



Full wwPDB EM Validation Report ⓘ

Jun 26, 2026 – 08:57 AM EDT

PDB ID : 9O3W / pdb_00009o3w
EMDB ID : EMD-70084
Title : Human 80S ribosome bound to IDB-001 stalled on MYC nascent chain
Authors : Sauer, P.V.; Schuller, A.P.; Hamann, L.G.
Deposited on : 2025-04-07
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

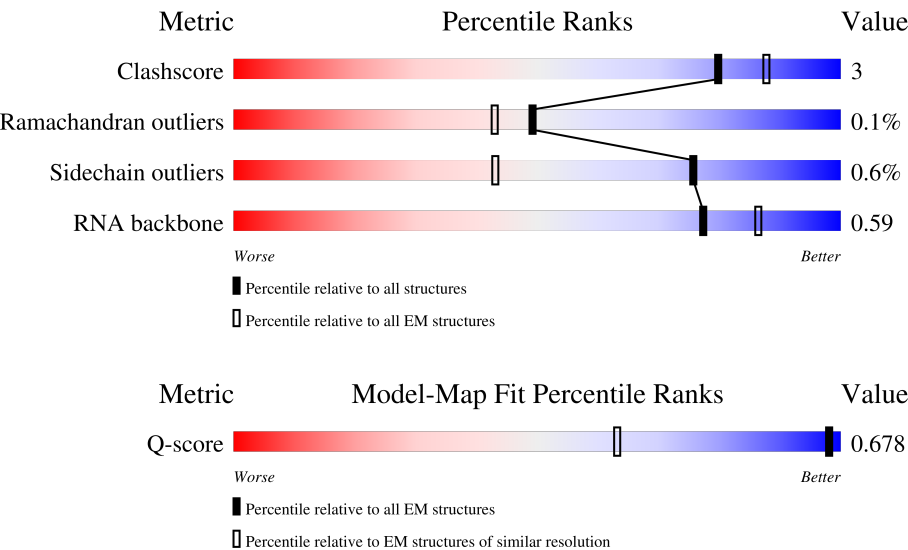
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 1.90 Å.

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



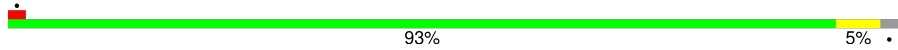
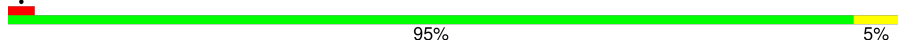
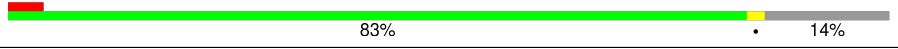
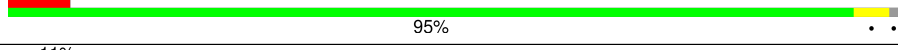
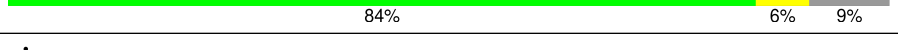
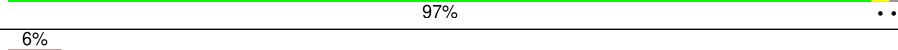
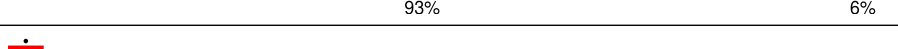
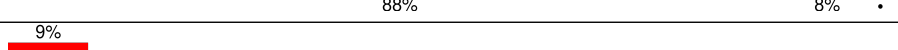
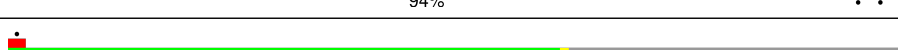
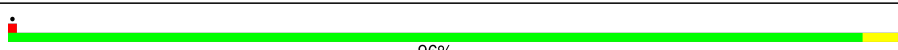
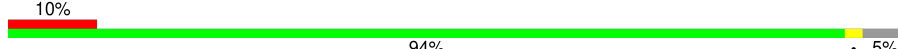
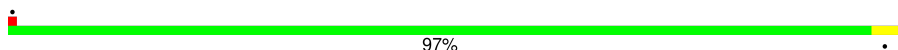
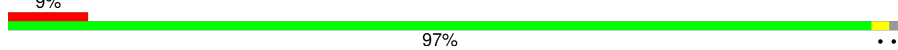
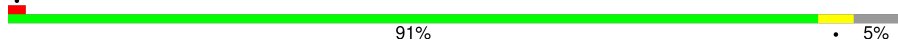
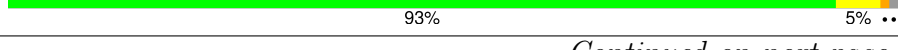
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1185 (1.40 - 2.40)

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	L5	5069	9% 51% 17% 30%
2	L7	120	87% 12%
3	L8	156	6% 74% 24%

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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	

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Mol	Chain	Length	Quality of chain
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	NC	19	
47	Pt	75	
48	S2	1869	
49	SA	295	
50	SB	264	
51	SC	293	
52	SD	243	
53	SE	263	

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Mol	Chain	Length	Quality of chain
54	SF	204	
55	SG	249	
56	SH	194	
57	SI	208	
58	SJ	194	
59	SK	165	
60	SL	158	
61	SM	132	
62	SN	151	
63	SO	151	
64	SP	145	
65	SQ	146	
66	SR	135	
67	SS	152	
68	ST	145	
69	SU	119	
70	SV	84	
71	SW	130	
72	SX	143	
73	SY	133	
74	SZ	125	
75	Sa	115	
76	Sb	84	
77	Sc	69	
78	Sd	56	

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Mol	Chain	Length	Quality of chain
79	Se	133	8%37%62% .
80	Sf	156	40%31%8%60% .
81	Sg	317	84%86%12% ..
82	mR	832	99% .

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 219527 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 RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3546	Total	C	N	O	P	2	0
			76136	33944	13925	24720	3547		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	251	Total	C	N	O	S	0	0
			1921	1204	393	318	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	0	0
			3240	2061	608	557	14		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	366	Total	C	N	O	S	0	0
			2914	1832	581	487	14		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	223	Total	C	N	O	S	0	0
			1787	1150	339	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 10 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1716	1086	331	285	14		

- Molecule 13 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 14 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 15 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 16 is a protein called Large ribosomal subunit protein eL15.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	202	Total	C	N	O	S	0	0
			1655	1066	322	262	5		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 22 is a protein called Large ribosomal subunit protein eL21.

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

- Molecule 23 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	133	Total	C	N	O	S	0	0
			989	623	186	175	5		

- Molecule 25 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	68	Total	C	N	O	S	0	0
			562	356	111	92	3		

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 28 is a protein called Large ribosomal subunit protein eL27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	111	Total	C	N	O	S	0	0
			898	560	195	139	4		

- Molecule 31 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	99	Total	C	N	O	S	0	0
			770	488	136	140	6		

- Molecule 32 is a protein called Large ribosomal subunit protein eL31.

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

- Molecule 33 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 34 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	110	Total	C	N	O	S	0	0
			884	560	175	145	4		

- Molecule 35 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 37 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 38 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 39 is a protein called Large ribosomal subunit protein eL38.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 42 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	0	0
			864	543	175	140	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

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

- Molecule 45 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	126	Total	C	N	O	S	0	0
			1005	624	207	169	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	2	ACE	-	acetylation	UNP P46779

- Molecule 46 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	NC	19	Total	C	N	O	0	0
			118	68	20	30		

- Molecule 47 is a RNA chain called P-site glutamyl-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Pt	75	Total	C	N	O	P	0	0
			1597	713	275	534	75		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1672	Total	C	N	O	P	0	0
			35736	15981	6403	11681	1671		

- Molecule 49 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SA	223	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	ACE	-	acetylation	UNP P08865

- Molecule 50 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SB	223	Total	C	N	O	S	0	0
			1806	1145	325	322	14		

- Molecule 51 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 52 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		

- Molecule 53 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 55 is a protein called Small ribosomal subunit protein eS6.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SH	189	Total	C	N	O	S	0	0
			1517	966	279	271	1		

- Molecule 57 is a protein called Small ribosomal subunit protein eS8.

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

- Molecule 58 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS10.

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

- Molecule 60 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SL	146	Total	C	N	O	S	0	0
			1200	766	226	202	6		

- Molecule 61 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SM	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 62 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 63 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 64 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP	131	Total	C	N	O	S	0	0
			1078	684	204	183	7		

- Molecule 65 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 66 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SR	134	Total	C	N	O	S	0	0
			1083	680	201	198	4		

- Molecule 67 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 68 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	ST	142	Total	C	N	O	S	0	0
			1103	691	212	197	3		

- Molecule 69 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 70 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SV	84	Total	C	N	O	S	0	0
			640	395	117	123	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SV	0	ACE	-	acetylation	UNP P63220

- Molecule 71 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 72 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SX	140	Total	C	N	O	S	0	0
			1088	687	215	183	3		

- Molecule 73 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 74 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SZ	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 75 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 76 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 77 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sc	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 78 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 79 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Se	50	Total	C	N	O	S	0	0
			395	241	88	65	1		

- Molecule 80 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 81 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	mR	6	Total	C	N	O	P	0	0
			133	59	27	41	6		

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

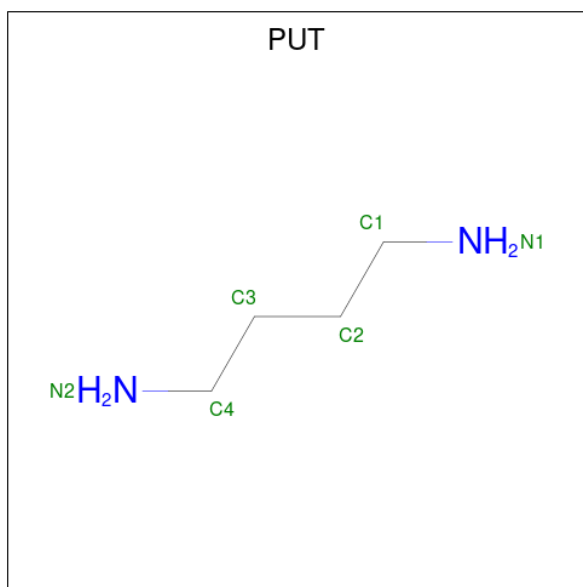
Mol	Chain	Residues	Atoms		AltConf
83	L5	114	Total	K	0
			114	114	
83	L7	3	Total	K	0
			3	3	
83	L8	5	Total	K	0
			5	5	
83	LA	3	Total	K	0
			3	3	
83	LH	1	Total	K	0
			1	1	
83	LI	1	Total	K	0
			1	1	
83	LL	1	Total	K	0
			1	1	
83	LN	1	Total	K	0
			1	1	
83	LQ	1	Total	K	0
			1	1	
83	Lb	1	Total	K	0
			1	1	
83	Le	1	Total	K	0
			1	1	
83	Lf	1	Total	K	0
			1	1	
83	Ll	1	Total	K	0
			1	1	
83	S2	32	Total	K	0
			32	32	
83	SL	1	Total	K	0
			1	1	
83	SO	1	Total	K	0
			1	1	

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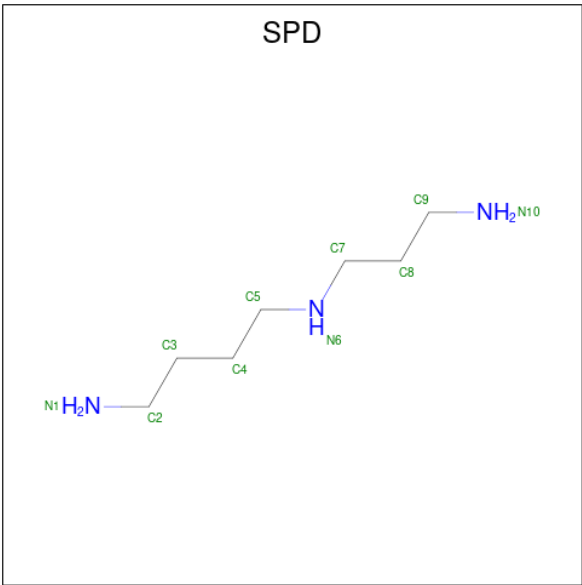
Mol	Chain	Residues	Atoms		AltConf
83	ST	1	Total	K	0
			1	1	
83	Sa	1	Total	K	0
			1	1	

- Molecule 84 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



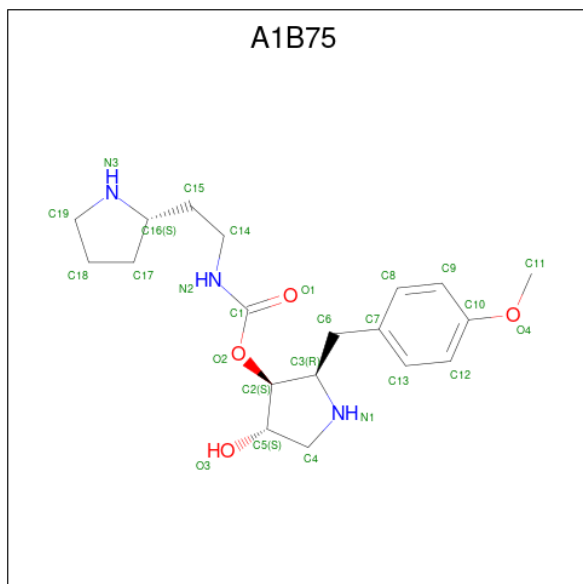
Mol	Chain	Residues	Atoms			AltConf
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



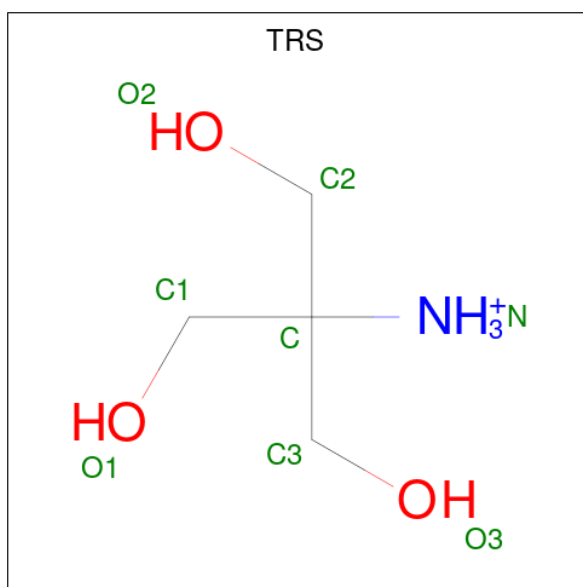
Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			10	7	3	
			Total	C	N	
			10	7	3	
			Total	C	N	
			10	7	3	
			Total	C	N	
			10	7	3	
			Total	C	N	
			10	7	3	
			Total	C	N	
			10	7	3	
			Total	C	N	
			10	7	3	
85	S2	1	Total	C	N	0
			10	7	3	

- Molecule 86 is (2R,3S,4S)-4-hydroxy-2-[(4-methoxyphenyl)methyl]pyrrolidin-3-yl {2-[(2S)-pyrrolidin-2-yl]ethyl}carbamate (CCD ID: A1B75) (formula: $C_{19}H_{29}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
86	L5	1	Total	C	N	O	0
			26	19	3	4	

- Molecule 87 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
87	L5	1	Total	C	N	O	0
			8	4	1	3	
87	L5	1	Total	C	N	O	0
			8	4	1	3	

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	L5	271	Total	Mg	0
			271	271	
88	L7	5	Total	Mg	0
			5	5	
88	L8	6	Total	Mg	0
			6	6	
88	LL	1	Total	Mg	0
			1	1	
88	LN	2	Total	Mg	0
			2	2	
88	Lj	1	Total	Mg	0
			1	1	
88	Lo	1	Total	Mg	0
			1	1	
88	S2	83	Total	Mg	0
			83	83	
88	Sd	1	Total	Mg	0
			1	1	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	Lg	1	Total	Zn	0
			1	1	
89	Lj	1	Total	Zn	0
			1	1	
89	Lm	1	Total	Zn	0
			1	1	
89	Lo	1	Total	Zn	0
			1	1	
89	Lp	1	Total	Zn	0
			1	1	
89	Sa	1	Total	Zn	0
			1	1	
89	Sd	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
89	Sf	1	Total 1	Zn 1	0

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	L5	337	Total 337	O 337	0
90	L5	60	Total 60	O 60	0
90	L5	1	Total 1	O 1	0
90	L5	1	Total 1	O 1	0
90	L5	1	Total 1	O 1	0
90	L5	42	Total 42	O 42	0
90	L5	1	Total 1	O 1	0
90	L5	24	Total 24	O 24	0
90	L5	3910	Total 3910	O 3910	0
90	L5	65	Total 65	O 65	0
90	L7	33	Total 33	O 33	0
90	L7	48	Total 48	O 48	0
90	L8	1	Total 1	O 1	0
90	L8	11	Total 11	O 11	0
90	L8	3	Total 3	O 3	0
90	LA	90	Total 90	O 90	0
90	LA	40	Total 40	O 40	0
90	LB	142	Total 142	O 142	0

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Mol	Chain	Residues	Atoms		AltConf
90	LC	116	Total 116	O 116	0
90	LD	38	Total 38	O 38	0
90	LE	7	Total 7	O 7	0
90	LF	54	Total 54	O 54	0
90	LG	17	Total 17	O 17	0
90	LH	2	Total 2	O 2	0
90	LH	15	Total 15	O 15	0
90	LI	22	Total 22	O 22	0
90	LI	40	Total 40	O 40	0
90	LJ	3	Total 3	O 3	0
90	LL	28	Total 28	O 28	0
90	LL	11	Total 11	O 11	0
90	LL	18	Total 18	O 18	0
90	LM	11	Total 11	O 11	0
90	LN	7	Total 7	O 7	0
90	LN	92	Total 92	O 92	0
90	LN	22	Total 22	O 22	0
90	LO	79	Total 79	O 79	0
90	LP	62	Total 62	O 62	0
90	LQ	41	Total 41	O 41	0
90	LQ	46	Total 46	O 46	0

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Mol	Chain	Residues	Atoms		AltConf
90	LR	57	Total 57	O 57	0
90	LS	46	Total 46	O 46	0
90	LT	64	Total 64	O 64	0
90	LV	43	Total 43	O 43	0
90	LW	12	Total 12	O 12	0
90	LX	22	Total 22	O 22	0
90	LY	16	Total 16	O 16	0
90	LZ	5	Total 5	O 5	0
90	La	87	Total 87	O 87	0
90	Lb	33	Total 33	O 33	0
90	Lc	8	Total 8	O 8	0
90	Ld	29	Total 29	O 29	0
90	Le	21	Total 21	O 21	0
90	Le	67	Total 67	O 67	0
90	Lf	4	Total 4	O 4	0
90	Lf	34	Total 34	O 34	0
90	Lg	33	Total 33	O 33	0
90	Lg	27	Total 27	O 27	0
90	Lh	15	Total 15	O 15	0
90	Li	11	Total 11	O 11	0
90	Lj	26	Total 26	O 26	0

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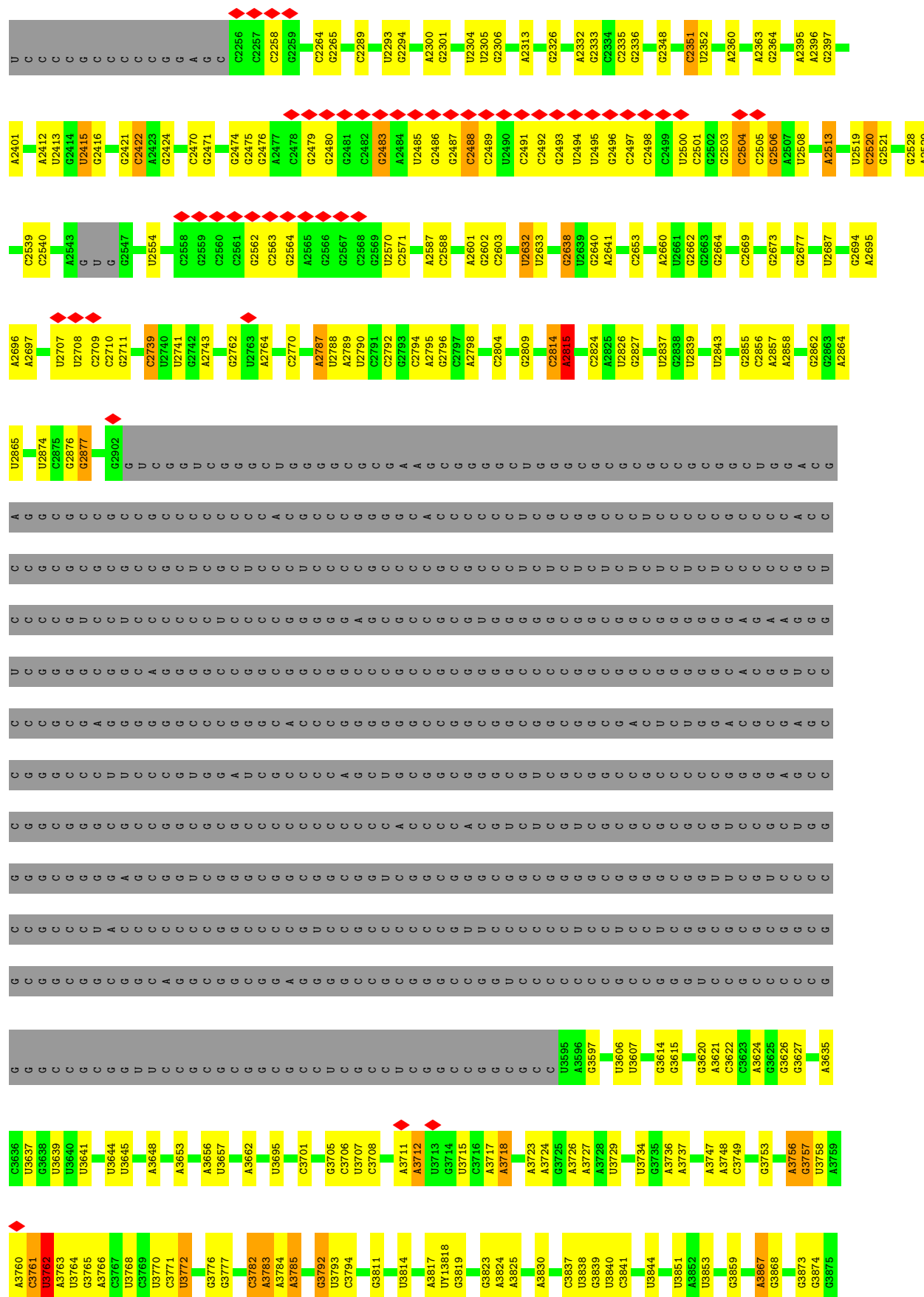
Mol	Chain	Residues	Atoms		AltConf
90	Lj	19	Total 19	O 19	0
90	Lj	16	Total 16	O 16	0
90	Lk	1	Total 1	O 1	0
90	Ll	33	Total 33	O 33	0
90	Lm	16	Total 16	O 16	0
90	Ln	13	Total 13	O 13	0
90	Lo	28	Total 28	O 28	0
90	Lo	1	Total 1	O 1	0
90	Lo	13	Total 13	O 13	0
90	Lp	29	Total 29	O 29	0
90	Lp	1	Total 1	O 1	0
90	Lr	19	Total 19	O 19	0
90	NC	5	Total 5	O 5	0
90	Pt	3	Total 3	O 3	0
90	S2	80	Total 80	O 80	0
90	S2	111	Total 111	O 111	0
90	S2	10	Total 10	O 10	0
90	S2	105	Total 105	O 105	0
90	S2	76	Total 76	O 76	0
90	S2	23	Total 23	O 23	0
90	S2	2	Total 2	O 2	0

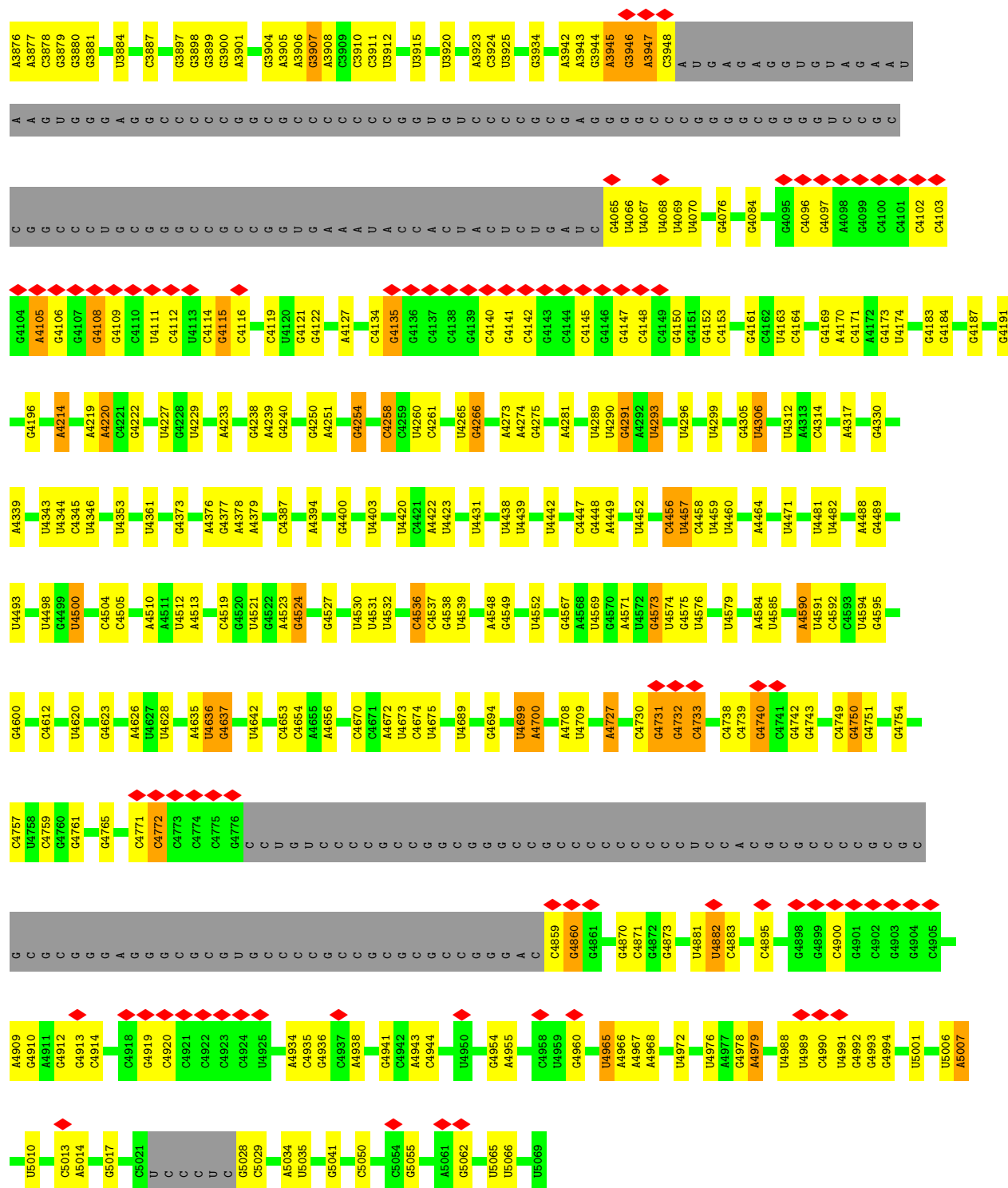
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Mol	Chain	Residues	Atoms		AltConf
90	S2	44	Total 44	O 44	0
90	S2	281	Total 281	O 281	0
90	S2	1	Total 1	O 1	0
90	S2	18	Total 18	O 18	0
90	S2	97	Total 97	O 97	0
90	S2	2	Total 2	O 2	0
90	Sb	6	Total 6	O 6	0
90	Se	2	Total 2	O 2	0
90	mR	3	Total 3	O 3	0





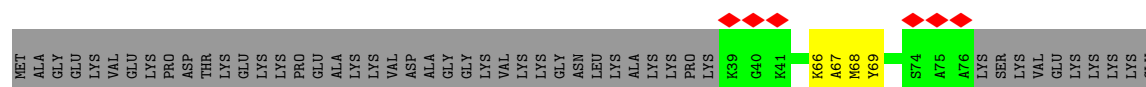
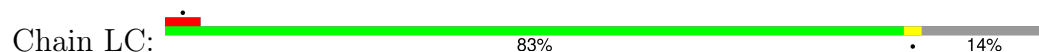
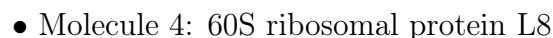


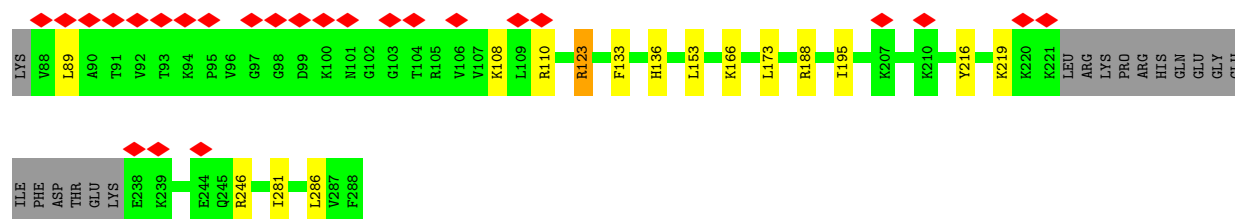
• Molecule 2: 5S rRNA

Chain L7: 87% 12%



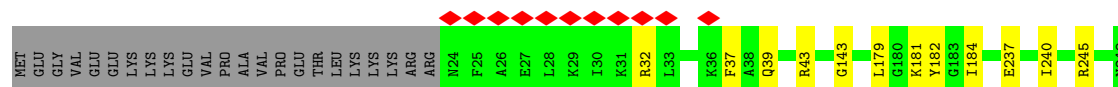
Chain L8:





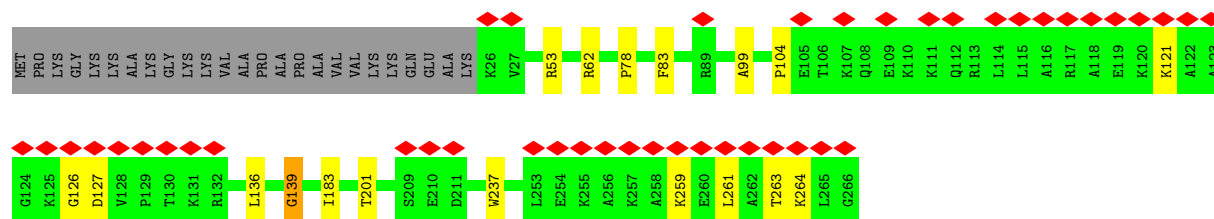
- Molecule 9: 60S ribosomal protein L7

Chain LF: 86% 5% 9%



- Molecule 10: Large ribosomal subunit protein eL8

Chain LG: 17% 84% 6% 9%



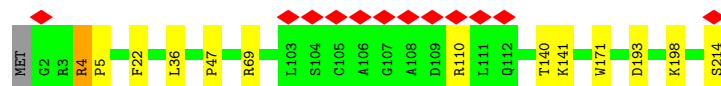
- Molecule 11: Large ribosomal subunit protein uL6

Chain LH: 97% ..



