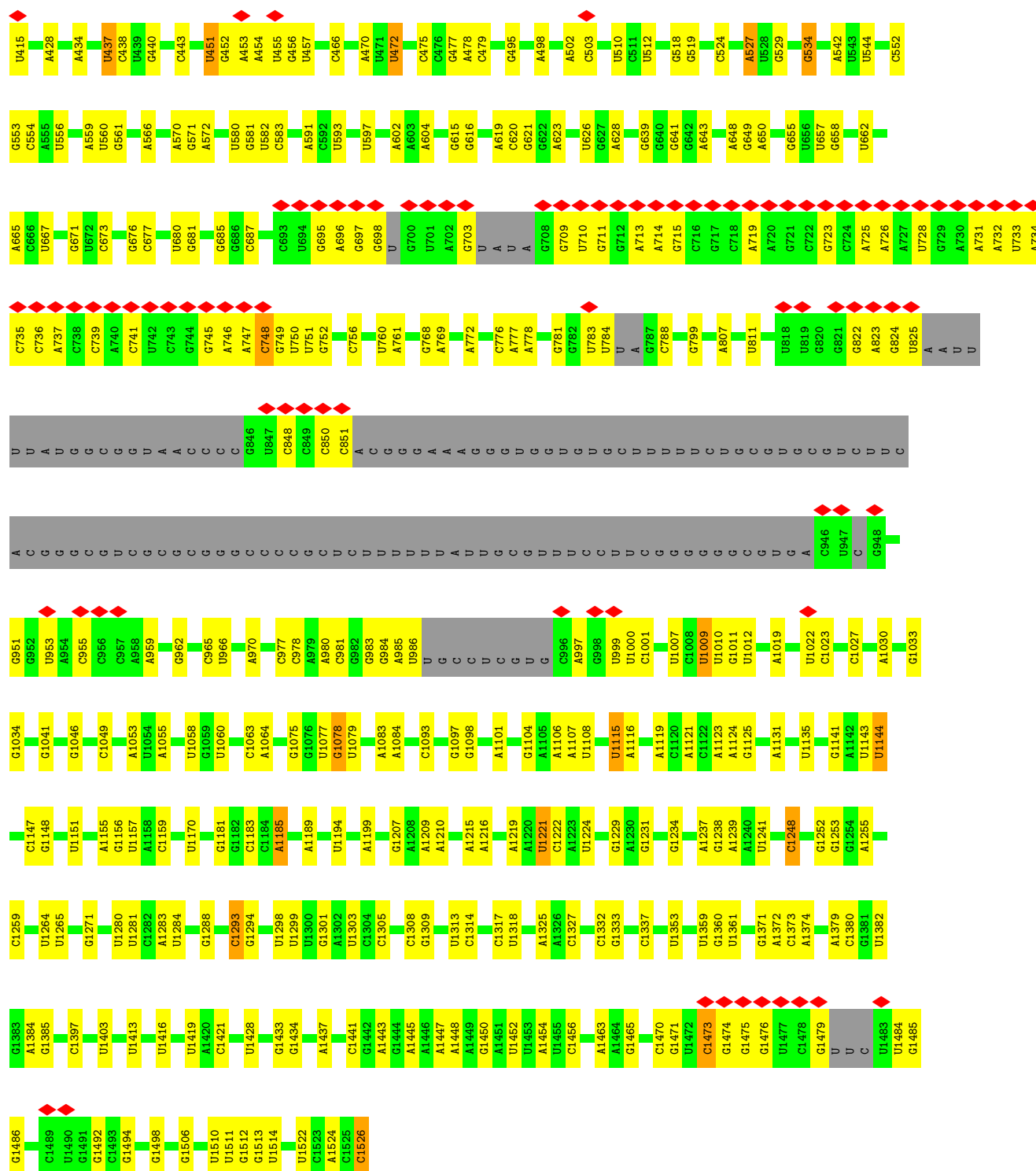


• Molecule 85: 5.8S_rRNA_chain_7



• Molecule 86: LSUb_rRNA_chain_2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134493	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 ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	358.56, 358.56, 358.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.747, 0.747, 0.747	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 7MG, MA6, OMG, NA, A2M, MG, K, 5MC, 1MA, OMC, C4J, OMU

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	SB	0.26	0/1660	0.50	0/2246
2	SC	0.26	0/1658	0.50	0/2219
3	SD	0.25	0/1509	0.54	0/2026
4	SE	0.26	0/2088	0.53	0/2814
5	SF	0.26	0/1706	0.48	0/2311
6	SG	0.26	0/1853	0.56	0/2475
7	SH	0.24	0/1458	0.50	0/1955
8	SI	0.25	0/1649	0.52	0/2220
9	SJ	0.26	0/1038	0.51	0/1391
10	SK	0.27	0/1465	0.58	0/1964
11	SL	0.25	0/1145	0.48	0/1540
12	SM	0.24	0/806	0.52	0/1093
13	SN	0.26	0/836	0.47	0/1134
14	SO	0.26	0/1030	0.54	0/1384
15	SP	0.26	0/1120	0.51	0/1500
16	SQ	0.23	0/658	0.52	0/890
17	SR	0.25	0/1099	0.53	0/1477
18	SS	0.25	0/458	0.52	0/607
19	ST	0.28	0/1178	0.53	0/1580
20	SU	0.27	0/1208	0.51	0/1622
21	SV	0.24	0/856	0.50	0/1141
22	SW	0.26	0/945	0.49	0/1271
23	SX	0.26	0/1233	0.51	0/1656
24	SY	0.24	0/650	0.49	0/883
25	SZ	0.26	0/1051	0.49	0/1399
26	Sa	0.25	0/563	0.53	0/757
27	Sb	0.28	0/837	0.58	0/1120
28	Sc	0.31	0/660	0.57	0/888
29	Sd	0.26	0/476	0.57	0/640
30	Se	0.25	0/411	0.51	0/544
31	Sf	0.25	0/544	0.48	0/723
32	Sg	0.25	0/2274	0.48	0/3100

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sh	0.27	0/532	0.51	0/718
34	S4	0.31	0/1613	1.25	8/2506 (0.3%)
35	S1	0.37	0/42994	0.85	41/66965 (0.1%)
36	SA	0.26	0/1848	0.53	0/2487
37	4	0.47	0/4397	0.95	27/6854 (0.4%)
38	6	0.35	0/1683	0.86	1/2618 (0.0%)
39	8	0.39	0/2829	0.86	5/4405 (0.1%)
40	A	0.29	0/1969	0.57	0/2643
41	B	0.27	0/3212	0.54	0/4324
42	C	0.27	0/2849	0.54	0/3835
43	D	0.26	0/1313	0.52	0/1766
44	E	0.27	0/1492	0.51	0/2011
45	H	0.27	0/1801	0.53	0/2419
46	I	0.26	0/1678	0.53	0/2250
47	J	0.28	0/1013	0.53	0/1367
48	K	0.26	0/1332	0.51	0/1788
49	L	0.29	0/1137	0.53	0/1521
50	M	0.28	0/1744	0.58	0/2329
51	P	0.28	0/1557	0.56	0/2084
52	Q	0.26	0/1546	0.56	0/2047
53	R	0.29	0/1486	0.52	0/2003
54	S	0.29	0/1282	0.53	0/1728
55	T	0.29	0/1239	0.54	0/1660
56	U	0.23	0/80	0.60	0/105
57	V	0.27	0/949	0.52	0/1277
58	W	0.26	0/969	0.55	0/1294
59	X	0.29	0/569	0.53	0/767
60	Y	0.28	0/1069	0.54	0/1434
61	Z	0.26	0/1137	0.55	0/1521
62	a	0.26	0/1039	0.55	0/1379
63	b	0.26	0/557	0.50	0/743
64	c	0.28	0/1900	0.53	0/2544
65	d	0.28	0/715	0.49	0/968
66	f	0.28	0/1043	0.57	0/1395
67	g	0.29	0/1172	0.58	0/1573
68	h	0.27	0/1027	0.57	0/1368
69	i	0.28	0/792	0.53	0/1059
70	j	0.29	0/686	0.62	0/915
71	k	0.27	0/623	0.51	0/833
72	l	0.27	0/463	0.55	0/617
73	m	0.29	0/416	0.55	0/553
74	n	0.28	0/296	0.73	0/386
75	o	0.28	0/701	0.58	0/934

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	p	0.32	0/800	0.53	0/1058
77	F	0.27	0/1140	0.52	0/1546
78	G	0.26	0/1817	0.53	0/2447
79	N	0.28	0/1647	0.57	0/2203
80	O	0.27	0/2164	0.50	0/2904
81	e	0.26	0/1474	0.54	0/1959
82	1	0.44	1/38669 (0.0%)	0.86	54/60289 (0.1%)
83	3	0.39	0/4189	0.89	19/6510 (0.3%)
84	5	0.46	0/2785	0.97	11/4330 (0.3%)
85	7	0.41	0/3712	0.82	1/5778 (0.0%)
86	2	0.44	0/27120	0.90	46/42264 (0.1%)
All	All	0.36	1/220388 (0.0%)	0.76	213/323851 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	157	U	C1'-N1	6.28	1.58	1.48

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	S4	12	U	O5'-P-OP1	-26.31	79.13	110.70
34	S4	12	U	O5'-P-OP2	-16.96	90.35	110.70
34	S4	11	C	OP1-P-O3'	-15.32	71.50	105.20
34	S4	12	U	OP1-P-OP2	15.27	142.50	119.60
86	2	55	C	OP1-P-O3'	-14.02	74.35	105.20
86	2	55	C	OP2-P-O3'	-12.58	77.52	105.20
34	S4	11	C	OP2-P-O3'	-11.62	79.64	105.20
84	5	88	C	P-O3'-C3'	-10.01	107.69	119.70
37	4	4	A	P-O3'-C3'	-9.88	107.85	119.70
37	4	20	U	P-O3'-C3'	-9.66	108.11	119.70
82	1	750	G	O4'-C1'-N9	9.47	115.78	108.20
37	4	3	G	P-O3'-C3'	-9.38	108.45	119.70
86	2	451	U	O4'-C1'-N1	9.32	115.66	108.20
84	5	89	C	P-O3'-C3'	-9.24	108.61	119.70
37	4	8[A]	U	O3'-P-O5'	-9.03	86.85	104.00
37	4	8[B]	U	O3'-P-O5'	-9.03	86.85	104.00
82	1	447	G	O4'-C1'-N9	8.97	115.38	108.20
84	5	87	U	P-O3'-C3'	-8.64	109.34	119.70
84	5	86	G	P-O3'-C3'	-8.59	109.39	119.70
86	2	56	U	OP1-P-OP2	8.55	132.43	119.60
84	5	85	C	P-O3'-C3'	-8.49	109.51	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	2	61	C	C2-N1-C1'	8.27	127.90	118.80
37	4	2	U	P-O3'-C3'	-8.18	109.88	119.70
37	4	7	U	P-O3'-C3'	-7.90	110.22	119.70
84	5	90	C	P-O3'-C3'	-7.76	110.39	119.70
86	2	61	C	N1-C2-O2	7.64	123.48	118.90
37	4	5	G	P-O3'-C3'	-7.63	110.54	119.70
37	4	9	G	O5'-P-OP1	7.52	119.72	110.70
37	4	21	C	P-O3'-C3'	-7.41	110.81	119.70
34	S4	11	C	C5-C6-N1	7.37	124.69	121.00
82	1	973	U	C2-N1-C1'	7.22	126.37	117.70
83	3	34	C	C2-N1-C1'	7.21	126.73	118.80
83	3	112	C	C2-N1-C1'	7.08	126.59	118.80
86	2	1063	C	C2-N1-C1'	7.04	126.54	118.80
86	2	44	C	C2-N1-C1'	6.94	126.44	118.80
35	S1	1426	U	C2-N1-C1'	6.87	125.94	117.70
84	5	112	U	N3-C2-O2	-6.80	117.44	122.20
37	4	8[A]	U	OP2-P-O3'	-6.78	90.28	105.20
37	4	8[B]	U	OP2-P-O3'	-6.78	90.28	105.20
86	2	748	C	N1-C2-O2	6.73	122.94	118.90
35	S1	1181	C	C2-N1-C1'	6.68	126.15	118.80
83	3	112	C	N1-C2-O2	6.65	122.89	118.90
82	1	437	A	OP1-P-OP2	-6.64	109.63	119.60
35	S1	1904	U	C2-N1-C1'	6.64	125.67	117.70
82	1	886	G	O4'-C1'-N9	6.58	113.47	108.20
84	5	112	U	N1-C2-O2	6.56	127.39	122.80
35	S1	549	U	C2-N1-C1'	6.55	125.56	117.70
82	1	1600	U	C2-N1-C1'	6.53	125.53	117.70
35	S1	1816	U	C2-N1-C1'	6.53	125.53	117.70
82	1	939	C	OP1-P-O3'	6.48	119.47	105.20
86	2	15	C	C2-N1-C1'	6.48	125.92	118.80
37	4	8[A]	U	P-O3'-C3'	-6.47	111.94	119.70
37	4	8[B]	U	P-O3'-C3'	-6.47	111.94	119.70
84	5	135	U	P-O3'-C3'	-6.44	111.98	119.70
83	3	112	C	N3-C2-O2	-6.43	117.40	121.90
82	1	421	U	OP1-P-O3'	6.41	119.31	105.20
82	1	1574	C	C2-N1-C1'	6.40	125.84	118.80
82	1	29	C	C2-N1-C1'	6.40	125.84	118.80
82	1	1252	C	C2-N1-C1'	6.37	125.81	118.80
83	3	34	C	N1-C2-O2	6.36	122.72	118.90
39	8	71	C	N3-C2-O2	-6.36	117.45	121.90
37	4	9	G	O5'-P-OP2	6.32	118.28	110.70
82	1	1238	C	C2-N1-C1'	6.31	125.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	1	1401	U	OP1-P-O3'	6.31	119.09	105.20
35	S1	509	G	OP1-P-OP2	-6.30	110.14	119.60
82	1	1376	C	N3-C2-O2	-6.30	117.49	121.90
82	1	1571	C	C6-N1-C2	-6.25	117.80	120.30
83	3	125	U	N1-C2-O2	6.25	127.18	122.80
35	S1	1788	U	N3-C2-O2	-6.24	117.83	122.20
82	1	993	U	N3-C2-O2	-6.24	117.83	122.20
82	1	948	U	N3-C2-O2	-6.22	117.84	122.20
82	1	949	U	N3-C2-O2	-6.22	117.84	122.20
86	2	748	C	N3-C2-O2	-6.19	117.57	121.90
82	1	1552	C	OP1-P-OP2	-6.19	110.32	119.60
37	4	161	C	C2-N1-C1'	6.18	125.59	118.80
35	S1	354	C	C2-N1-C1'	6.17	125.58	118.80
82	1	1376	C	C2-N1-C1'	6.17	125.58	118.80
37	4	19	C	P-O3'-C3'	-6.13	112.34	119.70
82	1	1600	U	N1-C2-O2	6.11	127.08	122.80
82	1	238	A	OP1-P-O3'	6.11	118.64	105.20
37	4	8[A]	U	OP1-P-O3'	-6.10	91.78	105.20
37	4	8[B]	U	OP1-P-O3'	-6.10	91.78	105.20
39	8	71	C	C6-N1-C2	-6.07	117.87	120.30
86	2	1115	U	N3-C2-O2	-6.06	117.95	122.20
86	2	479	C	C2-N1-C1'	6.06	125.47	118.80
86	2	61	C	N3-C2-O2	-6.06	117.66	121.90
86	2	1049	C	C2-N1-C1'	6.04	125.44	118.80
37	4	18	U	P-O3'-C3'	-6.03	112.46	119.70
86	2	1143	U	C2-N1-C1'	6.00	124.90	117.70
86	2	673	C	C2-N1-C1'	5.98	125.38	118.80
86	2	1063	C	N1-C2-O2	5.98	122.49	118.90
86	2	44	C	N3-C2-O2	-5.97	117.72	121.90
37	4	85	C	N3-C2-O2	-5.97	117.72	121.90
86	2	61	C	C6-N1-C1'	-5.97	113.64	120.80
83	3	131	C	C2-N1-C1'	5.92	125.31	118.80
35	S1	1572	C	N3-C2-O2	-5.91	117.76	121.90
82	1	1746	C	O4'-C1'-N1	5.90	112.92	108.20
34	S4	11	C	C6-N1-C2	-5.89	117.94	120.30
35	S1	630	U	C2-N1-C1'	5.85	124.72	117.70
83	3	34	C	N3-C2-O2	-5.85	117.81	121.90
86	2	1023	C	C2-N1-C1'	5.84	125.23	118.80
82	1	1358	C	C2-N1-C1'	5.81	125.19	118.80
82	1	1232	U	N3-C2-O2	-5.78	118.16	122.20
82	1	853	C	C2-N1-C1'	5.78	125.15	118.80
39	8	39	C	C2-N1-C1'	5.76	125.13	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	1600	C	N3-C2-O2	-5.75	117.88	121.90
37	4	1	G	P-O3'-C3'	-5.72	112.83	119.70
86	2	1456	C	C2-N1-C1'	5.71	125.08	118.80
82	1	1600	U	N3-C2-O2	-5.71	118.21	122.20
82	1	1354	C	C2-N1-C1'	5.70	125.07	118.80
83	3	112	C	C6-N1-C2	-5.67	118.03	120.30
35	S1	2040	C	N3-C2-O2	-5.65	117.94	121.90
37	4	161	C	N3-C2-O2	-5.65	117.94	121.90
83	3	119	C	N3-C2-O2	-5.62	117.97	121.90
86	2	1526	C	C2-N1-C1'	5.62	124.98	118.80
35	S1	1181	C	N1-C2-O2	5.61	122.26	118.90
82	1	1358	C	N3-C2-O2	-5.60	117.98	121.90
86	2	1151	U	N3-C2-O2	-5.59	118.29	122.20
83	3	188	C	C2-N1-C1'	5.58	124.94	118.80
84	5	112	U	C2-N1-C1'	5.58	124.39	117.70
35	S1	1572	C	C2-N1-C1'	5.57	124.93	118.80
86	2	79	C	C2-N1-C1'	-5.56	112.68	118.80
37	4	145	C	C2-N1-C1'	5.55	124.91	118.80
82	1	1277	G	P-O3'-C3'	5.55	126.36	119.70
82	1	1402	U	C2-N1-C1'	5.55	124.36	117.70
82	1	1355	C	C2-N1-C1'	5.54	124.90	118.80
35	S1	549	U	N1-C2-O2	5.54	126.68	122.80
82	1	853	C	N3-C2-O2	-5.54	118.02	121.90
35	S1	1788	U	N1-C2-O2	5.54	126.68	122.80
35	S1	748	C	C6-N1-C2	-5.53	118.09	120.30
82	1	1446	C	C2-N1-C1'	5.52	124.87	118.80
35	S1	1510	C	N3-C2-O2	-5.52	118.04	121.90
82	1	1089	C	C2-N1-C1'	5.52	124.87	118.80
86	2	1473	C	C2-N1-C1'	5.49	124.84	118.80
35	S1	2202	U	C2-N1-C1'	5.46	124.26	117.70
82	1	613	C	N3-C2-O2	-5.45	118.08	121.90
82	1	1277	G	OP1-P-O3'	5.45	117.19	105.20
82	1	1232	U	C2-N1-C1'	5.44	124.23	117.70
37	4	33	G	O4'-C1'-N9	5.44	112.55	108.20
35	S1	1212	C	C2-N1-C1'	5.42	124.77	118.80
83	3	188	C	N1-C2-O2	5.42	122.15	118.90
35	S1	1956	C	N1-C2-O2	5.41	122.15	118.90
86	2	7	C	C2-N1-C1'	5.41	124.75	118.80
35	S1	1904	U	C6-N1-C1'	-5.41	113.63	121.20
82	1	80	C	N3-C2-O2	-5.39	118.12	121.90
35	S1	2040	C	C6-N1-C2	-5.38	118.15	120.30
35	S1	1911	U	C2-N1-C1'	5.36	124.13	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	1609	U	C2-N1-C1'	5.35	124.11	117.70
83	3	20	C	C2-N1-C1'	5.34	124.67	118.80
35	S1	748	C	N3-C2-O2	-5.33	118.17	121.90
83	3	20	C	C6-N1-C2	-5.32	118.17	120.30
82	1	950	U	C2-N1-C1'	5.29	124.05	117.70
82	1	948	U	C2-N1-C1'	5.29	124.04	117.70
39	8	39	C	N1-C2-O2	5.28	122.07	118.90
35	S1	1788	U	C2-N1-C1'	5.27	124.03	117.70
82	1	1216	U	C2-N1-C1'	5.27	124.03	117.70
35	S1	1797	A	O4'-C1'-N9	5.26	112.41	108.20
85	7	164	U	C2-N1-C1'	5.25	123.99	117.70
86	2	1222	C	C2-N1-C1'	5.24	124.56	118.80
86	2	345	C	N3-C2-O2	-5.23	118.24	121.90
86	2	756	C	C2-N1-C1'	5.23	124.55	118.80
34	S4	10	G	N3-C4-C5	-5.22	125.99	128.60
83	3	119	C	N1-C2-O2	5.22	122.03	118.90
82	1	196	C	C2-N1-C1'	5.21	124.53	118.80
86	2	3	C	C2-N1-C1'	5.21	124.53	118.80
86	2	1353	U	OP1-P-O3'	-5.20	93.77	105.20
86	2	673	C	N3-C2-O2	-5.19	118.27	121.90
82	1	1046	U	N3-C2-O2	-5.19	118.57	122.20
37	4	6	A	P-O3'-C3'	-5.19	113.47	119.70
86	2	2	C	C2-N1-C1'	5.19	124.51	118.80
35	S1	1467	U	C2-N1-C1'	5.18	123.92	117.70
82	1	1376	C	N1-C2-O2	5.17	122.00	118.90
86	2	1222	C	N3-C2-O2	-5.17	118.28	121.90
86	2	1157	U	N3-C2-O2	-5.17	118.58	122.20
82	1	704	G	P-O3'-C3'	5.16	125.89	119.70
35	S1	734	U	C2-N1-C1'	5.15	123.88	117.70
39	8	71	C	C2-N1-C1'	5.15	124.47	118.80
82	1	853	C	N1-C2-O2	5.15	121.99	118.90
35	S1	1973	C	N1-C2-O2	5.14	121.98	118.90
82	1	1217	U	C2-N1-C1'	5.14	123.87	117.70
86	2	379	U	C2-N1-C1'	5.14	123.87	117.70
35	S1	1510	C	C2-N1-C1'	5.14	124.45	118.80
82	1	613	C	C2-N1-C1'	5.13	124.45	118.80
83	3	33	A	P-O3'-C3'	5.13	125.86	119.70
86	2	1293	C	P-O3'-C3'	5.13	125.86	119.70
83	3	20	C	N3-C2-O2	-5.13	118.31	121.90
82	1	1046	U	C2-N1-C1'	5.12	123.85	117.70
86	2	7	C	N1-C2-O2	5.12	121.97	118.90
84	5	4	C	C2-N1-C1'	5.12	124.43	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	1	725	U	C2-N1-C1'	5.11	123.83	117.70
35	S1	747	C	C2-N1-C1'	5.11	124.42	118.80
83	3	34	C	C6-N1-C2	-5.10	118.26	120.30
86	2	345	C	N1-C2-O2	5.10	121.96	118.90
83	3	172	G	N3-C2-N2	-5.09	116.33	119.90
35	S1	748	C	N1-C2-O2	5.09	121.95	118.90
35	S1	630	U	N1-C2-O2	5.09	126.36	122.80
82	1	950	U	N3-C2-O2	-5.09	118.64	122.20
82	1	1574	C	N1-C2-O2	5.08	121.95	118.90
37	4	85	C	C6-N1-C2	-5.08	118.27	120.30
35	S1	254	A	P-O3'-C3'	5.08	125.79	119.70
86	2	1009	U	N3-C2-O2	-5.08	118.64	122.20
35	S1	659	G	C4-N9-C1'	5.07	133.09	126.50
86	2	1221	U	C2-N1-C1'	5.05	123.76	117.70
86	2	851	C	O4'-C1'-N1	5.04	112.23	108.20
86	2	1115	U	C2-N1-C1'	5.04	123.75	117.70
35	S1	1973	C	C2-N1-C1'	5.04	124.34	118.80
86	2	1143	U	N3-C2-O2	-5.04	118.68	122.20
35	S1	147	U	C2-N1-C1'	5.02	123.73	117.70
38	6	11	G	O4'-C1'-N9	5.01	112.21	108.20
35	S1	1904	U	OP1-P-O3'	5.01	116.23	105.20
86	2	1157	U	C2-N1-C1'	5.01	123.71	117.70
82	1	208	C	C2-N1-C1'	5.01	124.31	118.80
35	S1	2040	C	C2-N1-C1'	5.00	124.31	118.80

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	SB	206/246 (84%)	196 (95%)	10 (5%)	0	100	100
2	SC	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
3	SD	180/190 (95%)	179 (99%)	1 (1%)	0	100	100
4	SE	258/273 (94%)	254 (98%)	4 (2%)	0	100	100
5	SF	217/265 (82%)	214 (99%)	3 (1%)	0	100	100
6	SG	229/249 (92%)	222 (97%)	6 (3%)	1 (0%)	30	53
7	SH	178/190 (94%)	174 (98%)	4 (2%)	0	100	100
8	SI	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
9	SJ	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
10	SK	178/220 (81%)	178 (100%)	0	0	100	100
11	SL	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
12	SM	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
13	SN	98/168 (58%)	94 (96%)	4 (4%)	0	100	100
14	SO	134/144 (93%)	130 (97%)	4 (3%)	0	100	100
15	SP	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
16	SQ	87/141 (62%)	78 (90%)	9 (10%)	0	100	100
17	SR	134/153 (88%)	128 (96%)	6 (4%)	0	100	100
18	SS	54/57 (95%)	54 (100%)	0	0	100	100
19	ST	140/151 (93%)	139 (99%)	1 (1%)	0	100	100
20	SU	144/173 (83%)	141 (98%)	3 (2%)	0	100	100
21	SV	103/143 (72%)	98 (95%)	5 (5%)	0	100	100
22	SW	113/152 (74%)	111 (98%)	2 (2%)	0	100	100
23	SX	150/161 (93%)	145 (97%)	5 (3%)	0	100	100
24	SY	85/164 (52%)	81 (95%)	4 (5%)	0	100	100
25	SZ	125/137 (91%)	124 (99%)	1 (1%)	0	100	100
26	Sa	69/120 (58%)	67 (97%)	2 (3%)	0	100	100
27	Sb	101/112 (90%)	97 (96%)	4 (4%)	0	100	100
28	Sc	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
29	Sd	63/87 (72%)	63 (100%)	0	0	100	100
30	Se	47/66 (71%)	46 (98%)	1 (2%)	0	100	100
31	Sf	59/152 (39%)	56 (95%)	3 (5%)	0	100	100
32	Sg	286/312 (92%)	273 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Sh	67/235 (28%)	62 (92%)	5 (8%)	0	100	100
36	SA	224/264 (85%)	216 (96%)	8 (4%)	0	100	100
40	A	254/260 (98%)	246 (97%)	8 (3%)	0	100	100
41	B	399/419 (95%)	392 (98%)	7 (2%)	0	100	100
42	C	364/373 (98%)	356 (98%)	8 (2%)	0	100	100
43	D	171/188 (91%)	165 (96%)	6 (4%)	0	100	100
44	E	184/190 (97%)	178 (97%)	6 (3%)	0	100	100
45	H	219/222 (99%)	217 (99%)	2 (1%)	0	100	100
46	I	207/220 (94%)	204 (99%)	3 (1%)	0	100	100
47	J	132/139 (95%)	130 (98%)	2 (2%)	0	100	100
48	K	168/175 (96%)	162 (96%)	6 (4%)	0	100	100
49	L	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
50	M	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
51	P	195/198 (98%)	187 (96%)	8 (4%)	0	100	100
52	Q	183/254 (72%)	182 (100%)	1 (0%)	0	100	100
53	R	176/179 (98%)	175 (99%)	1 (1%)	0	100	100
54	S	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
55	T	149/166 (90%)	147 (99%)	2 (1%)	0	100	100
56	U	10/129 (8%)	10 (100%)	0	0	100	100
57	V	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
58	W	118/143 (82%)	115 (98%)	3 (2%)	0	100	100
59	X	62/124 (50%)	61 (98%)	1 (2%)	0	100	100
60	Y	131/134 (98%)	129 (98%)	2 (2%)	0	100	100
61	Z	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
62	a	122/127 (96%)	119 (98%)	3 (2%)	0	100	100
63	b	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
64	c	227/252 (90%)	221 (97%)	6 (3%)	0	100	100
65	d	90/104 (86%)	89 (99%)	1 (1%)	0	100	100
66	f	124/133 (93%)	120 (97%)	4 (3%)	0	100	100
67	g	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
68	h	123/168 (73%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	i	96/105 (91%)	96 (100%)	0	0	100	100
70	j	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
71	k	75/83 (90%)	75 (100%)	0	0	100	100
72	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
73	m	49/128 (38%)	49 (100%)	0	0	100	100
74	n	31/34 (91%)	26 (84%)	5 (16%)	0	100	100
75	o	86/92 (94%)	81 (94%)	5 (6%)	0	100	100
76	p	96/106 (91%)	94 (98%)	2 (2%)	0	100	100
77	F	144/195 (74%)	140 (97%)	4 (3%)	0	100	100
78	G	224/264 (85%)	221 (99%)	3 (1%)	0	100	100
79	N	195/213 (92%)	188 (96%)	7 (4%)	0	100	100
80	O	274/305 (90%)	270 (98%)	4 (2%)	0	100	100
81	e	181/188 (96%)	175 (97%)	6 (3%)	0	100	100
All	All	11077/12926 (86%)	10807 (98%)	269 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	SG	172	ASP

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	SB	173/202 (86%)	165 (95%)	8 (5%)	23	47
2	SC	171/184 (93%)	164 (96%)	7 (4%)	26	52
3	SD	154/164 (94%)	150 (97%)	4 (3%)	41	69
4	SE	215/225 (96%)	211 (98%)	4 (2%)	52	77
5	SF	175/208 (84%)	171 (98%)	4 (2%)	45	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	SG	189/208 (91%)	181 (96%)	8 (4%)	25	51
7	SH	151/159 (95%)	146 (97%)	5 (3%)	33	61
8	SI	175/186 (94%)	173 (99%)	2 (1%)	70	87
9	SJ	110/111 (99%)	107 (97%)	3 (3%)	40	68
10	SK	141/176 (80%)	135 (96%)	6 (4%)	25	50
11	SL	113/120 (94%)	111 (98%)	2 (2%)	54	78
12	SM	92/104 (88%)	90 (98%)	2 (2%)	47	74
13	SN	86/128 (67%)	82 (95%)	4 (5%)	22	47
14	SO	103/113 (91%)	100 (97%)	3 (3%)	37	65
15	SP	114/117 (97%)	111 (97%)	3 (3%)	41	69
16	SQ	59/120 (49%)	54 (92%)	5 (8%)	8	20
17	SR	111/130 (85%)	108 (97%)	3 (3%)	40	68
18	SS	47/49 (96%)	47 (100%)	0	100	100
19	ST	124/132 (94%)	121 (98%)	3 (2%)	44	71
20	SU	125/152 (82%)	119 (95%)	6 (5%)	21	46
21	SV	89/126 (71%)	86 (97%)	3 (3%)	32	59
22	SW	97/130 (75%)	92 (95%)	5 (5%)	19	42
23	SX	121/131 (92%)	117 (97%)	4 (3%)	33	61
24	SY	67/116 (58%)	65 (97%)	2 (3%)	36	64
25	SZ	109/118 (92%)	108 (99%)	1 (1%)	75	89
26	Sa	63/95 (66%)	61 (97%)	2 (3%)	34	62
27	Sb	85/93 (91%)	82 (96%)	3 (4%)	31	58
28	Sc	70/76 (92%)	63 (90%)	7 (10%)	6	15
29	Sd	48/75 (64%)	46 (96%)	2 (4%)	25	51
30	Se	42/54 (78%)	42 (100%)	0	100	100
31	Sf	56/126 (44%)	52 (93%)	4 (7%)	12	29
32	Sg	235/265 (89%)	225 (96%)	10 (4%)	25	50
33	Sh	47/177 (27%)	42 (89%)	5 (11%)	5	13
36	SA	197/222 (89%)	189 (96%)	8 (4%)	26	52
40	A	195/204 (96%)	193 (99%)	2 (1%)	73	88
41	B	324/351 (92%)	320 (99%)	4 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	C	286/301 (95%)	279 (98%)	7 (2%)	44	71
43	D	121/162 (75%)	115 (95%)	6 (5%)	20	44
44	E	164/172 (95%)	158 (96%)	6 (4%)	29	56
45	H	181/188 (96%)	177 (98%)	4 (2%)	47	74
46	I	171/183 (93%)	169 (99%)	2 (1%)	67	85
47	J	103/111 (93%)	102 (99%)	1 (1%)	73	88
48	K	129/145 (89%)	122 (95%)	7 (5%)	18	41
49	L	109/114 (96%)	107 (98%)	2 (2%)	54	78
50	M	176/180 (98%)	170 (97%)	6 (3%)	32	59
51	P	160/164 (98%)	158 (99%)	2 (1%)	65	84
52	Q	152/198 (77%)	150 (99%)	2 (1%)	65	84
53	R	156/159 (98%)	155 (99%)	1 (1%)	84	93
54	S	130/134 (97%)	128 (98%)	2 (2%)	60	82
55	T	128/143 (90%)	126 (98%)	2 (2%)	58	81
56	U	7/114 (6%)	6 (86%)	1 (14%)	2	6
57	V	98/124 (79%)	93 (95%)	5 (5%)	20	43
58	W	102/122 (84%)	98 (96%)	4 (4%)	27	54
59	X	58/104 (56%)	56 (97%)	2 (3%)	32	59
60	Y	104/116 (90%)	102 (98%)	2 (2%)	52	77
61	Z	115/118 (98%)	113 (98%)	2 (2%)	56	80
62	a	110/118 (93%)	107 (97%)	3 (3%)	40	68
63	b	56/58 (97%)	54 (96%)	2 (4%)	30	57
64	c	192/209 (92%)	188 (98%)	4 (2%)	48	75
65	d	80/89 (90%)	76 (95%)	4 (5%)	20	44
66	f	108/115 (94%)	106 (98%)	2 (2%)	52	77
67	g	120/121 (99%)	115 (96%)	5 (4%)	25	51
68	h	105/146 (72%)	103 (98%)	2 (2%)	52	77
69	i	79/88 (90%)	78 (99%)	1 (1%)	65	84
70	j	68/70 (97%)	66 (97%)	2 (3%)	37	65
71	k	67/74 (90%)	67 (100%)	0	100	100
72	l	46/47 (98%)	45 (98%)	1 (2%)	47	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	m	44/113 (39%)	44 (100%)	0	100	100
74	n	30/32 (94%)	29 (97%)	1 (3%)	33	61
75	o	70/74 (95%)	67 (96%)	3 (4%)	25	50
76	p	83/92 (90%)	79 (95%)	4 (5%)	21	46
77	F	113/153 (74%)	108 (96%)	5 (4%)	24	49
78	G	183/221 (83%)	178 (97%)	5 (3%)	40	68
79	N	168/179 (94%)	159 (95%)	9 (5%)	18	41
80	O	195/242 (81%)	192 (98%)	3 (2%)	60	82
81	e	152/158 (96%)	143 (94%)	9 (6%)	16	37
All	All	9192/10798 (85%)	8917 (97%)	275 (3%)	37	64

