



Full wwPDB EM Validation Report ⓘ

Dec 14, 2023 – 08:51 am GMT

PDB ID : 8A3W
EMDB ID : EMD-15124
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
WILD TYPE
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2022-06-09
Resolution : 2.89 Å (reported)
Based on initial models : 6AZ3, 6AZ1, 5T2A

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:

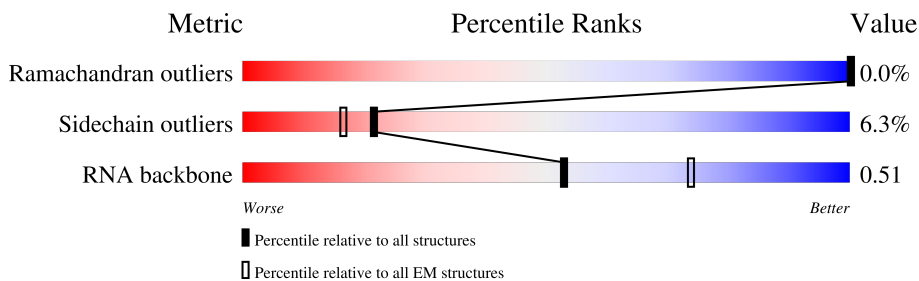
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.89 Å.

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



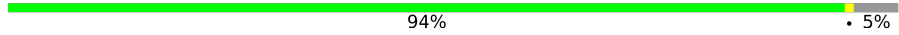



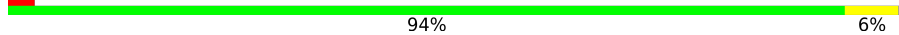










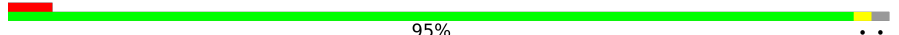








Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	SD	190	78% 8% 14%
2	SE	273	93% 5%
3	SF	265	14% 74% 23%
4	SG	249	89% 6%
5	SH	190	92% 5%
6	SI	200	93% 6%
7	SJ	130	97%
8	SK	220	5% 80% 16%

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Mol	Chain	Length	Quality of chain
9	SL	149	 94% 5%
10	SM	116	 81% 6% 12%
11	SN	168	 54% 42%
12	SO	144	 90% 7%
13	SP	143	 94% 6%
14	SR	153	 82% 7% 12%
15	SS	57	 89% 5% 5%
16	ST	151	 91% 7%
17	SU	173	 84% 5% 11% 6%
18	SV	143	 48% 50%
19	SW	152	 68% 5% 27%
20	SX	161	 80% 7% 13%
21	SY	164	 51% 46% 26%
22	SZ	137	 82% 7% 11%
23	Sa	120	 56% 42%
24	Sb	112	 65% 10% 25%
25	Sc	86	 95%
26	Sd	87	 57% 5% 38%
27	Se	66	 67% 30% 8%
28	Sg	312	 86% 7% 7%
29	S1	2204	 57% 16% 25%
30	SA	264	 72% 5% 23%
31	SB	246	 79% 6% 15% 2%
32	SC	219	 87% 5% 8%
33	Sh	235	 36% 60% 18%


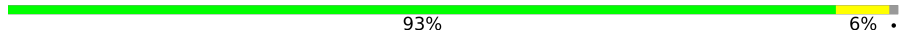


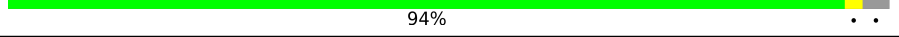



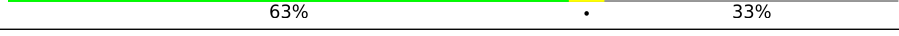
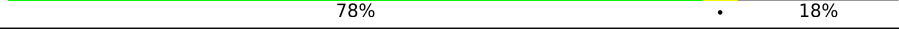
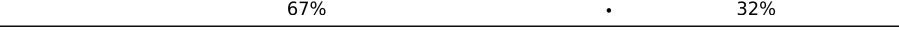

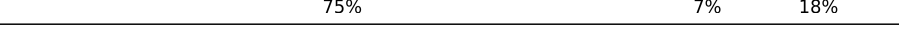
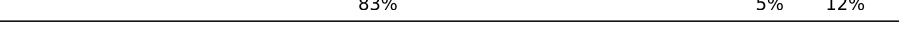
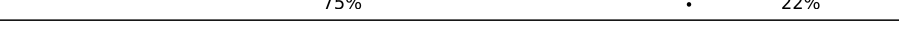

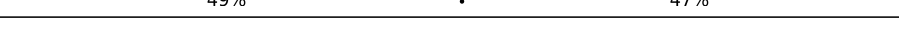
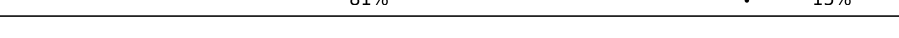
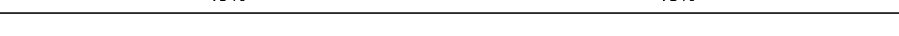

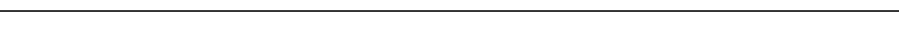

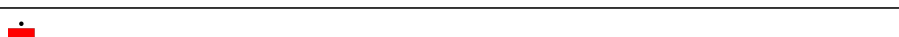
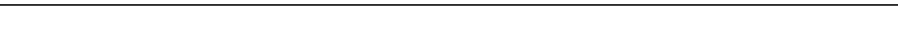
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Mol	Chain	Length	Quality of chain
34	S4	20	
35	8	123	
36	6	73	
37	2	1522	
38	7	171	
39	5	135	
40	4	183	
41	3	216	
42	1	1782	
43	B	419	
44	C	373	
45	A	260	
46	c	252	
47	O	305	
48	M	204	
49	H	222	
50	G	264	
51	P	198	
52	R	179	
53	I	220	
54	Q	254	
55	T	166	
56	S	159	
57	L	145	
58	F	195	

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Mol	Chain	Length	Quality of chain
59	E	190	 73% 5% 22%
60	Y	134	 93% 6%
61	f	133	 89% 8%
62	g	144	 82% 14%
63	a	127	 94%
64	J	139	 91% 7%
65	W	143	 80% 18%
66	V	145	 76% 6% 19%
67	h	168	 63% 33%
68	Z	147	 78% 18%
69	K	175	 67% 32%
70	j	83	 90% 6%
71	i	105	 75% 7% 18%
72	U	129	 83% 5% 12%
73	p	106	 75% 22%
74	o	92	 89% 7%
75	D	188	 49% 47%
76	d	104	 81% 15%
77	X	124	 49% 48%
78	b	70	 89% 6% 6%
79	k	83	 86% 14%
80	l	51	 88% 10%
81	n	34	 44% 74% 26%
82	e	188	 76% 20%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 183881 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 Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	SD	163	1347	852	266	221	8	1	0

- Molecule 2 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SE	260	2060	1307	397	347	9	2	0

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SF	205	1555	1000	279	267	9	0	0

- Molecule 4 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SG	233	1810	1132	370	305	3	1	0

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SH	183	1404	876	263	258	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SI	199	1583	1010	301	265	7	0	0

- Molecule 7 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SJ	129	1017	644	188	177	8	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SK	184	1453	912	307	232	2	0	0

- Molecule 9 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SL	142	1112	715	205	189	3	0	0

- Molecule 10 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SM	102	807	503	150	152	2	2	0

- Molecule 11 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SN	98	791	507	139	138	7	0	0

- Molecule 12 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SO	134	975	602	192	174	7	0	0

- Molecule 13 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SP	142	1119	706	223	187	3	3	0

- Molecule 14 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SR	135	1077	681	212	180	4	1	0

- Molecule 15 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	SS	54	417	257	84	71	5	0	0

- Molecule 16 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	ST	140	1140	720	227	185	8	0	0

- Molecule 17 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SU	154	1218	771	241	201	5	0	0

- Molecule 18 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SV	71	577	368	110	97	2	0	0

- Molecule 19 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	SW	111	866	553	164	145	4	0	0

- Molecule 20 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	SX	140	1092	694	211	183	4	0	0

- Molecule 21 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SY	88	Total	C	N	O	S	0	0
			622	382	116	121	3		

- Molecule 22 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SZ	122	Total	C	N	O	S	0	0
			972	623	187	160	2		

- Molecule 23 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sa	70	Total	C	N	O	S	0	0
			549	351	97	98	3		

- Molecule 24 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sb	84	Total	C	N	O	S	0	0
			661	410	138	106	7		

- Molecule 25 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Sc	84	Total	C	N	O	S	0	0
			624	390	118	112	4		

- Molecule 26 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sd	54	Total	C	N	O	S	0	0
			390	240	80	66	4		

- Molecule 27 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Se	46	Total	C	N	O	S	0	0
			350	221	71	57	1		

- Molecule 28 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sg	290	Total	C	N	O	S	1	0
			2173	1369	381	411	12		

- Molecule 29 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S1	1663	Total	C	N	O	P	0	0
			35569	15906	6433	11567	1663		

- Molecule 30 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SA	204	Total	C	N	O	S	1	0
			1653	1043	314	287	9		

- Molecule 31 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SB	210	Total	C	N	O	S	0	0
			1595	1015	281	287	12		

- Molecule 32 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SC	202	Total	C	N	O	S	1	0
			1525	974	272	266	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sh	95	Total	C	N	O	S	0	0
			668	413	128	125	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S4	17	Total	C	N	O	P	0	0
			359	161	66	116	16		

- Molecule 35 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	8	119	2531	1132	452	828	119	0	0

- Molecule 36 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
36	6	63	1329	595	238	433	63	0	0

- Molecule 37 is a RNA chain called LSub_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	2	947	20228	9057	3635	6589	947	0	0

- Molecule 38 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	7	163	3463	1551	613	1137	162	0	0

- Molecule 39 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	5	98	2096	934	381	683	98	0	0

- Molecule 40 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	4	158	3378	1507	611	1102	158	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	4	G	A	conflict	GB 321438308

- Molecule 41 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	153	Total	C	N	O	P	0	0
			3252	1454	570	1075	153		

- Molecule 42 is a RNA chain called LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1	1467	Total	C	N	O	P	1	0
			31495	14076	5781	10171	1467		

- Molecule 43 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	B	395	Total	C	N	O	S	4	0
			2955	1874	575	494	12		

- Molecule 44 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	C	325	Total	C	N	O	S	0	0
			2343	1481	447	401	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A	254	Total	C	N	O	S	1	0
			1852	1153	375	314	10		

- Molecule 46 is a protein called uL30_chain_c.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	c	227	Total	C	N	O	S	0	0
			1779	1134	340	294	11		

- Molecule 47 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	243	Total	C	N	O	S	1	0
			1764	1130	333	298	3		

- Molecule 48 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	M	203	1692	1068	360	256	8	0	0

- Molecule 49 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	H	220	1690	1071	340	272	7	0	0

- Molecule 50 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	G	212	1635	1036	324	268	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	P	196	1513	952	303	252	6	0	0

- Molecule 52 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	R	178	1399	894	267	233	5	0	0

- Molecule 53 is a protein called eL13_chain_I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	I	169	1299	822	262	208	7	0	0

- Molecule 54 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Q	168	1290	802	276	206	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	T	152	1217	761	241	204	11	0	0

- Molecule 56 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	S	151	1164	738	228	195	3	0	0

- Molecule 57 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	L	144	1114	703	226	179	6	0	0

- Molecule 58 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	F	142	1032	658	191	181	2	0	0

- Molecule 59 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	E	148	1032	659	191	179	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	Y	132	1008	649	198	159	2	0	0

- Molecule 61 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	f	123	993	624	197	168	4	0	0

- Molecule 62 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	g	124	989	618	207	159	5	0	0

- Molecule 63 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	a	123	955	597	199	157	2	0	0

- Molecule 64 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	J	129	933	590	174	163	6	0	0

- Molecule 65 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	W	117	928	580	193	151	4	0	0

- Molecule 66 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	V	118	917	582	174	159	2	0	0

- Molecule 67 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	h	112	889	548	195	142	4	0	0

- Molecule 68 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Z	120	892	548	182	157	5	0	0

- Molecule 69 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	K	119	883	557	176	146	4	0	0

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	j	80	659	401	152	100	6	0	0

- Molecule 71 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	i	86	660	421	133	104	2	0	0

- Molecule 72 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	U	114	795	508	147	138	2	0	0

- Molecule 73 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	p	83	640	410	126	102	2	0	0

- Molecule 74 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	o	88	659	410	135	108	6	0	0

- Molecule 75 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	D	100	649	406	129	109	5	0	0

- Molecule 76 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	d	88	Total	C	N	O	S	0	0
			607	379	109	114	5		

- Molecule 77 is a protein called Putative ribosomal protein L24.

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

- Molecule 78 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	b	66	Total	C	N	O		0	0
			520	318	120	82			

- Molecule 79 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	k	71	Total	C	N	O	S	0	0
			508	323	96	86	3		

- Molecule 80 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	l	50	Total	C	N	O	S	0	0
			440	285	91	63	1		

- Molecule 81 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms				AltConf	Trace	
81	n	25	Total	C	N	O		0	0
			159	97	36	26			

- Molecule 82 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	151	Total	C	N	O	S	0	0
			1103	698	210	193	2		

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	SD	1	Total Mg 1 1	0
83	S1	30	Total Mg 30 30	0
83	2	25	Total Mg 25 25	0
83	7	2	Total Mg 2 2	0
83	5	1	Total Mg 1 1	0
83	3	1	Total Mg 1 1	0
83	1	52	Total Mg 52 52	0
83	C	1	Total Mg 1 1	0
83	T	1	Total Mg 1 1	0

- Molecule 84 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
84	SO	1	Total Na 1 1	0
84	S1	23	Total Na 23 23	0
84	2	9	Total Na 9 9	0
84	4	1	Total Na 1 1	0
84	1	22	Total Na 22 22	0
84	J	1	Total Na 1 1	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
85	SS	1	Total Zn 1 1	0
85	Sb	1	Total Zn 1 1	0
85	j	1	Total Zn 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
85	o	1	Total 1	Zn 1	0

- Molecule 86 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
86	Sb	1	Total 1	K 1	0
86	S1	4	Total 4	K 4	0
86	8	1	Total 1	K 1	0
86	2	3	Total 3	K 3	0
86	4	1	Total 1	K 1	0
86	1	3	Total 3	K 3	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	SH	1	Total 1	O 1	0
87	SN	2	Total 2	O 2	0
87	SR	1	Total 1	O 1	0
87	ST	1	Total 1	O 1	0
87	SX	1	Total 1	O 1	0
87	S1	36	Total 36	O 36	0
87	8	5	Total 5	O 5	0
87	6	1	Total 1	O 1	0
87	2	148	Total 148	O 148	0
87	7	40	Total 40	O 40	0

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Mol	Chain	Residues	Atoms		AltConf
87	5	19	Total 19	O 19	0
87	4	29	Total 29	O 29	0
87	3	17	Total 17	O 17	0
87	1	283	Total 283	O 283	0
87	B	9	Total 9	O 9	0
87	C	11	Total 11	O 11	0
87	A	10	Total 10	O 10	0
87	c	3	Total 3	O 3	0
87	M	9	Total 9	O 9	0
87	H	3	Total 3	O 3	0
87	G	3	Total 3	O 3	0
87	P	8	Total 8	O 8	0
87	R	1	Total 1	O 1	0
87	I	4	Total 4	O 4	0
87	Q	4	Total 4	O 4	0
87	T	7	Total 7	O 7	0
87	S	1	Total 1	O 1	0
87	L	3	Total 3	O 3	0
87	f	2	Total 2	O 2	0
87	g	1	Total 1	O 1	0
87	a	1	Total 1	O 1	0

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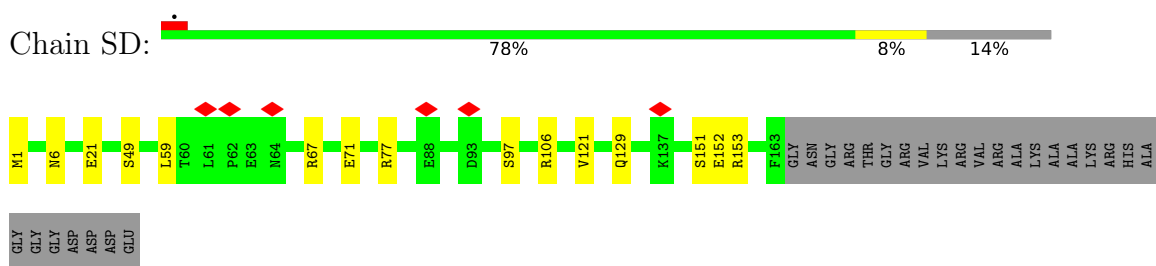
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Mol	Chain	Residues	Atoms		AltConf
87	J	1	Total 1	O 1	0
87	W	1	Total 1	O 1	0
87	V	2	Total 2	O 2	0
87	h	3	Total 3	O 3	0
87	j	7	Total 7	O 7	0
87	d	1	Total 1	O 1	0
87	X	1	Total 1	O 1	0
87	l	4	Total 4	O 4	0
87	e	3	Total 3	O 3	0

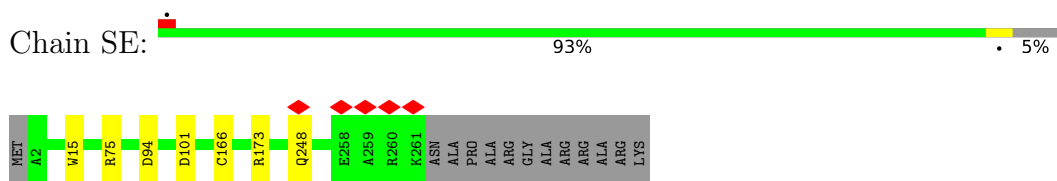
3 Residue-property plots

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

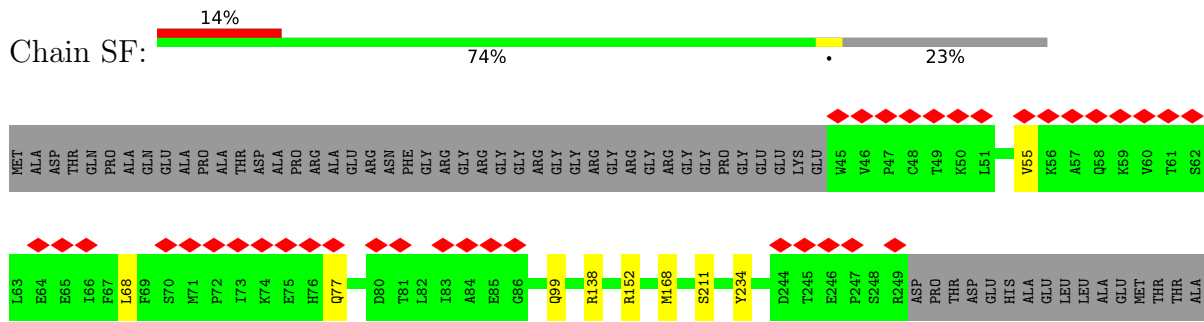
- Molecule 1: Putative 40S ribosomal protein S9



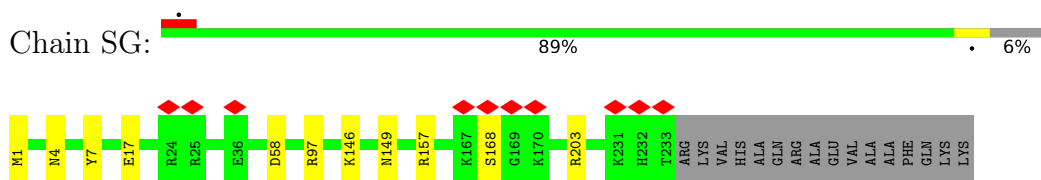
- Molecule 2: 40S ribosomal protein S4



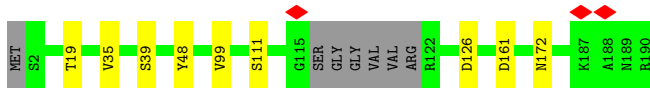
- Molecule 3: 40S ribosomal protein S2



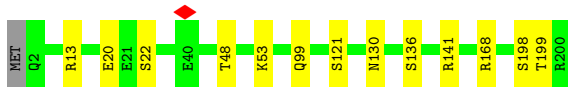
- Molecule 4: 40S ribosomal protein S6



- Molecule 5: 40S ribosomal protein S5



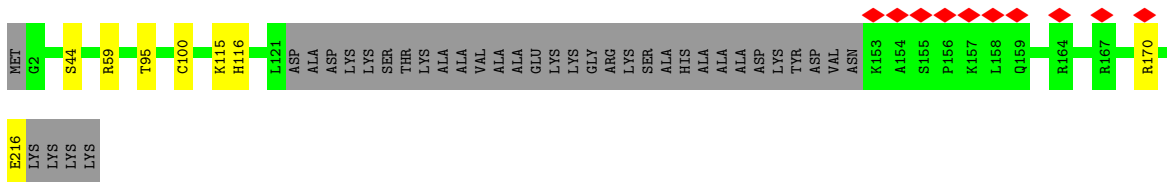
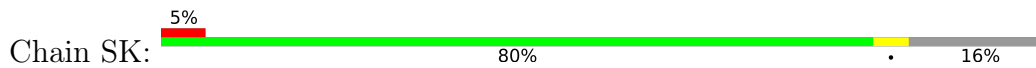
- Molecule 6: 40S ribosomal protein S7



- Molecule 7: Putative 40S ribosomal protein S15A



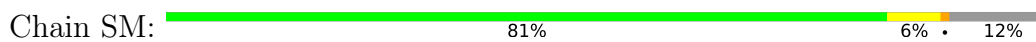
- Molecule 8: 40S ribosomal protein S8



- Molecule 9: Putative 40S ribosomal protein S16



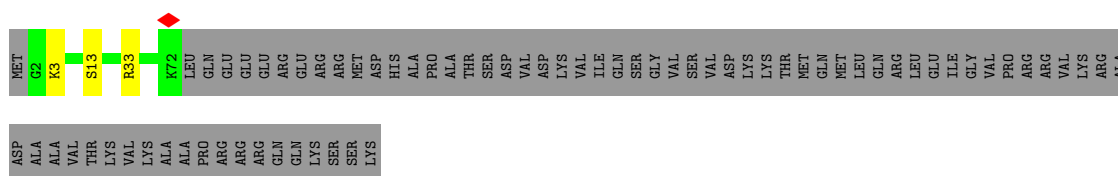
- Molecule 10: Putative ribosomal protein S20



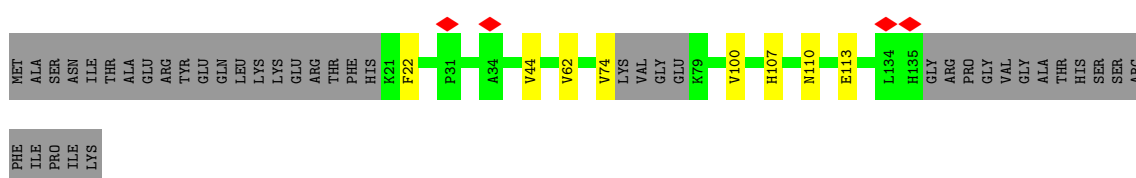
- Molecule 11: Putative 40S ribosomal protein S10



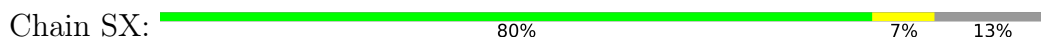
- Molecule 18: Putative 40S ribosomal protein S17



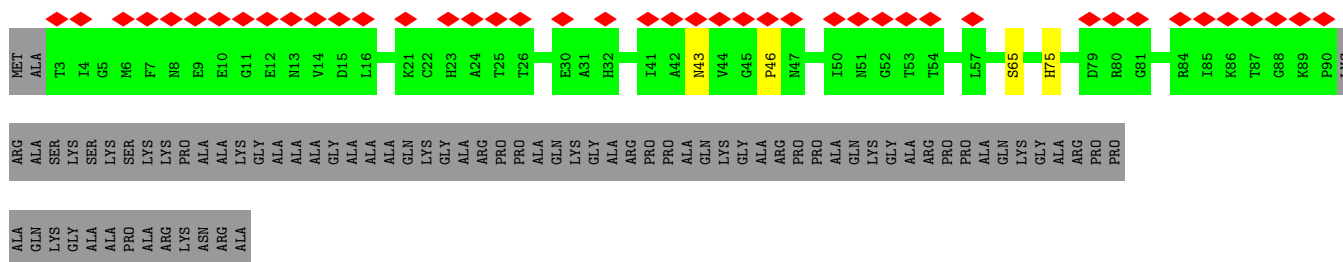
- Molecule 19: Putative 40S ribosomal protein S15



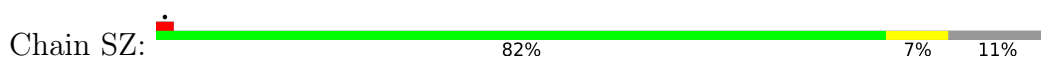
- Molecule 20: 40S ribosomal protein S19-like protein



- Molecule 21: Putative 40S ribosomal protein S21

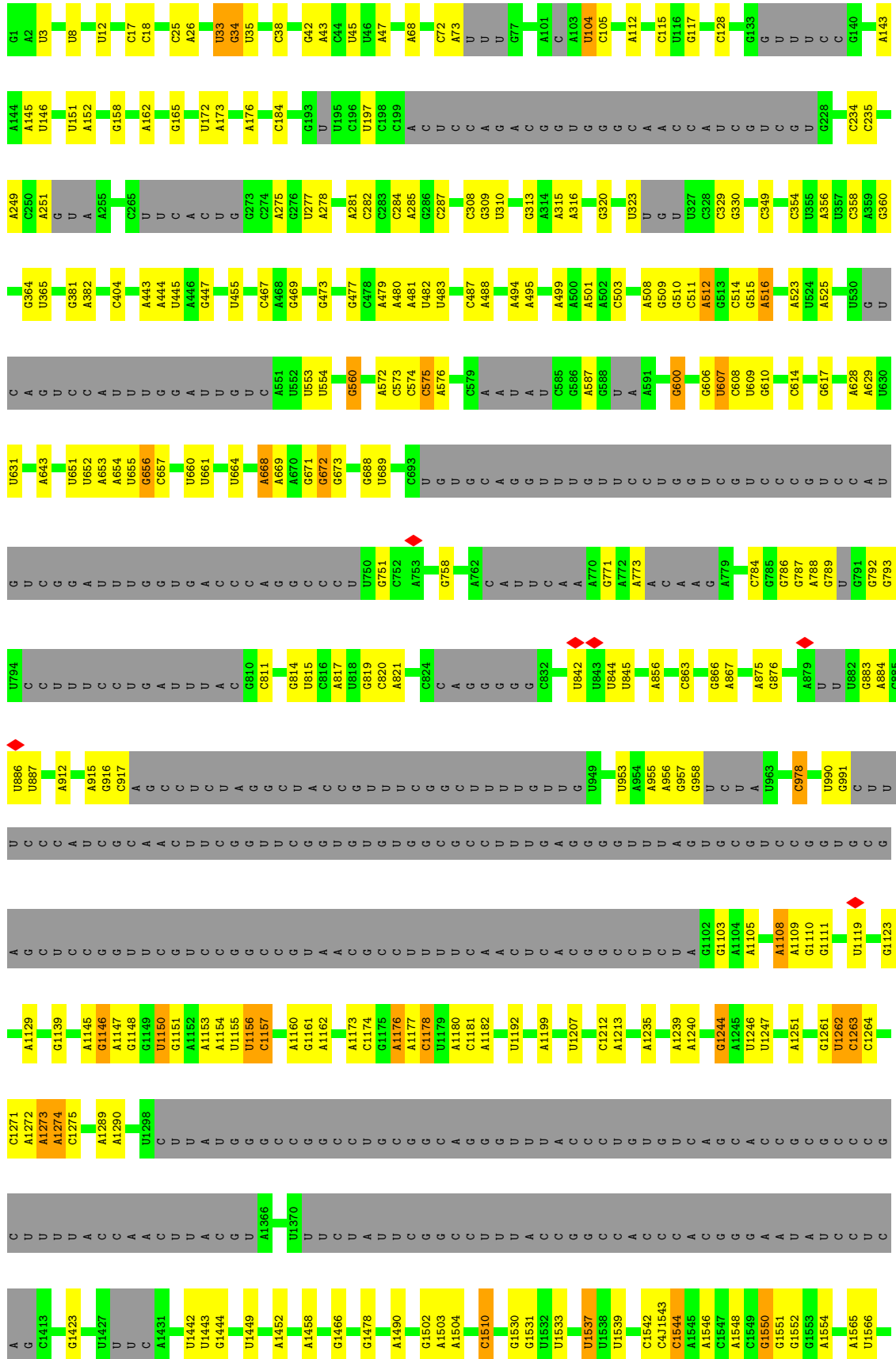


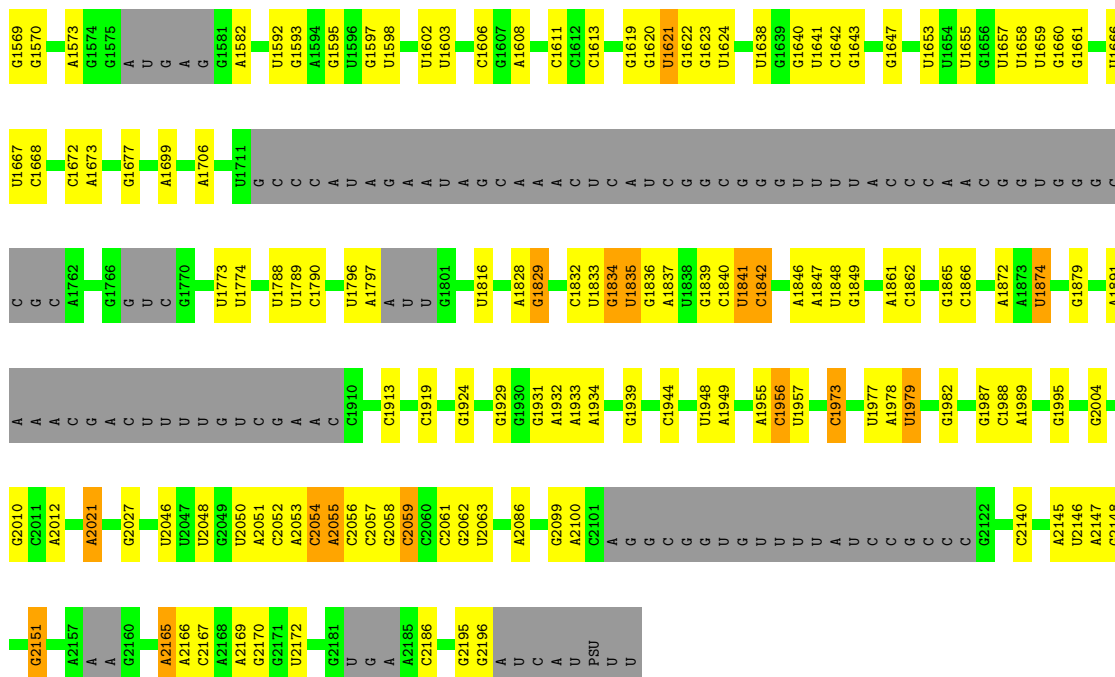
- Molecule 22: 40S ribosomal protein S24



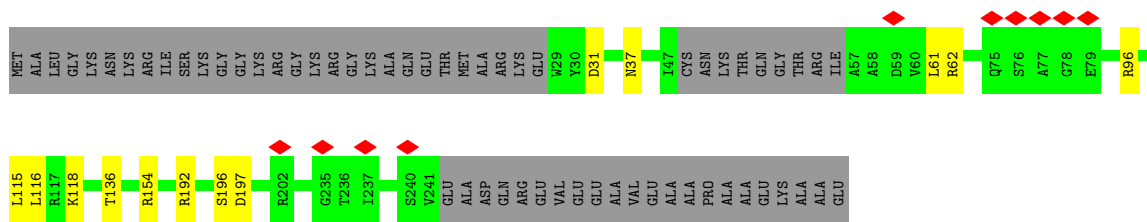
- Molecule 23: 40S ribosomal protein S25



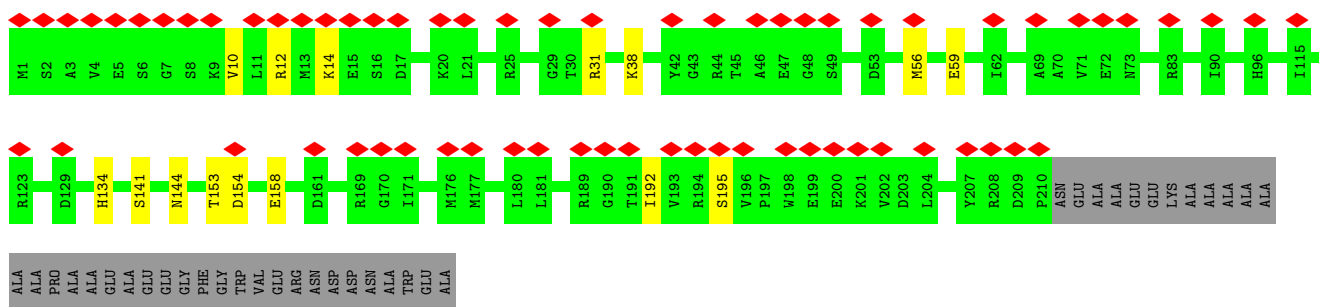
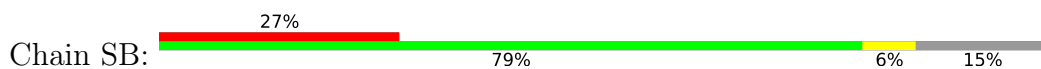




● Molecule 30: 40S ribosomal protein S3a

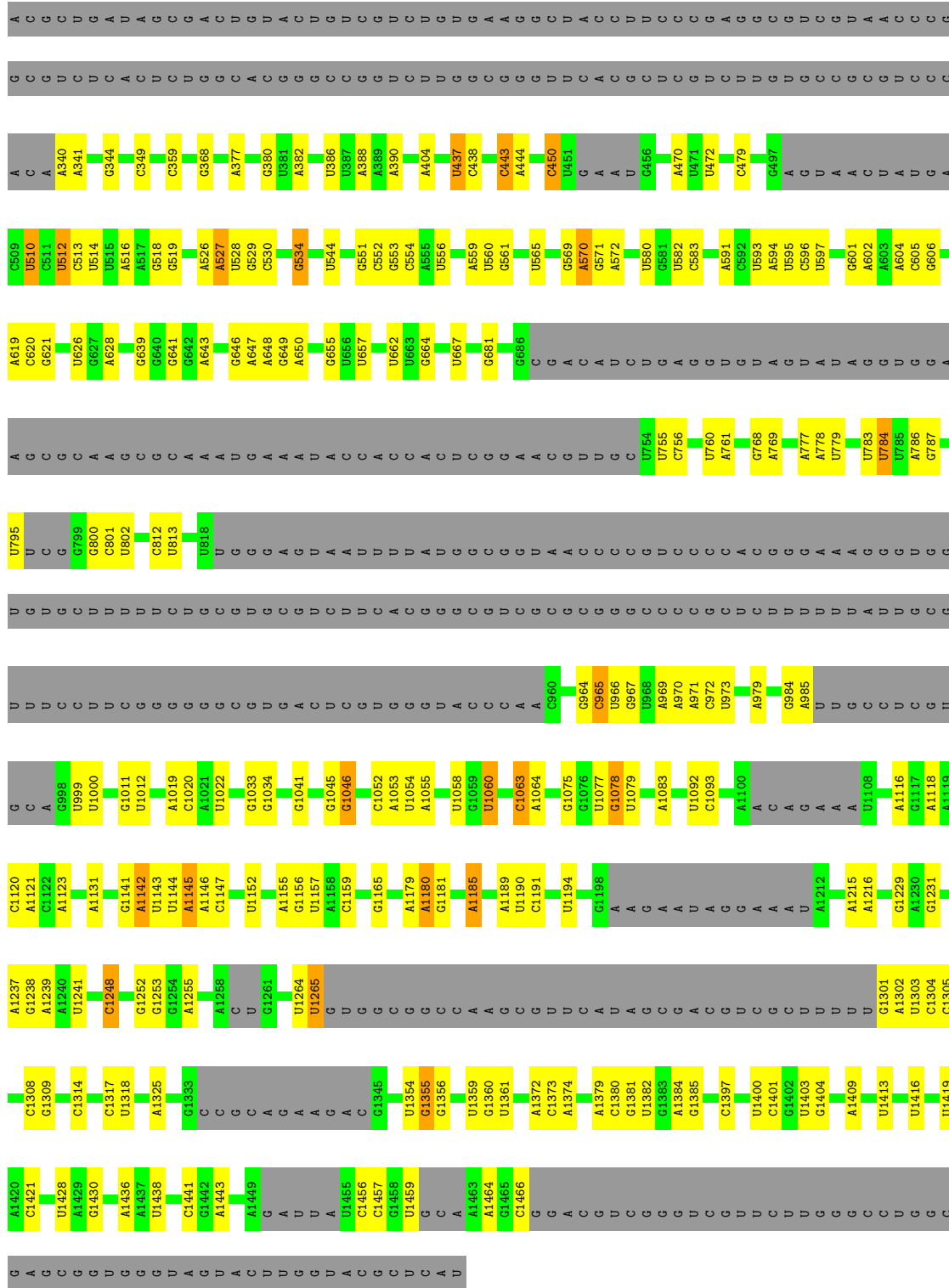


● Molecule 31: 40S ribosomal protein SA



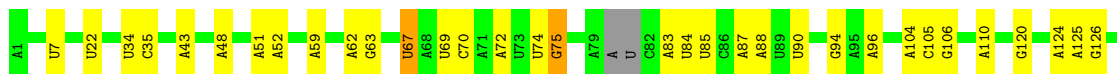
● Molecule 32: Putative 40S ribosomal protein S3