- Molecule 12: Large ribosomal subunit protein uL16

Chain LI: 6% 93% 6%

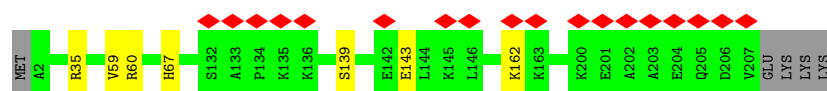


- Molecule 13: Large ribosomal subunit protein uL5

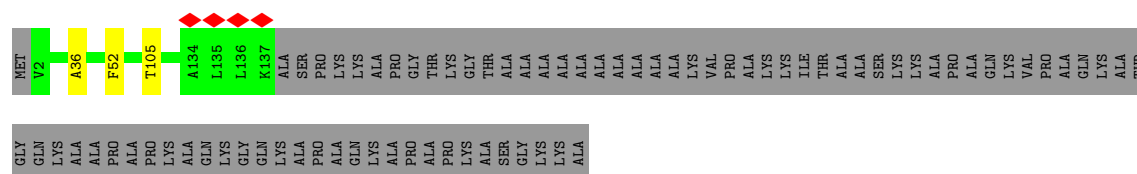
Chain LJ: 88% 8% .

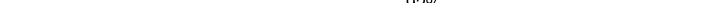


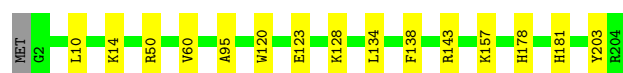
- Molecule 14: Large ribosomal subunit protein eL13

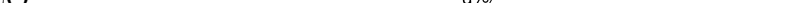


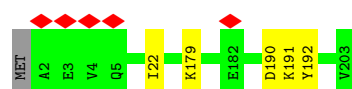
- Chain LM:



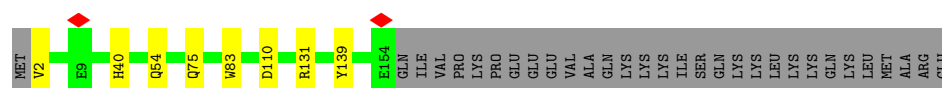
- Chain LN: 

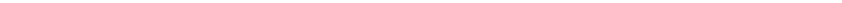


- Chain LO: 



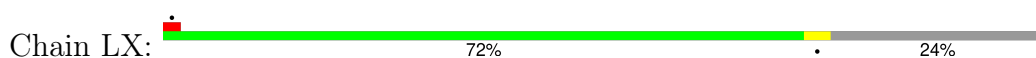
- Chain LP: 79% 17%

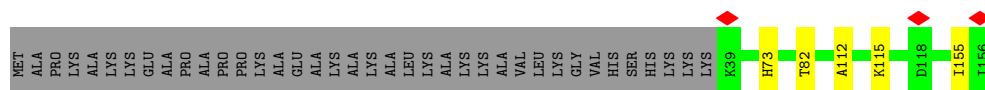


- Chain LQ:  96%

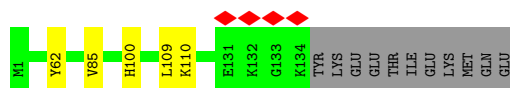
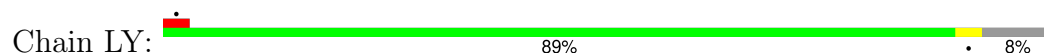


- Chain LB: 10% 94% 5%

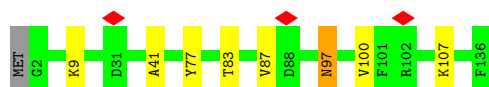




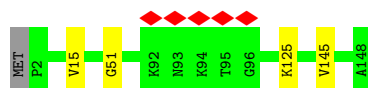
- Molecule 27: Large ribosomal subunit protein uL24



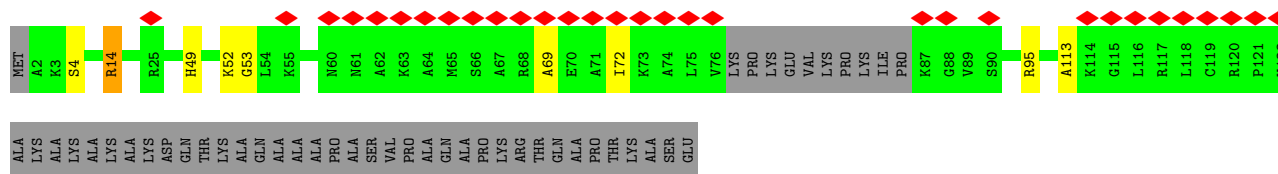
- Molecule 28: Large ribosomal subunit protein eL27



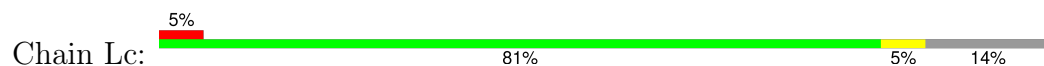
- Molecule 29: 60S ribosomal protein L27a



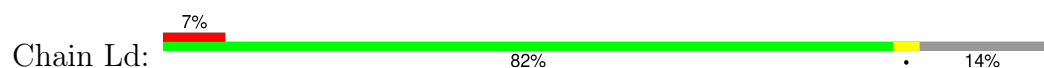
- Molecule 30: Large ribosomal subunit protein eL29

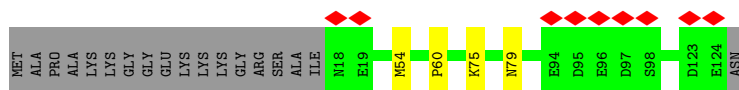


- Molecule 31: Large ribosomal subunit protein eL30



- Molecule 32: Large ribosomal subunit protein eL31





- Molecule 33: Large ribosomal subunit protein eL32



- Molecule 34: Large ribosomal subunit protein eL33



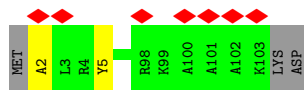
- Molecule 35: Large ribosomal subunit protein eL34



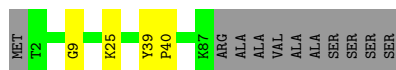
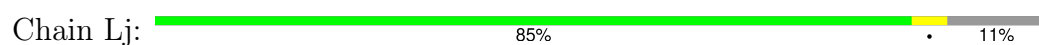
- Molecule 36: Large ribosomal subunit protein uL29



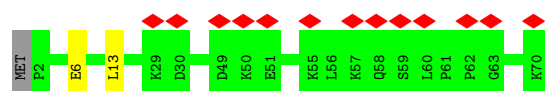
- Molecule 37: Large ribosomal subunit protein eL36



- Molecule 38: Large ribosomal subunit protein eL37



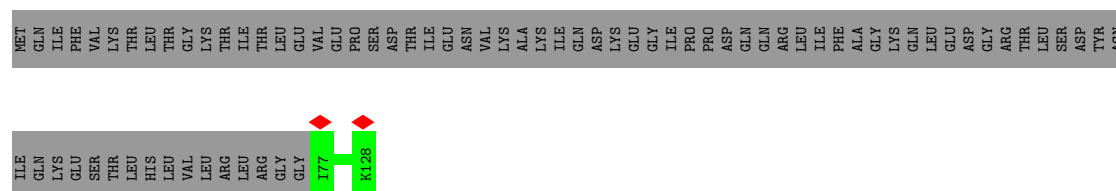
- Molecule 39: Large ribosomal subunit protein eL38



- Molecule 40: Large ribosomal subunit protein eL39



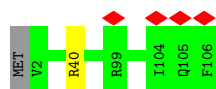
- Molecule 41: Ubiquitin-ribosomal protein eL40 fusion protein



- Molecule 42: Small ribosomal subunit protein eS32



- Molecule 43: Large ribosomal subunit protein eL42



- Molecule 44: Large ribosomal subunit protein eL43



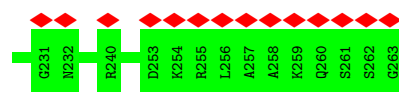
- Molecule 45: Large ribosomal subunit protein eL28



[illegible]

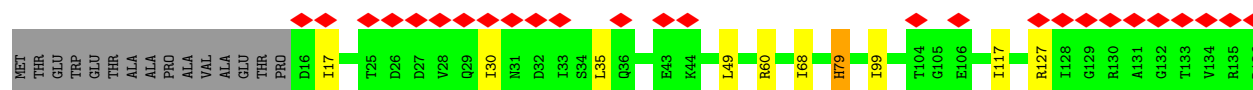
Number of genes in each category

Category	Number of genes	Red Diamond
MET	1	No
A2	1	No
R3	1	No
M19	1	No
L20	1	No
D21	1	No
T24	1	No
P31	1	No
L38	1	No
K53	1	Yes
M66	1	No
F69	1	No
D73	1	Yes
G74	1	Yes
D93	1	Yes
K94	1	Yes
T95	1	Yes
G96	1	Yes
E97	1	Yes
R100	1	Yes
G107	1	No
R108	1	No
F109	1	Yes
A110	1	Yes
E118	1	Yes
C124	1	No
R127	1	Yes
H142	1	No
D163	1	Yes
L154	1	Yes
E165	1	Yes
T166	1	No
I169	1	Yes
M192	1	No
L189	1	No
G190	1	No
A213	1	Yes
N214	1	Yes
G215	1	Yes
G216	1	Yes



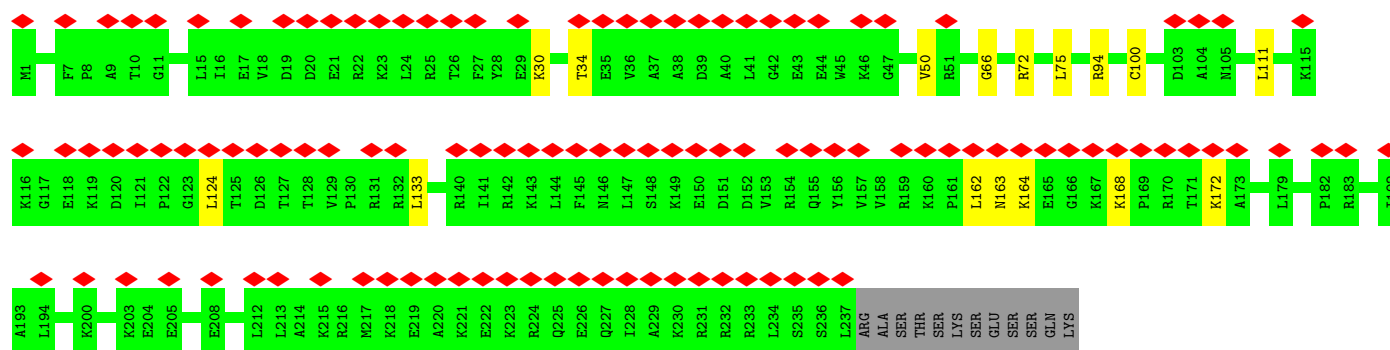
- Molecule 54: Small ribosomal subunit protein uS7

Chain SF:



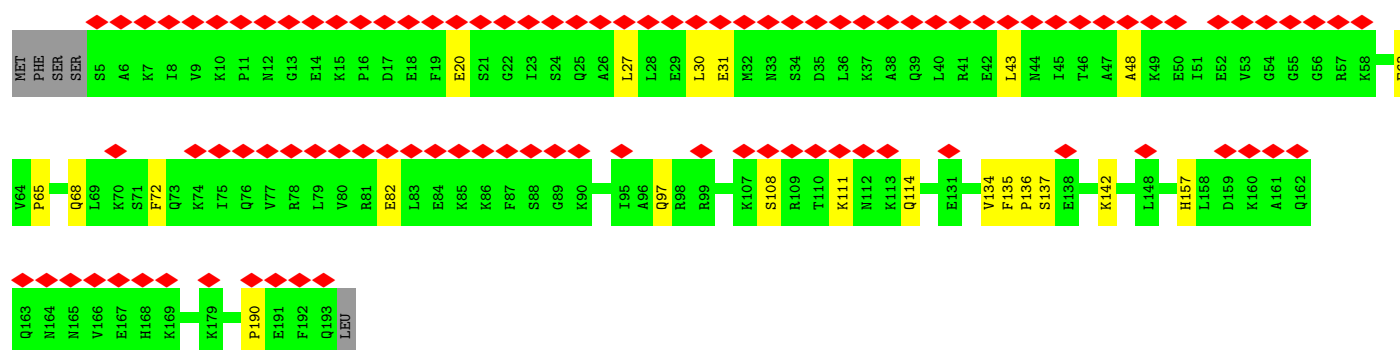
- Molecule 55: Small ribosomal subunit protein eS6

Chain SG:



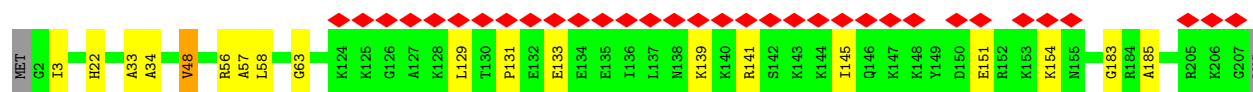
- Molecule 56: Small ribosomal subunit protein eS7

Chain SH:

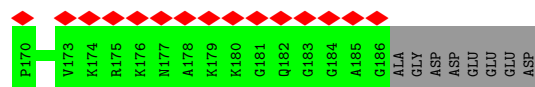
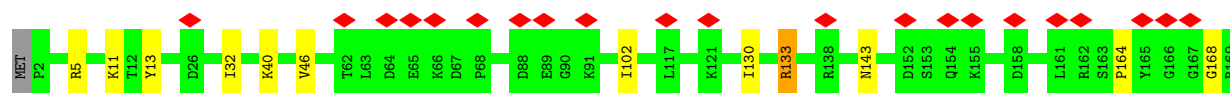
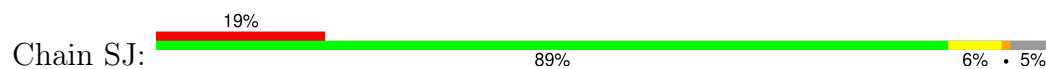


- Molecule 57: Small ribosomal subunit protein eS8

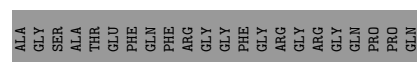
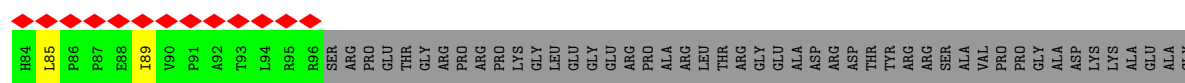
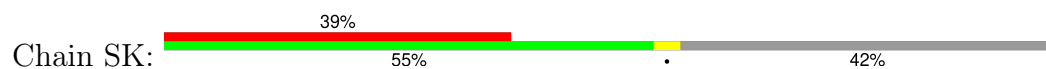
Chain SI:



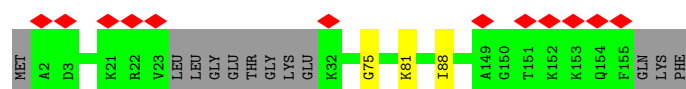
- Molecule 58: Small ribosomal subunit protein uS4



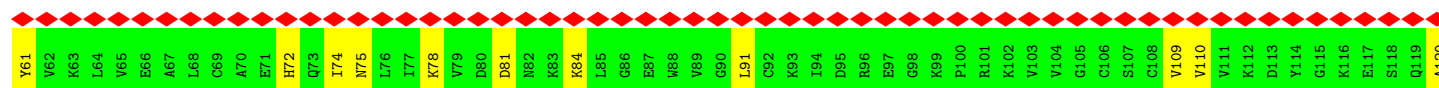
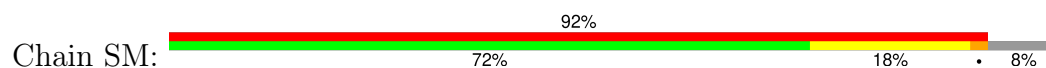
- Molecule 59: Small ribosomal subunit protein eS10

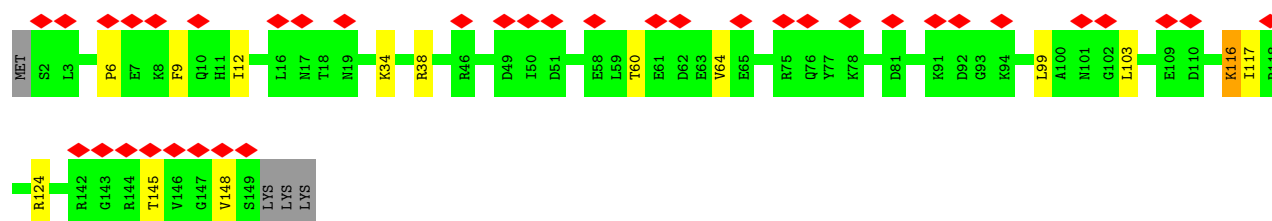
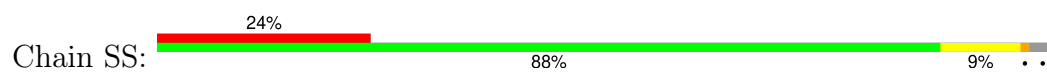


- Molecule 60: Small ribosomal subunit protein uS17

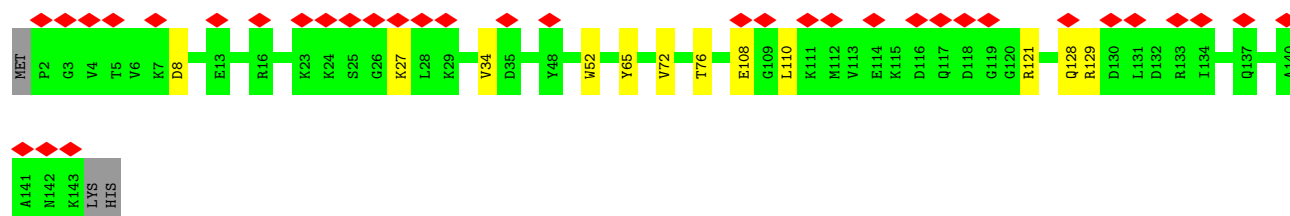


- Molecule 61: Small ribosomal subunit protein eS12

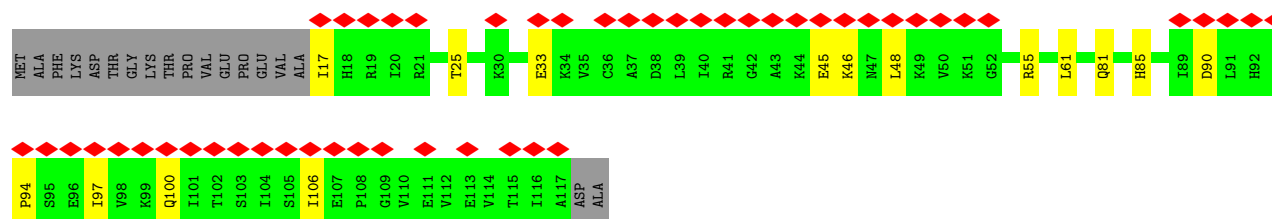
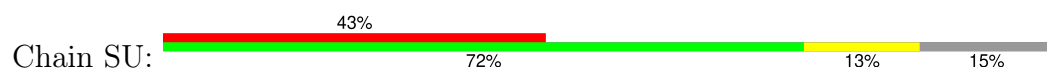




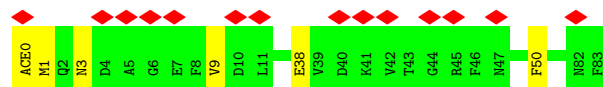
- Molecule 68: Small ribosomal subunit protein eS19



- Molecule 69: Small ribosomal subunit protein uS10



- Molecule 70: 40S ribosomal protein S21

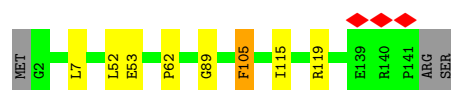


- Molecule 71: Small ribosomal subunit protein uS8

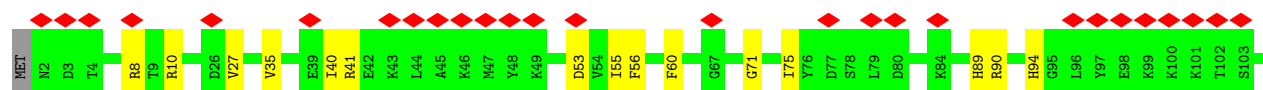
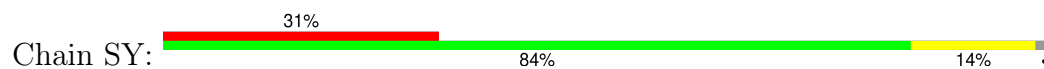


- Molecule 72: Small ribosomal subunit protein uS12

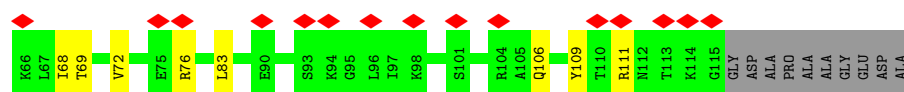




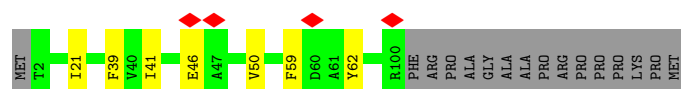
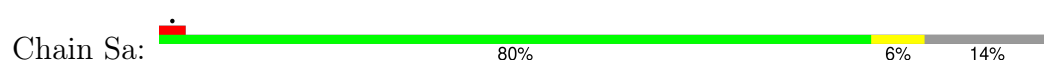
- Molecule 73: 40S ribosomal protein S24



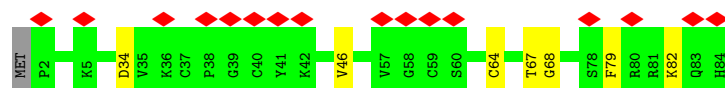
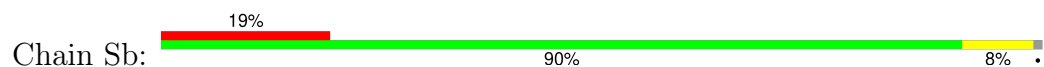
- Molecule 74: Small ribosomal subunit protein eS25



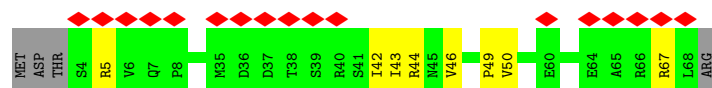
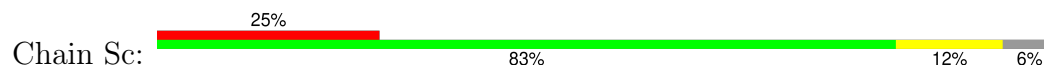
- Molecule 75: Small ribosomal subunit protein eS26



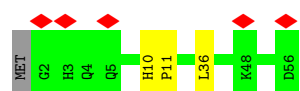
- Molecule 76: Small ribosomal subunit protein eS27



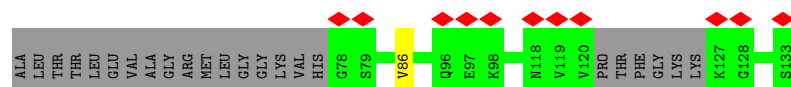
- Molecule 77: Small ribosomal subunit protein eS28



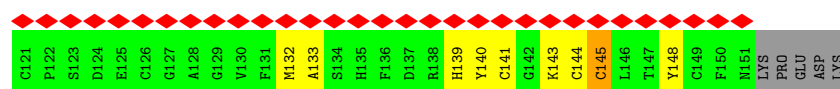
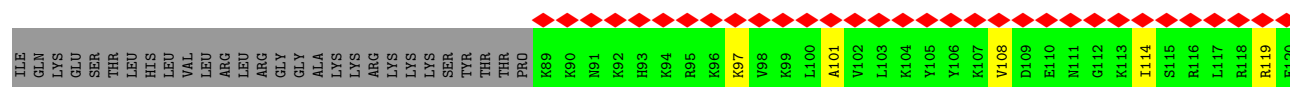
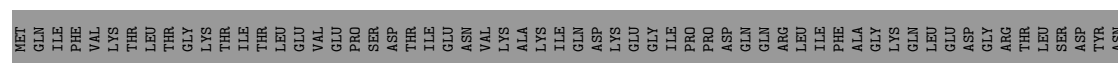
- Molecule 78: Small ribosomal subunit protein uS14



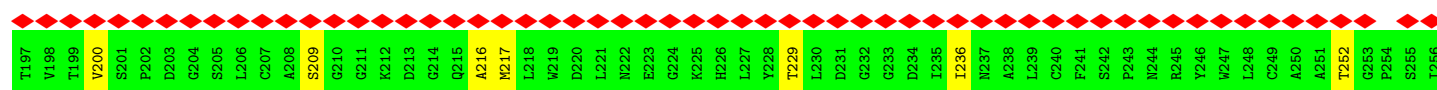
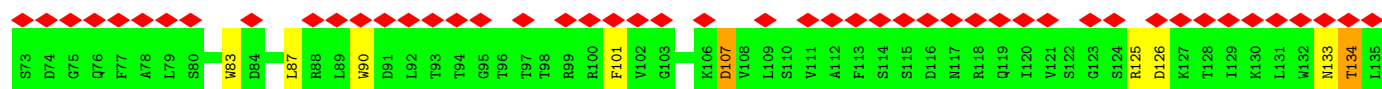
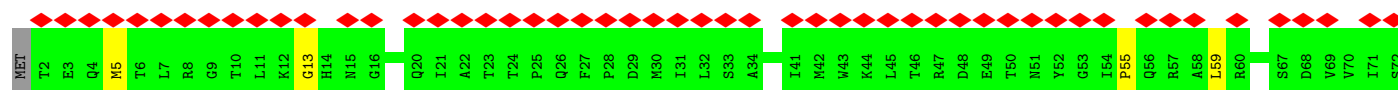
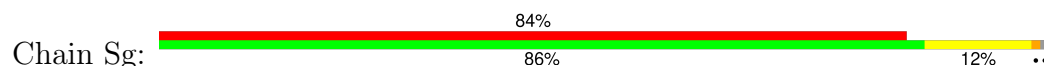
- Molecule 79: FAU ubiquitin-like and ribosomal protein S30



- Molecule 80: Ubiquitin-ribosomal protein eS31 fusion protein



- Molecule 81: Receptor of activated protein C kinase 1





Chain mR: 99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	538472	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.479	Depositor
Minimum map value	-0.471	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.112	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, OMG, TRS, K, MLZ, MG, ACE, PUT, 4AC, PSU, 6MZ, H2U, ZN, G7M, OMU, A1B75, 5MC, HY3, MA6, B8N, M3L, A2M, 2MU, 1MA, UY1, 2MG, SPD, HIC, OMC

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	L5	0.52	4/82102 (0.0%)	0.65	8/128082 (0.0%)
2	L7	0.51	0/2858	0.63	2/4455 (0.0%)
3	L8	0.52	0/3609	0.63	0/5623
4	LA	0.41	0/1959	0.62	0/2627
5	LB	0.36	0/3295	0.59	0/4406
6	LC	0.37	0/2968	0.56	0/3985
7	LD	0.33	0/2437	0.52	0/3263
8	LE	0.31	0/1821	0.52	0/2442
9	LF	0.37	0/1905	0.53	0/2539
10	LG	0.31	0/1960	0.61	2/2637 (0.1%)
11	LH	0.34	0/1537	0.52	0/2066
12	LI	0.34	0/1755	0.53	0/2344
13	LJ	0.30	0/1385	0.54	0/1852
14	LL	0.31	0/1695	0.51	0/2270
15	LM	0.34	0/1142	0.51	0/1527
16	LN	0.41	0/1746	0.59	0/2338
17	LO	0.37	0/1687	0.54	0/2257
18	LP	0.40	0/1268	0.58	0/1701
19	LQ	0.37	0/1537	0.58	0/2052
20	LR	0.33	0/1582	0.48	0/2091
21	LS	0.36	0/1501	0.51	0/2013
22	LT	0.36	0/1326	0.56	0/1770
23	LU	0.31	0/822	0.53	0/1103
24	LV	0.37	0/1003	0.54	0/1345
25	LW	0.36	0/574	0.55	0/763
26	LX	0.34	0/984	0.54	0/1323
27	LY	0.34	0/1132	0.54	0/1504
28	LZ	0.36	0/1130	0.58	0/1507
29	La	0.41	0/1191	0.59	0/1591
30	Lb	0.33	0/900	0.52	0/1187
31	Lc	0.36	0/780	0.54	0/1046

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.36	0/903	0.54	0/1216
33	Le	0.39	0/1071	0.57	0/1429
34	Lf	0.39	0/903	0.60	0/1208
35	Lg	0.35	0/916	0.52	0/1220
36	Lh	0.32	0/1023	0.49	0/1351
37	Li	0.31	0/843	0.48	0/1115
38	Lj	0.42	0/720	0.65	0/952
39	Lk	0.30	0/575	0.51	0/761
40	Ll	0.38	0/454	0.60	0/599
41	Lm	0.35	0/426	0.52	0/564
42	Ln	0.38	0/241	0.59	0/305
43	Lo	0.37	0/867	0.55	0/1141
44	Lp	0.39	0/718	0.61	0/953
45	Lr	0.36	0/1018	0.49	0/1366
46	NC	0.31	0/52	0.73	0/68
47	Pt	0.37	0/1640	0.71	1/2555 (0.0%)
48	S2	0.45	2/37935 (0.0%)	0.61	4/59125 (0.0%)
49	SA	0.29	0/1785	0.48	0/2426
50	SB	0.33	0/1832	0.50	0/2449
51	SC	0.32	0/1762	0.47	0/2381
52	SD	0.26	0/1784	0.46	0/2403
53	SE	0.31	0/2118	0.53	0/2849
54	SF	0.28	0/1516	0.53	0/2037
55	SG	0.26	0/1946	0.51	0/2590
56	SH	0.27	0/1540	0.51	0/2064
57	SI	0.33	0/1715	0.53	0/2287
58	SJ	0.30	0/1550	0.54	0/2069
59	SK	0.24	0/834	0.47	0/1125
60	SL	0.34	0/1221	0.50	0/1632
61	SM	0.20	0/960	0.50	0/1286
62	SN	0.31	0/1232	0.49	0/1656
63	SO	0.34	0/1023	0.57	0/1372
64	SP	0.25	0/1100	0.54	0/1470
65	SQ	0.29	0/1142	0.51	0/1528
66	SR	0.26	0/1098	0.50	0/1474
67	SS	0.27	0/1232	0.50	0/1651
68	ST	0.27	0/1122	0.49	0/1504
69	SU	0.28	0/813	0.51	0/1092
70	SV	0.38	1/645 (0.2%)	0.54	0/862
71	SW	0.34	0/1051	0.48	0/1406
72	SX	0.34	0/1096	0.57	0/1461
73	SY	0.26	0/1083	0.53	0/1438
74	SZ	0.25	0/691	0.57	0/922