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SB	17	ASP
1	SB	27	HIS
1	SB	31	ARG
1	SB	77	VAL
1	SB	84	LEU
1	SB	95	GLN
1	SB	126	VAL
1	SB	202	VAL
2	SC	44	ARG
2	SC	63	ARG
2	SC	75	ARG
2	SC	115	ARG
2	SC	127	GLU
2	SC	136	THR
2	SC	213	LYS
3	SD	24	ASP
3	SD	89	LYS
3	SD	92	LEU
3	SD	171	VAL
4	SE	68	HIS
4	SE	133	VAL
4	SE	178	VAL
4	SE	208	LYS
5	SF	106	GLN
5	SF	151	VAL

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Mol	Chain	Res	Type
5	SF	153	ARG
5	SF	234	TYR
6	SG	1	MET
6	SG	7	TYR
6	SG	9	ARG
6	SG	27	GLN
6	SG	114	VAL
6	SG	149	ASN
6	SG	210	ARG
6	SG	230	LYS
7	SH	64	PHE
7	SH	67	ARG
7	SH	121	ARG
7	SH	142	LYS
7	SH	161	ASP
8	SI	12	LYS
8	SI	157	LEU
9	SJ	23	ARG
9	SJ	49	GLU
9	SJ	105	THR
10	SK	29	LEU
10	SK	43	VAL
10	SK	58	LEU
10	SK	79	LEU
10	SK	81	VAL
10	SK	184	VAL
11	SL	20	THR
11	SL	96	ILE
12	SM	16	THR
12	SM	44	LYS
13	SN	17	PHE
13	SN	32	THR
13	SN	37	LEU
13	SN	98	GLN
14	SO	45	THR
14	SO	118	LYS
14	SO	124	ASP
15	SP	19	ARG
15	SP	105	PHE
15	SP	135	ARG
16	SQ	35	GLN
16	SQ	87	ASP

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Mol	Chain	Res	Type
16	SQ	94	ARG
16	SQ	123	ILE
16	SQ	126	PHE
17	SR	87	ARG
17	SR	135	GLN
17	SR	136	HIS
19	ST	2	VAL
19	ST	104	ARG
19	ST	132	VAL
20	SU	13	VAL
20	SU	19	HIS
20	SU	39	LYS
20	SU	82	ARG
20	SU	117	LYS
20	SU	153	ASN
21	SV	5	ARG
21	SV	8	THR
21	SV	111	ARG
22	SW	22	PHE
22	SW	50	ARG
22	SW	75	LYS
22	SW	91	VAL
22	SW	107	HIS
23	SX	19	LEU
23	SX	113	LEU
23	SX	114	HIS
23	SX	138	ARG
24	SY	26	THR
24	SY	56	THR
25	SZ	56	VAL
26	Sa	67	ASP
26	Sa	82	GLN
27	Sb	17	ARG
27	Sb	98	ILE
27	Sb	103	LYS
28	Sc	14	ARG
28	Sc	42	ARG
28	Sc	53	THR
28	Sc	58	LYS
28	Sc	60	CYS
28	Sc	68	THR
28	Sc	78	CYS

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Mol	Chain	Res	Type
29	Sd	71	ASP
29	Sd	78	THR
31	Sf	80	PHE
31	Sf	81	THR
31	Sf	137	ARG
31	Sf	148	LYS
32	Sg	6	HIS
32	Sg	87	ARG
32	Sg	111	LEU
32	Sg	115	PHE
32	Sg	146	ARG
32	Sg	147	ASP
32	Sg	153	VAL
32	Sg	158	PHE
32	Sg	174	ASN
32	Sg	189	THR
33	Sh	138	VAL
33	Sh	163	GLN
33	Sh	169	ARG
33	Sh	177	LEU
33	Sh	200	LEU
36	SA	51	THR
36	SA	121	THR
36	SA	133	ASP
36	SA	159	LYS
36	SA	166	LEU
36	SA	222	THR
36	SA	226	ASP
36	SA	236	THR
40	A	106	GLN
40	A	108	THR
41	B	26	ARG
41	B	282	GLN
41	B	323	THR
41	B	381	LYS
42	C	62	SER
42	C	121	PHE
42	C	171	LYS
42	C	192	ARG
42	C	198	ARG
42	C	203	ARG
42	C	225	LEU

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Mol	Chain	Res	Type
43	D	15	VAL
43	D	109	ASP
43	D	110	GLU
43	D	111	HIS
43	D	131	VAL
43	D	167	LYS
44	E	50	LYS
44	E	83	VAL
44	E	127	ASN
44	E	171	ILE
44	E	172	ARG
44	E	180	VAL
45	H	85	THR
45	H	86	LYS
45	H	149	ARG
45	H	182	LYS
46	I	137	LYS
46	I	152	THR
47	J	47	ARG
48	K	17	ARG
48	K	42	GLU
48	K	95	ARG
48	K	131	LYS
48	K	135	THR
48	K	153	LYS
48	K	154	MET
49	L	39	HIS
49	L	117	VAL
50	M	29	GLU
50	M	117	ASN
50	M	154	SER
50	M	164	LEU
50	M	189	ARG
50	M	202	ARG
51	P	144	TYR
51	P	150	LYS
52	Q	43	LYS
52	Q	180	LYS
53	R	157	ARG
54	S	24	VAL
54	S	116	LEU
55	T	66	LYS

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Mol	Chain	Res	Type
55	T	79	THR
56	U	7	LYS
57	V	32	ARG
57	V	34	GLN
57	V	39	HIS
57	V	58	LYS
57	V	141	LYS
58	W	9	ARG
58	W	41	ASN
58	W	109	THR
58	W	121	ARG
59	X	3	THR
59	X	30	LYS
60	Y	99	VAL
60	Y	119	ARG
61	Z	17	ARG
61	Z	136	LYS
62	a	5	MET
62	a	92	THR
62	a	100	LYS
63	b	29	LEU
63	b	69	LYS
64	c	129	MET
64	c	131	LYS
64	c	164	LEU
64	c	246	ARG
65	d	26	VAL
65	d	86	HIS
65	d	90	CYS
65	d	94	VAL
66	f	56	LYS
66	f	127	LEU
67	g	3	THR
67	g	52	GLN
67	g	63	THR
67	g	66	ASP
67	g	143	GLN
68	h	12	MET
68	h	110	GLU
69	i	31	ASP
70	j	33	ARG
70	j	80	THR

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Mol	Chain	Res	Type
72	l	5	LYS
74	n	24	LEU
75	o	41	PHE
75	o	42	CYS
75	o	47	PHE
76	p	72	LEU
76	p	81	ARG
76	p	97	LYS
76	p	99	THR
77	F	45	ARG
77	F	84	VAL
77	F	145	LEU
77	F	148	ASP
77	F	172	LYS
78	G	49	ARG
78	G	69	ARG
78	G	76	LEU
78	G	167	MET
78	G	183	ASP
79	N	24	ARG
79	N	28	ASP
79	N	43	VAL
79	N	54	SER
79	N	128	ARG
79	N	193	ARG
79	N	198	LYS
79	N	209	ARG
79	N	211	VAL
80	O	93	THR
80	O	126	ASP
80	O	233	SER
81	e	30	ARG
81	e	80	LYS
81	e	119	LEU
81	e	140	VAL
81	e	141	LYS
81	e	154	LYS
81	e	158	THR
81	e	179	LYS
81	e	187	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
7	SH	189	ASN
21	SV	107	GLN
21	SV	110	GLN
22	SW	121	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	S4	64/76 (84%)	31 (48%)	2 (3%)
35	S1	1819/2204 (82%)	442 (24%)	12 (0%)
37	4	182/184 (98%)	35 (19%)	2 (1%)
38	6	70/73 (95%)	24 (34%)	2 (2%)
39	8	118/123 (95%)	9 (7%)	0
82	1	1636/1782 (91%)	391 (23%)	13 (0%)
83	3	173/216 (80%)	41 (23%)	4 (2%)
84	5	112/135 (82%)	30 (26%)	3 (2%)
85	7	160/171 (93%)	32 (20%)	2 (1%)
86	2	1181/1526 (77%)	311 (26%)	6 (0%)
All	All	5515/6490 (84%)	1346 (24%)	46 (0%)

All (1346) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	S4	4	C
34	S4	5	G
34	S4	6	G
34	S4	7	A
34	S4	8	U
34	S4	9	A
34	S4	10	G
34	S4	11	C
34	S4	12	U
34	S4	13	C
34	S4	14	A
34	S4	16	U
34	S4	21	A
34	S4	23	A
34	S4	27	G
34	S4	28	G
34	S4	30	G
34	S4	31	A
34	S4	45	U

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Mol	Chain	Res	Type
34	S4	46	G
34	S4	49	C
34	S4	50	U
34	S4	52	G
34	S4	60	U
34	S4	61	C
34	S4	65	G
34	S4	70	C
34	S4	71	G
34	S4	73	A
34	S4	74	C
34	S4	76	A
35	S1	3	U
35	S1	11	A
35	S1	17	C
35	S1	26	A
35	S1	27	U
35	S1	33	PSU
35	S1	34	G
35	S1	35	U
35	S1	42	G
35	S1	44	C
35	S1	45	U
35	S1	47	A
35	S1	57	G
35	S1	60	U
35	S1	61	C
35	S1	65	A
35	S1	98	A2M
35	S1	102	A
35	S1	103	A
35	S1	112	A
35	S1	114	U
35	S1	117	G
35	S1	122	A
35	S1	145	A
35	S1	146	U
35	S1	150	A
35	S1	158	G
35	S1	165	G
35	S1	167	C
35	S1	171	C

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Mol	Chain	Res	Type
35	S1	174	A
35	S1	176	A
35	S1	181	A
35	S1	192	U
35	S1	193	G
35	S1	194	U
35	S1	195	U
35	S1	198	C
35	S1	200	A
35	S1	201	C
35	S1	227	U
35	S1	228	G
35	S1	231	A
35	S1	235	C
35	S1	236	C
35	S1	238	G
35	S1	245	A
35	S1	249	A
35	S1	252	G
35	S1	254	A
35	S1	255	A
35	S1	263	G
35	S1	264	C
35	S1	275	A
35	S1	276	G
35	S1	281	A
35	S1	282	C
35	S1	284	C
35	S1	286	G
35	S1	287	C
35	S1	288	A
35	S1	308	C
35	S1	310	U
35	S1	313	G
35	S1	315	A
35	S1	316	A
35	S1	320	G
35	S1	321	G
35	S1	322	C
35	S1	327	U
35	S1	329	C
35	S1	333	G

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Mol	Chain	Res	Type
35	S1	340	G
35	S1	356	A
35	S1	358	C
35	S1	360	G
35	S1	364	G
35	S1	377	A
35	S1	381	G
35	S1	382	A
35	S1	404	C
35	S1	405	G
35	S1	433	G
35	S1	443	A
35	S1	444	A
35	S1	445	U
35	S1	447	G
35	S1	461	G
35	S1	466	G
35	S1	467	C
35	S1	469	G
35	S1	470	C
35	S1	471	A
35	S1	473	G
35	S1	477	G
35	S1	481	A
35	S1	482	U
35	S1	487	C
35	S1	495	A
35	S1	499	A
35	S1	501	A
35	S1	503	C
35	S1	516	A
35	S1	525	A
35	S1	527	A
35	S1	528	G
35	S1	549	U
35	S1	550	C
35	S1	551	A
35	S1	553	U
35	S1	554	U
35	S1	556	A
35	S1	559	G
35	S1	566	A

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Mol	Chain	Res	Type
35	S1	576	A
35	S1	580	A
35	S1	581	A
35	S1	582	U
35	S1	585	C
35	S1	588	G
35	S1	591	A
35	S1	600	OMG
35	S1	606	G
35	S1	614	C
35	S1	617	G
35	S1	627	U
35	S1	628	A
35	S1	631	U
35	S1	643	A
35	S1	660	U
35	S1	668	A2M
35	S1	669	A
35	S1	671	G
35	S1	672	G
35	S1	673	G
35	S1	678	U
35	S1	679	A
35	S1	689	U
35	S1	691	G
35	S1	692	G
35	S1	697	G
35	S1	701	G
35	S1	702	U
35	S1	703	U
35	S1	712	G
35	S1	713	U
35	S1	714	C
35	S1	715	G
35	S1	716	U
35	S1	735	G
35	S1	736	G
35	S1	737	U
35	S1	738	G
35	S1	739	A
35	S1	741	C
35	S1	743	A

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Mol	Chain	Res	Type
35	S1	744	G
35	S1	745	G
35	S1	746	C
35	S1	747	C
35	S1	752	C
35	S1	756	C
35	S1	757	C
35	S1	758	G
35	S1	769	A
35	S1	770	A
35	S1	771	G
35	S1	772	A
35	S1	773	A
35	S1	777	A
35	S1	778	G
35	S1	779	A
35	S1	780	A
35	S1	782	C
35	S1	783	A
35	S1	785	G
35	S1	787	G
35	S1	788	A
35	S1	789	G
35	S1	792	G
35	S1	793	G
35	S1	794	U
35	S1	814	G
35	S1	817	A
35	S1	818	U
35	S1	819	G
35	S1	833	G
35	S1	834	U
35	S1	838	U
35	S1	840	A
35	S1	854	C
35	S1	856	A
35	S1	866	G
35	S1	867	A
35	S1	876	G
35	S1	881	U
35	S1	882	U
35	S1	883	G

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Mol	Chain	Res	Type
35	S1	886	U
35	S1	887	U
35	S1	892	U
35	S1	895	A
35	S1	916	G
35	S1	918	A2M
35	S1	953	U
35	S1	954	A
35	S1	955	A
35	S1	956	A
35	S1	957	G
35	S1	958	G
35	S1	961	U
35	S1	962	A
35	S1	963	U
35	S1	969	A2M
35	S1	970	U
35	S1	975	G
35	S1	977	G
35	S1	978	C
35	S1	986	C
35	S1	987	A
35	S1	989	A
35	S1	990	U
35	S1	991	G
35	S1	992	C
35	S1	994	U
35	S1	998	C
35	S1	1000	U
35	S1	1014	C
35	S1	1038	U
35	S1	1040	A
35	S1	1041	G
35	S1	1042	U
35	S1	1097	C
35	S1	1098	U
35	S1	1100	U
35	S1	1101	A
35	S1	1102	G
35	S1	1105	A
35	S1	1109	A
35	S1	1119	U

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Mol	Chain	Res	Type
35	S1	1123	G
35	S1	1139	G
35	S1	1160	A
35	S1	1161	G
35	S1	1169	C
35	S1	1171	A
35	S1	1180	A
35	S1	1181	C
35	S1	1182	A
35	S1	1191	A
35	S1	1196	U
35	S1	1197	C
35	S1	1198	A
35	S1	1199	A
35	S1	1207	U
35	S1	1210	C
35	S1	1211	U
35	S1	1213	A
35	S1	1217	A
35	S1	1235	A
35	S1	1239	A
35	S1	1240	A
35	S1	1245	A
35	S1	1248	A
35	S1	1251	A
35	S1	1252	A
35	S1	1272	A
35	S1	1273	A
35	S1	1275	C
35	S1	1277	A
35	S1	1284	C
35	S1	1290	A
35	S1	1296	G
35	S1	1371	U
35	S1	1410	C
35	S1	1411	A
35	S1	1443	U
35	S1	1444	G
35	S1	1448	U
35	S1	1449	U
35	S1	1452	A
35	S1	1461	G

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Mol	Chain	Res	Type
35	S1	1463	G
35	S1	1465	A
35	S1	1466	G
35	S1	1467	U
35	S1	1478	OMG
35	S1	1490	A
35	S1	1493	A
35	S1	1502	G
35	S1	1503	A
35	S1	1510	C
35	S1	1516	G
35	S1	1518	C
35	S1	1537	U
35	S1	1538	U
35	S1	1542	C
35	S1	1546	A
35	S1	1548	A
35	S1	1551	G
35	S1	1552	G
35	S1	1554	A
35	S1	1566	PSU
35	S1	1569	G
35	S1	1570	G
35	S1	1580	G
35	S1	1581	G
35	S1	1595	G
35	S1	1597	G
35	S1	1598	U
35	S1	1600	C
35	S1	1603	U
35	S1	1604	C
35	S1	1608	A
35	S1	1609	U
35	S1	1614	U
35	S1	1617	A
35	S1	1621	OMU
35	S1	1638	U
35	S1	1643	G
35	S1	1653	U
35	S1	1658	U
35	S1	1659	U
35	S1	1666	U

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Mol	Chain	Res	Type
35	S1	1667	U
35	S1	1673	A
35	S1	1674	A
35	S1	1676	G
35	S1	1688	A
35	S1	1689	G
35	S1	1690	C
35	S1	1695	C
35	S1	1696	A
35	S1	1697	G
35	S1	1699	A
35	S1	1700	G
35	S1	1705	C
35	S1	1712	G
35	S1	1713	C
35	S1	1715	C
35	S1	1716	A
35	S1	1724	G
35	S1	1725	C
35	S1	1762	A
35	S1	1768	U
35	S1	1770	G
35	S1	1775	C
35	S1	1776	U
35	S1	1782	G
35	S1	1787	A
35	S1	1788	U
35	S1	1789	U
35	S1	1795	G
35	S1	1796	U
35	S1	1797	A
35	S1	1798	U
35	S1	1799	U
35	S1	1800	U
35	S1	1806	A
35	S1	1813	A
35	S1	1814	U
35	S1	1826	G
35	S1	1828	A
35	S1	1829	OMG
35	S1	1833	OMU
35	S1	1846	A

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Mol	Chain	Res	Type
35	S1	1847	A
35	S1	1860	C
35	S1	1872	A
35	S1	1874	U
35	S1	1884	A
35	S1	1887	A
35	S1	1889	G
35	S1	1890	A
35	S1	1891	A
35	S1	1894	A
35	S1	1895	C
35	S1	1896	G
35	S1	1905	C
35	S1	1906	G
35	S1	1907	A
35	S1	1915	U
35	S1	1916	G
35	S1	1917	A
35	S1	1919	C
35	S1	1920	A
35	S1	1923	A
35	S1	1926	G
35	S1	1928	G
35	S1	1932	A
35	S1	1933	A
35	S1	1942	A
35	S1	1944	C
35	S1	1948	U
35	S1	1949	A
35	S1	1950	G
35	S1	1955	A
35	S1	1956	C
35	S1	1961	G
35	S1	1963	C
35	S1	1966	A
35	S1	1976	U
35	S1	1978	A
35	S1	1989	A
35	S1	1991	C
35	S1	2004	G
35	S1	2010	G
35	S1	2015	U

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Mol	Chain	Res	Type
35	S1	2016	C
35	S1	2017	A
35	S1	2021	A2M
35	S1	2031	A
35	S1	2039	C
35	S1	2052	C
35	S1	2055	A
35	S1	2057	C
35	S1	2058	G
35	S1	2063	U
35	S1	2070	U
35	S1	2100	A
35	S1	2118	G
35	S1	2120	C
35	S1	2122	G
35	S1	2157	A
35	S1	2159	A
35	S1	2160	G
35	S1	2163	G
35	S1	2165	A
35	S1	2166	A
35	S1	2169	A
35	S1	2170	G
35	S1	2172	U
35	S1	2177	G
35	S1	2183	G
35	S1	2195	G
35	S1	2196	G
35	S1	2197	G
35	S1	2198	A
35	S1	2199	C
35	S1	2202	U
35	S1	2203	U
35	S1	2204	U
37	4	4	A
37	4	7	U
37	4	9	G
37	4	10	U
37	4	11	G
37	4	14	G
37	4	15	G
37	4	16	G

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Mol	Chain	Res	Type
37	4	20	U
37	4	31	G
37	4	40	G
37	4	50	G
37	4	58	G
37	4	60	A
37	4	76	C
37	4	85	C
37	4	86	U
37	4	92	U
37	4	93	U
37	4	97	G
37	4	102	G
37	4	114	A
37	4	120	U
37	4	121	C
37	4	127	G
37	4	128	U
37	4	132	U
37	4	148	C
37	4	155	A
37	4	156	G
37	4	158	A
37	4	159	G
37	4	168	A
37	4	171	A
37	4	173	C
38	6	5	C
38	6	7	A
38	6	12	C
38	6	15	C
38	6	22	G
38	6	24	C
38	6	25	U
38	6	26	G
38	6	31	U
38	6	39	U
38	6	42	A
38	6	43	A
38	6	44	G
38	6	45	G
38	6	51	A

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Mol	Chain	Res	Type
38	6	52	G
38	6	54	A
38	6	63	A
38	6	64	U
38	6	65	C
38	6	70	G
38	6	71	A
38	6	72	C
38	6	73	A
39	8	22	A
39	8	37	U
39	8	46	A
39	8	53	A
39	8	57	U
39	8	67	C
39	8	68	A
39	8	104	A
39	8	114	G
82	1	20	G
82	1	24	A
82	1	25	C
82	1	32	A
82	1	38	A
82	1	41	A
82	1	47	C
82	1	58	A
82	1	64	A
82	1	70	C
82	1	71	C
82	1	75	A
82	1	81	U
82	1	84	G
82	1	86	G
82	1	87	A
82	1	91	G
82	1	98	A
82	1	108	G
82	1	109	A
82	1	110	A
82	1	111	C
82	1	117	G
82	1	119	C

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Mol	Chain	Res	Type
82	1	127	G
82	1	131	U
82	1	132	A
82	1	135	A
82	1	136	G
82	1	138	C
82	1	140	U
82	1	141	U
82	1	142	G
82	1	143	A
82	1	156	A
82	1	165	U
82	1	166	G
82	1	169	G
82	1	170	U
82	1	171	U
82	1	175	G
82	1	187	A
82	1	191	U
82	1	192	C
82	1	199	A
82	1	200	A
82	1	201	A
82	1	208	C
82	1	212	U
82	1	218	A
82	1	223	A
82	1	233	U
82	1	234	G
82	1	238	A
82	1	243	G
82	1	245	C
82	1	251	A
82	1	255	G
82	1	256	U
82	1	264	U
82	1	267	A
82	1	273	A
82	1	280	A
82	1	281	G
82	1	291	A
82	1	292	A

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Mol	Chain	Res	Type
82	1	301	A
82	1	302	G
82	1	303	C
82	1	306	G
82	1	307	U
82	1	310	C
82	1	314	G
82	1	323	U
82	1	330	U
82	1	331	C
82	1	332	A
82	1	334	G
82	1	335	U
82	1	336	U
82	1	337	G
82	1	343	U
82	1	348	G
82	1	351	U
82	1	352	G
82	1	357	A
82	1	361	A
82	1	363	A
82	1	367	A
82	1	368	G
82	1	369	A
82	1	374	G
82	1	376	A
82	1	383	U
82	1	390	C
82	1	391	A
82	1	392	A
82	1	406	A
82	1	407	A2M
82	1	409	U
82	1	410	U
82	1	417	G
82	1	426	A
82	1	438	A
82	1	440	A
82	1	442	A
82	1	443	A
82	1	445	C

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Mol	Chain	Res	Type
82	1	461	G
82	1	463	C
82	1	464	A
82	1	469	A
82	1	477	C
82	1	478	C
82	1	479	A
82	1	481	U
82	1	483	C
82	1	485	A
82	1	486	C
82	1	488	G
82	1	502	U
82	1	508	A
82	1	516	G
82	1	522	G
82	1	525	C
82	1	526	A
82	1	527	A
82	1	528	A
82	1	529	A
82	1	539	C
82	1	543	G
82	1	546	G
82	1	547	U
82	1	548	G
82	1	551	A
82	1	552	G
82	1	553	A
82	1	554	A
82	1	555	U
82	1	563	C
82	1	568	U
82	1	569	G
82	1	571	A
82	1	572	A
82	1	575	A
82	1	581	G
82	1	582	U
82	1	586	U
82	1	609	C
82	1	610	A

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Mol	Chain	Res	Type
82	1	611	C
82	1	616	U
82	1	617	G
82	1	620	U
82	1	625	C
82	1	626	U
82	1	628	C
82	1	630	U
82	1	631	G
82	1	632	A
82	1	635	C
82	1	640	U
82	1	641	G
82	1	648	A
82	1	649	U
82	1	658	G
82	1	659	G
82	1	668	C
82	1	669	C
82	1	681	A2M
82	1	692	A
82	1	705	C
82	1	709	A
82	1	713	A
82	1	718	A
82	1	719	U
82	1	721	U
82	1	723	G
82	1	728	C
82	1	736	C
82	1	748	A
82	1	751	G
82	1	753	A
82	1	754	G
82	1	763	U
82	1	769	U
82	1	771	U
82	1	772	G
82	1	778	C
82	1	779	A
82	1	795	U
82	1	803	C

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Mol	Chain	Res	Type
82	1	818	C
82	1	825	G
82	1	828	U
82	1	832	G
82	1	835	G
82	1	836	G
82	1	838	G
82	1	850	G
82	1	867	A
82	1	868	A
82	1	889	G
82	1	895	G
82	1	900	C
82	1	912	C
82	1	916	U
82	1	925	U
82	1	930	U
82	1	948	U
82	1	957	C
82	1	959	OMG
82	1	965	A
82	1	967	G
82	1	968	A
82	1	972	A
82	1	974	C
82	1	975	G
82	1	976	A
82	1	985	G
82	1	988	G
82	1	995	C
82	1	1010	OMC
82	1	1011	PSU
82	1	1016	A
82	1	1025	G
82	1	1029	G
82	1	1031	A
82	1	1042	G
82	1	1045	G
82	1	1048	A
82	1	1053	A
82	1	1057	A
82	1	1086	G

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Mol	Chain	Res	Type
82	1	1091	A
82	1	1092	U
82	1	1098	A
82	1	1104	A
82	1	1107	OMU
82	1	1108	G
82	1	1116	A
82	1	1122	U
82	1	1123	G
82	1	1128	A
82	1	1129	G
82	1	1134	C
82	1	1135	U
82	1	1140	G
82	1	1141	G
82	1	1148	A
82	1	1149	G
82	1	1153	A
82	1	1156	A
82	1	1159	A
82	1	1161	A
82	1	1162	G
82	1	1165	A
82	1	1169	A
82	1	1170	G
82	1	1174	G
82	1	1175	C
82	1	1181	PSU
82	1	1188	G
82	1	1196	G
82	1	1201	U
82	1	1202	G
82	1	1207	A
82	1	1210	A
82	1	1211	A
82	1	1217	U
82	1	1221	G
82	1	1225	U
82	1	1235	A
82	1	1238	C
82	1	1240	U
82	1	1242	U

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Mol	Chain	Res	Type
82	1	1251	U
82	1	1257	U
82	1	1258	A
82	1	1261	U
82	1	1263	A
82	1	1271	G
82	1	1277	G
82	1	1278	G
82	1	1279	A
82	1	1285	A
82	1	1289	U
82	1	1346	C
82	1	1347	G
82	1	1348	A
82	1	1349	A
82	1	1369	G
82	1	1371	OMU
82	1	1378	U
82	1	1379	A
82	1	1385	A
82	1	1388	U
82	1	1389	A
82	1	1390	G
82	1	1391	U
82	1	1392	G
82	1	1393	A
82	1	1395	U
82	1	1396	G
82	1	1401	U
82	1	1402	U
82	1	1413	U
82	1	1416	G
82	1	1417	G
82	1	1421	G
82	1	1422	A
82	1	1424	A
82	1	1426	A
82	1	1428	A
82	1	1438	A
82	1	1441	U
82	1	1444	A
82	1	1445	G

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Mol	Chain	Res	Type
82	1	1446	C
82	1	1451	C
82	1	1455	U
82	1	1464	G
82	1	1472	G
82	1	1473	G
82	1	1476	A
82	1	1479	A
82	1	1480	C
82	1	1482	A
82	1	1483	A
82	1	1484	G
82	1	1489	U
82	1	1490	G
82	1	1495	G
82	1	1504	A
82	1	1505	U
82	1	1507	G
82	1	1509	C
82	1	1521	G
82	1	1527	OMC
82	1	1536	C
82	1	1540	OMG
82	1	1545	G
82	1	1547	U
82	1	1557	A
82	1	1561	A
82	1	1563	U
82	1	1566	A
82	1	1568	A
82	1	1570	G
82	1	1574	C
82	1	1575	G
82	1	1579	G
82	1	1586	G
82	1	1588	G
82	1	1592	G
82	1	1607	C
82	1	1612	G
82	1	1613	C
82	1	1639	U
82	1	1654	A

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Mol	Chain	Res	Type
82	1	1655	U
82	1	1660	U
82	1	1661	U
82	1	1662	G
82	1	1663	U
82	1	1666	G
82	1	1667	G
82	1	1669	A
82	1	1676	G
82	1	1683	C
82	1	1722	A
82	1	1723	A
82	1	1724	C
82	1	1726	G
82	1	1727	A
82	1	1730	A
82	1	1734	G
82	1	1737	A
82	1	1739	A
82	1	1744	A
82	1	1745	C
82	1	1746	C
82	1	1747	U
82	1	1750	G
82	1	1763	A
82	1	1766	G
82	1	1771	U
82	1	1772	G
82	1	1774	A
82	1	1775	U
82	1	1780	G
83	3	8	G
83	3	10	U
83	3	17	A
83	3	20	C
83	3	24	U
83	3	28	A
83	3	34	C
83	3	35	A
83	3	37	A
83	3	41	A
83	3	51	G

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Mol	Chain	Res	Type
83	3	75	C
83	3	109	U
83	3	110	U
83	3	111	A
83	3	124	U
83	3	126	C
83	3	146	G
83	3	149	A
83	3	150	A
83	3	151	A
83	3	156	G
83	3	159	C
83	3	160	U
83	3	168	U
83	3	169	A
83	3	172	G
83	3	180	U
83	3	181	G
83	3	183	G
83	3	185	G
83	3	187	U
83	3	192	G
83	3	193	C
83	3	194	A
83	3	195	U
83	3	196	U
83	3	199	A
83	3	201	C
83	3	202	A
83	3	204	A
84	5	5	G
84	5	14	C
84	5	23	G
84	5	28	U
84	5	41	A
84	5	49	C
84	5	52	G
84	5	67	G
84	5	68	G
84	5	70	C
84	5	72	C
84	5	73	G

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Mol	Chain	Res	Type
84	5	86	G
84	5	87	U
84	5	88	C
84	5	89	C
84	5	90	C
84	5	99	G
84	5	105	U
84	5	106	G
84	5	108	G
84	5	109	G
84	5	113	G
84	5	116	A
84	5	122	U
84	5	123	G
84	5	124	C
84	5	134	C
84	5	135	U
84	5	136	A
85	7	3	C
85	7	6	G
85	7	16	A
85	7	20	C
85	7	21	U
85	7	33	U
85	7	34	U
85	7	43	A2M
85	7	59	A
85	7	62	A
85	7	63	G
85	7	69	PSU
85	7	70	C
85	7	84	U
85	7	88	A
85	7	89	U
85	7	94	G
85	7	95	A
85	7	103	A
85	7	105	C
85	7	110	A
85	7	115	G
85	7	117	A
85	7	120	G

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Mol	Chain	Res	Type
85	7	124	A
85	7	129	C
85	7	140	U
85	7	157	U
85	7	158	U
85	7	159	C
85	7	164	U
85	7	168	G
86	2	5	A
86	2	6	A
86	2	7	C
86	2	12	G
86	2	13	A
86	2	18	A
86	2	25	A
86	2	29	C
86	2	33	A
86	2	61	C
86	2	62	A
86	2	63	U
86	2	68	A
86	2	69	A
86	2	75	C
86	2	76	A
86	2	80	A
86	2	81	G
86	2	90	G
86	2	97	A
86	2	106	A
86	2	119	C
86	2	121	U
86	2	340	A
86	2	344	G
86	2	345	C
86	2	346	C
86	2	348	A
86	2	349	C
86	2	350	U
86	2	351	C
86	2	358	G
86	2	359	OMC
86	2	360	U

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Mol	Chain	Res	Type
86	2	365	G
86	2	368	G
86	2	377	A
86	2	383	U
86	2	386	U
86	2	390	A
86	2	395	A
86	2	396	G
86	2	397	G
86	2	404	A
86	2	406	G
86	2	415	U
86	2	428	A
86	2	434	A
86	2	437	PSU
86	2	438	C
86	2	440	G
86	2	451	U
86	2	452	G
86	2	453	A
86	2	454	A
86	2	455	U
86	2	456	G
86	2	457	U
86	2	466	C
86	2	470	A
86	2	472	PSU
86	2	475	C
86	2	477	G
86	2	478	A
86	2	495	G
86	2	498	A
86	2	502	A
86	2	503	C
86	2	518	G
86	2	519	G
86	2	527	A2M
86	2	529	G
86	2	534	OMG
86	2	542	A
86	2	544	U
86	2	552	C

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Mol	Chain	Res	Type
86	2	553	G
86	2	554	C
86	2	556	U
86	2	559	A
86	2	561	G
86	2	566	A
86	2	571	G
86	2	580	U
86	2	581	G
86	2	582	U
86	2	602	A
86	2	615	G
86	2	616	G
86	2	619	A
86	2	620	C
86	2	621	G
86	2	623	A
86	2	639	G
86	2	643	A
86	2	648	A
86	2	649	G
86	2	650	A
86	2	657	U
86	2	658	G
86	2	665	A
86	2	671	G
86	2	676	G
86	2	677	C
86	2	680	U
86	2	681	G
86	2	685	G
86	2	687	C
86	2	695	G
86	2	696	A
86	2	697	G
86	2	698	G
86	2	703	G
86	2	709	G
86	2	710	U
86	2	711	G
86	2	713	A
86	2	714	A

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Mol	Chain	Res	Type
86	2	715	G
86	2	719	A
86	2	723	G
86	2	725	A
86	2	726	A
86	2	728	U
86	2	731	A
86	2	732	A
86	2	733	U
86	2	734	A
86	2	735	C
86	2	736	C
86	2	737	A
86	2	739	C
86	2	741	C
86	2	745	G
86	2	746	A
86	2	747	A
86	2	748	C
86	2	749	G
86	2	750	U
86	2	751	U
86	2	752	G
86	2	760	U
86	2	761	A
86	2	768	G
86	2	769	A
86	2	772	A
86	2	776	C
86	2	777	A
86	2	778	A
86	2	781	G
86	2	783	U
86	2	784	U
86	2	788	C
86	2	799	G
86	2	807	A
86	2	811	U
86	2	822	G
86	2	823	A
86	2	824	G
86	2	825	U