• Molecule 38: 5.8S_rRNA_chain_7

Chain 7: 72% 22% • 5%

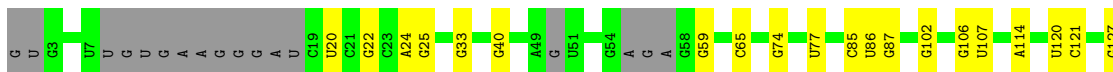




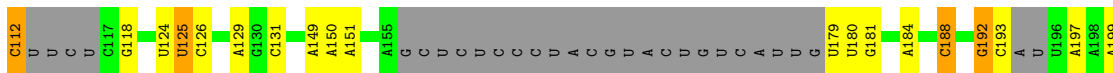
• Molecule 39: SR4_chain_5



• Molecule 40: SR2_chain_4

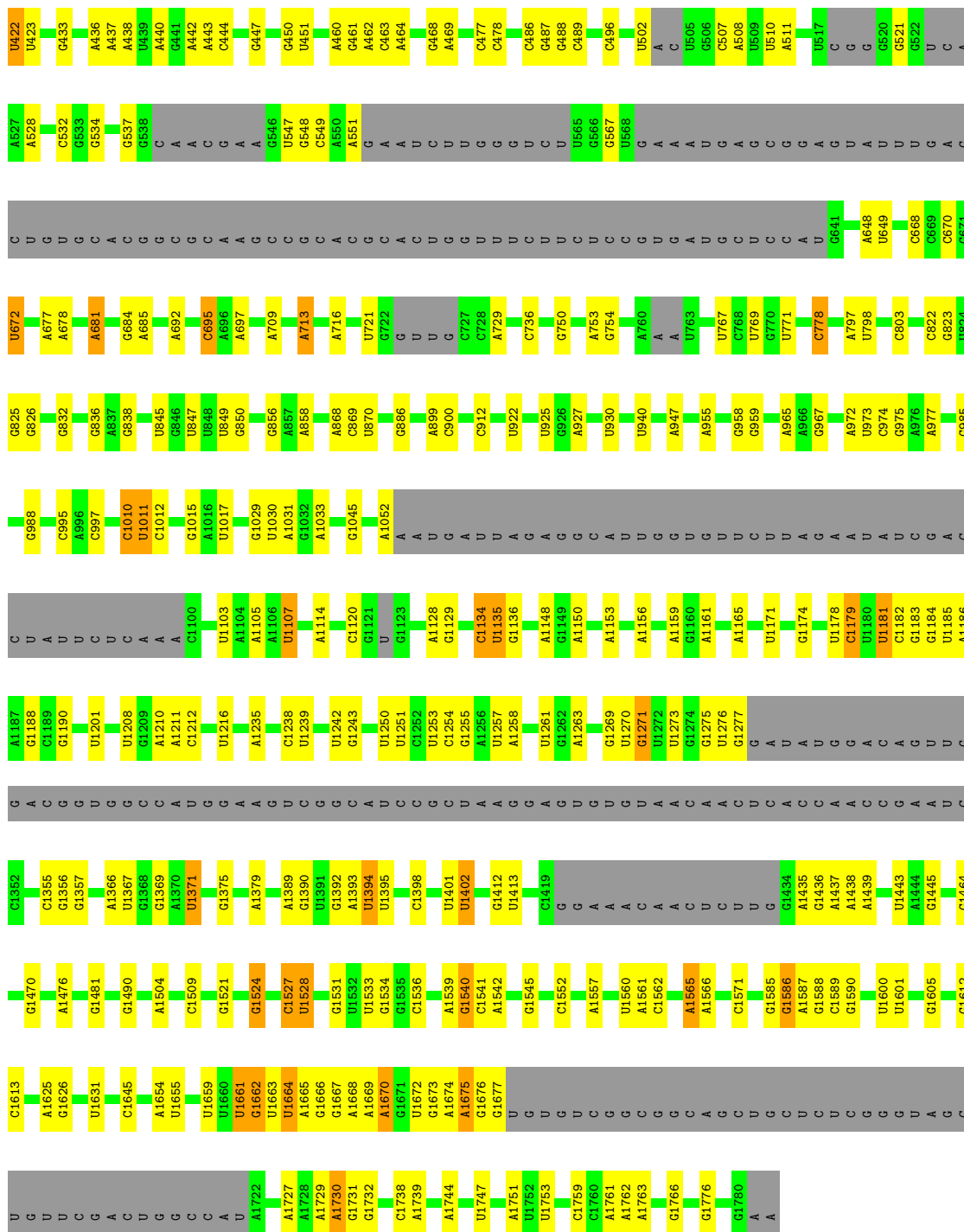


• Molecule 41: SR1_chain_3



• Molecule 42: LSUa_rRNA_chain_1



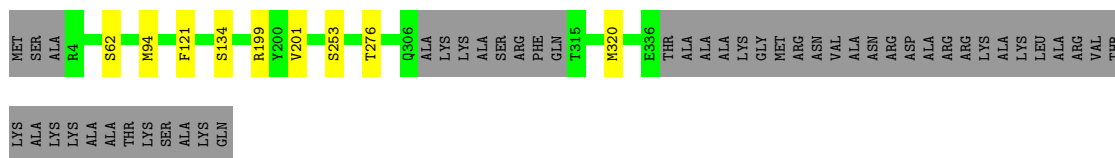
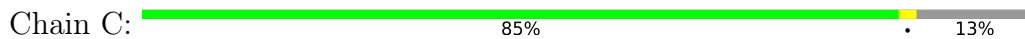


• Molecule 43: Putative ribosomal protein L3



MET	LYS	R209	R26	K170	R209	S217	I287	K310	D327	R402	LYS	GLU	ARG	ALA	ALA	ALA	ALA	ALA	LYS
-----	-----	------	-----	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

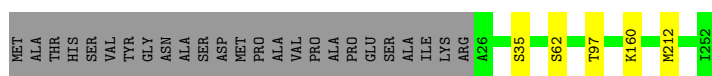
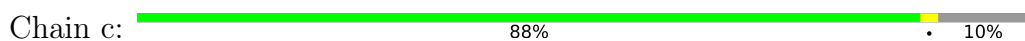
• Molecule 44: Putative ribosomal protein L1a



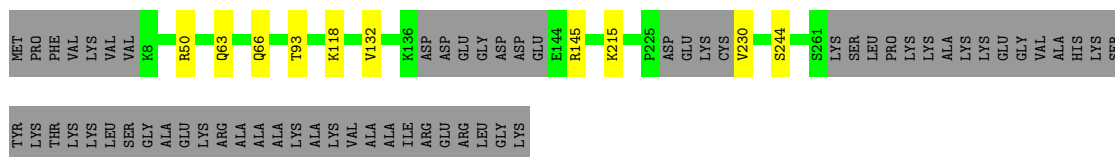
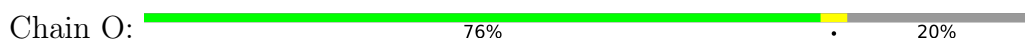
- Molecule 45: Putative 60S ribosomal protein L2



- Molecule 46: uL30_chain_c



- Molecule 47: Putative 60S ribosomal protein L5



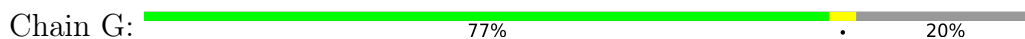
- Molecule 48: Ribosomal protein L15

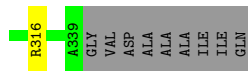


- Molecule 49: Putative 60S ribosomal protein L13a



- Molecule 50: 60S ribosomal protein L7a





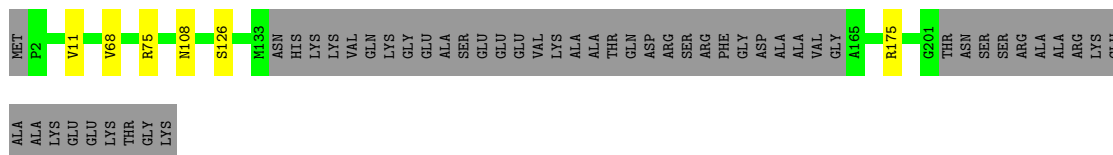
- Molecule 51: 60S ribosomal protein L18



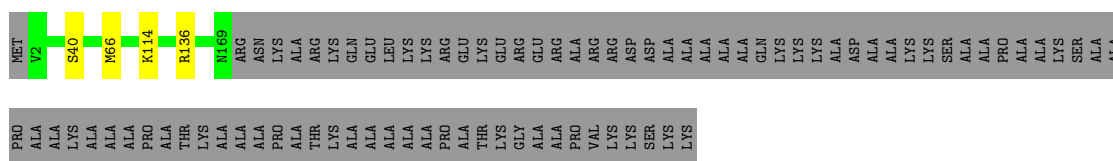
- Molecule 52: 60S ribosomal protein L18a



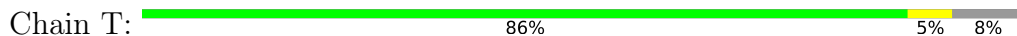
- Molecule 53: eL13_chain_I



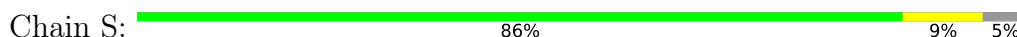
- Molecule 54: Putative 60S ribosomal protein L19



- Molecule 55: Putative 60S ribosomal protein L17



- Molecule 56: Putative 60S ribosomal protein L21





- Molecule 57: Putative 60S ribosomal protein L27A/L29

Chain L: 96%



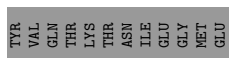
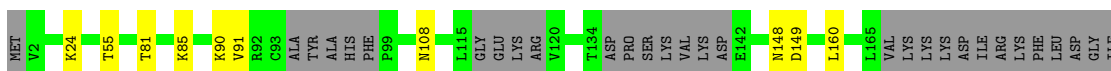
- Molecule 58: Putative 60S ribosomal protein L6

Chain F: 67% 6% 27%



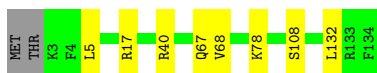
- Molecule 59: Putative 60S ribosomal protein L9

Chain E: 73% 5% 22%



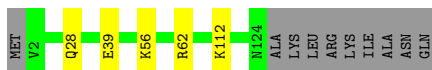
- Molecule 60: 60S ribosomal protein L27

Chain Y: 93% 6%



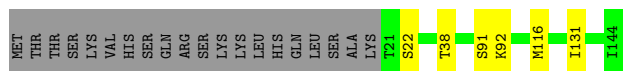
- Molecule 61: 60S ribosomal protein L32

Chain f: 89% 8%



- Molecule 62: Putative ribosomal protein l35a

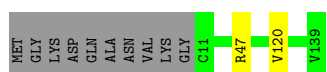
Chain g: 82% 14%



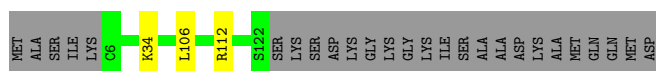
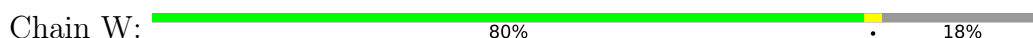
• Molecule 63: Putative 60S ribosomal protein L35



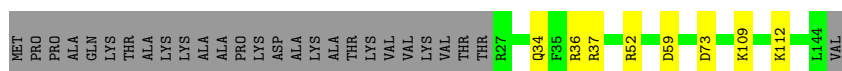
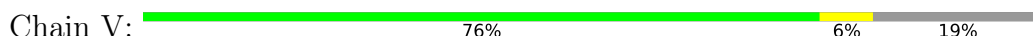
• Molecule 64: Putative 60S ribosomal protein L23



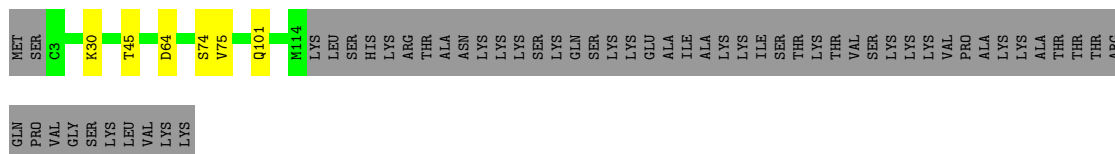
• Molecule 65: Putative 60S ribosomal protein L26



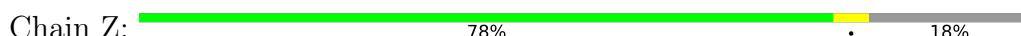
• Molecule 66: Putative 60S ribosomal protein L23a



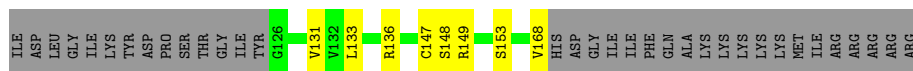
• Molecule 67: Putative 60S ribosomal protein L34



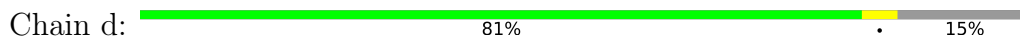
• Molecule 68: Putative 60S ribosomal protein L28



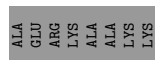
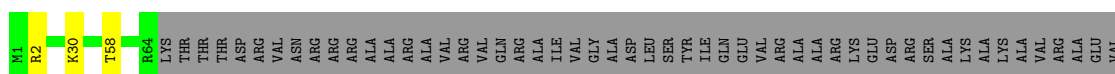
• Molecule 69: Putative 40S ribosomal protein L14



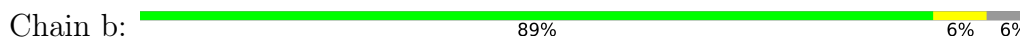
• Molecule 76: 60S ribosomal protein L30



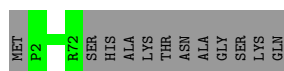
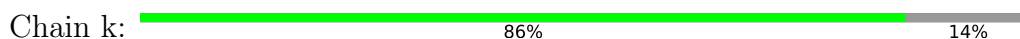
• Molecule 77: Putative ribosomal protein L24



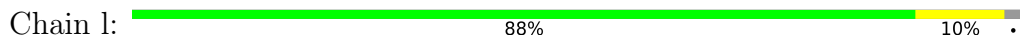
• Molecule 78: 60S ribosomal protein L29



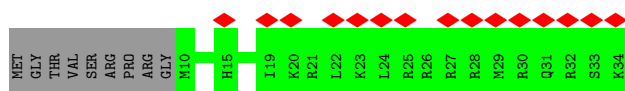
• Molecule 79: Putative ribosomal protein L38



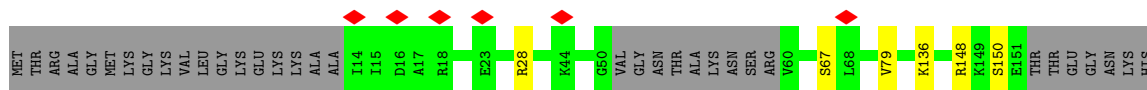
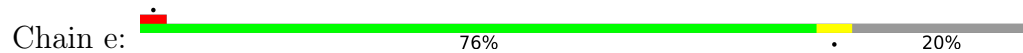
• Molecule 80: Putative 60S ribosomal protein L39



• Molecule 81: 60S ribosomal protein L41



• Molecule 82: Putative 60S ribosomal subunit protein L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	742580	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.85, 0.85, 0.85	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, OMC, OMG, MG, OMU, K, ZN, 5MC, PSU, NA, C4J, G7M

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	SD	0.26	0/1374	0.56	0/1850
2	SE	0.29	0/2104	0.55	0/2834
3	SF	0.26	0/1589	0.50	0/2152
4	SG	0.26	0/1836	0.57	0/2462
5	SH	0.35	0/1426	0.51	0/1919
6	SI	0.26	0/1613	0.51	0/2179
7	SJ	0.28	0/1034	0.51	0/1386
8	SK	0.27	0/1475	0.59	0/1978
9	SL	0.34	0/1132	0.49	0/1522
10	SM	0.29	0/817	0.58	1/1109 (0.1%)
11	SN	0.60	2/813 (0.2%)	0.97	4/1103 (0.4%)
12	SO	0.32	0/989	0.56	0/1333
13	SP	0.27	0/1148	0.52	0/1538
14	SR	0.34	0/1099	0.55	0/1477
15	SS	0.35	0/422	0.54	0/565
16	ST	0.30	0/1163	0.57	0/1560
17	SU	0.29	0/1245	0.51	0/1677
18	SV	0.32	0/584	0.51	0/777
19	SW	0.33	0/885	0.52	0/1197
20	SX	0.35	0/1121	0.53	0/1512
21	SY	0.65	2/631 (0.3%)	0.90	3/863 (0.3%)
22	SZ	0.39	1/991 (0.1%)	0.68	2/1324 (0.2%)
23	Sa	0.35	0/554	0.56	0/745
24	Sb	0.32	0/676	0.56	0/906
25	Sc	0.27	0/637	0.53	0/862
26	Sd	0.32	0/388	0.58	0/517
27	Se	0.24	0/355	0.49	0/474
28	Sg	0.31	0/2225	0.52	1/3035 (0.0%)
29	S1	0.50	0/38833	0.90	117/60463 (0.2%)
30	SA	0.28	0/1677	0.54	0/2260
31	SB	0.24	0/1629	0.50	0/2215
32	SC	0.30	0/1551	0.53	0/2080

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sh	0.26	0/676	0.53	0/920
34	S4	0.51	0/399	0.91	1/618 (0.2%)
35	8	0.63	0/2829	0.87	1/4405 (0.0%)
36	6	0.76	0/1484	1.03	6/2306 (0.3%)
37	2	1.01	0/21251	1.00	56/33095 (0.2%)
38	7	1.04	0/3723	0.95	5/5795 (0.1%)
39	5	1.01	0/2340	1.00	6/3640 (0.2%)
40	4	0.95	0/3746	0.93	1/5829 (0.0%)
41	3	0.86	0/3605	0.97	14/5602 (0.2%)
42	1	1.06	0/34332	0.99	79/53510 (0.1%)
43	B	0.47	0/3026	0.60	0/4105
44	C	0.46	0/2391	0.57	0/3249
45	A	0.49	0/1893	0.59	0/2556
46	c	0.48	0/1812	0.56	0/2440
47	O	0.35	0/1798	0.52	0/2435
48	M	0.53	0/1732	0.61	0/2316
49	H	0.46	0/1724	0.60	1/2330 (0.0%)
50	G	0.42	0/1660	0.57	0/2241
51	P	0.50	0/1537	0.61	0/2057
52	R	0.45	0/1433	0.54	0/1943
53	I	0.43	0/1328	0.57	0/1792
54	Q	0.41	0/1307	0.57	0/1751
55	T	0.53	0/1241	0.58	0/1665
56	S	0.43	0/1190	0.54	0/1609
57	L	0.50	0/1141	0.57	0/1525
58	F	0.39	0/1051	0.54	0/1434
59	E	0.26	0/1042	0.49	0/1418
60	Y	0.42	0/1029	0.55	0/1389
61	f	0.56	0/1013	0.60	0/1358
62	g	0.55	0/1010	0.67	0/1360
63	a	0.39	0/965	0.56	0/1295
64	J	0.45	0/950	0.57	0/1291
65	W	0.41	0/941	0.60	0/1257
66	V	0.44	0/932	0.53	0/1259
67	h	0.45	0/903	0.62	0/1207
68	Z	0.38	0/905	0.56	0/1221
69	K	0.36	0/897	0.53	0/1220
70	j	0.58	0/673	0.69	0/899
71	i	0.35	0/668	0.54	0/889
72	U	0.33	0/803	0.56	0/1082
73	p	0.44	0/649	0.54	0/864
74	o	0.46	0/670	0.63	0/897
75	D	0.27	0/658	0.51	0/889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	d	0.36	0/617	0.46	0/848
77	X	0.47	0/569	0.58	0/767
78	b	0.39	0/531	0.55	0/712
79	k	0.36	0/515	0.52	0/699
80	l	0.54	0/453	0.58	0/606
81	n	0.25	0/159	0.49	0/215
82	e	0.43	0/1117	0.55	0/1505
All	All	0.71	5/193334 (0.0%)	0.83	298/284189 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	SY	46	PRO	CG-CD	-14.00	1.04	1.50
11	SN	95	PRO	CG-CD	-12.66	1.08	1.50
22	SZ	35	PRO	CG-CD	-7.35	1.26	1.50
11	SN	95	PRO	N-CD	5.65	1.55	1.47
21	SY	46	PRO	N-CD	5.45	1.55	1.47

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1265	U	O5'-P-OP2	-24.45	81.36	110.70
11	SN	95	PRO	N-CD-CG	-18.11	76.04	103.20
21	SY	46	PRO	N-CD-CG	-17.03	77.65	103.20
37	2	1264	PSU	O3'-P-O5'	14.59	131.71	104.00
11	SN	95	PRO	CA-N-CD	-13.50	92.60	111.50
37	2	1264	PSU	OP2-P-O3'	-12.21	78.34	105.20
11	SN	95	PRO	CA-CB-CG	-11.84	81.50	104.00
22	SZ	35	PRO	CA-N-CD	-11.74	95.06	111.50
42	1	1185	U	P-O3'-C3'	-10.79	106.75	119.70
29	S1	1834	G	P-O3'-C3'	-10.57	107.02	119.70
29	S1	2062	G	P-O3'-C3'	-10.50	107.09	119.70
29	S1	607	PSU	P-O3'-C3'	-10.27	107.38	119.70
29	S1	2058	G	P-O3'-C3'	-10.23	107.42	119.70
29	S1	512	A2M	P-O3'-C3'	-10.15	107.51	119.70
37	2	472	PSU	P-O3'-C3'	-10.11	107.56	119.70
29	S1	2059	C	P-O3'-C3'	-10.11	107.57	119.70
37	2	1403	PSU	P-O3'-C3'	-10.09	107.59	119.70
37	2	71	OMG	P-O3'-C3'	-9.90	107.82	119.70
29	S1	2050	U	P-O3'-C3'	-9.78	107.97	119.70
29	S1	2048	PSU	P-O3'-C3'	-9.78	107.97	119.70
29	S1	1247	U	P-O3'-C3'	-9.61	108.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1246	PSU	P-O3'-C3'	-9.59	108.19	119.70
42	1	1184	G	P-O3'-C3'	-9.58	108.20	119.70
29	S1	2055	A	P-O3'-C3'	-9.55	108.24	119.70
29	S1	1264	C	P-O3'-C3'	-9.54	108.25	119.70
29	S1	1620	G	OP2-P-O3'	9.54	126.19	105.20
42	1	1661	U	P-O3'-C3'	-9.53	108.26	119.70
42	1	1730	A	P-O3'-C3'	-9.50	108.30	119.70
29	S1	1642	C	P-O3'-C3'	-9.48	108.32	119.70
29	S1	35	U	P-O3'-C3'	-9.46	108.35	119.70
29	S1	673	G	P-O3'-C3'	-9.45	108.36	119.70
29	S1	33	PSU	P-O3'-C3'	-9.39	108.43	119.70
39	5	106	G	N7-C8-N9	9.39	117.79	113.10
39	5	106	G	C8-N9-C4	-9.38	102.65	106.40
29	S1	656	G	P-O3'-C3'	-9.38	108.45	119.70
29	S1	2166	A	P-O3'-C3'	-9.32	108.52	119.70
29	S1	1533	PSU	P-O3'-C3'	-9.30	108.53	119.70
29	S1	1839	G	P-O3'-C3'	-9.30	108.54	119.70
29	S1	2046	PSU	P-O3'-C3'	-9.29	108.55	119.70
42	1	239	PSU	P-O3'-C3'	-9.29	108.55	119.70
29	S1	653	A	P-O3'-C3'	-9.29	108.56	119.70
29	S1	1147	A	P-O3'-C3'	-9.27	108.57	119.70
42	1	1664	PSU	P-O3'-C3'	-9.22	108.64	119.70
42	1	1531	G	P-O3'-C3'	-9.20	108.66	119.70
29	S1	2063	U	P-O3'-C3'	-9.19	108.67	119.70
29	S1	1531	G	P-O3'-C3'	-9.17	108.70	119.70
29	S1	575	C	P-O3'-C3'	-9.13	108.74	119.70
21	SY	46	PRO	CA-CB-CG	-9.13	86.66	104.00
29	S1	1841	PSU	P-O3'-C3'	-9.12	108.76	119.70
21	SY	46	PRO	CA-N-CD	-9.12	98.74	111.50
37	2	1144	PSU	P-O3'-C3'	-9.11	108.77	119.70
29	S1	515	G	P-O3'-C3'	-9.10	108.78	119.70
29	S1	609	PSU	P-O3'-C3'	-9.04	108.85	119.70
42	1	1017	PSU	P-O3'-C3'	-9.03	108.86	119.70
38	7	69	PSU	P-O3'-C3'	-9.02	108.88	119.70
37	2	1060	PSU	P-O3'-C3'	-9.01	108.89	119.70
29	S1	1156	PSU	P-O3'-C3'	-9.01	108.89	119.70
42	1	1533	PSU	P-O3'-C3'	-8.94	108.97	119.70
42	1	447	G	O4'-C1'-N9	8.94	115.35	108.20
29	S1	1154	A	P-O3'-C3'	-8.93	108.99	119.70
37	2	597	PSU	P-O3'-C3'	-8.92	108.99	119.70
29	S1	1539	PSU	P-O3'-C3'	-8.91	109.01	119.70
29	S1	572	A	P-O3'-C3'	-8.87	109.05	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	1179	C	P-O3'-C3'	-8.86	109.06	119.70
29	S1	573	C	P-O3'-C3'	-8.83	109.10	119.70
29	S1	1619	G	P-O3'-C3'	-8.74	109.21	119.70
29	S1	2146	U	P-O3'-C3'	-8.73	109.22	119.70
37	2	1058	PSU	P-O3'-C3'	-8.73	109.22	119.70
38	7	70	C	P-O3'-C3'	-8.70	109.26	119.70
41	3	34	C	C2-N1-C1'	8.66	128.32	118.80
29	S1	1842	C	P-O3'-C3'	-8.65	109.32	119.70
29	S1	1641	U	P-O3'-C3'	-8.64	109.33	119.70
29	S1	1192	PSU	P-O3'-C3'	-8.61	109.37	119.70
22	SZ	35	PRO	N-CD-CG	-8.60	90.30	103.20
29	S1	2147	A	P-O3'-C3'	-8.59	109.40	119.70
37	2	1303	PSU	P-O3'-C3'	-8.54	109.45	119.70
37	2	1401	C	P-O3'-C3'	-8.49	109.52	119.70
29	S1	1146	G	P-O3'-C3'	-8.47	109.53	119.70
29	S1	560	G	P-O3'-C3'	-8.46	109.56	119.70
42	1	1528	PSU	P-O3'-C3'	-8.38	109.65	119.70
37	2	78	PSU	P-O3'-C3'	-8.36	109.67	119.70
29	S1	2057	C	P-O3'-C3'	-8.35	109.68	119.70
38	7	67	U	P-O3'-C3'	-8.33	109.70	119.70
37	2	1179	A	P-O3'-C3'	-8.29	109.75	119.70
29	S1	1623	OMG	P-O3'-C3'	-8.25	109.80	119.70
37	2	1301	G	P-O3'-C3'	-8.24	109.82	119.70
42	1	451	U	P-O3'-C3'	-8.19	109.87	119.70
29	S1	576	A	P-O3'-C3'	-8.18	109.89	119.70
29	S1	1148	G	P-O3'-C3'	-8.13	109.94	119.70
29	S1	1643	G	P-O3'-C3'	-8.13	109.94	119.70
42	1	1534	G	P-O3'-C3'	-8.13	109.95	119.70
41	3	34	C	N1-C2-O2	8.11	123.77	118.90
29	S1	1263	C	P-O3'-C3'	-8.09	110.00	119.70
29	S1	1244	G	P-O3'-C3'	-8.05	110.03	119.70
41	3	34	C	N3-C2-O2	-8.05	116.26	121.90
29	S1	1273	A	P-O3'-C3'	-8.03	110.07	119.70
29	S1	2054	C	P-O3'-C3'	-8.02	110.08	119.70
29	S1	1510	C	N3-C2-O2	-8.01	116.29	121.90
29	S1	1832	C	P-O3'-C3'	-8.01	110.09	119.70
29	S1	654	A	P-O3'-C3'	-7.99	110.11	119.70
42	1	1732	G	P-O3'-C3'	-7.99	110.11	119.70
29	S1	672	G	P-O3'-C3'	-7.95	110.16	119.70
42	1	1181	PSU	P-O3'-C3'	-7.89	110.23	119.70
29	S1	1261	G	P-O3'-C3'	-7.88	110.24	119.70
29	S1	510	G	P-O3'-C3'	-7.86	110.27	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1271	C	P-O3'-C3'	-7.84	110.29	119.70
29	S1	651	U	P-O3'-C3'	-7.82	110.31	119.70
29	S1	2167	C	P-O3'-C3'	-7.82	110.32	119.70
29	S1	1176	A	P-O3'-C3'	-7.80	110.34	119.70
38	7	72	A	P-O3'-C3'	-7.80	110.34	119.70
37	2	591	A2M	P-O3'-C3'	-7.79	110.35	119.70
42	1	1186	A	P-O3'-C3'	-7.79	110.35	119.70
29	S1	1157	C	P-O3'-C3'	-7.76	110.39	119.70
42	1	1600	U	C2-N1-C1'	7.71	126.96	117.70
37	2	75	C	P-O3'-C3'	-7.66	110.51	119.70
37	2	76	A	P-O3'-C3'	-7.63	110.54	119.70
42	1	450	G	P-O3'-C3'	-7.61	110.57	119.70
42	1	437	A	OP1-P-OP2	-7.60	108.20	119.60
29	S1	516	A	P-O3'-C3'	-7.57	110.62	119.70
37	2	965	C	C2-N1-C1'	7.53	127.09	118.80
29	S1	2051	A	P-O3'-C3'	-7.45	110.76	119.70
29	S1	2165	A	P-O3'-C3'	-7.41	110.81	119.70
42	1	685	A	P-O3'-C3'	-7.39	110.83	119.70
42	1	1541	C	P-O3'-C3'	-7.38	110.84	119.70
11	SN	95	PRO	CB-CG-CD	7.37	135.26	106.50
29	S1	1510	C	C6-N1-C2	-7.36	117.36	120.30
29	S1	1262	U	P-O3'-C3'	-7.35	110.88	119.70
29	S1	1510	C	C2-N1-C1'	7.33	126.86	118.80
42	1	237	U	P-O3'-C3'	-7.30	110.94	119.70
37	2	91	C	C6-N1-C2	-7.30	117.38	120.30
29	S1	1274	A	P-O3'-C3'	-7.22	111.04	119.70
29	S1	1620	G	P-O3'-C3'	-7.21	111.05	119.70
37	2	1190	U	N3-C2-O2	-7.17	117.18	122.20
29	S1	1832	C	OP2-P-O3'	7.15	120.93	105.20
42	1	670	C	P-O3'-C3'	-7.14	111.14	119.70
29	S1	2052	C	P-O3'-C3'	-7.13	111.14	119.70
29	S1	1272	A	P-O3'-C3'	-7.11	111.16	119.70
37	2	91	C	N3-C2-O2	-7.10	116.93	121.90
37	2	595	U	P-O3'-C3'	-7.09	111.19	119.70
29	S1	509	G	OP1-P-OP2	-6.99	109.11	119.60
42	1	436	A	OP1-P-O3'	6.98	120.56	105.20
29	S1	1956	C	N1-C2-O2	6.96	123.08	118.90
37	2	1191	C	N3-C2-O2	-6.94	117.04	121.90
42	1	672	PSU	P-O3'-C3'	-6.94	111.38	119.70
37	2	1191	C	C6-N1-C2	-6.91	117.54	120.30
41	3	125	U	O4'-C1'-N1	6.87	113.70	108.20
42	1	1731	G	P-O3'-C3'	-6.87	111.46	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	886	G	O4'-C1'-N9	6.85	113.68	108.20
29	S1	1177	A	P-O3'-C3'	-6.85	111.48	119.70
29	S1	1174	C	P-O3'-C3'	-6.84	111.49	119.70
37	2	470	A	P-O3'-C3'	-6.83	111.50	119.70
29	S1	1835	U	P-O3'-C3'	-6.81	111.53	119.70
42	1	420	C	P-O3'-C3'	-6.80	111.54	119.70
29	S1	1655	U	P-O3'-C3'	-6.79	111.56	119.70
29	S1	1657	PSU	P-O3'-C3'	-6.78	111.56	119.70
37	2	605	C	P-O3'-C3'	-6.78	111.57	119.70
29	S1	1510	C	N1-C2-O2	6.76	122.96	118.90
41	3	34	C	C6-N1-C2	-6.75	117.60	120.30
29	S1	115	C	OP1-P-OP2	-6.74	109.49	119.60
42	1	973	U	C2-N1-C1'	6.73	125.78	117.70
42	1	1135	U	C2-N1-C1'	6.73	125.77	117.70
42	1	1670	A	P-O3'-C3'	-6.73	111.63	119.70
37	2	593	PSU	P-O3'-C3'	-6.72	111.63	119.70
42	1	1015	G	P-O3'-C3'	-6.68	111.69	119.70
39	5	106	G	C5-N7-C8	-6.66	100.97	104.30
37	2	965	C	N1-C2-O2	6.64	122.88	118.90
41	3	192	G	O4'-C1'-N9	6.62	113.49	108.20
29	S1	34	G	P-O3'-C3'	-6.58	111.80	119.70
37	2	1191	C	C2-N1-C1'	6.55	126.01	118.80
42	1	1542	A	P-O3'-C3'	-6.53	111.86	119.70
42	1	40	C	C6-N1-C2	-6.53	117.69	120.30
37	2	1145	A	P-O3'-C3'	-6.49	111.92	119.70
29	S1	1956	C	C2-N1-C1'	6.48	125.93	118.80
37	2	1142	A	P-O3'-C3'	-6.48	111.92	119.70
41	3	131	C	C2-N1-C1'	6.40	125.84	118.80
29	S1	1640	G	P-O3'-C3'	-6.40	112.02	119.70
42	1	778	C	N3-C2-O2	-6.39	117.43	121.90
29	S1	514	C	P-O3'-C3'	-6.38	112.04	119.70
37	2	1355	G	O4'-C1'-N9	6.32	113.25	108.20
42	1	1135	U	N1-C2-O2	6.25	127.18	122.80
42	1	1394	U	C2-N1-C1'	6.25	125.19	117.70
29	S1	1537	U	P-O3'-C3'	-6.20	112.26	119.70
29	S1	2061	5MC	P-O3'-C3'	-6.20	112.26	119.70
42	1	1669	A	P-O3'-C3'	-6.13	112.35	119.70
37	2	1404	G	P-O3'-C3'	-6.10	112.38	119.70
42	1	1588	G	O4'-C1'-N9	6.10	113.08	108.20
29	S1	1874	U	C2-N1-C1'	6.08	125.00	117.70
29	S1	1956	C	N3-C2-O2	-6.03	117.68	121.90
37	2	1190	U	C2-N1-C1'	6.02	124.93	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	3	188	C	C2-N1-C1'	5.98	125.38	118.80
28	Sg	300	ASP	CB-CG-OD2	5.97	123.67	118.30
37	2	479	C	N3-C2-O2	-5.97	117.72	121.90
42	1	1662	G	C3'-C2'-C1'	-5.93	96.75	101.50
29	S1	1178	C	P-O3'-C3'	-5.91	112.61	119.70
42	1	684	G	P-O3'-C3'	-5.89	112.64	119.70
29	S1	1151	G	P-O3'-C3'	-5.88	112.64	119.70
29	S1	354	C	C2-N1-C1'	5.86	125.25	118.80
42	1	1183	G	P-O3'-C3'	-5.84	112.69	119.70
37	2	1180	A	P-O3'-C3'	-5.83	112.71	119.70
38	7	164	U	C2-N1-C1'	5.82	124.68	117.70
36	6	6	G	N3-C4-C5	5.79	131.50	128.60
37	2	784	U	C2-N1-C1'	5.79	124.65	117.70
42	1	1759	C	C2-N1-C1'	5.79	125.17	118.80
42	1	1601	U	C2-N1-C1'	5.77	124.62	117.70
42	1	240	U	P-O3'-C3'	-5.76	112.78	119.70
42	1	1178	U	P-O3'-C3'	-5.75	112.80	119.70
29	S1	2148	G	P-O3'-C3'	-5.73	112.83	119.70
37	2	965	C	C6-N1-C1'	-5.72	113.93	120.80
42	1	1552	C	OP1-P-OP2	-5.72	111.02	119.60
41	3	34	C	C6-N1-C1'	-5.64	114.03	120.80
37	2	965	C	N3-C2-O2	-5.63	117.96	121.90
42	1	1271	G	N3-C2-N2	-5.62	115.96	119.90
42	1	736	C	C2-N1-C1'	5.62	124.98	118.80
37	2	1304	C	P-O3'-C3'	-5.60	112.98	119.70
40	4	33	G	O4'-C1'-N9	5.59	112.67	108.20
42	1	1729	A	P-O3'-C3'	-5.59	112.99	119.70
34	S4	70	C	C2-N1-C1'	5.58	124.93	118.80
41	3	179	U	N3-C2-O2	-5.57	118.30	122.20
36	6	7	A	O4'-C1'-N9	5.57	112.65	108.20
29	S1	2145	A	P-O3'-C3'	-5.56	113.03	119.70
42	1	713	A	O4'-C1'-N9	5.51	112.61	108.20
41	3	76	C	C2-N1-C1'	5.49	124.84	118.80
37	2	1063	C	C2-N1-C1'	5.49	124.83	118.80
42	1	1585	G	O4'-C1'-N9	5.49	112.59	108.20
42	1	419	A	P-O3'-C3'	-5.48	113.12	119.70
42	1	736	C	C6-N1-C2	-5.48	118.11	120.30
29	S1	657	C	P-O3'-C3'	-5.48	113.13	119.70
29	S1	1212	C	C2-N1-C1'	5.47	124.82	118.80
37	2	606	G	P-O3'-C3'	-5.46	113.14	119.70
37	2	450	C	C2-N1-C1'	5.46	124.81	118.80
42	1	869	C	C6-N1-C2	-5.45	118.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1150	U	P-O3'-C3'	-5.45	113.16	119.70
42	1	1565	A	C4-N9-C1'	5.42	136.06	126.30
41	3	188	C	N1-C2-O2	5.39	122.14	118.90
39	5	106	G	C6-C5-N7	-5.39	127.17	130.40
42	1	1600	U	C5-C6-N1	5.38	125.39	122.70
29	S1	508	A	OP2-P-O3'	5.37	117.02	105.20
42	1	736	C	N3-C2-O2	-5.37	118.14	121.90
42	1	100	G	O4'-C1'-N9	5.37	112.49	108.20
49	H	167	LYS	CA-C-N	5.36	129.00	117.20
42	1	100	G	C8-N9-C1'	-5.36	120.03	127.00
37	2	479	C	C2-N1-C1'	5.35	124.68	118.80
29	S1	655	U	P-O3'-C3'	-5.34	113.29	119.70
37	2	784	U	N3-C2-O2	-5.34	118.46	122.20
37	2	479	C	N1-C2-O2	5.33	122.10	118.90
37	2	802	U	N3-C2-O2	-5.32	118.47	122.20
42	1	100	G	C4-N9-C1'	5.32	133.42	126.50
42	1	191	U	O4'-C1'-N1	5.31	112.45	108.20
42	1	1255	G	N7-C8-N9	5.31	115.75	113.10
29	S1	1530	G	P-O3'-C3'	-5.31	113.33	119.70
37	2	784	U	N1-C2-O2	5.30	126.51	122.80
42	1	1394	U	N1-C2-O2	5.30	126.51	122.80
29	S1	1108	A	P-O3'-C3'	5.30	126.06	119.70
29	S1	1173	A	P-O3'-C3'	-5.30	113.34	119.70
29	S1	1973	C	C2-N1-C1'	5.29	124.62	118.80
42	1	1586	G	P-O3'-C3'	5.29	126.05	119.70
35	8	39	C	C2-N1-C1'	5.29	124.62	118.80
41	3	112	C	N1-C2-O2	5.29	122.07	118.90
42	1	1135	U	N3-C2-O2	-5.28	118.50	122.20
42	1	1212	C	C2-N1-C1'	5.26	124.59	118.80
42	1	1134	C	P-O3'-C3'	5.25	126.00	119.70
37	2	1063	C	C6-N1-C2	-5.24	118.20	120.30
29	S1	1153	A	P-O3'-C3'	-5.23	113.43	119.70
29	S1	652	U	P-O3'-C3'	-5.22	113.43	119.70
39	5	106	G	C4-N9-C1'	5.22	133.28	126.50
42	1	1394	U	N3-C2-O2	-5.21	118.55	122.20
37	2	1400	U	P-O3'-C3'	-5.21	113.45	119.70
37	2	1264	PSU	OP1-P-O3'	5.21	116.65	105.20
37	2	569	G	N3-C4-C5	-5.19	126.01	128.60
36	6	65	C	N3-C2-O2	-5.18	118.27	121.90
42	1	778	C	C6-N1-C2	-5.18	118.23	120.30
29	S1	1913	C	C2-N1-C1'	5.18	124.50	118.80
42	1	1565	A	C4-C5-C6	5.18	119.59	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	6	7	A	C5-N7-C8	-5.18	101.31	103.90
42	1	778	C	C2-N1-C1'	5.17	124.49	118.80
41	3	179	U	N1-C2-O2	5.17	126.42	122.80
36	6	6	G	N3-C4-N9	-5.15	122.91	126.00
37	2	594	A	P-O3'-C3'	-5.15	113.52	119.70
29	S1	1788	U	C2-N1-C1'	5.14	123.87	117.70
29	S1	1956	C	C6-N1-C2	-5.14	118.24	120.30
29	S1	1973	C	N3-C2-O2	-5.14	118.30	121.90
42	1	1571	C	C6-N1-C2	-5.14	118.24	120.30
29	S1	978	C	N3-C2-O2	-5.13	118.31	121.90
42	1	217	A	OP2-P-O3'	5.13	116.48	105.20
37	2	1190	U	C6-N1-C2	-5.12	117.92	121.00
42	1	1134	C	OP1-P-O3'	5.11	116.44	105.20
29	S1	1987	G	O4'-C1'-N9	5.11	112.29	108.20
36	6	67	C	N3-C2-O2	-5.11	118.33	121.90
10	SM	108	ASP	CB-CG-OD1	5.10	122.89	118.30
39	5	4	C	C2-N1-C1'	5.10	124.41	118.80
29	S1	1973	C	N1-C2-O2	5.07	121.94	118.90
29	S1	574	C	P-O3'-C3'	-5.06	113.62	119.70
37	2	479	C	C6-N1-C2	-5.06	118.28	120.30
42	1	1255	G	C5-N7-C8	-5.04	101.78	104.30
42	1	1675	A	O4'-C1'-N9	5.04	112.23	108.20
29	S1	1621	U	OP1-P-OP2	-5.04	112.04	119.60
29	S1	1874	U	N1-C2-O2	5.03	126.32	122.80
42	1	778	C	N1-C2-O2	5.03	121.92	118.90