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sa	0.35	0/805	0.54	0/1079
76	Sb	0.30	0/665	0.55	0/891
77	Sc	0.29	0/514	0.59	0/688
78	Sd	0.28	0/470	0.50	0/623
79	Se	0.28	0/397	0.54	0/519
80	Sf	0.21	0/525	0.58	0/695
81	Sg	0.22	0/2493	0.51	0/3394
82	mR	0.37	0/149	0.97	0/231
All	All	0.43	7/221805 (0.0%)	0.60	17/325191 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	LC	0	1
8	LE	0	1
9	LF	0	1
10	LG	0	2
12	LI	0	1
13	LJ	0	1
14	LL	0	1
16	LN	0	1
18	LP	0	1
23	LU	0	1
30	Lb	0	1
34	Lf	0	2
43	Lo	0	1
50	SB	0	1
58	SJ	0	1
63	SO	0	2
65	SQ	0	1
67	SS	0	2
72	SX	0	1
All	All	0	23

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	SV	0	ACE	C-N	5.97	1.45	1.33
1	L5	4590	A2M	O3'-P	5.29	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	1871	A2M	O3'-P	5.23	1.61	1.56
1	L5	3718	A2M	O3'-P	5.12	1.61	1.56
48	S2	1804	OMU	O3'-P	5.07	1.61	1.56
48	S2	99	A2M	O3'-P	5.05	1.61	1.56
1	L5	3724	A2M	O3'-P	5.03	1.61	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	417	G	O4'-C1'-N9	5.81	116.92	108.20
1	L5	3756	A	O4'-C1'-N9	5.78	116.87	108.20
1	L5	1444	G	N9-C1'-C2'	5.74	120.60	112.00
1	L5	1523	A	N9-C1'-C2'	5.63	120.44	112.00
48	S2	1247	C	C4'-C3'-O3'	5.57	117.75	109.40
48	S2	482	G	P-O5'-C5'	5.51	129.16	120.90
1	L5	2304	U	O4'-C1'-C2'	5.49	111.29	105.80
2	L7	53	U	C5'-C4'-C3'	-5.47	106.99	115.20
2	L7	7	G	O5'-C5'-C4'	-5.31	103.54	111.50
1	L5	312	G	C5'-C4'-C3'	-5.25	108.12	116.00
10	LG	104	PRO	CA-C-N	5.21	129.48	121.19
10	LG	104	PRO	C-N-CA	5.21	129.48	121.19
1	L5	311	G	O3'-P-O5'	-5.20	96.20	104.00
48	S2	666	U	N1-C1'-C2'	5.15	119.73	112.00
1	L5	4510	A	N9-C1'-C2'	5.14	119.72	112.00
48	S2	1371	U	C5'-C4'-O4'	5.14	116.81	109.10
47	Pt	1	U	N1-C1'-C2'	5.09	119.63	112.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LC	201	ARG	Sidechain
8	LE	123	ARG	Sidechain
9	LF	245	ARG	Sidechain
10	LG	139	GLY	Peptide
10	LG	62	ARG	Sidechain
12	LI	4	ARG	Sidechain
13	LJ	75	ARG	Peptide
14	LL	35	ARG	Sidechain
16	LN	50	ARG	Sidechain
18	LP	131	ARG	Sidechain
23	LU	101	ARG	Sidechain