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Mol	Chain	Res	Type
86	2	848	C
86	2	850	C
86	2	951	G
86	2	953	U
86	2	955	C
86	2	959	A
86	2	962	G
86	2	965	C
86	2	966	U
86	2	970	A
86	2	977	C
86	2	978	C
86	2	980	A
86	2	981	C
86	2	983	G
86	2	984	G
86	2	985	A
86	2	986	U
86	2	997	A
86	2	999	U
86	2	1000	U
86	2	1001	C
86	2	1007	U
86	2	1009	U
86	2	1010	U
86	2	1011	G
86	2	1012	U
86	2	1019	A
86	2	1022	U
86	2	1027	C
86	2	1030	A
86	2	1033	G
86	2	1034	G
86	2	1041	G
86	2	1053	A
86	2	1055	A
86	2	1064	A
86	2	1075	G
86	2	1078	OMG
86	2	1079	U
86	2	1083	A
86	2	1084	A

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Mol	Chain	Res	Type
86	2	1093	C
86	2	1097	G
86	2	1098	G
86	2	1101	A
86	2	1104	G
86	2	1106	A
86	2	1107	A
86	2	1108	U
86	2	1115	U
86	2	1116	A
86	2	1119	A
86	2	1121	A
86	2	1123	A
86	2	1124	A
86	2	1125	G
86	2	1131	A
86	2	1135	U
86	2	1141	G
86	2	1144	PSU
86	2	1147	C
86	2	1148	G
86	2	1155	A
86	2	1156	G
86	2	1170	U
86	2	1181	G
86	2	1183	C
86	2	1185	A2M
86	2	1189	A
86	2	1199	A
86	2	1207	G
86	2	1209	A
86	2	1210	A
86	2	1215	A
86	2	1216	A
86	2	1219	A
86	2	1221	U
86	2	1224	U
86	2	1234	G
86	2	1237	A
86	2	1238	G
86	2	1239	A
86	2	1241	U

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Mol	Chain	Res	Type
86	2	1248	OMC
86	2	1252	G
86	2	1255	A
86	2	1259	C
86	2	1271	G
86	2	1280	U
86	2	1281	U
86	2	1283	A
86	2	1284	U
86	2	1288	G
86	2	1294	G
86	2	1298	U
86	2	1299	U
86	2	1301	G
86	2	1305	C
86	2	1309	G
86	2	1313	U
86	2	1314	C
86	2	1325	A
86	2	1327	C
86	2	1332	C
86	2	1333	G
86	2	1337	C
86	2	1371	G
86	2	1373	C
86	2	1374	A
86	2	1379	A
86	2	1380	C
86	2	1385	G
86	2	1416	U
86	2	1421	C
86	2	1428	U
86	2	1433	G
86	2	1434	G
86	2	1437	A
86	2	1441	C
86	2	1443	A
86	2	1445	A
86	2	1447	A
86	2	1448	A
86	2	1450	G
86	2	1452	U

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Mol	Chain	Res	Type
86	2	1454	A
86	2	1463	A
86	2	1465	G
86	2	1470	C
86	2	1471	G
86	2	1473	C
86	2	1474	G
86	2	1475	G
86	2	1476	G
86	2	1479	G
86	2	1484	U
86	2	1485	G
86	2	1486	G
86	2	1492	G
86	2	1494	G
86	2	1498	G
86	2	1506	G
86	2	1510	U
86	2	1511	U
86	2	1512	G
86	2	1513	G
86	2	1514	U
86	2	1522	U
86	2	1524	A
86	2	1526	C

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	S4	11	C
34	S4	12	U
35	S1	254	A
35	S1	550	C
35	S1	702	U
35	S1	736	G
35	S1	740	C
35	S1	961	U
35	S1	1209	C
35	S1	1672	C
35	S1	1889	G
35	S1	1904	U
35	S1	1915	U

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Mol	Chain	Res	Type
35	S1	2119	C
37	4	85	C
37	4	92	U
38	6	51	A
38	6	71	A
82	1	217	A
82	1	468	G
82	1	574	G
82	1	704	G
82	1	967	G
82	1	1011	PSU
82	1	1030	U
82	1	1090	U
82	1	1277	G
82	1	1391	U
82	1	1479	A
82	1	1562	C
82	1	1662	G
83	3	33	A
83	3	150	A
83	3	167	G
83	3	180	U
84	5	71	U
84	5	107	A
84	5	134	C
85	7	69	PSU
85	7	93	C
86	2	11	A
86	2	350	U
86	2	455	U
86	2	747	A
86	2	1293	C
86	2	1475	G

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

151 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	$\# Z > 2$
86	A2M	2	604	86,82	18,25,26	4.34	6 (33%)	18,36,39	2.68	3 (16%)
35	OMU	S1	661	35	19,22,23	3.01	8 (42%)	26,31,34	1.69	5 (19%)
35	5MC	S1	2061	35	18,22,23	3.55	7 (38%)	26,32,35	1.03	2 (7%)
86	PSU	2	597	86	18,21,22	4.48	7 (38%)	22,30,33	2.06	5 (22%)
82	PSU	1	1039	82	18,21,22	4.52	7 (38%)	22,30,33	1.73	4 (18%)
35	MA6	S1	2185	35	18,26,27	1.15	3 (16%)	19,38,41	3.14	2 (10%)
85	OMG	7	75	85	18,26,27	2.56	8 (44%)	19,38,41	1.54	4 (21%)
86	A2M	2	1372	86	18,25,26	4.34	6 (33%)	18,36,39	2.44	3 (16%)
35	OMG	S1	2151	35	18,26,27	2.50	8 (44%)	19,38,41	1.49	4 (21%)
86	OMC	2	1248	86	19,22,23	2.97	8 (42%)	26,31,34	0.87	1 (3%)
86	PSU	2	662	86,87	18,21,22	4.43	7 (38%)	22,30,33	1.79	5 (22%)
82	OMG	1	1524	82	18,26,27	2.54	8 (44%)	19,38,41	1.64	4 (21%)
85	A2M	7	162	85,82	18,25,26	4.36	8 (44%)	18,36,39	2.72	3 (16%)
35	OMU	S1	1979	35	19,22,23	3.01	8 (42%)	26,31,34	1.72	5 (19%)
35	PSU	S1	104	35	18,21,22	4.49	7 (38%)	22,30,33	1.71	5 (22%)
86	5MC	2	524	86,87	18,22,23	3.50	7 (38%)	26,32,35	1.04	2 (7%)
35	OMU	S1	1621	87,35	19,22,23	3.00	8 (42%)	26,31,34	1.69	5 (19%)
85	PSU	7	69	85	18,21,22	4.48	9 (50%)	22,30,33	1.69	4 (18%)
35	A2M	S1	479	35	18,25,26	4.23	7 (38%)	18,36,39	2.76	3 (16%)
86	PSU	2	626	86	18,21,22	4.43	7 (38%)	22,30,33	1.72	4 (18%)
86	OMG	2	655	86	18,26,27	2.46	8 (44%)	19,38,41	1.35	3 (15%)
86	A2M	2	527	86,87	18,25,26	4.03	8 (44%)	18,36,39	2.65	3 (16%)
35	PSU	S1	12	35	18,21,22	4.45	7 (38%)	22,30,33	1.76	5 (22%)
86	PSU	2	593	86	18,21,22	4.36	7 (38%)	22,30,33	1.71	5 (22%)
86	OMG	2	1229	86	18,26,27	2.50	8 (44%)	19,38,41	1.52	4 (21%)
86	OMC	2	1317	86	19,22,23	3.02	8 (42%)	26,31,34	0.98	1 (3%)
86	OMU	2	73	86	19,22,23	2.95	8 (42%)	26,31,34	1.55	4 (15%)
82	A2M	1	955	82	18,25,26	4.29	7 (38%)	18,36,39	2.81	3 (16%)
35	PSU	S1	1657	35	18,21,22	4.43	7 (38%)	22,30,33	1.70	3 (13%)
35	A2M	S1	98	87,35	18,25,26	4.32	7 (38%)	18,36,39	2.66	3 (16%)
35	A2M	S1	918	35	18,25,26	4.22	7 (38%)	18,36,39	2.55	3 (16%)
86	PSU	2	1194	86	18,21,22	4.45	7 (38%)	22,30,33	1.66	4 (18%)
35	A2M	S1	753	35	18,25,26	4.35	7 (38%)	18,36,39	2.69	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	PSU	1	1177	82	18,21,22	4.47	7 (38%)	22,30,33	1.80	5 (22%)
86	PSU	2	1144	86	18,21,22	4.60	8 (44%)	22,30,33	1.91	4 (18%)
86	OMG	2	1078	86	18,26,27	2.47	8 (44%)	19,38,41	1.69	5 (26%)
86	PSU	2	1058	86	18,21,22	4.46	7 (38%)	22,30,33	2.13	5 (22%)
35	OMG	S1	600	35	18,26,27	2.54	8 (44%)	19,38,41	1.51	4 (21%)
35	PSU	S1	1539	35	18,21,22	4.47	7 (38%)	22,30,33	1.72	4 (18%)
35	OMC	S1	1866	35	19,22,23	2.97	8 (42%)	26,31,34	0.81	0
35	A2M	S1	28	87,35	18,25,26	4.26	6 (33%)	18,36,39	2.77	3 (16%)
82	OMC	1	1527	82	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
35	PSU	S1	1246	35	18,21,22	4.45	7 (38%)	22,30,33	1.83	5 (22%)
86	OMC	2	1397	86	19,22,23	2.95	8 (42%)	26,31,34	0.79	0
35	7MG	S1	1995	35	22,26,27	4.28	10 (45%)	29,39,42	2.03	9 (31%)
82	1MA	1	677	87,82	16,25,26	3.66	5 (31%)	18,37,40	1.87	4 (22%)
86	5MC	2	1308	86,88	18,22,23	4.65	13 (72%)	26,32,35	1.32	2 (7%)
82	A2M	1	858	82	18,25,26	4.22	7 (38%)	18,36,39	3.12	4 (22%)
86	OMC	2	443	86,87,88	19,22,23	2.88	8 (42%)	26,31,34	0.82	0
82	PSU	1	1011	86,82	18,21,22	4.38	9 (50%)	22,30,33	1.73	6 (27%)
86	OMC	2	359	86	19,22,23	3.01	8 (42%)	26,31,34	0.77	0
85	A2M	7	43	85	18,25,26	4.33	7 (38%)	18,36,39	2.73	4 (22%)
35	OMG	S1	1478	35	18,26,27	2.45	8 (44%)	19,38,41	1.61	5 (26%)
35	OMC	S1	2140	35	19,22,23	2.98	8 (42%)	26,31,34	0.81	0
86	OMU	2	1419	86	19,22,23	2.96	8 (42%)	26,31,34	1.66	4 (15%)
86	PSU	2	1265	86,87	18,21,22	4.45	7 (38%)	22,30,33	1.84	5 (22%)
82	OMG	1	1626	82	18,26,27	2.53	8 (44%)	19,38,41	1.53	4 (21%)
82	OMU	1	1107	82	19,22,23	2.98	8 (42%)	26,31,34	1.74	5 (19%)
35	OMG	S1	1550	35	18,26,27	2.54	8 (44%)	19,38,41	1.48	4 (21%)
35	MA6	S1	2184	35	18,26,27	1.15	1 (5%)	19,38,41	3.00	2 (10%)
35	OMU	S1	29	35	19,22,23	3.01	8 (42%)	26,31,34	1.69	4 (15%)
86	PSU	2	437	86,88	18,21,22	4.47	8 (44%)	22,30,33	1.81	5 (22%)
86	OMG	2	1360	86	18,26,27	2.55	8 (44%)	19,38,41	1.51	4 (21%)
86	PSU	2	1382	86,87,88	18,21,22	4.42	8 (44%)	22,30,33	2.06	6 (27%)
35	PSU	S1	1566	35	18,21,22	4.47	8 (44%)	22,30,33	1.68	4 (18%)
82	PSU	1	672	87,82	18,21,22	4.47	7 (38%)	22,30,33	1.88	6 (27%)
37	OMG	4	74	37	18,26,27	2.46	8 (44%)	19,38,41	1.46	5 (26%)
86	OMG	2	641	86,87	18,26,27	2.49	8 (44%)	19,38,41	1.60	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	PSU	1	1664	82	18,21,22	4.51	7 (38%)	22,30,33	1.75	5 (22%)
86	A2M	2	572	86	18,25,26	4.32	7 (38%)	18,36,39	2.74	3 (16%)
82	PSU	1	870	87,82	18,21,22	4.45	7 (38%)	22,30,33	2.02	5 (22%)
83	OMU	3	13	83	19,22,23	3.01	8 (42%)	26,31,34	1.72	4 (15%)
86	PSU	2	1403	86	18,21,22	4.52	7 (38%)	22,30,33	1.79	6 (27%)
85	OMU	7	7	85,82	19,22,23	3.03	8 (42%)	26,31,34	1.71	4 (15%)
35	PSU	S1	2046	35	18,21,22	4.53	7 (38%)	22,30,33	1.94	4 (18%)
35	OMU	S1	1833	35	19,22,23	3.04	8 (42%)	26,31,34	1.82	5 (19%)
82	A2M	1	678	86,82	18,25,26	4.35	8 (44%)	18,36,39	2.75	3 (16%)
82	OMU	1	847	82	19,22,23	3.00	8 (42%)	26,31,34	1.77	5 (19%)
35	OMC	S1	2059	35	19,22,23	2.97	8 (42%)	26,31,34	1.16	2 (7%)
86	OMG	2	534	86	18,26,27	2.50	8 (44%)	19,38,41	1.48	3 (15%)
35	A2M	S1	969	35	18,25,26	4.30	7 (38%)	18,36,39	2.80	4 (22%)
86	A2M	2	1185	86	18,25,26	4.36	7 (38%)	18,36,39	2.67	3 (16%)
86	OMG	2	71	86	18,26,27	2.52	8 (44%)	19,38,41	1.55	3 (15%)
35	A2M	S1	897	35	18,25,26	4.29	8 (44%)	18,36,39	2.68	3 (16%)
35	5MC	S1	1544	35	18,22,23	3.58	7 (38%)	26,32,35	1.03	1 (3%)
35	OMU	S1	8	35	19,22,23	2.96	8 (42%)	26,31,34	1.81	5 (19%)
35	A2M	S1	2021	35	18,25,26	4.13	7 (38%)	18,36,39	2.74	3 (16%)
35	OMG	S1	1829	87,35	18,26,27	2.52	8 (44%)	19,38,41	1.51	3 (15%)
82	PSU	1	1528	82	18,21,22	4.51	7 (38%)	22,30,33	1.98	5 (22%)
35	PSU	S1	1533	35	18,21,22	4.46	7 (38%)	22,30,33	1.85	5 (22%)
82	OMU	1	845	82	19,22,23	2.98	8 (42%)	26,31,34	2.24	8 (30%)
82	OMG	1	1190	87,82	18,26,27	2.46	8 (44%)	19,38,41	1.64	4 (21%)
86	PSU	2	1318	86	18,21,22	4.51	7 (38%)	22,30,33	1.99	6 (27%)
82	A2M	1	235	82	18,25,26	4.43	7 (38%)	18,36,39	2.73	4 (22%)
82	A2M	1	697	82	18,25,26	4.36	6 (33%)	18,36,39	2.61	3 (16%)
35	OMG	S1	1865	35	18,26,27	2.58	8 (44%)	19,38,41	1.57	4 (21%)
86	A2M	2	382	86	18,25,26	4.44	6 (33%)	18,36,39	2.55	3 (16%)
82	OMC	1	695	82	19,22,23	2.91	8 (42%)	26,31,34	0.68	0
82	A2M	1	681	82	18,25,26	4.24	6 (33%)	18,36,39	2.75	3 (16%)
86	OMU	2	1077	86	19,22,23	3.04	8 (42%)	26,31,34	1.68	4 (15%)
35	PSU	S1	609	35	18,21,22	4.51	7 (38%)	22,30,33	1.80	5 (22%)
86	A2M	2	591	86	18,25,26	4.34	6 (33%)	18,36,39	2.74	3 (16%)
82	PSU	1	1181	82	18,21,22	4.50	8 (44%)	22,30,33	2.00	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	PSU	2	1303	86	18,21,22	4.51	7 (38%)	22,30,33	2.17	6 (27%)
35	OMC	S1	38	35	19,22,23	2.97	8 (42%)	26,31,34	0.76	0
82	OMG	1	1540	86,82	18,26,27	2.48	8 (44%)	19,38,41	1.50	4 (21%)
86	PSU	2	510	86	18,21,22	4.51	7 (38%)	22,30,33	1.76	5 (22%)
35	PSU	S1	2048	35	18,21,22	4.48	7 (38%)	22,30,33	2.06	5 (22%)
86	OMC	2	1159	86	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
82	OMU	1	1371	82	19,22,23	3.05	8 (42%)	26,31,34	1.96	7 (26%)
82	PSU	1	1017	82	18,21,22	4.44	7 (38%)	22,30,33	1.86	5 (22%)
86	OMC	2	583	86	19,22,23	3.04	8 (42%)	26,31,34	0.84	1 (3%)
86	PSU	2	512	86	18,21,22	4.51	7 (38%)	22,30,33	1.83	5 (22%)
82	PSU	1	1171	82	18,21,22	4.42	7 (38%)	22,30,33	1.76	6 (27%)
82	OMG	1	856	82	18,26,27	2.50	8 (44%)	19,38,41	1.51	6 (31%)
86	PSU	2	1060	86	18,21,22	4.48	7 (38%)	22,30,33	2.07	5 (22%)
86	PSU	2	78	86	18,21,22	4.49	7 (38%)	22,30,33	1.99	4 (18%)
35	OMG	S1	1623	35	18,26,27	2.53	8 (44%)	19,38,41	1.52	5 (26%)
82	A2M	1	407	87,82	18,25,26	4.30	8 (44%)	18,36,39	2.62	4 (22%)
86	OMG	2	1231	86	18,26,27	2.52	8 (44%)	19,38,41	1.50	4 (21%)
82	OMG	1	959	82	18,26,27	2.51	8 (44%)	19,38,41	1.47	4 (21%)
35	PSU	S1	1841	35	18,21,22	4.50	7 (38%)	22,30,33	1.81	5 (22%)
86	PSU	2	1264	86	18,21,22	4.41	7 (38%)	22,30,33	1.79	6 (27%)
35	A2M	S1	912	35	18,25,26	4.39	7 (38%)	18,36,39	2.80	4 (22%)
82	PSU	1	1533	86,82	18,21,22	4.49	7 (38%)	22,30,33	1.82	6 (27%)
35	A2M	S1	668	87,35	18,25,26	3.92	8 (44%)	18,36,39	2.72	4 (22%)
82	A2M	1	927	82	18,25,26	4.33	6 (33%)	18,36,39	2.76	3 (16%)
82	A2M	1	305	82	18,25,26	4.15	7 (38%)	18,36,39	2.95	3 (16%)
82	A2M	1	1539	86,87,82	18,25,26	4.29	8 (44%)	18,36,39	2.60	3 (16%)
82	OMU	1	1659	87,82	19,22,23	3.01	8 (42%)	26,31,34	1.68	4 (15%)
86	OMG	2	1046	86	18,26,27	2.42	8 (44%)	19,38,41	1.39	5 (26%)
35	OMC	S1	115	35	19,22,23	2.96	8 (42%)	26,31,34	0.71	0
86	PSU	2	1413	86,87	18,21,22	4.41	7 (38%)	22,30,33	1.75	4 (18%)
35	OMC	S1	18	35	19,22,23	2.95	8 (42%)	26,31,34	0.74	0
86	PSU	2	1361	86	18,21,22	4.49	7 (38%)	22,30,33	1.82	4 (18%)
85	PSU	7	101	85	18,21,22	4.44	7 (38%)	22,30,33	1.82	6 (27%)
35	OMG	S1	1647	35	18,26,27	2.52	8 (44%)	19,38,41	1.59	3 (15%)
35	C4J	S1	1543	35	24,29,30	2.96	8 (33%)	29,42,45	1.28	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	A2M	2	570	86,82	18,25,26	4.15	7 (38%)	18,36,39	2.73	5 (27%)
86	A2M	2	95	86	18,25,26	4.35	7 (38%)	18,36,39	2.70	4 (22%)
86	OMU	2	667	86	19,22,23	3.04	8 (42%)	26,31,34	1.74	4 (15%)
86	A2M	2	1384	86,87	18,25,26	4.27	6 (33%)	18,36,39	2.57	3 (16%)
86	A2M	2	628	86	18,25,26	4.28	7 (38%)	18,36,39	2.72	3 (16%)
86	OMU	2	560	86,87	19,22,23	2.97	8 (42%)	26,31,34	1.79	5 (19%)
86	PSU	2	472	86	18,21,22	4.52	8 (44%)	22,30,33	1.78	4 (18%)
86	OMG	2	1253	86	18,26,27	2.46	8 (44%)	19,38,41	1.51	4 (21%)
85	PSU	7	74	85	18,21,22	4.49	7 (38%)	22,30,33	1.76	5 (22%)
86	OMU	2	1359	86	19,22,23	3.03	8 (42%)	26,31,34	1.73	4 (15%)
35	PSU	S1	33	35	18,21,22	4.61	8 (44%)	22,30,33	1.82	3 (13%)
35	A2M	S1	512	87,35	18,25,26	4.32	8 (44%)	18,36,39	2.74	3 (16%)
82	OMC	1	1010	87,82	19,22,23	2.95	8 (42%)	26,31,34	0.86	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	A2M	2	604	86,82	-	0/5/27/28	0/3/3/3
35	OMU	S1	661	35	-	0/9/27/28	0/2/2/2
35	5MC	S1	2061	35	-	2/7/25/26	0/2/2/2
86	PSU	2	597	86	-	0/7/25/26	0/2/2/2
82	PSU	1	1039	82	-	1/7/25/26	0/2/2/2
35	MA6	S1	2185	35	-	3/7/29/30	0/3/3/3
85	OMG	7	75	85	-	0/5/27/28	0/3/3/3
86	A2M	2	1372	86	-	0/5/27/28	0/3/3/3
35	OMG	S1	2151	35	-	0/5/27/28	0/3/3/3
86	OMC	2	1248	86	-	1/9/27/28	0/2/2/2
86	PSU	2	662	86,87	-	0/7/25/26	0/2/2/2
82	OMG	1	1524	82	-	1/5/27/28	0/3/3/3
85	A2M	7	162	85,82	-	2/5/27/28	0/3/3/3
35	OMU	S1	1979	35	-	0/9/27/28	0/2/2/2
35	PSU	S1	104	35	-	0/7/25/26	0/2/2/2
86	5MC	2	524	86,87	-	0/7/25/26	0/2/2/2
35	OMU	S1	1621	87,35	-	1/9/27/28	0/2/2/2
85	PSU	7	69	85	-	2/7/25/26	0/2/2/2
35	A2M	S1	479	35	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PSU	2	626	86	-	0/7/25/26	0/2/2/2
86	OMG	2	655	86	-	0/5/27/28	0/3/3/3
86	A2M	2	527	86,87	-	2/5/27/28	0/3/3/3
35	PSU	S1	12	35	-	0/7/25/26	0/2/2/2
86	PSU	2	593	86	-	0/7/25/26	0/2/2/2
86	OMG	2	1229	86	-	0/5/27/28	0/3/3/3
86	OMC	2	1317	86	-	0/9/27/28	0/2/2/2
86	OMU	2	73	86	-	1/9/27/28	0/2/2/2
82	A2M	1	955	82	-	1/5/27/28	0/3/3/3
35	PSU	S1	1657	35	-	2/7/25/26	0/2/2/2
35	A2M	S1	98	87,35	-	3/5/27/28	0/3/3/3
35	A2M	S1	918	35	-	1/5/27/28	0/3/3/3
86	PSU	2	1194	86	-	0/7/25/26	0/2/2/2
35	A2M	S1	753	35	-	0/5/27/28	0/3/3/3
82	PSU	1	1177	82	-	0/7/25/26	0/2/2/2
86	PSU	2	1144	86	-	2/7/25/26	0/2/2/2
86	OMG	2	1078	86	-	1/5/27/28	0/3/3/3
86	PSU	2	1058	86	-	0/7/25/26	0/2/2/2
35	OMG	S1	600	35	-	2/5/27/28	0/3/3/3
35	PSU	S1	1539	35	-	1/7/25/26	0/2/2/2
35	OMC	S1	1866	35	-	3/9/27/28	0/2/2/2
35	A2M	S1	28	87,35	-	1/5/27/28	0/3/3/3
82	OMC	1	1527	82	-	2/9/27/28	0/2/2/2
35	PSU	S1	1246	35	-	0/7/25/26	0/2/2/2
86	OMC	2	1397	86	-	0/9/27/28	0/2/2/2
35	7MG	S1	1995	35	-	2/7/37/38	0/3/3/3
82	1MA	1	677	87,82	-	0/3/25/26	0/3/3/3
86	5MC	2	1308	86,88	-	4/7/25/26	0/2/2/2
82	A2M	1	858	82	-	1/5/27/28	0/3/3/3
86	OMC	2	443	86,87,88	-	4/9/27/28	0/2/2/2
82	PSU	1	1011	86,82	-	2/7/25/26	0/2/2/2
86	OMC	2	359	86	-	2/9/27/28	0/2/2/2
85	A2M	7	43	85	-	2/5/27/28	0/3/3/3
35	OMG	S1	1478	35	-	1/5/27/28	0/3/3/3
35	OMC	S1	2140	35	-	0/9/27/28	0/2/2/2
86	OMU	2	1419	86	-	1/9/27/28	0/2/2/2
86	PSU	2	1265	86,87	-	0/7/25/26	0/2/2/2
82	OMG	1	1626	82	-	0/5/27/28	0/3/3/3
82	OMU	1	1107	82	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	OMG	S1	1550	35	-	0/5/27/28	0/3/3/3
35	MA6	S1	2184	35	-	0/7/29/30	0/3/3/3
35	OMU	S1	29	35	-	1/9/27/28	0/2/2/2
86	PSU	2	437	86,88	-	2/7/25/26	0/2/2/2
86	OMG	2	1360	86	-	0/5/27/28	0/3/3/3
86	PSU	2	1382	86,87,88	-	0/7/25/26	0/2/2/2
35	PSU	S1	1566	35	-	2/7/25/26	0/2/2/2
82	PSU	1	672	87,82	-	0/7/25/26	0/2/2/2
37	OMG	4	74	37	-	2/5/27/28	0/3/3/3
86	OMG	2	641	86,87	-	0/5/27/28	0/3/3/3
82	PSU	1	1664	82	-	0/7/25/26	0/2/2/2
86	A2M	2	572	86	-	0/5/27/28	0/3/3/3
82	PSU	1	870	87,82	-	0/7/25/26	0/2/2/2
83	OMU	3	13	83	-	1/9/27/28	0/2/2/2
86	PSU	2	1403	86	-	0/7/25/26	0/2/2/2
85	OMU	7	7	85,82	-	1/9/27/28	0/2/2/2
35	PSU	S1	2046	35	-	0/7/25/26	0/2/2/2
35	OMU	S1	1833	35	-	2/9/27/28	0/2/2/2
82	A2M	1	678	86,82	-	0/5/27/28	0/3/3/3
82	OMU	1	847	82	-	0/9/27/28	0/2/2/2
35	OMC	S1	2059	35	-	2/9/27/28	0/2/2/2
86	OMG	2	534	86	-	2/5/27/28	0/3/3/3
35	A2M	S1	969	35	-	2/5/27/28	0/3/3/3
86	A2M	2	1185	86	-	3/5/27/28	0/3/3/3
86	OMG	2	71	86	-	0/5/27/28	0/3/3/3
35	A2M	S1	897	35	-	0/5/27/28	0/3/3/3
35	5MC	S1	1544	35	-	0/7/25/26	0/2/2/2
35	OMU	S1	8	35	-	4/9/27/28	0/2/2/2
35	A2M	S1	2021	35	-	3/5/27/28	0/3/3/3
35	OMG	S1	1829	87,35	-	3/5/27/28	0/3/3/3
82	PSU	1	1528	82	-	0/7/25/26	0/2/2/2
35	PSU	S1	1533	35	-	0/7/25/26	0/2/2/2
82	OMU	1	845	82	-	3/9/27/28	0/2/2/2
82	OMG	1	1190	87,82	-	0/5/27/28	0/3/3/3
86	PSU	2	1318	86	-	0/7/25/26	0/2/2/2
82	A2M	1	235	82	-	0/5/27/28	0/3/3/3
82	A2M	1	697	82	-	0/5/27/28	0/3/3/3
35	OMG	S1	1865	35	-	0/5/27/28	0/3/3/3
86	A2M	2	382	86	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	OMC	1	695	82	-	1/9/27/28	0/2/2/2
82	A2M	1	681	82	-	3/5/27/28	0/3/3/3
86	OMU	2	1077	86	-	0/9/27/28	0/2/2/2
35	PSU	S1	609	35	-	0/7/25/26	0/2/2/2
86	A2M	2	591	86	-	0/5/27/28	0/3/3/3
82	PSU	1	1181	82	-	2/7/25/26	0/2/2/2
86	PSU	2	1303	86	-	0/7/25/26	0/2/2/2
35	OMC	S1	38	35	-	0/9/27/28	0/2/2/2
82	OMG	1	1540	86,82	-	2/5/27/28	0/3/3/3
86	PSU	2	510	86	-	0/7/25/26	0/2/2/2
35	PSU	S1	2048	35	-	0/7/25/26	0/2/2/2
86	OMC	2	1159	86	-	0/9/27/28	0/2/2/2
82	OMU	1	1371	82	-	4/9/27/28	0/2/2/2
82	PSU	1	1017	82	-	0/7/25/26	0/2/2/2
86	OMC	2	583	86	-	0/9/27/28	0/2/2/2
86	PSU	2	512	86	-	0/7/25/26	0/2/2/2
82	PSU	1	1171	82	-	0/7/25/26	0/2/2/2
82	OMG	1	856	82	-	0/5/27/28	0/3/3/3
86	PSU	2	1060	86	-	0/7/25/26	0/2/2/2
86	PSU	2	78	86	-	0/7/25/26	0/2/2/2
35	OMG	S1	1623	35	-	0/5/27/28	0/3/3/3
82	A2M	1	407	87,82	-	3/5/27/28	0/3/3/3
86	OMG	2	1231	86	-	0/5/27/28	0/3/3/3
82	OMG	1	959	82	-	2/5/27/28	0/3/3/3
35	PSU	S1	1841	35	-	0/7/25/26	0/2/2/2
86	PSU	2	1264	86	-	0/7/25/26	0/2/2/2
35	A2M	S1	912	35	-	1/5/27/28	0/3/3/3
82	PSU	1	1533	86,82	-	0/7/25/26	0/2/2/2
35	A2M	S1	668	87,35	-	2/5/27/28	0/3/3/3
82	A2M	1	927	82	-	1/5/27/28	0/3/3/3
82	A2M	1	305	82	-	0/5/27/28	0/3/3/3
82	A2M	1	1539	86,87,82	-	0/5/27/28	0/3/3/3
82	OMU	1	1659	87,82	-	0/9/27/28	0/2/2/2
86	OMG	2	1046	86	-	1/5/27/28	0/3/3/3
35	OMC	S1	115	35	-	0/9/27/28	0/2/2/2
86	PSU	2	1413	86,87	-	0/7/25/26	0/2/2/2
35	OMC	S1	18	35	-	0/9/27/28	0/2/2/2
86	PSU	2	1361	86	-	1/7/25/26	0/2/2/2
85	PSU	7	101	85	-	0/7/25/26	0/2/2/2
35	OMG	S1	1647	35	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	C4J	S1	1543	35	-	7/16/34/35	0/2/2/2
86	A2M	2	570	86,82	-	1/5/27/28	0/3/3/3
86	A2M	2	95	86	-	0/5/27/28	0/3/3/3
86	OMU	2	667	86	-	1/9/27/28	0/2/2/2
86	A2M	2	1384	86,87	-	1/5/27/28	0/3/3/3
86	A2M	2	628	86	-	0/5/27/28	0/3/3/3
86	OMU	2	560	86,87	-	1/9/27/28	0/2/2/2
86	PSU	2	472	86	-	2/7/25/26	0/2/2/2
86	OMG	2	1253	86	-	0/5/27/28	0/3/3/3
85	PSU	7	74	85	-	0/7/25/26	0/2/2/2
86	OMU	2	1359	86	-	0/9/27/28	0/2/2/2
35	PSU	S1	33	35	-	2/7/25/26	0/2/2/2
35	A2M	S1	512	87,35	-	2/5/27/28	0/3/3/3
82	OMC	1	1010	87,82	-	1/9/27/28	0/2/2/2