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	SD	162/190 (85%)	154 (95%)	8 (5%)	0	100	100
2	SE	260/273 (95%)	254 (98%)	6 (2%)	0	100	100
3	SF	203/265 (77%)	198 (98%)	5 (2%)	0	100	100
4	SG	232/249 (93%)	231 (100%)	1 (0%)	0	100	100
5	SH	179/190 (94%)	171 (96%)	8 (4%)	0	100	100
6	SI	197/200 (98%)	191 (97%)	6 (3%)	0	100	100
7	SJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
8	SK	180/220 (82%)	178 (99%)	2 (1%)	0	100	100
9	SL	140/149 (94%)	132 (94%)	8 (6%)	0	100	100
10	SM	102/116 (88%)	99 (97%)	3 (3%)	0	100	100
11	SN	96/168 (57%)	88 (92%)	7 (7%)	1 (1%)	15	45
12	SO	132/144 (92%)	126 (96%)	6 (4%)	0	100	100
13	SP	143/143 (100%)	140 (98%)	3 (2%)	0	100	100
14	SR	134/153 (88%)	131 (98%)	3 (2%)	0	100	100
15	SS	52/57 (91%)	50 (96%)	2 (4%)	0	100	100
16	ST	138/151 (91%)	137 (99%)	1 (1%)	0	100	100
17	SU	152/173 (88%)	148 (97%)	4 (3%)	0	100	100
18	SV	69/143 (48%)	67 (97%)	2 (3%)	0	100	100
19	SW	107/152 (70%)	102 (95%)	5 (5%)	0	100	100
20	SX	138/161 (86%)	131 (95%)	7 (5%)	0	100	100
21	SY	86/164 (52%)	84 (98%)	2 (2%)	0	100	100
22	SZ	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
23	Sa	68/120 (57%)	65 (96%)	3 (4%)	0	100	100
24	Sb	82/112 (73%)	77 (94%)	5 (6%)	0	100	100
25	Sc	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
26	Sd	48/87 (55%)	45 (94%)	3 (6%)	0	100	100
27	Se	42/66 (64%)	40 (95%)	2 (5%)	0	100	100
28	Sg	281/312 (90%)	265 (94%)	16 (6%)	0	100	100
30	SA	201/264 (76%)	197 (98%)	4 (2%)	0	100	100
31	SB	208/246 (85%)	204 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	SC	199/219 (91%)	195 (98%)	4 (2%)	0	100	100
33	Sh	93/235 (40%)	84 (90%)	9 (10%)	0	100	100
43	B	397/419 (95%)	381 (96%)	16 (4%)	0	100	100
44	C	321/373 (86%)	308 (96%)	13 (4%)	0	100	100
45	A	253/260 (97%)	245 (97%)	8 (3%)	0	100	100
46	c	225/252 (89%)	215 (96%)	10 (4%)	0	100	100
47	O	238/305 (78%)	225 (94%)	13 (6%)	0	100	100
48	M	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
49	H	218/222 (98%)	215 (99%)	3 (1%)	0	100	100
50	G	208/264 (79%)	199 (96%)	9 (4%)	0	100	100
51	P	194/198 (98%)	187 (96%)	7 (4%)	0	100	100
52	R	176/179 (98%)	173 (98%)	3 (2%)	0	100	100
53	I	165/220 (75%)	157 (95%)	8 (5%)	0	100	100
54	Q	166/254 (65%)	163 (98%)	3 (2%)	0	100	100
55	T	150/166 (90%)	140 (93%)	10 (7%)	0	100	100
56	S	149/159 (94%)	145 (97%)	4 (3%)	0	100	100
57	L	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
58	F	138/195 (71%)	131 (95%)	7 (5%)	0	100	100
59	E	140/190 (74%)	134 (96%)	6 (4%)	0	100	100
60	Y	130/134 (97%)	127 (98%)	3 (2%)	0	100	100
61	f	121/133 (91%)	116 (96%)	5 (4%)	0	100	100
62	g	122/144 (85%)	114 (93%)	8 (7%)	0	100	100
63	a	121/127 (95%)	120 (99%)	1 (1%)	0	100	100
64	J	127/139 (91%)	124 (98%)	3 (2%)	0	100	100
65	W	115/143 (80%)	113 (98%)	2 (2%)	0	100	100
66	V	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
67	h	110/168 (66%)	105 (96%)	5 (4%)	0	100	100
68	Z	116/147 (79%)	114 (98%)	2 (2%)	0	100	100
69	K	115/175 (66%)	113 (98%)	2 (2%)	0	100	100
70	j	78/83 (94%)	75 (96%)	3 (4%)	0	100	100
71	i	82/105 (78%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	U	110/129 (85%)	106 (96%)	4 (4%)	0	100	100
73	p	79/106 (74%)	74 (94%)	5 (6%)	0	100	100
74	o	86/92 (94%)	78 (91%)	8 (9%)	0	100	100
75	D	94/188 (50%)	91 (97%)	3 (3%)	0	100	100
76	d	86/104 (83%)	85 (99%)	1 (1%)	0	100	100
77	X	62/124 (50%)	60 (97%)	2 (3%)	0	100	100
78	b	64/70 (91%)	64 (100%)	0	0	100	100
79	k	69/83 (83%)	67 (97%)	2 (3%)	0	100	100
80	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
81	n	23/34 (68%)	23 (100%)	0	0	100	100
82	e	145/188 (77%)	134 (92%)	11 (8%)	0	100	100
All	All	10153/12292 (83%)	9786 (96%)	366 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	SN	94	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SD	142/164 (87%)	127 (89%)	15 (11%)	6	20
2	SE	216/225 (96%)	208 (96%)	8 (4%)	34	68
3	SF	162/208 (78%)	153 (94%)	9 (6%)	21	52
4	SG	181/208 (87%)	170 (94%)	11 (6%)	18	48
5	SH	145/159 (91%)	136 (94%)	9 (6%)	18	47
6	SI	167/186 (90%)	154 (92%)	13 (8%)	12	34
7	SJ	109/111 (98%)	106 (97%)	3 (3%)	43	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	SK	141/176 (80%)	133 (94%)	8 (6%)	20	51
9	SL	112/120 (93%)	110 (98%)	2 (2%)	59	85
10	SM	92/104 (88%)	84 (91%)	8 (9%)	10	30
11	SN	82/128 (64%)	77 (94%)	5 (6%)	18	48
12	SO	95/113 (84%)	90 (95%)	5 (5%)	22	54
13	SP	115/117 (98%)	107 (93%)	8 (7%)	15	41
14	SR	111/130 (85%)	101 (91%)	10 (9%)	9	29
15	SS	41/49 (84%)	38 (93%)	3 (7%)	14	38
16	ST	122/132 (92%)	119 (98%)	3 (2%)	47	78
17	SU	126/152 (83%)	117 (93%)	9 (7%)	14	40
18	SV	62/126 (49%)	59 (95%)	3 (5%)	25	58
19	SW	87/130 (67%)	79 (91%)	8 (9%)	9	27
20	SX	109/131 (83%)	97 (89%)	12 (11%)	6	19
21	SY	62/116 (53%)	59 (95%)	3 (5%)	25	58
22	SZ	101/118 (86%)	93 (92%)	8 (8%)	12	34
23	Sa	62/95 (65%)	59 (95%)	3 (5%)	25	58
24	Sb	69/93 (74%)	58 (84%)	11 (16%)	2	7
25	Sc	62/76 (82%)	60 (97%)	2 (3%)	39	73
26	Sd	40/75 (53%)	36 (90%)	4 (10%)	7	23
27	Se	35/54 (65%)	33 (94%)	2 (6%)	20	51
28	Sg	226/265 (85%)	206 (91%)	20 (9%)	10	30
30	SA	178/222 (80%)	165 (93%)	13 (7%)	14	38
31	SB	165/202 (82%)	150 (91%)	15 (9%)	9	28
32	SC	156/184 (85%)	145 (93%)	11 (7%)	14	40
33	Sh	60/177 (34%)	50 (83%)	10 (17%)	2	6
43	B	283/351 (81%)	276 (98%)	7 (2%)	47	78
44	C	222/301 (74%)	213 (96%)	9 (4%)	30	64
45	A	178/204 (87%)	174 (98%)	4 (2%)	52	81
46	c	174/209 (83%)	169 (97%)	5 (3%)	42	76
47	O	150/242 (62%)	140 (93%)	10 (7%)	16	43
48	M	173/180 (96%)	164 (95%)	9 (5%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	H	165/188 (88%)	157 (95%)	8 (5%)	25	58
50	G	162/221 (73%)	154 (95%)	8 (5%)	25	57
51	P	157/164 (96%)	151 (96%)	6 (4%)	33	67
52	R	143/159 (90%)	136 (95%)	7 (5%)	25	57
53	I	130/183 (71%)	124 (95%)	6 (5%)	27	60
54	Q	117/198 (59%)	113 (97%)	4 (3%)	37	71
55	T	127/143 (89%)	118 (93%)	9 (7%)	14	40
56	S	117/134 (87%)	103 (88%)	14 (12%)	5	15
57	L	110/114 (96%)	105 (96%)	5 (4%)	27	61
58	F	99/153 (65%)	88 (89%)	11 (11%)	6	19
59	E	92/172 (54%)	82 (89%)	10 (11%)	6	19
60	Y	96/116 (83%)	88 (92%)	8 (8%)	11	32
61	f	104/115 (90%)	99 (95%)	5 (5%)	25	58
62	g	100/121 (83%)	94 (94%)	6 (6%)	19	49
63	a	93/118 (79%)	90 (97%)	3 (3%)	39	73
64	J	93/111 (84%)	91 (98%)	2 (2%)	52	81
65	W	98/122 (80%)	95 (97%)	3 (3%)	40	74
66	V	94/124 (76%)	86 (92%)	8 (8%)	10	31
67	h	87/146 (60%)	81 (93%)	6 (7%)	15	41
68	Z	89/118 (75%)	83 (93%)	6 (7%)	16	43
69	K	80/145 (55%)	78 (98%)	2 (2%)	47	78
70	j	66/70 (94%)	61 (92%)	5 (8%)	13	36
71	i	64/88 (73%)	57 (89%)	7 (11%)	6	19
72	U	64/114 (56%)	57 (89%)	7 (11%)	6	19
73	p	61/92 (66%)	58 (95%)	3 (5%)	25	57
74	o	62/74 (84%)	56 (90%)	6 (10%)	8	25
75	D	42/162 (26%)	34 (81%)	8 (19%)	1	4
76	d	58/89 (65%)	54 (93%)	4 (7%)	15	41
77	X	58/104 (56%)	55 (95%)	3 (5%)	23	55
78	b	52/58 (90%)	48 (92%)	4 (8%)	13	35
79	k	47/74 (64%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	l	44/47 (94%)	39 (89%)	5 (11%)	5	17
81	n	8/32 (25%)	8 (100%)	0	100	100
82	e	104/158 (66%)	96 (92%)	8 (8%)	13	35
All	All	7896/10260 (77%)	7401 (94%)	495 (6%)	21	46

All (495) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SD	1	MET
1	SD	6	ASN
1	SD	21	GLU
1	SD	49	SER
1	SD	59	LEU
1	SD	67	ARG
1	SD	71	GLU
1	SD	77	ARG
1	SD	97	SER
1	SD	106	ARG
1	SD	121	VAL
1	SD	129	GLN
1	SD	151	SER
1	SD	152	GLU
1	SD	153	ARG
2	SE	15	TRP
2	SE	75[A]	ARG
2	SE	75[B]	ARG
2	SE	94	ASP
2	SE	101	ASP
2	SE	166	CYS
2	SE	173	ARG
2	SE	248	GLN
3	SF	55	VAL
3	SF	68	LEU
3	SF	77	GLN
3	SF	99	GLN
3	SF	138	ARG
3	SF	152	ARG
3	SF	168	MET
3	SF	211	SER
3	SF	234	TYR
4	SG	1	MET

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Mol	Chain	Res	Type
4	SG	4	ASN
4	SG	7	TYR
4	SG	17	GLU
4	SG	58	ASP
4	SG	97	ARG
4	SG	146	LYS
4	SG	149	ASN
4	SG	157	ARG
4	SG	168	SER
4	SG	203	ARG
5	SH	19	THR
5	SH	35	VAL
5	SH	39	SER
5	SH	48	TYR
5	SH	99	VAL
5	SH	111	SER
5	SH	126	ASP
5	SH	161	ASP
5	SH	172	ASN
6	SI	13	ARG
6	SI	20	GLU
6	SI	22	SER
6	SI	48	THR
6	SI	53	LYS
6	SI	99	GLN
6	SI	121	SER
6	SI	130	ASN
6	SI	136	SER
6	SI	141	ARG
6	SI	168	ARG
6	SI	198	SER
6	SI	199	THR
7	SJ	83	THR
7	SJ	91	LYS
7	SJ	119	ARG
8	SK	44	SER
8	SK	59	ARG
8	SK	95	THR
8	SK	100	CYS
8	SK	115	LYS
8	SK	116	HIS
8	SK	170	ARG

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Mol	Chain	Res	Type
8	SK	216	GLU
9	SL	55	MET
9	SL	104	ASN
10	SM	20	THR
10	SM	31	SER
10	SM	46	THR
10	SM	87	ASP
10	SM	100	SER
10	SM	108	ASP
10	SM	113	ILE
10	SM	115	ASP
11	SN	4	TYR
11	SN	13	VAL
11	SN	17	PHE
11	SN	23	ILE
11	SN	96	ASN
12	SO	59	ARG
12	SO	60	ASP
12	SO	73	ASP
12	SO	77	ARG
12	SO	126	THR
13	SP	33	PHE
13	SP	34	SER
13	SP	64	SER
13	SP	98	ASP
13	SP	105	PHE
13	SP	115	ILE
13	SP	126	SER
13	SP	136	GLN
14	SR	5	LEU
14	SR	11	GLN
14	SR	26	LYS
14	SR	40	ARG
14	SR	60	LEU
14	SR	61	THR
14	SR	63	GLU
14	SR	74	ASP
14	SR	93	THR
14	SR	101	SER
15	SS	4	LEU
15	SS	22	CYS
15	SS	41	ARG

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Mol	Chain	Res	Type
16	ST	3	ARG
16	ST	9	ARG
16	ST	64	LYS
17	SU	31	GLU
17	SU	55	LEU
17	SU	62	LYS
17	SU	80	VAL
17	SU	82	ARG
17	SU	92	SER
17	SU	102	ARG
17	SU	133	LYS
17	SU	153	ASN
18	SV	3	LYS
18	SV	13	SER
18	SV	33	ARG
19	SW	22	PHE
19	SW	44	VAL
19	SW	62	VAL
19	SW	74	VAL
19	SW	100	VAL
19	SW	107	HIS
19	SW	110	ASN
19	SW	113	GLU
20	SX	47	THR
20	SX	52	SER
20	SX	58	ARG
20	SX	61	GLN
20	SX	69	ARG
20	SX	109	SER
20	SX	113	LEU
20	SX	114	HIS
20	SX	136	LEU
20	SX	141	HIS
20	SX	151	VAL
20	SX	154	ARG
21	SY	43	ASN
21	SY	65	SER
21	SY	75	HIS
22	SZ	13	ARG
22	SZ	30	VAL
22	SZ	33	ASN
22	SZ	44	GLN

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Mol	Chain	Res	Type
22	SZ	60	SER
22	SZ	62	VAL
22	SZ	103	PHE
22	SZ	107	ARG
23	Sa	40	VAL
23	Sa	85	ARG
23	Sa	93	SER
24	Sb	34	LYS
24	Sb	38	VAL
24	Sb	40	ARG
24	Sb	44	ARG
24	Sb	45	ARG
24	Sb	68	MET
24	Sb	71	LEU
24	Sb	72	TYR
24	Sb	73	MET
24	Sb	75	GLN
24	Sb	79	ILE
25	Sc	61	SER
25	Sc	82	ARG
26	Sd	23	VAL
26	Sd	28	LYS
26	Sd	32	ARG
26	Sd	74	SER
27	Se	10	ARG
27	Se	39	LYS
28	Sg	1	MET
28	Sg	39	ILE
28	Sg	46	ASP
28	Sg	95	ARG
28	Sg	115	PHE
28	Sg	128	ASP
28	Sg	134	TRP
28	Sg	136	VAL
28	Sg	139	GLU
28	Sg	167	VAL
28	Sg	174	ASN
28	Sg	187	GLU
28	Sg	199	THR
28	Sg	214	LYS
28	Sg	234	VAL
28	Sg	248	PHE

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Mol	Chain	Res	Type
28	Sg	260	VAL
28	Sg	265	SER
28	Sg	281	GLU
28	Sg	282	CYS
30	SA	31	ASP
30	SA	37	ASN
30	SA	61	LEU
30	SA	62	ARG
30	SA	96	ARG
30	SA	115	LEU
30	SA	116	LEU
30	SA	118	LYS
30	SA	136	THR
30	SA	154	ARG
30	SA	192	ARG
30	SA	196	SER
30	SA	197	ASP
31	SB	10	VAL
31	SB	12	ARG
31	SB	14	LYS
31	SB	31	ARG
31	SB	38	LYS
31	SB	56	MET
31	SB	59	GLU
31	SB	134	HIS
31	SB	141	SER
31	SB	144	ASN
31	SB	153	THR
31	SB	154	ASP
31	SB	158	GLU
31	SB	192	ILE
31	SB	195	SER
32	SC	45	THR
32	SC	46	GLU
32	SC	75	ARG
32	SC	92	VAL
32	SC	106	PHE
32	SC	147	LYS
32	SC	155	TYR
32	SC	173	HIS
32	SC	180	CYS
32	SC	208	THR

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Mol	Chain	Res	Type
32	SC	211	GLU
33	Sh	154	MET
33	Sh	162	VAL
33	Sh	163	GLN
33	Sh	172	PHE
33	Sh	174	TYR
33	Sh	202	VAL
33	Sh	207	ARG
33	Sh	212	LEU
33	Sh	221	VAL
33	Sh	226	HIS
43	B	26	ARG
43	B	170	LYS
43	B	209	ARG
43	B	217	SER
43	B	287	ILE
43	B	310	LYS
43	B	327	ASP
44	C	62	SER
44	C	94	MET
44	C	121	PHE
44	C	134	SER
44	C	199	ARG
44	C	201	VAL
44	C	253	SER
44	C	276	THR
44	C	320	MET
45	A	60	ARG
45	A	96	LEU
45	A	188	ARG
45	A	245	ARG
46	c	35	SER
46	c	62	SER
46	c	97	THR
46	c	160	LYS
46	c	212	MET
47	O	50	ARG
47	O	63	GLN
47	O	66	GLN
47	O	93	THR
47	O	118	LYS
47	O	132	VAL

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Mol	Chain	Res	Type
47	O	145	ARG
47	O	215	LYS
47	O	230	VAL
47	O	244	SER
48	M	31	ARG
48	M	43	THR
48	M	60	CYS
48	M	83	LYS
48	M	126	THR
48	M	135	VAL
48	M	166	SER
48	M	189	ARG
48	M	193	ARG
49	H	64	THR
49	H	77	ARG
49	H	82	THR
49	H	95	SER
49	H	119	SER
49	H	136	ARG
49	H	169	SER
49	H	199	SER
50	G	124	ASP
50	G	160	LEU
50	G	172	ARG
50	G	177	LYS
50	G	178	LEU
50	G	230	LYS
50	G	288	VAL
50	G	316	ARG
51	P	115	SER
51	P	118	GLN
51	P	139	THR
51	P	144	TYR
51	P	162	SER
51	P	192	ARG
52	R	7	ARG
52	R	18	SER
52	R	75	ASN
52	R	89	TYR
52	R	97	ARG
52	R	114	SER
52	R	175	ARG

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Mol	Chain	Res	Type
53	I	11	VAL
53	I	68	VAL
53	I	75	ARG
53	I	108	ASN
53	I	126	SER
53	I	175	ARG
54	Q	40	SER
54	Q	66	MET
54	Q	114	LYS
54	Q	136	ARG
55	T	13	LYS
55	T	19	VAL
55	T	20	SER
55	T	22	LEU
55	T	43	LYS
55	T	57	CYS
55	T	85	ARG
55	T	125	MET
55	T	148	LEU
56	S	4	SER
56	S	9	SER
56	S	43	VAL
56	S	55	LYS
56	S	83	ARG
56	S	90	CYS
56	S	98	LYS
56	S	111	GLN
56	S	115	TYR
56	S	119	LYS
56	S	148	ARG
56	S	150	VAL
56	S	152	ASP
56	S	153	TYR
57	L	8	CYS
57	L	9	ARG
57	L	26	ARG
57	L	30	SER
57	L	103	SER
58	F	23	SER
58	F	32	SER
58	F	70	LYS
58	F	84	VAL

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Mol	Chain	Res	Type
58	F	91	VAL
58	F	95	SER
58	F	144	THR
58	F	146	VAL
58	F	154	GLN
58	F	161	LEU
58	F	174	LYS
59	E	24	LYS
59	E	55	THR
59	E	81	THR
59	E	85	LYS
59	E	90	LYS
59	E	91	VAL
59	E	108	ASN
59	E	148	ASN
59	E	149	ASP
59	E	160	LEU
60	Y	5	LEU
60	Y	17	ARG
60	Y	40	ARG
60	Y	67	GLN
60	Y	68	VAL
60	Y	78	LYS
60	Y	108	SER
60	Y	132	LEU
61	f	28	GLN
61	f	39	GLU
61	f	56	LYS
61	f	62	ARG
61	f	112	LYS
62	g	22	SER
62	g	38	THR
62	g	91	SER
62	g	92	LYS
62	g	116	MET
62	g	131	ILE
63	a	21	THR
63	a	30	SER
63	a	68	SER
64	J	47	ARG
64	J	120	VAL
65	W	34	LYS

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Mol	Chain	Res	Type
65	W	106	LEU
65	W	112	ARG
66	V	34	GLN
66	V	36	ARG
66	V	37	ARG
66	V	52	ARG
66	V	59	ASP
66	V	73	ASP
66	V	109	LYS
66	V	112	LYS
67	h	30	LYS
67	h	45	THR
67	h	64	ASP
67	h	74	SER
67	h	75	VAL
67	h	101	GLN
68	Z	6	ASP
68	Z	53	VAL
68	Z	62	CYS
68	Z	72	ASN
68	Z	75	ARG
68	Z	123	LYS
69	K	3	SER
69	K	22	ARG
70	j	14	ARG
70	j	43	SER
70	j	58	ARG
70	j	63	ARG
70	j	69	VAL
71	i	5	THR
71	i	21	THR
71	i	49	ASP
71	i	69	GLU
71	i	84	THR
71	i	89	LYS
71	i	91	SER
72	U	30	CYS
72	U	46	ASN
72	U	75	ASN
72	U	81	THR
72	U	102	ASP
72	U	103	LEU

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Mol	Chain	Res	Type
72	U	116	THR
73	p	38	ARG
73	p	55	LYS
73	p	77	CYS
74	o	7	LYS
74	o	13	ARG
74	o	32	SER
74	o	41	PHE
74	o	57	CYS
74	o	58	ASP
75	D	131	VAL
75	D	133	LEU
75	D	136	ARG
75	D	147	CYS
75	D	148	SER
75	D	149	ARG
75	D	153	SER
75	D	168	VAL
76	d	10	ASP
76	d	89	THR
76	d	95	THR
76	d	97	VAL
77	X	2	ARG
77	X	30	LYS
77	X	58	THR
78	b	4	SER
78	b	13	SER
78	b	18	ARG
78	b	37	TRP
80	l	5	LYS
80	l	31	THR
80	l	38	ASN
80	l	39	GLU
80	l	51	TYR
82	e	28	ARG
82	e	67	SER
82	e	79	VAL
82	e	136	LYS
82	e	148	ARG
82	e	150	SER
82	e	172	SER
82	e	180	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
7	SJ	98	GLN
12	SO	31	ASN
44	C	115	ASN
58	F	191	HIS
60	Y	117	GLN
70	j	77	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	S1	1627/2204 (73%)	310 (19%)	19 (1%)
34	S4	15/20 (75%)	6 (40%)	0
35	8	118/123 (95%)	18 (15%)	0
36	6	61/73 (83%)	30 (49%)	2 (3%)
37	2	933/1522 (61%)	185 (19%)	12 (1%)
38	7	160/171 (93%)	32 (20%)	1 (0%)
39	5	94/135 (69%)	18 (19%)	0
40	4	153/183 (83%)	23 (15%)	1 (0%)
41	3	148/216 (68%)	29 (19%)	6 (4%)
42	1	1446/1782 (81%)	308 (21%)	20 (1%)
All	All	4755/6429 (73%)	959 (20%)	61 (1%)

All (959) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	S1	3	U
29	S1	17	C
29	S1	25	C
29	S1	26	A
29	S1	33	PSU
29	S1	34	G
29	S1	42	G
29	S1	43	A
29	S1	45	U
29	S1	47	A
29	S1	68	A
29	S1	73	A
29	S1	104	PSU
29	S1	105	C
29	S1	112	A

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Mol	Chain	Res	Type
29	S1	117	G
29	S1	128	C
29	S1	143	A
29	S1	145	A
29	S1	146	U
29	S1	151	U
29	S1	152	A
29	S1	158	G
29	S1	162	A
29	S1	165	G
29	S1	172	U
29	S1	173	A
29	S1	176	A
29	S1	184	C
29	S1	197	U
29	S1	235	C
29	S1	249	A
29	S1	251	A
29	S1	275	A
29	S1	278	A
29	S1	281	A
29	S1	282	C
29	S1	284	C
29	S1	285	A
29	S1	287	C
29	S1	308	C
29	S1	309	G
29	S1	310	U
29	S1	313	G
29	S1	315	A
29	S1	316	A
29	S1	320	G
29	S1	323	U
29	S1	329	C
29	S1	330	G
29	S1	349	C
29	S1	356	A
29	S1	358	C
29	S1	360	G
29	S1	364	G
29	S1	365	U
29	S1	381	G

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Mol	Chain	Res	Type
29	S1	382	A
29	S1	404	C
29	S1	443	A
29	S1	444	A
29	S1	445	U
29	S1	447	G
29	S1	467	C
29	S1	469	G
29	S1	473	G
29	S1	477	G
29	S1	479	A
29	S1	480	A
29	S1	481	A
29	S1	482	U
29	S1	483	U
29	S1	487	C
29	S1	488	A
29	S1	495	A
29	S1	499	A
29	S1	501	A
29	S1	503	C
29	S1	511	C
29	S1	512	A2M
29	S1	516	A
29	S1	523	A
29	S1	525	A
29	S1	553	U
29	S1	554	U
29	S1	560	G
29	S1	575	C
29	S1	587	A
29	S1	600	OMG
29	S1	606	G
29	S1	607	PSU
29	S1	608	C
29	S1	610	G
29	S1	614	C
29	S1	617	G
29	S1	628	A
29	S1	629	A
29	S1	631	U
29	S1	643	A

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Mol	Chain	Res	Type
29	S1	656	G
29	S1	660	U
29	S1	664	U
29	S1	668	A2M
29	S1	669	A
29	S1	671	G
29	S1	672	G
29	S1	688	G
29	S1	689	U
29	S1	751	G
29	S1	758	G
29	S1	771	G
29	S1	773	A
29	S1	784	C
29	S1	786	G
29	S1	787	G
29	S1	788	A
29	S1	789	G
29	S1	792	G
29	S1	793	G
29	S1	811	C
29	S1	814	G
29	S1	815	U
29	S1	817	A
29	S1	819	G
29	S1	820	C
29	S1	821	A
29	S1	842	U
29	S1	844	U
29	S1	845	U
29	S1	856	A
29	S1	863	C
29	S1	866	G
29	S1	867	A
29	S1	875	A
29	S1	876	G
29	S1	883	G
29	S1	884	A
29	S1	886	U
29	S1	887	U
29	S1	912	A
29	S1	915	A

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Mol	Chain	Res	Type
29	S1	916	G
29	S1	917	C
29	S1	953	U
29	S1	955	A
29	S1	956	A
29	S1	957	G
29	S1	958	G
29	S1	978	C
29	S1	990	U
29	S1	991	G
29	S1	1103	G
29	S1	1105	A
29	S1	1109	A
29	S1	1110	G
29	S1	1111	G
29	S1	1119	U
29	S1	1123	G
29	S1	1129	A
29	S1	1139	G
29	S1	1145	A
29	S1	1146	G
29	S1	1150	U
29	S1	1155	U
29	S1	1156	PSU
29	S1	1157	C
29	S1	1160	A
29	S1	1161	G
29	S1	1162	A
29	S1	1176	A
29	S1	1178	C
29	S1	1180	A
29	S1	1181	C
29	S1	1182	A
29	S1	1199	A
29	S1	1207	U
29	S1	1213	A
29	S1	1235	A
29	S1	1239	A
29	S1	1240	A
29	S1	1244	G
29	S1	1251	A
29	S1	1262	U

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Mol	Chain	Res	Type
29	S1	1263	C
29	S1	1273	A
29	S1	1274	A
29	S1	1275	C
29	S1	1289	A
29	S1	1290	A
29	S1	1423	G
29	S1	1442	U
29	S1	1443	U
29	S1	1444	G
29	S1	1449	U
29	S1	1452	A
29	S1	1458	A
29	S1	1466	G
29	S1	1490	A
29	S1	1502	G
29	S1	1503	A
29	S1	1504	A
29	S1	1510	C
29	S1	1537	U
29	S1	1542	C
29	S1	1544	5MC
29	S1	1546	A
29	S1	1548	A
29	S1	1550	OMG
29	S1	1551	G
29	S1	1552	G
29	S1	1554	A
29	S1	1565	A
29	S1	1569	G
29	S1	1570	G
29	S1	1573	A
29	S1	1582	A
29	S1	1592	U
29	S1	1593	G
29	S1	1595	G
29	S1	1597	G
29	S1	1598	U
29	S1	1602	U
29	S1	1603	U
29	S1	1606	C
29	S1	1608	A

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Mol	Chain	Res	Type
29	S1	1611	C
29	S1	1613	C
29	S1	1621	U
29	S1	1622	G
29	S1	1624	U
29	S1	1638	U
29	S1	1653	U
29	S1	1658	U
29	S1	1659	U
29	S1	1660	G
29	S1	1661	G
29	S1	1666	U
29	S1	1667	U
29	S1	1668	C
29	S1	1673	A
29	S1	1677	G
29	S1	1699	A
29	S1	1706	A
29	S1	1773	U
29	S1	1774	U
29	S1	1789	U
29	S1	1790	C
29	S1	1796	U
29	S1	1797	A
29	S1	1816	U
29	S1	1828	A
29	S1	1829	OMG
29	S1	1833	U
29	S1	1834	G
29	S1	1835	U
29	S1	1836	G
29	S1	1837	A
29	S1	1840	C
29	S1	1842	C
29	S1	1846	A
29	S1	1847	A
29	S1	1848	U
29	S1	1849	G
29	S1	1861	A
29	S1	1862	C
29	S1	1872	A
29	S1	1874	U

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Mol	Chain	Res	Type
29	S1	1891	A
29	S1	1919	C
29	S1	1924	G
29	S1	1929	G
29	S1	1931	G
29	S1	1932	A
29	S1	1933	A
29	S1	1934	A
29	S1	1939	G
29	S1	1944	C
29	S1	1948	U
29	S1	1949	A
29	S1	1955	A
29	S1	1956	C
29	S1	1957	U
29	S1	1973	C
29	S1	1977	U
29	S1	1978	A
29	S1	1979	OMU
29	S1	1982	G
29	S1	1988	C
29	S1	1989	A
29	S1	2004	G
29	S1	2010	G
29	S1	2012	A
29	S1	2021	A2M
29	S1	2027	G
29	S1	2053	A
29	S1	2054	C
29	S1	2055	A
29	S1	2056	C
29	S1	2059	C
29	S1	2086	A
29	S1	2099	G
29	S1	2100	A
29	S1	2151	OMG
29	S1	2165	A
29	S1	2169	A
29	S1	2170	G
29	S1	2172	U
29	S1	2186	C
29	S1	2195	G

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Mol	Chain	Res	Type
29	S1	2196	G
34	S4	3	G
34	S4	4	C
34	S4	5	G
34	S4	70	C
34	S4	73	A
34	S4	76	A
35	8	11	G
35	8	31	A
35	8	32	C
35	8	37	U
35	8	38	C
35	8	46	A
35	8	53	A
35	8	54	A
35	8	56	U
35	8	67	C
35	8	68	A
35	8	69	G
35	8	70	G
35	8	94	A
35	8	95	U
35	8	104	A
35	8	114	G
35	8	123	C
36	6	5	C
36	6	7	A
36	6	11	G
36	6	12	C
36	6	13	C
36	6	14	A
36	6	15	C
36	6	24	C
36	6	25	U
36	6	26	G
36	6	30	C
36	6	31	U
36	6	32	U
36	6	33	G
36	6	51	A
36	6	52	G
36	6	53	U

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Mol	Chain	Res	Type
36	6	54	A
36	6	55	U
36	6	56	A
36	6	57	U
36	6	58	U
36	6	60	A
36	6	64	U
36	6	65	C
36	6	67	C
36	6	68	A
36	6	69	A
36	6	72	C
36	6	73	A
37	2	6	A
37	2	22	A
37	2	25	A
37	2	29	C
37	2	50	A
37	2	54	U
37	2	61	C
37	2	63	U
37	2	64	A
37	2	68	A
37	2	69	A
37	2	72	G
37	2	75	C
37	2	76	A
37	2	78	PSU
37	2	90	G
37	2	91	C
37	2	135	A
37	2	136	A
37	2	341	A
37	2	344	G
37	2	349	C
37	2	368	G
37	2	377	A
37	2	380	G
37	2	386	U
37	2	388	A
37	2	390	A
37	2	404	A

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Mol	Chain	Res	Type
37	2	437	PSU
37	2	438	C
37	2	443	OMC
37	2	444	A
37	2	450	C
37	2	510	PSU
37	2	512	PSU
37	2	513	C
37	2	514	U
37	2	516	A
37	2	518	G
37	2	519	G
37	2	526	A
37	2	527	A2M
37	2	528	U
37	2	529	G
37	2	530	C
37	2	534	OMG
37	2	544	U
37	2	551	G
37	2	552	C
37	2	553	G
37	2	554	C
37	2	556	U
37	2	559	A
37	2	561	G
37	2	565	U
37	2	570	A2M
37	2	571	G
37	2	580	U
37	2	582	U
37	2	596	C
37	2	601	G
37	2	602	A
37	2	619	A
37	2	620	C
37	2	621	G
37	2	639	G
37	2	643	A
37	2	647	A
37	2	648	A
37	2	649	G

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Mol	Chain	Res	Type
37	2	650	A
37	2	657	U
37	2	664	G
37	2	681	G
37	2	755	U
37	2	756	C
37	2	760	U
37	2	761	A
37	2	768	G
37	2	769	A
37	2	777	A
37	2	778	A
37	2	779	U
37	2	783	U
37	2	784	U
37	2	786	A
37	2	787	G
37	2	795	U
37	2	800	G
37	2	801	C
37	2	812	C
37	2	813	U
37	2	964	G
37	2	965	C
37	2	966	U
37	2	967	G
37	2	969	A
37	2	970	A
37	2	971	A
37	2	972	C
37	2	973	U
37	2	979	A
37	2	984	G
37	2	985	A
37	2	999	U
37	2	1000	U
37	2	1011	G
37	2	1012	U
37	2	1019	A
37	2	1020	C
37	2	1022	U
37	2	1033	G

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Mol	Chain	Res	Type
37	2	1034	G
37	2	1041	G
37	2	1045	G
37	2	1046	OMG
37	2	1053	A
37	2	1054	U
37	2	1055	A
37	2	1060	PSU
37	2	1063	C
37	2	1064	A
37	2	1075	G
37	2	1078	OMG
37	2	1079	U
37	2	1083	A
37	2	1093	C
37	2	1116	A
37	2	1118	A
37	2	1120	C
37	2	1121	A
37	2	1123	A
37	2	1131	A
37	2	1141	G
37	2	1142	A
37	2	1143	U
37	2	1145	A
37	2	1146	A
37	2	1147	C
37	2	1155	A
37	2	1156	G
37	2	1157	U
37	2	1165	G
37	2	1180	A
37	2	1181	G
37	2	1185	A2M
37	2	1189	A
37	2	1215	A
37	2	1216	A
37	2	1237	A
37	2	1238	G
37	2	1239	A
37	2	1241	U
37	2	1248	OMC

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Mol	Chain	Res	Type
37	2	1252	G
37	2	1255	A
37	2	1265	U
37	2	1302	A
37	2	1305	C
37	2	1309	G
37	2	1314	C
37	2	1325	A
37	2	1355	G
37	2	1356	G
37	2	1373	C
37	2	1374	A
37	2	1379	A
37	2	1380	C
37	2	1381	G
37	2	1385	G
37	2	1409	A
37	2	1416	U
37	2	1421	C
37	2	1428	U
37	2	1430	G
37	2	1436	A
37	2	1438	U
37	2	1441	C
37	2	1443	A
37	2	1456	C
37	2	1457	C
37	2	1459	U
37	2	1464	A
37	2	1466	C
38	7	22	U
38	7	34	U
38	7	35	C
38	7	48	A
38	7	51	A
38	7	52	A
38	7	59	A
38	7	62	A
38	7	63	G
38	7	67	U
38	7	75	OMG
38	7	83	A

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Mol	Chain	Res	Type
38	7	84	U
38	7	85	U
38	7	87	A
38	7	88	A
38	7	90	U
38	7	94	G
38	7	96	A
38	7	104	A
38	7	105	C
38	7	106	G
38	7	110	A
38	7	120	G
38	7	124	A
38	7	125	A
38	7	126	G
38	7	135	U
38	7	136	G
38	7	157	U
38	7	158	U
38	7	169	A
39	5	5	G
39	5	14	C
39	5	23	G
39	5	28	U
39	5	38	G
39	5	43	G
39	5	67	G
39	5	70	U
39	5	71	C
39	5	87	U
39	5	99	G
39	5	101	A
39	5	106	G
39	5	108	G
39	5	109	G
39	5	113	G
39	5	125	U
39	5	134	C
40	4	20	U
40	4	22	G
40	4	24	A
40	4	25	G