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Mol	Chain	Res	Type	Group
30	Lb	14	ARG	Sidechain
34	Lf	44	GLY	Peptide
34	Lf	98	GLY	Peptide
43	Lo	40	ARG	Sidechain
50	SB	51	ARG	Sidechain
58	SJ	5	ARG	Sidechain
63	SO	137	SER	Peptide
63	SO	138	ASP	Peptide
65	SQ	58	LEU	Peptide
67	SS	38	ARG	Sidechain
67	SS	99	LEU	Peptide
72	SX	89	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L5	76136	0	38528	396	0
2	L7	2558	0	1295	8	0
3	L8	3316	0	1687	17	0
4	LA	1921	0	2022	11	0
5	LB	3240	0	3377	16	0
6	LC	2914	0	3087	6	0
7	LD	2391	0	2426	7	0
8	LE	1787	0	1945	12	0
9	LF	1870	0	1996	9	0
10	LG	1927	0	2074	10	0
11	LH	1518	0	1600	3	0
12	LI	1716	0	1765	9	0
13	LJ	1362	0	1399	10	0
14	LL	1664	0	1773	3	0
15	LM	1120	0	1187	1	0
16	LN	1701	0	1749	9	0
17	LO	1655	0	1799	3	0
18	LP	1242	0	1269	5	0
19	LQ	1513	0	1628	5	0
20	LR	1566	0	1729	1	0
21	LS	1461	0	1502	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	LT	1298	0	1366	3	0
23	LU	808	0	831	5	0
24	LV	989	0	1047	3	0
25	LW	562	0	569	1	0
26	LX	967	0	1040	3	0
27	LY	1115	0	1205	3	0
28	LZ	1107	0	1182	5	0
29	La	1162	0	1213	3	0
30	Lb	898	0	983	7	0
31	Lc	770	0	809	5	0
32	Ld	888	0	930	2	0
33	Le	1053	0	1147	3	0
34	Lf	884	0	923	2	0
35	Lg	906	0	998	1	0
36	Lh	1015	0	1148	4	0
37	Li	832	0	917	2	0
38	Lj	705	0	737	2	0
39	Lk	569	0	637	1	0
40	Ll	444	0	482	3	0
41	Lm	432	0	471	0	0
42	Ln	240	0	289	0	0
43	Lo	864	0	929	0	0
44	Lp	708	0	756	5	0
45	Lr	1005	0	1072	2	0
46	NC	118	0	55	2	0
47	Pt	1597	0	817	13	0
48	S2	35736	0	18083	224	0
49	SA	1750	0	1755	11	0
50	SB	1806	0	1888	6	0
51	SC	1725	0	1813	16	0
52	SD	1756	0	1852	12	0
53	SE	2076	0	2177	13	0
54	SF	1495	0	1549	12	0
55	SG	1923	0	2089	11	0
56	SH	1517	0	1605	12	0
57	SI	1686	0	1772	10	0
58	SJ	1525	0	1640	6	0
59	SK	810	0	836	3	0
60	SL	1200	0	1271	4	0
61	SM	950	0	987	16	0
62	SN	1208	0	1293	5	0
63	SO	1010	0	1034	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	SP	1078	0	1121	11	0
65	SQ	1124	0	1193	9	0
66	SR	1083	0	1137	9	0
67	SS	1214	0	1275	9	0
68	ST	1103	0	1133	8	0
69	SU	803	0	873	7	0
70	SV	640	0	638	5	0
71	SW	1034	0	1080	7	0
72	SX	1088	0	1149	3	0
73	SY	1065	0	1142	13	0
74	SZ	683	0	761	7	0
75	Sa	792	0	841	4	0
76	Sb	651	0	672	4	0
77	Sc	512	0	541	6	0
78	Sd	459	0	448	2	0
79	Se	395	0	434	1	0
80	Sf	515	0	521	12	0
81	Sg	2436	0	2393	22	0
82	mR	133	0	66	0	0
83	L5	114	0	0	0	0
83	L7	3	0	0	0	0
83	L8	5	0	0	0	0
83	LA	3	0	0	0	0
83	LH	1	0	0	0	0
83	LI	1	0	0	0	0
83	LL	1	0	0	0	0
83	LN	1	0	0	0	0
83	LQ	1	0	0	0	0
83	Lb	1	0	0	0	0
83	Le	1	0	0	0	0
83	Lf	1	0	0	0	0
83	Ll	1	0	0	0	0
83	S2	32	0	0	0	0
83	SL	1	0	0	0	0
83	SO	1	0	0	0	0
83	ST	1	0	0	0	0
83	Sa	1	0	0	0	0
84	L5	42	0	84	5	0
85	L5	120	0	228	2	0
85	S2	20	0	38	0	0
86	L5	26	0	0	1	0
87	L5	16	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	L5	271	0	0	0	0
88	L7	5	0	0	0	0
88	L8	6	0	0	0	0
88	LL	1	0	0	0	0
88	LN	2	0	0	0	0
88	Lj	1	0	0	0	0
88	Lo	1	0	0	0	0
88	S2	83	0	0	0	0
88	Sd	1	0	0	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	1	0	0	0	0
89	Sf	1	0	0	0	0
90	L5	4442	0	0	1	0
90	L7	81	0	0	0	0
90	L8	15	0	0	0	0
90	LA	130	0	0	0	0
90	LB	142	0	0	1	0
90	LC	116	0	0	0	0
90	LD	38	0	0	0	0
90	LE	7	0	0	0	0
90	LF	54	0	0	0	0
90	LG	17	0	0	0	0
90	LH	17	0	0	0	0
90	LI	62	0	0	0	0
90	LJ	3	0	0	0	0
90	LL	57	0	0	0	0
90	LM	11	0	0	0	0
90	LN	121	0	0	0	0
90	LO	79	0	0	0	0
90	LP	62	0	0	0	0
90	LQ	87	0	0	0	0
90	LR	57	0	0	0	0
90	LS	46	0	0	0	0
90	LT	64	0	0	0	0
90	LV	43	0	0	0	0
90	LW	12	0	0	0	0
90	LX	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	LY	16	0	0	0	0
90	LZ	5	0	0	0	0
90	La	87	0	0	0	0
90	Lb	33	0	0	0	0
90	Lc	8	0	0	0	0
90	Ld	29	0	0	0	0
90	Le	88	0	0	0	0
90	Lf	38	0	0	0	0
90	Lg	60	0	0	0	0
90	Lh	15	0	0	0	0
90	Li	11	0	0	0	0
90	Lj	61	0	0	0	0
90	Lk	1	0	0	0	0
90	Ll	33	0	0	0	0
90	Lm	16	0	0	0	0
90	Ln	13	0	0	0	0
90	Lo	42	0	0	0	0
90	Lp	30	0	0	0	0
90	Lr	19	0	0	0	0
90	NC	5	0	0	0	0
90	Pt	3	0	0	0	0
90	S2	850	0	0	2	0
90	Sb	6	0	0	0	0
90	Se	2	0	0	0	0
90	mR	3	0	0	0	0
All	All	219527	0	157826	989	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (989) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2485:U:H3	1:L5:2493:G:H1	1.09	0.99
1:L5:3946:G:N2	1:L5:4067:U:O2	2.06	0.87
47:Pt:18:G:H1	47:Pt:55:PSU:HN3	1.25	0.84
1:L5:3944:OMG:HM22	1:L5:3945:A:H5''	1.62	0.81
61:SM:52:LEU:HB2	61:SM:78:LYS:HE3	1.62	0.81
1:L5:4108:G:H2'	1:L5:4109:G:C8	2.18	0.79
48:S2:73:C:H42	55:SG:168:LYS:HD3	1.48	0.79
48:S2:925:G:H1	48:S2:1017:U:H3	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1285:G:H1	61:SM:57:ASP:HB3	1.50	0.76
1:L5:517:C:H2'	1:L5:518:G:C8	2.21	0.74
48:S2:1286:G:H21	48:S2:1313:A:H62	1.35	0.74
1:L5:1100:U:H3	1:L5:1195:G:H1	1.36	0.73
48:S2:903:A:H2'	48:S2:904:A:C8	2.23	0.73
48:S2:1286:G:N2	48:S2:1313:A:H62	1.86	0.73
61:SM:81:ASP:HB3	61:SM:84:LYS:HG2	1.71	0.73
48:S2:928:G:H1	48:S2:1013:U:H3	1.35	0.72
1:L5:3946:G:H1	1:L5:4067:U:H3	1.39	0.71
48:S2:1228:A:H2'	48:S2:1229:G:C8	2.25	0.71
48:S2:546:G:H2'	48:S2:547:G:H8	1.56	0.69
1:L5:3756:A:HO2'	1:L5:3757:G:H8	1.41	0.68
48:S2:145:G:H2'	48:S2:146:G:C8	2.28	0.68
1:L5:517:C:H2'	1:L5:518:G:N7	2.09	0.67
1:L5:1339:U:H2'	1:L5:1340:OMC:C6	2.29	0.67
73:SY:114:MET:HE2	73:SY:122:LYS:HE2	1.75	0.67
48:S2:1091:C:HO2'	71:SW:2:VAL:N	1.92	0.66
48:S2:367:U:H4'	48:S2:371:A:C8	2.30	0.66
62:SN:16:LEU:HD12	62:SN:17:PRO:HD2	1.78	0.66
40:LI:9:ILE:HD12	40:LI:51:LEU:HD11	1.77	0.66
52:SD:40:ARG:HB2	52:SD:47:GLU:HB2	1.78	0.65
57:SI:34:ALA:HB2	57:SI:56:ARG:HD2	1.78	0.65
66:SR:17:ILE:HD11	66:SR:54:VAL:HG13	1.77	0.65
1:L5:3653:A:H4'	4:LA:179:ILE:O	1.97	0.65
81:Sg:236:ILE:HG22	81:Sg:252:THR:HG22	1.77	0.64
13:LJ:15:LEU:HD21	13:LJ:134:LEU:HD13	1.80	0.64
1:L5:1404:G:H2'	1:L5:1405:C:C6	2.32	0.64
1:L5:3908[A]:A:H61	46:NC:27:GLU:HB3	1.60	0.64
1:L5:2351:OMC:HM22	1:L5:2352:U:H5'	1.78	0.63
16:LN:123:GLU:HG2	16:LN:128:LYS:HG2	1.81	0.63
81:Sg:5:MET:HE3	81:Sg:270:LEU:HD11	1.80	0.63
1:L5:496:G:H2'	1:L5:497:G:C8	2.34	0.63
48:S2:546:G:H2'	48:S2:547:G:C8	2.34	0.63
48:S2:1371:U:H5''	48:S2:1372:U:H5	1.64	0.62
1:L5:490:C:H2'	1:L5:491:G:H8	1.65	0.62
67:SS:34:LYS:HG2	67:SS:103:LEU:HD23	1.82	0.62
1:L5:2495:U:H2'	1:L5:2496:G:H8	1.65	0.62
31:Lc:17:ARG:HD3	31:Lc:104:ILE:HA	1.82	0.61
1:L5:1400:G:H2'	1:L5:1401:C:C6	2.35	0.61
48:S2:319:C:H2'	48:S2:320:G:C8	2.35	0.61
1:L5:492:U:H2'	1:L5:493:G:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:888:U:H3'	48:S2:889:U:H5'	1.82	0.61
1:L5:664:G:N2	1:L5:667:A:H61	1.98	0.61
48:S2:494:C:N4	48:S2:509:OMG:HN22	1.97	0.61
54:SF:30:ILE:HG23	54:SF:117:ILE:HD11	1.82	0.61
3:L8:128:C:H2'	3:L8:129:C:C6	2.35	0.61
48:S2:115:U:H2'	48:S2:116:OMU:C6	2.32	0.60
1:L5:492:U:H2'	1:L5:493:G:H8	1.66	0.60
51:SC:263:LYS:HE2	70:SV:50:PHE:HZ	1.66	0.60
1:L5:4727:A:H5'	5:LB:129:ALA:O	2.01	0.60
1:L5:4935:C:H2'	1:L5:4936:G:C8	2.36	0.60
81:Sg:133:ASN:O	81:Sg:134:THR:HG22	2.01	0.60
52:SD:16:ILE:HD11	78:Sd:36:LEU:HD23	1.84	0.60
1:L5:4260:U:H2'	1:L5:4261:C:C6	2.37	0.60
1:L5:4220:6MZ:O5'	1:L5:4220:6MZ:H8	2.02	0.60
48:S2:1417:C:H2'	48:S2:1418:C:C6	2.37	0.60
9:LF:143:GLY:HA3	9:LF:240:ILE:HB	1.82	0.59
48:S2:145:G:H2'	48:S2:146:G:H8	1.67	0.59
48:S2:441:C:H4'	48:S2:1737:G:O2'	2.02	0.59
1:L5:4873:G:C8	17:LO:179:LYS:HE3	2.37	0.59
1:L5:516:C:H2'	1:L5:517:C:C6	2.38	0.59
1:L5:2492:C:H2'	1:L5:2493:G:H8	1.66	0.59
48:S2:877:C:H2'	48:S2:878:G:C8	2.37	0.59
48:S2:981:A:H2'	48:S2:982:G:C8	2.36	0.59
1:L5:488:G:H2'	1:L5:489:C:C6	2.38	0.59
48:S2:74:G:H1'	48:S2:76:U:C4	2.38	0.59
1:L5:1278:C:H2'	1:L5:1279:A:O4'	2.02	0.59
1:L5:4881:U:H4'	1:L5:4882:U:C5	2.38	0.59
47:Pt:34:C:H2'	47:Pt:35:U:H5''	1.85	0.59
48:S2:394:G:H5''	60:SL:81:LYS:HB3	1.83	0.59
48:S2:1667:U:H2'	48:S2:1668:U:C6	2.38	0.59
1:L5:4400:G:H4'	84:L5:5615:PUT:H41	1.85	0.58
48:S2:382:C:H2'	48:S2:383:G:H8	1.69	0.58
48:S2:195:C:H2'	48:S2:196:C:C6	2.37	0.58
1:L5:4067:U:H2'	1:L5:4068:U:C6	2.38	0.58
81:Sg:87:LEU:HB2	81:Sg:101:PHE:HB2	1.86	0.58
58:SJ:130:ILE:O	58:SJ:143:ASN:HA	2.04	0.57
1:L5:1411:C:H2'	1:L5:1412:G:C8	2.39	0.57
48:S2:903:A:H2'	48:S2:904:A:H8	1.70	0.57
48:S2:1778:C:H2'	48:S2:1779:G:C8	2.40	0.57
81:Sg:191:HIS:CG	81:Sg:195:LEU:HD21	2.39	0.57
1:L5:1205:G:H2'	1:L5:1206:C:C6	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1404:G:H2'	1:L5:1405:C:H6	1.70	0.57
1:L5:1437:C:H1'	1:L5:2098:G:H3'	1.85	0.57
48:S2:1588:A:H2'	48:S2:1589:A:C8	2.39	0.57
59:SK:15:LEU:HD22	59:SK:49:MET:HE1	1.86	0.57
59:SK:85:LEU:HD22	59:SK:89:ILE:HD12	1.87	0.56
1:L5:490:C:H2'	1:L5:491:G:C8	2.39	0.56
1:L5:4919:G:H2'	1:L5:4920:C:C6	2.40	0.56
48:S2:555:A:H2'	48:S2:556:U:C6	2.41	0.56
81:Sg:174:VAL:HB	81:Sg:188:HIS:HB2	1.86	0.56
1:L5:4935:C:H2'	1:L5:4936:G:H8	1.71	0.56
48:S2:1801:A:H2'	48:S2:1802:C:C6	2.41	0.56
1:L5:664:G:H21	1:L5:667:A:H61	1.53	0.56
48:S2:140:C:H42	48:S2:313:A:H61	1.53	0.56
23:LU:26:THR:HA	23:LU:68:SER:HB3	1.88	0.56
48:S2:1390:U:H2'	48:S2:1391:OMC:C6	2.41	0.56
48:S2:550:C:H2'	48:S2:551:U:C6	2.41	0.55
48:S2:1679:A:C2	54:SF:60:ARG:HA	2.42	0.55
1:L5:2809:G:N7	85:L5:5607:SPD:H92	2.20	0.55
23:LU:28:PRO:HB2	23:LU:34:MET:HG2	1.89	0.55
48:S2:545:A:H3'	48:S2:546:G:C8	2.41	0.55
68:ST:65:TYR:HE2	68:ST:128:GLN:HG3	1.71	0.55
21:LS:164:LYS:HE3	34:Lf:34:TYR:HB2	1.89	0.55
58:SJ:164:PRO:HA	58:SJ:168:GLY:HA2	1.87	0.55
48:S2:455:A:H2'	48:S2:456:C:C6	2.42	0.55
50:SB:136:ARG:HB2	50:SB:218:LEU:HD11	1.89	0.55
81:Sg:165:ILE:HG23	81:Sg:179:LEU:HD11	1.87	0.55
1:L5:4591:U:H2'	1:L5:4592:C:C6	2.41	0.55
50:SB:22:VAL:HG11	63:SO:84:ARG:HH22	1.71	0.55
1:L5:2491:C:H2'	1:L5:2492:C:C6	2.42	0.55
54:SF:17:ILE:HD11	65:SQ:57:LEU:HD21	1.88	0.55
48:S2:382:C:H2'	48:S2:383:G:C8	2.42	0.55
71:SW:28:ARG:HG3	71:SW:60:LYS:HE3	1.89	0.55
1:L5:959:G:C8	8:LE:123:ARG:HG2	2.41	0.55
1:L5:3717:A:H2'	1:L5:3718:A2M:C8	2.36	0.55
1:L5:982:U:H2'	1:L5:983:C:C6	2.42	0.54
1:L5:496:G:H2'	1:L5:497:G:H8	1.70	0.54
26:LX:73:HIS:CE1	26:LX:115:LYS:HD3	2.41	0.54
48:S2:1421:A:H1'	48:S2:1422:G:H2'	1.90	0.54
1:L5:1280:C:O2	87:L5:5618:TRS:H22	2.06	0.54
1:L5:3923:A:H2'	1:L5:3924:C:C6	2.42	0.54
1:L5:4265:U:O2	7:LD:16:TYR:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2018:C:H2'	1:L5:2019:C:C6	2.43	0.54
21:LS:11:LYS:HE3	21:LS:29:ARG:HD3	1.89	0.54
1:L5:1789:C:H2'	1:L5:1790:U:C6	2.43	0.54
1:L5:2562:G:O5'	1:L5:2562:G:H8	1.91	0.54
1:L5:5034:A:H2'	1:L5:5035:U:O4'	2.08	0.54
31:Lc:27:TYR:HE1	31:Lc:29:LEU:HD11	1.73	0.54
48:S2:116:OMU:H6	48:S2:116:OMU:O5'	2.08	0.54
76:Sb:34:ASP:O	76:Sb:79:PHE:HA	2.07	0.54
1:L5:691:C:H2'	1:L5:692:A:C8	2.43	0.54
1:L5:4266:G:N3	1:L5:4266:G:H2'	2.21	0.54
1:L5:4934:A:H2'	1:L5:4935:C:C6	2.43	0.54
48:S2:1737:G:H2'	48:S2:1738:C:C6	2.43	0.53
1:L5:1719:A:H2'	1:L5:1720:C:H1'	1.89	0.53
1:L5:1617:G:H1'	1:L5:2513:A:N6	2.23	0.53
1:L5:1755:C:N3	7:LD:3:PHE:HB3	2.23	0.53
1:L5:4731:G:H1'	1:L5:4732:G:C2	2.43	0.53
29:La:125:LYS:HG2	29:La:145:VAL:HB	1.90	0.53
48:S2:525:A:H2'	48:S2:526:A:H8	1.73	0.53
1:L5:93:G:H2'	1:L5:94:A:C8	2.44	0.53
1:L5:4274:A:H2'	1:L5:4275:G:C8	2.44	0.53
48:S2:1536:G:H2'	48:S2:1537:A:C8	2.43	0.53
1:L5:970:G:C2	8:LE:123:ARG:HD3	2.44	0.53
1:L5:1300:G:H2'	1:L5:1301:C:C6	2.43	0.53
1:L5:4488:A:H4'	1:L5:4489:G:C8	2.43	0.53
48:S2:1628:C:H2'	48:S2:1629:C:C6	2.43	0.53
51:SC:196:ILE:HB	51:SC:223:TYR:HB2	1.91	0.53
52:SD:51:LEU:HD23	52:SD:89:GLU:HB2	1.91	0.53
3:L8:128:C:H2'	3:L8:129:C:H6	1.73	0.53
1:L5:4739:C:H2'	1:L5:4740:G:H5'	1.91	0.53
48:S2:562:U:H2'	48:S2:563:G:C8	2.44	0.53
48:S2:640:A:H2'	48:S2:641:A:C8	2.43	0.53
77:Sc:46:VAL:HG11	77:Sc:50:VAL:HG11	1.91	0.53
1:L5:1766:A:C2'	67:SS:116:LYS:HB2	2.39	0.53
1:L5:4105:A:H1'	1:L5:4106:G:N2	2.24	0.53
1:L5:106:A:H2'	1:L5:107:G:O4'	2.09	0.53
1:L5:280:G:H5''	16:LN:14:LYS:HE2	1.91	0.53
77:Sc:42:ILE:HD12	77:Sc:44:ARG:HD3	1.91	0.53
48:S2:1849:G:H2'	48:S2:1850:MA6:C8	2.38	0.52
49:SA:63:ARG:NH1	70:SV:38:GLU:HA	2.24	0.52
48:S2:1203:G:H2'	48:S2:1204:A:C8	2.44	0.52
1:L5:3736:A:H2'	1:L5:3737:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:3749:C:H4'	4:LA:221:LYS:O	2.09	0.52
1:L5:3756:A:O2'	1:L5:3757:G:H8	1.92	0.52
32:Ld:54:MET:HE2	32:Ld:60:PRO:HA	1.90	0.52
1:L5:1760:G:H5''	1:L5:1761:G:OP2	2.10	0.52
48:S2:118:C:H1'	48:S2:445:A:C5	2.45	0.52
68:ST:27:LYS:HB2	68:ST:110:LEU:HD21	1.91	0.52
18:LP:54:GLN:HA	18:LP:83:TRP:CD1	2.44	0.52
54:SF:99:ILE:HD11	74:SZ:106:GLN:HE21	1.73	0.52
1:L5:5065:U:H1'	18:LP:75:GLN:NE2	2.25	0.52
48:S2:12:U:H2'	48:S2:13:C:C6	2.44	0.52
48:S2:1181:A:H2'	48:S2:1182:A:C8	2.44	0.52
65:SQ:50:LYS:HA	65:SQ:50:LYS:HE2	1.91	0.52
1:L5:4573:G:H2'	1:L5:4574:U:C6	2.45	0.52
1:L5:4771:C:H2'	1:L5:4772:C:C6	2.45	0.52
48:S2:1289:U:H4'	59:SK:2:LEU:HD11	1.92	0.52
1:L5:952:G:H4'	34:Lf:75:THR:HG23	1.92	0.52
48:S2:484:A2M:O5'	48:S2:484:A2M:H8	2.10	0.52
48:S2:394:G:H5''	60:SL:81:LYS:CB	2.39	0.52
48:S2:433:A:H5''	57:SI:22:HIS:HB3	1.92	0.52
48:S2:1536:G:H2'	48:S2:1537:A:H8	1.74	0.52
1:L5:4152:G:H2'	1:L5:4153:C:C6	2.45	0.52
48:S2:191:A:H2'	48:S2:192:C:O4'	2.10	0.52
28:LZ:100:VAL:HG13	28:LZ:107:LYS:HA	1.91	0.51
51:SC:69:LEU:HD21	51:SC:273:LEU:HG	1.92	0.51
48:S2:67:C:C5	55:SG:162:LEU:HB3	2.45	0.51
1:L5:1410:U:H4'	1:L5:1411:C:H4'	1.92	0.51
1:L5:2479:G:H2'	1:L5:2480:G:H8	1.75	0.51
1:L5:4992:G:H2'	1:L5:4993:G:C8	2.46	0.51
48:S2:1217:A:H2'	48:S2:1218:C:C6	2.44	0.51
1:L5:1762:C:H42	1:L5:1770:A:H61	1.58	0.51
1:L5:2485:U:H2'	1:L5:2486:G:C8	2.46	0.51
1:L5:4954:G:H2'	1:L5:4955:A:C8	2.44	0.51
47:Pt:65:U:H2'	47:Pt:66:C:C6	2.46	0.51
48:S2:381:C:H5'	57:SI:48:VAL:HG13	1.93	0.51
1:L5:1074:G:H2'	1:L5:1075:G:H8	1.76	0.51
1:L5:2492:C:H2'	1:L5:2493:G:C8	2.45	0.51
1:L5:3747:A:C8	4:LA:245:ARG:HD3	2.46	0.51
4:LA:180:LEU:HG	44:Lp:18:TYR:CG	2.46	0.51
48:S2:59:U:H5''	48:S2:503:C:N4	2.26	0.51
48:S2:70:G:H21	48:S2:79:A:H2	1.59	0.51
61:SM:32:ALA:HB3	61:SM:110:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1662:C:H2'	1:L5:1663:C:C6	2.45	0.51
1:L5:3868:G:H22	1:L5:3900:G:H1'	1.75	0.51
1:L5:4459:U:H2'	1:L5:4460:U:C6	2.46	0.51
14:LL:60:ARG:HD2	14:LL:67:HIS:O	2.11	0.51
48:S2:1037:G:H4'	48:S2:1845:A:H4'	1.91	0.51
58:SJ:32:ILE:HD11	58:SJ:40:LYS:HD3	1.91	0.51
1:L5:2483:G:C6	1:L5:2496:G:C6	2.99	0.51
1:L5:4069:U:H2'	1:L5:4070:U:C6	2.45	0.51
1:L5:4111:U:H2'	1:L5:4112:C:C6	2.46	0.51
51:SC:137:VAL:HG22	51:SC:217:ALA:HA	1.91	0.51
1:L5:1730:U:H1'	22:LT:101:SER:HB3	1.91	0.51
1:L5:2602:G:H2'	1:L5:2603:C:C6	2.46	0.51
1:L5:4859:C:H3'	1:L5:4860:G:H8	1.75	0.51
48:S2:1407:U:H2'	48:S2:1408:U:C6	2.46	0.51
47:Pt:34:C:C2'	47:Pt:35:U:H5''	2.41	0.51
49:SA:2(A):SER:O	49:SA:8:LEU:HD12	2.10	0.51
74:SZ:64:ASN:O	74:SZ:111:ARG:HG2	2.11	0.51
1:L5:4065:G:H2'	1:L5:4066:U:C6	2.46	0.50
1:L5:4771:C:H6	1:L5:4771:C:O5'	1.94	0.50
32:Ld:75:LYS:HE3	32:Ld:79:ASN:O	2.12	0.50
48:S2:5:U:H2'	48:S2:6:G:H8	1.77	0.50
47:Pt:18:G:H3'	47:Pt:19:U:H5''	1.93	0.50
48:S2:67:C:C5	55:SG:164:LYS:HB2	2.46	0.50
52:SD:142:LEU:HD13	52:SD:150:MET:SD	2.51	0.50
53:SE:124:CYS:HA	53:SE:142:HIS:CE1	2.46	0.50
9:LF:43:ARG:HG3	9:LF:43:ARG:HH11	1.76	0.50
48:S2:74:G:H1'	48:S2:76:U:C5	2.46	0.50
48:S2:838:G:O6	73:SY:10:ARG:HA	2.11	0.50
1:L5:385:A:N3	1:L5:387:G:H5''	2.27	0.50
1:L5:469:C:H2'	1:L5:470:A:C8	2.46	0.50
1:L5:489:C:H2'	1:L5:490:C:C6	2.47	0.50
1:L5:3718:A2M:O5'	1:L5:3718:A2M:H8	2.11	0.50
48:S2:79:A:H3'	48:S2:80:G:H8	1.75	0.50
48:S2:467:G:H5'	55:SG:72:ARG:NH2	2.25	0.50
1:L5:1762:C:H2'	1:L5:1763:C:C6	2.47	0.50
1:L5:1898:C:O3'	84:L5:5616:PUT:H11	2.11	0.50
1:L5:1920:C:H3'	1:L5:1921:C:H5''	1.93	0.50
1:L5:2485:U:O4	1:L5:2493:G:O6	2.30	0.50
1:L5:2504:C:H5	1:L5:2506:G:H21	1.56	0.50
1:L5:3911:C:H2'	1:L5:3912:U:C6	2.46	0.50
81:Sg:191:HIS:CD2	81:Sg:195:LEU:HD21	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Pt:35:U:H6	47:Pt:35:U:C5'	2.25	0.50
48:S2:528:A:H2'	48:S2:529:A:H8	1.77	0.50
48:S2:1308:U:H2'	48:S2:1309:C:C6	2.47	0.50
61:SM:72:HIS:HB3	61:SM:74:ILE:HD13	1.94	0.50
48:S2:1101:U:H2'	48:S2:1102:G:C8	2.46	0.50
54:SF:144:LEU:HD23	77:Sc:49:PRO:HG2	1.94	0.50
1:L5:455:C:H2'	1:L5:456:C:C6	2.47	0.49
4:LA:178:PRO:HG2	44:Lp:26:VAL:HG23	1.94	0.49
40:Ll:51:LEU:HD13	40:Ll:51:LEU:O	2.12	0.49
48:S2:1597:C:H4'	48:S2:1603:G:O6	2.12	0.49
52:SD:26:THR:O	52:SD:30:ALA:HB2	2.12	0.49
53:SE:31:PRO:HG2	53:SE:38:LEU:HG	1.94	0.49
1:L5:134:G:O6	36:Lh:74:LYS:HE2	2.12	0.49
1:L5:457:G:H2'	1:L5:458:C:C6	2.46	0.49
10:LG:83:PHE:HA	10:LG:183:ILE:HD13	1.93	0.49
10:LG:121:LYS:HG2	10:LG:127:ASP:HA	1.94	0.49
80:Sf:132:MET:SD	80:Sf:141:CYS:HB2	2.52	0.49
1:L5:455:C:H2'	1:L5:456:C:H6	1.76	0.49
1:L5:2351:OMC:HM23	6:LC:95:MET:HG3	1.95	0.49
1:L5:4966:A:H5''	5:LB:128:LYS:HG3	1.93	0.49
3:L8:141:C:H2'	3:L8:142:U:C6	2.47	0.49
12:LI:140:THR:HG23	12:LI:141:LYS:O	2.11	0.49
51:SC:137:VAL:O	51:SC:162:ILE:HA	2.13	0.49
56:SH:65:PRO:HB2	56:SH:68:GLN:HG3	1.94	0.49
64:SP:45:LEU:HD21	64:SP:84:ILE:HD11	1.94	0.49
74:SZ:68:ILE:HB	74:SZ:109:TYR:HB2	1.94	0.49
61:SM:31:LEU:HD23	61:SM:109:VAL:HG21	1.94	0.49
1:L5:469:C:H2'	1:L5:470:A:H8	1.77	0.49
1:L5:1672:U:H2'	1:L5:1673:U:C6	2.47	0.49
1:L5:2792:C:O2	38:Lj:9:GLY:HA2	2.12	0.49
1:L5:4524:G:C2	5:LB:252:ALA:HB1	2.47	0.49
48:S2:354:OMU:HM22	48:S2:355:G:O4'	2.13	0.49
48:S2:1228:A:H2'	48:S2:1229:G:H8	1.77	0.49
1:L5:1566:C:H2'	1:L5:1567:U:H6	1.78	0.49
1:L5:2874:U:O4	1:L5:3823:G:C8	2.65	0.49
48:S2:552:G:H2'	48:S2:553:U:C5	2.46	0.49
80:Sf:119:ARG:O	80:Sf:132:MET:HG2	2.13	0.49
1:L5:4238:G:H2'	1:L5:4239:A:C8	2.47	0.49
1:L5:4859:C:H3'	1:L5:4860:G:C8	2.48	0.49
48:S2:1597:C:H4'	48:S2:1603:G:C6	2.48	0.49
64:SP:34:MET:CG	64:SP:42:ARG:HG3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Sg:163:PRO:HB2	81:Sg:179:LEU:HB2	1.93	0.49
1:L5:963:G:N2	9:LF:32:ARG:HH12	2.11	0.49
1:L5:1079:C:H2'	1:L5:1080:C:H5'	1.94	0.49
1:L5:2065:G:H2'	1:L5:2066:C:O4'	2.13	0.49
1:L5:2539:C:H2'	1:L5:2540:C:C6	2.48	0.49
1:L5:3707:U:H2'	1:L5:3708:C:C6	2.48	0.49
48:S2:1712:A:H2'	48:S2:1713:C:C6	2.48	0.49
49:SA:38:ILE:HD11	49:SA:150:THR:HG22	1.94	0.49
1:L5:4504:C:H2'	1:L5:4505:C:C6	2.48	0.48
80:Sf:139:HIS:CE1	80:Sf:148:TYR:HB2	2.47	0.48
1:L5:4161:G:C6	10:LG:53:ARG:HD2	2.47	0.48
7:LD:291:GLN:NE2	12:LI:214:SER:HA	2.28	0.48
48:S2:804:U:H2'	48:S2:805:U:C6	2.48	0.48
1:L5:711:A:H2'	1:L5:712:C:C6	2.49	0.48
1:L5:2493:G:H2'	1:L5:2494:U:C6	2.49	0.48
1:L5:3946:G:H2'	1:L5:3947:A:C8	2.49	0.48
48:S2:107:A:H2'	48:S2:108:G:C8	2.48	0.48
48:S2:1284:A:C5	61:SM:91:LEU:HD22	2.48	0.48
48:S2:1418:C:H2'	48:S2:1419:C:O4'	2.13	0.48
48:S2:1545:A:H5''	65:SQ:74:GLY:HA2	1.95	0.48
1:L5:187:U:H1'	1:L5:188:G:N7	2.28	0.48
1:L5:2487:G:C2	1:L5:2488:C:H1'	2.49	0.48
4:LA:46:LYS:HE2	4:LA:62:VAL:HG21	1.95	0.48
52:SD:163:PRO:HA	52:SD:166:TYR:CZ	2.48	0.48
53:SE:107:GLY:HA2	53:SE:189:LEU:HG	1.94	0.48
62:SN:33:VAL:HG21	62:SN:66:VAL:HG11	1.95	0.48
68:ST:108:GLU:OE2	68:ST:121:ARG:HD3	2.12	0.48
1:L5:664:G:H2'	1:L5:667:A:H62	1.79	0.48
1:L5:3910:C:H2'	1:L5:3911:C:C6	2.48	0.48
1:L5:4065:G:H2'	1:L5:4066:U:H6	1.78	0.48
1:L5:5065:U:H1'	18:LP:75:GLN:HE21	1.78	0.48
10:LG:259:LYS:O	10:LG:263:THR:HG23	2.13	0.48
48:S2:1406:G:H2'	48:S2:1407:U:C6	2.49	0.48
51:SC:188:CYS:SG	51:SC:238:LYS:HE3	2.53	0.48
54:SF:188:TYR:CZ	54:SF:192:LYS:HE2	2.48	0.48
51:SC:74:LYS:HB3	51:SC:269:PHE:CE1	2.47	0.48
1:L5:4187:G:OP1	85:L5:5610:SPD:H52	2.13	0.48
12:LI:110:ARG:HG2	47:Pt:73:C:C5	2.49	0.48
16:LN:138:PHE:HA	16:LN:143:ARG:HD2	1.95	0.48
48:S2:1371:U:H5''	48:S2:1372:U:C5	2.48	0.48
1:L5:116:G:H2'	1:L5:117:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:659:G:H2'	1:L5:660:A:C8	2.49	0.48
1:L5:2029:A:H2'	1:L5:2030:A:C8	2.48	0.48
48:S2:872:A:H2'	48:S2:872:A:N3	2.28	0.48
48:S2:1692:PSU:H2'	48:S2:1693:G:C8	2.49	0.48
1:L5:1074:G:H2'	1:L5:1075:G:C8	2.49	0.48
1:L5:1846:G:H2'	1:L5:1847:C:C6	2.48	0.48
3:L8:87:G:H8	3:L8:87:G:OP2	1.97	0.48
58:SJ:133:ARG:HH11	58:SJ:133:ARG:HG2	1.78	0.48
81:Sg:83:TRP:HA	81:Sg:107:ASP:HB3	1.95	0.48
1:L5:690:C:H2'	1:L5:691:C:H6	1.79	0.47
8:LE:281:ILE:HG23	8:LE:286:LEU:HD21	1.96	0.47
48:S2:608:C:H5'	48:S2:608:C:C6	2.49	0.47
48:S2:940:U:H2'	48:S2:941:C:C6	2.49	0.47
48:S2:1421:A:H4'	48:S2:1422:G:H5'	1.96	0.47
51:SC:263:LYS:HE2	70:SV:50:PHE:CZ	2.48	0.47
1:L5:1186:U:H2'	1:L5:1187:G:N3	2.29	0.47
1:L5:1637:A:OP1	1:L5:1639:U:H5	1.97	0.47
1:L5:4254:G:N3	1:L5:4254:G:H2'	2.29	0.47
1:L5:4978:G:H2'	1:L5:4979:A:H5''	1.97	0.47
48:S2:99:A2M:H2'	48:S2:100:U:O4'	2.15	0.47
48:S2:1227:G:C2	48:S2:1228:A:C8	3.01	0.47
62:SN:31:ASP:O	62:SN:35:GLU:HG2	2.14	0.47
1:L5:182:G:N2	1:L5:256:G:H1'	2.29	0.47
1:L5:288:G:H2'	1:L5:289:C:C6	2.50	0.47
1:L5:1786:A:H2'	1:L5:1789:C:C5	2.49	0.47
1:L5:3705:G:H2'	1:L5:3706:C:C6	2.48	0.47
1:L5:4169:G:H4'	1:L5:4171:C:C2	2.48	0.47
80:Sf:119:ARG:H	80:Sf:119:ARG:HD2	1.80	0.47
48:S2:195:C:C2	48:S2:196:C:C5	3.03	0.47
48:S2:928:G:H2'	48:S2:929:G:C8	2.50	0.47
56:SH:30:LEU:HD21	56:SH:82:GLU:HG3	1.96	0.47
70:SV:1:MET:O	70:SV:9:VAL:HG22	2.14	0.47
84:L5:5616:PUT:H21	90:L5:8556:HOH:O	2.14	0.47
16:LN:60:VAL:HG22	16:LN:134:LEU:HB2	1.96	0.47
48:S2:532:C:H2'	48:S2:533:A:C8	2.49	0.47
64:SP:108:LYS:HB2	67:SS:117:ILE:HD11	1.95	0.47
76:Sb:46:VAL:HG11	76:Sb:64:CYS:SG	2.54	0.47
1:L5:1265:G:H5''	30:Lb:95:ARG:HH12	1.80	0.47
1:L5:1308:C:H2'	1:L5:1309:C:C6	2.50	0.47
1:L5:2486:G:H2'	1:L5:2487:G:C8	2.50	0.47
1:L5:3782:5MC:H2'	1:L5:3783:A:H5''	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SM:49:LEU:HG	61:SM:127:TYR:OH	2.15	0.47
61:SM:121:LYS:HA	61:SM:124:ILE:HB	1.97	0.47
1:L5:325:U:H2'	1:L5:326:C:C6	2.49	0.47
1:L5:445:U:H2'	1:L5:446:C:O4'	2.14	0.47
1:L5:1766:A:H2'	67:SS:116:LYS:HB2	1.96	0.47
1:L5:2091:C:H4'	1:L5:2092:G:H5'	1.96	0.47
1:L5:4488:A:H4'	1:L5:4489:G:H8	1.79	0.47
8:LE:173:LEU:O	8:LE:188:ARG:HA	2.14	0.47
53:SE:182:MET:HE2	53:SE:190:GLY:HA2	1.97	0.47
65:SQ:59:GLY:HA2	65:SQ:63:PHE:HD1	1.79	0.47
74:SZ:69:THR:H	74:SZ:72:VAL:HG12	1.80	0.47
1:L5:3908[A]:A:N6	46:NC:27:GLU:HB3	2.29	0.47
47:Pt:19:U:O2	47:Pt:19:U:H2'	2.15	0.47
48:S2:542:U:H2'	48:S2:543:C:C6	2.50	0.47
54:SF:35:LEU:HD12	54:SF:117:ILE:HG12	1.97	0.47
55:SG:162:LEU:HD11	55:SG:172:LYS:HG3	1.95	0.47
1:L5:984:C:H2'	1:L5:985:C:H6	1.80	0.47
1:L5:3867:A2M:HM'3	1:L5:3880:G:N2	2.30	0.47
1:L5:4289:U:H2'	1:L5:4290:U:C6	2.50	0.47
2:L7:55:A:H4'	13:LJ:155:HIS:HB2	1.97	0.47
16:LN:178:HIS:HA	16:LN:181:HIS:NE2	2.28	0.47
48:S2:1845:A:H2'	48:S2:1846:G:C8	2.50	0.47
64:SP:60:LEU:HD22	64:SP:92:SER:OG	2.15	0.47
66:SR:66:VAL:HG12	66:SR:67:ARG:N	2.30	0.47
69:SU:33:GLU:CD	69:SU:55:ARG:HH12	2.23	0.47
1:L5:3765:G:H1'	1:L5:3766:A:C2	2.50	0.47
8:LE:216:TYR:OH	8:LE:246:ARG:HD3	2.15	0.47
9:LF:181:LYS:HE3	9:LF:182:TYR:CZ	2.50	0.47
48:S2:1274:G:H5'	48:S2:1274:G:N3	2.30	0.47
48:S2:1374:C:H2'	48:S2:1375:G:O4'	2.15	0.47
49:SA:39:TYR:CE2	66:SR:105:MET:HB2	2.50	0.47
55:SG:30:LYS:HE3	55:SG:34:THR:HG21	1.97	0.47
23:LU:20:LYS:HB2	23:LU:20:LYS:HE2	1.76	0.46
48:S2:5:U:H2'	48:S2:6:G:C8	2.51	0.46
48:S2:615:C:H2'	48:S2:616:A:O4'	2.15	0.46
65:SQ:41:MET:HE3	68:ST:8:ASP:O	2.15	0.46
1:L5:260:C:H2'	1:L5:261:G:H8	1.81	0.46
1:L5:5065:U:H2'	1:L5:5066:U:O4'	2.15	0.46
28:LZ:97:ASN:C	28:LZ:97:ASN:HD22	2.22	0.46
48:S2:159:A2M:O5'	48:S2:159:A2M:H8	2.15	0.46
48:S2:528:A:H2'	48:S2:529:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:896:U:H5	48:S2:898:U:C4	2.34	0.46
48:S2:1831:A:H2'	48:S2:1832:6MZ:H8	1.96	0.46
48:S2:1849:G:H2'	48:S2:1850:MA6:H8	1.96	0.46
76:Sb:67:THR:HG22	76:Sb:68:GLY:N	2.31	0.46
9:LF:37:PHE:HZ	30:Lb:113:ALA:HB1	1.80	0.46
10:LG:121:LYS:HA	10:LG:126:GLY:O	2.15	0.46
48:S2:1347:PSU:H2'	48:S2:1348:G:N3	2.30	0.46
1:L5:454:U:H2'	1:L5:455:C:C6	2.50	0.46
1:L5:1720:C:H3'	1:L5:1721:G:H5''	1.96	0.46
1:L5:3911:C:H2'	1:L5:3912:U:H6	1.79	0.46
1:L5:4524:G:N3	5:LB:252:ALA:HB1	2.31	0.46
48:S2:394:G:C5'	60:SL:81:LYS:HB3	2.44	0.46
48:S2:1595:U:H2'	48:S2:1596:U:C6	2.50	0.46
1:L5:4584:A:H2'	1:L5:4585:U:O4'	2.16	0.46
8:LE:108:LYS:HE3	8:LE:110:ARG:O	2.15	0.46
12:LI:36:LEU:HD13	12:LI:69:ARG:NH1	2.31	0.46
23:LU:45:GLU:O	23:LU:53:ALA:HB1	2.15	0.46
48:S2:29:G:H2'	48:S2:30:C:C6	2.51	0.46
48:S2:1523:C:H4'	67:SS:145:THR:HA	1.98	0.46
48:S2:1804:OMU:H1'	48:S2:1804:OMU:HM23	1.61	0.46
1:L5:18:C:H4'	16:LN:138:PHE:CD1	2.51	0.46
1:L5:184:U:H2'	1:L5:186:G:C8	2.51	0.46
1:L5:964:A:N3	1:L5:964:A:H2'	2.29	0.46
33:Le:35:TRP:CZ2	33:Le:56:PRO:HD2	2.50	0.46
48:S2:159:A2M:HM'3	48:S2:159:A2M:H1'	1.46	0.46
48:S2:379:C:H5'	57:SI:33:ALA:HA	1.98	0.46
48:S2:888:U:C3'	48:S2:889:U:H5'	2.45	0.46
81:Sg:158:PRO:HD3	81:Sg:200:VAL:HG21	1.96	0.46
1:L5:111:C:OP1	36:Lh:110:LYS:HE3	2.15	0.46
1:L5:4239:A:H2'	1:L5:4240:G:C8	2.50	0.46
10:LG:261:LEU:O	10:LG:264:LYS:HB3	2.15	0.46
48:S2:15:U:H2'	48:S2:16:G:O4'	2.16	0.46
48:S2:576:A2M:HM'3	48:S2:576:A2M:H1'	1.66	0.46
56:SH:63:PHE:HB3	56:SH:97:GLN:HG3	1.98	0.46
60:SL:75:GLY:HA3	60:SL:88:ILE:HD12	1.97	0.46
64:SP:135:ALA:HB3	67:SS:148:VAL:CG2	2.46	0.46
68:ST:72:VAL:O	68:ST:76:THR:HG23	2.16	0.46
1:L5:2351:OMC:HM23	6:LC:95:MET:CG	2.46	0.46
24:LV:60:MET:HE3	24:LV:129:TRP:CH2	2.51	0.46
47:Pt:42:C:H2'	47:Pt:43:G:O4'	2.15	0.46
48:S2:467:G:H5'	55:SG:72:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1232:PSU:H2'	48:S2:1233:G:C8	2.51	0.46
65:SQ:59:GLY:HA2	65:SQ:63:PHE:CD1	2.50	0.46
1:L5:1788:A:H2'	12:LI:22:PHE:CZ	2.51	0.46
1:L5:2673:G:H5'	1:L5:2673:G:N3	2.30	0.46
1:L5:2876:OMG:HM22	1:L5:2877:G:H5'	1.98	0.46
1:L5:4536:OMC:HM23	1:L5:4536:OMC:H1'	1.79	0.46
73:SY:89:HIS:CE1	73:SY:90:ARG:HG3	2.50	0.46
1:L5:187:U:O4	1:L5:1365:C:C2	2.69	0.46
1:L5:664:G:H21	1:L5:667:A:N6	2.14	0.46
1:L5:2815:A2M:H3'	1:L5:2815:A2M:OP1	2.16	0.46
1:L5:3946:G:H2'	1:L5:3947:A:H8	1.81	0.46
48:S2:1406:G:H2'	48:S2:1407:U:H6	1.79	0.46
1:L5:1401:C:H2'	1:L5:1402:C:C6	2.50	0.45
1:L5:2396:A:C8	1:L5:2814:C:H2'	2.51	0.45
1:L5:4456:OMC:HM21	5:LB:241:PRO:HD3	1.98	0.45
40:LI:9:ILE:CD1	40:LI:51:LEU:HD11	2.46	0.45
48:S2:867:OMG:HM23	48:S2:867:OMG:H1'	1.58	0.45
48:S2:1035:A:H2'	48:S2:1036:A:O4'	2.15	0.45
51:SC:173:LYS:O	70:SV:3:ASN:HB2	2.15	0.45
75:Sa:21:ILE:C	75:Sa:21:ILE:HD12	2.40	0.45
81:Sg:217:MET:HG2	81:Sg:229:THR:HG23	1.98	0.45
1:L5:1566:C:H2'	1:L5:1567:U:C6	2.50	0.45
1:L5:4740:G:C6	1:L5:4960:G:C6	3.05	0.45
1:L5:4750:G:H2'	1:L5:4751:G:C8	2.50	0.45
48:S2:79:A:N3	48:S2:79:A:H5'	2.31	0.45
52:SD:46:THR:HG23	52:SD:84:VAL:HG12	1.98	0.45
81:Sg:59:LEU:HD23	81:Sg:90:TRP:CD2	2.51	0.45
1:L5:1762:C:H42	1:L5:1770:A:N6	2.13	0.45
1:L5:3761:C:H2'	1:L5:3762:PSU:C6	2.52	0.45
37:Li:2:ALA:HB3	37:Li:5:TYR:CZ	2.51	0.45
47:Pt:12:C:H2'	47:Pt:13:PSU:C6	2.51	0.45
69:SU:46:LYS:HB2	69:SU:48:LEU:HG	1.99	0.45
13:LJ:15:LEU:HD22	13:LJ:165:TRP:CD1	2.51	0.45
15:LM:36:ALA:HB2	15:LM:52:PHE:CE1	2.51	0.45
47:Pt:35:U:H5'	47:Pt:35:U:C6	2.52	0.45
48:S2:468:A2M:HM'3	48:S2:468:A2M:H1'	1.81	0.45
56:SH:142:LYS:HE2	56:SH:142:LYS:HB3	1.76	0.45
1:L5:516:C:H2'	1:L5:517:C:C5	2.52	0.45
1:L5:3873:G:H2'	1:L5:3874:G:C8	2.51	0.45
1:L5:3907:G:H5'	1:L5:4449:A:N1	2.31	0.45
1:L5:4967:A:H2'	1:L5:4968:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SA:80:ARG:NH2	49:SA:82:THR:HG21	2.31	0.45
61:SM:11:VAL:O	61:SM:14:VAL:HG22	2.16	0.45
74:SZ:65:TYR:OH	74:SZ:76:ARG:HG2	2.16	0.45
3:L8:92:U:H2'	3:L8:93:C:O4'	2.17	0.45
16:LN:120:TRP:HE1	16:LN:123:GLU:HG3	1.82	0.45
53:SE:19:MET:SD	53:SE:108:ARG:HD2	2.56	0.45
53:SE:165:GLU:HG3	53:SE:166:THR:HG23	1.99	0.45
55:SG:50:VAL:CG1	55:SG:111:LEU:HB3	2.47	0.45
1:L5:384:A:N1	1:L5:405:U:H4'	2.31	0.45
1:L5:690:C:H2'	1:L5:691:C:C6	2.52	0.45
2:L7:110:G:H2'	2:L7:111:C:C6	2.52	0.45
4:LA:178:PRO:HG2	44:Lp:26:VAL:CG2	2.47	0.45
48:S2:552:G:O5'	48:S2:552:G:H8	1.99	0.45
65:SQ:102:GLU:HB3	81:Sg:55:PRO:O	2.16	0.45
71:SW:77:PRO:HB2	72:SX:7:LEU:HG	1.98	0.45
75:Sa:46:GLU:O	75:Sa:50:VAL:HG23	2.16	0.45
1:L5:980:U:H2'	1:L5:981:C:C6	2.51	0.45
1:L5:3942:A:H2'	1:L5:3943:A:C8	2.52	0.45
1:L5:4732:G:H1'	1:L5:4733:C:C6	2.52	0.45
5:LB:258:HIS:HA	5:LB:259:PRO:C	2.40	0.45
10:LG:78:PRO:HD3	10:LG:237:TRP:CE2	2.52	0.45
1:L5:4343:U:H2'	1:L5:4344:U:C6	2.52	0.45
1:L5:4537:C:H2'	1:L5:4538:G:C8	2.52	0.45
12:LI:4:ARG:HB2	12:LI:5:PRO:HD2	1.99	0.45
13:LJ:44:THR:HG21	13:LJ:72:CYS:SG	2.57	0.45
48:S2:376:A:H2'	48:S2:377:G:O4'	2.16	0.45
48:S2:1044:G:HO2'	48:S2:1045:U:H5	1.65	0.45
53:SE:124:CYS:HA	53:SE:142:HIS:HE1	1.82	0.45
1:L5:669:C:H5'	45:Lr:68:SER:HB2	1.99	0.45
1:L5:924:C:H5''	1:L5:925:C:OP2	2.16	0.45
1:L5:2528:G:H2'	1:L5:2529:A:O4'	2.17	0.45
1:L5:4147:G:H2'	1:L5:4148:C:C6	2.52	0.45
48:S2:674:C:H2'	48:S2:675:U:C6	2.52	0.45
1:L5:3792:OMG:H2'	1:L5:3793:U:C6	2.52	0.44