All (1126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	382	A2M	O4'-C1'	16.06	1.63	1.41
82	1	235	A2M	O4'-C1'	16.01	1.63	1.41
35	S1	912	A2M	O4'-C1'	15.84	1.63	1.41
86	2	1185	A2M	O4'-C1'	15.73	1.63	1.41
82	1	697	A2M	O4'-C1'	15.69	1.63	1.41
85	7	162	A2M	O4'-C1'	15.65	1.62	1.41
86	2	1372	A2M	O4'-C1'	15.65	1.62	1.41
35	S1	98	A2M	O4'-C1'	15.63	1.62	1.41
86	2	604	A2M	O4'-C1'	15.59	1.62	1.41
86	2	591	A2M	O4'-C1'	15.58	1.62	1.41
86	2	95	A2M	O4'-C1'	15.58	1.62	1.41
82	1	407	A2M	O4'-C1'	15.57	1.62	1.41
35	S1	753	A2M	O4'-C1'	15.55	1.62	1.41
82	1	927	A2M	O4'-C1'	15.50	1.62	1.41
86	2	572	A2M	O4'-C1'	15.46	1.62	1.41
86	2	1384	A2M	O4'-C1'	15.46	1.62	1.41
35	S1	969	A2M	O4'-C1'	15.44	1.62	1.41
85	7	43	A2M	O4'-C1'	15.43	1.62	1.41
35	S1	512	A2M	O4'-C1'	15.42	1.62	1.41
82	1	678	A2M	O4'-C1'	15.38	1.62	1.41
35	S1	897	A2M	O4'-C1'	15.38	1.62	1.41
35	S1	28	A2M	O4'-C1'	15.37	1.62	1.41
82	1	1539	A2M	O4'-C1'	15.35	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	955	A2M	O4'-C1'	15.33	1.62	1.41
86	2	628	A2M	O4'-C1'	15.32	1.62	1.41
35	S1	479	A2M	O4'-C1'	15.32	1.62	1.41
82	1	858	A2M	O4'-C1'	15.17	1.62	1.41
35	S1	918	A2M	O4'-C1'	15.03	1.62	1.41
82	1	681	A2M	O4'-C1'	15.03	1.62	1.41
82	1	305	A2M	O4'-C1'	14.92	1.61	1.41
86	2	570	A2M	O4'-C1'	14.75	1.61	1.41
35	S1	2021	A2M	O4'-C1'	14.69	1.61	1.41
86	2	527	A2M	O4'-C1'	14.30	1.61	1.41
35	S1	668	A2M	O4'-C1'	13.45	1.59	1.41
82	1	677	1MA	C2-N3	12.78	1.44	1.29
86	2	1144	PSU	C6-C5	12.05	1.49	1.35
35	S1	33	PSU	C6-C5	12.00	1.49	1.35
86	2	472	PSU	C6-C5	11.90	1.49	1.35
82	1	1039	PSU	C6-C5	11.83	1.49	1.35
86	2	437	PSU	C6-C5	11.78	1.49	1.35
35	S1	609	PSU	C6-C5	11.76	1.49	1.35
82	1	1528	PSU	C6-C5	11.74	1.49	1.35
82	1	1664	PSU	C6-C5	11.72	1.49	1.35
35	S1	1566	PSU	C6-C5	11.72	1.49	1.35
85	7	69	PSU	C6-C5	11.69	1.48	1.35
86	2	78	PSU	C6-C5	11.68	1.48	1.35
85	7	74	PSU	C6-C5	11.68	1.48	1.35
86	2	1403	PSU	C6-C5	11.65	1.48	1.35
86	2	510	PSU	C6-C5	11.64	1.48	1.35
86	2	1194	PSU	C6-C5	11.64	1.48	1.35
86	2	1361	PSU	C6-C5	11.64	1.48	1.35
35	S1	1539	PSU	C6-C5	11.63	1.48	1.35
35	S1	104	PSU	C6-C5	11.62	1.48	1.35
35	S1	1841	PSU	C6-C5	11.62	1.48	1.35
35	S1	2048	PSU	C6-C5	11.62	1.48	1.35
86	2	1318	PSU	C6-C5	11.61	1.48	1.35
86	2	626	PSU	C6-C5	11.61	1.48	1.35
35	S1	2046	PSU	C6-C5	11.61	1.48	1.35
35	S1	12	PSU	C6-C5	11.60	1.48	1.35
82	1	1017	PSU	C6-C5	11.60	1.48	1.35
86	2	1060	PSU	C6-C5	11.60	1.48	1.35
82	1	1533	PSU	C6-C5	11.59	1.48	1.35
82	1	1177	PSU	C6-C5	11.59	1.48	1.35
86	2	1413	PSU	C6-C5	11.58	1.48	1.35
82	1	672	PSU	C6-C5	11.57	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S1	1533	PSU	C6-C5	11.55	1.48	1.35
86	2	512	PSU	C6-C5	11.55	1.48	1.35
86	2	597	PSU	C6-C5	11.54	1.48	1.35
86	2	1265	PSU	C6-C5	11.54	1.48	1.35
86	2	1058	PSU	C6-C5	11.54	1.48	1.35
86	2	1303	PSU	C6-C5	11.51	1.48	1.35
35	S1	1657	PSU	C6-C5	11.51	1.48	1.35
82	1	1171	PSU	C6-C5	11.50	1.48	1.35
86	2	1382	PSU	C6-C5	11.48	1.48	1.35
82	1	870	PSU	C6-C5	11.47	1.48	1.35
85	7	101	PSU	C6-C5	11.47	1.48	1.35
86	2	662	PSU	C6-C5	11.45	1.48	1.35
82	1	1181	PSU	C6-C5	11.37	1.48	1.35
35	S1	1246	PSU	C6-C5	11.37	1.48	1.35
86	2	593	PSU	C6-C5	11.34	1.48	1.35
35	S1	1995	7MG	C8-N9	11.31	1.52	1.46
86	2	1264	PSU	C6-C5	11.30	1.48	1.35
82	1	1011	PSU	C6-C5	11.05	1.48	1.35
35	S1	2046	PSU	C2-N1	10.11	1.50	1.36
86	2	1318	PSU	C2-N1	10.06	1.50	1.36
35	S1	33	PSU	C2-N1	10.05	1.50	1.36
86	2	78	PSU	C2-N1	9.94	1.50	1.36
82	1	1181	PSU	C2-N1	9.91	1.50	1.36
82	1	1528	PSU	C2-N1	9.88	1.50	1.36
86	2	1303	PSU	C2-N1	9.86	1.50	1.36
86	2	1144	PSU	C2-N1	9.81	1.50	1.36
86	2	1060	PSU	C2-N1	9.80	1.50	1.36
35	S1	2048	PSU	C2-N1	9.80	1.50	1.36
82	1	870	PSU	C2-N1	9.79	1.50	1.36
86	2	512	PSU	C2-N1	9.78	1.50	1.36
86	2	597	PSU	C2-N1	9.77	1.49	1.36
82	1	1664	PSU	C2-N1	9.75	1.49	1.36
86	2	1058	PSU	C2-N1	9.74	1.49	1.36
35	S1	1543	C4J	C6-C5	9.73	1.48	1.34
82	1	1011	PSU	C2-N1	9.72	1.49	1.36
82	1	1039	PSU	C2-N1	9.71	1.49	1.36
35	S1	1841	PSU	C2-N1	9.71	1.49	1.36
85	7	74	PSU	C2-N1	9.70	1.49	1.36
86	2	1382	PSU	C2-N1	9.70	1.49	1.36
86	2	1361	PSU	C2-N1	9.69	1.49	1.36
86	2	510	PSU	C2-N1	9.68	1.49	1.36
86	2	437	PSU	C2-N1	9.66	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S1	609	PSU	C2-N1	9.65	1.49	1.36
82	1	672	PSU	C2-N1	9.65	1.49	1.36
35	S1	104	PSU	C2-N1	9.65	1.49	1.36
86	2	1403	PSU	C2-N1	9.65	1.49	1.36
82	1	1177	PSU	C2-N1	9.62	1.49	1.36
35	S1	1657	PSU	C2-N1	9.61	1.49	1.36
85	7	101	PSU	C2-N1	9.59	1.49	1.36
82	1	1533	PSU	C2-N1	9.59	1.49	1.36
35	S1	1533	PSU	C2-N1	9.56	1.49	1.36
35	S1	12	PSU	C2-N1	9.55	1.49	1.36
35	S1	1246	PSU	C2-N1	9.52	1.49	1.36
35	S1	1566	PSU	C2-N1	9.51	1.49	1.36
86	2	1194	PSU	C2-N1	9.48	1.49	1.36
35	S1	1539	PSU	C2-N1	9.47	1.49	1.36
86	2	1265	PSU	C2-N1	9.47	1.49	1.36
86	2	1264	PSU	C2-N1	9.46	1.49	1.36
35	S1	1995	7MG	C5-N7	9.45	1.46	1.35
86	2	662	PSU	C2-N1	9.44	1.49	1.36
86	2	472	PSU	C2-N1	9.44	1.49	1.36
82	1	1017	PSU	C2-N1	9.41	1.49	1.36
85	7	69	PSU	C2-N1	9.41	1.49	1.36
86	2	1413	PSU	C2-N1	9.41	1.49	1.36
86	2	626	PSU	C2-N1	9.38	1.49	1.36
82	1	1171	PSU	C2-N1	9.37	1.49	1.36
35	S1	1544	5MC	C6-C5	9.30	1.49	1.34
86	2	1308	5MC	C6-C5	9.21	1.49	1.34
86	2	593	PSU	C2-N1	9.17	1.49	1.36
86	2	524	5MC	C6-C5	9.12	1.49	1.34
35	S1	2061	5MC	C6-C5	9.06	1.49	1.34
86	2	1308	5MC	C3'-C4'	-8.73	1.30	1.53
82	1	1371	OMU	C2-N1	7.81	1.51	1.38
86	2	512	PSU	C2-N3	7.65	1.50	1.37
86	2	1144	PSU	C2-N3	7.61	1.50	1.37
86	2	1403	PSU	C2-N3	7.58	1.50	1.37
86	2	510	PSU	C2-N3	7.57	1.50	1.37
86	2	472	PSU	C2-N3	7.57	1.50	1.37
35	S1	1246	PSU	C2-N3	7.57	1.50	1.37
82	1	1181	PSU	C2-N3	7.56	1.50	1.37
35	S1	33	PSU	C2-N3	7.54	1.50	1.37
82	1	1533	PSU	C2-N3	7.53	1.50	1.37
82	1	1177	PSU	C2-N3	7.52	1.50	1.37
35	S1	1841	PSU	C2-N3	7.52	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S1	104	PSU	C2-N3	7.50	1.50	1.37
35	S1	609	PSU	C2-N3	7.49	1.50	1.37
82	1	845	OMU	C2-N1	7.49	1.50	1.38
82	1	1039	PSU	C2-N3	7.47	1.50	1.37
86	2	1303	PSU	C2-N3	7.45	1.50	1.37
35	S1	1539	PSU	C2-N3	7.45	1.50	1.37
85	7	69	PSU	C2-N3	7.44	1.50	1.37
35	S1	1533	PSU	C2-N3	7.43	1.50	1.37
35	S1	1566	PSU	C2-N3	7.42	1.50	1.37
86	2	1361	PSU	C2-N3	7.41	1.50	1.37
82	1	1664	PSU	C2-N3	7.40	1.50	1.37
82	1	672	PSU	C2-N3	7.39	1.50	1.37
82	1	1011	PSU	C2-N3	7.38	1.50	1.37
86	2	662	PSU	C2-N3	7.38	1.50	1.37
35	S1	1995	7MG	C4-N9	7.37	1.46	1.37
86	2	597	PSU	C2-N3	7.36	1.50	1.37
86	2	1264	PSU	C2-N3	7.36	1.50	1.37
85	7	101	PSU	C2-N3	7.36	1.50	1.37
86	2	1308	5MC	O4'-C4'	7.34	1.61	1.45
82	1	1017	PSU	C2-N3	7.33	1.50	1.37
86	2	626	PSU	C2-N3	7.33	1.50	1.37
86	2	1265	PSU	C2-N3	7.32	1.50	1.37
86	2	1194	PSU	C2-N3	7.32	1.50	1.37
35	S1	12	PSU	C2-N3	7.32	1.50	1.37
85	7	74	PSU	C2-N3	7.31	1.50	1.37
82	1	1171	PSU	C2-N3	7.30	1.50	1.37
86	2	437	PSU	C2-N3	7.29	1.50	1.37
35	S1	2046	PSU	C2-N3	7.29	1.50	1.37
82	1	1528	PSU	C2-N3	7.27	1.50	1.37
86	2	1058	PSU	C2-N3	7.26	1.49	1.37
86	2	1318	PSU	C2-N3	7.23	1.49	1.37
86	2	593	PSU	C2-N3	7.22	1.49	1.37
35	S1	2048	PSU	C2-N3	7.22	1.49	1.37
86	2	1413	PSU	C2-N3	7.20	1.49	1.37
86	2	1359	OMU	C2-N1	7.19	1.50	1.38
86	2	1060	PSU	C2-N3	7.18	1.49	1.37
86	2	667	OMU	C2-N1	7.17	1.50	1.38
35	S1	1657	PSU	C2-N3	7.16	1.49	1.37
35	S1	1833	OMU	C2-N1	7.16	1.49	1.38
82	1	870	PSU	C2-N3	7.15	1.49	1.37
35	S1	29	OMU	C2-N1	7.14	1.49	1.38
85	7	7	OMU	C2-N1	7.13	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	1077	OMU	C2-N1	7.12	1.49	1.38
86	2	78	PSU	C2-N3	7.09	1.49	1.37
86	2	1382	PSU	C2-N3	7.08	1.49	1.37
82	1	847	OMU	C2-N1	7.06	1.49	1.38
82	1	1659	OMU	C2-N1	7.02	1.49	1.38
35	S1	1979	OMU	C2-N1	6.96	1.49	1.38
86	2	560	OMU	C2-N1	6.87	1.49	1.38
83	3	13	OMU	C2-N1	6.87	1.49	1.38
35	S1	1833	OMU	C2-N3	6.87	1.50	1.38
35	S1	661	OMU	C2-N1	6.86	1.49	1.38
82	1	1107	OMU	C2-N1	6.85	1.49	1.38
82	1	847	OMU	C2-N3	6.82	1.50	1.38
86	2	73	OMU	C2-N1	6.81	1.49	1.38
35	S1	1621	OMU	C2-N1	6.81	1.49	1.38
35	S1	1621	OMU	C2-N3	6.81	1.50	1.38
35	S1	1979	OMU	C2-N3	6.78	1.50	1.38
86	2	1419	OMU	C2-N1	6.77	1.49	1.38
35	S1	8	OMU	C2-N3	6.73	1.50	1.38
86	2	1077	OMU	C2-N3	6.72	1.49	1.38
82	1	1659	OMU	C2-N3	6.72	1.49	1.38
85	7	7	OMU	C2-N3	6.72	1.49	1.38
35	S1	668	A2M	O4'-C4'	-6.72	1.30	1.45
35	S1	661	OMU	C2-N3	6.72	1.49	1.38
86	2	560	OMU	C2-N3	6.69	1.49	1.38
86	2	667	OMU	C2-N3	6.68	1.49	1.38
82	1	1107	OMU	C2-N3	6.67	1.49	1.38
35	S1	8	OMU	C2-N1	6.67	1.49	1.38
86	2	1359	OMU	C2-N3	6.62	1.49	1.38
82	1	1371	OMU	C2-N3	6.62	1.49	1.38
83	3	13	OMU	C2-N3	6.58	1.49	1.38
35	S1	29	OMU	C2-N3	6.57	1.49	1.38
82	1	678	A2M	O4'-C4'	-6.57	1.30	1.45
86	2	73	OMU	C2-N3	6.56	1.49	1.38
82	1	858	A2M	O4'-C4'	-6.51	1.30	1.45
82	1	681	A2M	O4'-C4'	-6.48	1.30	1.45
82	1	955	A2M	O4'-C4'	-6.45	1.30	1.45
82	1	235	A2M	O4'-C4'	-6.44	1.30	1.45
86	2	1419	OMU	C2-N3	6.43	1.49	1.38
85	7	43	A2M	O4'-C4'	-6.42	1.30	1.45
86	2	628	A2M	O4'-C4'	-6.42	1.30	1.45
82	1	845	OMU	C2-N3	6.40	1.49	1.38
35	S1	2061	5MC	C4-N3	6.39	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S1	912	A2M	O4'-C4'	-6.39	1.30	1.45
86	2	591	A2M	O4'-C4'	-6.38	1.30	1.45
35	S1	28	A2M	O4'-C4'	-6.38	1.30	1.45
82	1	1539	A2M	O4'-C4'	-6.38	1.30	1.45
86	2	604	A2M	O4'-C4'	-6.37	1.30	1.45
82	1	927	A2M	O4'-C4'	-6.36	1.30	1.45
35	S1	2021	A2M	O4'-C4'	-6.35	1.30	1.45
82	1	697	A2M	O4'-C4'	-6.34	1.30	1.45
86	2	359	OMC	C2-N3	6.34	1.49	1.36
35	S1	1544	5MC	C4-N3	6.33	1.44	1.34
86	2	1372	A2M	O4'-C4'	-6.33	1.30	1.45
35	S1	753	A2M	O4'-C4'	-6.32	1.30	1.45
86	2	1159	OMC	C2-N3	6.31	1.49	1.36
82	1	1010	OMC	C2-N3	6.31	1.49	1.36
35	S1	1995	7MG	C2-N3	6.31	1.48	1.33
35	S1	512	A2M	O4'-C4'	-6.30	1.30	1.45
86	2	572	A2M	O4'-C4'	-6.30	1.30	1.45
86	2	583	OMC	C2-N3	6.28	1.49	1.36
35	S1	2140	OMC	C2-N3	6.27	1.49	1.36
86	2	95	A2M	O4'-C4'	-6.26	1.31	1.45
85	7	162	A2M	O4'-C4'	-6.26	1.31	1.45
35	S1	897	A2M	O4'-C4'	-6.26	1.31	1.45
35	S1	115	OMC	C2-N3	6.24	1.49	1.36
35	S1	969	A2M	O4'-C4'	-6.23	1.31	1.45
35	S1	479	A2M	O4'-C4'	-6.23	1.31	1.45
35	S1	918	A2M	O4'-C4'	-6.22	1.31	1.45
86	2	382	A2M	O4'-C4'	-6.22	1.31	1.45
35	S1	18	OMC	C2-N3	6.20	1.48	1.36
86	2	1317	OMC	C2-N3	6.20	1.48	1.36
35	S1	98	A2M	O4'-C4'	-6.19	1.31	1.45
86	2	570	A2M	O4'-C4'	-6.19	1.31	1.45
35	S1	38	OMC	C2-N3	6.19	1.48	1.36
35	S1	1866	OMC	C2-N3	6.19	1.48	1.36
86	2	1185	A2M	O4'-C4'	-6.18	1.31	1.45
35	S1	1543	C4J	C2-N3	6.17	1.49	1.38
82	1	407	A2M	O4'-C4'	-6.13	1.31	1.45
86	2	1384	A2M	O4'-C4'	-6.13	1.31	1.45
86	2	524	5MC	C4-N3	6.11	1.44	1.34
86	2	583	OMC	C6-C5	6.08	1.49	1.35
82	1	1527	OMC	C2-N3	6.07	1.48	1.36
86	2	1248	OMC	C2-N3	6.07	1.48	1.36
86	2	1317	OMC	C6-C5	6.05	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	695	OMC	C2-N3	6.03	1.48	1.36
86	2	443	OMC	C6-C5	6.03	1.49	1.35
82	1	305	A2M	O4'-C4'	-6.03	1.31	1.45
35	S1	1544	5MC	C2-N3	6.02	1.48	1.36
86	2	1397	OMC	C2-N3	6.02	1.48	1.36
86	2	1397	OMC	C6-C5	6.00	1.49	1.35
35	S1	2059	OMC	C6-C5	5.99	1.49	1.35
35	S1	2059	OMC	C2-N3	5.98	1.48	1.36
35	S1	2061	5MC	C2-N3	5.97	1.48	1.36
82	1	1527	OMC	C6-C5	5.97	1.48	1.35
35	S1	38	OMC	C6-C5	5.97	1.48	1.35
35	S1	115	OMC	C6-C5	5.96	1.48	1.35
86	2	527	A2M	O4'-C4'	-5.95	1.31	1.45
86	2	359	OMC	C6-C5	5.93	1.48	1.35
86	2	1248	OMC	C6-C5	5.93	1.48	1.35
35	S1	1866	OMC	C6-C5	5.91	1.48	1.35
35	S1	2140	OMC	C6-C5	5.90	1.48	1.35
35	S1	18	OMC	C6-C5	5.90	1.48	1.35
86	2	1308	5MC	C4-N3	5.85	1.44	1.34
86	2	524	5MC	C2-N3	5.84	1.48	1.36
82	1	695	OMC	C6-C5	5.83	1.48	1.35
86	2	1159	OMC	C6-C5	5.83	1.48	1.35
86	2	443	OMC	C2-N3	5.82	1.48	1.36
82	1	1010	OMC	C6-C5	5.81	1.48	1.35
35	S1	661	OMU	C6-C5	5.72	1.48	1.35
86	2	1419	OMU	C6-C5	5.70	1.48	1.35
35	S1	29	OMU	C6-C5	5.69	1.48	1.35
83	3	13	OMU	C6-C5	5.66	1.48	1.35
86	2	667	OMU	C6-C5	5.66	1.48	1.35
86	2	1077	OMU	C6-C5	5.66	1.48	1.35
86	2	1359	OMU	C6-C5	5.65	1.48	1.35
35	S1	1621	OMU	C6-C5	5.62	1.48	1.35
35	S1	33	PSU	C6-N1	5.62	1.45	1.36
86	2	1308	5MC	C2-N3	5.61	1.47	1.36
35	S1	1979	OMU	C6-C5	5.61	1.48	1.35
82	1	1107	OMU	C6-C5	5.61	1.48	1.35
86	2	1144	PSU	C6-N1	5.58	1.45	1.36
86	2	73	OMU	C6-C5	5.57	1.48	1.35
82	1	847	OMU	C6-C5	5.57	1.48	1.35
35	S1	8	OMU	C6-C5	5.56	1.48	1.35
82	1	1659	OMU	C6-C5	5.55	1.47	1.35
35	S1	2046	PSU	C6-N1	5.54	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	7	7	OMU	C6-C5	5.50	1.47	1.35
82	1	1371	OMU	C6-C5	5.49	1.47	1.35
35	S1	1833	OMU	C6-C5	5.48	1.47	1.35
35	S1	1995	7MG	C4-N3	5.48	1.47	1.34
86	2	560	OMU	C6-C5	5.48	1.47	1.35
35	S1	104	PSU	C6-N1	5.42	1.45	1.36
86	2	1318	PSU	C6-N1	5.41	1.45	1.36
86	2	1060	PSU	C6-N1	5.41	1.45	1.36
35	S1	2048	PSU	C6-N1	5.40	1.45	1.36
35	S1	609	PSU	C6-N1	5.40	1.45	1.36
86	2	512	PSU	C6-N1	5.40	1.45	1.36
86	2	1361	PSU	C6-N1	5.39	1.45	1.36
85	7	74	PSU	C6-N1	5.38	1.45	1.36
82	1	1533	PSU	C6-N1	5.38	1.45	1.36
82	1	1039	PSU	C6-N1	5.37	1.45	1.36
86	2	78	PSU	C6-N1	5.35	1.45	1.36
82	1	1528	PSU	C6-N1	5.34	1.45	1.36
35	S1	1566	PSU	C6-N1	5.33	1.45	1.36
35	S1	1539	PSU	C6-N1	5.32	1.45	1.36
86	2	1360	OMG	C2-N3	5.31	1.46	1.33
86	2	510	PSU	C6-N1	5.30	1.45	1.36
35	S1	1841	PSU	C6-N1	5.30	1.45	1.36
82	1	1010	OMC	C4-N3	5.29	1.45	1.34
86	2	1403	PSU	C6-N1	5.28	1.45	1.36
85	7	69	PSU	C6-N1	5.27	1.45	1.36
86	2	597	PSU	C6-N1	5.26	1.45	1.36
35	S1	1657	PSU	C6-N1	5.26	1.45	1.36
35	S1	1246	PSU	C6-N1	5.24	1.44	1.36
35	S1	12	PSU	C6-N1	5.23	1.44	1.36
82	1	959	OMG	C2-N3	5.23	1.45	1.33
86	2	583	OMC	C4-N3	5.23	1.45	1.34
82	1	1664	PSU	C6-N1	5.22	1.44	1.36
86	2	662	PSU	C6-N1	5.22	1.44	1.36
35	S1	1865	OMG	C2-N3	5.21	1.45	1.33
35	S1	1533	PSU	C6-N1	5.21	1.44	1.36
86	2	1058	PSU	C6-N1	5.20	1.44	1.36
86	2	359	OMC	C4-N3	5.20	1.45	1.34
86	2	1303	PSU	C6-N1	5.20	1.44	1.36
86	2	1382	PSU	C6-N1	5.20	1.44	1.36
35	S1	600	OMG	C2-N3	5.20	1.45	1.33
82	1	1181	PSU	C6-N1	5.19	1.44	1.36
86	2	1194	PSU	C6-N1	5.19	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	1413	PSU	C6-N1	5.18	1.44	1.36
86	2	1264	PSU	C6-N1	5.18	1.44	1.36
86	2	1265	PSU	C6-N1	5.18	1.44	1.36
35	S1	2151	OMG	C2-N3	5.18	1.45	1.33
82	1	1524	OMG	C2-N3	5.18	1.45	1.33
82	1	1177	PSU	C6-N1	5.17	1.44	1.36
82	1	870	PSU	C6-N1	5.17	1.44	1.36
86	2	534	OMG	C2-N3	5.16	1.45	1.33
35	S1	1550	OMG	C2-N3	5.16	1.45	1.33
85	7	101	PSU	C6-N1	5.14	1.44	1.36
86	2	655	OMG	C2-N3	5.14	1.45	1.33
82	1	845	OMU	C6-C5	5.14	1.47	1.35
86	2	472	PSU	C6-N1	5.13	1.44	1.36
86	2	71	OMG	C2-N3	5.13	1.45	1.33
35	S1	38	OMC	C4-N3	5.13	1.44	1.34
35	S1	1623	OMG	C2-N3	5.12	1.45	1.33
35	S1	2140	OMC	C4-N3	5.12	1.44	1.34
35	S1	1829	OMG	C2-N3	5.12	1.45	1.33
82	1	1171	PSU	C6-N1	5.11	1.44	1.36
86	2	593	PSU	C6-N1	5.11	1.44	1.36
82	1	672	PSU	C6-N1	5.10	1.44	1.36
86	2	1159	OMC	C4-N3	5.10	1.44	1.34
85	7	75	OMG	C2-N3	5.09	1.45	1.33
35	S1	1866	OMC	C4-N3	5.07	1.44	1.34
82	1	1017	PSU	C6-N1	5.07	1.44	1.36
86	2	626	PSU	C6-N1	5.06	1.44	1.36
86	2	1231	OMG	C2-N3	5.06	1.45	1.33
82	1	1626	OMG	C2-N3	5.05	1.45	1.33
86	2	1229	OMG	C2-N3	5.05	1.45	1.33
86	2	437	PSU	C6-N1	5.04	1.44	1.36
35	S1	1647	OMG	C2-N3	5.03	1.45	1.33
35	S1	115	OMC	C4-N3	5.03	1.44	1.34
35	S1	18	OMC	C4-N3	5.02	1.44	1.34
86	2	1317	OMC	C4-N3	5.02	1.44	1.34
86	2	1248	OMC	C4-N3	5.02	1.44	1.34
82	1	856	OMG	C2-N3	4.98	1.45	1.33
82	1	1527	OMC	C4-N3	4.97	1.44	1.34
82	1	1011	PSU	C6-N1	4.94	1.44	1.36
86	2	1397	OMC	C4-N3	4.93	1.44	1.34
86	2	583	OMC	C4-N4	4.92	1.45	1.33
82	1	1540	OMG	C2-N3	4.91	1.45	1.33
86	2	1253	OMG	C2-N3	4.89	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S1	1865	OMG	C4-N3	4.89	1.49	1.37
86	2	1317	OMC	C4-N4	4.88	1.45	1.33
86	2	1308	5MC	O4'-C1'	-4.86	1.30	1.42
82	1	695	OMC	C4-N3	4.86	1.44	1.34
86	2	641	OMG	C2-N3	4.84	1.45	1.33
82	1	1527	OMC	C4-N4	4.84	1.45	1.33
86	2	359	OMC	C4-N4	4.84	1.45	1.33
86	2	71	OMG	C4-N3	4.83	1.49	1.37
35	S1	1550	OMG	C4-N3	4.83	1.49	1.37
35	S1	600	OMG	C4-N3	4.83	1.49	1.37
35	S1	2059	OMC	C4-N4	4.82	1.45	1.33
82	1	959	OMG	C4-N3	4.82	1.49	1.37
35	S1	2151	OMG	C4-N3	4.82	1.49	1.37
86	2	1303	PSU	C1'-C5	-4.80	1.39	1.50
37	4	74	OMG	C2-N3	4.80	1.44	1.33
82	1	1010	OMC	C4-N4	4.78	1.45	1.33
86	2	1046	OMG	C2-N3	4.78	1.44	1.33
35	S1	2140	OMC	C4-N4	4.77	1.45	1.33
35	S1	115	OMC	C4-N4	4.77	1.45	1.33
86	2	1248	OMC	C4-N4	4.76	1.45	1.33
82	1	1626	OMG	C4-N3	4.76	1.48	1.37
86	2	1159	OMC	C4-N4	4.76	1.45	1.33
35	S1	1829	OMG	C4-N3	4.76	1.48	1.37
35	S1	38	OMC	C4-N4	4.75	1.45	1.33
86	2	1360	OMG	C4-N3	4.75	1.48	1.37
85	7	75	OMG	C4-N3	4.75	1.48	1.37
35	S1	1647	OMG	C4-N3	4.75	1.48	1.37
86	2	1231	OMG	C4-N3	4.74	1.48	1.37
35	S1	1866	OMC	C4-N4	4.74	1.45	1.33
85	7	75	OMG	C2-N2	4.74	1.45	1.34
86	2	443	OMC	C4-N3	4.73	1.44	1.34
35	S1	2059	OMC	C4-N3	4.73	1.44	1.34
86	2	1360	OMG	C2-N2	4.73	1.45	1.34
82	1	856	OMG	C4-N3	4.73	1.48	1.37
86	2	1229	OMG	C4-N3	4.73	1.48	1.37
35	S1	1478	OMG	C2-N3	4.73	1.44	1.33
35	S1	18	OMC	C4-N4	4.71	1.45	1.33
86	2	534	OMG	C4-N3	4.71	1.48	1.37
35	S1	1865	OMG	C2-N2	4.71	1.45	1.34
86	2	1058	PSU	C1'-C5	-4.71	1.39	1.50
82	1	695	OMC	C4-N4	4.70	1.45	1.33
86	2	1317	OMC	C2-N1	4.70	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	1190	OMG	C2-N3	4.70	1.44	1.33
86	2	1060	PSU	C1'-C5	-4.70	1.39	1.50
35	S1	1623	OMG	C4-N3	4.70	1.48	1.37
35	S1	1544	5MC	C6-N1	4.68	1.46	1.38
86	2	1397	OMC	C4-N4	4.68	1.44	1.33
86	2	1078	OMG	C2-N3	4.68	1.44	1.33
86	2	597	PSU	C1'-C5	-4.67	1.39	1.50
82	1	1524	OMG	C4-N3	4.67	1.48	1.37
35	S1	1550	OMG	C2-N2	4.67	1.45	1.34
86	2	1253	OMG	C4-N3	4.66	1.48	1.37
35	S1	1647	OMG	C2-N2	4.66	1.45	1.34
82	1	870	PSU	C1'-C5	-4.66	1.39	1.50
82	1	1540	OMG	C4-N3	4.64	1.48	1.37
86	2	655	OMG	C4-N3	4.64	1.48	1.37
82	1	1181	PSU	C1'-C5	-4.64	1.39	1.50
35	S1	2048	PSU	C1'-C5	-4.63	1.39	1.50
82	1	1524	OMG	C2-N2	4.63	1.45	1.34
86	2	78	PSU	C1'-C5	-4.62	1.39	1.50
86	2	1231	OMG	C2-N2	4.62	1.45	1.34
35	S1	600	OMG	C2-N2	4.61	1.45	1.34
86	2	443	OMC	C4-N4	4.60	1.44	1.33
82	1	959	OMG	C2-N2	4.60	1.45	1.34
37	4	74	OMG	C4-N3	4.60	1.48	1.37
82	1	1626	OMG	C2-N2	4.59	1.45	1.34
35	S1	1623	OMG	C2-N2	4.59	1.45	1.34
86	2	641	OMG	C4-N3	4.57	1.48	1.37
86	2	71	OMG	C2-N2	4.57	1.45	1.34
86	2	583	OMC	C2-N1	4.57	1.49	1.40
35	S1	1829	OMG	C2-N2	4.56	1.45	1.34
86	2	1248	OMC	C2-N1	4.56	1.49	1.40
86	2	1308	5MC	C6-N1	4.54	1.45	1.38
82	1	677	1MA	C4-N3	4.53	1.51	1.37
86	2	1229	OMG	C2-N2	4.53	1.45	1.34
82	1	856	OMG	C2-N2	4.53	1.45	1.34
37	4	74	OMG	C2-N2	4.53	1.45	1.34
35	S1	2151	OMG	C2-N2	4.52	1.44	1.34
35	S1	2059	OMC	C2-N1	4.52	1.49	1.40
86	2	1382	PSU	C1'-C5	-4.52	1.39	1.50
82	1	1540	OMG	C2-N2	4.52	1.44	1.34
35	S1	1478	OMG	C2-N2	4.52	1.44	1.34
35	S1	1246	PSU	C1'-C5	-4.52	1.39	1.50
35	S1	2046	PSU	C1'-C5	-4.52	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	1078	OMG	C4-N3	4.52	1.48	1.37
86	2	655	OMG	C2-N2	4.52	1.44	1.34
86	2	524	5MC	C6-N1	4.51	1.45	1.38
35	S1	1478	OMG	C4-N3	4.49	1.48	1.37
86	2	641	OMG	C2-N2	4.49	1.44	1.34
86	2	1046	OMG	C4-N3	4.49	1.48	1.37
35	S1	2140	OMC	C2-N1	4.49	1.49	1.40
82	1	672	PSU	C1'-C5	-4.49	1.39	1.50
82	1	1190	OMG	C4-N3	4.49	1.48	1.37
35	S1	2061	5MC	C6-N1	4.49	1.45	1.38
86	2	359	OMC	C2-N1	4.49	1.49	1.40
86	2	1078	OMG	C2-N2	4.47	1.44	1.34
86	2	1253	OMG	C2-N2	4.45	1.44	1.34
35	S1	1866	OMC	C2-N1	4.45	1.49	1.40
86	2	1265	PSU	C1'-C5	-4.44	1.40	1.50
86	2	1046	OMG	C2-N2	4.44	1.44	1.34
86	2	534	OMG	C2-N2	4.42	1.44	1.34
35	S1	1841	PSU	C1'-C5	-4.38	1.40	1.50
35	S1	1533	PSU	C1'-C5	-4.36	1.40	1.50
86	2	1318	PSU	C1'-C5	-4.36	1.40	1.50
35	S1	1544	5MC	C4-N4	4.36	1.45	1.34
35	S1	2061	5MC	C4-N4	4.36	1.45	1.34
82	1	1190	OMG	C2-N2	4.34	1.44	1.34
86	2	1397	OMC	C2-N1	4.34	1.49	1.40
35	S1	38	OMC	C2-N1	4.34	1.49	1.40
86	2	1403	PSU	C1'-C5	-4.33	1.40	1.50
86	2	1361	PSU	C1'-C5	-4.33	1.40	1.50
86	2	593	PSU	C1'-C5	-4.33	1.40	1.50
82	1	1528	PSU	C1'-C5	-4.32	1.40	1.50
86	2	1159	OMC	C2-N1	4.31	1.49	1.40
82	1	695	OMC	C2-N1	4.31	1.49	1.40
35	S1	12	PSU	C1'-C5	-4.31	1.40	1.50
82	1	1017	PSU	C1'-C5	-4.30	1.40	1.50
82	1	1171	PSU	C1'-C5	-4.30	1.40	1.50
35	S1	18	OMC	C2-N1	4.29	1.49	1.40
85	7	74	PSU	C1'-C5	-4.28	1.40	1.50
86	2	1308	5MC	C4-N4	4.27	1.45	1.34
35	S1	609	PSU	C1'-C5	-4.26	1.40	1.50
35	S1	115	OMC	C2-N1	4.26	1.49	1.40
86	2	1264	PSU	C1'-C5	-4.25	1.40	1.50
82	1	1011	PSU	C1'-C5	-4.24	1.40	1.50
82	1	1533	PSU	C1'-C5	-4.24	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	510	PSU	C1'-C5	-4.24	1.40	1.50
82	1	1527	OMC	C2-N1	4.23	1.49	1.40
35	S1	2061	5MC	C2-N1	4.23	1.49	1.40
86	2	512	PSU	C1'-C5	-4.22	1.40	1.50
35	S1	33	PSU	C1'-C5	-4.22	1.40	1.50
86	2	1413	PSU	C1'-C5	-4.21	1.40	1.50
82	1	1177	PSU	C1'-C5	-4.21	1.40	1.50
35	S1	1539	PSU	C1'-C5	-4.20	1.40	1.50
86	2	524	5MC	C4-N4	4.20	1.45	1.34
35	S1	1833	OMU	C4-N3	4.19	1.46	1.38
86	2	626	PSU	C1'-C5	-4.18	1.40	1.50
35	S1	104	PSU	C1'-C5	-4.18	1.40	1.50
35	S1	29	OMU	C4-N3	4.17	1.46	1.38
85	7	101	PSU	C1'-C5	-4.17	1.40	1.50
35	S1	1543	C4J	C6-N1	4.17	1.47	1.36
86	2	662	PSU	C1'-C5	-4.16	1.40	1.50
86	2	524	5MC	C2-N1	4.16	1.49	1.40
85	7	7	OMU	C4-N3	4.16	1.46	1.38
82	1	1664	PSU	C1'-C5	-4.13	1.40	1.50
35	S1	1544	5MC	C2-N1	4.13	1.49	1.40
86	2	437	PSU	C1'-C5	-4.13	1.40	1.50
86	2	1194	PSU	C1'-C5	-4.13	1.40	1.50
35	S1	1979	OMU	C4-N3	4.10	1.45	1.38
35	S1	1657	PSU	C1'-C5	-4.08	1.40	1.50
82	1	1039	PSU	C1'-C5	-4.08	1.40	1.50
86	2	472	PSU	C1'-C5	-4.08	1.40	1.50
35	S1	1621	OMU	C4-N3	4.07	1.45	1.38
83	3	13	OMU	C4-N3	4.06	1.45	1.38
86	2	510	PSU	C4-N3	4.04	1.46	1.38
86	2	443	OMC	C2-N1	4.02	1.48	1.40
35	S1	661	OMU	C4-N3	4.02	1.45	1.38
82	1	1659	OMU	C4-N3	4.01	1.45	1.38
86	2	1077	OMU	C4-N3	4.01	1.45	1.38
86	2	1419	OMU	C4-N3	3.99	1.45	1.38
86	2	560	OMU	C4-N3	3.99	1.45	1.38
35	S1	1566	PSU	C1'-C5	-3.98	1.41	1.50
86	2	472	PSU	C4-N3	3.98	1.46	1.38
86	2	512	PSU	C4-N3	3.98	1.46	1.38
86	2	1144	PSU	C4-N3	3.97	1.46	1.38
86	2	1403	PSU	C4-N3	3.95	1.46	1.38
82	1	1010	OMC	C2-N1	3.92	1.48	1.40
86	2	667	OMU	C4-N3	3.92	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S1	8	OMU	C4-N3	3.91	1.45	1.38
82	1	1177	PSU	C4-N3	3.91	1.46	1.38
35	S1	1539	PSU	C4-N3	3.90	1.46	1.38
85	7	69	PSU	C4-N3	3.90	1.46	1.38
35	S1	1246	PSU	C4-N3	3.90	1.46	1.38
82	1	847	OMU	C4-N3	3.89	1.45	1.38
82	1	1039	PSU	C4-N3	3.89	1.46	1.38
86	2	1359	OMU	C4-N3	3.89	1.45	1.38
86	2	1194	PSU	C4-N3	3.87	1.46	1.38
35	S1	104	PSU	C4-N3	3.86	1.46	1.38
35	S1	512	A2M	O3'-C3'	-3.84	1.33	1.43
85	7	69	PSU	C1'-C5	-3.84	1.41	1.50
86	2	1144	PSU	C1'-C5	-3.84	1.41	1.50
35	S1	1566	PSU	C4-N3	3.83	1.46	1.38
35	S1	609	PSU	C4-N3	3.83	1.45	1.38
35	S1	1841	PSU	C4-N3	3.83	1.45	1.38
85	7	74	PSU	C4-N3	3.82	1.45	1.38
86	2	1308	5MC	C2-N1	3.81	1.48	1.40
85	7	75	OMG	C6-N1	3.81	1.43	1.37
86	2	1264	PSU	C4-N3	3.81	1.45	1.38
82	1	1664	PSU	C4-N3	3.80	1.45	1.38
82	1	1533	PSU	C4-N3	3.80	1.45	1.38
35	S1	1533	PSU	C4-N3	3.79	1.45	1.38
85	7	43	A2M	O3'-C3'	-3.78	1.34	1.43
82	1	1107	OMU	C4-N3	3.78	1.45	1.38
86	2	662	PSU	C4-N3	3.78	1.45	1.38
82	1	1524	OMG	C6-N1	3.78	1.43	1.37
82	1	678	A2M	O3'-C3'	-3.77	1.34	1.43
82	1	681	A2M	O3'-C3'	-3.77	1.34	1.43
82	1	672	PSU	C4-N3	3.77	1.45	1.38
35	S1	33	PSU	C4-N3	3.77	1.45	1.38
86	2	73	OMU	C4-N3	3.76	1.45	1.38
82	1	1171	PSU	C4-N3	3.74	1.45	1.38
86	2	626	PSU	C4-N3	3.73	1.45	1.38
35	S1	753	A2M	O3'-C3'	-3.73	1.34	1.43
35	S1	1865	OMG	C6-N1	3.73	1.43	1.37
86	2	382	A2M	O3'-C3'	-3.72	1.34	1.43
82	1	1626	OMG	C6-N1	3.72	1.43	1.37
35	S1	1623	OMG	C6-N1	3.72	1.43	1.37
82	1	677	1MA	C2-N1	3.72	1.42	1.35
82	1	1190	OMG	C6-N1	3.71	1.43	1.37
86	2	1078	OMG	C6-N1	3.70	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	1011	PSU	C4-N3	3.70	1.45	1.38
82	1	1371	OMU	C4-N3	3.70	1.45	1.38
35	S1	1478	OMG	C6-N1	3.70	1.43	1.37
86	2	437	PSU	C4-N3	3.69	1.45	1.38
35	S1	600	OMG	C6-N1	3.69	1.43	1.37
82	1	1017	PSU	C4-N3	3.69	1.45	1.38
82	1	856	OMG	C6-N1	3.68	1.43	1.37
85	7	101	PSU	C4-N3	3.67	1.45	1.38
86	2	1265	PSU	C4-N3	3.67	1.45	1.38
35	S1	1657	PSU	C4-N3	3.66	1.45	1.38
35	S1	1550	OMG	C6-N1	3.65	1.43	1.37
86	2	95	A2M	O3'-C3'	-3.64	1.34	1.43
86	2	593	PSU	C4-N3	3.63	1.45	1.38
82	1	927	A2M	O3'-C3'	-3.62	1.34	1.43
37	4	74	OMG	C6-N1	3.61	1.43	1.37
86	2	1361	PSU	C4-N3	3.61	1.45	1.38
86	2	1413	PSU	C4-N3	3.61	1.45	1.38
82	1	1181	PSU	C4-N3	3.60	1.45	1.38
35	S1	1995	7MG	C6-N1	3.60	1.45	1.38
86	2	591	A2M	O3'-C3'	-3.60	1.34	1.43
86	2	1185	A2M	O3'-C3'	-3.60	1.34	1.43
86	2	1360	OMG	C6-N1	3.60	1.43	1.37
86	2	1231	OMG	C6-N1	3.58	1.43	1.37
35	S1	1829	OMG	C6-N1	3.58	1.43	1.37
86	2	534	OMG	C6-N1	3.58	1.43	1.37
86	2	641	OMG	C6-N1	3.58	1.43	1.37
86	2	604	A2M	O3'-C3'	-3.57	1.34	1.43
35	S1	12	PSU	C4-N3	3.57	1.45	1.38
86	2	1229	OMG	C6-N1	3.57	1.43	1.37
86	2	572	A2M	O3'-C3'	-3.56	1.34	1.43
82	1	955	A2M	O3'-C3'	-3.55	1.34	1.43
82	1	1528	PSU	C4-N3	3.55	1.45	1.38
86	2	1046	OMG	C6-N1	3.54	1.43	1.37
35	S1	897	A2M	O3'-C3'	-3.53	1.34	1.43
35	S1	2046	PSU	C4-N3	3.52	1.45	1.38
85	7	162	A2M	O3'-C3'	-3.52	1.34	1.43
82	1	697	A2M	O3'-C3'	-3.52	1.34	1.43
35	S1	1995	7MG	C2-N1	3.52	1.46	1.37
82	1	1540	OMG	C6-N1	3.50	1.43	1.37
86	2	1303	PSU	C4-N3	3.50	1.45	1.38
35	S1	912	A2M	O3'-C3'	-3.49	1.34	1.43
86	2	628	A2M	O3'-C3'	-3.49	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	1318	PSU	C4-N3	3.48	1.45	1.38
82	1	959	OMG	C6-N1	3.48	1.43	1.37
35	S1	1995	7MG	C5-C6	3.46	1.52	1.43
35	S1	2059	OMC	O2-C2	-3.45	1.17	1.23
35	S1	2151	OMG	C6-N1	3.45	1.43	1.37
82	1	1527	OMC	C6-N1	3.44	1.46	1.38
35	S1	98	A2M	O3'-C3'	-3.44	1.34	1.43
82	1	1539	A2M	O3'-C3'	-3.44	1.34	1.43
82	1	235	A2M	O3'-C3'	-3.43	1.34	1.43
86	2	71	OMG	C6-N1	3.39	1.42	1.37
86	2	1253	OMG	C6-N1	3.38	1.42	1.37
35	S1	2048	PSU	C4-N3	3.37	1.45	1.38
82	1	845	OMU	O2-C2	-3.37	1.16	1.23
35	S1	1543	C4J	C4-N3	3.37	1.46	1.40
35	S1	28	A2M	O3'-C3'	-3.36	1.35	1.43
86	2	1058	PSU	C4-N3	3.36	1.45	1.38
86	2	583	OMC	C6-N1	3.36	1.46	1.38
35	S1	1647	OMG	C6-N1	3.35	1.42	1.37
86	2	597	PSU	C4-N3	3.35	1.45	1.38
82	1	870	PSU	C4-N3	3.34	1.45	1.38
86	2	1060	PSU	C4-N3	3.34	1.45	1.38
86	2	1397	OMC	C6-N1	3.33	1.46	1.38
86	2	1384	A2M	O3'-C3'	-3.31	1.35	1.43
86	2	1372	A2M	O3'-C3'	-3.31	1.35	1.43
86	2	1382	PSU	C4-N3	3.31	1.45	1.38
82	1	407	A2M	O3'-C3'	-3.30	1.35	1.43
35	S1	918	A2M	O3'-C3'	-3.29	1.35	1.43
86	2	655	OMG	C6-N1	3.29	1.42	1.37
86	2	1317	OMC	C6-N1	3.28	1.45	1.38
35	S1	1995	7MG	C2-N2	3.28	1.42	1.34
35	S1	1543	C4J	C2-N1	3.28	1.48	1.39
35	S1	969	A2M	O3'-C3'	-3.28	1.35	1.43
82	1	845	OMU	O4-C4	-3.27	1.18	1.24
86	2	1248	OMC	C6-N1	3.27	1.45	1.38
82	1	845	OMU	C4-N3	3.27	1.44	1.38
35	S1	18	OMC	C6-N1	3.25	1.45	1.38
35	S1	2059	OMC	C6-N1	3.25	1.45	1.38
35	S1	1543	C4J	C31-C3	3.25	1.59	1.52
35	S1	1866	OMC	C6-N1	3.24	1.45	1.38
82	1	677	1MA	C5-C4	-3.24	1.34	1.43
35	S1	8	OMU	O4-C4	-3.23	1.18	1.24
86	2	359	OMC	C6-N1	3.23	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	678	A2M	O2'-C2'	3.22	1.50	1.42
86	2	1159	OMC	C6-N1	3.22	1.45	1.38
82	1	695	OMC	C6-N1	3.22	1.45	1.38
35	S1	1833	OMU	O4-C4	-3.21	1.18	1.24
86	2	95	A2M	C6-N6	3.20	1.45	1.34
35	S1	753	A2M	C6-N6	3.20	1.45	1.34
35	S1	38	OMC	C6-N1	3.20	1.45	1.38
82	1	1190	OMG	C5-C6	3.20	1.53	1.47
86	2	78	PSU	C4-N3	3.20	1.44	1.38
35	S1	115	OMC	C6-N1	3.19	1.45	1.38
83	3	13	OMU	O4-C4	-3.18	1.18	1.24
35	S1	2140	OMC	C6-N1	3.16	1.45	1.38
82	1	1659	OMU	O4-C4	-3.16	1.18	1.24
82	1	858	A2M	O3'-C3'	-3.16	1.35	1.43
35	S1	969	A2M	C6-N6	3.15	1.45	1.34
35	S1	918	A2M	C6-N6	3.15	1.45	1.34
82	1	1107	OMU	O4-C4	-3.15	1.18	1.24
35	S1	2021	A2M	C6-N6	3.15	1.45	1.34
35	S1	912	A2M	C6-N6	3.15	1.45	1.34
82	1	858	A2M	C6-N6	3.14	1.45	1.34
35	S1	512	A2M	C6-N6	3.14	1.45	1.34
82	1	678	A2M	C6-N6	3.13	1.45	1.34
86	2	443	OMC	C6-N1	3.13	1.45	1.38
85	7	43	A2M	C6-N6	3.12	1.45	1.34
86	2	71	OMG	C5-C6	3.12	1.53	1.47
35	S1	1623	OMG	C5-C6	3.12	1.53	1.47
86	2	73	OMU	O4-C4	-3.12	1.18	1.24
85	7	162	A2M	C6-N6	3.12	1.45	1.34
86	2	1185	A2M	C6-N6	3.12	1.45	1.34
86	2	641	OMG	C5-C6	3.11	1.53	1.47
35	S1	969	A2M	O2'-C2'	3.11	1.50	1.42
35	S1	897	A2M	C6-N6	3.11	1.45	1.34
35	S1	668	A2M	C6-N6	3.10	1.45	1.34
86	2	1359	OMU	O4-C4	-3.10	1.18	1.24
35	S1	1865	OMG	C5-C6	3.10	1.53	1.47
35	S1	661	OMU	O4-C4	-3.10	1.18	1.24
86	2	1078	OMG	C5-C6	3.10	1.53	1.47
85	7	75	OMG	C5-C6	3.10	1.53	1.47
82	1	1524	OMG	C5-C6	3.10	1.53	1.47
82	1	1626	OMG	C5-C6	3.10	1.53	1.47
35	S1	1647	OMG	C5-C6	3.10	1.53	1.47
35	S1	1995	7MG	O6-C6	-3.09	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	534	OMG	C5-C6	3.09	1.53	1.47
86	2	570	A2M	O3'-C3'	-3.08	1.35	1.43
82	1	955	A2M	C6-N6	3.08	1.45	1.34
86	2	570	A2M	O2'-C2'	3.08	1.50	1.42
82	1	927	A2M	C6-N6	3.07	1.45	1.34
35	S1	28	A2M	O2'-C2'	3.07	1.50	1.42
86	2	560	OMU	O4-C4	-3.07	1.18	1.24
86	2	1384	A2M	O2'-C2'	3.07	1.50	1.42
86	2	382	A2M	C6-N6	3.07	1.45	1.34
86	2	641	OMG	C5-C4	-3.07	1.35	1.43
86	2	1253	OMG	C5-C6	3.07	1.53	1.47
86	2	604	A2M	C6-N6	3.06	1.45	1.34
86	2	570	A2M	C6-N6	3.06	1.45	1.34
82	1	1540	OMG	C5-C6	3.06	1.53	1.47
86	2	1372	A2M	C6-N6	3.06	1.45	1.34
35	S1	1829	OMG	C5-C6	3.06	1.53	1.47
82	1	697	A2M	C6-N6	3.06	1.45	1.34
86	2	443	OMC	O2-C2	-3.06	1.18	1.23
35	S1	98	A2M	O2'-C2'	3.06	1.50	1.42
35	S1	753	A2M	O2'-C2'	3.06	1.50	1.42
35	S1	1621	OMU	O4-C4	-3.06	1.18	1.24
86	2	1360	OMG	C5-C6	3.06	1.53	1.47
82	1	235	A2M	C6-N6	3.05	1.45	1.34
35	S1	600	OMG	C5-C6	3.05	1.53	1.47
86	2	591	A2M	C6-N6	3.05	1.45	1.34
86	2	95	A2M	O2'-C2'	3.04	1.50	1.42
82	1	305	A2M	C6-N6	3.04	1.45	1.34
82	1	681	A2M	O2'-C2'	3.04	1.50	1.42
86	2	667	OMU	O4-C4	-3.04	1.18	1.24
86	2	628	A2M	C6-N6	3.04	1.45	1.34
82	1	1539	A2M	C6-N6	3.04	1.45	1.34
85	7	7	OMU	O4-C4	-3.03	1.18	1.24
35	S1	1478	OMG	C5-C4	-3.02	1.35	1.43
82	1	681	A2M	C6-N6	3.02	1.45	1.34
35	S1	918	A2M	O2'-C2'	3.02	1.50	1.42
86	2	1308	5MC	O2-C2	-3.01	1.18	1.23
82	1	847	OMU	O4-C4	-3.01	1.18	1.24
35	S1	1543	C4J	O4-C4	-3.01	1.16	1.23
86	2	604	A2M	O2'-C2'	3.01	1.50	1.42
86	2	1308	5MC	O2'-C2'	-3.00	1.35	1.43
85	7	162	A2M	O2'-C2'	3.00	1.50	1.42
35	S1	1657	PSU	O4-C4	-3.00	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	305	A2M	O3'-C3'	-2.99	1.35	1.43
82	1	927	A2M	O2'-C2'	2.99	1.50	1.42
35	S1	2151	OMG	C5-C6	2.99	1.53	1.47
86	2	572	A2M	O2'-C2'	2.99	1.50	1.42
86	2	572	A2M	C6-N6	2.99	1.44	1.34
86	2	1077	OMU	O4-C4	-2.99	1.18	1.24
82	1	1190	OMG	C5-C4	-2.98	1.35	1.43
35	S1	479	A2M	O3'-C3'	-2.98	1.35	1.43
86	2	1231	OMG	C5-C6	2.98	1.53	1.47
35	S1	1550	OMG	C5-C6	2.98	1.53	1.47
35	S1	1979	OMU	O4-C4	-2.98	1.18	1.24
82	1	955	A2M	O2'-C2'	2.97	1.50	1.42
35	S1	479	A2M	C6-N6	2.96	1.44	1.34
35	S1	98	A2M	C6-N6	2.96	1.44	1.34
86	2	591	A2M	O2'-C2'	2.96	1.50	1.42
86	2	382	A2M	O2'-C2'	2.95	1.50	1.42
83	3	13	OMU	C6-N1	2.95	1.45	1.38
86	2	1078	OMG	C5-C4	-2.95	1.35	1.43
82	1	1664	PSU	O4-C4	-2.94	1.18	1.23
86	2	667	OMU	C6-N1	2.94	1.45	1.38
35	S1	661	OMU	C6-N1	2.94	1.45	1.38
82	1	1371	OMU	O4-C4	-2.94	1.18	1.24
86	2	1077	OMU	C6-N1	2.94	1.45	1.38
82	1	407	A2M	C6-N6	2.93	1.44	1.34
35	S1	1647	OMG	C5-C4	-2.93	1.35	1.43
35	S1	479	A2M	O2'-C2'	2.93	1.50	1.42
85	7	7	OMU	C6-N1	2.93	1.45	1.38
82	1	856	OMG	C5-C6	2.92	1.53	1.47
82	1	959	OMG	C5-C6	2.92	1.53	1.47
35	S1	28	A2M	C6-N6	2.92	1.44	1.34
82	1	695	OMC	O2-C2	-2.92	1.18	1.23
86	2	1046	OMG	C2-N1	2.92	1.44	1.37
82	1	1010	OMC	C6-N1	2.92	1.45	1.38
82	1	1171	PSU	O4-C4	-2.92	1.18	1.23
86	2	1419	OMU	O4-C4	-2.91	1.18	1.24
86	2	1359	OMU	C6-N1	2.91	1.45	1.38
82	1	235	A2M	O2'-C2'	2.91	1.50	1.42
82	1	1659	OMU	C6-N1	2.91	1.45	1.38
86	2	1229	OMG	C5-C6	2.91	1.53	1.47
35	S1	512	A2M	O2'-C2'	2.90	1.50	1.42
37	4	74	OMG	C5-C4	-2.90	1.35	1.43
86	2	527	A2M	C6-N6	2.90	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S1	2021	A2M	O3'-C3'	-2.90	1.36	1.43
35	S1	1979	OMU	C6-N1	2.89	1.45	1.38
82	1	1527	OMC	O2-C2	-2.89	1.18	1.23
86	2	1231	OMG	C5-C4	-2.89	1.35	1.43
86	2	1248	OMC	O2-C2	-2.89	1.18	1.23
37	4	74	OMG	C5-C6	2.88	1.53	1.47
86	2	1384	A2M	C6-N6	2.88	1.44	1.34
35	S1	2061	5MC	O2-C2	-2.88	1.18	1.23
35	S1	912	A2M	O2'-C2'	2.88	1.50	1.42
35	S1	38	OMC	O2-C2	-2.87	1.18	1.23
86	2	527	A2M	O2'-C2'	2.87	1.50	1.42
82	1	407	A2M	O2'-C2'	2.87	1.50	1.42
86	2	1265	PSU	O4-C4	-2.87	1.18	1.23
82	1	1017	PSU	O4-C4	-2.87	1.18	1.23
82	1	1539	A2M	O2'-C2'	2.86	1.49	1.42
86	2	1397	OMC	O2-C2	-2.86	1.18	1.23
86	2	1229	OMG	C5-C4	-2.85	1.35	1.43
86	2	1159	OMC	O2-C2	-2.85	1.18	1.23
86	2	1046	OMG	C5-C4	-2.85	1.35	1.43
35	S1	897	A2M	O2'-C2'	2.85	1.49	1.42
35	S1	1621	OMU	C6-N1	2.85	1.44	1.38
82	1	1540	OMG	C5-C4	-2.85	1.35	1.43
86	2	1308	5MC	O3'-C3'	2.84	1.49	1.43
85	7	101	PSU	O4-C4	-2.84	1.18	1.23
35	S1	29	OMU	C6-N1	2.84	1.44	1.38
86	2	1419	OMU	C6-N1	2.84	1.44	1.38
35	S1	2140	OMC	O2-C2	-2.83	1.18	1.23
35	S1	18	OMC	O2-C2	-2.83	1.18	1.23
86	2	626	PSU	O4-C4	-2.82	1.18	1.23
86	2	662	PSU	O4-C4	-2.82	1.18	1.23
35	S1	12	PSU	O4-C4	-2.82	1.18	1.23
86	2	628	A2M	O2'-C2'	2.82	1.49	1.42
82	1	305	A2M	C5-C4	-2.82	1.33	1.40
82	1	1107	OMU	C6-N1	2.82	1.44	1.38
86	2	1253	OMG	C5-C4	-2.81	1.35	1.43
86	2	655	OMG	C5-C6	2.81	1.53	1.47
86	2	73	OMU	C6-N1	2.81	1.44	1.38
86	2	1317	OMC	O2-C2	-2.81	1.18	1.23
86	2	572	A2M	C5-C4	-2.80	1.33	1.40
82	1	927	A2M	C5-C4	-2.80	1.33	1.40
86	2	560	OMU	C6-N1	2.80	1.44	1.38
82	1	305	A2M	O2'-C2'	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	524	5MC	O2-C2	-2.79	1.18	1.23
82	1	856	OMG	C5-C4	-2.79	1.36	1.43
86	2	1264	PSU	O4-C4	-2.79	1.18	1.23
82	1	697	A2M	O2'-C2'	2.79	1.49	1.42
35	S1	1478	OMG	C5-C6	2.79	1.53	1.47
35	S1	115	OMC	O2-C2	-2.78	1.18	1.23
86	2	1194	PSU	O4-C4	-2.78	1.18	1.23
35	S1	1833	OMU	C6-N1	2.78	1.44	1.38
35	S1	1623	OMG	C2-N1	2.78	1.44	1.37
86	2	527	A2M	O3'-C3'	-2.78	1.36	1.43
86	2	655	OMG	C2-N1	2.78	1.44	1.37
35	S1	2021	A2M	O2'-C2'	2.78	1.49	1.42
82	1	1524	OMG	C5-C4	-2.78	1.36	1.43
82	1	1010	OMC	O2-C2	-2.77	1.18	1.23
82	1	847	OMU	C6-N1	2.77	1.44	1.38
86	2	1361	PSU	O4-C4	-2.77	1.18	1.23
82	1	1371	OMU	C6-N1	2.77	1.44	1.38
82	1	697	A2M	C5-C4	-2.77	1.33	1.40
86	2	527	A2M	C5-C4	-2.77	1.33	1.40
86	2	1372	A2M	C5-C4	-2.77	1.33	1.40
86	2	1078	OMG	C2-N1	2.76	1.44	1.37
86	2	359	OMC	O2-C2	-2.76	1.18	1.23
85	7	75	OMG	C2-N1	2.76	1.44	1.37
82	1	1533	PSU	O4-C4	-2.76	1.18	1.23
35	S1	8	OMU	C6-N1	2.76	1.44	1.38
35	S1	600	OMG	C2-N1	2.76	1.44	1.37
82	1	235	A2M	C5-C4	-2.76	1.33	1.40
82	1	1626	OMG	C2-N1	2.76	1.44	1.37
86	2	71	OMG	C5-C4	-2.76	1.36	1.43
35	S1	1544	5MC	O2-C2	-2.76	1.18	1.23
35	S1	1478	OMG	C2-N1	2.75	1.44	1.37
86	2	628	A2M	C5-C4	-2.75	1.33	1.40
82	1	1039	PSU	O4-C4	-2.75	1.18	1.23
35	S1	1865	OMG	C5-C4	-2.74	1.36	1.43
35	S1	1865	OMG	C2-N1	2.74	1.44	1.37
82	1	856	OMG	C2-N1	2.74	1.44	1.37
82	1	1524	OMG	C2-N1	2.74	1.44	1.37
85	7	75	OMG	C5-C4	-2.74	1.36	1.43
82	1	1626	OMG	C5-C4	-2.74	1.36	1.43
35	S1	1829	OMG	C5-C4	-2.74	1.36	1.43
86	2	1231	OMG	C2-N1	2.73	1.44	1.37
35	S1	1550	OMG	C2-N1	2.73	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S1	2151	OMG	C5-C4	-2.73	1.36	1.43
35	S1	668	A2M	C5-C4	-2.73	1.33	1.40
86	2	1403	PSU	O4-C4	-2.72	1.18	1.23
35	S1	1866	OMC	O2-C2	-2.72	1.18	1.23
86	2	534	OMG	C5-C4	-2.72	1.36	1.43
82	1	681	A2M	C5-C4	-2.72	1.33	1.40
86	2	604	A2M	C5-C4	-2.72	1.33	1.40
35	S1	1623	OMG	C5-C4	-2.72	1.36	1.43
35	S1	29	OMU	O4-C4	-2.72	1.19	1.24
82	1	1539	A2M	C5-C4	-2.72	1.33	1.40
82	1	672	PSU	O4-C4	-2.71	1.18	1.23
86	2	1185	A2M	C5-C4	-2.71	1.33	1.40
35	S1	1550	OMG	C5-C4	-2.71	1.36	1.43
86	2	1360	OMG	C2-N1	2.71	1.44	1.37
35	S1	2184	MA6	C5-C4	-2.71	1.33	1.40
86	2	570	A2M	C5-C4	-2.71	1.33	1.40
86	2	593	PSU	O4-C4	-2.71	1.18	1.23
86	2	1413	PSU	O4-C4	-2.71	1.18	1.23
86	2	382	A2M	C5-C4	-2.70	1.33	1.40
37	4	74	OMG	C2-N1	2.70	1.44	1.37
86	2	437	PSU	O4-C4	-2.70	1.18	1.23
86	2	78	PSU	O4-C4	-2.69	1.18	1.23
86	2	1185	A2M	O2'-C2'	2.69	1.49	1.42
35	S1	600	OMG	C5-C4	-2.69	1.36	1.43
82	1	870	PSU	O4-C4	-2.69	1.18	1.23
85	7	162	A2M	C5-C4	-2.69	1.33	1.40
86	2	591	A2M	C5-C4	-2.69	1.33	1.40
86	2	1372	A2M	O2'-C2'	2.68	1.49	1.42
85	7	43	A2M	O2'-C2'	2.68	1.49	1.42
35	S1	918	A2M	C5-C4	-2.68	1.33	1.40
86	2	1360	OMG	C5-C4	-2.68	1.36	1.43
35	S1	1829	OMG	C2-N1	2.68	1.44	1.37
86	2	583	OMC	O2-C2	-2.68	1.18	1.23
86	2	1229	OMG	C2-N1	2.67	1.44	1.37
86	2	655	OMG	C5-C4	-2.67	1.36	1.43
82	1	1540	OMG	C2-N1	2.67	1.44	1.37
35	S1	1841	PSU	O4-C4	-2.67	1.18	1.23
82	1	858	A2M	C5-C4	-2.66	1.33	1.40
35	S1	668	A2M	O3'-C3'	-2.66	1.36	1.43
86	2	641	OMG	C2-N1	2.65	1.44	1.37
82	1	1177	PSU	O4-C4	-2.65	1.18	1.23
86	2	597	PSU	O4-C4	-2.65	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	71	OMG	C2-N1	2.65	1.44	1.37
35	S1	912	A2M	C5-C4	-2.65	1.33	1.40
35	S1	2021	A2M	C5-C4	-2.65	1.33	1.40
86	2	534	OMG	C2-N1	2.64	1.44	1.37
85	7	69	PSU	O4-C4	-2.64	1.18	1.23
35	S1	104	PSU	O4-C4	-2.64	1.18	1.23
82	1	959	OMG	C2-N1	2.64	1.44	1.37
86	2	95	A2M	C5-C4	-2.63	1.34	1.40
35	S1	668	A2M	O2'-C2'	2.63	1.49	1.42
85	7	74	PSU	O4-C4	-2.62	1.18	1.23
35	S1	1533	PSU	O4-C4	-2.62	1.18	1.23
82	1	858	A2M	O2'-C2'	2.62	1.49	1.42
86	2	1318	PSU	O4-C4	-2.62	1.18	1.23
86	2	1046	OMG	C5-C6	2.62	1.52	1.47
82	1	1190	OMG	C2-N1	2.62	1.44	1.37
35	S1	609	PSU	O4-C4	-2.62	1.18	1.23
35	S1	897	A2M	C5-C4	-2.62	1.34	1.40
85	7	69	PSU	O4'-C1'	-2.61	1.40	1.43
86	2	1382	PSU	O4-C4	-2.61	1.18	1.23
35	S1	2185	MA6	C5-C4	-2.61	1.34	1.40
85	7	43	A2M	C5-C4	-2.61	1.34	1.40
35	S1	512	A2M	C5-C4	-2.61	1.34	1.40
35	S1	1647	OMG	C2-N1	2.61	1.44	1.37
86	2	583	OMC	C5-C4	2.61	1.48	1.42
86	2	1253	OMG	C2-N1	2.60	1.44	1.37
82	1	959	OMG	C5-C4	-2.60	1.36	1.43
35	S1	2151	OMG	C2-N1	2.59	1.44	1.37
82	1	955	A2M	C5-C4	-2.59	1.34	1.40
85	7	43	A2M	O5'-C5'	-2.58	1.38	1.44
35	S1	2048	PSU	O4-C4	-2.58	1.18	1.23
35	S1	1246	PSU	O4-C4	-2.58	1.18	1.23
35	S1	1539	PSU	O4-C4	-2.58	1.18	1.23
86	2	1317	OMC	C5-C4	2.58	1.48	1.42
35	S1	753	A2M	C5-C4	-2.58	1.34	1.40
82	1	1527	OMC	C5-C4	2.57	1.48	1.42
86	2	510	PSU	O4-C4	-2.57	1.18	1.23
86	2	1058	PSU	O4-C4	-2.56	1.18	1.23
35	S1	1566	PSU	O4-C4	-2.56	1.18	1.23
82	1	407	A2M	C5-C4	-2.55	1.34	1.40
35	S1	29	OMU	C5-C4	2.55	1.49	1.43
86	2	1060	PSU	O4-C4	-2.55	1.18	1.23
86	2	1397	OMC	C5-C4	2.54	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	667	OMU	O2-C2	-2.54	1.18	1.23
82	1	678	A2M	C5-C4	-2.53	1.34	1.40
86	2	512	PSU	O4-C4	-2.53	1.18	1.23
83	3	13	OMU	O2-C2	-2.52	1.18	1.23
82	1	1010	OMC	C5-C4	2.52	1.48	1.42
86	2	472	PSU	O4-C4	-2.51	1.18	1.23
86	2	1419	OMU	C5-C4	2.51	1.49	1.43
86	2	1253	OMG	O6-C6	-2.50	1.18	1.23
86	2	443	OMC	C5-C4	2.50	1.48	1.42
86	2	1419	OMU	O2-C2	-2.50	1.18	1.23
86	2	1303	PSU	O4-C4	-2.49	1.18	1.23
35	S1	969	A2M	C5-C4	-2.49	1.34	1.40
86	2	1144	PSU	O4-C4	-2.48	1.18	1.23
82	1	1659	OMU	O2-C2	-2.47	1.18	1.23
86	2	1077	OMU	C5-C4	2.47	1.49	1.43
86	2	1077	OMU	O2-C2	-2.44	1.18	1.23
86	2	1359	OMU	O2-C2	-2.44	1.18	1.23
82	1	845	OMU	C6-N1	2.44	1.43	1.38
35	S1	2046	PSU	O4-C4	-2.44	1.18	1.23
35	S1	1543	C4J	O2-C2	-2.44	1.18	1.22
86	2	73	OMU	O2-C2	-2.43	1.18	1.23
35	S1	1866	OMC	C5-C4	2.43	1.48	1.42
35	S1	661	OMU	O2-C2	-2.42	1.18	1.23
86	2	641	OMG	O6-C6	-2.42	1.18	1.23
35	S1	38	OMC	C5-C4	2.41	1.48	1.42
35	S1	8	OMU	O2-C2	-2.41	1.18	1.23
86	2	1384	A2M	C5-C4	-2.41	1.34	1.40
86	2	1248	OMC	C5-C4	2.41	1.48	1.42
35	S1	18	OMC	C5-C4	2.41	1.48	1.42
82	1	1107	OMU	C5-C4	2.40	1.48	1.43
82	1	1528	PSU	O4-C4	-2.39	1.19	1.23
86	2	560	OMU	O2-C2	-2.39	1.18	1.23
82	1	959	OMG	O6-C6	-2.39	1.18	1.23
35	S1	668	A2M	O5'-C5'	-2.39	1.38	1.44
35	S1	479	A2M	C5-C4	-2.39	1.34	1.40
82	1	1540	OMG	O6-C6	-2.39	1.18	1.23
86	2	1229	OMG	O6-C6	-2.39	1.18	1.23
82	1	1181	PSU	O4-C4	-2.39	1.19	1.23
86	2	359	OMC	C5-C4	2.39	1.48	1.42
82	1	1190	OMG	O6-C6	-2.38	1.18	1.23
35	S1	115	OMC	C5-C4	2.38	1.48	1.42
86	2	1159	OMC	C5-C4	2.38	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	534	OMG	O6-C6	-2.37	1.18	1.23
82	1	1107	OMU	O2-C2	-2.37	1.18	1.23
83	3	13	OMU	C5-C4	2.37	1.48	1.43
86	2	1078	OMG	O6-C6	-2.37	1.18	1.23
86	2	667	OMU	C5-C4	2.36	1.48	1.43
35	S1	1621	OMU	O2-C2	-2.36	1.18	1.23
35	S1	661	OMU	C5-C4	2.36	1.48	1.43
82	1	1011	PSU	O4-C4	-2.35	1.19	1.23
82	1	847	OMU	O2-C2	-2.35	1.18	1.23
35	S1	1979	OMU	O2-C2	-2.35	1.18	1.23
35	S1	1829	OMG	O6-C6	-2.35	1.18	1.23
35	S1	1478	OMG	O6-C6	-2.35	1.18	1.23
86	2	1231	OMG	O6-C6	-2.34	1.18	1.23
35	S1	2059	OMC	C5-C4	2.34	1.48	1.42
35	S1	1647	OMG	O6-C6	-2.34	1.18	1.23
82	1	856	OMG	O6-C6	-2.33	1.18	1.23
86	2	1359	OMU	C5-C4	2.33	1.48	1.43
35	S1	2140	OMC	C5-C4	2.33	1.48	1.42
35	S1	98	A2M	C5-C4	-2.33	1.34	1.40
37	4	74	OMG	O6-C6	-2.33	1.18	1.23
86	2	71	OMG	O6-C6	-2.33	1.18	1.23
35	S1	33	PSU	O4-C4	-2.32	1.19	1.23
35	S1	1621	OMU	C5-C4	2.32	1.48	1.43
35	S1	1865	OMG	O6-C6	-2.32	1.18	1.23
86	2	1360	OMG	O6-C6	-2.32	1.18	1.23
85	7	7	OMU	C5-C4	2.31	1.48	1.43
35	S1	1979	OMU	C5-C4	2.31	1.48	1.43
82	1	695	OMC	C5-C4	2.31	1.48	1.42
35	S1	969	A2M	C2-N3	2.31	1.35	1.32
35	S1	918	A2M	C2-N3	2.30	1.35	1.32
82	1	1626	OMG	O6-C6	-2.29	1.18	1.23
35	S1	600	OMG	O6-C6	-2.28	1.18	1.23
85	7	7	OMU	O2-C2	-2.28	1.18	1.23
35	S1	28	A2M	C5-C4	-2.28	1.34	1.40
35	S1	1623	OMG	O6-C6	-2.28	1.18	1.23
35	S1	8	OMU	C5-C4	2.28	1.48	1.43
86	2	73	OMU	C5-C4	2.27	1.48	1.43
85	7	75	OMG	O6-C6	-2.26	1.18	1.23
82	1	1181	PSU	C4-C5	2.25	1.50	1.44
82	1	407	A2M	O5'-C5'	-2.25	1.39	1.44
35	S1	2151	OMG	O6-C6	-2.25	1.18	1.23
82	1	678	A2M	C2-N3	2.24	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	1371	OMU	C5-C4	2.23	1.48	1.43
35	S1	1833	OMU	O2-C2	-2.23	1.19	1.23
86	2	527	A2M	O5'-C5'	-2.23	1.39	1.44
35	S1	1833	OMU	C5-C4	2.23	1.48	1.43
82	1	1659	OMU	C5-C4	2.23	1.48	1.43
35	S1	1550	OMG	O6-C6	-2.21	1.18	1.23
82	1	1371	OMU	O2-C2	-2.21	1.19	1.23
35	S1	512	A2M	O5'-C5'	-2.20	1.39	1.44
82	1	847	OMU	C5-C4	2.19	1.48	1.43
86	2	560	OMU	C5-C4	2.18	1.48	1.43
86	2	472	PSU	O4'-C1'	-2.18	1.40	1.43
82	1	1524	OMG	O6-C6	-2.17	1.18	1.23
86	2	655	OMG	O6-C6	-2.17	1.18	1.23
82	1	845	OMU	C5-C4	2.17	1.48	1.43
82	1	1011	PSU	C4-C5	2.16	1.50	1.44
35	S1	29	OMU	O2-C2	-2.16	1.19	1.23
35	S1	668	A2M	C2-N3	2.16	1.35	1.32
35	S1	912	A2M	C2-N3	2.14	1.35	1.32
85	7	162	A2M	O5'-C5'	-2.13	1.39	1.44
35	S1	2185	MA6	C2-N3	2.13	1.35	1.32
82	1	955	A2M	O5'-C5'	-2.12	1.39	1.44
82	1	305	A2M	O5'-C5'	-2.11	1.39	1.44
82	1	235	A2M	C2-N3	2.11	1.35	1.32
82	1	1539	A2M	O5'-C5'	-2.11	1.39	1.44
35	S1	2021	A2M	C2-N3	2.10	1.35	1.32
35	S1	2185	MA6	C10-N6	2.09	1.50	1.45
86	2	572	A2M	O5'-C5'	-2.09	1.39	1.44
85	7	162	A2M	C2-N3	2.09	1.35	1.32
86	2	95	A2M	C2-N3	2.09	1.35	1.32
35	S1	1566	PSU	C4-C5	2.09	1.50	1.44
35	S1	98	A2M	C2-N3	2.08	1.35	1.32
86	2	527	A2M	C2-N3	2.07	1.35	1.32
86	2	1382	PSU	O2-C2	-2.06	1.19	1.23
82	1	677	1MA	CM1-N1	-2.06	1.42	1.46
35	S1	897	A2M	O5'-C5'	-2.05	1.39	1.44
82	1	858	A2M	O5'-C5'	-2.05	1.39	1.44
35	S1	897	A2M	C2-N3	2.05	1.35	1.32
82	1	1011	PSU	O4'-C1'	-2.05	1.41	1.43
35	S1	479	A2M	C2-N3	2.05	1.35	1.32
35	S1	33	PSU	C4-C5	2.04	1.50	1.44
86	2	1308	5MC	O5'-C5'	-2.04	1.39	1.44
86	2	1185	A2M	C2-N3	2.04	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	1046	OMG	O6-C6	-2.04	1.19	1.23
82	1	678	A2M	O5'-C5'	-2.04	1.39	1.44
86	2	628	A2M	O5'-C5'	-2.03	1.39	1.44
35	S1	753	A2M	C2-N3	2.03	1.35	1.32
35	S1	512	A2M	C2-N3	2.02	1.35	1.32
85	7	69	PSU	C4-C5	2.02	1.49	1.44
82	1	1539	A2M	C2-N3	2.01	1.35	1.32
86	2	1144	PSU	C4-C5	2.01	1.49	1.44
86	2	570	A2M	O5'-C5'	-2.01	1.39	1.44
86	2	437	PSU	C4-C5	2.00	1.49	1.44
82	1	407	A2M	C2-N3	2.00	1.35	1.32