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Mol	Chain	Res	Type
40	4	40	G
40	4	59	G
40	4	65	C
40	4	77	U
40	4	85	C
40	4	86	U
40	4	87	G
40	4	102	G
40	4	107	U
40	4	114	A
40	4	120	U
40	4	121	C
40	4	127	G
40	4	131	U
40	4	137	G
40	4	158	A
40	4	168	A
40	4	171	A
40	4	173	C
41	3	35	A
41	3	42	U
41	3	51	G
41	3	72	A
41	3	99	U
41	3	100	U
41	3	101	G
41	3	104	C
41	3	110	U
41	3	112	C
41	3	118	G
41	3	124	U
41	3	125	U
41	3	126	C
41	3	129	A
41	3	149	A
41	3	150	A
41	3	151	A
41	3	180	U
41	3	181	G
41	3	184	A
41	3	188	C
41	3	192	G

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Mol	Chain	Res	Type
41	3	193	C
41	3	197	A
41	3	199	A
41	3	201	C
41	3	202	A
41	3	210	G
42	1	24	A
42	1	29	C
42	1	38	A
42	1	41	A
42	1	47	C
42	1	58	A
42	1	64	A
42	1	73	U
42	1	84	G
42	1	86	G
42	1	87	A
42	1	88	G
42	1	91	G
42	1	92	C
42	1	98	A
42	1	110	A
42	1	127	G
42	1	131	U
42	1	132	A
42	1	134	A
42	1	135	A
42	1	136	G
42	1	141	U
42	1	142	G
42	1	153	C
42	1	175	G
42	1	176	C
42	1	177	A
42	1	191	U
42	1	192	C
42	1	200	A
42	1	205	A
42	1	206	A
42	1	209	C
42	1	211	U
42	1	212	U

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Mol	Chain	Res	Type
42	1	213	G
42	1	214	C
42	1	215	U
42	1	217	A
42	1	218	A
42	1	219	U
42	1	220	A
42	1	223	A
42	1	230	A
42	1	231	U
42	1	237	U
42	1	238	A
42	1	250	A
42	1	251	A
42	1	255	G
42	1	256	U
42	1	257	U
42	1	258	A
42	1	261	C
42	1	266	G
42	1	267	A
42	1	273	A
42	1	279	G
42	1	280	A
42	1	283	G
42	1	292	A
42	1	293	C
42	1	294	U
42	1	301	A
42	1	305	A2M
42	1	306	G
42	1	323	U
42	1	332	A
42	1	343	U
42	1	349	U
42	1	361	A
42	1	367	A
42	1	368	G
42	1	369	A
42	1	374	G
42	1	378	A
42	1	383	U

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Mol	Chain	Res	Type
42	1	390	C
42	1	392	A
42	1	407	A2M
42	1	409	U
42	1	410	U
42	1	417	G
42	1	422	PSU
42	1	423	U
42	1	433	G
42	1	438	A
42	1	440	A
42	1	442	A
42	1	444	C
42	1	460	A
42	1	461	G
42	1	462	A
42	1	463	C
42	1	464	A
42	1	469	A
42	1	477	C
42	1	478	C
42	1	486	C
42	1	487	G
42	1	488	G
42	1	489	C
42	1	496	C
42	1	502	U
42	1	507	C
42	1	508	A
42	1	510	U
42	1	511	A
42	1	521	G
42	1	528	A
42	1	532	C
42	1	534	G
42	1	537	G
42	1	547	U
42	1	548	G
42	1	549	C
42	1	551	A
42	1	567	G
42	1	649	U

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Mol	Chain	Res	Type
42	1	668	C
42	1	672	PSU
42	1	677	A
42	1	681	A2M
42	1	692	A
42	1	695	OMC
42	1	709	A
42	1	713	A
42	1	716	A
42	1	721	U
42	1	729	A
42	1	750	G
42	1	753	A
42	1	754	G
42	1	767	U
42	1	769	U
42	1	771	U
42	1	778	C
42	1	797	A
42	1	798	U
42	1	803	C
42	1	822	C
42	1	823	G
42	1	825	G
42	1	826	G
42	1	832	G
42	1	836	G
42	1	838	G
42	1	849	U
42	1	850	G
42	1	868	A
42	1	899	A
42	1	900	C
42	1	912	C
42	1	922	U
42	1	925	U
42	1	930	U
42	1	947	A
42	1	958	G
42	1	965	A
42	1	967	G
42	1	972	A

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Mol	Chain	Res	Type
42	1	974	C
42	1	975	G
42	1	977	A
42	1	985	G
42	1	988	G
42	1	995	C
42	1	997	C
42	1	1010	OMC
42	1	1011	PSU
42	1	1012	C
42	1	1029	G
42	1	1030	U
42	1	1031	A
42	1	1033	A
42	1	1045	G
42	1	1052	A
42	1	1103	U
42	1	1105	A
42	1	1107	OMU
42	1	1114	A
42	1	1120	C
42	1	1128	A
42	1	1129	G
42	1	1135	U
42	1	1136	G
42	1	1148	A
42	1	1150	A
42	1	1153	A
42	1	1156	A
42	1	1159	A
42	1	1161	A
42	1	1165	A
42	1	1174	G
42	1	1179	C
42	1	1181	PSU
42	1	1182	C
42	1	1188	G
42	1	1201	U
42	1	1208	U
42	1	1210	A
42	1	1211	A
42	1	1216	U

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Mol	Chain	Res	Type
42	1	1235	A
42	1	1238	C
42	1	1239	U
42	1	1242	U
42	1	1243	G
42	1	1250	U
42	1	1251	U
42	1	1253	U
42	1	1254	C
42	1	1257	U
42	1	1258	A
42	1	1261	U
42	1	1263	A
42	1	1269	G
42	1	1270	U
42	1	1271	G
42	1	1273	U
42	1	1275	G
42	1	1277	G
42	1	1355	C
42	1	1357	G
42	1	1366	A
42	1	1367	U
42	1	1369	G
42	1	1371	OMU
42	1	1375	G
42	1	1379	A
42	1	1389	A
42	1	1390	G
42	1	1392	G
42	1	1394	U
42	1	1395	U
42	1	1398	C
42	1	1401	U
42	1	1402	PSU
42	1	1412	G
42	1	1413	U
42	1	1435	A
42	1	1436	G
42	1	1437	A
42	1	1438	A
42	1	1439	A

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Mol	Chain	Res	Type
42	1	1443	U
42	1	1445	G
42	1	1464	G
42	1	1470	G
42	1	1476	A
42	1	1481	G
42	1	1490	G
42	1	1504	A
42	1	1509	C
42	1	1521	G
42	1	1524	OMG
42	1	1527	OMC
42	1	1528	PSU
42	1	1536	C
42	1	1540	OMG
42	1	1545	G
42	1	1557	A
42	1	1560	U
42	1	1561	A
42	1	1562	C
42	1	1565	A
42	1	1566	A
42	1	1586	G
42	1	1587	A
42	1	1589	C
42	1	1590	G
42	1	1605	G
42	1	1612	G
42	1	1613	C
42	1	1625	A
42	1	1631	U
42	1	1645	C
42	1	1654	A
42	1	1655	U
42	1	1661	U
42	1	1662	G
42	1	1663	U
42	1	1664	PSU
42	1	1665	A
42	1	1666	G
42	1	1667	G
42	1	1668	A

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Mol	Chain	Res	Type
42	1	1670	A
42	1	1672	U
42	1	1673	G
42	1	1674	A
42	1	1675	A
42	1	1676	G
42	1	1677	G
42	1	1727	A
42	1	1730	A
42	1	1738	C
42	1	1739	A
42	1	1744	A
42	1	1747	U
42	1	1751	A
42	1	1753	U
42	1	1761	A
42	1	1762	A
42	1	1763	A
42	1	1766	G
42	1	1776	G

All (61) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	S1	33	PSU
29	S1	72	C
29	S1	234	C
29	S1	277	U
29	S1	309	G
29	S1	494	A
29	S1	607	PSU
29	S1	656	G
29	S1	916	G
29	S1	1108	A
29	S1	1145	A
29	S1	1156	PSU
29	S1	1621	U
29	S1	1667	U
29	S1	1672	C
29	S1	1833	U
29	S1	1841	PSU
29	S1	2053	A

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Mol	Chain	Res	Type
29	S1	2054	C
36	6	51	A
36	6	72	C
37	2	68	A
37	2	340	A
37	2	443	OMC
37	2	646	G
37	2	648	A
37	2	755	U
37	2	984	G
37	2	1052	C
37	2	1053	A
37	2	1092	U
37	2	1239	A
37	2	1456	C
38	7	157	U
40	4	106	G
41	3	98	C
41	3	111	A
41	3	150	A
41	3	180	U
41	3	192	G
41	3	201	C
42	1	141	U
42	1	191	U
42	1	214	C
42	1	217	A
42	1	219	U
42	1	422	PSU
42	1	443	A
42	1	468	G
42	1	510	U
42	1	648	A
42	1	947	A
42	1	1011	PSU
42	1	1134	C
42	1	1135	U
42	1	1269	G
42	1	1276	U
42	1	1356	G
42	1	1393	A
42	1	1586	G

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Mol	Chain	Res	Type
42	1	1664	PSU

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

142 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
42	PSU	1	1011	42	18,21,22	4.32	9 (50%)	22,30,33	1.96	5 (22%)
29	PSU	S1	12	29	18,21,22	4.39	7 (38%)	22,30,33	1.82	5 (22%)
37	OMC	2	1397	37	19,22,23	2.63	7 (36%)	26,31,34	0.81	0
37	A2M	2	95	37	18,25,26	3.67	7 (38%)	18,36,39	3.60	4 (22%)
37	A2M	2	1185	37	18,25,26	3.66	7 (38%)	18,36,39	3.55	4 (22%)
29	OMU	S1	1979	29	19,22,23	2.91	8 (42%)	26,31,34	1.73	5 (19%)
42	A2M	1	235	42	18,25,26	3.70	7 (38%)	18,36,39	3.74	4 (22%)
37	OMG	2	534	37	18,26,27	2.35	8 (44%)	19,38,41	1.54	5 (26%)
37	PSU	2	1264	37	18,21,22	1.48	4 (22%)	22,30,33	1.98	4 (18%)
37	A2M	2	382	37	18,25,26	3.71	7 (38%)	18,36,39	3.74	4 (22%)
42	PSU	1	672	84,42,83	18,21,22	1.44	3 (16%)	22,30,33	2.11	5 (22%)
29	OMG	S1	2151	29	18,26,27	2.48	8 (44%)	19,38,41	1.57	4 (21%)
42	PSU	1	940	42	18,21,22	3.96	8 (44%)	22,30,33	2.02	4 (18%)
42	OMC	1	1010	42	19,22,23	2.84	8 (42%)	26,31,34	0.87	1 (3%)
37	PSU	2	512	37	18,21,22	4.47	7 (38%)	22,30,33	1.84	5 (22%)
29	A2M	S1	512	29,84	18,25,26	0.96	1 (5%)	18,36,39	1.31	3 (16%)
29	PSU	S1	2046	29	18,21,22	1.44	3 (16%)	22,30,33	1.97	4 (18%)
29	OMG	S1	1865	29	18,26,27	2.48	8 (44%)	19,38,41	1.60	5 (26%)
42	A2M	1	697	42	18,25,26	3.75	8 (44%)	18,36,39	3.76	4 (22%)
42	OMG	1	1540	42,37	18,26,27	2.31	8 (44%)	19,38,41	1.60	6 (31%)
29	OMG	S1	1550	29	18,26,27	2.52	8 (44%)	19,38,41	1.56	4 (21%)
37	OMU	2	667	37	19,22,23	2.72	7 (36%)	26,31,34	1.91	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PSU	2	1354	37	18,21,22	4.21	8 (44%)	22,30,33	1.88	5 (22%)
42	OMC	1	695	42	19,22,23	2.61	7 (36%)	26,31,34	0.87	1 (3%)
42	PSU	1	239	42	18,21,22	1.40	3 (16%)	22,30,33	2.09	5 (22%)
37	5MC	2	1308	37	18,22,23	4.58	13 (72%)	26,32,35	1.34	2 (7%)
37	PSU	2	1361	37	18,21,22	4.33	8 (44%)	22,30,33	1.84	4 (18%)
37	OMU	2	1077	37	19,22,23	2.84	8 (42%)	26,31,34	1.81	5 (19%)
42	OMG	1	856	42	18,26,27	2.32	8 (44%)	19,38,41	1.69	5 (26%)
37	OMG	2	1078	37	18,26,27	2.36	8 (44%)	19,38,41	1.72	5 (26%)
37	OMC	2	1248	37	19,22,23	2.72	7 (36%)	26,31,34	0.97	1 (3%)
42	OMU	1	1107	42	19,22,23	2.83	8 (42%)	26,31,34	1.87	5 (19%)
29	PSU	S1	1566	29	18,21,22	4.40	8 (44%)	22,30,33	1.69	3 (13%)
37	PSU	2	78	37	18,21,22	1.46	4 (22%)	22,30,33	2.02	5 (22%)
37	A2M	2	527	37	18,25,26	3.79	8 (44%)	18,36,39	3.79	5 (27%)
37	PSU	2	597	37	18,21,22	1.45	3 (16%)	22,30,33	2.06	5 (22%)
37	OMG	2	1360	37	18,26,27	2.42	8 (44%)	19,38,41	1.56	4 (21%)
29	OMC	S1	1866	29	19,22,23	2.81	8 (42%)	26,31,34	0.70	0
38	A2M	7	162	42,38	18,25,26	3.64	8 (44%)	18,36,39	3.78	4 (22%)
42	OMU	1	845	42	19,22,23	2.69	6 (31%)	26,31,34	2.44	7 (26%)
37	A2M	2	1372	37	18,25,26	3.69	7 (38%)	18,36,39	4.02	4 (22%)
29	OMG	S1	1829	84,29,83	18,26,27	2.49	8 (44%)	19,38,41	1.48	4 (21%)
42	OMG	1	959[A]	42	18,26,27	2.49	8 (44%)	19,38,41	1.56	4 (21%)
42	PSU	1	1533	42,37	18,21,22	1.44	3 (16%)	22,30,33	2.15	5 (22%)
37	PSU	2	1403	37	18,21,22	1.43	3 (16%)	22,30,33	2.12	5 (22%)
38	OMG	7	75	38	18,26,27	1.04	1 (5%)	19,38,41	1.15	2 (10%)
37	A2M	2	1384	37	18,25,26	3.70	7 (38%)	18,36,39	3.68	4 (22%)
37	OMC	2	583	37	19,22,23	2.66	7 (36%)	26,31,34	0.75	0
37	PSU	2	1413	37	18,21,22	4.08	8 (44%)	22,30,33	1.89	4 (18%)
37	A2M	2	572	37	18,25,26	3.69	8 (44%)	18,36,39	3.95	5 (27%)
37	A2M	2	604	42,37	18,25,26	3.70	7 (38%)	18,36,39	3.56	4 (22%)
42	OMC	1	1527	42	19,22,23	0.88	0	26,31,34	0.90	1 (3%)
29	OMU	S1	8	29	19,22,23	2.94	8 (42%)	26,31,34	1.75	5 (19%)
37	PSU	2	1060	37	18,21,22	1.44	3 (16%)	22,30,33	2.09	5 (22%)
29	PSU	S1	1192	29	18,21,22	1.37	2 (11%)	22,30,33	2.13	5 (22%)
37	OMC	2	1159	37	19,22,23	2.69	7 (36%)	26,31,34	0.79	0
37	PSU	2	1382	86,37	18,21,22	4.20	9 (50%)	22,30,33	1.84	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PSU	2	510	37	18,21,22	4.58	9 (50%)	22,30,33	1.62	4 (18%)
37	OMG	2	655	37	18,26,27	2.34	8 (44%)	19,38,41	1.69	4 (21%)
29	PSU	S1	1539	29	18,21,22	1.43	3 (16%)	22,30,33	2.05	5 (22%)
29	PSU	S1	609	29	18,21,22	1.38	3 (16%)	22,30,33	2.03	5 (22%)
37	PSU	2	437	37	18,21,22	4.18	8 (44%)	22,30,33	1.89	5 (22%)
29	PSU	S1	1841	29	18,21,22	1.43	3 (16%)	22,30,33	2.06	5 (22%)
37	OMU	2	73	37	19,22,23	1.33	3 (15%)	26,31,34	1.84	5 (19%)
42	A2M	1	305	42	18,25,26	3.75	9 (50%)	18,36,39	4.04	6 (33%)
29	OMG	S1	600	29	18,26,27	2.52	8 (44%)	19,38,41	1.50	4 (21%)
29	A2M	S1	2021	29	18,25,26	3.64	7 (38%)	18,36,39	3.91	4 (22%)
42	OMG	1	1190	42	18,26,27	2.48	8 (44%)	19,38,41	1.66	5 (26%)
37	OMU	2	560	84,37	19,22,23	2.78	7 (36%)	26,31,34	1.77	4 (15%)
29	A2M	S1	668	29,83	18,25,26	3.66	8 (44%)	18,36,39	3.84	4 (22%)
29	OMC	S1	18	29	19,22,23	2.90	8 (42%)	26,31,34	0.75	0
42	A2M	1	858	42	18,25,26	3.69	8 (44%)	18,36,39	3.96	5 (27%)
37	A2M	2	570	42,37	18,25,26	3.74	8 (44%)	18,36,39	3.74	6 (33%)
42	OMG	1	1524	42	18,26,27	2.40	8 (44%)	19,38,41	1.78	5 (26%)
37	A2M	2	591	37	18,25,26	0.95	1 (5%)	18,36,39	1.22	2 (11%)
42	A2M	1	681	42	18,25,26	3.64	7 (38%)	18,36,39	3.69	4 (22%)
37	OMC	2	1317	37	19,22,23	2.69	7 (36%)	26,31,34	0.78	1 (3%)
37	PSU	2	472	37	18,21,22	1.40	3 (16%)	22,30,33	2.06	5 (22%)
37	PSU	2	626	37	18,21,22	4.10	8 (44%)	22,30,33	1.86	4 (18%)
37	OMG	2	1046	37	18,26,27	2.50	8 (44%)	19,38,41	1.56	5 (26%)
42	A2M	1	678	42,37	18,25,26	3.62	7 (38%)	18,36,39	3.55	4 (22%)
41	OMU	3	13	41	19,22,23	2.83	7 (36%)	26,31,34	2.24	7 (26%)
42	A2M	1	1539	42,83,37	18,25,26	3.70	7 (38%)	18,36,39	3.81	5 (27%)
29	OMC	S1	2140	29	19,22,23	2.95	8 (42%)	26,31,34	0.84	0
42	OMU	1	1371	42	19,22,23	2.87	8 (42%)	26,31,34	2.02	7 (26%)
42	PSU	1	1664	42	18,21,22	1.46	4 (22%)	22,30,33	2.11	4 (18%)
37	OMU	2	1419	37	19,22,23	2.77	7 (36%)	26,31,34	1.79	5 (19%)
42	OMU	1	847	42	19,22,23	2.74	7 (36%)	26,31,34	1.86	5 (19%)
42	OMG	1	959[B]	42	18,26,27	2.39	8 (44%)	19,38,41	1.48	5 (26%)
29	OMG	S1	1623	29	18,26,27	1.01	1 (5%)	19,38,41	1.22	2 (10%)
38	PSU	7	69	38	18,21,22	1.38	3 (16%)	22,30,33	2.16	5 (22%)
42	PSU	1	1171	42	18,21,22	4.19	9 (50%)	22,30,33	2.05	7 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PSU	2	593	37	18,21,22	1.49	3 (16%)	22,30,33	2.11	5 (22%)
42	PSU	1	1181	42	18,21,22	1.38	2 (11%)	22,30,33	2.05	5 (22%)
29	OMG	S1	1879	29	18,26,27	2.47	8 (44%)	19,38,41	1.60	4 (21%)
42	PSU	1	870	42,83	18,21,22	4.12	8 (44%)	22,30,33	1.86	4 (18%)
42	A2M	1	955	42	18,25,26	3.70	8 (44%)	18,36,39	3.65	4 (22%)
37	PSU	2	1303	37	18,21,22	1.35	2 (11%)	22,30,33	2.05	5 (22%)
37	OMU	2	1359	37	19,22,23	2.81	8 (42%)	26,31,34	1.82	4 (15%)
42	OMG	1	1626	42	18,26,27	2.26	8 (44%)	19,38,41	1.65	5 (26%)
37	OMG	2	1229	37	18,26,27	2.39	8 (44%)	19,38,41	1.67	6 (31%)
29	5MC	S1	2061	29	18,22,23	0.97	2 (11%)	26,32,35	1.22	3 (11%)
29	OMG	S1	1647	29	18,26,27	2.55	8 (44%)	19,38,41	1.58	4 (21%)
29	PSU	S1	1657	29	18,21,22	1.41	3 (16%)	22,30,33	2.07	4 (18%)
37	PSU	2	1058	37	18,21,22	1.42	3 (16%)	22,30,33	2.01	5 (22%)
37	A2M	2	628	37	18,25,26	3.69	8 (44%)	18,36,39	3.99	4 (22%)
37	PSU	2	1144	37	18,21,22	1.42	3 (16%)	22,30,33	2.08	5 (22%)
29	PSU	S1	607	29	18,21,22	1.34	2 (11%)	22,30,33	2.10	5 (22%)
42	PSU	1	1528	42	18,21,22	1.45	3 (16%)	22,30,33	2.09	5 (22%)
37	OMG	2	1253	37	18,26,27	2.30	8 (44%)	19,38,41	1.62	4 (21%)
37	OMU	2	1152	37	19,22,23	2.78	7 (36%)	26,31,34	1.80	5 (19%)
37	OMG	2	1231	37	18,26,27	2.37	8 (44%)	19,38,41	1.61	6 (31%)
29	OMU	S1	661	29	19,22,23	2.96	8 (42%)	26,31,34	1.72	5 (19%)
37	PSU	2	1318	37	18,21,22	4.09	8 (44%)	22,30,33	1.86	4 (18%)
29	PSU	S1	2048	29	18,21,22	1.42	3 (16%)	22,30,33	2.09	5 (22%)
29	PSU	S1	33	29	18,21,22	1.38	2 (11%)	22,30,33	1.98	4 (18%)
38	A2M	7	43	38	18,25,26	3.69	7 (38%)	18,36,39	3.90	4 (22%)
37	OMC	2	359	37	19,22,23	2.82	8 (42%)	26,31,34	0.71	0
38	OMU	7	7	42,38	19,22,23	2.82	7 (36%)	26,31,34	1.73	4 (15%)
37	OMC	2	443	86,37	19,22,23	2.81	8 (42%)	26,31,34	0.88	0
40	OMG	4	74	40	18,26,27	2.31	8 (44%)	19,38,41	1.62	5 (26%)
29	G7M	S1	1995	29	20,26,27	4.06	9 (45%)	17,39,42	0.98	1 (5%)
37	PSU	2	662	84,37	18,21,22	4.07	8 (44%)	22,30,33	1.78	4 (18%)
29	PSU	S1	1156	29	18,21,22	1.37	2 (11%)	22,30,33	2.10	4 (18%)
42	A2M	1	927	42	18,25,26	3.71	8 (44%)	18,36,39	3.69	4 (22%)
42	PSU	1	422	42	18,21,22	1.50	4 (22%)	22,30,33	2.20	5 (22%)
37	PSU	2	1194	37	18,21,22	4.21	8 (44%)	22,30,33	1.80	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	OMG	2	71	37	18,26,27	1.06	1 (5%)	19,38,41	1.10	2 (10%)
29	PSU	S1	104	29	18,21,22	4.45	7 (38%)	22,30,33	1.79	5 (22%)
42	OMU	1	1659	42	19,22,23	2.73	7 (36%)	26,31,34	1.75	5 (19%)
29	PSU	S1	1533	29	18,21,22	1.43	3 (16%)	22,30,33	1.99	5 (22%)
37	OMG	2	641	37	18,26,27	2.31	8 (44%)	19,38,41	1.74	5 (26%)
42	PSU	1	1017	42,83	18,21,22	1.49	4 (22%)	22,30,33	2.09	5 (22%)
29	C4J	S1	1543	29	24,29,30	2.99	9 (37%)	29,42,45	1.38	4 (13%)
42	A2M	1	407	42	18,25,26	3.71	8 (44%)	18,36,39	3.78	5 (27%)
29	PSU	S1	455	29	18,21,22	4.45	7 (38%)	22,30,33	1.77	5 (22%)
29	5MC	S1	1544	29	18,22,23	3.49	7 (38%)	26,32,35	1.01	2 (7%)
38	PSU	7	74	38	18,21,22	1.42	3 (16%)	22,30,33	2.00	5 (22%)
42	PSU	1	1402	42	18,21,22	4.17	7 (38%)	22,30,33	1.77	4 (18%)
29	OMG	S1	1478	29	18,26,27	2.45	8 (44%)	19,38,41	1.56	4 (21%)
29	OMC	S1	38	29	19,22,23	2.94	8 (42%)	26,31,34	0.75	0
29	PSU	S1	1246	29	18,21,22	1.40	2 (11%)	22,30,33	1.99	5 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	PSU	1	1011	42	-	2/7/25/26	0/2/2/2
29	PSU	S1	12	29	-	0/7/25/26	0/2/2/2
37	OMC	2	1397	37	-	0/9/27/28	0/2/2/2
37	A2M	2	95	37	-	0/5/27/28	0/3/3/3
37	A2M	2	1185	37	-	2/5/27/28	0/3/3/3
29	OMU	S1	1979	29	-	1/9/27/28	0/2/2/2
42	A2M	1	235	42	-	1/5/27/28	0/3/3/3
37	OMG	2	534	37	-	2/5/27/28	0/3/3/3
37	PSU	2	1264	37	-	0/7/25/26	0/2/2/2
37	A2M	2	382	37	-	0/5/27/28	0/3/3/3
42	PSU	1	672	84,42,83	-	2/7/25/26	0/2/2/2
29	OMG	S1	2151	29	-	2/5/27/28	0/3/3/3
42	PSU	1	940	42	-	0/7/25/26	0/2/2/2
42	OMC	1	1010	42	-	1/9/27/28	0/2/2/2
37	PSU	2	512	37	-	2/7/25/26	0/2/2/2
29	A2M	S1	512	29,84	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PSU	S1	2046	29	-	2/7/25/26	0/2/2/2
29	OMG	S1	1865	29	-	1/5/27/28	0/3/3/3
42	A2M	1	697	42	-	0/5/27/28	0/3/3/3
42	OMG	1	1540	42,37	-	2/5/27/28	0/3/3/3
29	OMG	S1	1550	29	-	2/5/27/28	0/3/3/3
37	OMU	2	667	37	-	1/9/27/28	0/2/2/2
37	PSU	2	1354	37	-	0/7/25/26	0/2/2/2
42	OMC	1	695	42	-	2/9/27/28	0/2/2/2
42	PSU	1	239	42	-	0/7/25/26	0/2/2/2
37	5MC	2	1308	37	-	4/7/25/26	0/2/2/2
37	PSU	2	1361	37	-	3/7/25/26	0/2/2/2
37	OMU	2	1077	37	-	2/9/27/28	0/2/2/2
42	OMG	1	856	42	-	0/5/27/28	0/3/3/3
37	OMG	2	1078	37	-	0/5/27/28	0/3/3/3
37	OMC	2	1248	37	-	1/9/27/28	0/2/2/2
42	OMU	1	1107	42	-	2/9/27/28	0/2/2/2
29	PSU	S1	1566	29	-	2/7/25/26	0/2/2/2
37	PSU	2	78	37	-	2/7/25/26	0/2/2/2
37	A2M	2	527	37	-	0/5/27/28	0/3/3/3
37	PSU	2	597	37	-	2/7/25/26	0/2/2/2
37	OMG	2	1360	37	-	0/5/27/28	0/3/3/3
29	OMC	S1	1866	29	-	0/9/27/28	0/2/2/2
38	A2M	7	162	42,38	-	1/5/27/28	0/3/3/3
42	OMU	1	845	42	-	2/9/27/28	0/2/2/2
37	A2M	2	1372	37	-	0/5/27/28	0/3/3/3
29	OMG	S1	1829	84,29,83	-	1/5/27/28	0/3/3/3
42	OMG	1	959[A]	42	-	2/5/27/28	0/3/3/3
42	PSU	1	1533	42,37	-	1/7/25/26	0/2/2/2
37	PSU	2	1403	37	-	0/7/25/26	0/2/2/2
38	OMG	7	75	38	-	3/5/27/28	0/3/3/3
37	A2M	2	1384	37	-	0/5/27/28	0/3/3/3
37	OMC	2	583	37	-	1/9/27/28	0/2/2/2
37	PSU	2	1413	37	-	0/7/25/26	0/2/2/2
37	A2M	2	572	37	-	0/5/27/28	0/3/3/3
37	A2M	2	604	42,37	-	1/5/27/28	0/3/3/3
42	OMC	1	1527	42	-	2/9/27/28	0/2/2/2
29	OMU	S1	8	29	-	6/9/27/28	0/2/2/2
37	PSU	2	1060	37	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PSU	S1	1192	29	-	0/7/25/26	0/2/2/2
37	OMC	2	1159	37	-	0/9/27/28	0/2/2/2
37	PSU	2	1382	86,37	-	0/7/25/26	0/2/2/2
37	PSU	2	510	37	-	5/7/25/26	0/2/2/2
37	OMG	2	655	37	-	0/5/27/28	0/3/3/3
29	PSU	S1	1539	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	609	29	-	0/7/25/26	0/2/2/2
37	PSU	2	437	37	-	2/7/25/26	0/2/2/2
29	PSU	S1	1841	29	-	3/7/25/26	0/2/2/2
37	OMU	2	73	37	-	1/9/27/28	0/2/2/2
42	A2M	1	305	42	-	1/5/27/28	0/3/3/3
29	OMG	S1	600	29	-	2/5/27/28	0/3/3/3
29	A2M	S1	2021	29	-	2/5/27/28	0/3/3/3
42	OMG	1	1190	42	-	0/5/27/28	0/3/3/3
37	OMU	2	560	84,37	-	1/9/27/28	0/2/2/2
29	A2M	S1	668	29,83	-	3/5/27/28	0/3/3/3
29	OMC	S1	18	29	-	1/9/27/28	0/2/2/2
42	A2M	1	858	42	-	0/5/27/28	0/3/3/3
37	A2M	2	570	42,37	-	3/5/27/28	0/3/3/3
42	OMG	1	1524	42	-	2/5/27/28	0/3/3/3
37	A2M	2	591	37	-	1/5/27/28	0/3/3/3
42	A2M	1	681	42	-	2/5/27/28	0/3/3/3
37	OMC	2	1317	37	-	0/9/27/28	0/2/2/2
37	PSU	2	472	37	-	0/7/25/26	0/2/2/2
37	PSU	2	626	37	-	0/7/25/26	0/2/2/2
37	OMG	2	1046	37	-	3/5/27/28	0/3/3/3
42	A2M	1	678	42,37	-	0/5/27/28	0/3/3/3
41	OMU	3	13	41	-	3/9/27/28	0/2/2/2
42	A2M	1	1539	42,83,37	-	1/5/27/28	0/3/3/3
29	OMC	S1	2140	29	-	2/9/27/28	0/2/2/2
42	OMU	1	1371	42	-	4/9/27/28	0/2/2/2
42	PSU	1	1664	42	-	2/7/25/26	0/2/2/2
37	OMU	2	1419	37	-	0/9/27/28	0/2/2/2
42	OMU	1	847	42	-	0/9/27/28	0/2/2/2
42	OMG	1	959[B]	42	-	0/5/27/28	0/3/3/3
29	OMG	S1	1623	29	-	1/5/27/28	0/3/3/3
38	PSU	7	69	38	-	0/7/25/26	0/2/2/2
42	PSU	1	1171	42	-	2/7/25/26	0/2/2/2
37	PSU	2	593	37	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	PSU	1	1181	42	-	3/7/25/26	0/2/2/2
29	OMG	S1	1879	29	-	0/5/27/28	0/3/3/3
42	PSU	1	870	42,83	-	1/7/25/26	0/2/2/2
42	A2M	1	955	42	-	0/5/27/28	0/3/3/3
37	PSU	2	1303	37	-	0/7/25/26	0/2/2/2
37	OMU	2	1359	37	-	0/9/27/28	0/2/2/2
42	OMG	1	1626	42	-	1/5/27/28	0/3/3/3
37	OMG	2	1229	37	-	0/5/27/28	0/3/3/3
29	5MC	S1	2061	29	-	0/7/25/26	0/2/2/2
29	OMG	S1	1647	29	-	0/5/27/28	0/3/3/3
29	PSU	S1	1657	29	-	2/7/25/26	0/2/2/2
37	PSU	2	1058	37	-	1/7/25/26	0/2/2/2
37	A2M	2	628	37	-	0/5/27/28	0/3/3/3
37	PSU	2	1144	37	-	2/7/25/26	0/2/2/2
29	PSU	S1	607	29	-	5/7/25/26	0/2/2/2
42	PSU	1	1528	42	-	2/7/25/26	0/2/2/2
37	OMG	2	1253	37	-	0/5/27/28	0/3/3/3
37	OMU	2	1152	37	-	0/9/27/28	0/2/2/2
37	OMG	2	1231	37	-	0/5/27/28	0/3/3/3
29	OMU	S1	661	29	-	0/9/27/28	0/2/2/2
37	PSU	2	1318	37	-	0/7/25/26	0/2/2/2
29	PSU	S1	2048	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	33	29	-	4/7/25/26	0/2/2/2
38	A2M	7	43	38	-	0/5/27/28	0/3/3/3
37	OMC	2	359	37	-	0/9/27/28	0/2/2/2
38	OMU	7	7	42,38	-	0/9/27/28	0/2/2/2
37	OMC	2	443	86,37	-	5/9/27/28	0/2/2/2
40	OMG	4	74	40	-	0/5/27/28	0/3/3/3
29	G7M	S1	1995	29	-	2/3/25/26	0/3/3/3
37	PSU	2	662	84,37	-	0/7/25/26	0/2/2/2
29	PSU	S1	1156	29	-	0/7/25/26	0/2/2/2
42	A2M	1	927	42	-	0/5/27/28	0/3/3/3
42	PSU	1	422	42	-	2/7/25/26	0/2/2/2
37	PSU	2	1194	37	-	0/7/25/26	0/2/2/2
37	OMG	2	71	37	-	1/5/27/28	0/3/3/3
29	PSU	S1	104	29	-	2/7/25/26	0/2/2/2
42	OMU	1	1659	42	-	0/9/27/28	0/2/2/2
29	PSU	S1	1533	29	-	0/7/25/26	0/2/2/2
37	OMG	2	641	37	-	0/5/27/28	0/3/3/3
42	PSU	1	1017	42,83	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	C4J	S1	1543	29	-	8/16/34/35	0/2/2/2
42	A2M	1	407	42	-	2/5/27/28	0/3/3/3
29	PSU	S1	455	29	-	3/7/25/26	0/2/2/2
29	5MC	S1	1544	29	-	2/7/25/26	0/2/2/2
38	PSU	7	74	38	-	2/7/25/26	0/2/2/2
42	PSU	1	1402	42	-	5/7/25/26	0/2/2/2
29	OMG	S1	1478	29	-	0/5/27/28	0/3/3/3
29	OMC	S1	38	29	-	0/9/27/28	0/2/2/2
29	PSU	S1	1246	29	-	0/7/25/26	0/2/2/2