28:LZ:41:ALA:HB2	28:LZ:77:TYR:HE1	1.82	0.44
31:Lc:27:TYR:CE1	31:Lc:29:LEU:HD11	2.51	0.44
35:Lg:69:LYS:HA	35:Lg:72:LYS:HZ2	1.82	0.44
48:S2:160:U:O2'	48:S2:161:U:H3'	2.17	0.44
75:Sa:39:PHE:CE2	75:Sa:41:ILE:HD11	2.52	0.44
81:Sg:276:SER:OG	81:Sg:279:SER:HB2	2.17	0.44
1:L5:644:G:OP1	14:LL:162:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:665:C:H1'	1:L5:668:C:N4	2.32	0.44
1:L5:1095:A:H2'	1:L5:1096:C:C6	2.52	0.44
3:L8:8:U:H2'	3:L8:9:A:C8	2.52	0.44
3:L8:123:U:O2	3:L8:123:U:H2'	2.17	0.44
27:LY:109:LEU:O	27:LY:110:LYS:C	2.61	0.44
31:Lc:17:ARG:HG2	31:Lc:104:ILE:HB	1.99	0.44
48:S2:835:C:C4	73:SY:8:ARG:HD3	2.52	0.44
48:S2:1289:U:C5	80:Sf:97:LYS:HE3	2.52	0.44
51:SC:94:ILE:HG21	51:SC:162:ILE:HD12	1.99	0.44
62:SN:25:TRP:CE3	76:Sb:82:LYS:HE2	2.52	0.44
81:Sg:170:TRP:CG	81:Sg:194:TYR:HB2	2.52	0.44
1:L5:984:C:H2'	1:L5:985:C:C6	2.52	0.44
1:L5:1332:C:H2'	1:L5:1333:A:H8	1.81	0.44
5:LB:399:LYS:HD2	5:LB:400:GLU:N	2.31	0.44
12:LI:36:LEU:HD13	12:LI:69:ARG:HH11	1.83	0.44
1:L5:758:G:OP1	11:LH:52:LYS:HD2	2.17	0.44
1:L5:1701:A:H5'	6:LC:304:ALA:HB3	2.00	0.44
1:L5:4965:U:H4'	1:L5:4966:A:H5'	2.00	0.44
48:S2:533:A:N7	48:S2:534:G:C8	2.85	0.44
56:SH:27:LEU:O	56:SH:31:GLU:HG3	2.17	0.44
1:L5:1265:G:H5''	30:Lb:95:ARG:NH1	2.32	0.44
1:L5:1733:G:N3	1:L5:4214:A:H2'	2.33	0.44
27:LY:62:TYR:CG	27:LY:85:VAL:HG13	2.53	0.44
48:S2:449:A:H4'	53:SE:3:ARG:HD3	2.00	0.44
48:S2:1578:U:H5'	48:S2:1579:A:N3	2.33	0.44
81:Sg:126:ASP:C	81:Sg:126:ASP:OD1	2.60	0.44
1:L5:1554:A:H5'	44:Lp:9:GLY:C	2.42	0.44
1:L5:2097:U:H3	9:LF:39:GLN:NE2	2.15	0.44
1:L5:3765:G:H1'	1:L5:3766:A:H2	1.82	0.44
5:LB:288:GLY:HA3	5:LB:330:PHE:CE2	2.52	0.44
13:LJ:44:THR:HA	13:LJ:82:ILE:HD11	2.00	0.44
13:LJ:119:TYR:CE1	67:SS:12:ILE:HD12	2.53	0.44
23:LU:80:LYS:HE2	23:LU:110:TYR:CZ	2.52	0.44
48:S2:1550:G:H3'	48:S2:1579:A:H61	1.83	0.44
80:Sf:133:ALA:O	80:Sf:139:HIS:HA	2.18	0.44
1:L5:1380:G:H4'	1:L5:1381:U:H6	1.83	0.44
1:L5:2500:U:H2'	1:L5:2501:C:C6	2.53	0.44
1:L5:2638:G:N7	1:L5:2697:A:N1	2.66	0.44
1:L5:4637:OMG:HM23	1:L5:4637:OMG:H1'	1.78	0.44
1:L5:5013:C:H4'	1:L5:5014:A:C5'	2.47	0.44
7:LD:72:ASP:O	7:LD:73:MET:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1499:U:H4'	52:SD:176:LEU:HD13	1.98	0.44
64:SP:21:ASP:OD1	64:SP:21:ASP:C	2.60	0.44
1:L5:123:C:H2'	1:L5:124:C:C6	2.52	0.44
1:L5:2094:G:H2'	1:L5:2095:A:N3	2.33	0.44
1:L5:4457:PSU:H1'	5:LB:252:ALA:HB3	1.99	0.44
1:L5:4919:G:H2'	1:L5:4920:C:H6	1.82	0.44
7:LD:52:ILE:O	7:LD:62:CYS:HA	2.18	0.44
31:Lc:20:LEU:HD23	31:Lc:102:SER:HA	1.99	0.44
48:S2:862:A:C8	71:SW:107:SER:HA	2.51	0.44
64:SP:34:MET:HG3	64:SP:42:ARG:HG3	1.99	0.44
1:L5:123:C:H2'	1:L5:124:C:H6	1.83	0.44
1:L5:424:U:H2'	1:L5:425:U:C6	2.52	0.44
1:L5:653:U:H2'	1:L5:654:C:C6	2.53	0.44
1:L5:2864:A:H2'	1:L5:2865:U:C6	2.53	0.44
1:L5:3726:A:H2'	1:L5:3727:A:C8	2.53	0.44
1:L5:4612:C:N3	11:LH:120:GLU:O	2.51	0.44
48:S2:370:G:H1'	90:S2:8894:HOH:O	2.18	0.44
56:SH:43:LEU:HB3	56:SH:72:PHE:CE2	2.53	0.44
67:SS:6:PRO:HB2	67:SS:9:PHE:HB2	1.99	0.44
73:SY:41:ARG:NH2	73:SY:53:ASP:HA	2.32	0.44
5:LB:245:HIC:HD2	90:LB:6133:HOH:O	2.17	0.43
26:LX:82:THR:HG22	26:LX:155:ILE:HG23	1.98	0.43
28:LZ:9:LYS:HD2	28:LZ:83:THR:O	2.18	0.43
38:Lj:39:TYR:CD1	38:Lj:40:PRO:HA	2.52	0.43
48:S2:1797:U:H2'	48:S2:1798:C:C6	2.53	0.43
80:Sf:108:VAL:HG22	80:Sf:114:ILE:HG12	2.00	0.43
1:L5:233:U:C6	1:L5:234:G:H8	2.36	0.43
1:L5:2664:G:H4'	1:L5:2677:G:H4'	2.00	0.43
33:Le:82:VAL:HG13	33:Le:114:ARG:HG2	1.99	0.43
48:S2:996:A:H2'	48:S2:997:A:C8	2.53	0.43
51:SC:183:LYS:HD3	51:SC:194:ARG:NH2	2.34	0.43
66:SR:5:ARG:O	66:SR:10:LYS:HE2	2.18	0.43
73:SY:60:PHE:CD1	73:SY:71:GLY:HA3	2.53	0.43
1:L5:1631:A:N7	4:LA:199:VAL:HG21	2.33	0.43
1:L5:2739:C:H5''	44:Lp:69:TRP:CH2	2.53	0.43
48:S2:616:A:H1'	79:Se:86:VAL:HG23	2.00	0.43
57:SI:151:GLU:O	57:SI:154:LYS:HG2	2.19	0.43
1:L5:515:C:H2'	1:L5:516:C:C6	2.53	0.43
1:L5:2570:U:H2'	1:L5:2571:C:C6	2.54	0.43
1:L5:2815:A2M:HM'3	1:L5:2815:A2M:H1'	1.83	0.43
5:LB:107:ALA:HB2	5:LB:201:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:4:C:H4'	51:SC:207:ALA:HB2	2.01	0.43
48:S2:197:U:H5''	48:S2:198:U:OP2	2.18	0.43
49:SA:164:ASN:HB3	49:SA:170:SER:OG	2.19	0.43
77:Sc:43:ILE:HD11	77:Sc:67:ARG:HH21	1.82	0.43
1:L5:150:U:H4'	1:L5:151:G:OP2	2.18	0.43
1:L5:1754:U:H1'	1:L5:1755:C:H5	1.83	0.43
1:L5:1789:C:H2'	1:L5:1790:U:H6	1.81	0.43
1:L5:2497:C:H2'	1:L5:2498:C:H6	1.82	0.43
1:L5:3880:G:H2'	1:L5:3881:G:C8	2.53	0.43
45:Lr:4:HIS:O	45:Lr:8:MET:HG2	2.19	0.43
48:S2:178:C:H2'	48:S2:179:C:C6	2.53	0.43
48:S2:344:U:H2'	48:S2:345:U:C6	2.53	0.43
48:S2:1562:C:O2'	48:S2:1563:G:H5'	2.18	0.43
51:SC:65:LYS:HG2	51:SC:68:ARG:HH21	1.83	0.43
53:SE:31:PRO:CG	53:SE:38:LEU:HG	2.48	0.43
55:SG:66:GLY:N	55:SG:100:CYS:SG	2.91	0.43
68:ST:65:TYR:CE2	68:ST:128:GLN:HG3	2.50	0.43
1:L5:1510:G:H2'	1:L5:1511:U:C6	2.53	0.43
1:L5:2326:G:H5''	33:Le:127:ALA:HB2	2.00	0.43
1:L5:3712:A:C2	48:S2:970:G:C6	3.06	0.43
2:L7:75:G:H5''	21:LS:49:SER:O	2.18	0.43
48:S2:1025:U:H2'	48:S2:1026:C:O4'	2.18	0.43
56:SH:135:PHE:CG	56:SH:136:PRO:HA	2.53	0.43
64:SP:17:TYR:CD2	64:SP:18:ARG:HG2	2.54	0.43
73:SY:27:VAL:HG11	73:SY:35:VAL:HG11	1.99	0.43
73:SY:55:ILE:HD12	73:SY:75:ILE:HG12	2.01	0.43
1:L5:1332:C:H2'	1:L5:1333:A:C8	2.54	0.43
1:L5:1431:C:H2'	1:L5:1432:G:O4'	2.18	0.43
1:L5:5006:U:H4'	1:L5:5007:A:H5'	2.01	0.43
3:L8:6:C:H2'	3:L8:7:U:C6	2.54	0.43
10:LG:139:GLY:HA2	10:LG:201:THR:O	2.18	0.43
36:Lh:106:LYS:HG2	36:Lh:110:LYS:HE2	2.01	0.43
47:Pt:35:U:H6	47:Pt:35:U:H5'	1.84	0.43
48:S2:178:C:H2'	48:S2:179:C:H6	1.83	0.43
48:S2:829:C:OP1	53:SE:21:ASP:HB2	2.19	0.43
48:S2:874:G:H21	56:SH:114:GLN:HE22	1.66	0.43
48:S2:907:G:H2'	48:S2:908:A:C8	2.54	0.43
48:S2:1083:A:H4'	48:S2:1085:C:C4	2.54	0.43
56:SH:108:SER:HA	56:SH:111:LYS:HE3	2.01	0.43
61:SM:35:ILE:HD13	61:SM:61:TYR:CE1	2.53	0.43
1:L5:665:C:H1'	1:L5:668:C:H42	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Li:2:ALA:HB3	37:Li:5:TYR:CE1	2.52	0.43
48:S2:942:G:H2'	48:S2:943:U:C6	2.53	0.43
48:S2:1070:A:H2'	48:S2:1071:G:O4'	2.19	0.43
48:S2:1149:A:N3	48:S2:1149:A:H2'	2.33	0.43
58:SJ:11:LYS:HE3	58:SJ:13:TYR:O	2.18	0.43
73:SY:40:ILE:HD13	73:SY:60:PHE:CZ	2.53	0.43
73:SY:41:ARG:CZ	73:SY:94:HIS:CE1	3.01	0.43
75:Sa:59:PHE:HB2	75:Sa:62:TYR:HB2	2.00	0.43
81:Sg:168:CYS:HB2	81:Sg:195:LEU:HD13	2.01	0.43
1:L5:1359:G:H4'	16:LN:203:TYR:HB2	2.01	0.43
1:L5:3641:U:C6	1:L5:3645:U:C4	3.06	0.43
1:L5:3718:A2M:H2	1:L5:3934:G:O4'	2.19	0.43
1:L5:4250:G:H4'	13:LJ:106:GLY:C	2.43	0.43
1:L5:4594:U:H2'	1:L5:4595:G:H8	1.84	0.43
1:L5:4699:U:H1'	1:L5:4700:A:H5''	2.01	0.43
7:LD:265:ARG:HD3	7:LD:269:PRO:HD3	2.00	0.43
8:LE:67:ALA:HA	8:LE:69:TYR:CE2	2.53	0.43
50:SB:48:LEU:HD23	50:SB:48:LEU:H	1.84	0.43
1:L5:106:A:H1'	1:L5:336:A:N3	2.34	0.43
1:L5:1766:A:H1'	1:L5:1767:A:C5	2.54	0.43
1:L5:1773:U:H2'	1:L5:1774:C:C6	2.54	0.43
1:L5:2640:G:H2'	1:L5:2641:A:C8	2.54	0.43
1:L5:4134:C:H2'	1:L5:4135:G:O4'	2.18	0.43
1:L5:4771:C:H2'	1:L5:4772:C:C5	2.53	0.43
2:L7:3:C:H2'	2:L7:4:U:H6	1.84	0.43
48:S2:553:U:C5	48:S2:555:A:C8	3.06	0.43
48:S2:1728:U:H2'	48:S2:1729:U:O4'	2.19	0.43
48:S2:1737:G:H2'	48:S2:1738:C:H6	1.84	0.43
71:SW:83:LEU:HD11	71:SW:120:HIS:C	2.43	0.43
74:SZ:31:LYS:HB3	74:SZ:32:LYS:H	1.62	0.43
1:L5:975:C:OP1	9:LF:43:ARG:HD3	2.20	0.42
1:L5:2563:C:H3'	1:L5:2564:G:C8	2.53	0.42
1:L5:4114:C:H2'	1:L5:4115:G:N3	2.33	0.42
7:LD:38:ILE:HD12	22:LT:30:TYR:HB2	2.00	0.42
24:LV:75:LYS:HB3	24:LV:75:LYS:HE3	1.67	0.42
48:S2:572:PSU:H5''	73:SY:60:PHE:O	2.19	0.42
49:SA:39:TYR:CD2	66:SR:105:MET:HB2	2.54	0.42
50:SB:168:MET:HG2	50:SB:197:ILE:HG21	2.01	0.42
1:L5:665:C:H4'	1:L5:668:C:H41	1.83	0.42
1:L5:1804:A:O4'	1:L5:1806:G:C8	2.71	0.42
1:L5:2424:OMG:H1'	1:L5:2424:OMG:HM23	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2862:G:N3	1:L5:3624:A:H2'	2.33	0.42
1:L5:4438:U:H2'	1:L5:4439:U:O4'	2.19	0.42
1:L5:4749:C:H2'	1:L5:4750:G:O4'	2.19	0.42
48:S2:1223:A:H2'	48:S2:1224:G:O4'	2.19	0.42
54:SF:188:TYR:OH	54:SF:192:LYS:HE2	2.19	0.42
57:SI:129:LEU:HB2	57:SI:133:GLU:HB2	2.01	0.42
1:L5:231:U:H4'	27:LY:100:HIS:CD2	2.53	0.42
1:L5:495:C:H3'	1:L5:496:G:H5''	2.01	0.42
1:L5:658:C:H2'	1:L5:659:G:C8	2.55	0.42
1:L5:966:A:C2	1:L5:2092:G:C2	3.07	0.42
1:L5:2364:OMG:H1'	1:L5:2364:OMG:HM23	1.69	0.42
1:L5:2412:A:H2'	1:L5:2413:U:C6	2.54	0.42
1:L5:2486:G:C6	1:L5:2487:G:C6	3.08	0.42
3:L8:6:C:H2'	3:L8:7:U:H6	1.84	0.42
48:S2:191:A:OP2	57:SI:145:ILE:HD12	2.19	0.42
48:S2:464:A:H3'	48:S2:465:A:H8	1.83	0.42
48:S2:1552:G:O6	48:S2:1557:C:H2'	2.19	0.42
1:L5:1563:A:H2'	1:L5:1564:A:O4'	2.19	0.42
1:L5:1855:G:OP1	30:Lb:4:SER:HB2	2.19	0.42
1:L5:1866:U:H2'	1:L5:1867:A:O4'	2.19	0.42
1:L5:3837:C:H2'	1:L5:3838:U:O4'	2.18	0.42
1:L5:4111:U:H2'	1:L5:4112:C:H6	1.83	0.42
1:L5:5028:G:H2'	1:L5:5029:C:C6	2.54	0.42
48:S2:176:U:H2'	48:S2:177:G:C8	2.54	0.42
80:Sf:143:LYS:C	80:Sf:145:CYS:H	2.27	0.42
1:L5:423:G:H2'	1:L5:424:U:O4'	2.19	0.42
1:L5:750:U:H1'	1:L5:917:A:C8	2.54	0.42
1:L5:1249:C:H2'	1:L5:1250:C:C6	2.54	0.42
1:L5:1962:A:H2'	1:L5:1963:C:C6	2.55	0.42
1:L5:2874:U:O4	1:L5:3823:G:H8	2.02	0.42
1:L5:4524:G:H4'	1:L5:4524:G:OP2	2.19	0.42
1:L5:4539:U:O4	4:LA:216:HIS:HE1	2.02	0.42
10:LG:139:GLY:HA2	10:LG:201:THR:HG23	2.02	0.42
48:S2:836:G:H2'	48:S2:837:A:C6	2.55	0.42
48:S2:1052:A:H2'	48:S2:1053:C:O4'	2.20	0.42
81:Sg:290:ALA:O	81:Sg:298:LEU:HD12	2.19	0.42
1:L5:1247:U:H2'	1:L5:1248:C:C6	2.55	0.42
1:L5:1437:C:C2	1:L5:2098:G:C8	3.08	0.42
1:L5:1883:G:O6	1:L5:1896:A:H2	2.02	0.42
1:L5:4274:A:H2'	1:L5:4275:G:H8	1.84	0.42
1:L5:4941:G:OP1	8:LE:219:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:223:C:H2'	48:S2:224:A:C8	2.54	0.42
48:S2:555:A:H2'	48:S2:556:U:H6	1.84	0.42
48:S2:929:G:H2'	48:S2:930:C:O4'	2.19	0.42
48:S2:1807:C:H2'	48:S2:1808:U:O4'	2.20	0.42
50:SB:89:GLU:HG3	50:SB:228:LEU:HD13	2.00	0.42
54:SF:142:SER:HB2	77:Sc:50:VAL:HG13	2.02	0.42
69:SU:106:ILE:HD12	69:SU:106:ILE:HA	1.93	0.42
72:SX:52:LEU:HD12	72:SX:53:GLU:HG2	2.01	0.42
73:SY:130:LYS:HB3	73:SY:131:PRO:HD3	2.01	0.42
1:L5:1247:U:H2'	1:L5:1248:C:H6	1.84	0.42
1:L5:1363:C:H2'	1:L5:1364:U:O4'	2.19	0.42
1:L5:1468:C:H2'	1:L5:1469:C:C6	2.55	0.42
1:L5:1736:A:C2	1:L5:1794:A:C4	3.08	0.42
1:L5:1964:A:C2	1:L5:4694:G:C4	3.08	0.42
1:L5:2415:OMU:C4	1:L5:2416:G:C6	3.03	0.42
3:L8:14:OMU:H1'	3:L8:14:OMU:HM23	1.62	0.42
5:LB:24:ARG:HH11	5:LB:276:HIS:CD2	2.38	0.42
6:LC:174:LEU:HD23	6:LC:174:LEU:HA	1.78	0.42
18:LP:40:HIS:NE2	18:LP:110:ASP:O	2.47	0.42
29:La:125:LYS:HA	29:La:145:VAL:O	2.19	0.42
48:S2:155:G:H2'	48:S2:156:G:C8	2.55	0.42
48:S2:1223:A:OP1	54:SF:79:HIS:HA	2.20	0.42
48:S2:1842:4AC:H6	48:S2:1842:4AC:O5'	2.19	0.42
52:SD:106:ARG:CG	52:SD:175:VAL:HG22	2.50	0.42
52:SD:106:ARG:HG3	52:SD:175:VAL:HG22	2.02	0.42
56:SH:157:HIS:HB3	56:SH:190:PRO:HG3	2.01	0.42
1:L5:642:G:H2'	1:L5:643:C:C6	2.55	0.42
1:L5:2070:U:O4'	84:L5:5616:PUT:H31	2.20	0.42
1:L5:4345:C:H2'	1:L5:4346:U:C6	2.54	0.42
1:L5:4481:U:H2'	1:L5:4482:U:H6	1.85	0.42
4:LA:206:PRO:HD3	4:LA:213:GLY:CA	2.50	0.42
48:S2:441:C:H2'	48:S2:442:C:C6	2.55	0.42
48:S2:1286:G:OP1	80:Sf:101:ALA:HA	2.19	0.42
48:S2:1589:A:H2'	48:S2:1590:C:C6	2.55	0.42
54:SF:68:ILE:HD11	54:SF:151:ILE:HD11	2.00	0.42
48:S2:1201:U:H2'	48:S2:1202:U:C6	2.55	0.42
48:S2:1372:U:H2'	48:S2:1373:C:O4'	2.20	0.42
52:SD:138:VAL:HG13	52:SD:182:LEU:HD21	2.01	0.42
63:SO:83:GLN:NE2	77:Sc:5:ARG:HH21	2.17	0.42
80:Sf:143:LYS:O	80:Sf:144:CYS:SG	2.77	0.42
81:Sg:209:SER:O	81:Sg:216:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:417:G:N3	3:L8:16:G:C2	2.88	0.42
1:L5:489:C:H2'	1:L5:490:C:H6	1.84	0.42
1:L5:2305:U:H4'	1:L5:2306:G:OP2	2.20	0.42
1:L5:4674:C:H2'	1:L5:4675:U:C6	2.55	0.42
2:L7:111:C:H2'	2:L7:112:U:O4'	2.20	0.42
24:LV:43:LYS:HE2	24:LV:62:MET:SD	2.59	0.42
48:S2:121:OMU:H6	48:S2:121:OMU:O5'	2.19	0.42
48:S2:416:U:H2'	48:S2:417:C:O4'	2.19	0.42
48:S2:955:A:N3	48:S2:956:G:H1'	2.34	0.42
48:S2:1199:A:H2'	48:S2:1200:A:C8	2.54	0.42
53:SE:100:ARG:HH21	53:SE:118:GLU:HG2	1.85	0.42
64:SP:75:VAL:HG11	64:SP:104:GLN:HG2	2.02	0.42
69:SU:61:LEU:O	69:SU:81:GLN:HA	2.19	0.42
1:L5:268:G:H2'	1:L5:269:G:H8	1.84	0.41
1:L5:300:A:H5'	16:LN:95:ALA:O	2.20	0.41
1:L5:2520:C:H2'	1:L5:2521:G:C8	2.55	0.41
1:L5:2787:A2M:HM'1	1:L5:2789:A:H3'	2.02	0.41
1:L5:3771:C:H2'	1:L5:3772:U:O4'	2.19	0.41
84:L5:5621:PUT:H11	6:LC:202:ILE:HD12	2.02	0.41
8:LE:66:LYS:HE2	8:LE:68:MET:SD	2.59	0.41
13:LJ:15:LEU:HD13	13:LJ:165:TRP:HB2	2.02	0.41
22:LT:158:PHE:CE1	22:LT:159:MET:HE3	2.56	0.41
30:Lb:69:ALA:O	30:Lb:72:ILE:HB	2.19	0.41
48:S2:449:A:H5''	90:S2:6249:HOH:O	2.20	0.41
53:SE:21:ASP:OD2	53:SE:24:THR:HG23	2.20	0.41
58:SJ:46:VAL:HG12	58:SJ:102:ILE:HG13	2.00	0.41
62:SN:54:LEU:HB3	62:SN:60:VAL:HB	2.01	0.41
65:SQ:39:LEU:HD11	65:SQ:51:LEU:HB3	2.02	0.41
73:SY:56:PHE:CE2	73:SY:94:HIS:CD2	3.08	0.41
1:L5:1406:G:C2	1:L5:1412:G:C6	3.08	0.41
5:LB:245:HIC:C	5:LB:246:ARG:HG3	2.50	0.41
17:LO:190:ASP:OD1	17:LO:191:LYS:N	2.53	0.41
26:LX:73:HIS:CD2	26:LX:112:ALA:HA	2.55	0.41
48:S2:1293:A:H2'	48:S2:1294:G:C8	2.55	0.41
48:S2:1416:C:OP1	68:ST:129:ARG:HG3	2.20	0.41
57:SI:63:GLY:HA3	57:SI:185:ALA:O	2.20	0.41
64:SP:15:PHE:CE2	64:SP:109:PRO:HB2	2.55	0.41
1:L5:119:G:H3'	1:L5:120:A:H5''	2.02	0.41
1:L5:380:U:P	1:L5:413:G:H21	2.43	0.41
1:L5:717:U:H2'	1:L5:718:C:C6	2.56	0.41
1:L5:1501:C:O2	1:L5:1501:C:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1924:C:H2'	1:L5:1925:G:O4'	2.20	0.41
1:L5:3656:A:H2'	1:L5:3657:U:H6	1.85	0.41
1:L5:5013:C:H41	1:L5:5029:C:P	2.43	0.41
1:L5:1460:C:H5''	19:LQ:144:LYS:HG2	2.01	0.41
1:L5:3656:A:H2'	1:L5:3657:U:C6	2.56	0.41
5:LB:356:LYS:HE3	5:LB:356:LYS:HB2	1.87	0.41
54:SF:49:LEU:HD12	65:SQ:50:LYS:HG2	2.03	0.41
61:SM:124:ILE:HA	61:SM:127:TYR:CD2	2.56	0.41
69:SU:17:ILE:HG21	69:SU:94:PRO:HB3	2.02	0.41
72:SX:105:PHE:HB2	72:SX:119:ARG:C	2.45	0.41
1:L5:260:C:H2'	1:L5:261:G:C8	2.55	0.41
1:L5:2415:OMU:H1'	1:L5:2415:OMU:HM23	1.70	0.41
1:L5:2709:C:H1'	20:LR:39:GLN:HG2	2.02	0.41
2:L7:3:C:H2'	2:L7:4:U:C6	2.55	0.41
2:L7:89:G:H2'	2:L7:90:A:C8	2.55	0.41
8:LE:133:PHE:HA	8:LE:136:HIS:CE1	2.55	0.41
12:LI:193:ASP:OD2	12:LI:198:LYS:HE3	2.21	0.41
30:Lb:49:HIS:HB3	30:Lb:52:LYS:HE2	2.02	0.41
48:S2:204:G:C6	48:S2:205:G:C5	3.08	0.41
48:S2:1828:C:H2'	48:S2:1829:G:O4'	2.21	0.41
48:S2:1850:MA6:H8	48:S2:1850:MA6:O5'	2.21	0.41
71:SW:86:LEU:HD21	71:SW:113:HIS:HB2	2.02	0.41
81:Sg:176:VAL:CG2	81:Sg:186:THR:HB	2.50	0.41
1:L5:1405:C:C4	1:L5:1406:G:N7	2.88	0.41
1:L5:2264:C:H2'	1:L5:2265:G:O4'	2.21	0.41
1:L5:3620:G:C2	1:L5:4642:U:H5'	2.55	0.41
12:LI:47:PRO:HB3	12:LI:171:TRP:CZ2	2.56	0.41
25:LW:44:ARG:HG3	25:LW:44:ARG:HH11	1.86	0.41
39:Lk:13:LEU:HD23	39:Lk:13:LEU:HA	1.96	0.41
48:S2:1098:C:H2'	48:S2:1099:G:C8	2.55	0.41
48:S2:1289:U:H2'	48:S2:1290:G:C8	2.55	0.41
48:S2:1457:U:H2'	48:S2:1458:G:C8	2.55	0.41
49:SA:134:LEU:HD22	49:SA:144:THR:HG21	2.02	0.41
61:SM:35:ILE:HD13	61:SM:61:TYR:HE1	1.84	0.41
1:L5:2487:G:H2'	1:L5:2488:C:O4'	2.20	0.41
1:L5:2632:PSU:H2'	1:L5:2633:U:C6	2.55	0.41
3:L8:80:A:N3	3:L8:80:A:H2'	2.35	0.41
3:L8:85:U:H5''	3:L8:86:U:H3'	2.02	0.41
14:LL:139:SER:HB2	14:LL:143:GLU:OE2	2.20	0.41
48:S2:65:C:C2	55:SG:133:LEU:HD22	2.55	0.41
48:S2:462:OMC:HM23	48:S2:462:OMC:H1'	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1088:U:H4'	48:S2:1089:G:OP2	2.20	0.41
48:S2:1229:G:H2'	48:S2:1230:C:O4'	2.21	0.41
52:SD:113:LEU:HD23	52:SD:118:ALA:HB2	2.03	0.41
1:L5:968:C:O2'	1:L5:969:C:H3'	2.20	0.41
1:L5:1472:C:H2'	1:L5:1473:U:C6	2.55	0.41
1:L5:4967:A:H2'	1:L5:4968:A:H8	1.84	0.41
47:Pt:19:U:O2'	47:Pt:20:H2U:H5'	2.21	0.41
48:S2:166:A2M:H1'	48:S2:166:A2M:HM'3	1.88	0.41
48:S2:1735:A:H2'	48:S2:1736:G:O4'	2.21	0.41
49:SA:16:LEU:HD22	66:SR:96:ILE:HD12	2.03	0.41
50:SB:123:ALA:HB2	50:SB:165:ARG:HG3	2.02	0.41
74:SZ:48:VAL:C	74:SZ:83:LEU:HD22	2.46	0.41
1:L5:135:G:C5	36:Lh:97:LYS:HE3	2.55	0.41
1:L5:357:U:C2	1:L5:359:A:N7	2.89	0.41
1:L5:434:A:H2'	1:L5:435:A:O4'	2.20	0.41
1:L5:456:C:H2'	1:L5:457:G:C8	2.56	0.41
1:L5:1298:C:H2'	1:L5:1299:G:C8	2.55	0.41
1:L5:1433:A:H2'	1:L5:1434:G:O4'	2.21	0.41
1:L5:3793:U:H2'	1:L5:3794:C:C6	2.56	0.41
1:L5:4173:G:H2'	1:L5:4174:U:C6	2.56	0.41
1:L5:4219:A:H2'	1:L5:4220:6MZ:C8	2.51	0.41
1:L5:4258:C:OP1	13:LJ:53:ALA:HA	2.21	0.41
1:L5:4458:C:H2'	1:L5:4459:U:C6	2.56	0.41
2:L7:39:C:H4'	13:LJ:47:THR:HG23	2.01	0.41
5:LB:223:THR:O	5:LB:274:TYR:HA	2.21	0.41
9:LF:179:LEU:HB3	9:LF:184:ILE:HB	2.02	0.41
19:LQ:43:PHE:CD1	19:LQ:133:GLY:HA3	2.55	0.41
19:LQ:175:GLU:HA	29:La:51:GLY:C	2.46	0.41
48:S2:16:G:H2'	48:S2:17:C:C6	2.55	0.41
48:S2:495:U:H2'	48:S2:496:C:O4'	2.21	0.41
48:S2:538:U:H2'	48:S2:539:C:C6	2.56	0.41
48:S2:799:U:H2'	48:S2:800:U:C6	2.56	0.41
48:S2:1284:A:C6	61:SM:91:LEU:HD22	2.56	0.41
51:SC:79:GLU:OE1	51:SC:82:TYR:HD2	2.04	0.41
51:SC:182:CYS:HB2	71:SW:95:PRO:HB2	2.03	0.41
64:SP:107:ILE:HA	64:SP:111:MET:SD	2.60	0.41
66:SR:33:ARG:HD2	81:Sg:125:ARG:NH1	2.36	0.41
68:ST:34:VAL:HG23	68:ST:52:TRP:CZ2	2.56	0.41
1:L5:1246:G:H2'	1:L5:1247:U:C6	2.56	0.41
1:L5:3606:U:H2'	1:L5:3607:U:C6	2.56	0.41
1:L5:3946:G:C2	1:L5:4067:U:O2	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4291:G:H5''	1:L5:4293:PSU:C6	2.56	0.41
1:L5:4738:C:H2'	1:L5:4739:C:C6	2.56	0.41
19:LQ:49:LYS:HE2	19:LQ:49:LYS:HB3	1.78	0.41
61:SM:120:ALA:O	61:SM:123:VAL:HG22	2.21	0.41
80:Sf:141:CYS:SG	80:Sf:143:LYS:O	2.79	0.41
1:L5:1404:G:C2	1:L5:1405:C:C4	3.09	0.40
1:L5:1444:G:C2	1:L5:2102:G:C8	3.09	0.40
1:L5:2258:C:C2	8:LE:89:LEU:HD12	2.57	0.40
1:L5:2293:U:H2'	1:L5:2294:G:C8	2.55	0.40
1:L5:2497:C:H2'	1:L5:2498:C:C6	2.57	0.40
1:L5:3823:G:H2'	1:L5:3824:A:C8	2.56	0.40
3:L8:19:C:H2'	3:L8:20:A:C8	2.56	0.40
3:L8:75:OMG:HM23	3:L8:75:OMG:H1'	1.95	0.40
3:L8:129:C:H2'	3:L8:130:C:C6	2.56	0.40
5:LB:56:ILE:HD12	5:LB:56:ILE:C	2.46	0.40
9:LF:43:ARG:HG3	9:LF:43:ARG:NH1	2.36	0.40
11:LH:41:ILE:HG22	11:LH:43:VAL:HG13	2.03	0.40
48:S2:171:A:O2'	48:S2:172:OMU:H3'	2.21	0.40
48:S2:501:C:H2'	48:S2:502:C:H5''	2.03	0.40
48:S2:534:G:H4'	48:S2:534:G:OP1	2.20	0.40
56:SH:20:GLU:HG2	56:SH:48:ALA:HB3	2.03	0.40
57:SI:57:ALA:HB2	57:SI:183:GLY:HA2	2.04	0.40
1:L5:21:G:H1'	3:L8:103:A:N3	2.36	0.40
1:L5:440:U:H2'	1:L5:441:G:H8	1.86	0.40
1:L5:2335:C:H2'	1:L5:2336:G:H8	1.86	0.40
1:L5:2741:U:H2'	4:LA:50:HIS:CD2	2.56	0.40
1:L5:4238:G:H2'	1:L5:4239:A:H8	1.85	0.40
1:L5:4449:A:H1'	86:L5:5700:A1B75:O1	2.21	0.40
1:L5:4653:C:H2'	1:L5:4654:C:C6	2.57	0.40
10:LG:99:ALA:HB1	10:LG:136:LEU:HD11	2.03	0.40
19:LQ:154:LYS:HE3	19:LQ:154:LYS:HB3	1.90	0.40
48:S2:655:A:H5'	48:S2:655:A:N3	2.37	0.40
48:S2:943:U:C2	48:S2:944:A:C8	3.10	0.40
48:S2:953:C:H2'	48:S2:954:U:O4'	2.21	0.40
48:S2:1286:G:P	80:Sf:101:ALA:HA	2.61	0.40
48:S2:1390:U:H2'	48:S2:1391:OMC:H6	1.84	0.40
48:S2:1455:A:C2	48:S2:1456:G:C8	3.09	0.40
48:S2:1533:A:C8	48:S2:1604:G:H1'	2.56	0.40
48:S2:1558:C:H2'	48:S2:1559:C:C6	2.56	0.40
49:SA:10:MET:O	66:SR:111:PHE:HZ	2.04	0.40
56:SH:134:VAL:HG12	56:SH:137:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SM:75:ASN:OD1	61:SM:131:LYS:HE3	2.22	0.40
1:L5:10:A:H2'	1:L5:11:G:C8	2.56	0.40
1:L5:118:C:H5''	1:L5:119:G:OP2	2.21	0.40
1:L5:695:G:H3'	1:L5:696:C:H4'	2.03	0.40
1:L5:1812:C:O2'	30:Lb:53:GLY:HA3	2.22	0.40
1:L5:2804:OMC:H1'	1:L5:2804:OMC:HM23	1.74	0.40
1:L5:3621:A:H2'	1:L5:3622:C:O4'	2.22	0.40
8:LE:153:LEU:HD11	8:LE:195:ILE:HG13	2.02	0.40
17:LO:191:LYS:HE3	17:LO:192:TYR:CZ	2.56	0.40
48:S2:875:A:H2'	48:S2:876:C:C6	2.57	0.40
48:S2:985:G:H4'	63:SO:138:ASP:OD2	2.21	0.40
48:S2:1007:C:H2'	48:S2:1008:A:C8	2.56	0.40
51:SC:69:LEU:HD11	51:SC:273:LEU:HD11	2.03	0.40
55:SG:75:LEU:O	55:SG:94:ARG:HA	2.21	0.40
1:L5:964:A:C3'	1:L5:965:G:H4'	2.52	0.40
1:L5:1858:A:H2'	1:L5:1859:C:C6	2.56	0.40
1:L5:2857:A:H2'	1:L5:2858:A:O4'	2.22	0.40
1:L5:3859:G:H4'	18:LP:139:TYR:CE1	2.57	0.40
1:L5:4481:U:H2'	1:L5:4482:U:C6	2.55	0.40
28:LZ:87:VAL:HG23	28:LZ:87:VAL:O	2.22	0.40
48:S2:27:A2M:HM'3	48:S2:27:A2M:H1'	1.90	0.40
48:S2:502:C:O4'	53:SE:66:MET:HG3	2.21	0.40
48:S2:1309:C:C4	48:S2:1310:U:C4	3.10	0.40
49:SA:78:SER:OG	49:SA:83:GLY:HA3	2.22	0.40
66:SR:40:ILE:O	66:SR:40:ILE:HG13	2.22	0.40
67:SS:60:THR:O	67:SS:64:VAL:HG23	2.21	0.40
1:L5:384:A:C6	1:L5:386:A:C6	3.10	0.40
1:L5:946:C:H5'	6:LC:336:ARG:HD3	2.03	0.40
1:L5:1402:C:O5'	1:L5:1402:C:H6	2.05	0.40
1:L5:1443:A:C4	1:L5:1444:G:C8	3.10	0.40
1:L5:1754:U:H1'	1:L5:1755:C:C5	2.56	0.40
1:L5:2060:G:N2	21:LS:115:ALA:HB2	2.37	0.40
1:L5:2479:G:H2'	1:L5:2480:G:C8	2.54	0.40
48:S2:1293:A:H2'	48:S2:1294:G:H8	1.87	0.40
57:SI:139:LYS:O	57:SI:141:ARG:HD2	2.21	0.40
69:SU:25:THR:HA	69:SU:85:HIS:O	2.21	0.40
69:SU:97:ILE:O	69:SU:100:GLN:HG2	2.20	0.40
78:Sd:10:HIS:HA	78:Sd:11:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	249/257 (97%)	241 (97%)	8 (3%)	0	100	100
5	LB	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
6	LC	364/427 (85%)	357 (98%)	7 (2%)	0	100	100
7	LD	292/297 (98%)	284 (97%)	7 (2%)	1 (0%)	36	29
8	LE	217/288 (75%)	205 (94%)	11 (5%)	1 (0%)	24	16
9	LF	223/248 (90%)	218 (98%)	4 (2%)	1 (0%)	30	22
10	LG	239/266 (90%)	231 (97%)	8 (3%)	0	100	100
11	LH	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
12	LI	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
13	LJ	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
14	LL	204/211 (97%)	200 (98%)	4 (2%)	0	100	100
15	LM	134/215 (62%)	133 (99%)	1 (1%)	0	100	100
16	LN	201/204 (98%)	193 (96%)	7 (4%)	1 (0%)	24	16
17	LO	200/203 (98%)	195 (98%)	5 (2%)	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
20	LR	185/196 (94%)	185 (100%)	0	0	100	100
21	LS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
22	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
23	LU	97/128 (76%)	97 (100%)	0	0	100	100
24	LV	131/140 (94%)	127 (97%)	4 (3%)	0	100	100
25	LW	64/157 (41%)	63 (98%)	1 (2%)	0	100	100
26	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
27	LY	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
28	LZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	La	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	18	10
30	Lb	106/159 (67%)	103 (97%)	3 (3%)	0	100	100
31	Lc	97/115 (84%)	97 (100%)	0	0	100	100
32	Ld	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
33	Le	126/135 (93%)	126 (100%)	0	0	100	100
34	Lf	108/110 (98%)	108 (100%)	0	0	100	100
35	Lg	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
38	Lj	84/97 (87%)	81 (96%)	3 (4%)	0	100	100
39	Lk	67/70 (96%)	67 (100%)	0	0	100	100
40	Ll	48/51 (94%)	48 (100%)	0	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	23/25 (92%)	23 (100%)	0	0	100	100
43	Lo	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
44	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
45	Lr	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
46	NC	4/19 (21%)	3 (75%)	1 (25%)	0	100	100
49	SA	221/295 (75%)	219 (99%)	2 (1%)	0	100	100
50	SB	219/264 (83%)	215 (98%)	4 (2%)	0	100	100
51	SC	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
52	SD	224/243 (92%)	223 (100%)	1 (0%)	0	100	100
53	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
54	SF	187/204 (92%)	177 (95%)	9 (5%)	1 (0%)	24	16
55	SG	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
56	SH	187/194 (96%)	180 (96%)	7 (4%)	0	100	100
57	SI	204/208 (98%)	196 (96%)	7 (3%)	1 (0%)	24	16
58	SJ	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
59	SK	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
60	SL	142/158 (90%)	139 (98%)	3 (2%)	0	100	100
61	SM	120/132 (91%)	114 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
63	SO	133/151 (88%)	130 (98%)	3 (2%)	0	100	100
64	SP	129/145 (89%)	126 (98%)	3 (2%)	0	100	100
65	SQ	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
66	SR	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
67	SS	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
68	ST	140/145 (97%)	138 (99%)	2 (1%)	0	100	100
69	SU	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
70	SV	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
71	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
72	SX	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
73	SY	129/133 (97%)	127 (98%)	2 (2%)	0	100	100
74	SZ	83/125 (66%)	81 (98%)	2 (2%)	0	100	100
75	Sa	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
76	Sb	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
77	Sc	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
78	Sd	53/56 (95%)	53 (100%)	0	0	100	100
79	Se	46/133 (35%)	45 (98%)	1 (2%)	0	100	100
80	Sf	61/156 (39%)	55 (90%)	6 (10%)	0	100	100
81	Sg	311/317 (98%)	297 (96%)	12 (4%)	2 (1%)	21	13
All	All	11255/12782 (88%)	10989 (98%)	257 (2%)	9 (0%)	49	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	LE	166	LYS
57	SI	131	PRO
9	LF	237	GLU
16	LN	157	LYS
7	LD	17	GLN
54	SF	79	HIS
81	Sg	134	THR
29	La	15	VAL
81	Sg	13	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	193/199 (97%)	192 (100%)	1 (0%)	81	84
5	LB	347/348 (100%)	346 (100%)	1 (0%)	86	88
6	LC	305/348 (88%)	301 (99%)	4 (1%)	61	61
7	LD	247/250 (99%)	247 (100%)	0	100	100
8	LE	196/252 (78%)	196 (100%)	0	100	100
9	LF	194/215 (90%)	194 (100%)	0	100	100
10	LG	203/223 (91%)	203 (100%)	0	100	100
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	180/181 (99%)	180 (100%)	0	100	100
13	LJ	143/149 (96%)	141 (99%)	2 (1%)	59	59
14	LL	172/177 (97%)	171 (99%)	1 (1%)	78	81
15	LM	116/161 (72%)	115 (99%)	1 (1%)	70	73
16	LN	171/172 (99%)	170 (99%)	1 (1%)	78	81
17	LO	173/174 (99%)	172 (99%)	1 (1%)	78	81
18	LP	134/163 (82%)	133 (99%)	1 (1%)	76	78
19	LQ	164/165 (99%)	163 (99%)	1 (1%)	78	81
20	LR	166/175 (95%)	164 (99%)	2 (1%)	63	63
21	LS	157/157 (100%)	157 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	89/115 (77%)	89 (100%)	0	100	100
24	LV	102/107 (95%)	101 (99%)	1 (1%)	68	70
25	LW	58/126 (46%)	58 (100%)	0	100	100
26	LX	106/133 (80%)	106 (100%)	0	100	100
27	LY	124/135 (92%)	124 (100%)	0	100	100
28	LZ	117/118 (99%)	116 (99%)	1 (1%)	70	73
29	La	120/121 (99%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Lb	90/125 (72%)	89 (99%)	1 (1%)	65	67
31	Lc	84/97 (87%)	84 (100%)	0	100	100
32	Ld	98/110 (89%)	98 (100%)	0	100	100
33	Le	114/121 (94%)	113 (99%)	1 (1%)	70	73
34	Lf	89/89 (100%)	87 (98%)	2 (2%)	45	42
35	Lg	98/100 (98%)	97 (99%)	1 (1%)	68	70
36	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	73
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	73/80 (91%)	72 (99%)	1 (1%)	59	59
39	Lk	64/65 (98%)	63 (98%)	1 (2%)	55	54
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/115 (41%)	47 (100%)	0	100	100
42	Ln	24/24 (100%)	23 (96%)	1 (4%)	26	19
43	Lo	92/93 (99%)	92 (100%)	0	100	100
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/120 (91%)	109 (100%)	0	100	100
46	NC	6/6 (100%)	5 (83%)	1 (17%)	2	0
49	SA	184/242 (76%)	183 (100%)	1 (0%)	81	84
50	SB	202/231 (87%)	201 (100%)	1 (0%)	81	84
51	SC	188/225 (84%)	186 (99%)	2 (1%)	65	67
52	SD	189/202 (94%)	188 (100%)	1 (0%)	81	84
53	SE	224/225 (100%)	223 (100%)	1 (0%)	84	87
54	SF	159/170 (94%)	158 (99%)	1 (1%)	78	81
55	SG	207/218 (95%)	205 (99%)	2 (1%)	68	70
56	SH	168/174 (97%)	168 (100%)	0	100	100
57	SI	178/180 (99%)	175 (98%)	3 (2%)	53	52
58	SJ	161/168 (96%)	160 (99%)	1 (1%)	78	81
59	SK	87/136 (64%)	87 (100%)	0	100	100
60	SL	132/142 (93%)	132 (100%)	0	100	100
61	SM	104/108 (96%)	98 (94%)	6 (6%)	18	10
62	SN	130/131 (99%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	SO	105/119 (88%)	105 (100%)	0	100	100
64	SP	117/130 (90%)	116 (99%)	1 (1%)	70	73
65	SQ	117/121 (97%)	116 (99%)	1 (1%)	70	73
66	SR	121/122 (99%)	120 (99%)	1 (1%)	73	75
67	SS	128/132 (97%)	126 (98%)	2 (2%)	55	54
68	ST	112/115 (97%)	112 (100%)	0	100	100
69	SU	93/107 (87%)	91 (98%)	2 (2%)	45	42
70	SV	67/67 (100%)	67 (100%)	0	100	100
71	SW	112/113 (99%)	112 (100%)	0	100	100
72	SX	111/114 (97%)	109 (98%)	2 (2%)	51	50
73	SY	113/115 (98%)	113 (100%)	0	100	100
74	SZ	75/103 (73%)	74 (99%)	1 (1%)	61	61
75	Sa	86/98 (88%)	86 (100%)	0	100	100
76	Sb	75/76 (99%)	75 (100%)	0	100	100
77	Sc	58/62 (94%)	58 (100%)	0	100	100
78	Sd	48/49 (98%)	48 (100%)	0	100	100
79	Se	40/104 (38%)	40 (100%)	0	100	100
80	Sf	56/140 (40%)	54 (96%)	2 (4%)	31	23
81	Sg	272/275 (99%)	269 (99%)	3 (1%)	65	67
All	All	9808/10856 (90%)	9746 (99%)	62 (1%)	76	81