All (570) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	2185	MA6	N1-C6-N6	-12.27	104.14	117.06
35	S1	2184	MA6	N1-C6-N6	-11.49	104.97	117.06
82	1	858	A2M	C5-C6-N6	9.27	134.43	120.35
82	1	305	A2M	C5-C6-N6	8.78	133.70	120.35
35	S1	28	A2M	C5-C6-N6	8.68	133.55	120.35
35	S1	479	A2M	C5-C6-N6	8.54	133.34	120.35
82	1	955	A2M	C5-C6-N6	8.53	133.31	120.35
35	S1	98	A2M	C5-C6-N6	8.43	133.17	120.35
86	2	628	A2M	C5-C6-N6	8.30	132.97	120.35
86	2	591	A2M	C5-C6-N6	8.29	132.96	120.35
35	S1	912	A2M	C5-C6-N6	8.26	132.91	120.35
82	1	681	A2M	C5-C6-N6	8.24	132.88	120.35
82	1	678	A2M	C5-C6-N6	8.21	132.83	120.35
35	S1	512	A2M	C5-C6-N6	8.19	132.80	120.35
82	1	927	A2M	C5-C6-N6	8.19	132.80	120.35
86	2	572	A2M	C5-C6-N6	8.12	132.70	120.35
85	7	162	A2M	C5-C6-N6	8.11	132.68	120.35
86	2	95	A2M	C5-C6-N6	8.11	132.67	120.35
35	S1	753	A2M	C5-C6-N6	8.10	132.66	120.35
35	S1	2021	A2M	C5-C6-N6	8.06	132.60	120.35
35	S1	897	A2M	C5-C6-N6	8.06	132.59	120.35
86	2	1384	A2M	C5-C6-N6	8.03	132.55	120.35
86	2	604	A2M	C5-C6-N6	7.95	132.44	120.35
35	S1	969	A2M	C5-C6-N6	7.94	132.43	120.35
35	S1	668	A2M	C5-C6-N6	7.79	132.19	120.35
85	7	43	A2M	C5-C6-N6	7.78	132.18	120.35
82	1	697	A2M	C5-C6-N6	7.75	132.12	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	2	527	A2M	C5-C6-N6	7.74	132.12	120.35
86	2	1185	A2M	C5-C6-N6	7.72	132.09	120.35
82	1	235	A2M	C5-C6-N6	7.71	132.08	120.35
82	1	407	A2M	C5-C6-N6	7.66	131.99	120.35
82	1	1539	A2M	C5-C6-N6	7.60	131.90	120.35
86	2	382	A2M	C5-C6-N6	7.57	131.85	120.35
86	2	570	A2M	C5-C6-N6	7.50	131.74	120.35
35	S1	918	A2M	C5-C6-N6	7.48	131.71	120.35
86	2	1372	A2M	C5-C6-N6	7.03	131.04	120.35
82	1	845	OMU	C4-N3-C2	-6.44	118.08	126.58
82	1	677	1MA	N1-C2-N3	-6.19	118.80	126.02
82	1	858	A2M	N6-C6-N1	-6.16	105.78	118.57
82	1	858	A2M	N3-C2-N1	-6.00	119.29	128.68
82	1	305	A2M	N6-C6-N1	-5.75	106.64	118.57
35	S1	28	A2M	N6-C6-N1	-5.73	106.67	118.57
82	1	235	A2M	N3-C2-N1	-5.73	119.72	128.68
35	S1	479	A2M	N6-C6-N1	-5.72	106.71	118.57
35	S1	8	OMU	C4-N3-C2	-5.66	119.11	126.58
82	1	927	A2M	N3-C2-N1	-5.66	119.83	128.68
35	S1	668	A2M	N3-C2-N1	-5.62	119.89	128.68
35	S1	2184	MA6	N3-C2-N1	-5.60	119.92	128.68
86	2	572	A2M	N3-C2-N1	-5.59	119.94	128.68
86	2	560	OMU	C4-N3-C2	-5.58	119.22	126.58
82	1	1539	A2M	N3-C2-N1	-5.56	119.99	128.68
35	S1	512	A2M	N3-C2-N1	-5.54	120.02	128.68
86	2	591	A2M	N3-C2-N1	-5.49	120.09	128.68
82	1	847	OMU	C4-N3-C2	-5.48	119.35	126.58
86	2	1372	A2M	N3-C2-N1	-5.48	120.11	128.68
35	S1	2185	MA6	N3-C2-N1	-5.47	120.13	128.68
35	S1	1833	OMU	C4-N3-C2	-5.47	119.37	126.58
82	1	955	A2M	N3-C2-N1	-5.46	120.15	128.68
82	1	305	A2M	N3-C2-N1	-5.46	120.15	128.68
35	S1	2021	A2M	N3-C2-N1	-5.45	120.16	128.68
35	S1	98	A2M	N6-C6-N1	-5.44	107.28	118.57
86	2	570	A2M	N3-C2-N1	-5.44	120.18	128.68
86	2	1185	A2M	N3-C2-N1	-5.42	120.21	128.68
35	S1	897	A2M	N3-C2-N1	-5.41	120.23	128.68
85	7	162	A2M	N3-C2-N1	-5.40	120.24	128.68
86	2	527	A2M	N6-C6-N1	-5.40	107.37	118.57
82	1	681	A2M	N3-C2-N1	-5.37	120.28	128.68
35	S1	969	A2M	N3-C2-N1	-5.37	120.29	128.68
35	S1	912	A2M	N6-C6-N1	-5.36	107.45	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	2	628	A2M	N3-C2-N1	-5.35	120.32	128.68
82	1	697	A2M	N3-C2-N1	-5.34	120.33	128.68
82	1	1107	OMU	C4-N3-C2	-5.34	119.54	126.58
85	7	43	A2M	N3-C2-N1	-5.34	120.34	128.68
86	2	604	A2M	N3-C2-N1	-5.32	120.36	128.68
35	S1	1979	OMU	C4-N3-C2	-5.31	119.57	126.58
83	3	13	OMU	C4-N3-C2	-5.30	119.59	126.58
35	S1	1621	OMU	C4-N3-C2	-5.29	119.60	126.58
86	2	667	OMU	C4-N3-C2	-5.29	119.61	126.58
86	2	1384	A2M	N6-C6-N1	-5.28	107.61	118.57
86	2	1359	OMU	C4-N3-C2	-5.28	119.62	126.58
85	7	7	OMU	C4-N3-C2	-5.27	119.62	126.58
82	1	955	A2M	N6-C6-N1	-5.27	107.64	118.57
35	S1	912	A2M	N3-C2-N1	-5.25	120.48	128.68
82	1	678	A2M	N3-C2-N1	-5.24	120.48	128.68
35	S1	753	A2M	N3-C2-N1	-5.24	120.49	128.68
35	S1	661	OMU	C4-N3-C2	-5.24	119.67	126.58
86	2	1077	OMU	C4-N3-C2	-5.23	119.68	126.58
82	1	845	OMU	N3-C2-N1	5.23	121.83	114.89
82	1	927	A2M	N6-C6-N1	-5.22	107.73	118.57
86	2	570	A2M	N6-C6-N1	-5.21	107.77	118.57
35	S1	2021	A2M	N6-C6-N1	-5.20	107.77	118.57
82	1	235	A2M	N6-C6-N1	-5.20	107.78	118.57
86	2	527	A2M	N3-C2-N1	-5.20	120.55	128.68
35	S1	668	A2M	N6-C6-N1	-5.20	107.79	118.57
86	2	382	A2M	N3-C2-N1	-5.19	120.57	128.68
82	1	681	A2M	N6-C6-N1	-5.18	107.83	118.57
86	2	1419	OMU	C4-N3-C2	-5.17	119.75	126.58
86	2	591	A2M	N6-C6-N1	-5.16	107.86	118.57
85	7	162	A2M	N6-C6-N1	-5.16	107.87	118.57
86	2	628	A2M	N6-C6-N1	-5.15	107.88	118.57
82	1	1659	OMU	C4-N3-C2	-5.13	119.81	126.58
82	1	407	A2M	N6-C6-N1	-5.13	107.93	118.57
35	S1	29	OMU	C4-N3-C2	-5.12	119.82	126.58
82	1	678	A2M	N6-C6-N1	-5.11	107.97	118.57
35	S1	969	A2M	N6-C6-N1	-5.10	107.99	118.57
35	S1	918	A2M	N6-C6-N1	-5.09	108.01	118.57
86	2	572	A2M	N6-C6-N1	-5.08	108.03	118.57
35	S1	897	A2M	N6-C6-N1	-5.08	108.03	118.57
86	2	604	A2M	N6-C6-N1	-5.07	108.04	118.57
86	2	95	A2M	N3-C2-N1	-5.07	120.75	128.68
86	2	95	A2M	N6-C6-N1	-5.06	108.07	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	918	A2M	N3-C2-N1	-5.05	120.78	128.68
35	S1	512	A2M	N6-C6-N1	-5.05	108.09	118.57
86	2	1303	PSU	N1-C2-N3	5.03	120.83	115.13
35	S1	753	A2M	N6-C6-N1	-5.02	108.15	118.57
35	S1	1995	7MG	C5-C6-N1	5.01	119.82	110.99
86	2	1058	PSU	N1-C2-N3	4.97	120.77	115.13
82	1	697	A2M	N6-C6-N1	-4.95	108.31	118.57
86	2	1185	A2M	N6-C6-N1	-4.95	108.31	118.57
35	S1	2048	PSU	N1-C2-N3	4.91	120.70	115.13
82	1	1181	PSU	N1-C2-N3	4.88	120.66	115.13
86	2	597	PSU	N1-C2-N3	4.88	120.66	115.13
82	1	1539	A2M	N6-C6-N1	-4.88	108.45	118.57
86	2	1382	PSU	N1-C2-N3	4.86	120.63	115.13
86	2	1058	PSU	C4-N3-C2	-4.85	119.35	126.34
82	1	1528	PSU	N1-C2-N3	4.84	120.62	115.13
82	1	870	PSU	C4-N3-C2	-4.84	119.37	126.34
86	2	1318	PSU	C4-N3-C2	-4.84	119.37	126.34
35	S1	2048	PSU	C4-N3-C2	-4.82	119.39	126.34
35	S1	1657	PSU	C4-N3-C2	-4.82	119.40	126.34
86	2	1060	PSU	N1-C2-N3	4.82	120.59	115.13
82	1	870	PSU	N1-C2-N3	4.78	120.55	115.13
85	7	43	A2M	N6-C6-N1	-4.77	108.67	118.57
86	2	382	A2M	N6-C6-N1	-4.77	108.67	118.57
86	2	1303	PSU	C4-N3-C2	-4.74	119.51	126.34
35	S1	28	A2M	N3-C2-N1	-4.66	121.39	128.68
86	2	437	PSU	C4-N3-C2	-4.66	119.62	126.34
86	2	73	OMU	C4-N3-C2	-4.66	120.44	126.58
82	1	1371	OMU	C4-N3-C2	-4.65	120.45	126.58
82	1	1017	PSU	C4-N3-C2	-4.65	119.65	126.34
86	2	1060	PSU	C4-N3-C2	-4.64	119.65	126.34
86	2	597	PSU	C4-N3-C2	-4.64	119.65	126.34
82	1	1371	OMU	C1'-N1-C2	4.63	125.96	117.57
82	1	1664	PSU	C4-N3-C2	-4.62	119.68	126.34
35	S1	1841	PSU	C4-N3-C2	-4.62	119.68	126.34
86	2	1382	PSU	C4-N3-C2	-4.62	119.69	126.34
86	2	78	PSU	N1-C2-N3	4.62	120.36	115.13
35	S1	1533	PSU	C4-N3-C2	-4.61	119.69	126.34
35	S1	2046	PSU	C4-N3-C2	-4.61	119.69	126.34
35	S1	479	A2M	N3-C2-N1	-4.60	121.48	128.68
86	2	1144	PSU	N1-C2-N3	4.59	120.33	115.13
82	1	1181	PSU	C4-N3-C2	-4.58	119.74	126.34
82	1	407	A2M	N3-C2-N1	-4.58	121.52	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	1	1533	PSU	C4-N3-C2	-4.57	119.76	126.34
86	2	512	PSU	C4-N3-C2	-4.56	119.77	126.34
86	2	1303	PSU	C6-C5-C4	4.56	121.39	118.20
82	1	1039	PSU	C4-N3-C2	-4.56	119.77	126.34
86	2	1318	PSU	N1-C2-N3	4.55	120.28	115.13
35	S1	1246	PSU	C4-N3-C2	-4.53	119.81	126.34
35	S1	2046	PSU	N1-C2-N3	4.52	120.25	115.13
85	7	74	PSU	C4-N3-C2	-4.52	119.82	126.34
82	1	1177	PSU	C4-N3-C2	-4.52	119.82	126.34
86	2	1361	PSU	C4-N3-C2	-4.52	119.83	126.34
86	2	78	PSU	C4-N3-C2	-4.50	119.85	126.34
86	2	662	PSU	C4-N3-C2	-4.50	119.85	126.34
35	S1	98	A2M	N3-C2-N1	-4.50	121.65	128.68
35	S1	12	PSU	C4-N3-C2	-4.49	119.86	126.34
82	1	672	PSU	C4-N3-C2	-4.49	119.88	126.34
35	S1	609	PSU	C4-N3-C2	-4.48	119.88	126.34
86	2	1144	PSU	C4-N3-C2	-4.48	119.88	126.34
82	1	1528	PSU	C4-N3-C2	-4.48	119.89	126.34
35	S1	33	PSU	N1-C2-N3	4.47	120.19	115.13
86	2	1265	PSU	C4-N3-C2	-4.46	119.91	126.34
86	2	1194	PSU	C4-N3-C2	-4.45	119.93	126.34
86	2	1413	PSU	C4-N3-C2	-4.43	119.95	126.34
86	2	1264	PSU	C4-N3-C2	-4.42	119.98	126.34
86	2	510	PSU	C4-N3-C2	-4.40	120.00	126.34
86	2	1265	PSU	N1-C2-N3	4.40	120.11	115.13
35	S1	104	PSU	C4-N3-C2	-4.40	120.00	126.34
82	1	1017	PSU	N1-C2-N3	4.40	120.11	115.13
82	1	1171	PSU	C4-N3-C2	-4.39	120.01	126.34
86	2	1372	A2M	N6-C6-N1	-4.39	109.47	118.57
85	7	101	PSU	C4-N3-C2	-4.38	120.02	126.34
35	S1	1995	7MG	C2-N3-C4	4.38	120.11	112.30
86	2	626	PSU	C4-N3-C2	-4.38	120.03	126.34
35	S1	1539	PSU	C4-N3-C2	-4.38	120.03	126.34
86	2	1403	PSU	C4-N3-C2	-4.36	120.06	126.34
86	2	1384	A2M	N3-C2-N1	-4.33	121.91	128.68
82	1	672	PSU	N1-C2-N3	4.31	120.01	115.13
86	2	437	PSU	N1-C2-N3	4.30	120.00	115.13
86	2	1058	PSU	C6-C5-C4	4.28	121.19	118.20
86	2	472	PSU	N1-C2-N3	4.28	119.98	115.13
86	2	1361	PSU	N1-C2-N3	4.28	119.98	115.13
35	S1	1533	PSU	N1-C2-N3	4.28	119.97	115.13
35	S1	33	PSU	C4-N3-C2	-4.27	120.18	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	2	472	PSU	C4-N3-C2	-4.26	120.21	126.34
85	7	101	PSU	N1-C2-N3	4.25	119.94	115.13
82	1	1011	PSU	C4-N3-C2	-4.23	120.24	126.34
82	1	1533	PSU	N1-C2-N3	4.23	119.92	115.13
86	2	593	PSU	C4-N3-C2	-4.22	120.25	126.34
86	2	662	PSU	N1-C2-N3	4.21	119.90	115.13
86	2	1413	PSU	N1-C2-N3	4.20	119.89	115.13
35	S1	609	PSU	N1-C2-N3	4.20	119.89	115.13
86	2	1308	5MC	C5-C6-N1	-4.19	119.03	123.34
35	S1	1543	C4J	C4-N3-C2	-4.19	120.17	125.46
35	S1	1566	PSU	C4-N3-C2	-4.18	120.31	126.34
35	S1	1246	PSU	N1-C2-N3	4.18	119.86	115.13
86	2	1144	PSU	C6-N1-C2	-4.16	118.42	122.68
86	2	512	PSU	N1-C2-N3	4.16	119.84	115.13
35	S1	1841	PSU	N1-C2-N3	4.13	119.81	115.13
82	1	1177	PSU	N1-C2-N3	4.11	119.79	115.13
86	2	1264	PSU	N1-C2-N3	4.10	119.78	115.13
35	S1	12	PSU	N1-C2-N3	4.09	119.77	115.13
86	2	593	PSU	N1-C2-N3	4.07	119.75	115.13
82	1	845	OMU	C1'-N1-C2	4.07	124.94	117.57
85	7	74	PSU	N1-C2-N3	4.07	119.74	115.13
86	2	1060	PSU	C6-C5-C4	4.06	121.04	118.20
35	S1	1539	PSU	N1-C2-N3	4.06	119.73	115.13
35	S1	1657	PSU	N1-C2-N3	4.06	119.73	115.13
82	1	1171	PSU	N1-C2-N3	4.06	119.72	115.13
35	S1	1995	7MG	C5-C4-N3	-4.05	120.41	128.13
86	2	626	PSU	N1-C2-N3	4.04	119.70	115.13
85	7	69	PSU	C4-N3-C2	-4.02	120.54	126.34
35	S1	1566	PSU	N1-C2-N3	4.02	119.68	115.13
86	2	667	OMU	N3-C2-N1	4.01	120.22	114.89
82	1	1664	PSU	N1-C2-N3	4.01	119.67	115.13
86	2	1403	PSU	N1-C2-N3	3.99	119.65	115.13
82	1	1107	OMU	N3-C2-N1	3.97	120.17	114.89
86	2	510	PSU	N1-C2-N3	3.95	119.61	115.13
82	1	1039	PSU	N1-C2-N3	3.95	119.61	115.13
35	S1	33	PSU	C6-N1-C2	-3.94	118.66	122.68
86	2	1077	OMU	N3-C2-N1	3.93	120.10	114.89
82	1	1011	PSU	N1-C2-N3	3.92	119.58	115.13
82	1	847	OMU	N3-C2-N1	3.92	120.09	114.89
35	S1	104	PSU	N1-C2-N3	3.91	119.56	115.13
35	S1	661	OMU	N3-C2-N1	3.89	120.05	114.89
82	1	1528	PSU	C6-N1-C2	-3.88	118.71	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	2	78	PSU	C6-C5-C4	3.88	120.91	118.20
85	7	69	PSU	N1-C2-N3	3.88	119.53	115.13
86	2	1382	PSU	C6-C5-C4	3.88	120.91	118.20
35	S1	1979	OMU	N3-C2-N1	3.87	120.03	114.89
86	2	1359	OMU	N3-C2-N1	3.85	120.00	114.89
86	2	1194	PSU	N1-C2-N3	3.83	119.47	115.13
35	S1	8	OMU	N3-C2-N1	3.82	119.95	114.89
86	2	597	PSU	C6-C5-C4	3.81	120.86	118.20
35	S1	1833	OMU	C5-C4-N3	3.79	120.51	114.84
86	2	560	OMU	N3-C2-N1	3.79	119.92	114.89
35	S1	1544	5MC	C5-C6-N1	-3.73	119.51	123.34
82	1	1371	OMU	N3-C2-N1	3.68	119.78	114.89
35	S1	8	OMU	C5-C4-N3	3.65	120.31	114.84
86	2	1419	OMU	N3-C2-N1	3.64	119.72	114.89
35	S1	1833	OMU	O4-C4-C5	-3.64	118.76	125.16
83	3	13	OMU	C5-C4-N3	3.63	120.27	114.84
86	2	472	PSU	C6-N1-C2	-3.62	118.98	122.68
82	1	1181	PSU	C6-N1-C2	-3.62	118.98	122.68
83	3	13	OMU	N3-C2-N1	3.62	119.69	114.89
85	7	7	OMU	N3-C2-N1	3.58	119.65	114.89
82	1	870	PSU	C6-C5-C4	3.58	120.70	118.20
86	2	1419	OMU	C5-C4-N3	3.58	120.20	114.84
86	2	597	PSU	C6-N1-C2	-3.56	119.05	122.68
35	S1	1621	OMU	N3-C2-N1	3.55	119.61	114.89
35	S1	29	OMU	N3-C2-N1	3.55	119.60	114.89
82	1	1659	OMU	N3-C2-N1	3.54	119.59	114.89
35	S1	1621	OMU	C5-C4-N3	3.52	120.11	114.84
35	S1	2048	PSU	C6-N1-C2	-3.51	119.10	122.68
86	2	1382	PSU	C6-N1-C2	-3.51	119.10	122.68
82	1	1659	OMU	C5-C4-N3	3.50	120.08	114.84
86	2	1303	PSU	C6-N1-C2	-3.50	119.10	122.68
86	2	1359	OMU	C5-C4-N3	3.49	120.07	114.84
86	2	560	OMU	C5-C4-N3	3.49	120.06	114.84
85	7	7	OMU	C5-C4-N3	3.48	120.05	114.84
35	S1	1865	OMG	C5-C6-N1	3.48	120.09	113.95
35	S1	29	OMU	C5-C4-N3	3.44	119.99	114.84
86	2	1253	OMG	C5-C6-N1	3.42	119.98	113.95
86	2	73	OMU	N3-C2-N1	3.41	119.42	114.89
82	1	1626	OMG	C5-C6-N1	3.41	119.98	113.95
35	S1	1647	OMG	C5-C6-N1	3.40	119.96	113.95
35	S1	2046	PSU	C6-N1-C2	-3.39	119.21	122.68
35	S1	661	OMU	C5-C4-N3	3.36	119.87	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	1979	OMU	C5-C4-N3	3.36	119.87	114.84
82	1	1107	OMU	C5-C4-N3	3.36	119.87	114.84
86	2	641	OMG	C5-C6-N1	3.35	119.87	113.95
82	1	1190	OMG	C5-C6-N1	3.34	119.85	113.95
86	2	1229	OMG	C5-C6-N1	3.34	119.85	113.95
35	S1	1623	OMG	C5-C6-N1	3.34	119.84	113.95
82	1	847	OMU	C5-C4-N3	3.34	119.83	114.84
86	2	1077	OMU	C5-C4-N3	3.33	119.83	114.84
35	S1	1833	OMU	N3-C2-N1	3.33	119.32	114.89
86	2	1078	OMG	C5-C6-N1	3.33	119.83	113.95
86	2	71	OMG	C5-C6-N1	3.33	119.83	113.95
35	S1	2151	OMG	C5-C6-N1	3.33	119.83	113.95
35	S1	2059	OMC	O2-C2-N3	-3.32	116.93	122.33
35	S1	600	OMG	C5-C6-N1	3.32	119.81	113.95
86	2	1360	OMG	C5-C6-N1	3.32	119.81	113.95
35	S1	1478	OMG	C5-C6-N1	3.32	119.81	113.95
85	7	75	OMG	C5-C6-N1	3.31	119.80	113.95
86	2	667	OMU	C5-C4-N3	3.31	119.80	114.84
35	S1	1550	OMG	C5-C6-N1	3.29	119.77	113.95
86	2	1231	OMG	C5-C6-N1	3.29	119.76	113.95
86	2	524	5MC	C5-C6-N1	-3.29	119.96	123.34
86	2	78	PSU	C6-N1-C2	-3.28	119.33	122.68
82	1	959	OMG	C5-C6-N1	3.28	119.75	113.95
82	1	1524	OMG	C5-C6-N1	3.28	119.74	113.95
86	2	1058	PSU	C6-N1-C2	-3.28	119.33	122.68
82	1	1540	OMG	C5-C6-N1	3.28	119.74	113.95
82	1	856	OMG	C5-C6-N1	3.27	119.73	113.95
35	S1	1829	OMG	C5-C6-N1	3.27	119.72	113.95
86	2	534	OMG	C5-C6-N1	3.27	119.72	113.95
86	2	1318	PSU	C6-C5-C4	3.26	120.48	118.20
35	S1	2048	PSU	C6-C5-C4	3.26	120.48	118.20
86	2	1060	PSU	C6-N1-C2	-3.25	119.36	122.68
35	S1	1995	7MG	C4-C5-N7	3.25	110.04	105.53
85	7	69	PSU	C6-N1-C2	-3.22	119.39	122.68
82	1	1181	PSU	C6-C5-C4	3.20	120.44	118.20
86	2	73	OMU	C5-C4-N3	3.20	119.63	114.84
37	4	74	OMG	C5-C6-N1	3.19	119.58	113.95
82	1	407	A2M	C5'-C4'-C3'	-3.16	103.34	115.18
82	1	845	OMU	C5-C4-N3	3.14	119.53	114.84
86	2	1265	PSU	C6-N1-C2	-3.13	119.48	122.68
85	7	101	PSU	C6-N1-C2	-3.13	119.48	122.68
35	S1	2046	PSU	C6-C5-C4	3.12	120.38	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	1	672	PSU	C6-N1-C2	-3.10	119.51	122.68
82	1	672	PSU	C6-C5-C4	3.08	120.35	118.20
35	S1	1995	7MG	C5-C4-N9	3.08	110.35	106.35
35	S1	1647	OMG	C8-N7-C5	3.08	108.85	102.99
82	1	870	PSU	C6-N1-C2	-3.08	119.54	122.68
86	2	641	OMG	C8-N7-C5	3.07	108.84	102.99
86	2	1318	PSU	C6-N1-C2	-3.07	119.55	122.68
85	7	7	OMU	O4-C4-C5	-3.07	119.77	125.16
35	S1	2061	5MC	C5-C6-N1	-3.06	120.19	123.34
82	1	1177	PSU	C6-N1-C2	-3.05	119.56	122.68
35	S1	1566	PSU	C6-N1-C2	-3.04	119.57	122.68
86	2	560	OMU	O4-C4-C5	-3.04	119.81	125.16
82	1	1371	OMU	C5-C4-N3	3.03	119.38	114.84
82	1	1528	PSU	C6-C5-C4	3.02	120.31	118.20
82	1	1659	OMU	O4-C4-C5	-3.01	119.86	125.16
82	1	1190	OMG	C8-N7-C5	3.01	108.72	102.99
35	S1	8	OMU	O4-C4-C5	-3.00	119.89	125.16
82	1	1533	PSU	C6-N1-C2	-2.99	119.62	122.68
85	7	43	A2M	C5'-C4'-C3'	-2.98	104.00	115.18
86	2	1413	PSU	C6-N1-C2	-2.98	119.63	122.68
35	S1	1621	OMU	O4-C4-C5	-2.98	119.92	125.16
35	S1	609	PSU	C6-N1-C2	-2.98	119.64	122.68
86	2	512	PSU	C6-N1-C2	-2.96	119.66	122.68
35	S1	1829	OMG	C8-N7-C5	2.96	108.62	102.99
86	2	1361	PSU	C6-N1-C2	-2.94	119.68	122.68
35	S1	1246	PSU	C6-C5-C4	2.94	120.25	118.20
86	2	662	PSU	C6-N1-C2	-2.94	119.68	122.68
86	2	1360	OMG	C2-N1-C6	-2.93	119.70	125.10
86	2	71	OMG	C8-N7-C5	2.92	108.56	102.99
82	1	1540	OMG	C8-N7-C5	2.92	108.55	102.99
82	1	1524	OMG	C8-N7-C5	2.91	108.54	102.99
86	2	472	PSU	O2-C2-N1	-2.91	119.59	122.79
82	1	1011	PSU	C6-N1-C2	-2.90	119.71	122.68
86	2	1253	OMG	C8-N7-C5	2.90	108.52	102.99
83	3	13	OMU	O4-C4-C5	-2.90	120.06	125.16
86	2	1265	PSU	C6-C5-C4	2.90	120.23	118.20
86	2	1229	OMG	C8-N7-C5	2.89	108.50	102.99
35	S1	1865	OMG	C8-N7-C5	2.89	108.49	102.99
82	1	856	OMG	C8-N7-C5	2.88	108.48	102.99
35	S1	1533	PSU	C6-N1-C2	-2.88	119.74	122.68
37	4	74	OMG	C8-N7-C5	2.88	108.47	102.99
35	S1	1623	OMG	C2-N1-C6	-2.88	119.80	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	1979	OMU	O4-C4-C5	-2.87	120.11	125.16
86	2	534	OMG	C8-N7-C5	2.87	108.45	102.99
35	S1	1995	7MG	C2-N1-C6	-2.87	119.87	125.10
86	2	626	PSU	C6-N1-C2	-2.86	119.75	122.68
35	S1	12	PSU	C6-N1-C2	-2.86	119.76	122.68
35	S1	1478	OMG	C2-N1-C6	-2.86	119.83	125.10
35	S1	1539	PSU	C6-N1-C2	-2.86	119.76	122.68
86	2	1419	OMU	O4-C4-C5	-2.86	120.14	125.16
82	1	1626	OMG	C8-N7-C5	2.85	108.42	102.99
85	7	75	OMG	C8-N7-C5	2.85	108.42	102.99
82	1	1017	PSU	C6-C5-C4	2.85	120.19	118.20
86	2	1144	PSU	O2-C2-N1	-2.85	119.66	122.79
35	S1	600	OMG	C8-N7-C5	2.84	108.41	102.99
86	2	1078	OMG	C8-N7-C5	2.84	108.41	102.99
82	1	847	OMU	O4-C4-C5	-2.84	120.16	125.16
82	1	1626	OMG	C2-N1-C6	-2.84	119.87	125.10
35	S1	1550	OMG	C8-N7-C5	2.83	108.39	102.99
35	S1	1246	PSU	C6-N1-C2	-2.83	119.79	122.68
35	S1	29	OMU	O4-C4-C5	-2.83	120.18	125.16
35	S1	1478	OMG	C8-N7-C5	2.83	108.38	102.99
35	S1	1865	OMG	C2-N1-C6	-2.82	119.90	125.10
86	2	1231	OMG	C8-N7-C5	2.82	108.36	102.99
82	1	1171	PSU	C6-N1-C2	-2.82	119.80	122.68
35	S1	1623	OMG	C8-N7-C5	2.82	108.36	102.99
82	1	1017	PSU	C6-N1-C2	-2.81	119.81	122.68
86	2	1403	PSU	C6-N1-C2	-2.81	119.81	122.68
86	2	1360	OMG	C8-N7-C5	2.81	108.33	102.99
82	1	1190	OMG	C2-N1-C6	-2.80	119.93	125.10
35	S1	2151	OMG	C8-N7-C5	2.80	108.33	102.99
86	2	1359	OMU	O4-C4-C5	-2.80	120.23	125.16
35	S1	1533	PSU	C6-C5-C4	2.80	120.16	118.20
86	2	593	PSU	C6-N1-C2	-2.80	119.82	122.68
82	1	1524	OMG	C2-N1-C6	-2.80	119.94	125.10
86	2	1264	PSU	C6-N1-C2	-2.79	119.83	122.68
85	7	74	PSU	C6-N1-C2	-2.79	119.83	122.68
82	1	1371	OMU	O4-C4-C5	-2.79	120.26	125.16
82	1	677	1MA	C5-C6-N1	2.79	118.05	113.90
35	S1	1829	OMG	C2-N1-C6	-2.77	119.99	125.10
86	2	667	OMU	O4-C4-C5	-2.77	120.29	125.16
35	S1	1841	PSU	C6-N1-C2	-2.76	119.86	122.68
86	2	1253	OMG	C2-N1-C6	-2.76	120.02	125.10
35	S1	104	PSU	C6-N1-C2	-2.76	119.87	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	2	512	PSU	C6-C5-C4	2.75	120.12	118.20
35	S1	600	OMG	C2-N1-C6	-2.75	120.03	125.10
35	S1	1995	7MG	O6-C6-C5	-2.75	120.79	127.54
82	1	959	OMG	C8-N7-C5	2.75	108.22	102.99
86	2	1078	OMG	N2-C2-N1	2.75	122.56	116.71
86	2	1046	OMG	C8-N7-C5	2.75	108.22	102.99
86	2	534	OMG	C2-N1-C6	-2.74	120.05	125.10
35	S1	661	OMU	O4-C4-C5	-2.73	120.35	125.16
35	S1	2151	OMG	C2-N1-C6	-2.73	120.08	125.10
86	2	510	PSU	C6-N1-C2	-2.72	119.90	122.68
82	1	959	OMG	C2-N1-C6	-2.71	120.10	125.10
85	7	75	OMG	C2-N1-C6	-2.71	120.11	125.10
82	1	1010	OMC	CM2-O2'-C2'	2.70	121.61	114.52
82	1	845	OMU	O2-C2-N3	-2.70	116.48	121.50
82	1	1039	PSU	C6-N1-C2	-2.68	119.94	122.68
86	2	1077	OMU	O4-C4-C5	-2.68	120.45	125.16
86	2	71	OMG	C2-N1-C6	-2.68	120.17	125.10
86	2	641	OMG	C2-N1-C6	-2.67	120.17	125.10
86	2	510	PSU	O2-C2-N1	-2.67	119.85	122.79
86	2	1231	OMG	C2-N1-C6	-2.67	120.18	125.10
86	2	1265	PSU	O2-C2-N1	-2.67	119.85	122.79
35	S1	1647	OMG	C2-N1-C6	-2.66	120.20	125.10
86	2	437	PSU	C6-N1-C2	-2.65	119.98	122.68
86	2	1361	PSU	C6-C5-C4	2.64	120.05	118.20
35	S1	1550	OMG	C2-N1-C6	-2.63	120.25	125.10
82	1	1664	PSU	C6-N1-C2	-2.63	119.99	122.68
86	2	73	OMU	O4-C4-C5	-2.63	120.53	125.16
82	1	1181	PSU	O2-C2-N1	-2.63	119.89	122.79
82	1	1177	PSU	O2-C2-N1	-2.63	119.89	122.79
86	2	1229	OMG	C2-N1-C6	-2.63	120.26	125.10
35	S1	609	PSU	C6-C5-C4	2.62	120.03	118.20
85	7	101	PSU	C6-C5-C4	2.62	120.03	118.20
35	S1	969	A2M	C2'-C3'-C4'	2.61	107.67	101.99
82	1	1540	OMG	C2-N1-C6	-2.60	120.31	125.10
86	2	1078	OMG	C2-N1-C6	-2.60	120.31	125.10
35	S1	1246	PSU	O2-C2-N1	-2.59	119.93	122.79
86	2	655	OMG	C8-N7-C5	2.59	107.93	102.99
82	1	1107	OMU	O4-C4-C5	-2.59	120.60	125.16
86	2	1403	PSU	C6-C5-C4	2.59	120.01	118.20
35	S1	2048	PSU	O2-C2-N1	-2.58	119.94	122.79
86	2	1403	PSU	O2-C2-N1	-2.58	119.95	122.79
82	1	1190	OMG	N2-C2-N1	2.57	122.19	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	1841	PSU	C6-C5-C4	2.56	119.99	118.20
35	S1	8	OMU	O2-C2-N1	-2.56	119.38	122.79
82	1	672	PSU	O2-C2-N1	-2.56	119.97	122.79
35	S1	1539	PSU	O2-C2-N1	-2.55	119.98	122.79
86	2	662	PSU	O2-C2-N1	-2.55	119.98	122.79
35	S1	1533	PSU	O2-C2-N1	-2.54	120.00	122.79
86	2	1264	PSU	C6-C5-C4	2.54	119.97	118.20
82	1	845	OMU	O4-C4-C5	-2.53	120.71	125.16
35	S1	1995	7MG	N9-C4-N3	2.52	129.24	125.47
86	2	1264	PSU	O2-C2-N1	-2.52	120.01	122.79
35	S1	2059	OMC	C1'-N1-C2	2.52	124.04	118.42
86	2	1317	OMC	O2-C2-N3	-2.52	118.24	122.33
82	1	856	OMG	C2-N1-C6	-2.52	120.47	125.10
86	2	1194	PSU	C6-N1-C2	-2.51	120.12	122.68
86	2	1308	5MC	C4'-O4'-C1'	-2.50	103.95	109.47
86	2	1303	PSU	O2-C2-N1	-2.50	120.04	122.79
35	S1	1478	OMG	O6-C6-C5	-2.50	119.49	124.37
82	1	1017	PSU	O2-C2-N1	-2.50	120.04	122.79
37	4	74	OMG	C2-N1-C6	-2.49	120.51	125.10
86	2	626	PSU	O2-C2-N1	-2.49	120.05	122.79
35	S1	1478	OMG	N2-C2-N1	2.49	122.01	116.71
86	2	510	PSU	C6-C5-C4	2.49	119.94	118.20
82	1	1371	OMU	C1'-N1-C6	-2.48	115.42	120.84
35	S1	1657	PSU	C6-N1-C2	-2.47	120.16	122.68
35	S1	1543	C4J	N3-C2-N1	2.46	120.24	116.76
35	S1	1841	PSU	O2-C2-N1	-2.46	120.08	122.79
86	2	570	A2M	O2'-C2'-C1'	2.45	113.94	109.09
82	1	1533	PSU	O2-C2-N1	-2.44	120.10	122.79
86	2	655	OMG	C5-C6-N1	2.44	118.26	113.95
86	2	597	PSU	O2-C2-N1	-2.43	120.12	122.79
86	2	1058	PSU	O2-C2-N1	-2.43	120.12	122.79
86	2	512	PSU	O2-C2-N1	-2.43	120.12	122.79
82	1	1171	PSU	O2-C2-N1	-2.43	120.12	122.79
86	2	1382	PSU	O2-C2-N1	-2.42	120.12	122.79
82	1	1533	PSU	C6-C5-C4	2.41	119.89	118.20
82	1	677	1MA	C8-N7-C5	2.40	107.57	102.99
35	S1	912	A2M	C2'-C3'-C4'	2.40	107.20	101.99
35	S1	1995	7MG	N9-C8-N7	2.39	106.80	103.38
86	2	437	PSU	O2-C2-N1	-2.39	120.16	122.79
82	1	1171	PSU	C6-C5-C4	2.37	119.85	118.20
86	2	593	PSU	O2-C2-N1	-2.37	120.19	122.79
86	2	593	PSU	C6-C5-C4	2.36	119.85	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	2	570	A2M	C3'-C2'-C1'	2.36	107.32	102.89
86	2	437	PSU	C6-C5-C4	2.35	119.84	118.20
35	S1	668	A2M	C3'-C2'-C1'	2.34	107.29	102.89
86	2	641	OMG	N2-C2-N1	2.34	121.69	116.71
86	2	1060	PSU	O2-C2-N1	-2.32	120.23	122.79
35	S1	1833	OMU	C1'-N1-C2	2.32	121.77	117.57
86	2	655	OMG	C2-N1-C6	-2.32	120.83	125.10
86	2	1303	PSU	O4'-C1'-C2'	2.32	108.41	105.14
82	1	1528	PSU	O2-C2-N1	-2.31	120.25	122.79
35	S1	2061	5MC	CM5-C5-C6	-2.30	119.78	122.85
86	2	1318	PSU	O4'-C1'-C2'	2.30	108.39	105.14
82	1	845	OMU	C6-C5-C4	2.29	122.64	119.52
35	S1	609	PSU	O2-C2-N1	-2.29	120.27	122.79
82	1	1371	OMU	O2-C2-N3	-2.29	117.24	121.50
85	7	74	PSU	C6-C5-C4	2.29	119.80	118.20
85	7	69	PSU	O2-C2-N1	-2.28	120.28	122.79
82	1	1039	PSU	O2-C2-N1	-2.27	120.29	122.79
82	1	677	1MA	CM1-N1-C2	-2.27	115.77	120.55
82	1	1011	PSU	O2-C2-N1	-2.27	120.30	122.79
86	2	1046	OMG	C2-N1-C6	-2.26	120.93	125.10
86	2	95	A2M	C2'-C3'-C4'	2.25	106.89	101.99
86	2	560	OMU	O2-C2-N1	-2.25	119.79	122.79
85	7	101	PSU	O4'-C1'-C2'	2.25	108.32	105.14
86	2	524	5MC	CM5-C5-C6	-2.25	119.84	122.85
86	2	662	PSU	C6-C5-C4	2.25	119.77	118.20
86	2	1403	PSU	O4'-C1'-C2'	2.25	108.31	105.14
82	1	870	PSU	O2-C2-N1	-2.24	120.33	122.79
35	S1	12	PSU	O2-C2-N1	-2.24	120.33	122.79
82	1	1011	PSU	O4'-C1'-C2'	2.24	108.30	105.14
86	2	1413	PSU	O2-C2-N1	-2.23	120.34	122.79
82	1	1177	PSU	C6-C5-C4	2.23	119.75	118.20
86	2	1194	PSU	O2-C2-N1	-2.22	120.35	122.79
82	1	235	A2M	C2'-C3'-C4'	2.21	106.79	101.99
35	S1	1621	OMU	O2-C2-N1	-2.20	119.86	122.79
82	1	1664	PSU	O2-C2-N1	-2.20	120.37	122.79
35	S1	661	OMU	O2-C2-N1	-2.20	119.86	122.79
86	2	1382	PSU	O4'-C1'-C2'	2.18	108.22	105.14
86	2	1046	OMG	C5-C6-N1	2.18	117.80	113.95
86	2	1264	PSU	O4'-C1'-C2'	2.18	108.21	105.14
35	S1	1566	PSU	O2-C2-N1	-2.17	120.40	122.79
82	1	845	OMU	C1'-N1-C6	-2.17	116.11	120.84
85	7	74	PSU	O2-C2-N1	-2.17	120.41	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	2	1046	OMG	N2-C2-N1	2.17	121.32	116.71
82	1	1524	OMG	N2-C2-N1	2.16	121.31	116.71
35	S1	104	PSU	O2-C2-N1	-2.16	120.42	122.79
82	1	856	OMG	N2-C2-N1	2.16	121.31	116.71
86	2	1046	OMG	O6-C6-C5	-2.16	120.16	124.37
86	2	1360	OMG	O6-C6-C5	-2.13	120.21	124.37
85	7	101	PSU	O2-C2-N1	-2.12	120.45	122.79
82	1	858	A2M	O4'-C4'-C3'	-2.12	100.92	105.11
82	1	1626	OMG	O6-C6-C5	-2.12	120.23	124.37
37	4	74	OMG	N2-C2-N1	2.12	121.22	116.71
82	1	1011	PSU	C6-C5-C4	2.12	119.68	118.20
35	S1	1865	OMG	O6-C6-C5	-2.11	120.25	124.37
35	S1	1623	OMG	N2-C2-N1	2.10	121.19	116.71
82	1	959	OMG	O6-C6-C5	-2.10	120.27	124.37
86	2	1231	OMG	O6-C6-C5	-2.10	120.28	124.37
35	S1	104	PSU	C6-C5-C4	2.09	119.66	118.20
86	2	583	OMC	O2-C2-N3	-2.09	118.93	122.33
82	1	1540	OMG	N2-C2-N1	2.09	121.16	116.71
35	S1	12	PSU	C6-C5-C4	2.08	119.66	118.20
82	1	672	PSU	O4'-C1'-C2'	2.08	108.08	105.14
35	S1	1623	OMG	O6-C6-C5	-2.08	120.31	124.37
35	S1	1550	OMG	O6-C6-C5	-2.08	120.32	124.37
82	1	1533	PSU	O4'-C1'-C2'	2.07	108.07	105.14
86	2	1318	PSU	O2-C2-N1	-2.07	120.51	122.79
82	1	1107	OMU	O2-C2-N1	-2.07	120.04	122.79
35	S1	1979	OMU	O2-C2-N1	-2.06	120.04	122.79
86	2	1229	OMG	O6-C6-C5	-2.06	120.35	124.37
85	7	75	OMG	O6-C6-C5	-2.06	120.36	124.37
82	1	1664	PSU	C6-C5-C4	2.04	119.63	118.20
82	1	856	OMG	O6-C6-C5	-2.03	120.40	124.37
37	4	74	OMG	N1-C2-N3	-2.03	119.52	123.32
35	S1	600	OMG	O6-C6-C5	-2.02	120.42	124.37
35	S1	2151	OMG	O6-C6-C5	-2.02	120.42	124.37
86	2	1248	OMC	O2-C2-N3	-2.02	119.05	122.33
82	1	1171	PSU	O4'-C1'-C2'	2.02	107.99	105.14
86	2	1078	OMG	O6-C6-C5	-2.01	120.44	124.37
82	1	847	OMU	O2-C2-N1	-2.01	120.11	122.79
86	2	1253	OMG	N2-C2-N1	2.00	120.98	116.71
82	1	856	OMG	N1-C2-N3	-2.00	119.58	123.32