All (898) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	510	PSU	C6-C5	12.06	1.49	1.35
37	2	512	PSU	C6-C5	11.61	1.48	1.35
29	S1	455	PSU	C6-C5	11.55	1.48	1.35
29	S1	1566	PSU	C6-C5	11.38	1.48	1.35
29	S1	104	PSU	C6-C5	11.37	1.48	1.35
29	S1	12	PSU	C6-C5	11.27	1.48	1.35
37	2	1361	PSU	C6-C5	11.13	1.48	1.35
37	2	1194	PSU	C6-C5	11.01	1.48	1.35
37	2	626	PSU	C6-C5	10.93	1.48	1.35
37	2	1382	PSU	C6-C5	10.90	1.48	1.35
42	1	1171	PSU	C6-C5	10.89	1.48	1.35
37	2	662	PSU	C6-C5	10.89	1.48	1.35
37	2	437	PSU	C6-C5	10.87	1.48	1.35
37	2	1354	PSU	C6-C5	10.86	1.48	1.35
42	1	1402	PSU	C6-C5	10.81	1.47	1.35
37	2	1318	PSU	C6-C5	10.78	1.47	1.35
37	2	1413	PSU	C6-C5	10.69	1.47	1.35
42	1	1011	PSU	C6-C5	10.58	1.47	1.35
42	1	870	PSU	C6-C5	10.48	1.47	1.35
29	S1	1995	G7M	C8-N9	10.25	1.51	1.33
29	S1	1995	G7M	C8-N7	10.17	1.51	1.33
42	1	940	PSU	C6-C5	10.14	1.47	1.35
29	S1	1543	C4J	C6-C5	9.85	1.48	1.34
37	2	512	PSU	C2-N1	9.65	1.49	1.36
37	2	510	PSU	C2-N1	9.64	1.49	1.36
29	S1	1566	PSU	C2-N1	9.60	1.49	1.36
29	S1	104	PSU	C2-N1	9.57	1.49	1.36
42	1	1011	PSU	C2-N1	9.53	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	455	PSU	C2-N1	9.51	1.49	1.36
37	2	1361	PSU	C2-N1	9.43	1.49	1.36
29	S1	12	PSU	C2-N1	9.41	1.49	1.36
42	1	1402	PSU	C2-N1	9.33	1.49	1.36
42	1	407	A2M	C3'-C4'	-9.32	1.29	1.53
42	1	1171	PSU	C2-N1	9.26	1.49	1.36
42	1	697	A2M	C3'-C4'	-9.19	1.29	1.53
42	1	235	A2M	C3'-C4'	-9.19	1.29	1.53
38	7	43	A2M	C3'-C4'	-9.16	1.29	1.53
42	1	305	A2M	C3'-C4'	-9.13	1.29	1.53
37	2	628	A2M	C3'-C4'	-9.11	1.29	1.53
37	2	604	A2M	C3'-C4'	-9.11	1.29	1.53
42	1	858	A2M	C3'-C4'	-9.09	1.29	1.53
37	2	382	A2M	C3'-C4'	-9.06	1.29	1.53
42	1	955	A2M	C3'-C4'	-9.05	1.29	1.53
37	2	1384	A2M	C3'-C4'	-9.04	1.29	1.53
37	2	95	A2M	C3'-C4'	-9.03	1.29	1.53
42	1	1539	A2M	C3'-C4'	-9.02	1.30	1.53
42	1	927	A2M	C3'-C4'	-9.00	1.30	1.53
37	2	572	A2M	C3'-C4'	-8.98	1.30	1.53
29	S1	1544	5MC	C6-C5	8.96	1.49	1.34
37	2	1185	A2M	C3'-C4'	-8.96	1.30	1.53
37	2	1372	A2M	C3'-C4'	-8.93	1.30	1.53
37	2	1382	PSU	C2-N1	8.93	1.48	1.36
42	1	678	A2M	C3'-C4'	-8.91	1.30	1.53
37	2	1354	PSU	C2-N1	8.88	1.48	1.36
29	S1	2021	A2M	C3'-C4'	-8.86	1.30	1.53
42	1	870	PSU	C2-N1	8.86	1.48	1.36
38	7	162	A2M	C3'-C4'	-8.86	1.30	1.53
29	S1	668	A2M	C3'-C4'	-8.86	1.30	1.53
37	2	437	PSU	C2-N1	8.82	1.48	1.36
37	2	1308	5MC	C6-C5	8.80	1.49	1.34
37	2	1308	5MC	C3'-C4'	-8.77	1.30	1.53
42	1	681	A2M	C3'-C4'	-8.71	1.30	1.53
37	2	1194	PSU	C2-N1	8.69	1.48	1.36
37	2	527	A2M	C3'-C4'	-8.65	1.30	1.53
37	2	570	A2M	C3'-C4'	-8.64	1.30	1.53
37	2	527	A2M	O4'-C1'	-8.56	1.29	1.41
37	2	626	PSU	C2-N1	8.46	1.48	1.36
37	2	1318	PSU	C2-N1	8.44	1.48	1.36
37	2	1413	PSU	C2-N1	8.41	1.48	1.36
37	2	662	PSU	C2-N1	8.25	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	940	PSU	C2-N1	8.24	1.47	1.36
37	2	570	A2M	O4'-C1'	-8.06	1.29	1.41
42	1	858	A2M	O4'-C1'	-8.04	1.29	1.41
37	2	1372	A2M	O4'-C1'	-7.76	1.30	1.41
37	2	382	A2M	O4'-C1'	-7.75	1.30	1.41
42	1	1539	A2M	O4'-C1'	-7.73	1.30	1.41
42	1	927	A2M	O4'-C1'	-7.68	1.30	1.41
37	2	510	PSU	C2-N3	7.68	1.50	1.37
42	1	305	A2M	O4'-C4'	7.66	1.62	1.45
42	1	235	A2M	O4'-C1'	-7.65	1.30	1.41
37	2	572	A2M	O4'-C4'	7.61	1.62	1.45
37	2	570	A2M	O4'-C4'	7.60	1.62	1.45
29	S1	668	A2M	O4'-C1'	-7.57	1.30	1.41
42	1	681	A2M	O4'-C4'	7.56	1.61	1.45
42	1	697	A2M	O4'-C1'	-7.56	1.30	1.41
37	2	604	A2M	O4'-C1'	-7.54	1.30	1.41
29	S1	2021	A2M	O4'-C4'	7.54	1.61	1.45
42	1	305	A2M	O4'-C1'	-7.52	1.30	1.41
29	S1	104	PSU	C2-N3	7.52	1.50	1.37
42	1	955	A2M	O4'-C1'	-7.52	1.30	1.41
38	7	162	A2M	O4'-C1'	-7.51	1.30	1.41
38	7	43	A2M	O4'-C1'	-7.51	1.30	1.41
37	2	95	A2M	O4'-C1'	-7.50	1.30	1.41
37	2	1384	A2M	O4'-C1'	-7.50	1.30	1.41
29	S1	2021	A2M	O4'-C1'	-7.49	1.30	1.41
37	2	1384	A2M	O4'-C4'	7.45	1.61	1.45
37	2	1185	A2M	O4'-C1'	-7.45	1.30	1.41
37	2	604	A2M	O4'-C4'	7.43	1.61	1.45
37	2	512	PSU	C2-N3	7.43	1.50	1.37
37	2	572	A2M	O4'-C1'	-7.43	1.30	1.41
38	7	43	A2M	O4'-C4'	7.43	1.61	1.45
29	S1	668	A2M	O4'-C4'	7.42	1.61	1.45
42	1	407	A2M	O4'-C4'	7.42	1.61	1.45
29	S1	455	PSU	C2-N3	7.42	1.50	1.37
42	1	955	A2M	O4'-C4'	7.40	1.61	1.45
37	2	1308	5MC	O4'-C4'	7.39	1.61	1.45
42	1	697	A2M	O4'-C4'	7.38	1.61	1.45
37	2	382	A2M	O4'-C4'	7.36	1.61	1.45
37	2	95	A2M	O4'-C4'	7.34	1.61	1.45
37	2	527	A2M	O4'-C4'	7.34	1.61	1.45
42	1	681	A2M	O4'-C1'	-7.34	1.30	1.41
37	2	1185	A2M	O4'-C4'	7.33	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	628	A2M	O4'-C4'	7.31	1.61	1.45
42	1	235	A2M	O4'-C4'	7.31	1.61	1.45
37	2	1372	A2M	O4'-C4'	7.30	1.61	1.45
37	2	628	A2M	O4'-C1'	-7.29	1.30	1.41
42	1	678	A2M	O4'-C1'	-7.28	1.30	1.41
29	S1	12	PSU	C2-N3	7.27	1.50	1.37
38	7	162	A2M	O4'-C4'	7.24	1.61	1.45
42	1	927	A2M	O4'-C4'	7.19	1.61	1.45
29	S1	1566	PSU	C2-N3	7.15	1.49	1.37
42	1	678	A2M	O4'-C4'	7.14	1.61	1.45
42	1	1539	A2M	O4'-C4'	7.13	1.60	1.45
42	1	407	A2M	O4'-C1'	-7.10	1.31	1.41
42	1	1371	OMU	C2-N1	7.05	1.49	1.38
41	3	13	OMU	C2-N1	7.04	1.49	1.38
42	1	1011	PSU	C2-N3	6.95	1.49	1.37
42	1	858	A2M	O4'-C4'	6.90	1.60	1.45
37	2	1194	PSU	C2-N3	6.82	1.49	1.37
37	2	437	PSU	C2-N3	6.72	1.49	1.37
37	2	1354	PSU	C2-N3	6.70	1.49	1.37
29	S1	661	OMU	C2-N1	6.70	1.49	1.38
29	S1	8	OMU	C2-N1	6.69	1.49	1.38
37	2	1361	PSU	C2-N3	6.68	1.48	1.37
29	S1	8	OMU	C2-N3	6.60	1.49	1.38
42	1	845	OMU	C2-N1	6.58	1.49	1.38
37	2	1382	PSU	C2-N3	6.56	1.48	1.37
29	S1	661	OMU	C2-N3	6.56	1.49	1.38
29	S1	1979	OMU	C2-N1	6.54	1.48	1.38
37	2	1413	PSU	C2-N3	6.52	1.48	1.37
37	2	560	OMU	C2-N1	6.51	1.48	1.38
37	2	1419	OMU	C2-N1	6.51	1.48	1.38
29	S1	1979	OMU	C2-N3	6.51	1.49	1.38
37	2	1077	OMU	C2-N1	6.47	1.48	1.38
42	1	870	PSU	C2-N3	6.45	1.48	1.37
37	2	1318	PSU	C2-N3	6.44	1.48	1.37
37	2	662	PSU	C2-N3	6.39	1.48	1.37
42	1	1107	OMU	C2-N1	6.35	1.48	1.38
29	S1	1544	5MC	C4-N3	6.34	1.44	1.34
37	2	626	PSU	C2-N3	6.29	1.48	1.37
38	7	7	OMU	C2-N3	6.27	1.49	1.38
38	7	7	OMU	C2-N1	6.26	1.48	1.38
37	2	1359	OMU	C2-N1	6.26	1.48	1.38
42	1	940	PSU	C2-N3	6.24	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	38	OMC	C2-N3	6.23	1.49	1.36
29	S1	1995	G7M	C2-N3	6.21	1.48	1.33
37	2	667	OMU	C2-N1	6.20	1.48	1.38
29	S1	2140	OMC	C2-N3	6.19	1.48	1.36
37	2	1077	OMU	C2-N3	6.16	1.48	1.38
37	2	1152	OMU	C2-N3	6.12	1.48	1.38
42	1	1107	OMU	C2-N3	6.12	1.48	1.38
37	2	1152	OMU	C2-N1	6.12	1.48	1.38
42	1	1659	OMU	C2-N1	6.10	1.48	1.38
42	1	847	OMU	C2-N1	6.09	1.48	1.38
29	S1	18	OMC	C2-N3	6.09	1.48	1.36
42	1	1402	PSU	C2-N3	6.09	1.47	1.37
29	S1	1544	5MC	C2-N3	6.09	1.48	1.36
29	S1	1543	C4J	C2-N3	6.06	1.49	1.38
37	2	560	OMU	C2-N3	6.05	1.48	1.38
37	2	1359	OMU	C2-N3	6.03	1.48	1.38
42	1	1010	OMC	C2-N3	6.02	1.48	1.36
42	1	1371	OMU	C2-N3	6.01	1.48	1.38
42	1	1659	OMU	C2-N3	5.99	1.48	1.38
37	2	1419	OMU	C2-N3	5.98	1.48	1.38
41	3	13	OMU	C2-N3	5.95	1.48	1.38
37	2	359	OMC	C2-N3	5.94	1.48	1.36
29	S1	1866	OMC	C2-N3	5.92	1.48	1.36
42	1	847	OMU	C2-N3	5.88	1.48	1.38
29	S1	38	OMC	C6-C5	5.86	1.48	1.35
29	S1	2140	OMC	C6-C5	5.86	1.48	1.35
37	2	1248	OMC	C6-C5	5.84	1.48	1.35
29	S1	18	OMC	C6-C5	5.83	1.48	1.35
37	2	443	OMC	C6-C5	5.80	1.48	1.35
29	S1	1866	OMC	C6-C5	5.77	1.48	1.35
37	2	667	OMU	C2-N3	5.76	1.48	1.38
37	2	443	OMC	C2-N3	5.75	1.48	1.36
42	1	1171	PSU	C2-N3	5.75	1.47	1.37
42	1	1010	OMC	C6-C5	5.71	1.48	1.35
37	2	1159	OMC	C2-N3	5.68	1.47	1.36
29	S1	661	OMU	C6-C5	5.64	1.48	1.35
37	2	1308	5MC	C2-N3	5.62	1.47	1.36
37	2	1308	5MC	C4-N3	5.62	1.43	1.34
29	S1	8	OMU	C6-C5	5.59	1.48	1.35
37	2	1397	OMC	C2-N3	5.59	1.47	1.36
37	2	359	OMC	C6-C5	5.59	1.48	1.35
42	1	845	OMU	C2-N3	5.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	1979	OMU	C6-C5	5.55	1.47	1.35
37	2	1317	OMC	C2-N3	5.53	1.47	1.36
37	2	583	OMC	C2-N3	5.51	1.47	1.36
37	2	1317	OMC	C6-C5	5.51	1.47	1.35
37	2	510	PSU	C6-N1	5.50	1.45	1.36
37	2	1077	OMU	C6-C5	5.49	1.47	1.35
37	2	583	OMC	C6-C5	5.46	1.47	1.35
37	2	1159	OMC	C6-C5	5.44	1.47	1.35
37	2	1248	OMC	C2-N3	5.42	1.47	1.36
42	1	1107	OMU	C6-C5	5.39	1.47	1.35
38	7	7	OMU	C6-C5	5.35	1.47	1.35
42	1	1371	OMU	C6-C5	5.32	1.47	1.35
37	2	512	PSU	C6-N1	5.31	1.45	1.36
37	2	1397	OMC	C6-C5	5.29	1.47	1.35
37	2	1152	OMU	C6-C5	5.28	1.47	1.35
37	2	560	OMU	C6-C5	5.28	1.47	1.35
42	1	695	OMC	C2-N3	5.28	1.47	1.36
29	S1	600	OMG	C2-N3	5.26	1.46	1.33
29	S1	104	PSU	C6-N1	5.26	1.45	1.36
37	2	1359	OMU	C6-C5	5.26	1.47	1.35
42	1	695	OMC	C6-C5	5.24	1.47	1.35
29	S1	1566	PSU	C6-N1	5.23	1.44	1.36
29	S1	455	PSU	C6-N1	5.22	1.44	1.36
37	2	667	OMU	C6-C5	5.21	1.47	1.35
29	S1	1647	OMG	C2-N3	5.19	1.45	1.33
29	S1	12	PSU	C6-N1	5.19	1.44	1.36
42	1	847	OMU	C6-C5	5.17	1.47	1.35
42	1	959[A]	OMG	C2-N3	5.16	1.45	1.33
29	S1	1550	OMG	C2-N3	5.13	1.45	1.33
42	1	1659	OMU	C6-C5	5.12	1.46	1.35
29	S1	2140	OMC	C4-N3	5.11	1.44	1.34
29	S1	1829	OMG	C2-N3	5.11	1.45	1.33
37	2	1361	PSU	C6-N1	5.11	1.44	1.36
29	S1	2151	OMG	C2-N3	5.09	1.45	1.33
37	2	1419	OMU	C6-C5	5.08	1.46	1.35
29	S1	38	OMC	C4-N3	5.01	1.44	1.34
37	2	1046	OMG	C2-N3	5.01	1.45	1.33
41	3	13	OMU	C6-C5	5.00	1.46	1.35
42	1	1011	PSU	C6-N1	4.98	1.44	1.36
29	S1	1879	OMG	C2-N3	4.98	1.45	1.33
29	S1	1478	OMG	C2-N3	4.95	1.45	1.33
29	S1	1865	OMG	C2-N3	4.94	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1194	PSU	C6-N1	4.94	1.44	1.36
42	1	1402	PSU	C6-N1	4.93	1.44	1.36
29	S1	1995	G7M	C6-N1	4.93	1.45	1.37
42	1	1190	OMG	C2-N3	4.93	1.45	1.33
29	S1	1647	OMG	C4-N3	4.89	1.49	1.37
29	S1	18	OMC	C4-N3	4.88	1.44	1.34
37	2	1308	5MC	O4'-C1'	-4.87	1.30	1.42
37	2	1360	OMG	C2-N3	4.87	1.45	1.33
42	1	959[A]	OMG	C4-N3	4.82	1.49	1.37
42	1	959[B]	OMG	C2-N3	4.82	1.44	1.33
37	2	1354	PSU	C6-N1	4.82	1.44	1.36
29	S1	600	OMG	C4-N3	4.82	1.49	1.37
29	S1	2140	OMC	C4-N4	4.80	1.45	1.33
42	1	1171	PSU	C6-N1	4.79	1.44	1.36
42	1	1010	OMC	C4-N3	4.79	1.44	1.34
29	S1	38	OMC	C4-N4	4.78	1.45	1.33
37	2	437	PSU	C6-N1	4.78	1.44	1.36
37	2	1382	PSU	C6-N1	4.77	1.44	1.36
29	S1	1550	OMG	C2-N2	4.74	1.45	1.34
42	1	1011	PSU	C1'-C5	-4.73	1.39	1.50
29	S1	1865	OMG	C4-N3	4.72	1.48	1.37
37	2	1046	OMG	C4-N3	4.72	1.48	1.37
29	S1	18	OMC	C4-N4	4.71	1.45	1.33
29	S1	1866	OMC	C4-N3	4.71	1.44	1.34
37	2	1354	PSU	C1'-C5	-4.71	1.39	1.50
42	1	1190	OMG	C4-N3	4.71	1.48	1.37
37	2	359	OMC	C4-N3	4.70	1.44	1.34
29	S1	2151	OMG	C4-N3	4.69	1.48	1.37
29	S1	1829	OMG	C4-N3	4.68	1.48	1.37
42	1	870	PSU	C1'-C5	-4.68	1.39	1.50
42	1	1524	OMG	C2-N3	4.68	1.44	1.33
29	S1	1550	OMG	C4-N3	4.67	1.48	1.37
37	2	359	OMC	C4-N4	4.66	1.44	1.33
29	S1	1879	OMG	C4-N3	4.65	1.48	1.37
37	2	626	PSU	C6-N1	4.65	1.43	1.36
37	2	1229	OMG	C2-N3	4.64	1.44	1.33
29	S1	1829	OMG	C2-N2	4.63	1.45	1.34
42	1	940	PSU	C1'-C5	-4.62	1.39	1.50
42	1	845	OMU	C6-C5	4.61	1.45	1.35
37	2	534	OMG	C2-N3	4.61	1.44	1.33
29	S1	600	OMG	C2-N2	4.61	1.45	1.34
29	S1	1647	OMG	C2-N2	4.61	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	959[B]	OMG	C4-N3	4.61	1.48	1.37
37	2	1318	PSU	C6-N1	4.61	1.43	1.36
29	S1	1478	OMG	C4-N3	4.57	1.48	1.37
42	1	870	PSU	C6-N1	4.57	1.43	1.36
37	2	443	OMC	C4-N3	4.56	1.43	1.34
29	S1	1865	OMG	C2-N2	4.55	1.45	1.34
37	2	1360	OMG	C4-N3	4.54	1.48	1.37
37	2	1046	OMG	C2-N2	4.53	1.45	1.34
29	S1	1866	OMC	C4-N4	4.53	1.44	1.33
37	2	1231	OMG	C2-N3	4.53	1.44	1.33
29	S1	12	PSU	C1'-C5	-4.52	1.39	1.50
37	2	534	OMG	C4-N3	4.51	1.48	1.37
42	1	1190	OMG	C2-N2	4.50	1.44	1.34
29	S1	1879	OMG	C2-N2	4.49	1.44	1.34
29	S1	1478	OMG	C2-N2	4.49	1.44	1.34
29	S1	2151	OMG	C2-N2	4.47	1.44	1.34
42	1	1171	PSU	C1'-C5	-4.47	1.40	1.50
37	2	443	OMC	C4-N4	4.46	1.44	1.33
42	1	959[A]	OMG	C2-N2	4.46	1.44	1.34
37	2	655	OMG	C2-N3	4.46	1.44	1.33
37	2	1413	PSU	C6-N1	4.46	1.43	1.36
37	2	437	PSU	C1'-C5	-4.46	1.40	1.50
37	2	1382	PSU	C1'-C5	-4.45	1.40	1.50
37	2	1253	OMG	C2-N3	4.44	1.44	1.33
37	2	662	PSU	C6-N1	4.43	1.43	1.36
37	2	1360	OMG	C2-N2	4.43	1.44	1.34
37	2	1078	OMG	C4-N3	4.42	1.48	1.37
37	2	1231	OMG	C4-N3	4.41	1.48	1.37
37	2	1194	PSU	C1'-C5	-4.40	1.40	1.50
42	1	1010	OMC	C4-N4	4.40	1.44	1.33
42	1	1524	OMG	C2-N2	4.40	1.44	1.34
37	2	1159	OMC	C4-N4	4.39	1.44	1.33
37	2	1078	OMG	C2-N3	4.39	1.43	1.33
37	2	1229	OMG	C2-N2	4.39	1.44	1.34
37	2	655	OMG	C4-N3	4.38	1.48	1.37
37	2	1229	OMG	C4-N3	4.38	1.48	1.37
37	2	1231	OMG	C2-N2	4.37	1.44	1.34
37	2	662	PSU	C1'-C5	-4.37	1.40	1.50
37	2	1078	OMG	C2-N2	4.35	1.44	1.34
37	2	1159	OMC	C4-N3	4.33	1.43	1.34
37	2	1318	PSU	C1'-C5	-4.33	1.40	1.50
37	2	1361	PSU	C1'-C5	-4.33	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	2140	OMC	C2-N1	4.33	1.49	1.40
37	2	1248	OMC	C4-N4	4.32	1.44	1.33
29	S1	1544	5MC	C6-N1	4.32	1.45	1.38
37	2	583	OMC	C4-N4	4.32	1.44	1.33
42	1	959[B]	OMG	C2-N2	4.32	1.44	1.34
37	2	1253	OMG	C4-N3	4.32	1.47	1.37
42	1	856	OMG	C4-N3	4.31	1.47	1.37
37	2	1413	PSU	C1 ² -C5	-4.30	1.40	1.50
42	1	856	OMG	C2-N2	4.30	1.44	1.34
42	1	1540	OMG	C2-N2	4.30	1.44	1.34
42	1	1626	OMG	C4-N3	4.29	1.47	1.37
40	4	74	OMG	C2-N3	4.29	1.43	1.33
29	S1	104	PSU	C1 ² -C5	-4.28	1.40	1.50
42	1	1540	OMG	C4-N3	4.28	1.47	1.37
37	2	583	OMC	C4-N3	4.27	1.43	1.34
37	2	626	PSU	C1 ² -C5	-4.26	1.40	1.50
37	2	1317	OMC	C4-N3	4.26	1.43	1.34
37	2	1397	OMC	C4-N4	4.25	1.43	1.33
40	4	74	OMG	C4-N3	4.25	1.47	1.37
29	S1	38	OMC	C2-N1	4.24	1.49	1.40
29	S1	1544	5MC	C4-N4	4.23	1.45	1.34
42	1	856	OMG	C2-N3	4.23	1.43	1.33
42	1	1524	OMG	C4-N3	4.22	1.47	1.37
42	1	695	OMC	C4-N4	4.21	1.43	1.33
29	S1	18	OMC	C2-N1	4.21	1.49	1.40
42	1	940	PSU	C6-N1	4.20	1.43	1.36
37	2	1317	OMC	C4-N4	4.19	1.43	1.33
37	2	1253	OMG	C2-N2	4.19	1.44	1.34
37	2	1248	OMC	C4-N3	4.18	1.42	1.34
29	S1	455	PSU	C1 ² -C5	-4.17	1.40	1.50
37	2	534	OMG	C2-N2	4.17	1.44	1.34
37	2	641	OMG	C4-N3	4.17	1.47	1.37
37	2	1397	OMC	C4-N3	4.17	1.42	1.34
40	4	74	OMG	C2-N2	4.17	1.44	1.34
37	2	641	OMG	C2-N2	4.15	1.44	1.34
42	1	1540	OMG	C2-N3	4.13	1.43	1.33
37	2	641	OMG	C2-N3	4.12	1.43	1.33
37	2	655	OMG	C2-N2	4.11	1.44	1.34
42	1	1626	OMG	C2-N3	4.11	1.43	1.33
37	2	512	PSU	C1 ² -C5	-4.11	1.40	1.50
37	2	510	PSU	C4-N3	4.09	1.46	1.38
37	2	1308	5MC	C6-N1	4.08	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	695	OMC	C4-N3	4.07	1.42	1.34
37	2	1308	5MC	C4-N4	4.07	1.44	1.34
42	1	1402	PSU	C1'-C5	-4.05	1.40	1.50
29	S1	1566	PSU	C1'-C5	-4.03	1.41	1.50
37	2	443	OMC	C2-N1	4.01	1.48	1.40
29	S1	1543	C4J	C6-N1	3.99	1.46	1.36
29	S1	104	PSU	C4-N3	3.98	1.46	1.38
37	2	359	OMC	C2-N1	3.94	1.48	1.40
42	1	1626	OMG	C2-N2	3.93	1.43	1.34
37	2	1248	OMC	C2-N1	3.93	1.48	1.40
42	1	1010	OMC	C2-N1	3.92	1.48	1.40
29	S1	661	OMU	C4-N3	3.91	1.45	1.38
37	2	1317	OMC	C2-N1	3.90	1.48	1.40
29	S1	1995	G7M	C4-N3	3.89	1.46	1.37
29	S1	1544	5MC	C2-N1	3.89	1.48	1.40
29	S1	1979	OMU	C4-N3	3.87	1.45	1.38
29	S1	8	OMU	C4-N3	3.83	1.45	1.38
42	1	1171	PSU	O4-C4	-3.82	1.16	1.23
29	S1	455	PSU	C4-N3	3.82	1.45	1.38
37	2	512	PSU	C4-N3	3.80	1.45	1.38
37	2	1159	OMC	C2-N1	3.80	1.48	1.40
29	S1	1866	OMC	C2-N1	3.80	1.48	1.40
29	S1	12	PSU	C4-N3	3.80	1.45	1.38
42	1	845	OMU	O2-C2	-3.79	1.16	1.23
41	3	13	OMU	O4-C4	-3.75	1.17	1.24
29	S1	1566	PSU	C4-N3	3.75	1.45	1.38
37	2	1308	5MC	C2-N1	3.74	1.48	1.40
37	2	510	PSU	C1'-C5	-3.73	1.41	1.50
42	1	695	OMC	C2-N1	3.71	1.48	1.40
42	1	1540	OMG	C5-C4	-3.70	1.33	1.43
29	S1	1647	OMG	C6-N1	3.69	1.43	1.37
42	1	845	OMU	O4-C4	-3.65	1.17	1.24
37	2	641	OMG	C5-C4	-3.64	1.33	1.43
42	1	695	OMC	O2-C2	-3.62	1.17	1.23
37	2	583	OMC	C2-N1	3.60	1.47	1.40
37	2	1359	OMU	C4-N3	3.57	1.45	1.38
29	S1	1865	OMG	C6-N1	3.57	1.43	1.37
38	7	7	OMU	C4-N3	3.57	1.44	1.38
29	S1	1550	OMG	C6-N1	3.56	1.43	1.37
37	2	1397	OMC	C2-N1	3.55	1.47	1.40
42	1	856	OMG	C5-C4	-3.55	1.34	1.43
40	4	74	OMG	C5-C4	-3.53	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	667	OMU	O4-C4	-3.52	1.17	1.24
29	S1	1829	OMG	C6-N1	3.52	1.43	1.37
42	1	940	PSU	O4-C4	-3.51	1.16	1.23
37	2	1046	OMG	C6-N1	3.50	1.43	1.37
42	1	1371	OMU	O4-C4	-3.49	1.17	1.24
42	1	1107	OMU	C4-N3	3.49	1.44	1.38
42	1	1011	PSU	C4-N3	3.49	1.45	1.38
29	S1	600	OMG	C6-N1	3.48	1.43	1.37
42	1	847	OMU	O4-C4	-3.48	1.17	1.24
38	7	7	OMU	O4-C4	-3.48	1.17	1.24
37	2	1077	OMU	C4-N3	3.47	1.44	1.38
42	1	959[A]	OMG	C6-N1	3.46	1.43	1.37
42	1	1626	OMG	C5-C4	-3.46	1.34	1.43
37	2	583	OMC	O2-C2	-3.46	1.17	1.23
37	2	1317	OMC	O2-C2	-3.46	1.17	1.23
42	1	697	A2M	C5-C4	-3.45	1.31	1.40
37	2	527	A2M	C5-C4	-3.45	1.31	1.40
37	2	628	A2M	C5-C4	-3.45	1.31	1.40
37	2	1359	OMU	O4-C4	-3.43	1.17	1.24
37	2	1231	OMG	C5-C4	-3.42	1.34	1.43
37	2	1361	PSU	O4-C4	-3.41	1.17	1.23
37	2	1229	OMG	C5-C4	-3.41	1.34	1.43
29	S1	1478	OMG	C6-N1	3.41	1.42	1.37
42	1	1524	OMG	C6-N1	3.39	1.42	1.37
42	1	1659	OMU	O4-C4	-3.39	1.17	1.24
42	1	1659	OMU	C4-N3	3.37	1.44	1.38
42	1	847	OMU	C4-N3	3.37	1.44	1.38
29	S1	1879	OMG	C6-N1	3.37	1.42	1.37
37	2	1253	OMG	C5-C4	-3.36	1.34	1.43
42	1	959[B]	OMG	C6-N1	3.36	1.42	1.37
42	1	1524	OMG	C5-C4	-3.36	1.34	1.43
37	2	1419	OMU	C4-N3	3.35	1.44	1.38
29	S1	1995	G7M	C2-N1	3.35	1.46	1.37
42	1	1107	OMU	O4-C4	-3.34	1.18	1.24
42	1	927	A2M	C5-C4	-3.34	1.32	1.40
37	2	1248	OMC	O2-C2	-3.34	1.17	1.23
37	2	1152	OMU	C4-N3	3.33	1.44	1.38
37	2	1382	PSU	O4-C4	-3.33	1.17	1.23
42	1	407	A2M	C5-C4	-3.33	1.32	1.40
37	2	382	A2M	C5-C4	-3.32	1.32	1.40
42	1	955	A2M	C5-C4	-3.32	1.32	1.40
42	1	1539	A2M	C5-C4	-3.32	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	1190	OMG	C6-N1	3.32	1.42	1.37
37	2	655	OMG	C5-C4	-3.32	1.34	1.43
37	2	1318	PSU	O4-C4	-3.32	1.17	1.23
37	2	1413	PSU	O4-C4	-3.31	1.17	1.23
37	2	560	OMU	C4-N3	3.31	1.44	1.38
37	2	662	PSU	O4-C4	-3.31	1.17	1.23
37	2	1152	OMU	O4-C4	-3.30	1.18	1.24
37	2	1397	OMC	O2-C2	-3.30	1.17	1.23
37	2	1361	PSU	C4-N3	3.30	1.45	1.38
29	S1	2151	OMG	C6-N1	3.29	1.42	1.37
37	2	572	A2M	C5-C4	-3.29	1.32	1.40
37	2	593	PSU	C4-N3	-3.29	1.32	1.38
37	2	1194	PSU	C4-N3	3.28	1.44	1.38
42	1	870	PSU	O4-C4	-3.28	1.17	1.23
38	7	43	A2M	C5-C4	-3.27	1.32	1.40
37	2	1384	A2M	C5-C4	-3.27	1.32	1.40
37	2	1419	OMU	O4-C4	-3.27	1.18	1.24
37	2	1078	OMG	C5-C4	-3.26	1.34	1.43
42	1	1402	PSU	O4-C4	-3.25	1.17	1.23
29	S1	1543	C4J	C31-C3	3.24	1.59	1.52
37	2	570	A2M	O3'-C3'	3.22	1.50	1.43
38	7	162	A2M	C5-C4	-3.22	1.32	1.40
37	2	1360	OMG	C5-C4	-3.21	1.34	1.43
37	2	1229	OMG	C6-N1	3.20	1.42	1.37
37	2	534	OMG	C5-C4	-3.20	1.34	1.43
37	2	443	OMC	O2-C2	-3.19	1.17	1.23
37	2	1372	A2M	C5-C4	-3.19	1.32	1.40
29	S1	1995	G7M	C2-N2	3.18	1.41	1.34
37	2	560	OMU	O4-C4	-3.18	1.18	1.24
37	2	1308	5MC	O2'-C2'	-3.18	1.35	1.43
29	S1	1543	C4J	C4-N3	3.18	1.45	1.40
37	2	570	A2M	C5-C4	-3.18	1.32	1.40
37	2	1354	PSU	C4-N3	3.17	1.44	1.38
42	1	1017	PSU	C4-N3	-3.17	1.33	1.38
42	1	681	A2M	C5-C4	-3.15	1.32	1.40
37	2	626	PSU	C4-N3	3.15	1.44	1.38
29	S1	1979	OMU	O4-C4	-3.15	1.18	1.24
37	2	437	PSU	O4-C4	-3.15	1.17	1.23
37	2	1077	OMU	O4-C4	-3.14	1.18	1.24
37	2	1308	5MC	O2-C2	-3.14	1.17	1.23
29	S1	661	OMU	O4-C4	-3.14	1.18	1.24
29	S1	668	A2M	O3'-C3'	3.13	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1194	PSU	O4-C4	-3.12	1.17	1.23
29	S1	38	OMC	C6-N1	3.12	1.45	1.38
37	2	1360	OMG	C6-N1	3.12	1.42	1.37
42	1	422	PSU	C4-N3	-3.11	1.33	1.38
29	S1	1156	PSU	C6-C5	3.11	1.38	1.35
37	2	359	OMC	O2-C2	-3.11	1.18	1.23
37	2	1303	PSU	C6-C5	3.10	1.38	1.35
29	S1	8	OMU	O4-C4	-3.10	1.18	1.24
29	S1	1865	OMG	C5-C4	-3.10	1.35	1.43
42	1	1010	OMC	O2-C2	-3.10	1.18	1.23
37	2	1231	OMG	C6-N1	3.10	1.42	1.37
42	1	1010	OMC	C6-N1	3.10	1.45	1.38
37	2	1060	PSU	C4-N3	-3.10	1.33	1.38
42	1	1533	PSU	C4-N3	-3.09	1.33	1.38
37	2	1159	OMC	O2-C2	-3.09	1.18	1.23
37	2	597	PSU	C4-N3	-3.09	1.33	1.38
37	2	95	A2M	C5-C4	-3.08	1.32	1.40
37	2	1354	PSU	O4-C4	-3.08	1.17	1.23
37	2	534	OMG	C6-N1	3.08	1.42	1.37
29	S1	1879	OMG	C5-C4	-3.08	1.35	1.43
42	1	927	A2M	O2'-C2'	-3.08	1.34	1.42
42	1	678	A2M	C5-C4	-3.07	1.32	1.40
29	S1	1543	C4J	C2-N1	3.07	1.48	1.39
42	1	672	PSU	C4-N3	-3.07	1.33	1.38
42	1	1371	OMU	C4-N3	3.07	1.44	1.38
37	2	527	A2M	O3'-C3'	3.07	1.50	1.43
42	1	1528	PSU	C4-N3	-3.06	1.33	1.38
37	2	1403	PSU	C4-N3	-3.06	1.33	1.38
37	2	78	PSU	C4-N3	-3.06	1.33	1.38
42	1	1190	OMG	C5-C4	-3.05	1.35	1.43
37	2	1413	PSU	C4-N3	3.05	1.44	1.38
29	S1	18	OMC	C6-N1	3.05	1.45	1.38
37	2	71	OMG	C6-N1	-3.05	1.33	1.37
37	2	1185	A2M	C5-C4	-3.05	1.32	1.40
41	3	13	OMU	O2-C2	-3.05	1.17	1.23
37	2	1046	OMG	C5-C6	3.04	1.53	1.47
42	1	1659	OMU	O2-C2	-3.04	1.17	1.23
29	S1	2151	OMG	C5-C4	-3.04	1.35	1.43
42	1	858	A2M	C5-C4	-3.03	1.32	1.40
29	S1	2140	OMC	C6-N1	3.03	1.45	1.38
42	1	1664	PSU	C4-N3	-3.03	1.33	1.38
37	2	604	A2M	C5-C4	-3.03	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	628	A2M	O2'-C2'	-3.02	1.34	1.42
37	2	437	PSU	C4-N3	3.02	1.44	1.38
29	S1	668	A2M	C6-N6	3.02	1.45	1.34
29	S1	1866	OMC	O2-C2	-3.02	1.18	1.23
42	1	305	A2M	O2'-C2'	-3.02	1.34	1.42
29	S1	2048	PSU	C4-N3	-3.01	1.33	1.38
42	1	235	A2M	C5-C4	-3.01	1.33	1.40
42	1	1664	PSU	C6-C5	3.01	1.38	1.35
37	2	626	PSU	O4-C4	-3.01	1.17	1.23
29	S1	2021	A2M	C5-C4	-3.01	1.33	1.40
37	2	1152	OMU	O2-C2	-3.01	1.17	1.23
37	2	1078	OMG	C6-N1	3.01	1.42	1.37
42	1	697	A2M	O2'-C2'	-3.01	1.34	1.42
42	1	856	OMG	O6-C6	-3.00	1.17	1.23
37	2	667	OMU	O2-C2	-3.00	1.17	1.23
29	S1	2046	PSU	C4-N3	-3.00	1.33	1.38
37	2	359	OMC	C6-N1	3.00	1.45	1.38
42	1	858	A2M	C6-N6	3.00	1.45	1.34
38	7	74	PSU	C4-N3	-3.00	1.33	1.38
29	S1	600	OMG	C5-C6	3.00	1.53	1.47
29	S1	1841	PSU	C4-N3	-3.00	1.33	1.38
37	2	1308	5MC	O3'-C3'	3.00	1.50	1.43
42	1	235	A2M	C6-N6	2.99	1.45	1.34
42	1	1539	A2M	O2'-C2'	-2.99	1.35	1.42
42	1	407	A2M	O2'-C2'	-2.99	1.35	1.42
42	1	847	OMU	O2-C2	-2.99	1.17	1.23
29	S1	1543	C4J	O4-C4	-2.99	1.16	1.23
29	S1	607	PSU	C6-C5	2.99	1.38	1.35
37	2	472	PSU	C4-N3	-2.98	1.33	1.38
29	S1	2021	A2M	C6-N6	2.98	1.44	1.34
42	1	858	A2M	O3'-C3'	2.98	1.50	1.43
29	S1	1866	OMC	C6-N1	2.98	1.45	1.38
37	2	1144	PSU	C4-N3	-2.97	1.33	1.38
29	S1	1539	PSU	C4-N3	-2.97	1.33	1.38
38	7	69	PSU	C4-N3	-2.97	1.33	1.38
37	2	73	OMU	C4-N3	-2.97	1.33	1.38
37	2	1372	A2M	C6-N6	2.97	1.44	1.34
37	2	1264	PSU	C4-N3	-2.97	1.33	1.38
37	2	1185	A2M	O2'-C2'	-2.97	1.35	1.42
37	2	667	OMU	C4-N3	2.97	1.43	1.38
37	2	443	OMC	C6-N1	2.97	1.45	1.38
42	1	239	PSU	C4-N3	-2.97	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	681	A2M	O3'-C3'	2.95	1.49	1.43
37	2	1359	OMU	O2-C2	-2.95	1.17	1.23
37	2	1264	PSU	C6-C5	2.95	1.38	1.35
29	S1	609	PSU	C6-C5	2.95	1.38	1.35
29	S1	609	PSU	C4-N3	-2.94	1.33	1.38
29	S1	1647	OMG	C5-C6	2.94	1.53	1.47
29	S1	1533	PSU	C4-N3	-2.94	1.33	1.38
29	S1	1657	PSU	C4-N3	-2.94	1.33	1.38
29	S1	1539	PSU	C6-C5	2.93	1.38	1.35
29	S1	1478	OMG	C5-C4	-2.93	1.35	1.43
42	1	1402	PSU	C4-N3	2.93	1.44	1.38
37	2	1318	PSU	C4-N3	2.92	1.44	1.38
29	S1	1550	OMG	C5-C4	-2.92	1.35	1.43
37	2	95	A2M	C6-N6	2.92	1.44	1.34
42	1	678	A2M	O2'-C2'	-2.92	1.35	1.42
37	2	604	A2M	O3'-C3'	2.92	1.49	1.43
42	1	959[A]	OMG	C5-C4	-2.91	1.35	1.43
37	2	604	A2M	C6-N6	2.91	1.44	1.34
29	S1	1192	PSU	C4-N3	-2.91	1.33	1.38
37	2	1382	PSU	C4-N3	2.91	1.44	1.38
37	2	1078	OMG	C5-C6	2.91	1.53	1.47
42	1	422	PSU	C6-C5	2.91	1.38	1.35
37	2	1046	OMG	C5-C4	-2.91	1.35	1.43
29	S1	2021	A2M	O3'-C3'	2.91	1.49	1.43
29	S1	1543	C4J	O4'-C1'	-2.90	1.39	1.43
37	2	641	OMG	O6-C6	-2.90	1.17	1.23
37	2	1058	PSU	C6-C5	2.90	1.38	1.35
40	4	74	OMG	C6-N1	2.89	1.42	1.37
37	2	572	A2M	O2'-C2'	-2.89	1.35	1.42
37	2	382	A2M	O2'-C2'	-2.89	1.35	1.42
37	2	1058	PSU	C4-N3	-2.89	1.33	1.38
37	2	1185	A2M	C6-N6	2.88	1.44	1.34
42	1	305	A2M	O3'-C3'	2.88	1.49	1.43
29	S1	1533	PSU	C6-C5	2.88	1.38	1.35
42	1	235	A2M	O2'-C2'	-2.88	1.35	1.42
42	1	1181	PSU	C6-C5	2.87	1.38	1.35
37	2	662	PSU	C4-N3	2.87	1.44	1.38
42	1	678	A2M	C6-N6	2.87	1.44	1.34
37	2	1248	OMC	C6-N1	2.86	1.44	1.38
37	2	655	OMG	O6-C6	-2.86	1.17	1.23
37	2	641	OMG	C6-N1	2.86	1.42	1.37
42	1	1181	PSU	C4-N3	-2.86	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	1192	PSU	C6-C5	2.86	1.38	1.35
38	7	43	A2M	O2'-C2'	-2.86	1.35	1.42
37	2	1419	OMU	O2-C2	-2.86	1.17	1.23
37	2	527	A2M	C6-N6	2.86	1.44	1.34
37	2	655	OMG	C5-C6	2.86	1.53	1.47
37	2	570	A2M	C6-N6	2.85	1.44	1.34
29	S1	2046	PSU	C6-C5	2.85	1.38	1.35
37	2	1384	A2M	O2'-C2'	-2.85	1.35	1.42
42	1	305	A2M	C6-N6	2.84	1.44	1.34
37	2	78	PSU	C6-C5	2.84	1.38	1.35
29	S1	33	PSU	C6-C5	2.84	1.38	1.35
29	S1	18	OMC	O2-C2	-2.84	1.18	1.23
29	S1	1246	PSU	C4-N3	-2.84	1.33	1.38
37	2	1185	A2M	O3'-C3'	2.84	1.49	1.43
38	7	162	A2M	C6-N6	2.84	1.44	1.34
37	2	1384	A2M	C6-N6	2.83	1.44	1.34
37	2	655	OMG	C6-N1	2.83	1.42	1.37
42	1	1626	OMG	C6-N1	2.83	1.42	1.37
38	7	75	OMG	C6-N1	-2.83	1.33	1.37
42	1	1626	OMG	O6-C6	-2.83	1.17	1.23
29	S1	1995	G7M	O6-C6	-2.82	1.17	1.23
42	1	955	A2M	O3'-C3'	2.82	1.49	1.43
42	1	681	A2M	O2'-C2'	-2.82	1.35	1.42
38	7	69	PSU	C6-C5	2.82	1.38	1.35
37	2	1372	A2M	O3'-C3'	2.81	1.49	1.43
42	1	955	A2M	O2'-C2'	-2.81	1.35	1.42
29	S1	1647	OMG	C5-C4	-2.81	1.35	1.43
42	1	1107	OMU	O2-C2	-2.81	1.17	1.23
42	1	1371	OMU	O2-C2	-2.81	1.17	1.23
42	1	870	PSU	C4-N3	2.80	1.44	1.38
29	S1	33	PSU	C4-N3	-2.80	1.33	1.38
29	S1	38	OMC	O2-C2	-2.80	1.18	1.23
41	3	13	OMU	C4-N3	2.80	1.43	1.38
42	1	1540	OMG	O6-C6	-2.80	1.17	1.23
37	2	628	A2M	C6-N6	2.79	1.44	1.34
29	S1	668	A2M	C5-C4	-2.79	1.33	1.40
37	2	1253	OMG	O6-C6	-2.79	1.17	1.23
42	1	681	A2M	C6-N6	2.79	1.44	1.34
29	S1	1544	5MC	O2-C2	-2.79	1.18	1.23
29	S1	1156	PSU	C4-N3	-2.79	1.33	1.38
38	7	7	OMU	O2-C2	-2.79	1.18	1.23
38	7	162	A2M	O2'-C2'	-2.78	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	927	A2M	C6-N6	2.78	1.44	1.34
37	2	604	A2M	O2'-C2'	-2.78	1.35	1.42
29	S1	1829	OMG	C5-C6	2.78	1.53	1.47
37	2	628	A2M	O3'-C3'	2.78	1.49	1.43
42	1	959[B]	OMG	C5-C4	-2.78	1.36	1.43
29	S1	661	OMU	C6-N1	2.78	1.44	1.38
42	1	239	PSU	C6-C5	2.77	1.38	1.35
42	1	1528	PSU	C6-C5	2.77	1.38	1.35
37	2	572	A2M	C6-N6	2.77	1.44	1.34
42	1	955	A2M	C6-N6	2.77	1.44	1.34
37	2	1303	PSU	C4-N3	-2.77	1.33	1.38
29	S1	1246	PSU	C6-C5	2.76	1.38	1.35
37	2	1317	OMC	C6-N1	2.76	1.44	1.38
37	2	1159	OMC	C6-N1	2.76	1.44	1.38
42	1	1190	OMG	C5-C6	2.76	1.53	1.47
29	S1	8	OMU	C6-N1	2.76	1.44	1.38
29	S1	1550	OMG	C5-C6	2.76	1.53	1.47
38	7	43	A2M	C6-N6	2.76	1.44	1.34
29	S1	1879	OMG	C5-C6	2.75	1.53	1.47
38	7	162	A2M	O3'-C3'	2.74	1.49	1.43
29	S1	455	PSU	O4-C4	-2.74	1.18	1.23
42	1	678	A2M	O3'-C3'	2.74	1.49	1.43
29	S1	600	OMG	C5-C4	-2.74	1.36	1.43
42	1	697	A2M	C6-N6	2.74	1.44	1.34
29	S1	1829	OMG	C5-C4	-2.74	1.36	1.43
37	2	597	PSU	C6-C5	2.74	1.38	1.35
42	1	407	A2M	C6-N6	2.74	1.44	1.34
42	1	858	A2M	O2'-C2'	-2.73	1.35	1.42
29	S1	2151	OMG	C5-C6	2.73	1.53	1.47
42	1	1539	A2M	C6-N6	2.73	1.44	1.34
37	2	1384	A2M	O3'-C3'	2.73	1.49	1.43
29	S1	2140	OMC	O2-C2	-2.72	1.18	1.23
37	2	382	A2M	C6-N6	2.72	1.44	1.34
38	7	74	PSU	C6-C5	2.72	1.38	1.35
29	S1	1478	OMG	C5-C6	2.72	1.52	1.47
29	S1	1550	OMG	C2-N1	2.72	1.44	1.37
37	2	1046	OMG	C2-N1	2.72	1.44	1.37
37	2	1397	OMC	C6-N1	2.71	1.44	1.38
37	2	382	A2M	O3'-C3'	2.71	1.49	1.43
42	1	1540	OMG	C6-N1	2.71	1.41	1.37
37	2	593	PSU	C6-C5	2.71	1.38	1.35
42	1	940	PSU	C4-N3	2.71	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	1841	PSU	C6-C5	2.71	1.38	1.35
37	2	1144	PSU	C6-C5	2.71	1.38	1.35
37	2	95	A2M	O2'-C2'	-2.70	1.35	1.42
37	2	560	OMU	O2-C2	-2.70	1.18	1.23
40	4	74	OMG	O6-C6	-2.70	1.17	1.23
37	2	572	A2M	O3'-C3'	2.70	1.49	1.43
37	2	472	PSU	C6-C5	2.70	1.38	1.35
42	1	959[B]	OMG	C5-C6	2.70	1.52	1.47
42	1	1539	A2M	O3'-C3'	2.69	1.49	1.43
37	2	1372	A2M	O2'-C2'	-2.69	1.35	1.42
29	S1	1647	OMG	C2-N1	2.69	1.44	1.37
37	2	583	OMC	C6-N1	2.69	1.44	1.38
42	1	1011	PSU	O4-C4	-2.69	1.18	1.23
37	2	1403	PSU	C6-C5	2.69	1.38	1.35
29	S1	607	PSU	C4-N3	-2.69	1.33	1.38
37	2	1253	OMG	C6-N1	2.68	1.41	1.37
42	1	697	A2M	O3'-C3'	2.68	1.49	1.43
42	1	305	A2M	C5-C4	-2.68	1.33	1.40
37	2	1229	OMG	O6-C6	-2.67	1.17	1.23
37	2	1231	OMG	O6-C6	-2.67	1.17	1.23
29	S1	1829	OMG	C2-N1	2.67	1.44	1.37
37	2	95	A2M	O3'-C3'	2.67	1.49	1.43
42	1	1524	OMG	C5-C6	2.67	1.52	1.47
42	1	959[A]	OMG	C5-C6	2.66	1.52	1.47
37	2	527	A2M	O2'-C2'	-2.66	1.35	1.42
37	2	73	OMU	C2-N3	-2.66	1.33	1.38
37	2	534	OMG	O6-C6	-2.65	1.17	1.23
37	2	1060	PSU	C6-C5	2.65	1.38	1.35
42	1	1017	PSU	C6-C5	2.65	1.38	1.35
29	S1	1865	OMG	C2-N1	2.65	1.44	1.37
42	1	695	OMC	C6-N1	2.64	1.44	1.38
29	S1	1657	PSU	C6-C5	2.64	1.38	1.35
29	S1	12	PSU	O4-C4	-2.64	1.18	1.23
29	S1	2048	PSU	C6-C5	2.64	1.38	1.35
29	S1	1566	PSU	O4-C4	-2.64	1.18	1.23
42	1	407	A2M	O3'-C3'	2.63	1.49	1.43
29	S1	668	A2M	O2'-C2'	-2.63	1.35	1.42
29	S1	1979	OMU	C6-N1	2.63	1.44	1.38
29	S1	600	OMG	C2-N1	2.63	1.44	1.37
42	1	856	OMG	C5-C6	2.63	1.52	1.47
37	2	1077	OMU	O2-C2	-2.62	1.18	1.23
29	S1	1623	OMG	C6-N1	-2.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	672	PSU	C6-C5	2.62	1.38	1.35
37	2	1360	OMG	O6-C6	-2.61	1.18	1.23
37	2	510	PSU	O4-C4	-2.61	1.18	1.23
37	2	1077	OMU	C6-N1	2.61	1.44	1.38
29	S1	1543	C4J	O2-C2	-2.61	1.17	1.22
42	1	1190	OMG	C2-N1	2.60	1.44	1.37
42	1	1190	OMG	O6-C6	-2.60	1.18	1.23
42	1	1371	OMU	C6-N1	2.59	1.44	1.38
29	S1	661	OMU	O2-C2	-2.58	1.18	1.23
29	S1	104	PSU	O4-C4	-2.58	1.18	1.23
37	2	1359	OMU	C6-N1	2.58	1.44	1.38
29	S1	1478	OMG	C2-N1	2.57	1.44	1.37
29	S1	2151	OMG	C2-N1	2.57	1.44	1.37
37	2	512	PSU	O4-C4	-2.56	1.18	1.23
42	1	959[B]	OMG	C2-N1	2.55	1.44	1.37
42	1	1533	PSU	C6-C5	2.55	1.38	1.35
42	1	856	OMG	C6-N1	2.55	1.41	1.37
42	1	1626	OMG	C5-C6	2.54	1.52	1.47
42	1	927	A2M	O3'-C3'	2.54	1.49	1.43
38	7	7	OMU	C6-N1	2.54	1.44	1.38
29	S1	1979	OMU	O2-C2	-2.54	1.18	1.23
29	S1	2061	5MC	C6-C5	2.52	1.38	1.34
42	1	1107	OMU	C6-N1	2.52	1.44	1.38
38	7	43	A2M	O3'-C3'	2.51	1.48	1.43
42	1	407	A2M	O5'-C5'	-2.51	1.38	1.44
37	2	1078	OMG	O6-C6	-2.50	1.18	1.23
29	S1	1478	OMG	O6-C6	-2.50	1.18	1.23
37	2	560	OMU	C6-N1	2.48	1.44	1.38
37	2	534	OMG	C5-C6	2.48	1.52	1.47
29	S1	2151	OMG	O6-C6	-2.48	1.18	1.23
37	2	1360	OMG	C2-N1	2.47	1.43	1.37
29	S1	1995	G7M	C5-C6	2.47	1.51	1.45
42	1	235	A2M	O3'-C3'	2.47	1.48	1.43
42	1	1011	PSU	O4'-C1'	-2.46	1.40	1.43
42	1	959[A]	OMG	C2-N1	2.46	1.43	1.37
42	1	1524	OMG	O6-C6	-2.46	1.18	1.23
42	1	1540	OMG	C5-C6	2.45	1.52	1.47
42	1	1524	OMG	C2-N1	2.45	1.43	1.37
29	S1	1879	OMG	C2-N1	2.45	1.43	1.37
29	S1	8	OMU	O2-C2	-2.44	1.18	1.23
42	1	870	PSU	O2-C2	-2.43	1.18	1.23
29	S1	1865	OMG	O6-C6	-2.43	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	959[B]	OMG	O6-C6	-2.43	1.18	1.23
37	2	1152	OMU	C6-N1	2.42	1.43	1.38
37	2	1253	OMG	C5-C6	2.41	1.52	1.47
29	S1	1879	OMG	O6-C6	-2.41	1.18	1.23
29	S1	2140	OMC	C5-C4	2.41	1.48	1.42
37	2	1419	OMU	C6-N1	2.40	1.43	1.38
37	2	1229	OMG	C2-N1	2.40	1.43	1.37
42	1	305	A2M	O5'-C5'	-2.40	1.38	1.44
42	1	1171	PSU	C4-N3	2.40	1.43	1.38
29	S1	1865	OMG	C5-C6	2.40	1.52	1.47
37	2	1360	OMG	C5-C6	2.39	1.52	1.47
42	1	847	OMU	C6-N1	2.39	1.43	1.38
37	2	1231	OMG	C5-C6	2.38	1.52	1.47
37	2	593	PSU	C2-N3	-2.38	1.33	1.37
37	2	667	OMU	C6-N1	2.37	1.43	1.38
37	2	1229	OMG	C5-C6	2.36	1.52	1.47
37	2	641	OMG	C2-N1	2.36	1.43	1.37
37	2	1382	PSU	O4'-C1'	-2.36	1.40	1.43
37	2	570	A2M	O2'-C2'	-2.36	1.36	1.42
42	1	959[A]	OMG	O6-C6	-2.35	1.18	1.23
29	S1	38	OMC	C5-C4	2.35	1.48	1.42
37	2	1413	PSU	O2-C2	-2.35	1.18	1.23
37	2	1046	OMG	O6-C6	-2.35	1.18	1.23
29	S1	1550	OMG	O6-C6	-2.35	1.18	1.23
42	1	1171	PSU	O4'-C1'	-2.34	1.40	1.43
37	2	1078	OMG	C2-N1	2.34	1.43	1.37
40	4	74	OMG	C5-C6	2.34	1.52	1.47
37	2	641	OMG	C5-C6	2.34	1.52	1.47
42	1	927	A2M	O5'-C5'	-2.33	1.39	1.44
29	S1	1829	OMG	O6-C6	-2.33	1.18	1.23
29	S1	2021	A2M	O2'-C2'	-2.33	1.36	1.42
29	S1	512	A2M	C5-C4	2.30	1.47	1.40
42	1	1659	OMU	C6-N1	2.29	1.43	1.38
37	2	1077	OMU	C5-C4	2.29	1.48	1.43
29	S1	18	OMC	C5-C4	2.29	1.48	1.42
37	2	1231	OMG	C2-N1	2.29	1.43	1.37
37	2	662	PSU	O2-C2	-2.28	1.18	1.23
29	S1	2061	5MC	C6-N1	-2.28	1.34	1.38
37	2	626	PSU	O2-C2	-2.28	1.18	1.23
40	4	74	OMG	C2-N1	2.27	1.43	1.37
29	S1	600	OMG	O6-C6	-2.27	1.18	1.23
29	S1	1647	OMG	O6-C6	-2.27	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	655	OMG	C2-N1	2.26	1.43	1.37
29	S1	2046	PSU	C2-N3	-2.25	1.33	1.37
37	2	534	OMG	C2-N1	2.25	1.43	1.37
42	1	1528	PSU	C2-N3	-2.25	1.33	1.37
42	1	940	PSU	O2-C2	-2.24	1.18	1.23
42	1	1017	PSU	C2-N3	-2.23	1.33	1.37
37	2	570	A2M	O5'-C5'	-2.22	1.39	1.44
42	1	1171	PSU	O2-C2	-2.22	1.18	1.23
37	2	1318	PSU	O2-C2	-2.21	1.18	1.23
37	2	527	A2M	O5'-C5'	-2.20	1.39	1.44
42	1	672	PSU	C2-N3	-2.20	1.33	1.37
29	S1	8	OMU	C5-C4	2.20	1.48	1.43
37	2	78	PSU	C2-N3	-2.20	1.33	1.37
37	2	73	OMU	C5-C4	-2.20	1.38	1.43
41	3	13	OMU	C6-N1	2.20	1.43	1.38
37	2	1253	OMG	C2-N1	2.19	1.43	1.37
42	1	422	PSU	C2-N3	-2.18	1.33	1.37
29	S1	661	OMU	C5-C4	2.18	1.48	1.43
38	7	74	PSU	C2-N3	-2.18	1.33	1.37
37	2	597	PSU	C2-N3	-2.17	1.33	1.37
42	1	1540	OMG	C2-N1	2.16	1.43	1.37
37	2	1060	PSU	C2-N3	-2.15	1.33	1.37
37	2	1403	PSU	C2-N3	-2.15	1.33	1.37
29	S1	1657	PSU	C2-N3	-2.15	1.33	1.37
37	2	443	OMC	C5-C4	2.14	1.47	1.42
29	S1	1866	OMC	C5-C4	2.14	1.47	1.42
37	2	591	A2M	C5-C4	2.14	1.46	1.40
37	2	472	PSU	C2-N3	-2.14	1.33	1.37
37	2	510	PSU	C4-C5	2.14	1.50	1.44
42	1	858	A2M	O5'-C5'	-2.14	1.39	1.44
37	2	1361	PSU	O4'-C1'	-2.14	1.40	1.43
42	1	422	PSU	C2'-C1'	-2.12	1.51	1.53
29	S1	1979	OMU	C5-C4	2.12	1.48	1.43
37	2	359	OMC	C5-C4	2.11	1.47	1.42
42	1	856	OMG	C2-N1	2.11	1.42	1.37
42	1	1017	PSU	C2'-C1'	-2.11	1.51	1.53
42	1	845	OMU	C4-N3	2.10	1.42	1.38
42	1	1533	PSU	C2-N3	-2.10	1.33	1.37
42	1	305	A2M	C6-C5	-2.10	1.35	1.43
29	S1	668	A2M	O5'-C5'	-2.09	1.39	1.44
42	1	1664	PSU	C2-N3	-2.09	1.33	1.37
42	1	955	A2M	O5'-C5'	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1382	PSU	O2-C2	-2.09	1.19	1.23
42	1	1011	PSU	C4-C5	2.08	1.50	1.44
37	2	510	PSU	O4'-C1'	-2.08	1.40	1.43
42	1	1626	OMG	C2-N1	2.08	1.42	1.37
29	S1	1841	PSU	C2-N3	-2.08	1.33	1.37
42	1	697	A2M	O5'-C5'	-2.07	1.39	1.44
37	2	1264	PSU	C2-N3	-2.07	1.34	1.37
37	2	1058	PSU	C2-N3	-2.07	1.34	1.37
38	7	162	A2M	O5'-C5'	-2.07	1.39	1.44
37	2	1144	PSU	C2-N3	-2.06	1.34	1.37
37	2	437	PSU	O2-C2	-2.06	1.19	1.23
29	S1	609	PSU	C2-N3	-2.05	1.34	1.37
37	2	1264	PSU	C2'-C1'	-2.05	1.51	1.53
37	2	572	A2M	O5'-C5'	-2.04	1.39	1.44
42	1	1664	PSU	C2-N1	-2.04	1.34	1.36
38	7	69	PSU	C2-N3	-2.04	1.34	1.37
29	S1	1566	PSU	C4-C5	2.04	1.50	1.44
29	S1	1533	PSU	C2-N3	-2.04	1.34	1.37
42	1	1107	OMU	C5-C4	2.04	1.48	1.43
42	1	239	PSU	C2-N3	-2.03	1.34	1.37
37	2	1194	PSU	O2-C2	-2.03	1.19	1.23
37	2	628	A2M	O5'-C5'	-2.03	1.39	1.44
42	1	1010	OMC	C5-C4	2.03	1.47	1.42
37	2	1308	5MC	O5'-C5'	-2.03	1.39	1.44
37	2	1354	PSU	O2-C2	-2.02	1.19	1.23
37	2	1359	OMU	C5-C4	2.02	1.48	1.43
29	S1	1539	PSU	C2-N3	-2.02	1.34	1.37
42	1	1371	OMU	C5-C4	2.02	1.48	1.43
37	2	78	PSU	C2-N1	-2.01	1.34	1.36
29	S1	2048	PSU	C2-N3	-2.00	1.34	1.37