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	208	GLU
5	LB	19	ARG
6	LC	9	SER
6	LC	140	LYS
6	LC	189	MET
6	LC	366	ASP
13	LJ	26	VAL
13	LJ	169	LYS
14	LL	59	VAL
15	LM	105	THR
16	LN	10	LEU

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Mol	Chain	Res	Type
17	LO	22	ILE
18	LP	2	VAL
19	LQ	14	ARG
20	LR	34	ASN
20	LR	36	ASN
24	LV	92	ASP
28	LZ	97	ASN
30	Lb	14	ARG
33	Le	87	VAL
34	Lf	95	LYS
34	Lf	109	ARG
35	Lg	76	ARG
36	Lh	105	LYS
38	Lj	25	LYS
39	Lk	6	GLU
42	Ln	1	MET
46	NC	30	ASP
49	SA	2(A)	SER
50	SB	151	ARG
51	SC	120	GLN
51	SC	248	TYR
52	SD	156	LEU
53	SE	69	PHE
54	SF	127	ARG
55	SG	124	LEU
55	SG	163	ASN
57	SI	3	ILE
57	SI	48	VAL
57	SI	58	LEU
58	SJ	133	ARG
61	SM	14	VAL
61	SM	15	ASN
61	SM	36	ARG
61	SM	49	LEU
61	SM	55	ASN
61	SM	123	VAL
64	SP	24	GLN
65	SQ	16	LYS
66	SR	127	ASN
67	SS	116	LYS
67	SS	124	ARG
69	SU	45	GLU

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Mol	Chain	Res	Type
69	SU	90	ASP
72	SX	105	PHE
72	SX	115	ILE
74	SZ	50	PHE
80	Sf	140	TYR
80	Sf	145	CYS
81	Sg	107	ASP
81	Sg	155	ARG
81	Sg	177	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	216	HIS
5	LB	109	HIS
5	LB	184	GLN
5	LB	209	GLN
6	LC	43	ASN
6	LC	89	GLN
6	LC	310	HIS
7	LD	45	ASN
7	LD	291	GLN
10	LG	94	GLN
10	LG	236	HIS
11	LH	138	GLN
12	LI	59	GLN
12	LI	73	ASN
12	LI	123	GLN
12	LI	166	HIS
13	LJ	46	GLN
13	LJ	97	ASN
13	LJ	98	ASN
14	LL	149	GLN
15	LM	33	GLN
17	LO	26	GLN
17	LO	42	ASN
17	LO	199	HIS
18	LP	54	GLN
18	LP	56	GLN
18	LP	133	HIS
19	LQ	160	HIS
20	LR	34	ASN

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Mol	Chain	Res	Type
20	LR	40	GLN
22	LT	79	GLN
23	LU	95	ASN
26	LX	93	ASN
27	LY	18	HIS
27	LY	56	GLN
27	LY	96	HIS
28	LZ	97	ASN
29	La	67	GLN
30	Lb	49	HIS
30	Lb	60	ASN
31	Lc	19	GLN
32	Ld	116	ASN
35	Lg	73	HIS
36	Lh	20	GLN
38	Lj	66	HIS
40	Ll	19	GLN
40	Ll	33	ASN
42	Ln	22	GLN
43	Lo	25	GLN
43	Lo	90	HIS
43	Lo	102	GLN
50	SB	118	GLN
50	SB	179	ASN
50	SB	208	HIS
51	SC	113	GLN
52	SD	174	HIS
53	SE	36	HIS
53	SE	98	ASN
53	SE	138	HIS
53	SE	188	ASN
54	SF	179	ASN
55	SG	56	ASN
56	SH	39	GLN
56	SH	76	GLN
56	SH	114	GLN
56	SH	186	ASN
56	SH	193	GLN
57	SI	88	ASN
57	SI	116	HIS
60	SL	39	ASN
60	SL	94	HIS

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Mol	Chain	Res	Type
61	SM	46	GLN
61	SM	72	HIS
62	SN	69	ASN
62	SN	105	ASN
63	SO	83	GLN
64	SP	53	GLN
65	SQ	11	GLN
65	SQ	48	GLN
65	SQ	114	GLN
66	SR	127	ASN
67	SS	17	ASN
67	SS	101	ASN
68	ST	12	GLN
70	SV	35	ASN
72	SX	92	ASN
73	SY	94	HIS
74	SZ	46	ASN
81	Sg	117	ASN
81	Sg	178	ASN
81	Sg	222	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3529/5069 (69%)	454 (12%)	76 (2%)
2	L7	119/120 (99%)	6 (5%)	0
3	L8	155/156 (99%)	17 (10%)	4 (2%)
47	Pt	74/75 (98%)	15 (20%)	0
48	S2	1667/1869 (89%)	209 (12%)	31 (1%)
82	mR	5/832 (0%)	0	0
All	All	5549/8121 (68%)	701 (12%)	111 (2%)

All (701) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	25	A
1	L5	39	A
1	L5	42	A
1	L5	43	U
1	L5	48	G
1	L5	59	A

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Mol	Chain	Res	Type
1	L5	64	A
1	L5	65	A
1	L5	73	A
1	L5	85	G
1	L5	91	G
1	L5	109	G
1	L5	119	G
1	L5	120	A
1	L5	122	U
1	L5	132	G
1	L5	135	G
1	L5	136	C
1	L5	141	C
1	L5	142	G
1	L5	159	C
1	L5	160	G
1	L5	179	G
1	L5	180	C
1	L5	181	C
1	L5	184	U
1	L5	186	G
1	L5	189	G
1	L5	200	U
1	L5	201	C
1	L5	209	U
1	L5	218	A
1	L5	219	G
1	L5	220	C
1	L5	233	U
1	L5	234	G
1	L5	256	G
1	L5	257	C
1	L5	262	G
1	L5	266	C
1	L5	280	G
1	L5	294	G
1	L5	295	A
1	L5	296	A
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U

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Mol	Chain	Res	Type
1	L5	340	C
1	L5	349	A
1	L5	357	U
1	L5	387	G
1	L5	408	A
1	L5	409	G
1	L5	410	A
1	L5	412	G
1	L5	413	G
1	L5	450	G
1	L5	453	G
1	L5	454	U
1	L5	461	G
1	L5	484	U
1	L5	485	C
1	L5	489	C
1	L5	496	G
1	L5	498	C
1	L5	504	G
1	L5	509	A
1	L5	510	U
1	L5	513	U
1	L5	514	U
1	L5	518	G
1	L5	663	G
1	L5	664	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	692	A
1	L5	696	C
1	L5	697	G
1	L5	704	C
1	L5	705	G
1	L5	730	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	740	G
1	L5	915	A
1	L5	917	A
1	L5	925	C

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Mol	Chain	Res	Type
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	936	C
1	L5	937	U
1	L5	943	A
1	L5	944	A
1	L5	945	U
1	L5	955	G
1	L5	956	A
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	963	G
1	L5	964	A
1	L5	965	G
1	L5	967	C
1	L5	968	C
1	L5	1070	G
1	L5	1072	C
1	L5	1080	C
1	L5	1182	C
1	L5	1183	C
1	L5	1199	G
1	L5	1211	G
1	L5	1216	C
1	L5	1239	C
1	L5	1241	C
1	L5	1253	G
1	L5	1254	A
1	L5	1257	A
1	L5	1266	G
1	L5	1270	A
1	L5	1272	C
1	L5	1273	G
1	L5	1280	C
1	L5	1284	G
1	L5	1287	G
1	L5	1294	A
1	L5	1295	C
1	L5	1302	U

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Mol	Chain	Res	Type
1	L5	1303	A
1	L5	1304	C
1	L5	1313	C
1	L5	1326	A2M
1	L5	1337	A
1	L5	1354	A
1	L5	1359	G
1	L5	1366	G
1	L5	1380	G
1	L5	1381	U
1	L5	1387	A
1	L5	1397	A
1	L5	1398	A
1	L5	1408	G
1	L5	1411	C
1	L5	1412	G
1	L5	1415	G
1	L5	1420	A
1	L5	1444	G
1	L5	1445	U
1	L5	1484	G
1	L5	1498	G
1	L5	1501	C
1	L5	1502	G
1	L5	1533	A
1	L5	1534	A2M
1	L5	1547	A
1	L5	1566	C
1	L5	1578	U
1	L5	1591	U
1	L5	1596	U
1	L5	1613	A
1	L5	1614	C
1	L5	1624	G
1	L5	1625	OMG
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1654	G
1	L5	1661	C
1	L5	1676	C
1	L5	1677	PSU

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Mol	Chain	Res	Type
1	L5	1691	G
1	L5	1698	C
1	L5	1699	A
1	L5	1700	G
1	L5	1701	A
1	L5	1702	C
1	L5	1719	A
1	L5	1720	C
1	L5	1721	G
1	L5	1733	G
1	L5	1734	G
1	L5	1750	G
1	L5	1755	C
1	L5	1761	G
1	L5	1766	A
1	L5	1768	C
1	L5	1787	A
1	L5	1789	C
1	L5	1804	A
1	L5	1834	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1855	G
1	L5	1869	G
1	L5	1897	A
1	L5	1899	G
1	L5	1918	U
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1929	A
1	L5	1930	U
1	L5	1931	C
1	L5	1932	A
1	L5	1940	G
1	L5	1941	A
1	L5	1948	G
1	L5	1961	G
1	L5	1962	A
1	L5	1966	C

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Mol	Chain	Res	Type
1	L5	2024	G
1	L5	2026	A
1	L5	2042	A
1	L5	2043	A
1	L5	2046	G
1	L5	2048	U
1	L5	2055	G
1	L5	2056	G
1	L5	2069	A
1	L5	2084	C
1	L5	2092	G
1	L5	2093	A
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2102	G
1	L5	2103	G
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2313	A
1	L5	2332	A
1	L5	2333	G
1	L5	2348	G
1	L5	2351	OMC
1	L5	2360	A
1	L5	2395	A
1	L5	2397	G
1	L5	2421	G
1	L5	2422	OMC
1	L5	2470	C
1	L5	2471	G
1	L5	2474	G
1	L5	2475	G
1	L5	2476	G
1	L5	2483	G
1	L5	2489	C
1	L5	2503	G
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G

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Mol	Chain	Res	Type
1	L5	2513	A
1	L5	2519	U
1	L5	2520	C
1	L5	2554	U
1	L5	2587	A
1	L5	2588	C
1	L5	2601	A
1	L5	2638	G
1	L5	2653	C
1	L5	2660	A
1	L5	2662	G
1	L5	2669	C
1	L5	2687	U
1	L5	2694	G
1	L5	2695	A
1	L5	2696	A
1	L5	2708	U
1	L5	2710	C
1	L5	2711	G
1	L5	2739	C
1	L5	2743	A
1	L5	2762	G
1	L5	2764	A
1	L5	2770	C
1	L5	2788	U
1	L5	2790	U
1	L5	2794	C
1	L5	2795	A
1	L5	2796	G
1	L5	2798	A
1	L5	2814	C
1	L5	2815	A2M
1	L5	2826	U
1	L5	2827	G
1	L5	2855	G
1	L5	2856	C
1	L5	2877	G
1	L5	3597	G
1	L5	3614	G
1	L5	3615	G
1	L5	3626	G
1	L5	3635	A

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Mol	Chain	Res	Type
1	L5	3644	U
1	L5	3662	A
1	L5	3711	A
1	L5	3712	A
1	L5	3748	A
1	L5	3753	G
1	L5	3757	G
1	L5	3761	C
1	L5	3763	A
1	L5	3772	U
1	L5	3776	G
1	L5	3777	G
1	L5	3783	A
1	L5	3784	A
1	L5	3785	A2M
1	L5	3811	G
1	L5	3814	U
1	L5	3817	A
1	L5	3819	G
1	L5	3839	G
1	L5	3840	U
1	L5	3876	A
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3897	G
1	L5	3898	G
1	L5	3901	A
1	L5	3904	G
1	L5	3905	A
1	L5	3906	A
1	L5	3907	G
1	L5	3915	U
1	L5	3945	A
1	L5	3946	G
1	L5	3948	C
1	L5	4076	G
1	L5	4084	G
1	L5	4096	C
1	L5	4097	G
1	L5	4102	C
1	L5	4103	C

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Mol	Chain	Res	Type
1	L5	4105	A
1	L5	4108	G
1	L5	4115	G
1	L5	4116	C
1	L5	4119	C
1	L5	4121	G
1	L5	4122	G
1	L5	4127	A
1	L5	4135	G
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4145	C
1	L5	4150	G
1	L5	4163	U
1	L5	4164	C
1	L5	4170	A
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4214	A
1	L5	4222	G
1	L5	4229	U
1	L5	4233	A
1	L5	4251	A
1	L5	4254	G
1	L5	4258	C
1	L5	4266	G
1	L5	4273	A
1	L5	4281	A
1	L5	4291	G
1	L5	4305	G
1	L5	4306	OMU
1	L5	4314	C
1	L5	4317	A
1	L5	4330	G
1	L5	4339	A
1	L5	4373	G
1	L5	4376	A
1	L5	4377	G
1	L5	4378	A
1	L5	4379	A

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Mol	Chain	Res	Type
1	L5	4387	C
1	L5	4394	A
1	L5	4422	A
1	L5	4448	G
1	L5	4452	U
1	L5	4464	A
1	L5	4500	PSU
1	L5	4512	U
1	L5	4513	A
1	L5	4519	C
1	L5	4524	G
1	L5	4548	A
1	L5	4549	G
1	L5	4567	G
1	L5	4573	G
1	L5	4575	G
1	L5	4590	A2M
1	L5	4600	G
1	L5	4635	A
1	L5	4636	PSU
1	L5	4637	OMG
1	L5	4656	A
1	L5	4670	C
1	L5	4672	A
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4727	A
1	L5	4730	C
1	L5	4731	G
1	L5	4732	G
1	L5	4733	C
1	L5	4740	G
1	L5	4742	G
1	L5	4743	G
1	L5	4750	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4765	G
1	L5	4772	C

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Mol	Chain	Res	Type
1	L5	4860	G
1	L5	4870	G
1	L5	4871	C
1	L5	4882	U
1	L5	4883	C
1	L5	4895	C
1	L5	4900	C
1	L5	4909	A
1	L5	4910	G
1	L5	4912	G
1	L5	4913	G
1	L5	4914	C
1	L5	4938	A
1	L5	4943	A
1	L5	4944	C
1	L5	4976	U
1	L5	4979	A
1	L5	4988	U
1	L5	4989	U
1	L5	4990	C
1	L5	4991	U
1	L5	4994	G
1	L5	5007	A
1	L5	5017	G
1	L5	5041	G
1	L5	5050	C
1	L5	5055	G
1	L5	5062	G
2	L7	42	A
2	L7	53	U
2	L7	64	G
2	L7	100	A
2	L7	110	G
2	L7	120	U
3	L8	34	U
3	L8	35	C
3	L8	51	U
3	L8	52	A
3	L8	59	A
3	L8	62	A
3	L8	63	U
3	L8	84	A

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Mol	Chain	Res	Type
3	L8	87	G
3	L8	88	A
3	L8	104	A
3	L8	105	C
3	L8	110	U
3	L8	123	U
3	L8	124	U
3	L8	126	C
3	L8	127	U
47	Pt	7	G
47	Pt	8	U
47	Pt	9	G
47	Pt	10	2MG
47	Pt	17	G
47	Pt	18	G
47	Pt	19	U
47	Pt	20	H2U
47	Pt	35	U
47	Pt	36	C
47	Pt	47	C
47	Pt	48	C
47	Pt	73	C
47	Pt	74	C
47	Pt	75	A
48	S2	3	C
48	S2	4	C
48	S2	17	C
48	S2	33	G
48	S2	46	A
48	S2	55	U
48	S2	56	G
48	S2	67	C
48	S2	79	A
48	S2	80	G
48	S2	99	A2M
48	S2	102	A
48	S2	103	A
48	S2	113	G
48	S2	115	U
48	S2	126	G
48	S2	130	G
48	S2	140	C

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Mol	Chain	Res	Type
48	S2	143	U
48	S2	161	U
48	S2	162	C
48	S2	168	C
48	S2	184	G
48	S2	198	U
48	S2	199	C
48	S2	200	G
48	S2	202	G
48	S2	204	G
48	S2	205	G
48	S2	206	G
48	S2	215	G
48	S2	216	C
48	S2	309	G
48	S2	312	G
48	S2	319	C
48	S2	320	G
48	S2	326	C
48	S2	327	G
48	S2	328	U
48	S2	347	G
48	S2	362	C
48	S2	364	A
48	S2	370	G
48	S2	385	G
48	S2	386	C
48	S2	394	G
48	S2	407	G
48	S2	409	C
48	S2	448	A
48	S2	449	A
48	S2	450	C
48	S2	467	G
48	S2	472	C
48	S2	474	G
48	S2	482	G
48	S2	487	U
48	S2	492	C
48	S2	502	C
48	S2	516	A
48	S2	517	OMC

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Mol	Chain	Res	Type
48	S2	525	A
48	S2	534	G
48	S2	545	A
48	S2	546	G
48	S2	554	A
48	S2	561	A
48	S2	564	A
48	S2	587	A
48	S2	589	G
48	S2	590	A2M
48	S2	591	U
48	S2	606	G
48	S2	607	U
48	S2	608	C
48	S2	609	PSU
48	S2	614	C
48	S2	620	G
48	S2	621	C
48	S2	643	A
48	S2	644	OMG
48	S2	655	A
48	S2	668	A2M
48	S2	669	A
48	S2	671	A
48	S2	672	A
48	S2	673	G
48	S2	688	U
48	S2	821	G
48	S2	822	PSU
48	S2	830	A
48	S2	836	G
48	S2	838	G
48	S2	839	C
48	S2	840	C
48	S2	847	A
48	S2	870	A
48	S2	871	U
48	S2	872	A
48	S2	889	U
48	S2	891	G
48	S2	892	U
48	S2	896	U

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Mol	Chain	Res	Type
48	S2	897	U
48	S2	898	U
48	S2	910	G
48	S2	911	C
48	S2	912	C
48	S2	913	A
48	S2	920	A
48	S2	922	A
48	S2	933	G
48	S2	934	G
48	S2	990	A
48	S2	992	A
48	S2	1016	U
48	S2	1017	U
48	S2	1023	A
48	S2	1027	A
48	S2	1061	U
48	S2	1062	A
48	S2	1083	A
48	S2	1085	C
48	S2	1115	U
48	S2	1138	C
48	S2	1153	C
48	S2	1154	U
48	S2	1157	G
48	S2	1188	A
48	S2	1195	A
48	S2	1207	G
48	S2	1208	A
48	S2	1215	C
48	S2	1224	G
48	S2	1242	U
48	S2	1243	PSU
48	S2	1248	B8N
48	S2	1251	A
48	S2	1253	A
48	S2	1256	G
48	S2	1257	G
48	S2	1259	A
48	S2	1274	G
48	S2	1275	G
48	S2	1301	A