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	1	407	A2M	C3'-C4'-C5'-O5'
82	1	681	A2M	O4'-C4'-C5'-O5'
82	1	695	OMC	C1'-C2'-O2'-CM2
82	1	845	OMU	O4'-C1'-N1-C2
82	1	845	OMU	O4'-C1'-N1-C6
82	1	845	OMU	C1'-C2'-O2'-CM2
82	1	955	A2M	C1'-C2'-O2'-CM'
82	1	959	OMG	O4'-C4'-C5'-O5'
82	1	959	OMG	C3'-C4'-C5'-O5'
82	1	1010	OMC	C1'-C2'-O2'-CM2
82	1	1011	PSU	C2'-C1'-C5-C4
82	1	1011	PSU	C2'-C1'-C5-C6
82	1	1107	OMU	C3'-C4'-C5'-O5'
82	1	1107	OMU	O4'-C4'-C5'-O5'
82	1	1181	PSU	C3'-C4'-C5'-O5'
82	1	1181	PSU	O4'-C4'-C5'-O5'
82	1	1371	OMU	O4'-C1'-N1-C2
82	1	1371	OMU	O4'-C1'-N1-C6
82	1	1527	OMC	C1'-C2'-O2'-CM2
82	1	1540	OMG	O4'-C4'-C5'-O5'
82	1	1540	OMG	C3'-C4'-C5'-O5'
85	7	7	OMU	C1'-C2'-O2'-CM2
85	7	43	A2M	C3'-C4'-C5'-O5'
85	7	69	PSU	C3'-C4'-C5'-O5'
85	7	69	PSU	O4'-C4'-C5'-O5'
85	7	162	A2M	C1'-C2'-O2'-CM'
86	2	73	OMU	C1'-C2'-O2'-CM2
86	2	359	OMC	C3'-C4'-C5'-O5'
86	2	359	OMC	O4'-C4'-C5'-O5'
86	2	437	PSU	C3'-C4'-C5'-O5'
86	2	437	PSU	O4'-C4'-C5'-O5'
86	2	443	OMC	C2'-C1'-N1-C6
86	2	472	PSU	C3'-C4'-C5'-O5'
86	2	527	A2M	O4'-C4'-C5'-O5'
86	2	527	A2M	C3'-C4'-C5'-O5'
86	2	534	OMG	O4'-C4'-C5'-O5'
86	2	534	OMG	C3'-C4'-C5'-O5'
86	2	570	A2M	C1'-C2'-O2'-CM'
86	2	667	OMU	C1'-C2'-O2'-CM2
86	2	1144	PSU	C3'-C4'-C5'-O5'
86	2	1384	A2M	C1'-C2'-O2'-CM'
86	2	1419	OMU	C1'-C2'-O2'-CM2
35	S1	28	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
35	S1	29	OMU	C1'-C2'-O2'-CM2
35	S1	33	PSU	C3'-C4'-C5'-O5'
35	S1	98	A2M	C1'-C2'-O2'-CM'
35	S1	668	A2M	C1'-C2'-O2'-CM'
35	S1	912	A2M	C1'-C2'-O2'-CM'
35	S1	918	A2M	O4'-C4'-C5'-O5'
35	S1	969	A2M	C1'-C2'-O2'-CM'
35	S1	1543	C4J	C3-C31-C32-C34
35	S1	1543	C4J	C3-C31-C32-N33
35	S1	1543	C4J	N33-C32-C34-O36
35	S1	1566	PSU	C3'-C4'-C5'-O5'
35	S1	1657	PSU	O4'-C1'-C5-C4
35	S1	1657	PSU	O4'-C1'-C5-C6
35	S1	1866	OMC	C3'-C4'-C5'-O5'
35	S1	2021	A2M	C3'-C4'-C5'-O5'
35	S1	2021	A2M	C1'-C2'-O2'-CM'
35	S1	2059	OMC	O4'-C1'-N1-C2
35	S1	2059	OMC	O4'-C1'-N1-C6
86	2	443	OMC	C2'-C1'-N1-C2
82	1	681	A2M	C3'-C4'-C5'-O5'
85	7	43	A2M	O4'-C4'-C5'-O5'
86	2	1185	A2M	C3'-C4'-C5'-O5'
35	S1	600	OMG	O4'-C4'-C5'-O5'
35	S1	600	OMG	C3'-C4'-C5'-O5'
35	S1	1566	PSU	O4'-C4'-C5'-O5'
35	S1	1866	OMC	O4'-C4'-C5'-O5'
82	1	407	A2M	O4'-C4'-C5'-O5'
86	2	472	PSU	O4'-C4'-C5'-O5'
35	S1	33	PSU	O4'-C4'-C5'-O5'
35	S1	98	A2M	O4'-C4'-C5'-O5'
35	S1	1543	C4J	C3'-C4'-C5'-O5'
35	S1	2021	A2M	O4'-C4'-C5'-O5'
86	2	1078	OMG	C3'-C2'-O2'-CM2
35	S1	512	A2M	C3'-C4'-C5'-O5'
86	2	1308	5MC	C2'-C1'-N1-C6
37	4	74	OMG	C3'-C4'-C5'-O5'
82	1	1371	OMU	C3'-C4'-C5'-O5'
35	S1	2185	MA6	C3'-C4'-C5'-O5'
35	S1	1543	C4J	C4'-C5'-O5'-P
86	2	1144	PSU	O4'-C4'-C5'-O5'
35	S1	1995	7MG	O4'-C4'-C5'-O5'
35	S1	1543	C4J	N33-C32-C34-O35