All (581) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	305	A2M	C5-C6-N6	11.24	137.44	120.35
42	1	858	A2M	C5-C6-N6	11.22	137.40	120.35
37	2	1372	A2M	C5-C6-N6	11.00	137.07	120.35
37	2	628	A2M	C5-C6-N6	10.93	136.97	120.35
42	1	1539	A2M	C5-C6-N6	10.93	136.97	120.35
38	7	43	A2M	C5-C6-N6	10.92	136.95	120.35
37	2	572	A2M	C5-C6-N6	10.84	136.83	120.35
29	S1	2021	A2M	C5-C6-N6	10.71	136.62	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	668	A2M	C5-C6-N6	10.65	136.54	120.35
42	1	927	A2M	C5-C6-N6	10.58	136.42	120.35
37	2	570	A2M	C5-C6-N6	10.56	136.40	120.35
42	1	678	A2M	C5-C6-N6	10.52	136.35	120.35
42	1	697	A2M	C5-C6-N6	10.45	136.24	120.35
38	7	162	A2M	C5-C6-N6	10.43	136.20	120.35
37	2	95	A2M	C5-C6-N6	10.42	136.19	120.35
42	1	407	A2M	C5-C6-N6	10.41	136.16	120.35
42	1	235	A2M	C5-C6-N6	10.40	136.15	120.35
42	1	681	A2M	C5-C6-N6	10.32	136.03	120.35
37	2	604	A2M	C5-C6-N6	10.28	135.97	120.35
42	1	955	A2M	C5-C6-N6	10.16	135.80	120.35
37	2	527	A2M	C5-C6-N6	10.08	135.67	120.35
37	2	382	A2M	C5-C6-N6	10.04	135.61	120.35
37	2	1185	A2M	C5-C6-N6	9.97	135.50	120.35
37	2	1384	A2M	C5-C6-N6	9.86	135.33	120.35
37	2	1372	A2M	C1'-N9-C4	-8.60	111.53	126.64
37	2	628	A2M	C1'-N9-C4	-8.20	112.23	126.64
42	1	858	A2M	N6-C6-N1	-7.99	101.98	118.57
37	2	382	A2M	C1'-N9-C4	-7.99	112.60	126.64
29	S1	2021	A2M	C1'-N9-C4	-7.87	112.81	126.64
37	2	572	A2M	C1'-N9-C4	-7.75	113.02	126.64
37	2	628	A2M	N6-C6-N1	-7.73	102.53	118.57
38	7	43	A2M	N6-C6-N1	-7.73	102.54	118.57
37	2	1372	A2M	N6-C6-N1	-7.63	102.73	118.57
37	2	1384	A2M	C1'-N9-C4	-7.63	113.24	126.64
29	S1	668	A2M	C1'-N9-C4	-7.63	113.24	126.64
42	1	1539	A2M	N6-C6-N1	-7.59	102.83	118.57
37	2	572	A2M	N6-C6-N1	-7.52	102.96	118.57
29	S1	2021	A2M	N6-C6-N1	-7.48	103.04	118.57
38	7	162	A2M	C1'-N9-C4	-7.44	113.56	126.64
42	1	678	A2M	N6-C6-N1	-7.44	103.12	118.57
42	1	927	A2M	N6-C6-N1	-7.42	103.16	118.57
42	1	697	A2M	C1'-N9-C4	-7.39	113.66	126.64
38	7	43	A2M	C1'-N9-C4	-7.37	113.69	126.64
29	S1	668	A2M	N6-C6-N1	-7.35	103.32	118.57
42	1	955	A2M	N6-C6-N1	-7.30	103.41	118.57
42	1	235	A2M	N6-C6-N1	-7.28	103.47	118.57
42	1	407	A2M	N6-C6-N1	-7.28	103.47	118.57
37	2	527	A2M	C1'-N9-C4	-7.28	113.86	126.64
42	1	697	A2M	N6-C6-N1	-7.24	103.56	118.57
38	7	162	A2M	N6-C6-N1	-7.22	103.59	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	382	A2M	N6-C6-N1	-7.19	103.64	118.57
42	1	681	A2M	N6-C6-N1	-7.19	103.65	118.57
42	1	858	A2M	C1'-N9-C4	-7.17	114.04	126.64
37	2	95	A2M	N6-C6-N1	-7.17	103.69	118.57
37	2	570	A2M	N6-C6-N1	-7.17	103.70	118.57
42	1	235	A2M	C1'-N9-C4	-7.16	114.06	126.64
42	1	845	OMU	C4-N3-C2	-7.09	117.22	126.58
37	2	527	A2M	N6-C6-N1	-7.08	103.88	118.57
42	1	407	A2M	C1'-N9-C4	-7.04	114.27	126.64
42	1	305	A2M	N6-C6-N1	-7.01	104.02	118.57
37	2	604	A2M	N6-C6-N1	-6.98	104.08	118.57
37	2	1384	A2M	N6-C6-N1	-6.88	104.30	118.57
42	1	305	A2M	C1'-N9-C4	-6.86	114.58	126.64
37	2	1185	A2M	N6-C6-N1	-6.75	104.57	118.57
42	1	681	A2M	C1'-N9-C4	-6.74	114.80	126.64
42	1	1017	PSU	N1-C2-N3	6.70	122.72	115.13
29	S1	1657	PSU	N1-C2-N3	6.70	122.72	115.13
42	1	955	A2M	C1'-N9-C4	-6.66	114.95	126.64
42	1	1533	PSU	N1-C2-N3	6.63	122.64	115.13
37	2	1185	A2M	C1'-N9-C4	-6.63	115.00	126.64
42	1	1539	A2M	C1'-N9-C4	-6.58	115.08	126.64
42	1	422	PSU	N1-C2-N3	6.57	122.57	115.13
42	1	672	PSU	N1-C2-N3	6.53	122.53	115.13
37	2	593	PSU	N1-C2-N3	6.52	122.52	115.13
37	2	1060	PSU	N1-C2-N3	6.50	122.49	115.13
37	2	597	PSU	N1-C2-N3	6.48	122.48	115.13
37	2	1403	PSU	N1-C2-N3	6.46	122.45	115.13
37	2	604	A2M	C1'-N9-C4	-6.42	115.36	126.64
37	2	78	PSU	N1-C2-N3	6.41	122.39	115.13
29	S1	2048	PSU	N1-C2-N3	6.41	122.39	115.13
41	3	13	OMU	C4-N3-C2	-6.41	118.13	126.58
37	2	472	PSU	N1-C2-N3	6.40	122.38	115.13
42	1	239	PSU	N1-C2-N3	6.40	122.38	115.13
38	7	69	PSU	N1-C2-N3	6.37	122.35	115.13
42	1	1528	PSU	N1-C2-N3	6.34	122.32	115.13
37	2	1144	PSU	N1-C2-N3	6.32	122.29	115.13
37	2	1058	PSU	N1-C2-N3	6.32	122.29	115.13
29	S1	1246	PSU	N1-C2-N3	6.31	122.28	115.13
42	1	1181	PSU	N1-C2-N3	6.30	122.27	115.13
37	2	95	A2M	C1'-N9-C4	-6.30	115.57	126.64
37	2	1264	PSU	N1-C2-N3	6.30	122.26	115.13
29	S1	1533	PSU	N1-C2-N3	6.25	122.21	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1539	PSU	N1-C2-N3	6.25	122.21	115.13
29	S1	1192	PSU	N1-C2-N3	6.24	122.20	115.13
37	2	570	A2M	C1'-N9-C4	-6.23	115.70	126.64
29	S1	2046	PSU	N1-C2-N3	6.21	122.17	115.13
42	1	1664	PSU	N1-C2-N3	6.20	122.16	115.13
29	S1	1841	PSU	N1-C2-N3	6.15	122.09	115.13
38	7	74	PSU	N1-C2-N3	6.13	122.07	115.13
42	1	845	OMU	N3-C2-N1	6.12	123.01	114.89
29	S1	607	PSU	N1-C2-N3	6.11	122.05	115.13
37	2	1303	PSU	N1-C2-N3	6.09	122.03	115.13
29	S1	609	PSU	N1-C2-N3	6.06	122.00	115.13
29	S1	33	PSU	N1-C2-N3	6.05	121.98	115.13
29	S1	1156	PSU	N1-C2-N3	6.03	121.96	115.13
42	1	927	A2M	C1'-N9-C4	-6.01	116.09	126.64
37	2	572	A2M	N3-C2-N1	-5.95	119.38	128.68
38	7	162	A2M	N3-C2-N1	-5.92	119.43	128.68
37	2	667	OMU	C4-N3-C2	-5.88	118.83	126.58
42	1	681	A2M	N3-C2-N1	-5.86	119.52	128.68
42	1	407	A2M	N3-C2-N1	-5.81	119.60	128.68
37	2	1359	OMU	C4-N3-C2	-5.76	118.98	126.58
42	1	847	OMU	C4-N3-C2	-5.75	119.00	126.58
42	1	1107	OMU	C4-N3-C2	-5.74	119.01	126.58
38	7	43	A2M	N3-C2-N1	-5.74	119.71	128.68
37	2	1384	A2M	N3-C2-N1	-5.74	119.71	128.68
42	1	1371	OMU	C4-N3-C2	-5.67	119.10	126.58
42	1	697	A2M	N3-C2-N1	-5.66	119.82	128.68
37	2	1077	OMU	C4-N3-C2	-5.65	119.12	126.58
42	1	1171	PSU	C4-N3-C2	-5.64	118.21	126.34
37	2	527	A2M	N3-C2-N1	-5.61	119.91	128.68
42	1	927	A2M	N3-C2-N1	-5.61	119.91	128.68
37	2	628	A2M	N3-C2-N1	-5.59	119.95	128.68
37	2	1152	OMU	C4-N3-C2	-5.57	119.24	126.58
42	1	1539	A2M	N3-C2-N1	-5.56	120.00	128.68
42	1	955	A2M	N3-C2-N1	-5.53	120.03	128.68
42	1	858	A2M	N3-C2-N1	-5.53	120.03	128.68
42	1	235	A2M	N3-C2-N1	-5.52	120.06	128.68
37	2	1185	A2M	N3-C2-N1	-5.50	120.08	128.68
37	2	1372	A2M	N3-C2-N1	-5.50	120.08	128.68
37	2	1419	OMU	C4-N3-C2	-5.48	119.34	126.58
29	S1	2021	A2M	N3-C2-N1	-5.45	120.17	128.68
37	2	382	A2M	N3-C2-N1	-5.44	120.17	128.68
37	2	570	A2M	N3-C2-N1	-5.43	120.19	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	8	OMU	C4-N3-C2	-5.40	119.45	126.58
37	2	560	OMU	C4-N3-C2	-5.39	119.47	126.58
29	S1	1979	OMU	C4-N3-C2	-5.34	119.53	126.58
42	1	678	A2M	C1'-N9-C4	-5.33	117.28	126.64
29	S1	661	OMU	C4-N3-C2	-5.32	119.56	126.58
42	1	1659	OMU	C4-N3-C2	-5.25	119.66	126.58
29	S1	668	A2M	N3-C2-N1	-5.23	120.50	128.68
38	7	7	OMU	C4-N3-C2	-5.19	119.73	126.58
37	2	604	A2M	N3-C2-N1	-5.19	120.57	128.68
42	1	940	PSU	C4-N3-C2	-5.18	118.88	126.34
37	2	95	A2M	N3-C2-N1	-5.10	120.71	128.68
42	1	678	A2M	N3-C2-N1	-5.06	120.78	128.68
42	1	305	A2M	N3-C2-N1	-5.03	120.81	128.68
37	2	1361	PSU	C4-N3-C2	-5.00	119.14	126.34
42	1	940	PSU	N1-C2-N3	4.94	120.73	115.13
42	1	1402	PSU	C4-N3-C2	-4.91	119.27	126.34
42	1	1011	PSU	C4-N3-C2	-4.87	119.32	126.34
37	2	1382	PSU	C4-N3-C2	-4.86	119.33	126.34
42	1	870	PSU	C4-N3-C2	-4.84	119.36	126.34
37	2	1413	PSU	C4-N3-C2	-4.84	119.37	126.34
42	1	1171	PSU	N1-C2-N3	4.80	120.57	115.13
37	2	73	OMU	C4-N3-C2	-4.73	120.34	126.58
37	2	1354	PSU	C4-N3-C2	-4.72	119.53	126.34
37	2	1413	PSU	N1-C2-N3	4.72	120.48	115.13
37	2	437	PSU	C4-N3-C2	-4.71	119.56	126.34
42	1	1011	PSU	N1-C2-N3	4.67	120.43	115.13
37	2	626	PSU	C4-N3-C2	-4.66	119.62	126.34
41	3	13	OMU	N3-C2-N1	4.66	121.07	114.89
37	2	1318	PSU	C4-N3-C2	-4.64	119.65	126.34
37	2	1318	PSU	N1-C2-N3	4.61	120.35	115.13
37	2	626	PSU	N1-C2-N3	4.61	120.35	115.13
29	S1	12	PSU	C4-N3-C2	-4.58	119.74	126.34
37	2	667	OMU	N3-C2-N1	4.55	120.93	114.89
37	2	437	PSU	N1-C2-N3	4.55	120.28	115.13
37	2	1144	PSU	C4-N3-C2	-4.54	119.80	126.34
37	2	1194	PSU	C4-N3-C2	-4.49	119.87	126.34
37	2	73	OMU	N3-C2-N1	4.49	120.84	114.89
37	2	1354	PSU	N1-C2-N3	4.46	120.18	115.13
37	2	512	PSU	C4-N3-C2	-4.45	119.93	126.34
42	1	1017	PSU	C4-N3-C2	-4.44	119.94	126.34
29	S1	104	PSU	C4-N3-C2	-4.41	119.98	126.34
29	S1	2048	PSU	C4-N3-C2	-4.41	119.98	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1152	OMU	N3-C2-N1	4.40	120.73	114.89
42	1	422	PSU	C4-N3-C2	-4.39	120.01	126.34
37	2	662	PSU	N1-C2-N3	4.38	120.09	115.13
37	2	1382	PSU	N1-C2-N3	4.36	120.08	115.13
37	2	662	PSU	C4-N3-C2	-4.36	120.05	126.34
29	S1	1657	PSU	C4-N3-C2	-4.36	120.06	126.34
42	1	870	PSU	N1-C2-N3	4.36	120.07	115.13
29	S1	455	PSU	C4-N3-C2	-4.36	120.06	126.34
37	2	512	PSU	N1-C2-N3	4.34	120.05	115.13
38	7	69	PSU	C4-N3-C2	-4.33	120.11	126.34
29	S1	1566	PSU	C4-N3-C2	-4.32	120.11	126.34
42	1	1107	OMU	N3-C2-N1	4.32	120.62	114.89
37	2	1403	PSU	C4-N3-C2	-4.31	120.13	126.34
37	2	1060	PSU	C4-N3-C2	-4.31	120.13	126.34
42	1	1528	PSU	C4-N3-C2	-4.30	120.14	126.34
37	2	472	PSU	C4-N3-C2	-4.30	120.14	126.34
37	2	1194	PSU	N1-C2-N3	4.30	120.00	115.13
42	1	672	PSU	C4-N3-C2	-4.29	120.16	126.34
42	1	1533	PSU	C4-N3-C2	-4.29	120.16	126.34
37	2	1361	PSU	N1-C2-N3	4.29	119.99	115.13
37	2	597	PSU	C4-N3-C2	-4.28	120.17	126.34
37	2	593	PSU	C4-N3-C2	-4.27	120.19	126.34
42	1	847	OMU	N3-C2-N1	4.27	120.55	114.89
42	1	239	PSU	C4-N3-C2	-4.25	120.22	126.34
29	S1	1539	PSU	C4-N3-C2	-4.25	120.22	126.34
37	2	1058	PSU	C4-N3-C2	-4.22	120.26	126.34
42	1	1181	PSU	C4-N3-C2	-4.22	120.26	126.34
29	S1	1192	PSU	C4-N3-C2	-4.20	120.28	126.34
29	S1	1246	PSU	C4-N3-C2	-4.18	120.31	126.34
29	S1	12	PSU	N1-C2-N3	4.18	119.86	115.13
37	2	1419	OMU	N3-C2-N1	4.17	120.42	114.89
37	2	78	PSU	C4-N3-C2	-4.16	120.34	126.34
37	2	1077	OMU	N3-C2-N1	4.14	120.38	114.89
37	2	1308	5MC	C5-C6-N1	-4.13	119.09	123.34
29	S1	104	PSU	N1-C2-N3	4.12	119.80	115.13
42	1	1371	OMU	N3-C2-N1	4.11	120.34	114.89
29	S1	1543	C4J	C4-N3-C2	-4.11	120.27	125.46
29	S1	455	PSU	N1-C2-N3	4.10	119.78	115.13
38	7	74	PSU	C4-N3-C2	-4.10	120.44	126.34
42	1	1402	PSU	N1-C2-N3	4.09	119.77	115.13
37	2	560	OMU	N3-C2-N1	4.09	120.32	114.89
37	2	1359	OMU	N3-C2-N1	4.09	120.31	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1156	PSU	C3'-C2'-C1'	4.08	106.39	101.64
41	3	13	OMU	C1'-N1-C2	4.08	124.95	117.57
42	1	305	A2M	O4'-C1'-C2'	-4.08	99.52	106.59
29	S1	1533	PSU	C4-N3-C2	-4.07	120.47	126.34
42	1	1664	PSU	C4-N3-C2	-4.05	120.50	126.34
29	S1	8	OMU	N3-C2-N1	4.03	120.25	114.89
42	1	845	OMU	C1'-N1-C2	4.03	124.87	117.57
29	S1	1566	PSU	N1-C2-N3	4.00	119.66	115.13
29	S1	1657	PSU	O2-C2-N1	-3.99	118.39	122.79
37	2	510	PSU	C4-N3-C2	-3.99	120.59	126.34
37	2	1253	OMG	C5-C6-N1	3.99	121.00	113.95
37	2	1303	PSU	C4-N3-C2	-3.98	120.61	126.34
37	2	527	A2M	O4'-C1'-C2'	-3.95	99.73	106.59
29	S1	1841	PSU	C4-N3-C2	-3.95	120.65	126.34
37	2	1264	PSU	C4-N3-C2	-3.95	120.65	126.34
29	S1	2046	PSU	C4-N3-C2	-3.95	120.65	126.34
42	1	1371	OMU	C5-C4-N3	3.95	120.74	114.84
41	3	13	OMU	C5-C4-N3	3.90	120.67	114.84
37	2	1359	OMU	C5-C4-N3	3.90	120.67	114.84
29	S1	661	OMU	N3-C2-N1	3.89	120.06	114.89
29	S1	607	PSU	C4-N3-C2	-3.89	120.73	126.34
42	1	856	OMG	C5-C6-N1	3.89	120.82	113.95
29	S1	33	PSU	C4-N3-C2	-3.88	120.75	126.34
29	S1	1192	PSU	C3'-C2'-C1'	3.87	106.15	101.64
38	7	69	PSU	C3'-C2'-C1'	3.85	106.12	101.64
29	S1	609	PSU	C4-N3-C2	-3.85	120.80	126.34
29	S1	1156	PSU	C4-N3-C2	-3.84	120.80	126.34
37	2	73	OMU	C5-C4-N3	3.81	120.54	114.84
42	1	1659	OMU	N3-C2-N1	3.80	119.94	114.89
37	2	655	OMG	C5-C6-N1	3.78	120.62	113.95
38	7	7	OMU	N3-C2-N1	3.77	119.90	114.89
37	2	1229	OMG	C5-C6-N1	3.77	120.61	113.95
29	S1	1979	OMU	N3-C2-N1	3.77	119.90	114.89
42	1	672	PSU	O2-C2-N1	-3.74	118.67	122.79
42	1	422	PSU	O2-C2-N1	-3.74	118.67	122.79
37	2	667	OMU	C5-C4-N3	3.74	120.43	114.84
42	1	1533	PSU	O2-C2-N1	-3.73	118.68	122.79
29	S1	2048	PSU	O2-C2-N1	-3.72	118.69	122.79
42	1	847	OMU	C5-C4-N3	3.72	120.40	114.84
42	1	1626	OMG	C5-C6-N1	3.71	120.50	113.95
42	1	305	A2M	C3'-C2'-C1'	-3.70	95.92	102.89
37	2	1303	PSU	C3'-C2'-C1'	3.70	105.94	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	607	PSU	C3'-C2'-C1'	3.68	105.92	101.64
37	2	510	PSU	N1-C2-N3	3.68	119.30	115.13
37	2	1078	OMG	C5-C6-N1	3.66	120.42	113.95
42	1	1017	PSU	O2-C2-N1	-3.66	118.76	122.79
42	1	1371	OMU	C1'-N1-C2	3.66	124.19	117.57
37	2	1144	PSU	O2-C2-N1	-3.66	118.77	122.79
37	2	1360	OMG	C5-C6-N1	3.65	120.40	113.95
37	2	641	OMG	C5-C6-N1	3.65	120.40	113.95
29	S1	1879	OMG	C5-C6-N1	3.65	120.39	113.95
37	2	1077	OMU	C5-C4-N3	3.64	120.28	114.84
42	1	1524	OMG	C5-C6-N1	3.63	120.36	113.95
42	1	1107	OMU	C5-C4-N3	3.62	120.26	114.84
42	1	1540	OMG	C5-C6-N1	3.62	120.34	113.95
42	1	1190	OMG	C5-C6-N1	3.59	120.29	113.95
37	2	1231	OMG	C5-C6-N1	3.59	120.29	113.95
42	1	1181	PSU	O2-C2-N1	-3.59	118.84	122.79
42	1	1528	PSU	O2-C2-N1	-3.58	118.85	122.79
37	2	534	OMG	C5-C6-N1	3.57	120.26	113.95
42	1	1659	OMU	C5-C4-N3	3.56	120.17	114.84
38	7	7	OMU	C5-C4-N3	3.56	120.16	114.84
42	1	239	PSU	O2-C2-N1	-3.56	118.88	122.79
29	S1	1550	OMG	C5-C6-N1	3.56	120.23	113.95
40	4	74	OMG	C5-C6-N1	3.54	120.21	113.95
29	S1	1246	PSU	O2-C2-N1	-3.54	118.90	122.79
37	2	1264	PSU	O2-C2-N1	-3.54	118.90	122.79
37	2	1318	PSU	C6-N1-C2	-3.53	119.07	122.68
29	S1	33	PSU	O2-C2-N1	-3.53	118.91	122.79
29	S1	1647	OMG	C5-C6-N1	3.51	120.15	113.95
29	S1	2151	OMG	C5-C6-N1	3.50	120.14	113.95
29	S1	1478	OMG	C5-C6-N1	3.50	120.13	113.95
29	S1	1539	PSU	O2-C2-N1	-3.49	118.94	122.79
37	2	662	PSU	C6-N1-C2	-3.49	119.11	122.68
37	2	1060	PSU	O2-C2-N1	-3.49	118.95	122.79
29	S1	661	OMU	C5-C4-N3	3.48	120.04	114.84
37	2	1419	OMU	C5-C4-N3	3.47	120.03	114.84
42	1	1664	PSU	O2-C2-N1	-3.46	118.98	122.79
29	S1	1979	OMU	C5-C4-N3	3.46	120.02	114.84
29	S1	1865	OMG	C5-C6-N1	3.46	120.06	113.95
38	7	69	PSU	O2-C2-N1	-3.46	118.98	122.79
37	2	1152	OMU	C5-C4-N3	3.45	120.01	114.84
29	S1	1192	PSU	O2-C2-N1	-3.45	118.99	122.79
37	2	597	PSU	O2-C2-N1	-3.45	118.99	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1841	PSU	O2-C2-N1	-3.45	119.00	122.79
29	S1	607	PSU	O2-C2-N1	-3.44	119.00	122.79
37	2	1046	OMG	C5-C6-N1	3.43	120.02	113.95
37	2	78	PSU	O2-C2-N1	-3.42	119.02	122.79
29	S1	1533	PSU	O2-C2-N1	-3.42	119.03	122.79
29	S1	600	OMG	C5-C6-N1	3.41	119.97	113.95
37	2	1303	PSU	O2-C2-N1	-3.40	119.05	122.79
37	2	560	OMU	C5-C4-N3	3.40	119.92	114.84
37	2	1413	PSU	C6-N1-C2	-3.37	119.23	122.68
37	2	472	PSU	O2-C2-N1	-3.36	119.10	122.79
29	S1	512	A2M	N3-C2-N1	-3.35	123.44	128.68
42	1	1664	PSU	C3'-C2'-C1'	3.35	105.54	101.64
29	S1	1829	OMG	C5-C6-N1	3.35	119.86	113.95
37	2	1403	PSU	C3'-C2'-C1'	3.34	105.53	101.64
37	2	626	PSU	C6-N1-C2	-3.34	119.27	122.68
29	S1	8	OMU	C5-C4-N3	3.34	119.84	114.84
37	2	593	PSU	C3'-C2'-C1'	3.34	105.53	101.64
37	2	1058	PSU	O2-C2-N1	-3.34	119.12	122.79
29	S1	1544	5MC	C5-C6-N1	-3.31	119.94	123.34
29	S1	609	PSU	C3'-C2'-C1'	3.30	105.48	101.64
42	1	959[A]	OMG	C5-C6-N1	3.30	119.78	113.95
42	1	845	OMU	C5-C4-N3	3.29	119.76	114.84
37	2	1403	PSU	O2-C2-N1	-3.28	119.18	122.79
37	2	591	A2M	N3-C2-N1	-3.24	123.61	128.68
42	1	1533	PSU	C3'-C2'-C1'	3.24	105.41	101.64
37	2	1194	PSU	C6-N1-C2	-3.24	119.37	122.68
42	1	940	PSU	C6-N1-C2	-3.23	119.38	122.68
37	2	437	PSU	C6-N1-C2	-3.22	119.39	122.68
42	1	1524	OMG	C2-N1-C6	-3.22	119.17	125.10
37	2	593	PSU	O2-C2-N1	-3.21	119.25	122.79
29	S1	1841	PSU	C3'-C2'-C1'	3.18	105.34	101.64
38	7	74	PSU	O2-C2-N1	-3.18	119.29	122.79
37	2	1253	OMG	C2-N1-C6	-3.17	119.26	125.10
42	1	959[B]	OMG	C5-C6-N1	3.15	119.52	113.95
37	2	512	PSU	C6-N1-C2	-3.14	119.47	122.68
29	S1	104	PSU	C6-N1-C2	-3.11	119.50	122.68
29	S1	609	PSU	O2-C2-N1	-3.11	119.37	122.79
29	S1	2061	5MC	C5-C6-N1	-3.10	120.15	123.34
29	S1	2046	PSU	O2-C2-N1	-3.09	119.39	122.79
29	S1	1156	PSU	O2-C2-N1	-3.09	119.39	122.79
42	1	672	PSU	C3'-C2'-C1'	3.08	105.23	101.64
29	S1	1979	OMU	O4-C4-C5	-3.08	119.75	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	1011	PSU	C6-C5-C4	3.07	120.35	118.20
37	2	655	OMG	C2-N1-C6	-3.06	119.46	125.10
42	1	1528	PSU	C3'-C2'-C1'	3.06	105.20	101.64
37	2	1354	PSU	C6-N1-C2	-3.06	119.56	122.68
29	S1	455	PSU	C6-N1-C2	-3.05	119.57	122.68
37	2	510	PSU	C6-N1-C2	-3.02	119.59	122.68
42	1	239	PSU	C3'-C2'-C1'	3.02	105.15	101.64
37	2	641	OMG	C2-N1-C6	-3.02	119.55	125.10
29	S1	1995	G7M	C2-N1-C6	-3.00	119.56	125.10
29	S1	1566	PSU	C6-N1-C2	-3.00	119.61	122.68
42	1	1181	PSU	C3'-C2'-C1'	3.00	105.13	101.64
29	S1	2046	PSU	C3'-C2'-C1'	2.99	105.12	101.64
29	S1	1478	OMG	C2-N1-C6	-2.99	119.59	125.10
29	S1	2151	OMG	C2-N1-C6	-2.99	119.59	125.10
42	1	845	OMU	O2-C2-N3	-2.99	115.94	121.50
29	S1	1879	OMG	C2-N1-C6	-2.96	119.65	125.10
37	2	655	OMG	C8-N7-C5	2.95	108.61	102.99
29	S1	1550	OMG	C2-N1-C6	-2.94	119.69	125.10
42	1	1659	OMU	O4-C4-C5	-2.94	120.00	125.16
37	2	534	OMG	C2-N1-C6	-2.93	119.70	125.10
37	2	1360	OMG	C2-N1-C6	-2.93	119.71	125.10
42	1	1626	OMG	C2-N1-C6	-2.93	119.71	125.10
37	2	1078	OMG	C2-N1-C6	-2.92	119.72	125.10
37	2	1229	OMG	C2-N1-C6	-2.92	119.72	125.10
42	1	870	PSU	C6-N1-C2	-2.92	119.70	122.68
38	7	74	PSU	C3'-C2'-C1'	2.92	105.03	101.64
37	2	1046	OMG	C8-N7-C5	2.91	108.53	102.99
37	2	1382	PSU	C6-N1-C2	-2.90	119.72	122.68
37	2	73	OMU	O4-C4-C5	-2.90	120.06	125.16
37	2	1046	OMG	C2-N1-C6	-2.89	119.77	125.10
29	S1	12	PSU	C6-N1-C2	-2.89	119.73	122.68
42	1	847	OMU	O4-C4-C5	-2.89	120.08	125.16
37	2	1419	OMU	O4-C4-C5	-2.88	120.09	125.16
29	S1	1879	OMG	C8-N7-C5	2.88	108.47	102.99
42	1	940	PSU	O2-C2-N1	-2.88	119.62	122.79
42	1	1190	OMG	C8-N7-C5	2.87	108.47	102.99
42	1	1190	OMG	C2-N1-C6	-2.87	119.81	125.10
29	S1	600	OMG	C2-N1-C6	-2.87	119.81	125.10
29	S1	661	OMU	O4-C4-C5	-2.86	120.12	125.16
29	S1	1829	OMG	C2-N1-C6	-2.86	119.83	125.10
38	7	7	OMU	O4-C4-C5	-2.85	120.14	125.16
42	1	1011	PSU	C6-N1-C2	-2.85	119.77	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1647	OMG	C2-N1-C6	-2.84	119.86	125.10
37	2	1231	OMG	C2-N1-C6	-2.84	119.87	125.10
37	2	1359	OMU	O4-C4-C5	-2.84	120.17	125.16
40	4	74	OMG	C2-N1-C6	-2.83	119.88	125.10
29	S1	2151	OMG	C8-N7-C5	2.83	108.39	102.99
29	S1	600	OMG	C8-N7-C5	2.83	108.38	102.99
42	1	959[B]	OMG	C2-N1-C6	-2.83	119.89	125.10
37	2	667	OMU	O4-C4-C5	-2.82	120.19	125.16
42	1	1524	OMG	C8-N7-C5	2.81	108.35	102.99
37	2	1229	OMG	C8-N7-C5	2.81	108.35	102.99
42	1	959[A]	OMG	C8-N7-C5	2.81	108.35	102.99
37	2	597	PSU	C3'-C2'-C1'	2.81	104.90	101.64
37	2	1361	PSU	C6-N1-C2	-2.80	119.82	122.68
29	S1	1865	OMG	C2-N1-C6	-2.79	119.96	125.10
41	3	13	OMU	O4-C4-C5	-2.79	120.25	125.16
37	2	1078	OMG	C8-N7-C5	2.79	108.30	102.99
37	2	1231	OMG	C8-N7-C5	2.78	108.28	102.99
29	S1	2061	5MC	C5-C4-N3	-2.78	118.68	121.67
29	S1	1647	OMG	C8-N7-C5	2.77	108.27	102.99
29	S1	1550	OMG	C8-N7-C5	2.76	108.26	102.99
37	2	1060	PSU	C3'-C2'-C1'	2.75	104.83	101.64
42	1	1626	OMG	C8-N7-C5	2.74	108.22	102.99
29	S1	1478	OMG	C8-N7-C5	2.74	108.21	102.99
29	S1	8	OMU	O4-C4-C5	-2.74	120.34	125.16
37	2	641	OMG	N2-C2-N1	2.74	122.54	116.71
29	S1	1865	OMG	O6-C6-C5	-2.74	119.03	124.37
37	2	560	OMU	O4-C4-C5	-2.73	120.36	125.16
42	1	1107	OMU	O4-C4-C5	-2.72	120.37	125.16
42	1	1524	OMG	N2-C2-N1	2.71	122.49	116.71
37	2	641	OMG	C8-N7-C5	2.70	108.14	102.99
42	1	1371	OMU	O4-C4-C5	-2.70	120.41	125.16
40	4	74	OMG	C8-N7-C5	2.69	108.11	102.99
37	2	1078	OMG	N2-C2-N1	2.68	122.42	116.71
37	2	591	A2M	C4-C5-N7	-2.67	106.62	109.40
29	S1	1865	OMG	C8-N7-C5	2.66	108.06	102.99
37	2	472	PSU	C3'-C2'-C1'	2.65	104.72	101.64
29	S1	33	PSU	C3'-C2'-C1'	2.65	104.72	101.64
42	1	959[A]	OMG	C2-N1-C6	-2.64	120.23	125.10
37	2	1077	OMU	O4-C4-C5	-2.63	120.53	125.16
42	1	856	OMG	C8-N7-C5	2.63	108.01	102.99
29	S1	1539	PSU	C3'-C2'-C1'	2.63	104.70	101.64
29	S1	1829	OMG	C8-N7-C5	2.62	107.99	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1152	OMU	O4-C4-C5	-2.62	120.56	125.16
29	S1	12	PSU	C6-C5-C4	2.61	120.02	118.20
37	2	1360	OMG	C8-N7-C5	2.60	107.95	102.99
42	1	1540	OMG	C2-N1-C6	-2.59	120.33	125.10
37	2	570	A2M	O2'-C2'-C1'	2.59	114.23	109.09
29	S1	2061	5MC	C2'-C1'-N1	-2.59	105.89	113.22
37	2	512	PSU	C6-C5-C4	2.58	120.00	118.20
37	2	78	PSU	C3'-C2'-C1'	2.58	104.64	101.64
41	3	13	OMU	O2-C2-N3	-2.56	116.73	121.50
42	1	1540	OMG	C8-N7-C5	2.56	107.86	102.99
29	S1	104	PSU	O2-C2-N1	-2.55	119.98	122.79
42	1	1626	OMG	N2-C2-N1	2.54	122.12	116.71
37	2	1144	PSU	C3'-C2'-C1'	2.53	104.58	101.64
37	2	71	OMG	C5-C6-N1	2.53	118.41	113.95
29	S1	455	PSU	O2-C2-N1	-2.52	120.01	122.79
29	S1	512	A2M	C4-C5-N7	-2.52	106.77	109.40
37	2	1058	PSU	C3'-C2'-C1'	2.52	104.57	101.64
42	1	845	OMU	C6-C5-C4	2.52	122.96	119.52
29	S1	2048	PSU	C3'-C2'-C1'	2.52	104.57	101.64
37	2	1253	OMG	C8-N7-C5	2.52	107.78	102.99
37	2	626	PSU	O2-C2-N1	-2.52	120.02	122.79
42	1	856	OMG	C2-N1-C6	-2.52	120.47	125.10
37	2	534	OMG	C8-N7-C5	2.50	107.76	102.99
29	S1	2048	PSU	C5-C6-N1	-2.50	118.36	122.11
42	1	1171	PSU	C5-C4-N3	2.50	122.23	116.58
37	2	512	PSU	O2-C2-N1	-2.50	120.04	122.79
37	2	1194	PSU	O2-C2-N1	-2.50	120.04	122.79
42	1	1540	OMG	N2-C2-N1	2.49	122.02	116.71
37	2	1248	OMC	O2-C2-N3	-2.49	118.29	122.33
37	2	641	OMG	O6-C6-C5	-2.47	119.55	124.37
42	1	856	OMG	N2-C2-N1	2.47	121.97	116.71
29	S1	1533	PSU	C3'-C2'-C1'	2.47	104.51	101.64
37	2	1144	PSU	C5-C6-N1	-2.46	118.41	122.11
37	2	437	PSU	C6-C5-C4	2.46	119.92	118.20
37	2	1229	OMG	O6-C6-C5	-2.46	119.57	124.37
29	S1	1623	OMG	C8-N7-C5	2.44	107.64	102.99
37	2	71	OMG	C8-N7-C5	2.44	107.64	102.99
37	2	472	PSU	C5-C6-N1	-2.44	118.45	122.11
37	2	1152	OMU	O2-C2-N1	-2.44	119.55	122.79
42	1	856	OMG	N1-C2-N3	-2.44	118.77	123.32
37	2	1354	PSU	O2-C2-N1	-2.44	120.11	122.79
40	4	74	OMG	N2-C2-N1	2.44	121.90	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	3	13	OMU	C1'-N1-C6	-2.43	115.54	120.84
38	7	75	OMG	C5-C6-N1	2.43	118.24	113.95
29	S1	1192	PSU	C5-C6-N1	-2.42	118.49	122.11
29	S1	104	PSU	C6-C5-C4	2.41	119.88	118.20
38	7	75	OMG	C8-N7-C5	2.40	107.56	102.99
29	S1	12	PSU	O2-C2-N1	-2.40	120.15	122.79
37	2	1354	PSU	C6-C5-C4	2.38	119.86	118.20
37	2	1308	5MC	C3'-C2'-C1'	2.37	105.94	101.43
37	2	510	PSU	O2-C2-N1	-2.37	120.19	122.79
37	2	572	A2M	O4'-C1'-C2'	-2.37	102.48	106.59
29	S1	1543	C4J	N3-C2-N1	2.36	120.09	116.76
42	1	1524	OMG	O6-C6-C5	-2.35	119.77	124.37
37	2	1360	OMG	O6-C6-C5	-2.35	119.79	124.37
29	S1	1647	OMG	O6-C6-C5	-2.35	119.79	124.37
29	S1	1550	OMG	O6-C6-C5	-2.34	119.79	124.37
37	2	1229	OMG	N2-C2-N1	2.34	121.70	116.71
42	1	847	OMU	O2-C2-N1	-2.34	119.67	122.79
42	1	1371	OMU	O2-C2-N3	-2.34	117.14	121.50
37	2	1060	PSU	C5-C6-N1	-2.33	118.61	122.11
37	2	1253	OMG	O6-C6-C5	-2.33	119.81	124.37
42	1	1527	OMC	O2-C2-N3	-2.33	118.54	122.33
29	S1	1478	OMG	O6-C6-C5	-2.32	119.84	124.37
42	1	1011	PSU	O2-C2-N1	-2.32	120.24	122.79
37	2	1403	PSU	C5-C6-N1	-2.31	118.65	122.11
29	S1	609	PSU	C5-C6-N1	-2.30	118.66	122.11
37	2	1413	PSU	O2-C2-N1	-2.30	120.26	122.79
42	1	959[A]	OMG	O6-C6-C5	-2.30	119.88	124.37
42	1	1533	PSU	C5-C6-N1	-2.29	118.68	122.11
37	2	1231	OMG	O6-C6-C5	-2.28	119.91	124.37
42	1	1659	OMU	C1'-N1-C2	2.28	121.70	117.57
29	S1	1623	OMG	C5-C6-N1	2.28	117.98	113.95
42	1	1540	OMG	O6-C6-C5	-2.28	119.92	124.37
42	1	239	PSU	C5-C6-N1	-2.28	118.69	122.11
40	4	74	OMG	O6-C6-C5	-2.27	119.94	124.37
37	2	655	OMG	N2-C2-N1	2.27	121.54	116.71
29	S1	8	OMU	O2-C2-N1	-2.26	119.78	122.79
42	1	1017	PSU	C5-C6-N1	-2.26	118.72	122.11
37	2	593	PSU	C5-C6-N1	-2.26	118.72	122.11
37	2	437	PSU	O2-C2-N1	-2.25	120.31	122.79
42	1	1402	PSU	C6-N1-C2	-2.25	120.39	122.68
29	S1	1879	OMG	O6-C6-C5	-2.24	119.99	124.37
37	2	1077	OMU	O2-C2-N1	-2.24	119.81	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	1543	C4J	C5-C4-N3	2.24	120.32	116.17
29	S1	2151	OMG	O6-C6-C5	-2.23	120.01	124.37
29	S1	1539	PSU	C5-C6-N1	-2.23	118.76	122.11
37	2	1317	OMC	O2-C2-N3	-2.23	118.70	122.33
37	2	1318	PSU	O2-C2-N1	-2.22	120.34	122.79
38	7	69	PSU	C5-C6-N1	-2.22	118.78	122.11
42	1	672	PSU	C5-C6-N1	-2.21	118.80	122.11
42	1	1107	OMU	O2-C2-N1	-2.21	119.85	122.79
42	1	422	PSU	O3'-C3'-C2'	2.21	118.96	111.82
29	S1	1829	OMG	O6-C6-C5	-2.21	120.06	124.37
42	1	1171	PSU	C6-N1-C2	-2.20	120.43	122.68
42	1	1190	OMG	O6-C6-C5	-2.19	120.09	124.37
42	1	1171	PSU	O2-C2-N3	-2.19	117.69	121.82
42	1	959[B]	OMG	N2-C2-N1	2.19	121.37	116.71
42	1	1181	PSU	C5-C6-N1	-2.18	118.84	122.11
42	1	1402	PSU	C5-C4-N3	2.17	121.50	116.58
42	1	1540	OMG	N1-C2-N3	-2.17	119.26	123.32
29	S1	1246	PSU	C5-C6-N1	-2.16	118.87	122.11
29	S1	1979	OMU	O2-C2-N1	-2.16	119.92	122.79
42	1	959[B]	OMG	O6-C6-C5	-2.14	120.19	124.37
37	2	1229	OMG	N1-C2-N3	-2.14	119.32	123.32
42	1	422	PSU	C5-C6-N1	-2.14	118.91	122.11
29	S1	455	PSU	C6-C5-C4	2.14	119.69	118.20
29	S1	1657	PSU	C5-C6-N1	-2.13	118.91	122.11
37	2	1046	OMG	N2-C2-N1	2.12	121.24	116.71
37	2	662	PSU	O2-C2-N1	-2.12	120.46	122.79
37	2	1231	OMG	N2-C2-N1	2.12	121.22	116.71
37	2	78	PSU	C5-C6-N1	-2.12	118.94	122.11
42	1	1171	PSU	O4-C4-N3	-2.11	116.07	120.12
42	1	1539	A2M	O3'-C3'-C2'	-2.10	105.19	111.17
42	1	858	A2M	O4'-C4'-C3'	-2.10	100.96	105.11
37	2	1264	PSU	C5-C6-N1	-2.10	118.96	122.11
29	S1	1865	OMG	N2-C2-N1	2.09	121.17	116.71
29	S1	1544	5MC	CM5-C5-C6	-2.09	120.06	122.85
37	2	597	PSU	C5-C6-N1	-2.09	118.97	122.11
29	S1	1841	PSU	C5-C6-N1	-2.09	118.97	122.11
37	2	570	A2M	C3'-C2'-C1'	2.09	106.81	102.89
42	1	1171	PSU	O4'-C1'-C2'	2.08	108.08	105.14
29	S1	661	OMU	O2-C2-N1	-2.08	120.02	122.79
37	2	1303	PSU	C5-C6-N1	-2.08	118.99	122.11
42	1	1528	PSU	C5-C6-N1	-2.08	118.99	122.11
37	2	1058	PSU	C5-C6-N1	-2.08	118.99	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1361	PSU	C5-C4-N3	2.07	121.27	116.58
42	1	1010	OMC	CM2-O2'-C2'	2.07	119.96	114.52
29	S1	1533	PSU	C5-C6-N1	-2.07	119.01	122.11
42	1	1190	OMG	N2-C2-N1	2.06	121.11	116.71
29	S1	1246	PSU	C3'-C2'-C1'	2.06	104.04	101.64
37	2	1382	PSU	O4'-C1'-C2'	2.06	108.05	105.14
29	S1	600	OMG	O6-C6-C5	-2.06	120.35	124.37
42	1	1371	OMU	C1'-N1-C6	-2.06	116.35	120.84
42	1	695	OMC	O2-C2-N3	-2.06	118.99	122.33
37	2	1046	OMG	O6-C6-C5	-2.05	120.36	124.37
29	S1	607	PSU	O4'-C1'-C2'	2.04	108.03	105.14
37	2	534	OMG	O6-C6-C5	-2.04	120.38	124.37
37	2	667	OMU	O2-C2-N1	-2.04	120.07	122.79
42	1	1626	OMG	O6-C6-C5	-2.04	120.38	124.37
42	1	407	A2M	C5'-C4'-C3'	-2.04	107.55	115.18
37	2	1419	OMU	C1'-N1-C2	2.03	121.24	117.57
42	1	1017	PSU	C3'-C2'-C1'	2.03	104.00	101.64
42	1	845	OMU	O4-C4-C5	-2.02	121.61	125.16
29	S1	512	A2M	C2-N1-C6	2.02	122.21	118.75
37	2	534	OMG	N2-C2-N1	2.02	121.01	116.71
29	S1	1543	C4J	O35-C34-C32	2.02	120.26	113.38
42	1	870	PSU	O2-C2-N1	-2.02	120.57	122.79
38	7	74	PSU	C5-C6-N1	-2.01	119.09	122.11
37	2	1078	OMG	O6-C6-C5	-2.01	120.44	124.37
42	1	959[B]	OMG	C8-N7-C5	2.01	106.82	102.99
37	2	1231	OMG	N1-C2-N3	-2.01	119.56	123.32
37	2	73	OMU	C2'-C1'-N1	-2.00	110.34	114.22