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Mol	Chain	Res	Type
48	S2	1302	G
48	S2	1303	C
48	S2	1309	C
48	S2	1315	U
48	S2	1371	U
48	S2	1372	U
48	S2	1378	A
48	S2	1402	A
48	S2	1419	C
48	S2	1420	G
48	S2	1421	A
48	S2	1422	G
48	S2	1429	G
48	S2	1433	C
48	S2	1434	C
48	S2	1437	C
48	S2	1438	A
48	S2	1454	A
48	S2	1463	U
48	S2	1489	A
48	S2	1490	OMG
48	S2	1493	C
48	S2	1494	U
48	S2	1497	G
48	S2	1498	A
48	S2	1521	C
48	S2	1522	A
48	S2	1533	A
48	S2	1557	C
48	S2	1563	G
48	S2	1579	A
48	S2	1580	A
48	S2	1581	C
48	S2	1586	U
48	S2	1587	G
48	S2	1588	A
48	S2	1601	A
48	S2	1621	U
48	S2	1623	A
48	S2	1638	G
48	S2	1639	G7M
48	S2	1648	G

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Mol	Chain	Res	Type
48	S2	1654	G
48	S2	1665	G
48	S2	1721	U
48	S2	1722	G
48	S2	1752	C
48	S2	1754	G
48	S2	1777	G
48	S2	1778	C
48	S2	1783	C
48	S2	1785	C
48	S2	1800	A
48	S2	1808	U
48	S2	1825	A
48	S2	1826	G
48	S2	1829	G
48	S2	1835	A
48	S2	1837	G
48	S2	1838	U
48	S2	1861	G
48	S2	1862	G
48	S2	1863	A
48	S2	1864	U
48	S2	1865	C

All (111) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	42	A
1	L5	179	G
1	L5	183	C
1	L5	200	U
1	L5	218	A
1	L5	219	G
1	L5	278	G
1	L5	294	G
1	L5	296	A
1	L5	408	A
1	L5	413	G
1	L5	453	G
1	L5	483	G
1	L5	664	G
1	L5	704	C

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Mol	Chain	Res	Type
1	L5	738	C
1	L5	749	G
1	L5	936	C
1	L5	955	G
1	L5	959	G
1	L5	962	C
1	L5	964	A
1	L5	1253	G
1	L5	1266	G
1	L5	1294	A
1	L5	1324	A
1	L5	1380	G
1	L5	1444	G
1	L5	1501	C
1	L5	1590	C
1	L5	1613	A
1	L5	1625	OMG
1	L5	1633	G
1	L5	1654	G
1	L5	1698	C
1	L5	1699	A
1	L5	1700	G
1	L5	1701	A
1	L5	1719	A
1	L5	1733	G
1	L5	1754	U
1	L5	1898	C
1	L5	1929	A
1	L5	1961	G
1	L5	2042	A
1	L5	2055	G
1	L5	2095	A
1	L5	2475	G
1	L5	2488	C
1	L5	2587	A
1	L5	2707	U
1	L5	2794	C
1	L5	3614	G
1	L5	3648	A
1	L5	3762	PSU
1	L5	3876	A
1	L5	3878	C

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Mol	Chain	Res	Type
1	L5	3904	G
1	L5	3907	G
1	L5	3945	A
1	L5	3947	A
1	L5	4102	C
1	L5	4115	G
1	L5	4281	A
1	L5	4291	G
1	L5	4464	A
1	L5	4527	G
1	L5	4626	A
1	L5	4699	U
1	L5	4731	G
1	L5	4732	G
1	L5	4870	G
1	L5	4909	A
1	L5	4938	A
1	L5	4965	U
1	L5	4990	C
3	L8	51	U
3	L8	87	G
3	L8	94	G
3	L8	104	A
48	S2	102	A
48	S2	198	U
48	S2	215	G
48	S2	312	G
48	S2	326	C
48	S2	370	G
48	S2	448	A
48	S2	545	A
48	S2	560	A
48	S2	607	U
48	S2	620	G
48	S2	838	G
48	S2	870	A
48	S2	888	U
48	S2	889	U
48	S2	896	U
48	S2	910	G
48	S2	912	C
48	S2	1016	U

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Mol	Chain	Res	Type
48	S2	1061	U
48	S2	1165	G
48	S2	1215	C
48	S2	1371	U
48	S2	1437	C
48	S2	1493	C
48	S2	1519	U
48	S2	1520	G
48	S2	1646	C
48	S2	1777	G
48	S2	1784	G
48	S2	1825	A

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

229 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$
1	OMC	L5	1881	1,88	19,22,23	0.81	2 (10%)	25,31,34	0.82	0
1	A2M	L5	2787	1	22,25,26	1.27	1 (4%)	30,36,39	1.25	2 (6%)
1	OMC	L5	2804	1	19,22,23	0.77	0	25,31,34	0.50	0
1	A2M	L5	1871	1,88	22,25,26	1.25	1 (4%)	30,36,39	1.33	6 (20%)
1	A2M	L5	2401	1,88	22,25,26	1.25	1 (4%)	30,36,39	1.16	2 (6%)
1	OMG	L5	1522	1	23,26,27	0.69	0	32,38,41	0.80	1 (3%)
48	OMU	S2	116	48	19,22,23	0.70	0	25,31,34	1.11	2 (8%)
1	PSU	L5	5001	1,88	18,21,22	1.00	1 (5%)	21,30,33	1.74	4 (19%)
48	PSU	S2	406	48	18,21,22	1.06	2 (11%)	21,30,33	1.51	4 (19%)
47	2MG	Pt	10	47	23,26,27	1.30	2 (8%)	33,38,41	1.38	4 (12%)
48	PSU	S2	573	48	18,21,22	1.10	1 (5%)	21,30,33	1.59	4 (19%)
1	PSU	L5	3758	1	18,21,22	1.02	1 (5%)	21,30,33	1.47	4 (19%)
1	OMG	L5	1625	1,83	23,26,27	0.57	0	32,38,41	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	3729	1	18,21,22	1.25	2 (11%)	21,30,33	1.67	4 (19%)
47	2MU	Pt	54	47	20,23,24	1.42	2 (10%)	27,33,36	1.95	7 (25%)
48	PSU	S2	34	48	18,21,22	1.05	2 (11%)	21,30,33	1.50	4 (19%)
1	PSU	L5	3715	1	18,21,22	1.01	1 (5%)	21,30,33	1.64	4 (19%)
48	MA6	S2	1850	48	23,26,27	1.32	3 (13%)	33,38,41	2.94	13 (39%)
1	OMU	L5	4306	1	19,22,23	0.66	0	25,31,34	1.35	5 (20%)
1	OMG	L5	2424	1	23,26,27	0.66	0	32,38,41	0.54	0
1	PSU	L5	3920	1,88	18,21,22	1.28	2 (11%)	21,30,33	1.65	5 (23%)
48	PSU	S2	815	48	18,21,22	1.15	3 (16%)	21,30,33	1.62	4 (19%)
1	PSU	L5	4531	1	18,21,22	1.09	1 (5%)	21,30,33	1.91	3 (14%)
48	A2M	S2	1031	48	22,25,26	1.22	2 (9%)	30,36,39	1.19	4 (13%)
48	OMU	S2	121	48	19,22,23	0.64	0	25,31,34	1.12	2 (8%)
1	A2M	L5	1534	1,88	22,25,26	1.40	2 (9%)	30,36,39	1.31	1 (3%)
1	A2M	L5	3724	1	22,25,26	1.22	2 (9%)	30,36,39	1.40	5 (16%)
48	A2M	S2	1678	48	22,25,26	1.51	3 (13%)	30,36,39	1.50	7 (23%)
1	A2M	L5	3760	1,48	22,25,26	1.50	3 (13%)	30,36,39	1.68	10 (33%)
1	OMG	L5	4494	1	23,26,27	0.66	0	32,38,41	0.71	0
1	OMU	L5	4620	1	19,22,23	0.59	0	25,31,34	1.40	4 (16%)
48	PSU	S2	814	48	18,21,22	0.92	1 (5%)	21,30,33	1.49	3 (14%)
1	PSU	L5	4457	1	18,21,22	1.32	2 (11%)	21,30,33	1.28	4 (19%)
48	OMG	S2	509	48	23,26,27	0.60	0	32,38,41	0.58	0
48	PSU	S2	1243	48	18,21,22	1.20	2 (11%)	21,30,33	1.60	4 (19%)
48	PSU	S2	1232	48	18,21,22	1.08	2 (11%)	21,30,33	1.56	4 (19%)
1	PSU	L5	1744	1,83	18,21,22	1.13	2 (11%)	21,30,33	1.60	4 (19%)
1	OMC	L5	2861	1	19,22,23	0.59	0	25,31,34	0.52	0
1	PSU	L5	3770	1	18,21,22	1.13	2 (11%)	21,30,33	1.59	4 (19%)
1	A2M	L5	3830	1	22,25,26	1.30	3 (13%)	30,36,39	1.36	4 (13%)
1	PSU	L5	1781	1	18,21,22	0.94	1 (5%)	21,30,33	1.47	4 (19%)
1	OMG	L5	3744	1	23,26,27	0.71	0	32,38,41	0.57	0
1	OMC	L5	1340	1	19,22,23	0.86	2 (10%)	25,31,34	0.67	0
48	PSU	S2	609	48	18,21,22	0.99	1 (5%)	21,30,33	1.47	4 (19%)
1	PSU	L5	3639	1	18,21,22	1.39	2 (11%)	21,30,33	1.37	4 (19%)
3	PSU	L8	69	3	18,21,22	1.11	2 (11%)	21,30,33	1.58	5 (23%)
48	PSU	S2	1081	48	18,21,22	1.10	3 (16%)	21,30,33	1.42	4 (19%)
1	PSU	L5	1536	1	18,21,22	1.71	2 (11%)	21,30,33	1.71	6 (28%)
1	OMC	L5	3869	1	19,22,23	0.75	0	25,31,34	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	1367	48	18,21,22	0.99	1 (5%)	21,30,33	1.63	4 (19%)
48	PSU	S2	1136	48	18,21,22	1.11	2 (11%)	21,30,33	1.67	4 (19%)
1	PSU	L5	4972	1,83	18,21,22	1.15	2 (11%)	21,30,33	1.51	4 (19%)
1	A2M	L5	400	1	22,25,26	1.31	3 (13%)	30,36,39	1.27	3 (10%)
48	OMG	S2	683	48	23,26,27	0.69	0	32,38,41	0.68	0
47	PSU	Pt	13	47	18,21,22	1.06	2 (11%)	21,30,33	1.54	4 (19%)
48	A2M	S2	484	48	22,25,26	1.11	1 (4%)	30,36,39	1.29	5 (16%)
1	OMC	L5	2365	1	19,22,23	0.71	0	25,31,34	0.63	0
1	A2M	L5	3723	1	22,25,26	1.20	2 (9%)	30,36,39	1.48	7 (23%)
1	PSU	L5	4579	1	18,21,22	0.98	1 (5%)	21,30,33	1.68	4 (19%)
1	UR3	L5	4530	1	19,22,23	2.64	7 (36%)	26,32,35	1.76	4 (15%)
1	OMC	L5	2351	1,88	19,22,23	0.76	0	25,31,34	0.88	0
1	PSU	L5	3762	1	18,21,22	0.99	1 (5%)	21,30,33	1.38	4 (19%)
1	OMG	L5	1316	1	23,26,27	0.80	1 (4%)	32,38,41	0.73	1 (3%)
43	MLZ	Lo	53	43	8,9,10	0.66	0	4,9,11	0.70	0
1	1MA	L5	1322	1,88	21,25,26	0.75	0	30,37,40	0.89	1 (3%)
1	PSU	L5	4423	1	18,21,22	0.99	1 (5%)	21,30,33	1.50	4 (19%)
1	PSU	L5	1862	1	18,21,22	1.26	1 (5%)	21,30,33	1.67	4 (19%)
1	OMC	L5	4536	1,88	19,22,23	0.89	1 (5%)	25,31,34	0.68	0
48	PSU	S2	93	48	18,21,22	0.87	1 (5%)	21,30,33	1.52	4 (19%)
48	OMG	S2	644	48	23,26,27	0.63	0	32,38,41	0.65	0
48	6MZ	S2	1832	88,48,83	22,25,26	3.73	13 (59%)	29,36,39	2.79	12 (41%)
48	UY1	S2	1326	48,88	19,22,23	4.10	7 (36%)	21,31,34	2.27	5 (23%)
3	OMU	L8	14	1,83,3	19,22,23	0.65	1 (5%)	25,31,34	1.34	5 (20%)
48	PSU	S2	1239	48	18,21,22	1.23	3 (16%)	21,30,33	1.64	4 (19%)
48	B8N	S2	1248	48	25,29,30	0.64	0	28,42,45	1.14	2 (7%)
1	OMG	L5	4392	1	23,26,27	0.70	0	32,38,41	0.63	0
1	PSU	L5	1582	1	18,21,22	1.18	1 (5%)	21,30,33	1.36	4 (19%)
1	PSU	L5	1792	1,83	18,21,22	1.12	2 (11%)	21,30,33	1.52	4 (19%)
48	PSU	S2	801	48	18,21,22	1.06	1 (5%)	21,30,33	1.71	4 (19%)
48	PSU	S2	1692	48	18,21,22	1.06	2 (11%)	21,30,33	1.49	4 (19%)
48	A2M	S2	159	48	22,25,26	1.28	2 (9%)	30,36,39	1.67	6 (20%)
48	PSU	S2	119	48	18,21,22	1.13	1 (5%)	21,30,33	1.47	4 (19%)
1	A2M	L5	3825	1	22,25,26	1.18	1 (4%)	30,36,39	1.23	3 (10%)
1	PSU	L5	1677	1	18,21,22	1.18	3 (16%)	21,30,33	1.61	5 (23%)
1	PSU	L5	4420	1	18,21,22	1.20	4 (22%)	21,30,33	1.54	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A2M	S2	1383	48	22,25,26	1.15	2 (9%)	30,36,39	1.46	6 (20%)
1	OMC	L5	3701	1,83	19,22,23	0.72	1 (5%)	25,31,34	0.73	0
48	OMC	S2	1391	48	19,22,23	0.75	1 (5%)	25,31,34	0.61	0
1	PSU	L5	4576	1	18,21,22	1.03	1 (5%)	21,30,33	1.49	4 (19%)
1	PSU	L5	4442	1	18,21,22	0.99	2 (11%)	21,30,33	1.83	5 (23%)
48	OMU	S2	1288	48	19,22,23	0.70	0	25,31,34	1.39	5 (20%)
48	A2M	S2	590	48	22,25,26	1.41	2 (9%)	30,36,39	1.44	5 (16%)
1	OMG	L5	4228	1	23,26,27	0.64	0	32,38,41	0.72	0
1	6MZ	L5	4220	1	22,25,26	3.82	9 (40%)	29,36,39	2.74	12 (41%)
48	OMG	S2	1490	48,88	23,26,27	0.65	0	32,38,41	0.57	0
1	OMG	L5	2364	1	23,26,27	0.73	0	32,38,41	0.60	0
48	OMC	S2	517	48	19,22,23	0.73	1 (5%)	25,31,34	0.56	0
1	PSU	L5	3637	1,83	18,21,22	1.16	2 (11%)	21,30,33	1.35	4 (19%)
48	PSU	S2	1174	48,83	18,21,22	1.10	1 (5%)	21,30,33	1.43	4 (19%)
3	PSU	L8	55	3	18,21,22	1.13	2 (11%)	21,30,33	1.54	4 (19%)
1	A2M	L5	4590	1	22,25,26	1.04	1 (4%)	30,36,39	1.21	3 (10%)
1	A2M	L5	3718	1	22,25,26	1.29	2 (9%)	30,36,39	1.27	5 (16%)
1	PSU	L5	3851	1,83	18,21,22	1.48	2 (11%)	21,30,33	1.80	4 (19%)
1	5MC	L5	4447	1,83	19,22,23	3.53	8 (42%)	26,32,35	1.28	3 (11%)
47	H2U	Pt	20	47	18,21,22	0.55	0	19,30,33	1.18	1 (5%)
48	PSU	S2	651	48	18,21,22	0.94	1 (5%)	21,30,33	1.62	4 (19%)
48	PSU	S2	686	48	18,21,22	1.14	2 (11%)	21,30,33	1.53	4 (19%)
48	MA6	S2	1851	48	23,26,27	1.41	4 (17%)	33,38,41	2.95	14 (42%)
1	A2M	L5	3867	1	22,25,26	1.47	3 (13%)	30,36,39	1.26	3 (10%)
1	A2M	L5	398	1	22,25,26	1.20	1 (4%)	30,36,39	1.25	4 (13%)
1	OMG	L5	4499	1	23,26,27	0.56	0	32,38,41	0.62	0
1	PSU	L5	4312	1	18,21,22	0.96	1 (5%)	21,30,33	1.55	5 (23%)
48	PSU	S2	1004	48	18,21,22	1.21	2 (11%)	21,30,33	1.48	4 (19%)
1	PSU	L5	1683	1,83	18,21,22	1.20	1 (5%)	21,30,33	1.41	3 (14%)
1	OMU	L5	4498	1,83	19,22,23	0.72	0	25,31,34	1.34	4 (16%)
48	PSU	S2	105	48	18,21,22	0.92	0	21,30,33	1.71	4 (19%)
48	PSU	S2	1238	48	18,21,22	1.02	1 (5%)	21,30,33	1.58	4 (19%)
1	OMC	L5	2824	1	19,22,23	0.86	1 (5%)	25,31,34	0.56	0
1	PSU	L5	4552	1	18,21,22	1.35	1 (5%)	21,30,33	1.42	4 (19%)
1	OMG	L5	2876	1	23,26,27	0.73	0	32,38,41	0.74	0
48	PSU	S2	681	48	18,21,22	1.28	2 (11%)	21,30,33	1.36	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	1445	48	18,21,22	1.07	2 (11%)	21,30,33	1.57	4 (19%)
48	OMG	S2	867	48	23,26,27	0.51	0	32,38,41	0.50	0
1	PSU	L5	4569	1	18,21,22	1.27	4 (22%)	21,30,33	1.30	3 (14%)
48	A2M	S2	668	48,88	22,25,26	1.53	3 (13%)	30,36,39	1.28	4 (13%)
1	PSU	L5	3768	1	18,21,22	1.05	1 (5%)	21,30,33	1.64	4 (19%)
48	PSU	S2	1347	48	18,21,22	1.06	1 (5%)	21,30,33	1.59	4 (19%)
1	PSU	L5	4628	1	18,21,22	1.06	2 (11%)	21,30,33	1.66	4 (19%)
48	A2M	S2	512	48	22,25,26	1.24	2 (9%)	30,36,39	1.32	4 (13%)
48	PSU	S2	109	48	18,21,22	1.00	1 (5%)	21,30,33	1.69	4 (19%)
1	5MC	L5	3782	1,88	19,22,23	3.37	8 (42%)	26,32,35	1.11	2 (7%)
1	OMU	L5	3925	1	19,22,23	0.80	1 (5%)	25,31,34	1.31	4 (16%)
1	PSU	L5	4403	1,83	18,21,22	1.11	1 (5%)	21,30,33	1.60	4 (19%)
1	OMG	L5	4637	1,83	23,26,27	0.72	0	32,38,41	0.48	0
47	5MC	Pt	49	47	19,22,23	3.69	8 (42%)	26,32,35	0.99	1 (3%)
1	A2M	L5	2363	1,88	22,25,26	1.34	2 (9%)	30,36,39	1.39	5 (16%)
1	PSU	L5	4500	1	18,21,22	1.02	2 (11%)	21,30,33	1.77	4 (19%)
48	OMG	S2	1447	48	23,26,27	0.54	0	32,38,41	0.61	0
1	PSU	L5	5010	1	18,21,22	1.19	2 (11%)	21,30,33	1.53	4 (19%)
1	PSU	L5	1782	1	18,21,22	0.98	1 (5%)	21,30,33	1.54	4 (19%)
1	PSU	L5	4493	1,83	18,21,22	1.24	2 (11%)	21,30,33	1.48	4 (19%)
48	A2M	S2	468	48	22,25,26	1.18	2 (9%)	30,36,39	1.42	7 (23%)
48	OMU	S2	1442	48,88	19,22,23	0.62	0	25,31,34	1.31	6 (24%)
1	OMC	L5	3887	1	19,22,23	0.85	1 (5%)	25,31,34	0.72	0
1	OMC	L5	4456	1	19,22,23	0.80	1 (5%)	25,31,34	0.63	0
1	PSU	L5	3844	1	18,21,22	1.32	1 (5%)	21,30,33	1.48	4 (19%)
48	4AC	S2	1337	48	21,24,25	3.06	11 (52%)	28,34,37	1.13	2 (7%)
48	PSU	S2	866	48	18,21,22	1.10	1 (5%)	21,30,33	1.72	4 (19%)
48	PSU	S2	1625	48	18,21,22	0.97	1 (5%)	21,30,33	1.54	4 (19%)
48	4AC	S2	1842	48	21,24,25	2.93	11 (52%)	28,34,37	0.84	1 (3%)
1	OMU	L5	2415	1	19,22,23	0.58	0	25,31,34	1.31	5 (20%)
1	OMC	L5	3841	1	19,22,23	0.84	2 (10%)	25,31,34	0.81	1 (4%)
48	PSU	S2	966	48	18,21,22	0.84	1 (5%)	21,30,33	1.46	4 (19%)
1	OMG	L5	3944	1	23,26,27	0.52	0	32,38,41	0.53	0
1	PSU	L5	3695	1,83	18,21,22	1.00	1 (5%)	21,30,33	1.42	4 (19%)
48	PSU	S2	296	48	18,21,22	0.87	0	21,30,33	1.55	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	822	48	18,21,22	1.15	2 (11%)	21,30,33	1.49	5 (23%)
48	OMG	S2	436	48	23,26,27	0.63	0	32,38,41	0.59	0
48	PSU	S2	1177	48	18,21,22	1.08	2 (11%)	21,30,33	1.50	4 (19%)
1	OMC	L5	3808	1	19,22,23	0.75	0	25,31,34	0.67	0
48	PSU	S2	1244	48	18,21,22	1.03	1 (5%)	21,30,33	1.58	4 (19%)
48	PSU	S2	918	48	18,21,22	0.95	2 (11%)	21,30,33	1.72	5 (23%)
1	A2M	L5	1326	1	22,25,26	1.31	3 (13%)	30,36,39	1.27	3 (10%)
48	PSU	S2	572	48	18,21,22	1.01	2 (11%)	21,30,33	1.64	5 (23%)
1	PSU	L5	4296	1	18,21,22	1.24	3 (16%)	21,30,33	1.66	4 (19%)
48	OMU	S2	354	48	19,22,23	0.53	0	25,31,34	1.37	6 (24%)
1	A2M	L5	1524	1	22,25,26	1.34	3 (13%)	30,36,39	1.33	2 (6%)
48	OMU	S2	428	48	19,22,23	0.47	0	25,31,34	1.33	6 (24%)
1	PSU	L5	2839	1	18,21,22	1.24	2 (11%)	21,30,33	1.49	5 (23%)
48	PSU	S2	1643	48,88	18,21,22	1.00	2 (11%)	21,30,33	1.50	4 (19%)
1	A2M	L5	3785	1	22,25,26	1.50	3 (13%)	30,36,39	1.58	9 (30%)
1	PSU	L5	1779	1	18,21,22	1.10	2 (11%)	21,30,33	1.53	4 (19%)
1	PSU	L5	3764	1	18,21,22	1.66	2 (11%)	21,30,33	1.44	2 (9%)
1	OMG	L5	3899	1,88	23,26,27	0.79	0	32,38,41	0.77	1 (3%)
1	OMG	L5	4623	1	23,26,27	0.66	0	32,38,41	0.79	1 (3%)
48	OMU	S2	627	48	19,22,23	0.59	0	25,31,34	1.40	5 (20%)
41	M3L	Lm	98	41	10,11,12	0.47	0	9,14,16	0.46	0
1	A2M	L5	2815	1,88	22,25,26	1.18	3 (13%)	30,36,39	1.28	5 (16%)
1	PSU	L5	3853	1,88,83	18,21,22	1.38	3 (16%)	21,30,33	1.45	4 (19%)
48	OMC	S2	462	48	19,22,23	0.60	0	25,31,34	0.49	0
1	UY1	L5	3818	1,83	19,22,23	3.85	8 (42%)	21,31,34	2.53	6 (28%)
1	PSU	L5	1860	1	18,21,22	1.13	2 (11%)	21,30,33	1.65	4 (19%)
48	A2M	S2	27	48,88	22,25,26	1.25	1 (4%)	30,36,39	1.35	6 (20%)
1	PSU	L5	4361	1	18,21,22	1.19	2 (11%)	21,30,33	1.54	4 (19%)
48	OMG	S2	601	48	23,26,27	0.61	0	32,38,41	0.60	0
1	OMG	L5	4618	1,83	23,26,27	0.72	0	32,38,41	0.58	0
48	OMU	S2	1804	48	19,22,23	0.67	0	25,31,34	1.49	5 (20%)
30	MLZ	Lb	5	30,83	8,9,10	0.79	0	4,9,11	0.66	0
48	OMC	S2	174	48,88	19,22,23	0.63	0	25,31,34	0.64	0
48	A2M	S2	576	48	22,25,26	1.32	2 (9%)	30,36,39	1.39	6 (20%)
1	PSU	L5	4293	1	18,21,22	1.20	2 (11%)	21,30,33	1.53	4 (19%)
48	PSU	S2	649	48	18,21,22	1.07	2 (11%)	21,30,33	1.60	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L8	75	3	23,26,27	0.63	0	32,38,41	0.66	0
1	PSU	L5	4299	1	18,21,22	0.91	1 (5%)	21,30,33	1.34	3 (14%)
1	PSU	L5	4353	1	18,21,22	1.00	2 (11%)	21,30,33	1.68	4 (19%)
5	HIC	LB	245	5	10,11,12	0.57	0	9,14,16	0.88	0
1	PSU	L5	3734	1	18,21,22	0.91	1 (5%)	21,30,33	1.54	5 (23%)
72	HY3	SX	62	72	7,8,9	6.30	5 (71%)	7,10,12	1.29	1 (14%)
1	A2M	L5	4571	1	22,25,26	1.50	3 (13%)	30,36,39	1.38	6 (20%)
1	A2M	L5	4523	1,88	22,25,26	1.29	3 (13%)	30,36,39	1.31	3 (10%)
48	A2M	S2	166	48	22,25,26	1.32	2 (9%)	30,36,39	1.55	4 (13%)
1	OMU	L5	4227	1	19,22,23	0.84	1 (5%)	25,31,34	1.45	4 (16%)
48	PSU	S2	36	48	18,21,22	0.99	1 (5%)	21,30,33	1.43	3 (14%)
48	OMU	S2	172	48	19,22,23	0.50	0	25,31,34	1.45	6 (24%)
47	PSU	Pt	55	47	18,21,22	1.22	2 (11%)	21,30,33	1.55	4 (19%)
1	PSU	L5	2632	1	18,21,22	1.09	2 (11%)	21,30,33	1.55	4 (19%)
1	PSU	L5	4471	1	18,21,22	1.20	2 (11%)	21,30,33	1.59	4 (19%)
1	PSU	L5	4521	1,88,83	18,21,22	1.05	2 (11%)	21,30,33	1.62	4 (19%)
1	PSU	L5	3884	1	18,21,22	1.17	2 (11%)	21,30,33	1.62	4 (19%)
48	G7M	S2	1639	47,48	23,26,27	2.56	7 (30%)	34,39,42	2.41	9 (26%)
48	PSU	S2	1056	48	18,21,22	1.06	2 (11%)	21,30,33	1.69	5 (23%)
1	PSU	L5	4636	1	18,21,22	1.23	2 (11%)	21,30,33	1.42	4 (19%)
1	PSU	L5	4689	1	18,21,22	1.13	2 (11%)	21,30,33	1.42	3 (14%)
1	PSU	L5	2508	1	18,21,22	1.26	2 (11%)	21,30,33	1.49	4 (19%)
48	PSU	S2	218	48	18,21,22	0.95	1 (5%)	21,30,33	1.53	4 (19%)
48	A2M	S2	99	48,88	22,25,26	1.09	1 (4%)	30,36,39	1.21	1 (3%)
48	PSU	S2	863	48	18,21,22	0.92	0	21,30,33	1.44	4 (19%)
1	OMG	L5	3627	1	23,26,27	0.77	0	32,38,41	0.77	1 (3%)
1	OMG	L5	3792	1	23,26,27	0.76	1 (4%)	32,38,41	0.58	0
1	OMG	L5	4196	1,47,88	23,26,27	0.74	0	32,38,41	0.80	1 (3%)
1	OMG	L5	4370	1	23,26,27	0.65	0	32,38,41	0.63	0
1	OMC	L5	2422	1,88	19,22,23	0.84	1 (5%)	25,31,34	0.61	0
48	OMG	S2	1328	48	23,26,27	0.58	0	32,38,41	0.45	0
1	PSU	L5	4431	1	18,21,22	1.13	2 (11%)	21,30,33	1.66	4 (19%)
1	PSU	L5	2843	1	18,21,22	1.47	3 (16%)	21,30,33	1.52	4 (19%)
48	OMC	S2	1703	48,83	19,22,23	0.79	1 (5%)	25,31,34	0.58	0
1	PSU	L5	4532	1	18,21,22	0.99	1 (5%)	21,30,33	1.43	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	L5	2837	1	19,22,23	0.62	0	25,31,34	1.41	5 (20%)
1	PSU	L5	4673	1,88	18,21,22	1.31	1 (5%)	21,30,33	1.50	4 (19%)