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Mol	Chain	Res	Type	Atoms
82	1	1371	OMU	O4'-C4'-C5'-O5'
35	S1	1995	7MG	C3'-C4'-C5'-O5'
35	S1	1829	OMG	O4'-C4'-C5'-O5'
35	S1	969	A2M	C4'-C5'-O5'-P
37	4	74	OMG	O4'-C4'-C5'-O5'
86	2	1185	A2M	O4'-C4'-C5'-O5'
35	S1	1543	C4J	O4'-C4'-C5'-O5'
35	S1	2185	MA6	O4'-C4'-C5'-O5'
86	2	1046	OMG	C1'-C2'-O2'-CM2
86	2	1308	5MC	O4'-C1'-N1-C6
82	1	681	A2M	C4'-C5'-O5'-P
86	2	1248	OMC	C4'-C5'-O5'-P
35	S1	1478	OMG	C4'-C5'-O5'-P
86	2	443	OMC	O4'-C1'-N1-C2
35	S1	1866	OMC	C3'-C2'-O2'-CM2
86	2	443	OMC	O4'-C1'-N1-C6
35	S1	512	A2M	O4'-C4'-C5'-O5'
86	2	1308	5MC	C2'-C1'-N1-C2
83	3	13	OMU	C4'-C5'-O5'-P
86	2	560	OMU	C4'-C5'-O5'-P
86	2	1185	A2M	C4'-C5'-O5'-P
86	2	1308	5MC	O4'-C1'-N1-C2
86	2	1361	PSU	C4'-C5'-O5'-P
35	S1	2185	MA6	C4'-C5'-O5'-P
82	1	927	A2M	C3'-C2'-O2'-CM'
82	1	1524	OMG	C3'-C2'-O2'-CM2
35	S1	1829	OMG	C4'-C5'-O5'-P
35	S1	8	OMU	O4'-C4'-C5'-O5'
35	S1	1621	OMU	O4'-C4'-C5'-O5'
82	1	1039	PSU	O4'-C1'-C5-C4
35	S1	8	OMU	C2'-C1'-N1-C6
85	7	162	A2M	C3'-C4'-C5'-O5'
35	S1	668	A2M	O4'-C4'-C5'-O5'
35	S1	1539	PSU	C3'-C4'-C5'-O5'
35	S1	1833	OMU	O4'-C4'-C5'-O5'
35	S1	8	OMU	O4'-C1'-N1-C6
82	1	407	A2M	C3'-C2'-O2'-CM'
82	1	858	A2M	C3'-C4'-C5'-O5'
82	1	1527	OMC	O4'-C4'-C5'-O5'
35	S1	98	A2M	C3'-C4'-C5'-O5'
35	S1	8	OMU	C3'-C2'-O2'-CM2
35	S1	1829	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
35	S1	2061	5MC	O4'-C4'-C5'-O5'
35	S1	1833	OMU	C4'-C5'-O5'-P
35	S1	2061	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 391 ligands modelled in this entry, 391 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	S1	1
21	SV	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S1	1543:C4J	O3'	1544:5MC	P	4.41
1	SV	72:LYS	C	73:LEU	N	3.06

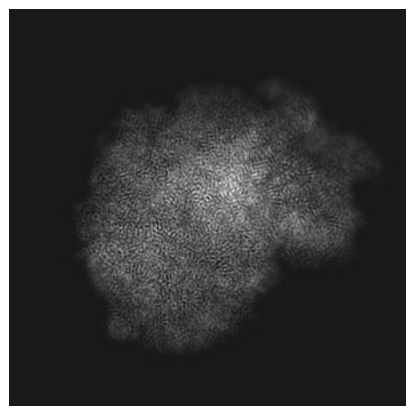
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18419. These allow visual inspection of the internal detail of the map and identification of artifacts.

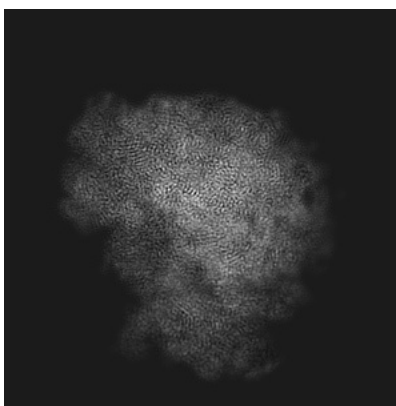
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

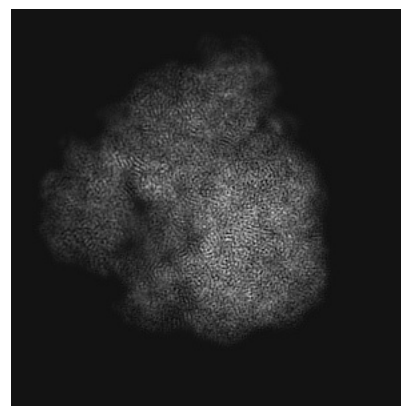
6.1.1 Primary map



X

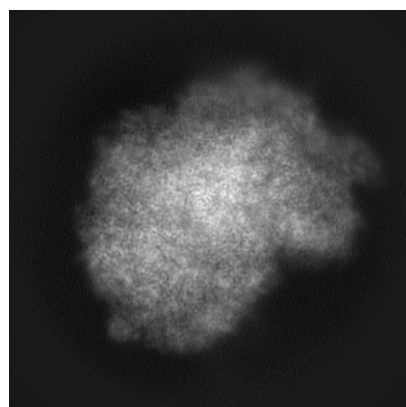


Y

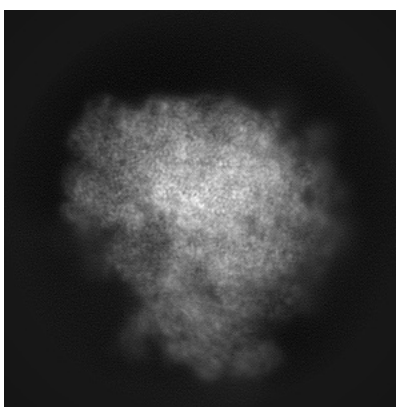


Z

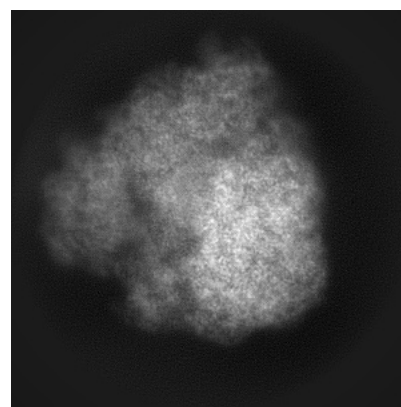
6.1.2 Raw map



X



Y

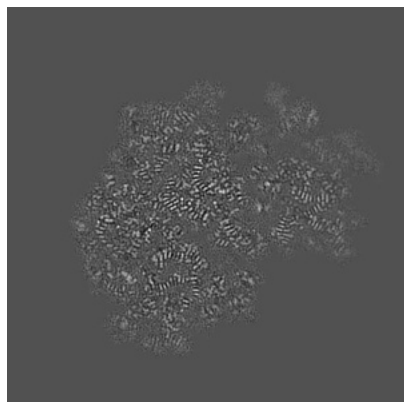


Z

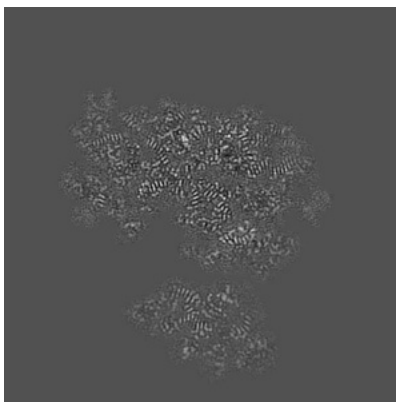
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

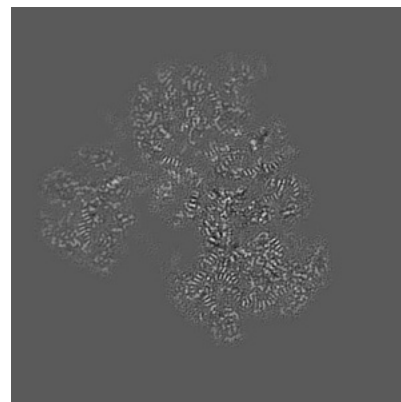
6.2.1 Primary map



X Index: 240

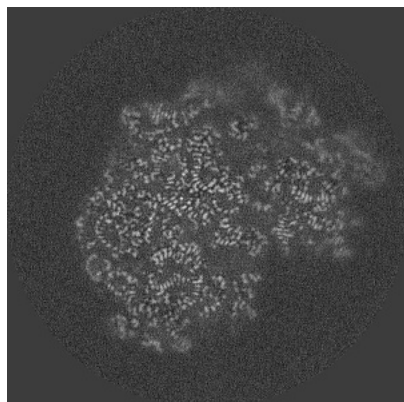


Y Index: 240

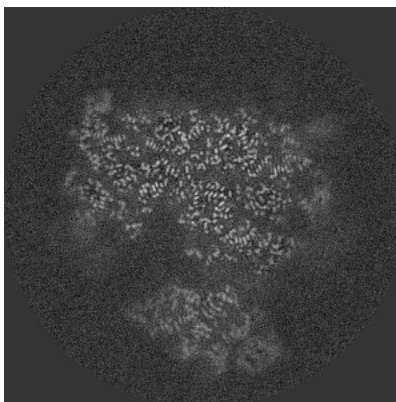


Z Index: 240

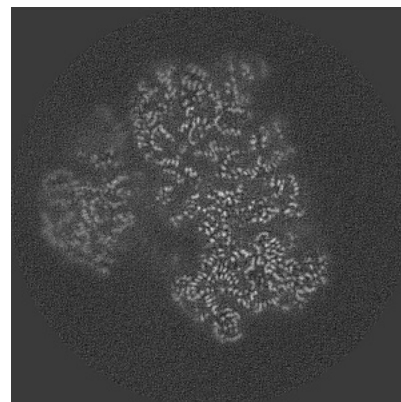
6.2.2 Raw map



X Index: 240



Y Index: 240

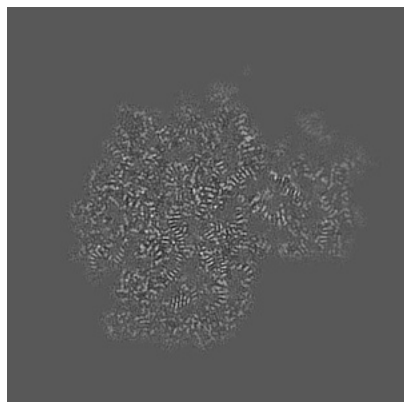


Z Index: 240

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

6.3 Largest variance slices [i](#)

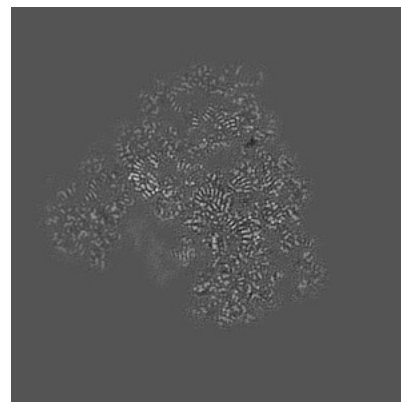
6.3.1 Primary map



X Index: 261

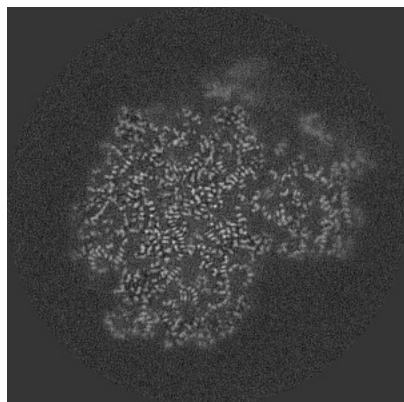


Y Index: 266

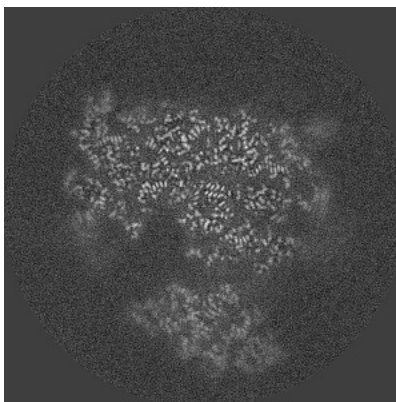


Z Index: 260

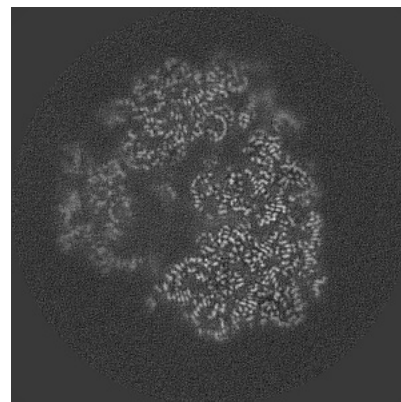
6.3.2 Raw map



X Index: 261



Y Index: 241

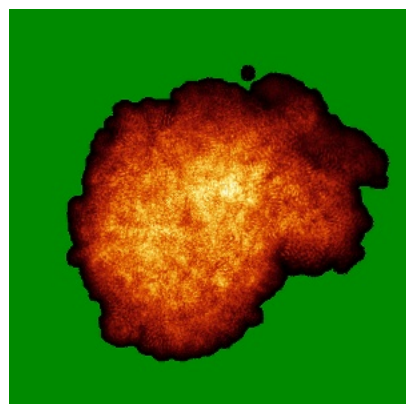


Z Index: 215

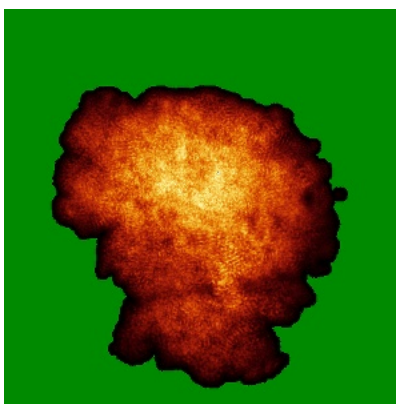
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