There are no chirality outliers.

All (170) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	71	OMG	C1'-C2'-O2'-CM2
37	2	73	OMU	C1'-C2'-O2'-CM2
37	2	78	PSU	O4'-C4'-C5'-O5'
37	2	437	PSU	C3'-C4'-C5'-O5'
37	2	437	PSU	O4'-C4'-C5'-O5'
37	2	443	OMC	C2'-C1'-N1-C2
37	2	443	OMC	C2'-C1'-N1-C6
37	2	510	PSU	O4'-C1'-C5-C4
37	2	510	PSU	O4'-C1'-C5-C6
37	2	510	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
37	2	510	PSU	O4'-C4'-C5'-O5'
37	2	534	OMG	O4'-C4'-C5'-O5'
37	2	534	OMG	C3'-C4'-C5'-O5'
37	2	570	A2M	C1'-C2'-O2'-CM'
37	2	591	A2M	C1'-C2'-O2'-CM'
37	2	604	A2M	C1'-C2'-O2'-CM'
37	2	667	OMU	C1'-C2'-O2'-CM2
37	2	1046	OMG	O4'-C4'-C5'-O5'
37	2	1046	OMG	C1'-C2'-O2'-CM2
37	2	1060	PSU	O4'-C4'-C5'-O5'
37	2	1361	PSU	O4'-C1'-C5-C4
37	2	1361	PSU	O4'-C1'-C5-C6
38	7	75	OMG	O4'-C4'-C5'-O5'
38	7	75	OMG	C3'-C4'-C5'-O5'
38	7	75	OMG	C1'-C2'-O2'-CM2
38	7	162	A2M	C1'-C2'-O2'-CM'
41	3	13	OMU	O4'-C1'-N1-C2
41	3	13	OMU	O4'-C1'-N1-C6
42	1	407	A2M	O4'-C4'-C5'-O5'
42	1	407	A2M	C3'-C4'-C5'-O5'
42	1	672	PSU	O4'-C4'-C5'-O5'
42	1	681	A2M	O4'-C4'-C5'-O5'
42	1	695	OMC	C3'-C4'-C5'-O5'
42	1	695	OMC	O4'-C4'-C5'-O5'
42	1	845	OMU	O4'-C1'-N1-C2
42	1	845	OMU	O4'-C1'-N1-C6
42	1	959[A]	OMG	O4'-C4'-C5'-O5'
42	1	959[A]	OMG	C3'-C4'-C5'-O5'
42	1	1010	OMC	C1'-C2'-O2'-CM2
42	1	1107	OMU	C3'-C4'-C5'-O5'
42	1	1107	OMU	O4'-C4'-C5'-O5'
42	1	1171	PSU	O4'-C1'-C5-C4
42	1	1171	PSU	O4'-C1'-C5-C6
42	1	1181	PSU	C3'-C4'-C5'-O5'
42	1	1371	OMU	O4'-C1'-N1-C2
42	1	1371	OMU	O4'-C1'-N1-C6
42	1	1371	OMU	C3'-C4'-C5'-O5'
42	1	1402	PSU	C2'-C1'-C5-C4
42	1	1402	PSU	O4'-C1'-C5-C4
42	1	1402	PSU	O4'-C1'-C5-C6
42	1	1402	PSU	C3'-C4'-C5'-O5'
42	1	1402	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
42	1	1540	OMG	O4'-C4'-C5'-O5'
42	1	1540	OMG	C3'-C4'-C5'-O5'
42	1	1664	PSU	C3'-C4'-C5'-O5'
29	S1	33	PSU	O4'-C1'-C5-C4
29	S1	33	PSU	O4'-C1'-C5-C6
29	S1	104	PSU	C3'-C4'-C5'-O5'
29	S1	104	PSU	O4'-C4'-C5'-O5'
29	S1	455	PSU	C2'-C1'-C5-C4
29	S1	455	PSU	O4'-C1'-C5-C4
29	S1	455	PSU	O4'-C1'-C5-C6
29	S1	512	A2M	O4'-C4'-C5'-O5'
29	S1	512	A2M	C1'-C2'-O2'-CM'
29	S1	600	OMG	O4'-C4'-C5'-O5'
29	S1	607	PSU	O4'-C1'-C5-C6
29	S1	607	PSU	C4'-C5'-O5'-P
29	S1	668	A2M	C1'-C2'-O2'-CM'
29	S1	1543	C4J	N3-C3-C31-C32
29	S1	1543	C4J	C3-C31-C32-N33
29	S1	1543	C4J	N33-C32-C34-O36
29	S1	1544	5MC	O4'-C4'-C5'-O5'
29	S1	1544	5MC	C3'-C4'-C5'-O5'
29	S1	1550	OMG	C3'-C4'-C5'-O5'
29	S1	1566	PSU	C3'-C4'-C5'-O5'
29	S1	1623	OMG	C1'-C2'-O2'-CM2
29	S1	1657	PSU	O4'-C1'-C5-C6
29	S1	1841	PSU	O4'-C1'-C5-C4
29	S1	1841	PSU	C2'-C1'-C5-C6
29	S1	1841	PSU	O4'-C1'-C5-C6
29	S1	1979	OMU	C1'-C2'-O2'-CM2
29	S1	2021	A2M	C1'-C2'-O2'-CM'
29	S1	2046	PSU	O4'-C1'-C5-C4
29	S1	2046	PSU	O4'-C1'-C5-C6
29	S1	2140	OMC	C3'-C4'-C5'-O5'
29	S1	2151	OMG	O4'-C4'-C5'-O5'
29	S1	2151	OMG	C3'-C4'-C5'-O5'
37	2	78	PSU	C3'-C4'-C5'-O5'
37	2	512	PSU	O4'-C4'-C5'-O5'
37	2	1046	OMG	C3'-C4'-C5'-O5'
37	2	1060	PSU	C3'-C4'-C5'-O5'
37	2	1185	A2M	C3'-C4'-C5'-O5'
42	1	672	PSU	C3'-C4'-C5'-O5'
42	1	681	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
42	1	1527	OMC	O4'-C4'-C5'-O5'
42	1	1528	PSU	O4'-C4'-C5'-O5'
29	S1	512	A2M	C3'-C4'-C5'-O5'
29	S1	600	OMG	C3'-C4'-C5'-O5'
29	S1	668	A2M	C3'-C4'-C5'-O5'
29	S1	1550	OMG	O4'-C4'-C5'-O5'
29	S1	1566	PSU	O4'-C4'-C5'-O5'
29	S1	2140	OMC	O4'-C4'-C5'-O5'
37	2	512	PSU	C3'-C4'-C5'-O5'
37	2	570	A2M	O4'-C4'-C5'-O5'
37	2	570	A2M	C3'-C4'-C5'-O5'
37	2	597	PSU	O4'-C4'-C5'-O5'
42	1	1011	PSU	O4'-C4'-C5'-O5'
42	1	1181	PSU	O4'-C4'-C5'-O5'
42	1	1371	OMU	O4'-C4'-C5'-O5'
42	1	1528	PSU	C3'-C4'-C5'-O5'
29	S1	33	PSU	C3'-C4'-C5'-O5'
29	S1	607	PSU	O4'-C4'-C5'-O5'
29	S1	1543	C4J	N33-C32-C34-O35
37	2	1308	5MC	C2'-C1'-N1-C6
29	S1	8	OMU	C2'-C1'-N1-C6
42	1	1527	OMC	C3'-C4'-C5'-O5'
29	S1	607	PSU	C3'-C4'-C5'-O5'
37	2	1185	A2M	O4'-C4'-C5'-O5'
42	1	422	PSU	O4'-C4'-C5'-O5'
42	1	1664	PSU	O4'-C4'-C5'-O5'
29	S1	668	A2M	O4'-C4'-C5'-O5'
29	S1	1995	G7M	O4'-C4'-C5'-O5'
38	7	74	PSU	C3'-C4'-C5'-O5'
42	1	422	PSU	C3'-C4'-C5'-O5'
42	1	1011	PSU	C3'-C4'-C5'-O5'
29	S1	1543	C4J	C31-C3-N3-C4
42	1	1626	OMG	O4'-C4'-C5'-O5'
37	2	597	PSU	C3'-C4'-C5'-O5'
29	S1	33	PSU	O4'-C4'-C5'-O5'
37	2	560	OMU	C4'-C5'-O5'-P
37	2	1361	PSU	C4'-C5'-O5'-P
38	7	74	PSU	O4'-C4'-C5'-O5'
29	S1	1995	G7M	C3'-C4'-C5'-O5'
29	S1	1543	C4J	C3-C31-C32-C34
42	1	235	A2M	C3'-C2'-O2'-CM'
37	2	1308	5MC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
37	2	1308	5MC	O4'-C1'-N1-C6
29	S1	8	OMU	O4'-C1'-N1-C6
37	2	443	OMC	O4'-C1'-N1-C2
37	2	443	OMC	C4'-C5'-O5'-P
29	S1	1543	C4J	C4'-C5'-O5'-P
37	2	1144	PSU	O4'-C4'-C5'-O5'
37	2	443	OMC	O4'-C1'-N1-C6
29	S1	8	OMU	O4'-C4'-C5'-O5'
29	S1	8	OMU	C2'-C1'-N1-C2
41	3	13	OMU	C4'-C5'-O5'-P
37	2	1308	5MC	O4'-C1'-N1-C2
29	S1	8	OMU	O4'-C1'-N1-C2
29	S1	607	PSU	O4'-C1'-C5-C4
29	S1	1657	PSU	O4'-C1'-C5-C4
37	2	1077	OMU	C3'-C2'-O2'-CM2
42	1	1524	OMG	C3'-C2'-O2'-CM2
29	S1	8	OMU	C3'-C2'-O2'-CM2
42	1	1181	PSU	C4'-C5'-O5'-P
37	2	583	OMC	O4'-C4'-C5'-O5'
42	1	870	PSU	O4'-C4'-C5'-O5'
42	1	1539	A2M	O4'-C4'-C5'-O5'
29	S1	2021	A2M	C3'-C4'-C5'-O5'
29	S1	1543	C4J	C31-C3-N3-C2
37	2	1058	PSU	O4'-C4'-C5'-O5'
42	1	1533	PSU	O4'-C4'-C5'-O5'
37	2	1077	OMU	C1'-C2'-O2'-CM2
29	S1	1865	OMG	C1'-C2'-O2'-CM2
42	1	305	A2M	O4'-C4'-C5'-O5'
29	S1	18	OMC	O4'-C4'-C5'-O5'
37	2	1248	OMC	C2'-C1'-N1-C2
37	2	1144	PSU	C3'-C4'-C5'-O5'
42	1	1524	OMG	C3'-C4'-C5'-O5'
29	S1	1829	OMG	O4'-C4'-C5'-O5'
37	2	510	PSU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 188 ligands modelled in this entry, 188 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

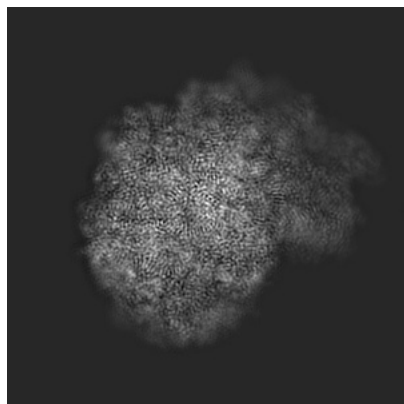
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15124. These allow visual inspection of the internal detail of the map and identification of artifacts.

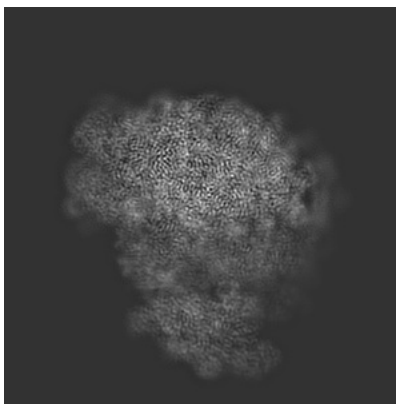
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

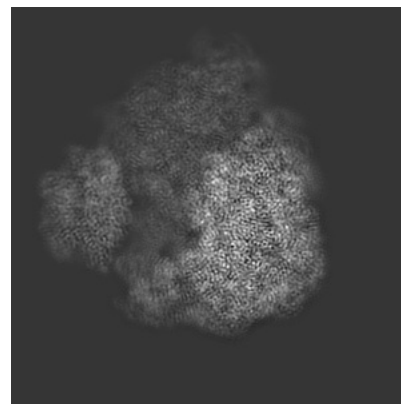
6.1.1 Primary map



X

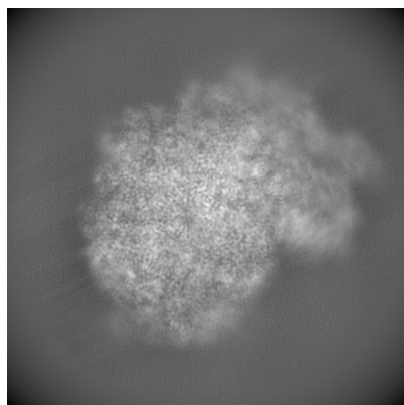


Y

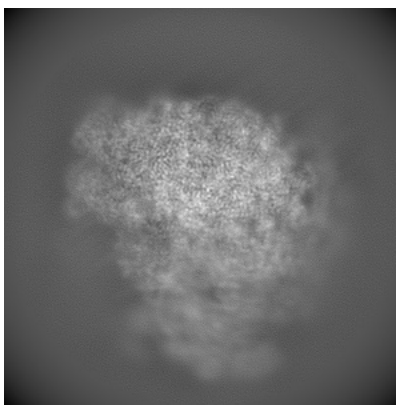


Z

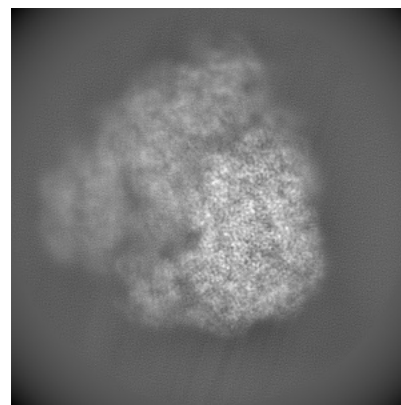
6.1.2 Raw map



X



Y

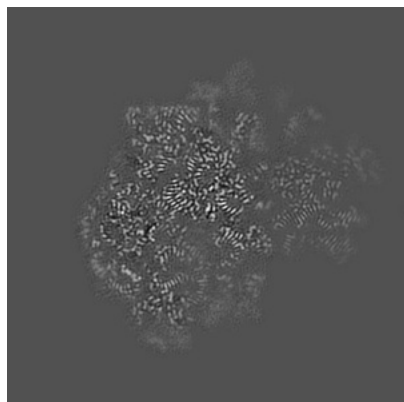


Z

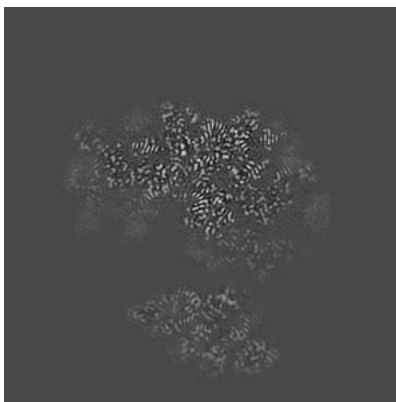
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

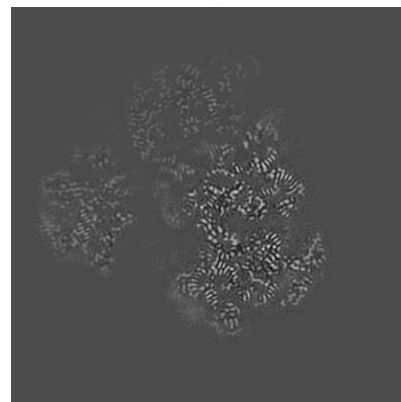
6.2.1 Primary map



X Index: 220

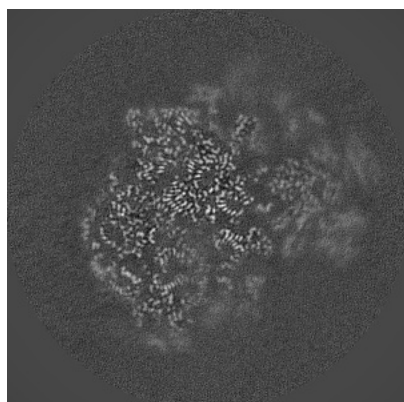


Y Index: 220

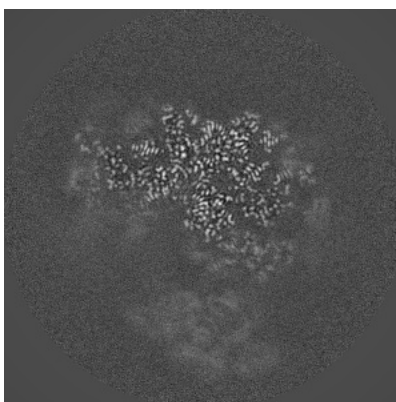


Z Index: 220

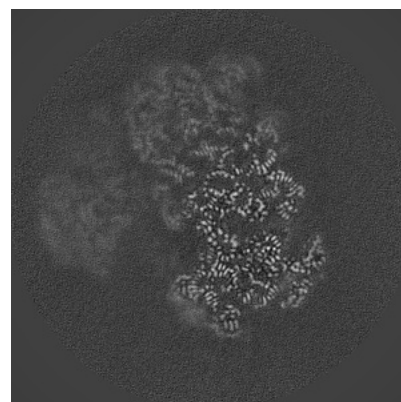
6.2.2 Raw map



X Index: 220



Y Index: 220

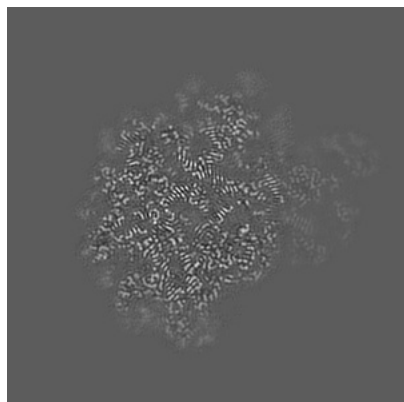


Z Index: 220

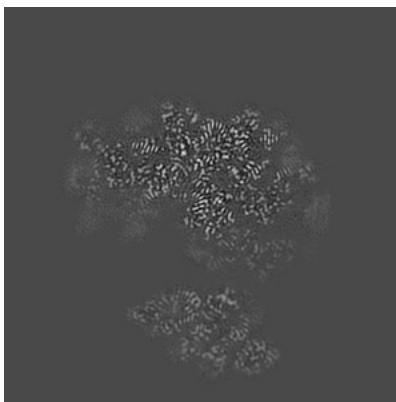
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

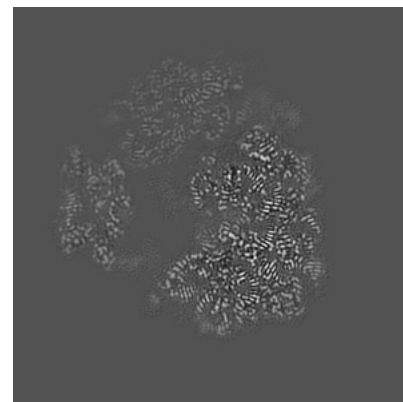
6.3.1 Primary map



X Index: 255

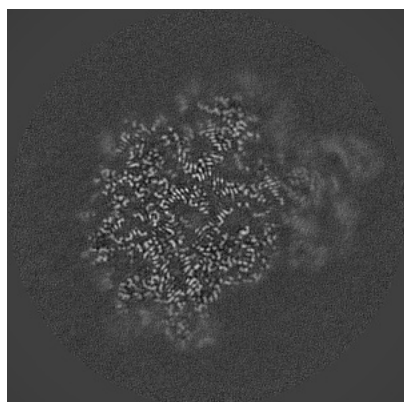


Y Index: 220

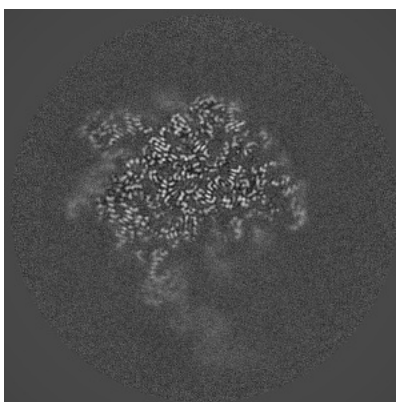


Z Index: 198

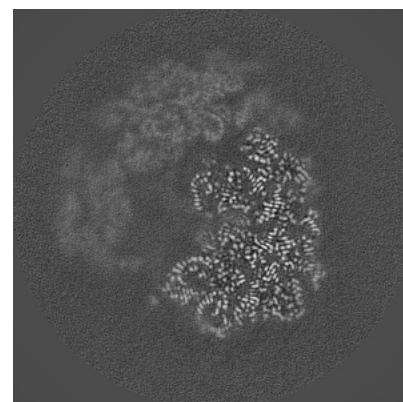
6.3.2 Raw map



X Index: 255



Y Index: 162

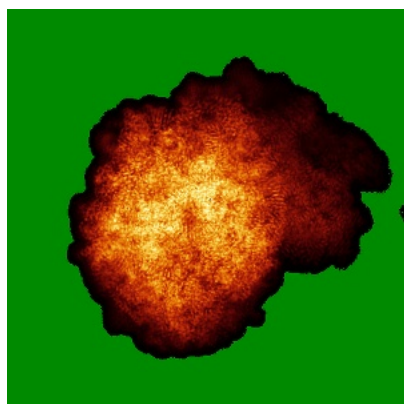


Z Index: 199

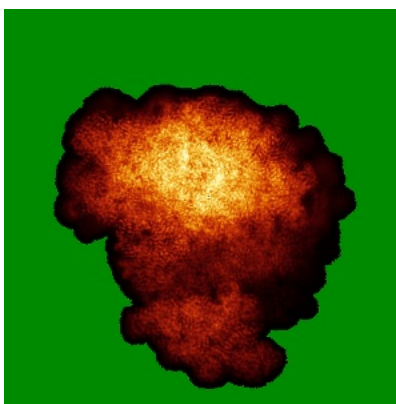
The images above show the largest variance slices of the map in three orthogonal directions.

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

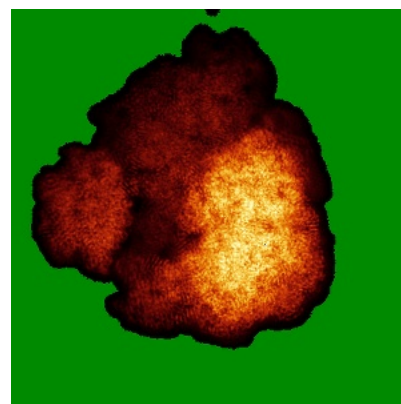
6.4.1 Primary map



X

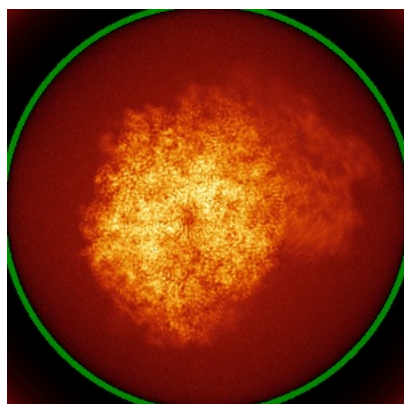


Y

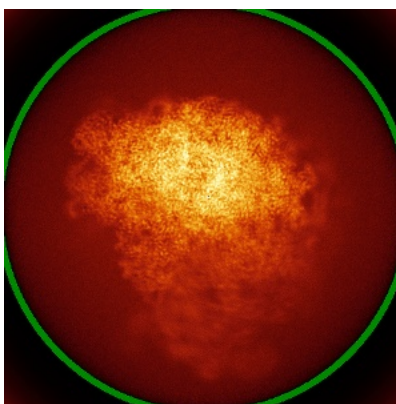


Z

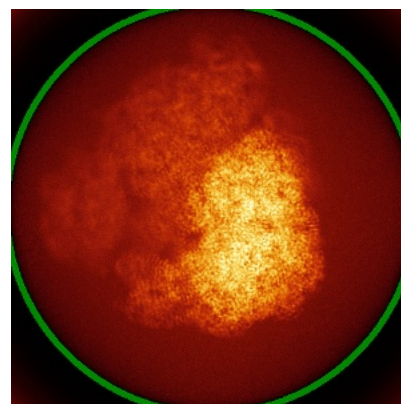
6.4.2 Raw map



X



Y

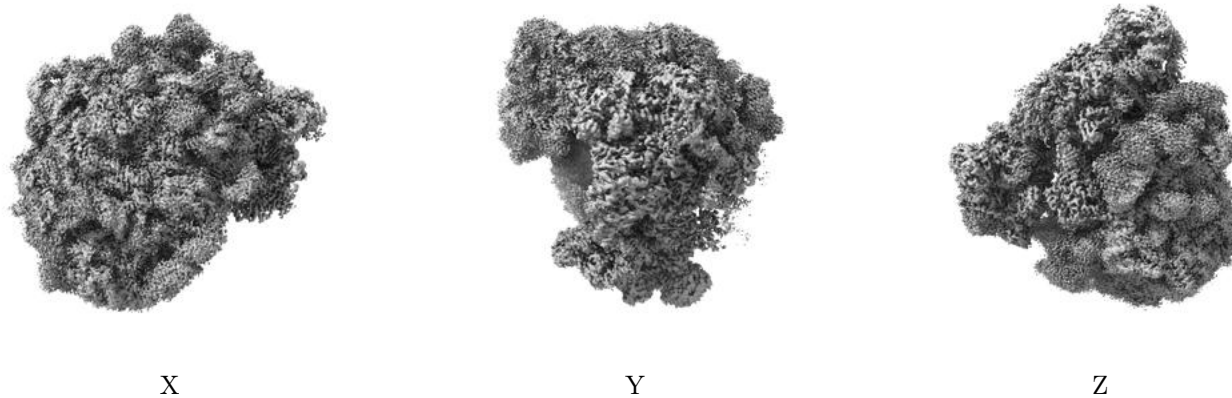


Z

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.

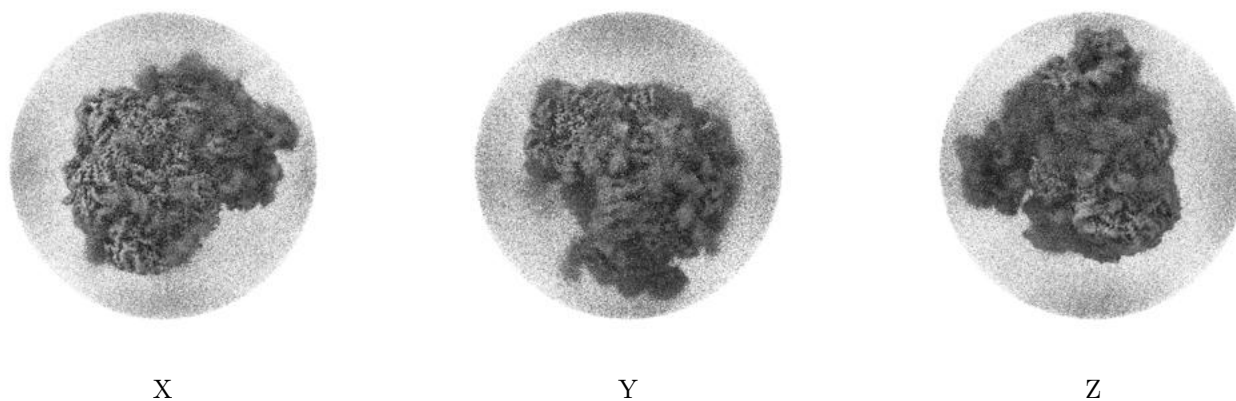
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

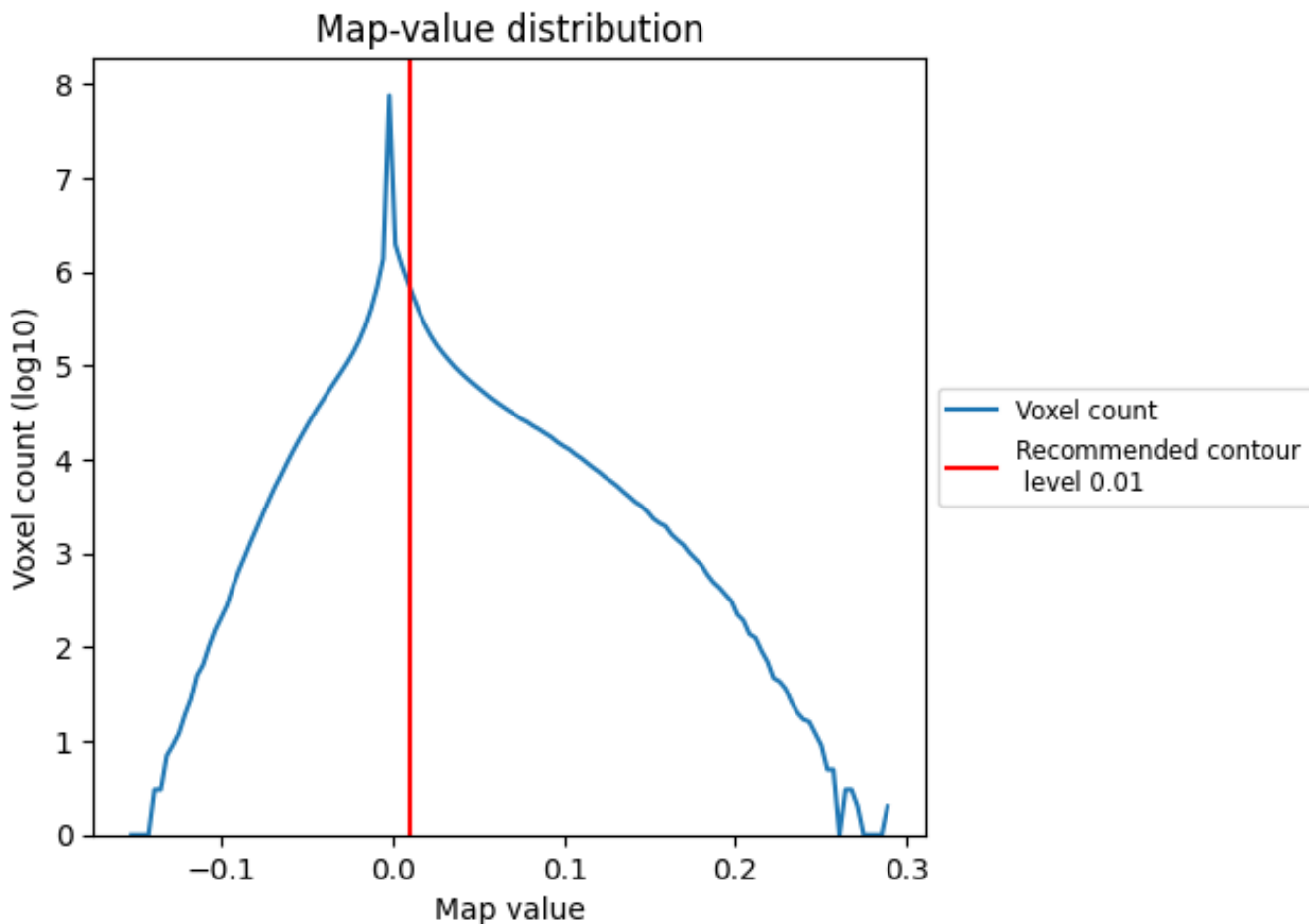
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

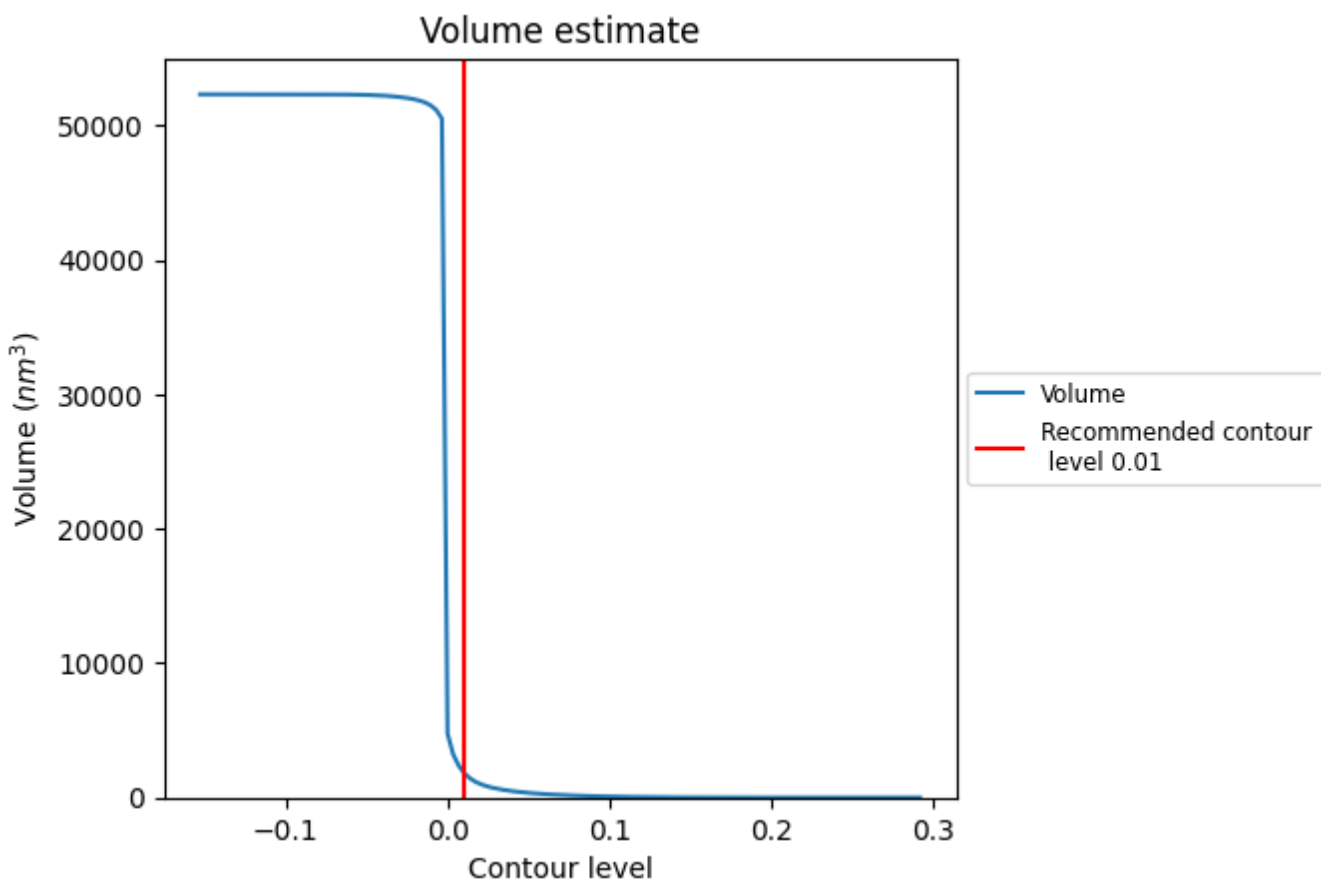
This section contains the results of statistical analysis of the map.

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.

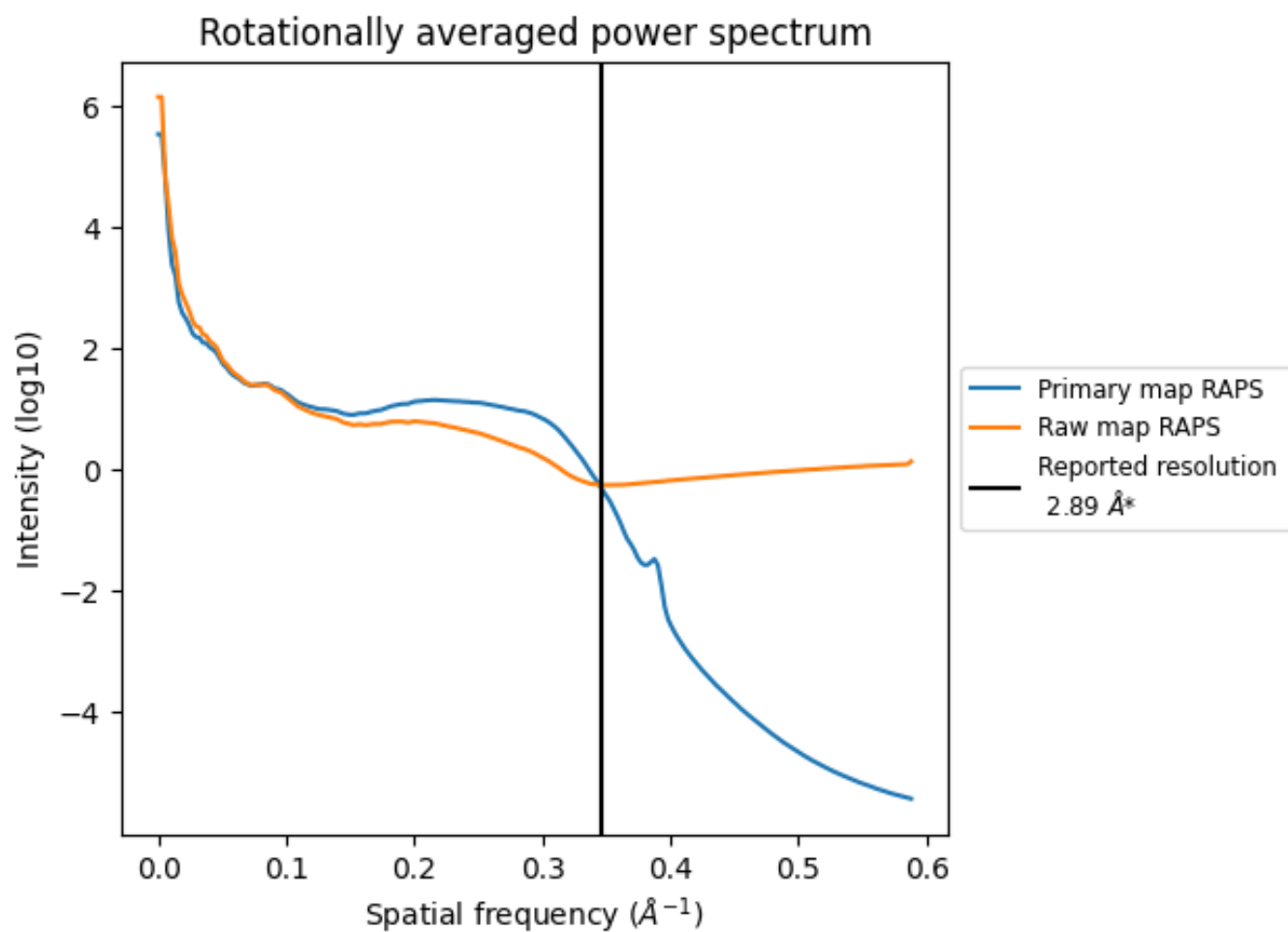
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1903 nm³; this corresponds to an approximate mass of 1719 kDa.

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

7.3 Rotationally averaged power spectrum i

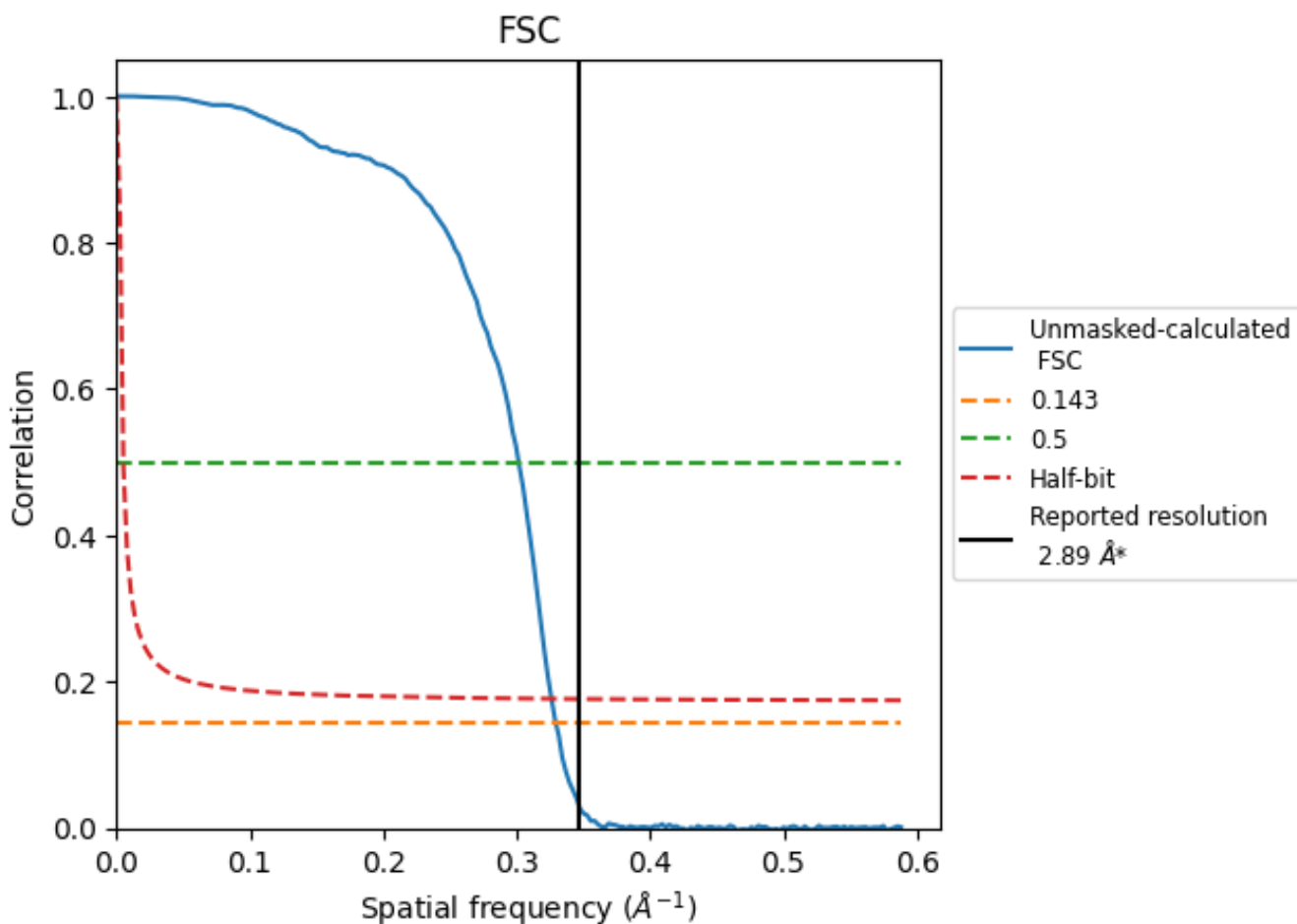


*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.346 \AA^{-1}

8.2 Resolution estimates [i](#)

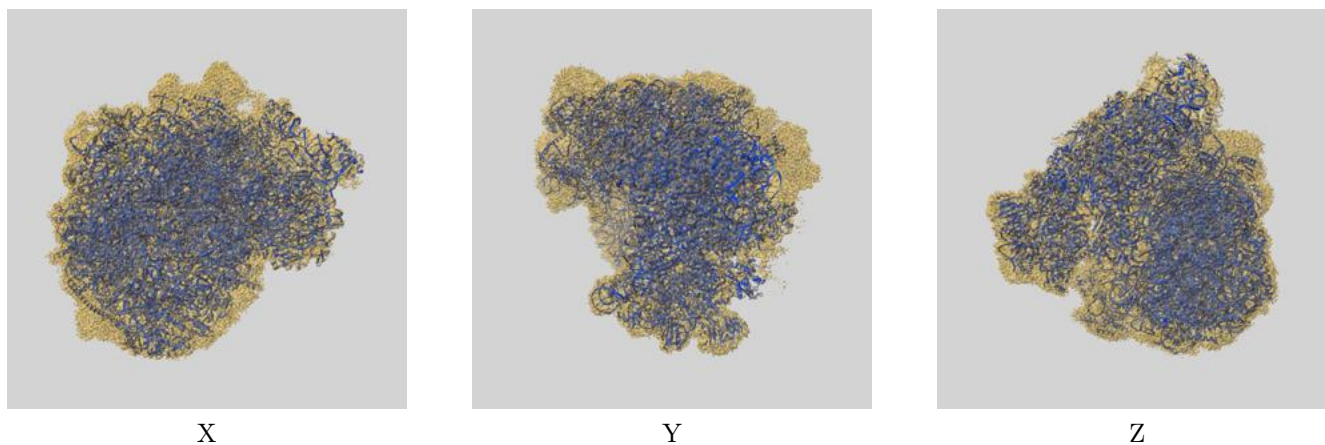
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.32	3.07

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

9 Map-model fit [i](#)

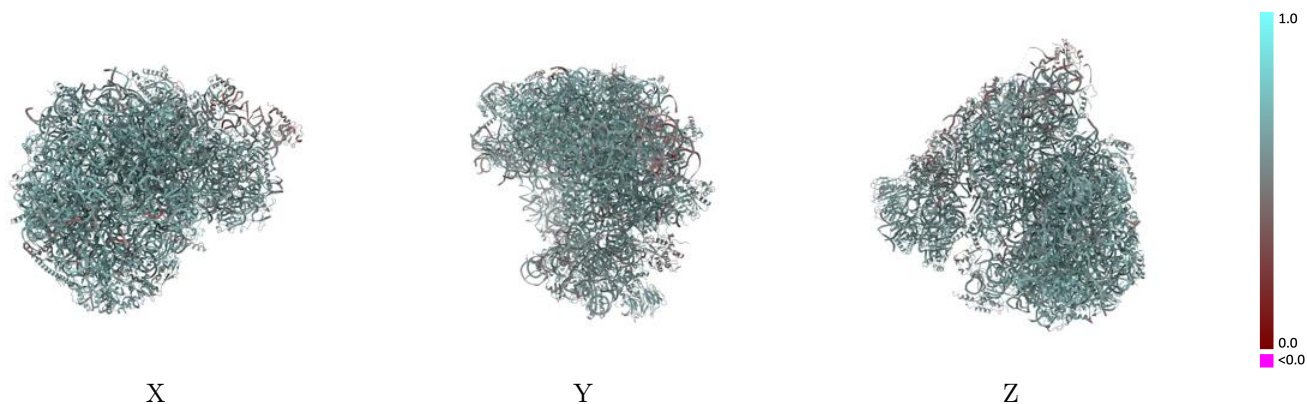
This section contains information regarding the fit between EMDB map EMD-15124 and PDB model 8A3W. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



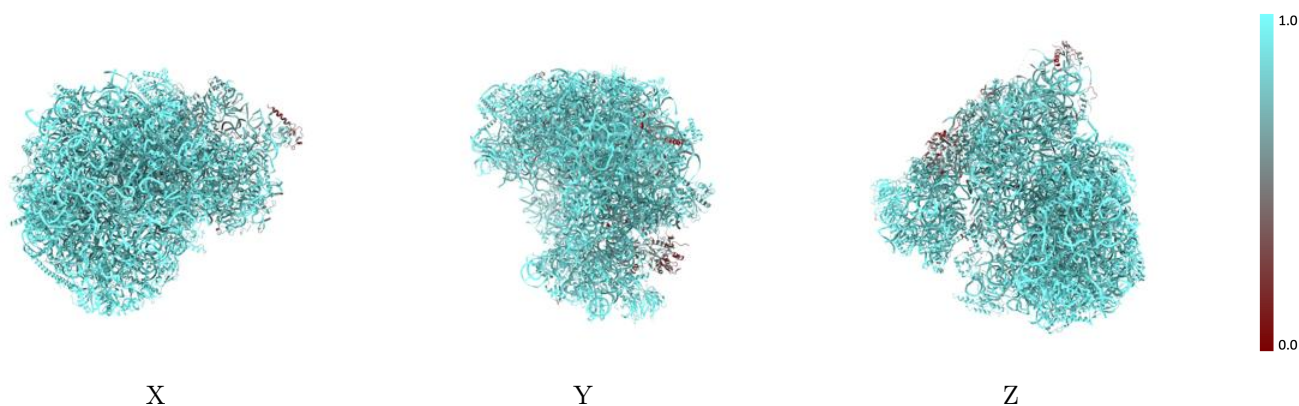
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



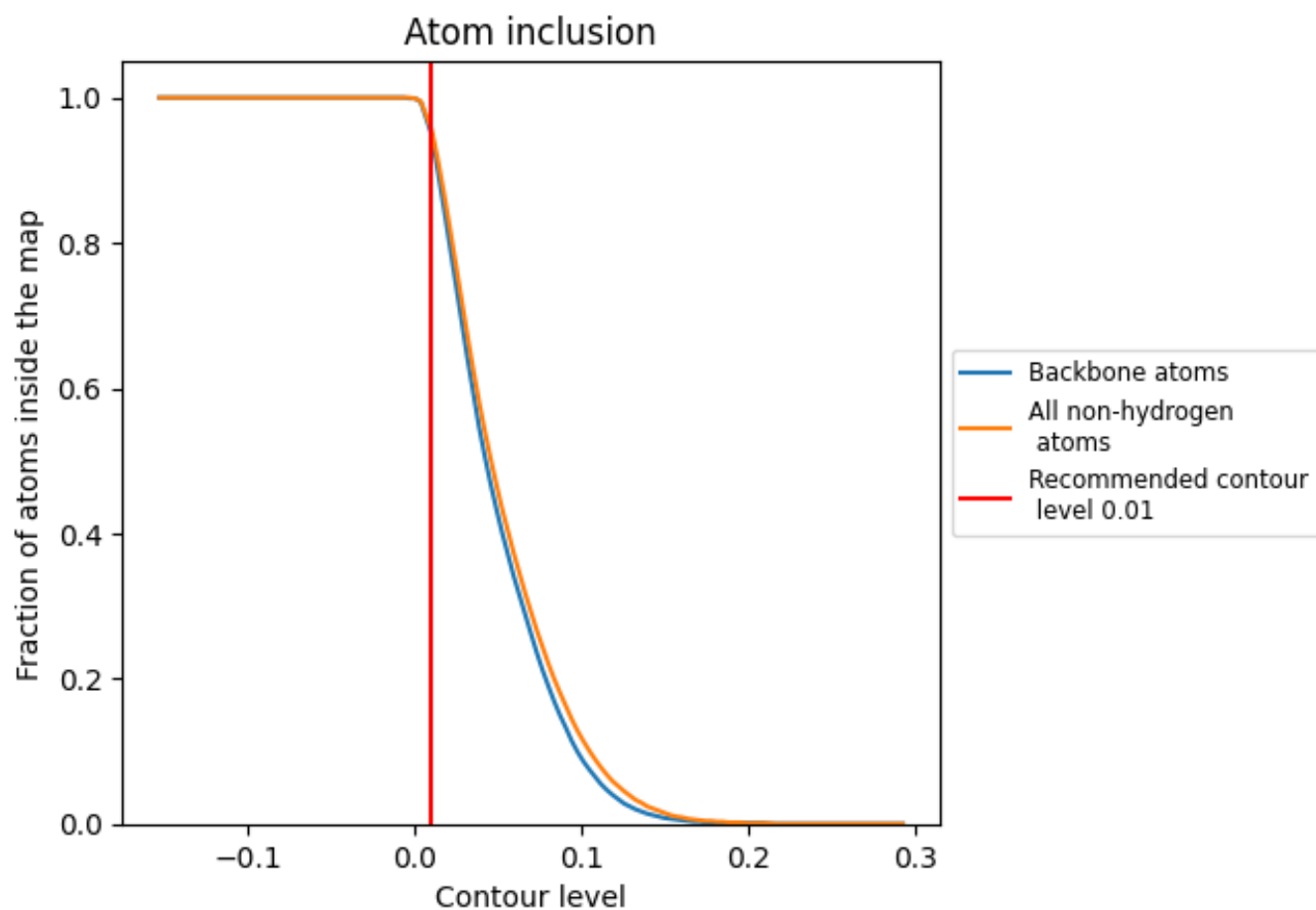
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.6070
1	 0.9940	 0.6260
2	 0.9950	 0.6320
3	 0.9930	 0.6170
4	 0.9940	 0.6100
5	 0.9980	 0.6360
6	 0.9860	 0.5860
7	 0.9950	 0.6330
8	 0.9950	 0.5830
A	 0.9960	 0.6570
B	 0.9980	 0.6500
C	 0.9980	 0.6510
D	 0.9890	 0.5400
E	 0.9550	 0.5610
F	 0.9930	 0.6110
G	 0.9940	 0.6280
H	 0.9900	 0.6350
I	 0.9900	 0.6360
J	 0.9980	 0.6450
K	 0.9920	 0.6130
L	 0.9940	 0.6520
M	 0.9970	 0.6620
O	 0.9930	 0.5900
P	 0.9970	 0.6510
Q	 0.9930	 0.6160
R	 0.9890	 0.6310
S	 0.9910	 0.6470
S1	 0.9470	 0.5790
S4	 0.8940	 0.5250
SA	 0.8050	 0.5800
SB	 0.5340	 0.4940
SC	 0.9190	 0.5410
SD	 0.8200	 0.5450
SE	 0.8660	 0.6010
SF	 0.7520	 0.5740















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Chain	Atom inclusion	Q-score
SG	0.7990	0.5780
SH	0.9550	0.5990
SI	0.8500	0.5790
SJ	0.9300	0.6260
SK	0.8990	0.6070
SL	0.9820	0.6110
SM	0.9530	0.5660
SN	0.9320	0.5410
SO	0.8740	0.5890
SP	0.8650	0.5990
SR	0.9680	0.5970
SS	0.9630	0.5810
ST	0.9320	0.6130
SU	0.8760	0.6190
SV	0.9610	0.5870
SW	0.9510	0.5870
SX	0.9930	0.6120
SY	0.4200	0.5030
SZ	0.8380	0.5770
Sa	0.9790	0.5880
Sb	0.8120	0.5750
Sc	0.8300	0.5680
Sd	0.9420	0.5800
Se	0.7240	0.5690
Sg	0.9640	0.5670
Sh	0.4360	0.4140
T	0.9940	0.6550
U	0.9850	0.5590
V	0.9960	0.6420
W	0.9920	0.6350
X	0.9940	0.6410
Y	0.9950	0.6130
Z	0.9880	0.6210
a	0.9960	0.6250
b	0.9920	0.6350
c	0.9940	0.6340
d	0.9880	0.5800
e	0.9350	0.5920
f	0.9960	0.6480
g	0.9890	0.6490
h	0.9880	0.6330
i	0.9830	0.6180

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Chain	Atom inclusion	Q-score
j	 1.0000	 0.6630
k	 0.9900	 0.5940
l	 0.9930	 0.6550
n	 0.3860	 0.4500
o	 0.9910	 0.6240
p	 0.9940	 0.6330