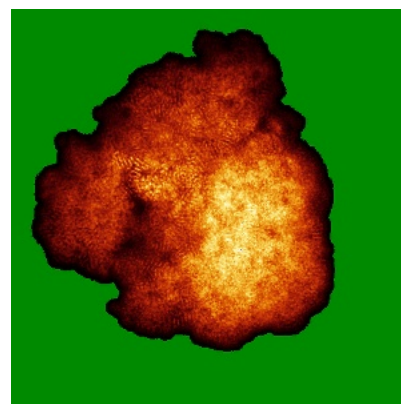
6.4.1 Primary map



X

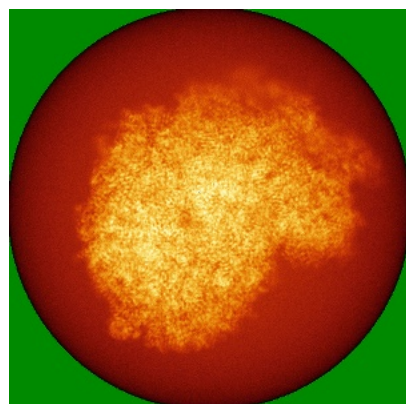


Y

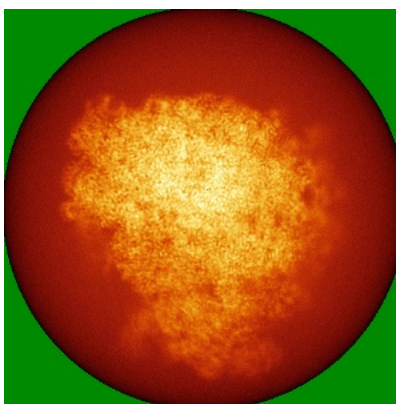


Z

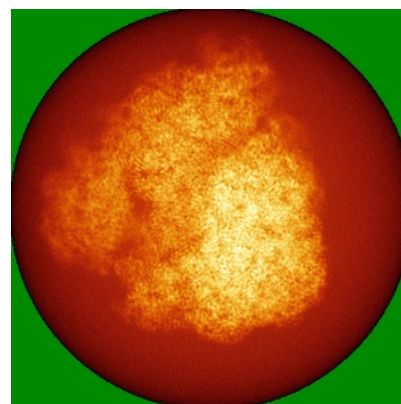
6.4.2 Raw map



X



Y

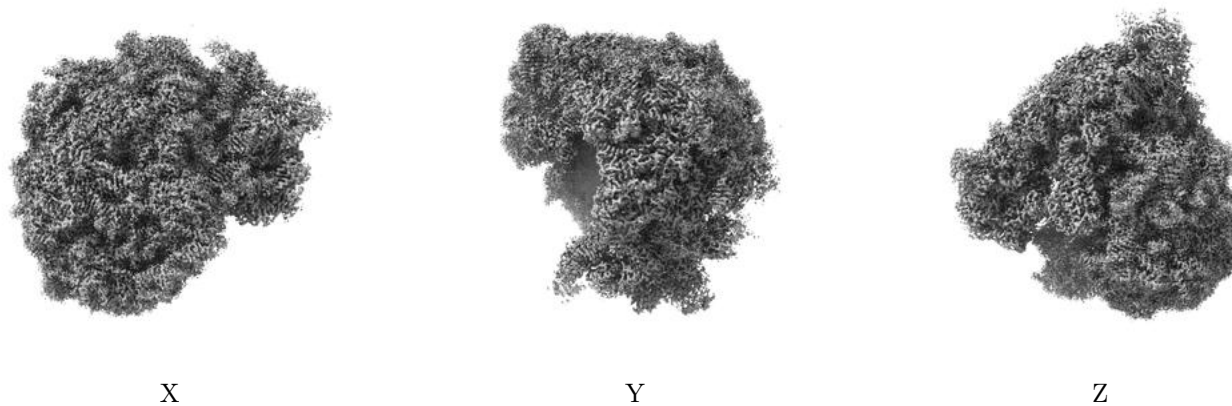


Z

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

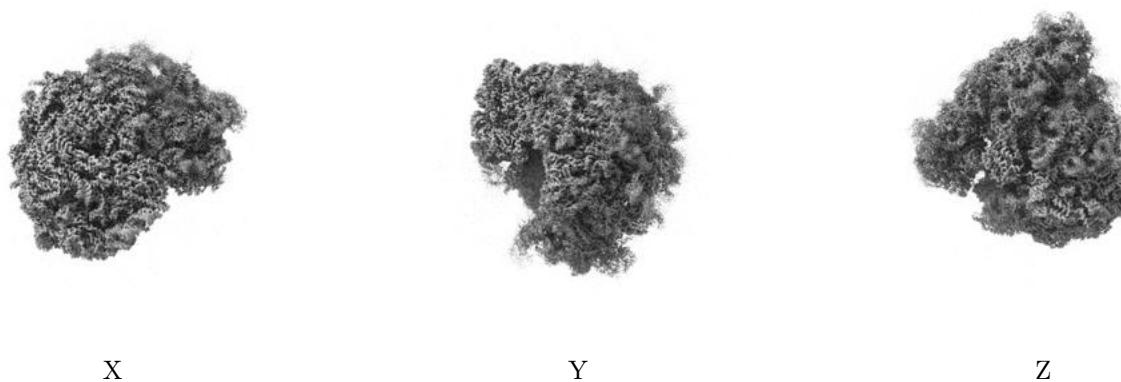
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

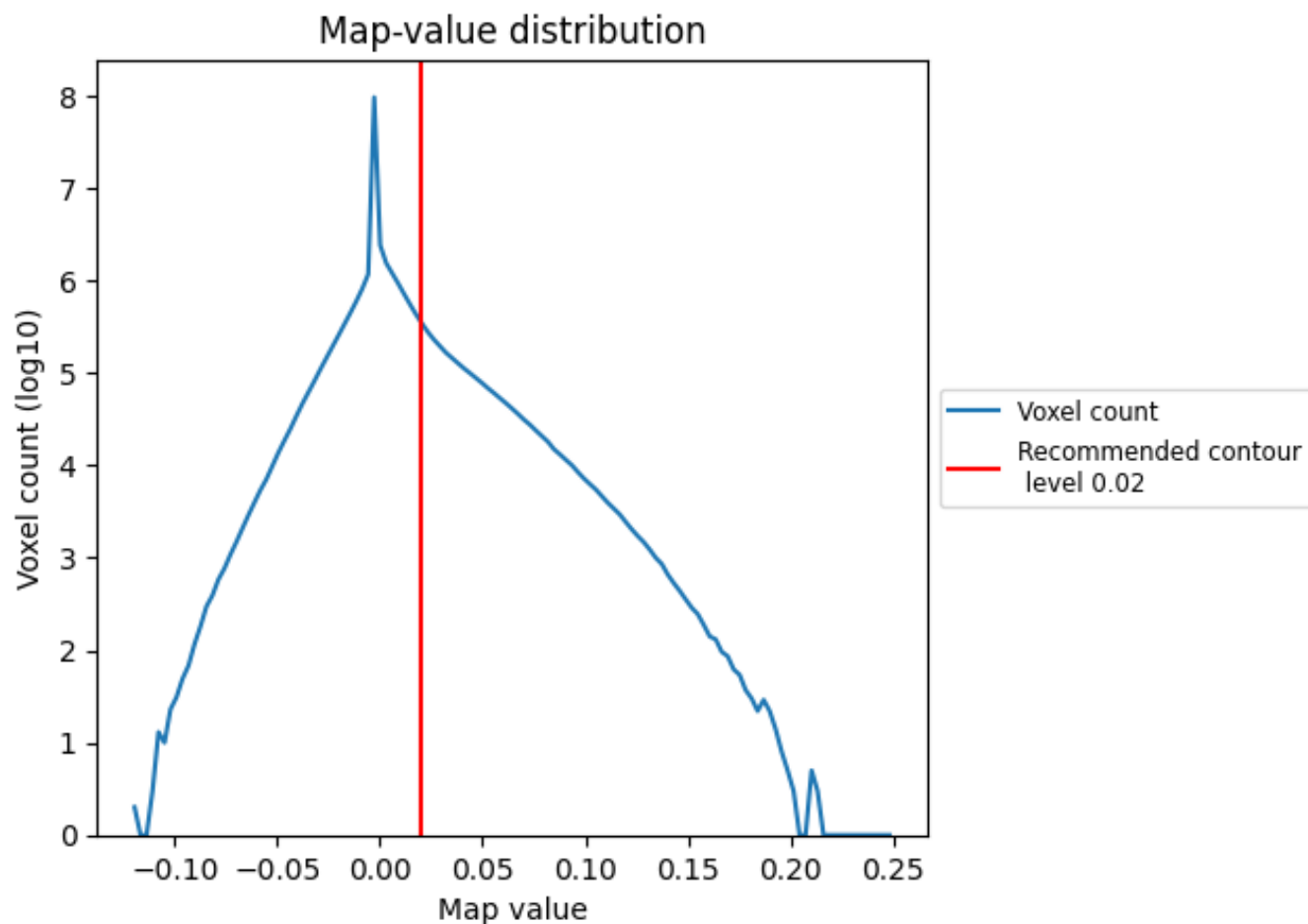
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

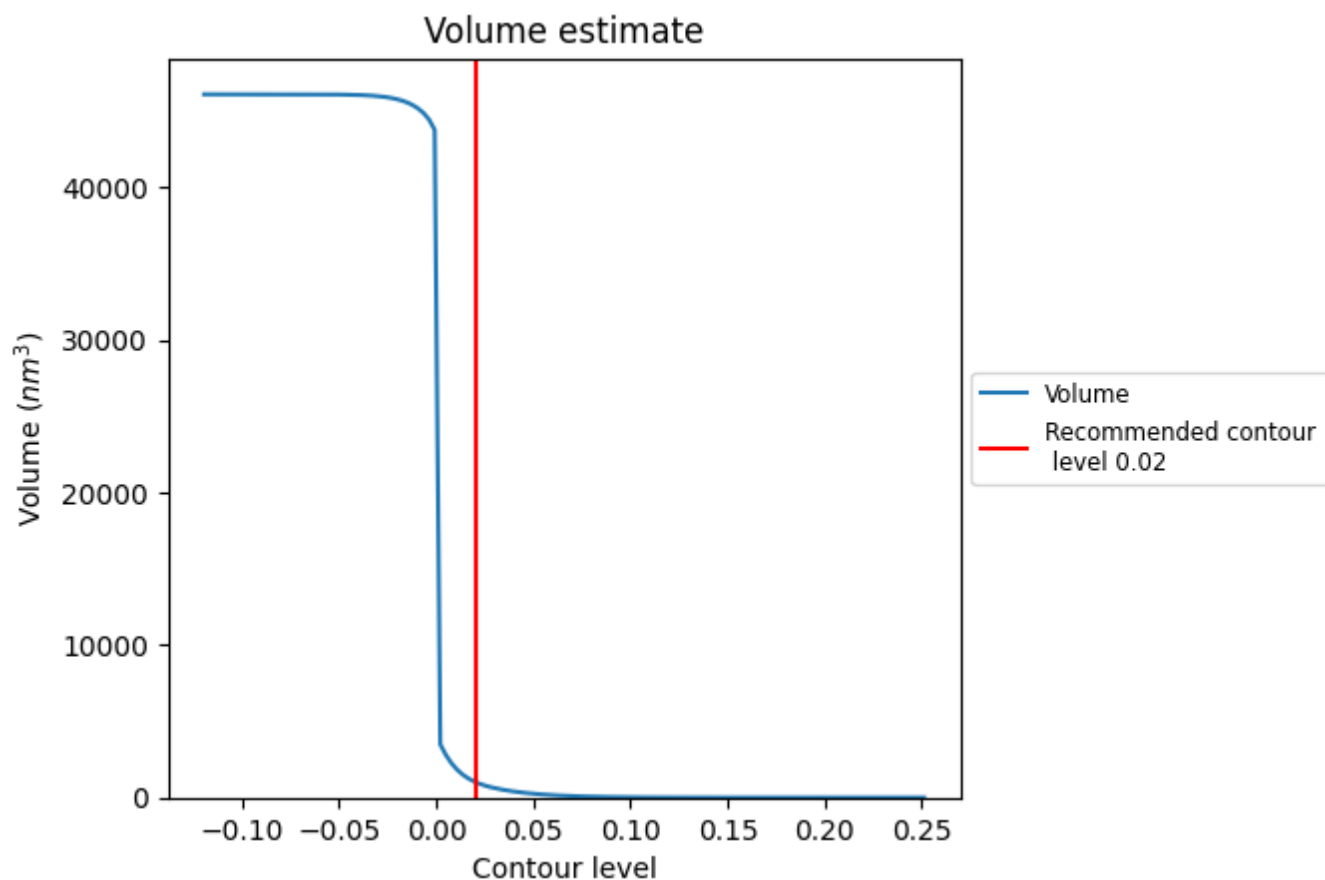
This section contains the results of statistical analysis of the map.

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.

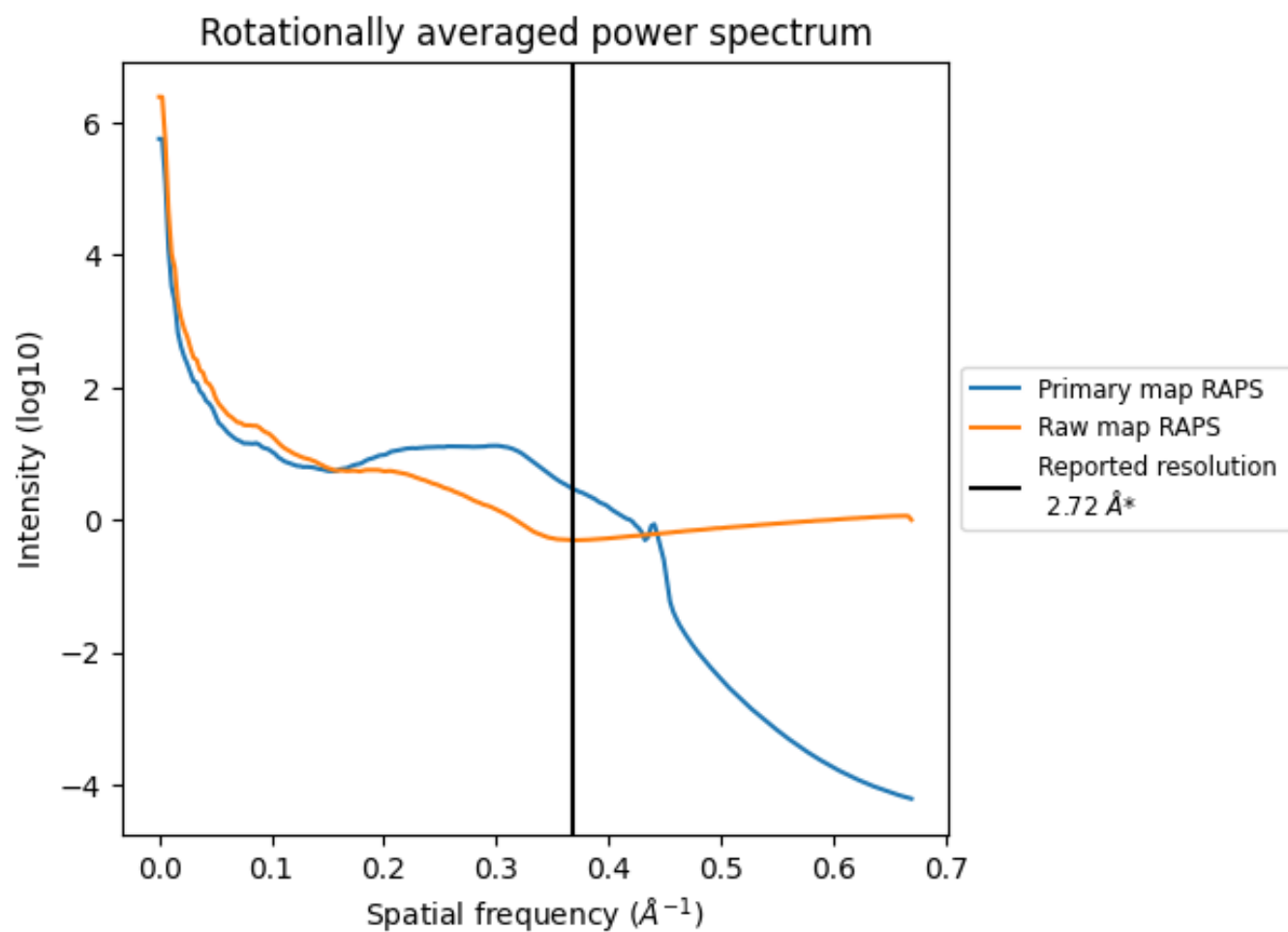
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1029 nm^3 ; this corresponds to an approximate mass of 929 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 ⓘ

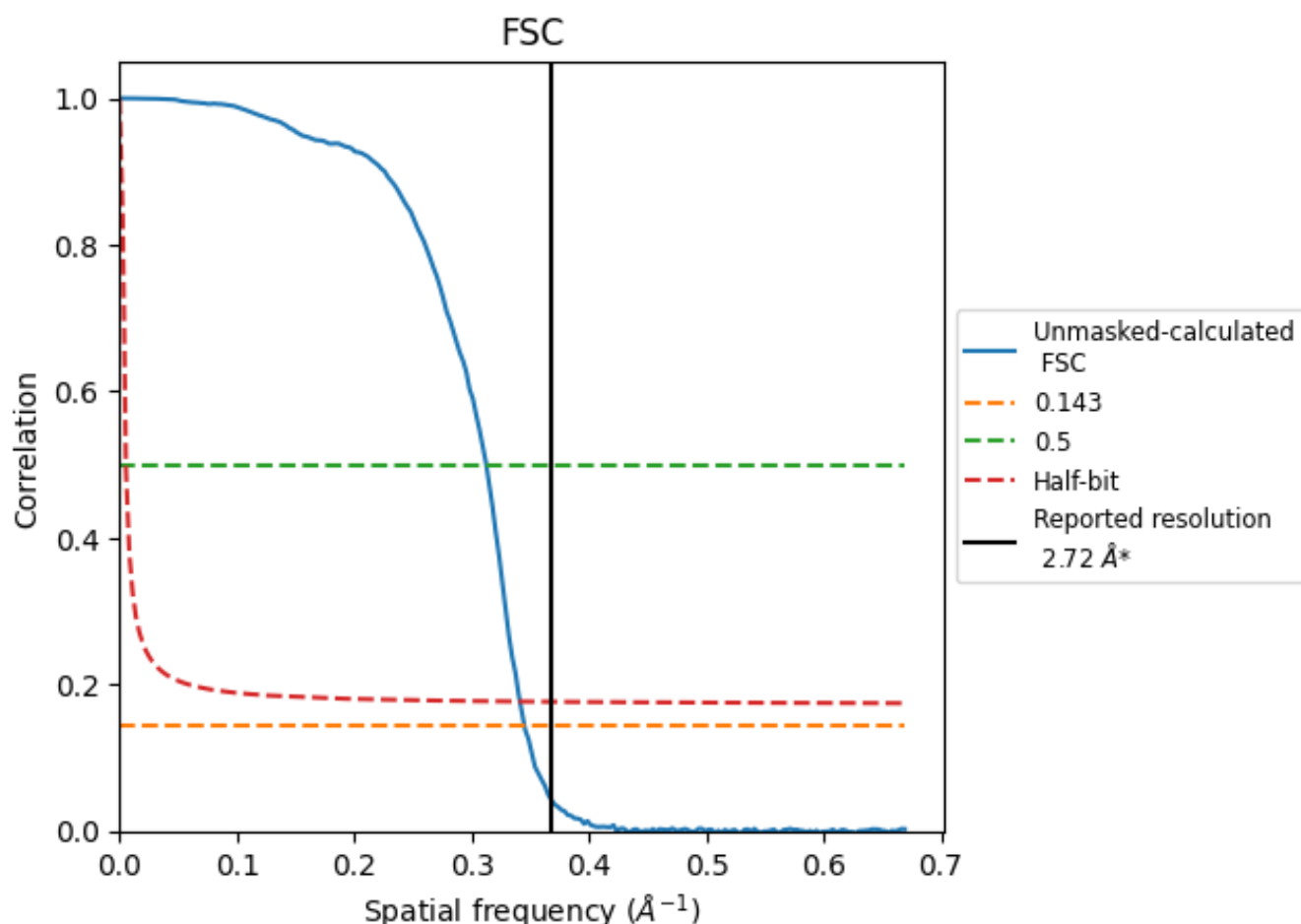


*Reported resolution corresponds to spatial frequency of 0.368 \AA^{-1}

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 0.368 \AA^{-1}

8.2 Resolution estimates [i](#)

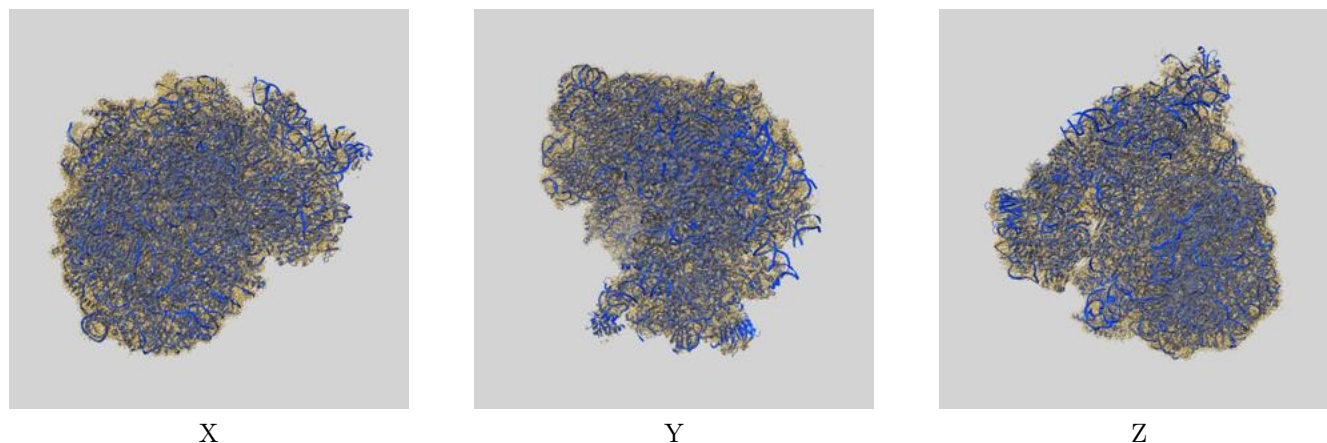
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.90	3.20	2.93

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

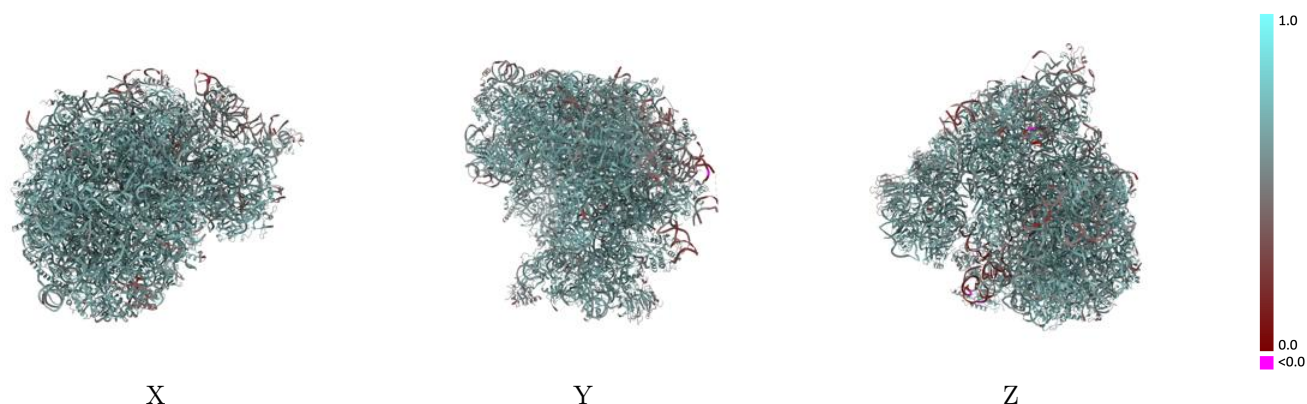
This section contains information regarding the fit between EMDB map EMD-18419 and PDB model 8QHU. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



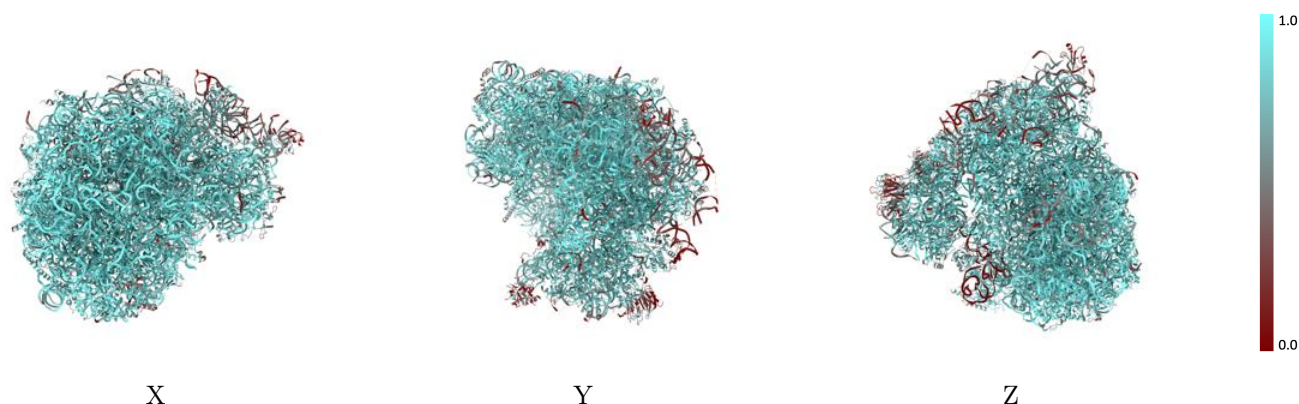
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



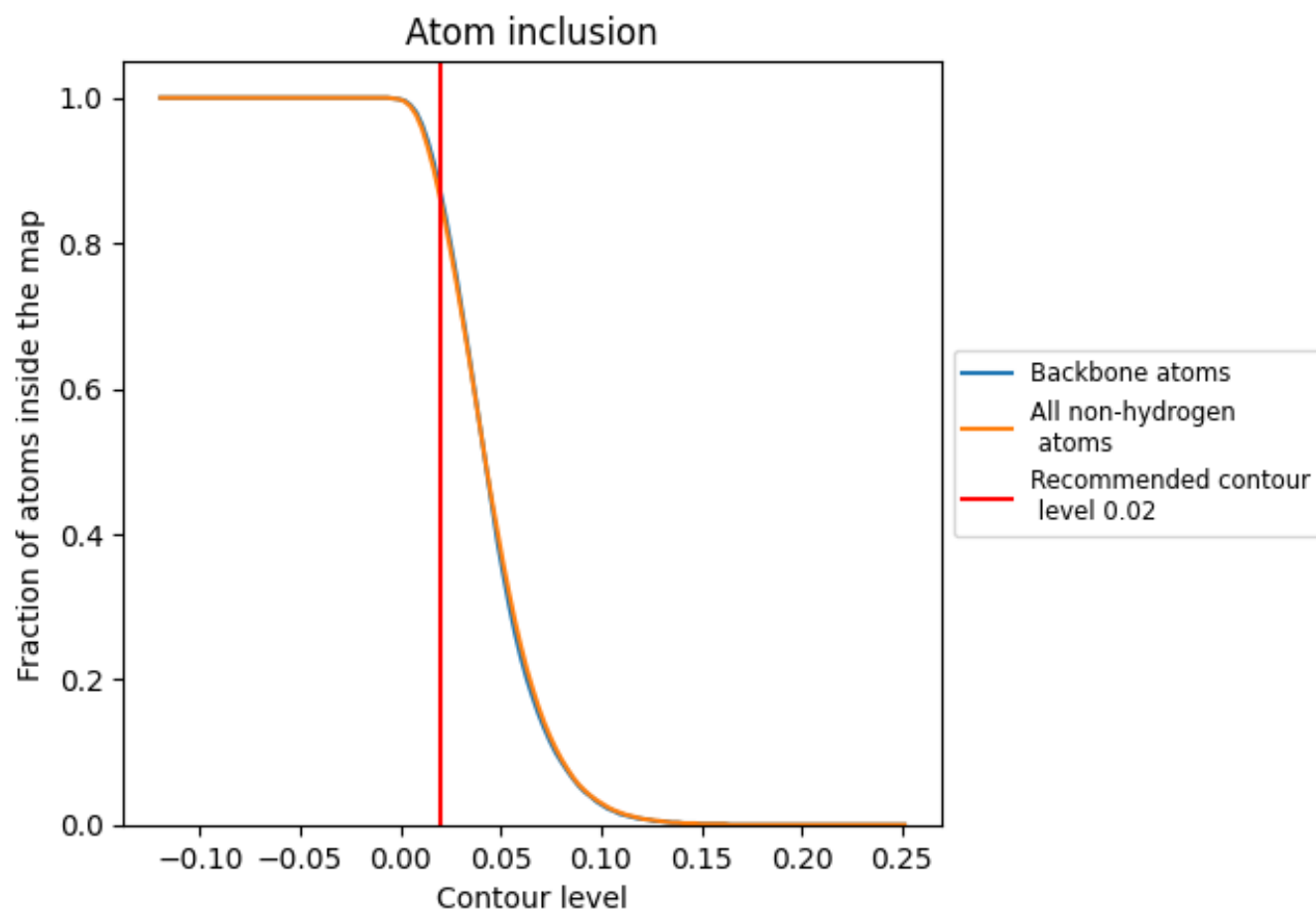
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.6220
1	 0.9280	 0.6380
2	 0.8730	 0.6080
3	 0.8700	 0.6040
4	 0.9500	 0.6550
5	 0.9040	 0.6120
6	 0.8570	 0.5870
7	 0.9230	 0.6360
8	 0.9430	 0.6380
A	 0.9680	 0.6840
B	 0.9470	 0.6820
C	 0.9290	 0.6540
D	 0.7250	 0.5510
E	 0.8810	 0.6450
F	 0.8220	 0.5990
G	 0.8810	 0.6240
H	 0.9390	 0.6700
I	 0.8840	 0.6420
J	 0.9350	 0.6700
K	 0.8220	 0.6040
L	 0.9380	 0.6700
M	 0.9810	 0.6850
N	 0.8900	 0.6490
O	 0.8470	 0.6100
P	 0.9390	 0.6640
Q	 0.8560	 0.6170
R	 0.9400	 0.6660
S	 0.8930	 0.6440
S1	 0.8400	 0.6000
S4	 0.2350	 0.2690
SA	 0.8060	 0.6210
SB	 0.7810	 0.6020
SC	 0.7150	 0.6090
SD	 0.8260	 0.6450
SE	 0.8240	 0.6480























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Chain	Atom inclusion	Q-score
SF	 0.8120	 0.6390
SG	 0.7250	 0.6150
SH	 0.8310	 0.6420
SI	 0.7500	 0.6100
SJ	 0.8880	 0.6620
SK	 0.8820	 0.6490
SL	 0.8660	 0.6540
SM	 0.6720	 0.6080
SN	 0.7240	 0.6130
SO	 0.8640	 0.6490
SP	 0.8780	 0.6580
SQ	 0.2120	 0.4660
SR	 0.7390	 0.6180
SS	 0.8740	 0.6570
ST	 0.8930	 0.6190
SU	 0.8660	 0.6540
SV	 0.5910	 0.5740
SW	 0.7230	 0.6150
SX	 0.8520	 0.6500
SY	 0.6860	 0.5960
SZ	 0.7720	 0.6310
Sa	 0.7420	 0.6180
Sb	 0.9130	 0.6470
Sc	 0.7510	 0.6090
Sd	 0.6950	 0.5920
Se	 0.7600	 0.6160
Sf	 0.3150	 0.5210
Sg	 0.4150	 0.5470
Sh	 0.3240	 0.4930
T	 0.9620	 0.6820
U	 0.3900	 0.4930
V	 0.9040	 0.6460
W	 0.9100	 0.6460
X	 0.9450	 0.6660
Y	 0.8520	 0.6130
Z	 0.8800	 0.6310
a	 0.8490	 0.6150
b	 0.9280	 0.6550
c	 0.9330	 0.6650
d	 0.8580	 0.6200
e	 0.8180	 0.6060
f	 0.9440	 0.6690

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Chain	Atom inclusion	Q-score
g	 0.9390	 0.6670
h	 0.8790	 0.6370
i	 0.8630	 0.6260
j	 0.9760	 0.6910
k	 0.7620	 0.5860
l	 0.9440	 0.6730
m	 0.9190	 0.6580
n	 0.8770	 0.5740
o	 0.9470	 0.6670
p	 0.9150	 0.6660