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
1	OMC	L5	1881	1,88	-	0/9/27/28	0/2/2/2
1	A2M	L5	2787	1	-	3/9/27/28	0/3/3/3
1	OMC	L5	2804	1	-	1/9/27/28	0/2/2/2
1	A2M	L5	1871	1,88	-	0/9/27/28	0/3/3/3
1	A2M	L5	2401	1,88	-	1/9/27/28	0/3/3/3
1	OMG	L5	1522	1	-	0/9/27/28	0/3/3/3
48	OMU	S2	116	48	-	0/9/27/28	0/2/2/2
1	PSU	L5	5001	1,88	-	0/7/25/26	0/2/2/2
48	PSU	S2	406	48	-	0/7/25/26	0/2/2/2
47	2MG	Pt	10	47	-	0/9/27/28	0/3/3/3
48	PSU	S2	573	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	3758	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	1625	1,83	-	1/9/27/28	0/3/3/3
1	PSU	L5	3729	1	-	0/7/25/26	0/2/2/2
47	2MU	Pt	54	47	-	1/9/27/28	0/2/2/2
48	PSU	S2	34	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	3715	1	-	0/7/25/26	0/2/2/2
48	MA6	S2	1850	48	-	0/11/29/30	0/3/3/3
1	OMU	L5	4306	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	2424	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	3920	1,88	-	0/7/25/26	0/2/2/2
48	PSU	S2	815	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4531	1	-	1/7/25/26	0/2/2/2
48	A2M	S2	1031	48	-	0/9/27/28	0/3/3/3
48	OMU	S2	121	48	-	0/9/27/28	0/2/2/2
1	A2M	L5	1534	1,88	-	1/9/27/28	0/3/3/3
1	A2M	L5	3724	1	-	0/9/27/28	0/3/3/3
48	A2M	S2	1678	48	-	1/9/27/28	0/3/3/3
1	A2M	L5	3760	1,48	-	4/9/27/28	0/3/3/3
1	OMG	L5	4494	1	-	0/9/27/28	0/3/3/3
1	OMU	L5	4620	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	814	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4457	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMG	S2	509	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	1243	48	-	3/7/25/26	0/2/2/2
48	PSU	S2	1232	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	1744	1,83	-	0/7/25/26	0/2/2/2
1	OMC	L5	2861	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	3770	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1781	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3744	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	1340	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	609	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	3639	1	-	0/7/25/26	0/2/2/2
3	PSU	L8	69	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	1081	48	-	1/7/25/26	0/2/2/2
1	PSU	L5	1536	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	3869	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	1367	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1136	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4972	1,83	-	0/7/25/26	0/2/2/2
1	A2M	L5	400	1	-	0/9/27/28	0/3/3/3
48	OMG	S2	683	48	-	0/9/27/28	0/3/3/3
47	PSU	Pt	13	47	-	1/7/25/26	0/2/2/2
48	A2M	S2	484	48	-	0/9/27/28	0/3/3/3
1	OMC	L5	2365	1	-	1/9/27/28	0/2/2/2
1	A2M	L5	3723	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	4579	1	-	0/7/25/26	0/2/2/2
1	UR3	L5	4530	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2351	1,88	-	1/9/27/28	0/2/2/2
1	PSU	L5	3762	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	1316	1	-	0/9/27/28	0/3/3/3
43	MLZ	Lo	53	43	-	0/7/8/10	-
1	1MA	L5	1322	1,88	-	2/7/25/26	0/3/3/3
1	PSU	L5	4423	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1862	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	4536	1,88	-	1/9/27/28	0/2/2/2
48	PSU	S2	93	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	644	48	-	3/9/27/28	0/3/3/3
48	6MZ	S2	1832	88,48,83	-	0/9/27/28	0/3/3/3
48	UY1	S2	1326	48,88	-	2/9/27/28	0/2/2/2
3	OMU	L8	14	1,83,3	-	1/9/27/28	0/2/2/2
48	PSU	S2	1239	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	B8N	S2	1248	48	-	5/16/34/35	0/2/2/2
1	OMG	L5	4392	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1582	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1792	1,83	-	0/7/25/26	0/2/2/2
48	PSU	S2	801	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1692	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	159	48	-	1/9/27/28	0/3/3/3
48	PSU	S2	119	48	-	0/7/25/26	0/2/2/2
1	A2M	L5	3825	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1677	1	-	3/7/25/26	0/2/2/2
1	PSU	L5	4420	1	-	2/7/25/26	0/2/2/2
48	A2M	S2	1383	48	-	0/9/27/28	0/3/3/3
1	OMC	L5	3701	1,83	-	4/9/27/28	0/2/2/2
48	OMC	S2	1391	48	-	0/9/27/28	0/2/2/2
1	PSU	L5	4576	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
48	OMU	S2	1288	48	-	0/9/27/28	0/2/2/2
48	A2M	S2	590	48	-	3/9/27/28	0/3/3/3
1	OMG	L5	4228	1	-	0/9/27/28	0/3/3/3
1	6MZ	L5	4220	1	-	0/9/27/28	0/3/3/3
48	OMG	S2	1490	48,88	-	4/9/27/28	0/3/3/3
1	OMG	L5	2364	1	-	1/9/27/28	0/3/3/3
48	OMC	S2	517	48	-	0/9/27/28	0/2/2/2
1	PSU	L5	3637	1,83	-	0/7/25/26	0/2/2/2
48	PSU	S2	1174	48,83	-	0/7/25/26	0/2/2/2
3	PSU	L8	55	3	-	0/7/25/26	0/2/2/2
1	A2M	L5	4590	1	-	1/9/27/28	0/3/3/3
1	A2M	L5	3718	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	3851	1,83	-	1/7/25/26	0/2/2/2
1	5MC	L5	4447	1,83	-	4/7/25/26	0/2/2/2
47	H2U	Pt	20	47	-	3/7/38/39	0/2/2/2
48	PSU	S2	651	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	686	48	-	0/7/25/26	0/2/2/2
48	MA6	S2	1851	48	-	3/11/29/30	0/3/3/3
1	A2M	L5	3867	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	398	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	4499	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4312	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	1004	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	1683	1,83	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	L5	4498	1,83	-	0/9/27/28	0/2/2/2
48	PSU	S2	105	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1238	48	-	0/7/25/26	0/2/2/2
1	OMC	L5	2824	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4552	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2876	1	-	0/9/27/28	0/3/3/3
48	PSU	S2	681	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1445	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	867	48	-	1/9/27/28	0/3/3/3
1	PSU	L5	4569	1	-	0/7/25/26	0/2/2/2
48	A2M	S2	668	48,88	-	2/9/27/28	0/3/3/3
1	PSU	L5	3768	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	1347	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
48	A2M	S2	512	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	109	48	-	0/7/25/26	0/2/2/2
1	5MC	L5	3782	1,88	-	0/7/25/26	0/2/2/2
1	OMU	L5	3925	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4403	1,83	-	0/7/25/26	0/2/2/2
1	OMG	L5	4637	1,83	-	1/9/27/28	0/3/3/3
47	5MC	Pt	49	47	-	0/7/25/26	0/2/2/2
1	A2M	L5	2363	1,88	-	0/9/27/28	0/3/3/3
1	PSU	L5	4500	1	-	1/7/25/26	0/2/2/2
48	OMG	S2	1447	48	-	1/9/27/28	0/3/3/3
1	PSU	L5	5010	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1782	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4493	1,83	-	0/7/25/26	0/2/2/2
48	A2M	S2	468	48	-	0/9/27/28	0/3/3/3
48	OMU	S2	1442	48,88	-	0/9/27/28	0/2/2/2
1	OMC	L5	3887	1	-	1/9/27/28	0/2/2/2
1	OMC	L5	4456	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	3844	1	-	1/7/25/26	0/2/2/2
48	4AC	S2	1337	48	-	0/11/29/30	0/2/2/2
48	PSU	S2	866	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1625	48	-	0/7/25/26	0/2/2/2
48	4AC	S2	1842	48	-	0/11/29/30	0/2/2/2
1	OMU	L5	2415	1	-	0/9/27/28	0/2/2/2
1	OMC	L5	3841	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	966	48	-	0/7/25/26	0/2/2/2
1	OMG	L5	3944	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	3695	1,83	-	0/7/25/26	0/2/2/2
48	PSU	S2	296	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	S2	822	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	436	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	1177	48	-	0/7/25/26	0/2/2/2
1	OMC	L5	3808	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	1244	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	918	48	-	0/7/25/26	0/2/2/2
1	A2M	L5	1326	1	-	2/9/27/28	0/3/3/3
48	PSU	S2	572	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4296	1	-	0/7/25/26	0/2/2/2
48	OMU	S2	354	48	-	0/9/27/28	0/2/2/2
1	A2M	L5	1524	1	-	1/9/27/28	0/3/3/3
48	OMU	S2	428	48	-	5/9/27/28	0/2/2/2
1	PSU	L5	2839	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	1643	48,88	-	0/7/25/26	0/2/2/2
1	A2M	L5	3785	1	-	2/9/27/28	0/3/3/3
1	PSU	L5	1779	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3764	1	-	2/7/25/26	0/2/2/2
1	OMG	L5	3899	1,88	-	0/9/27/28	0/3/3/3
1	OMG	L5	4623	1	-	0/9/27/28	0/3/3/3
48	OMU	S2	627	48	-	0/9/27/28	0/2/2/2
41	M3L	Lm	98	41	-	0/9/10/12	-
1	A2M	L5	2815	1,88	-	2/9/27/28	0/3/3/3
1	PSU	L5	3853	1,88,83	-	0/7/25/26	0/2/2/2
48	OMC	S2	462	48	-	1/9/27/28	0/2/2/2
1	UY1	L5	3818	1,83	-	2/9/27/28	0/2/2/2
1	PSU	L5	1860	1	-	0/7/25/26	0/2/2/2
48	A2M	S2	27	48,88	-	0/9/27/28	0/3/3/3
1	PSU	L5	4361	1	-	0/7/25/26	0/2/2/2
48	OMG	S2	601	48	-	1/9/27/28	0/3/3/3
1	OMG	L5	4618	1,83	-	0/9/27/28	0/3/3/3
48	OMU	S2	1804	48	-	1/9/27/28	0/2/2/2
30	MLZ	Lb	5	30,83	-	2/7/8/10	-
48	OMC	S2	174	48,88	-	0/9/27/28	0/2/2/2
48	A2M	S2	576	48	-	1/9/27/28	0/3/3/3
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	649	48	-	0/7/25/26	0/2/2/2
3	OMG	L8	75	3	-	0/9/27/28	0/3/3/3
1	PSU	L5	4299	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4353	1	-	0/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
1	PSU	L5	3734	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	HY3	SX	62	72	-	0/1/12/14	0/1/1/1
1	A2M	L5	4571	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	4523	1,88	-	0/9/27/28	0/3/3/3
48	A2M	S2	166	48	-	0/9/27/28	0/3/3/3
1	OMU	L5	4227	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	36	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	172	48	-	1/9/27/28	0/2/2/2
47	PSU	Pt	55	47	-	0/7/25/26	0/2/2/2
1	PSU	L5	2632	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4471	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4521	1,88,83	-	0/7/25/26	0/2/2/2
1	PSU	L5	3884	1	-	0/7/25/26	0/2/2/2
48	G7M	S2	1639	47,48	-	0/7/25/26	0/3/3/3
48	PSU	S2	1056	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4636	1	-	2/7/25/26	0/2/2/2
1	PSU	L5	4689	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	2508	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	218	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	99	48,88	-	1/9/27/28	0/3/3/3
48	PSU	S2	863	48	-	0/7/25/26	0/2/2/2
1	OMG	L5	3627	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	3792	1	-	1/9/27/28	0/3/3/3
1	OMG	L5	4196	1,47,88	-	1/9/27/28	0/3/3/3
1	OMG	L5	4370	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	2422	1,88	-	2/9/27/28	0/2/2/2
48	OMG	S2	1328	48	-	0/9/27/28	0/3/3/3
1	PSU	L5	4431	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	2843	1	-	0/7/25/26	0/2/2/2
48	OMC	S2	1703	48,83	-	0/9/27/28	0/2/2/2
1	PSU	L5	4532	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	2837	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4673	1,88	-	0/7/25/26	0/2/2/2

All (378) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1326	UY1	C6-C5	11.04	1.47	1.35
72	SX	62	HY3	C4-C3	-10.57	1.33	1.52
1	L5	4220	6MZ	C6-N6	10.16	1.45	1.34
1	L5	3818	UY1	C6-C5	9.56	1.45	1.35
48	S2	1326	UY1	C2-N1	9.39	1.48	1.36
72	SX	62	HY3	C3-CA	9.08	1.64	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3818	UY1	C2-N1	9.07	1.48	1.36
47	Pt	49	5MC	C6-C5	8.89	1.49	1.34
1	L5	4447	5MC	C6-C5	8.69	1.48	1.34
48	S2	1832	6MZ	C3'-C2'	-8.46	1.30	1.53
48	S2	1832	6MZ	C6-N6	8.41	1.43	1.34
1	L5	3782	5MC	C6-C5	8.38	1.48	1.34
72	SX	62	HY3	CA-N	-8.27	1.34	1.48
1	L5	4220	6MZ	C3'-C2'	-7.91	1.31	1.53
48	S2	1326	UY1	C2-N3	7.19	1.49	1.37
1	L5	3818	UY1	C2-N3	7.04	1.49	1.37
1	L5	4447	5MC	C5-C4	6.63	1.49	1.44
47	Pt	49	5MC	C5-C4	6.52	1.49	1.44
48	S2	1639	G7M	C4-N3	6.48	1.49	1.34
47	Pt	49	5MC	C4-N3	6.38	1.44	1.34
48	S2	1337	4AC	C4-N3	6.35	1.43	1.32
48	S2	1842	4AC	C4-N3	6.35	1.43	1.32
1	L5	3782	5MC	C4-N3	6.18	1.44	1.34
1	L5	1536	PSU	O4-C4	-6.18	1.11	1.23
1	L5	4530	UR3	C2-N1	6.12	1.47	1.38
1	L5	4530	UR3	C6-C5	6.06	1.49	1.35
48	S2	1337	4AC	C6-C5	5.99	1.49	1.35
48	S2	1832	6MZ	O4'-C1'	5.86	1.55	1.42
47	Pt	49	5MC	C2-N3	5.85	1.48	1.36
1	L5	3764	PSU	O4-C4	-5.82	1.12	1.23
48	S2	1842	4AC	C6-C5	5.78	1.48	1.35
48	S2	1832	6MZ	O4'-C4'	-5.77	1.32	1.45
1	L5	4220	6MZ	O4'-C1'	5.76	1.55	1.42
1	L5	4220	6MZ	O4'-C4'	-5.72	1.32	1.45
48	S2	1639	G7M	C2-N2	5.70	1.47	1.34
1	L5	4447	5MC	C4-N3	5.44	1.42	1.34
48	S2	1337	4AC	C2-N3	5.41	1.47	1.36
1	L5	4447	5MC	C2-N3	5.38	1.47	1.36
1	L5	3782	5MC	C5-C4	5.34	1.48	1.44
1	L5	4530	UR3	C2-N3	5.29	1.49	1.39
48	S2	1832	6MZ	C1'-N9	-5.12	1.32	1.46
1	L5	3782	5MC	C2-N3	5.06	1.46	1.36
48	S2	1639	G7M	C5-N7	-5.02	1.33	1.39
1	L5	4220	6MZ	C1'-N9	-4.86	1.32	1.46
48	S2	1842	4AC	C2-N3	4.83	1.45	1.36
48	S2	1326	UY1	C6-N1	4.77	1.44	1.36
1	L5	3844	PSU	O4-C4	-4.75	1.14	1.23
1	L5	3639	PSU	O4-C4	-4.71	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4220	6MZ	C3'-C4'	4.57	1.64	1.53
1	L5	4552	PSU	O4-C4	-4.54	1.14	1.23
47	Pt	10	2MG	C2-N2	4.48	1.42	1.33
1	L5	3785	A2M	O5'-C5'	-4.48	1.31	1.44
1	L5	3851	PSU	O4-C4	-4.45	1.15	1.23
47	Pt	54	2MU	O5'-C5'	-4.39	1.31	1.44
1	L5	1862	PSU	O4-C4	-4.39	1.15	1.23
47	Pt	49	5MC	C6-N1	4.39	1.45	1.38
1	L5	3867	A2M	O5'-C5'	-4.31	1.31	1.44
48	S2	1639	G7M	C2-N3	4.30	1.43	1.33
1	L5	1871	A2M	O5'-C5'	-4.28	1.31	1.44
1	L5	3818	UY1	C6-N1	4.25	1.43	1.36
48	S2	27	A2M	O5'-C5'	-4.25	1.31	1.44
47	Pt	49	5MC	C4-N4	4.21	1.44	1.34
1	L5	4523	A2M	O5'-C5'	-4.17	1.32	1.44
1	L5	4673	PSU	O4-C4	-4.13	1.15	1.23
48	S2	1337	4AC	C7-N4	4.12	1.45	1.37
48	S2	576	A2M	O5'-C5'	-4.10	1.32	1.44
48	S2	1832	6MZ	C3'-C4'	4.09	1.63	1.53
1	L5	2508	PSU	O4-C4	-4.08	1.15	1.23
48	S2	668	A2M	O4'-C4'	-4.08	1.35	1.45
48	S2	1842	4AC	O2-C2	-4.07	1.16	1.23
1	L5	2401	A2M	O5'-C5'	-4.04	1.32	1.44
1	L5	4571	A2M	O3'-C3'	-4.03	1.33	1.43
1	L5	4447	5MC	C6-N1	4.03	1.44	1.38
1	L5	3718	A2M	O5'-C5'	-4.02	1.32	1.44
1	L5	2843	PSU	C2-N1	4.01	1.41	1.36
48	S2	484	A2M	O5'-C5'	-3.92	1.32	1.44
48	S2	1337	4AC	C5-C4	3.92	1.49	1.41
1	L5	3920	PSU	O4-C4	-3.89	1.16	1.23
1	L5	1524	A2M	O5'-C5'	-3.88	1.32	1.44
1	L5	4457	PSU	O4-C4	-3.87	1.16	1.23
1	L5	4361	PSU	O4-C4	-3.87	1.16	1.23
1	L5	1534	A2M	O5'-C5'	-3.81	1.33	1.44
48	S2	1842	4AC	C7-N4	3.81	1.44	1.37
1	L5	1582	PSU	O4-C4	-3.80	1.16	1.23
1	L5	3825	A2M	O5'-C5'	-3.80	1.33	1.44
48	S2	1842	4AC	C5-C4	3.79	1.49	1.41
1	L5	2363	A2M	O5'-C5'	-3.78	1.33	1.44
48	S2	1678	A2M	O5'-C5'	-3.78	1.33	1.44
47	Pt	49	5MC	C2-N1	3.77	1.48	1.40
48	S2	681	PSU	O4-C4	-3.77	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4571	A2M	O5'-C5'	-3.74	1.33	1.44
1	L5	3782	5MC	C6-N1	3.73	1.44	1.38
48	S2	512	A2M	O5'-C5'	-3.71	1.33	1.44
1	L5	4447	5MC	O2-C2	-3.70	1.16	1.23
48	S2	1031	A2M	O5'-C5'	-3.70	1.33	1.44
48	S2	590	A2M	O5'-C5'	-3.70	1.33	1.44
1	L5	3724	A2M	O5'-C5'	-3.69	1.33	1.44
1	L5	400	A2M	O5'-C5'	-3.68	1.33	1.44
48	S2	1842	4AC	C2-N1	3.67	1.47	1.40
1	L5	3782	5MC	C2-N1	3.66	1.47	1.40
1	L5	4493	PSU	O4-C4	-3.63	1.16	1.23
1	L5	3830	A2M	O5'-C5'	-3.61	1.33	1.44
1	L5	4447	5MC	C4-N4	3.61	1.43	1.34
48	S2	1832	6MZ	C5-C4	-3.60	1.32	1.39
48	S2	1337	4AC	C4-N4	3.59	1.45	1.39
48	S2	1337	4AC	O2-C2	-3.56	1.17	1.23
1	L5	398	A2M	O5'-C5'	-3.55	1.33	1.44
1	L5	3760	A2M	O5'-C5'	-3.53	1.33	1.44
1	L5	3729	PSU	C2-N1	3.53	1.41	1.36
1	L5	4403	PSU	O4-C4	-3.52	1.16	1.23
1	L5	1683	PSU	O4-C4	-3.51	1.16	1.23
1	L5	4689	PSU	O4-C4	-3.50	1.16	1.23
48	S2	159	A2M	O5'-C5'	-3.50	1.34	1.44
1	L5	2839	PSU	C2-N1	3.49	1.41	1.36
1	L5	3782	5MC	C4-N4	3.49	1.43	1.34
48	S2	1383	A2M	O5'-C5'	-3.49	1.34	1.44
48	S2	1337	4AC	C2-N1	3.49	1.47	1.40
48	S2	1326	UY1	C4-N3	3.47	1.45	1.38
48	S2	1678	A2M	O3'-C3'	-3.46	1.34	1.43
48	S2	668	A2M	O5'-C5'	-3.46	1.34	1.44
1	L5	2843	PSU	O4-C4	-3.44	1.17	1.23
1	L5	3818	UY1	O4-C4	-3.40	1.17	1.23
48	S2	1639	G7M	C5-C6	3.39	1.52	1.43
1	L5	4447	5MC	C2-N1	3.37	1.47	1.40
1	L5	3782	5MC	O2-C2	-3.37	1.17	1.23
1	L5	1792	PSU	O4-C4	-3.37	1.17	1.23
1	L5	4293	PSU	O4-C4	-3.35	1.17	1.23
48	S2	1850	MA6	C6-N6	3.35	1.46	1.36
1	L5	3851	PSU	C2-N1	3.35	1.41	1.36
48	S2	1832	6MZ	C5-N7	-3.35	1.33	1.39
48	S2	468	A2M	O5'-C5'	-3.34	1.34	1.44
1	L5	3723	A2M	O5'-C5'	-3.33	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	166	A2M	O5'-C5'	-3.33	1.34	1.44
47	Pt	55	PSU	C2-N1	3.31	1.41	1.36
48	S2	406	PSU	O4-C4	-3.30	1.17	1.23
1	L5	4220	6MZ	C5-N7	-3.30	1.33	1.39
3	L8	55	PSU	O4-C4	-3.30	1.17	1.23
48	S2	801	PSU	C2-N1	3.29	1.41	1.36
1	L5	1860	PSU	O4-C4	-3.29	1.17	1.23
1	L5	4296	PSU	C2-N1	3.28	1.40	1.36
48	S2	1851	MA6	C5-C4	-3.27	1.33	1.39
1	L5	3853	PSU	C2-N1	3.27	1.40	1.36
1	L5	3818	UY1	O2-C2	-3.25	1.16	1.23
48	S2	1177	PSU	O4-C4	-3.25	1.17	1.23
48	S2	1851	MA6	C6-N6	3.25	1.45	1.36
48	S2	119	PSU	C2-N1	3.24	1.40	1.36
48	S2	1337	4AC	C6-N1	3.23	1.45	1.38
1	L5	2787	A2M	O5'-C5'	-3.23	1.34	1.44
1	L5	1779	PSU	O4-C4	-3.20	1.17	1.23
48	S2	1347	PSU	O4-C4	-3.18	1.17	1.23
48	S2	590	A2M	O4'-C4'	-3.16	1.38	1.45
1	L5	4471	PSU	O4-C4	-3.14	1.17	1.23
1	L5	1326	A2M	O5'-C5'	-3.09	1.35	1.44
1	L5	4628	PSU	O4-C4	-3.08	1.17	1.23
1	L5	3818	UY1	C4-N3	3.06	1.44	1.38
48	S2	1243	PSU	C2-N1	3.05	1.40	1.36
1	L5	4530	UR3	O4-C4	-3.05	1.17	1.23
48	S2	1239	PSU	C2-N1	3.04	1.40	1.36
47	Pt	49	5MC	O2-C2	-3.03	1.18	1.23
1	L5	4972	PSU	C2-N1	3.02	1.40	1.36
1	L5	5010	PSU	O4-C4	-3.02	1.17	1.23
1	L5	4576	PSU	O4-C4	-3.01	1.17	1.23
48	S2	1004	PSU	O4-C4	-3.01	1.17	1.23
48	S2	1639	G7M	C2-N1	2.99	1.44	1.37
1	L5	1744	PSU	O4-C4	-2.99	1.17	1.23
1	L5	3764	PSU	C2-N1	2.98	1.40	1.36
1	L5	2632	PSU	O4-C4	-2.97	1.17	1.23
48	S2	218	PSU	C2-N1	2.97	1.40	1.36
1	L5	3760	A2M	O3'-C3'	-2.96	1.35	1.43
48	S2	1850	MA6	C5-C4	-2.96	1.33	1.39
48	S2	1842	4AC	C6-N1	2.95	1.45	1.38
1	L5	4636	PSU	O4-C4	-2.95	1.18	1.23
1	L5	2363	A2M	O3'-C3'	-2.94	1.35	1.43
48	S2	34	PSU	C2-N1	2.93	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3637	PSU	C2-N1	2.92	1.40	1.36
48	S2	1136	PSU	C2-N1	2.90	1.40	1.36
1	L5	3770	PSU	O4-C4	-2.90	1.18	1.23
1	L5	4431	PSU	O4-C4	-2.90	1.18	1.23
1	L5	400	A2M	O3'-C3'	-2.87	1.35	1.43
48	S2	815	PSU	C2-N1	2.81	1.40	1.36
1	L5	4569	PSU	C2-N1	2.80	1.40	1.36
48	S2	1678	A2M	O4'-C4'	-2.80	1.38	1.45
1	L5	3884	PSU	O4-C4	-2.79	1.18	1.23
48	S2	166	A2M	O3'-C3'	-2.78	1.36	1.43
48	S2	109	PSU	O4-C4	-2.78	1.18	1.23
1	L5	4220	6MZ	C5-C4	-2.77	1.34	1.39
72	SX	62	HY3	C4-C5	2.76	1.57	1.53
1	L5	3715	PSU	C2-N1	2.75	1.40	1.36
1	L5	4972	PSU	O4-C4	-2.74	1.18	1.23
1	L5	4312	PSU	O4-C4	-2.74	1.18	1.23
1	L5	3867	A2M	O4'-C4'	-2.73	1.38	1.45
1	L5	5010	PSU	C2-N1	2.73	1.40	1.36
1	L5	4532	PSU	O4-C4	-2.72	1.18	1.23
1	L5	1326	A2M	O3'-C3'	-2.71	1.36	1.43
48	S2	1238	PSU	C2-N1	2.71	1.40	1.36
1	L5	4636	PSU	C2-N1	2.70	1.40	1.36
1	L5	3884	PSU	C2-N1	2.70	1.40	1.36
1	L5	2815	A2M	O4'-C4'	-2.70	1.39	1.45
48	S2	1326	UY1	O4-C4	-2.70	1.18	1.23
48	S2	686	PSU	O4-C4	-2.69	1.18	1.23
1	L5	1536	PSU	C2-N1	2.68	1.40	1.36
1	L5	3729	PSU	O4-C4	-2.68	1.18	1.23
1	L5	4590	A2M	O5'-C5'	-2.67	1.36	1.44
1	L5	3853	PSU	O4-C4	-2.67	1.18	1.23
1	L5	4521	PSU	C2-N1	2.67	1.40	1.36
48	S2	1850	MA6	C5-N7	-2.67	1.34	1.39
48	S2	1639	G7M	O6-C6	-2.66	1.18	1.23
1	L5	4420	PSU	C2-N1	2.65	1.40	1.36
1	L5	3723	A2M	O4'-C4'	-2.65	1.39	1.45
48	S2	1004	PSU	C2-N1	2.65	1.40	1.36
48	S2	822	PSU	O4'-C1'	-2.64	1.40	1.43
1	L5	1860	PSU	C2-N1	2.64	1.40	1.36
1	L5	3768	PSU	C2-N1	2.64	1.40	1.36
1	L5	3785	A2M	O4'-C1'	-2.63	1.35	1.42
1	L5	4530	UR3	C6-N1	2.63	1.44	1.38
48	S2	1243	PSU	O4-C4	-2.63	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3760	A2M	O4'-C4'	-2.61	1.39	1.45
1	L5	3867	A2M	O3'-C3'	-2.61	1.36	1.43
3	L8	69	PSU	O4-C4	-2.61	1.18	1.23
1	L5	4571	A2M	O4'-C4'	-2.60	1.39	1.45
48	S2	1445	PSU	C2-N1	2.58	1.40	1.36
48	S2	1031	A2M	O3'-C3'	-2.57	1.36	1.43
1	L5	1677	PSU	C2-N1	2.55	1.40	1.36
48	S2	1625	PSU	C2-N1	2.55	1.40	1.36
1	L5	4227	OMU	C2-N1	2.54	1.42	1.38
48	S2	822	PSU	C2-N1	2.54	1.40	1.36
48	S2	99	A2M	O5'-C5'	-2.54	1.36	1.44
48	S2	1367	PSU	C2-N1	2.53	1.40	1.36
48	S2	681	PSU	C2-N1	2.53	1.40	1.36
1	L5	4579	PSU	O4-C4	-2.53	1.18	1.23
48	S2	1174	PSU	C2-N1	2.52	1.40	1.36
48	S2	1851	MA6	C5-N7	-2.52	1.34	1.39
48	S2	1643	PSU	O4-C4	-2.52	1.18	1.23
48	S2	1326	UY1	O2-C2	-2.52	1.18	1.23
1	L5	2508	PSU	C2-N1	2.50	1.39	1.36
48	S2	576	A2M	O3'-C3'	-2.50	1.36	1.43
1	L5	4521	PSU	O4-C4	-2.50	1.18	1.23
48	S2	866	PSU	C2-N1	2.50	1.39	1.36
48	S2	573	PSU	C2-N1	2.49	1.39	1.36
3	L8	69	PSU	C2-N1	2.49	1.39	1.36
48	S2	1232	PSU	C2-N1	2.49	1.39	1.36
1	L5	3639	PSU	C2-N1	2.48	1.39	1.36
1	L5	4536	OMC	C4-N3	-2.48	1.29	1.34
48	S2	686	PSU	C2-N1	2.47	1.39	1.36
48	S2	814	PSU	C2-N1	2.46	1.39	1.36
48	S2	668	A2M	O3'-C3'	-2.46	1.36	1.43
48	S2	1692	PSU	C2-N1	2.46	1.39	1.36
47	Pt	13	PSU	C2-N1	2.44	1.39	1.36
48	S2	609	PSU	C2-N1	2.44	1.39	1.36
3	L8	55	PSU	C2-N1	2.44	1.39	1.36
48	S2	649	PSU	O4-C4	-2.44	1.18	1.23
1	L5	4442	PSU	O4'-C1'	-2.43	1.40	1.43
1	L5	4353	PSU	C2-N1	2.43	1.39	1.36
48	S2	918	PSU	C2-N1	2.43	1.39	1.36
48	S2	651	PSU	O4-C4	-2.43	1.19	1.23
1	L5	2815	A2M	C5'-C4'	2.43	1.58	1.51
1	L5	4442	PSU	C2-N1	2.42	1.39	1.36
1	L5	1340	OMC	C4-N3	-2.42	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	2843	PSU	C6-N1	2.41	1.40	1.36
48	S2	649	PSU	C2-N1	2.40	1.39	1.36
1	L5	4299	PSU	O4-C4	-2.40	1.19	1.23
48	S2	815	PSU	O4-C4	-2.39	1.19	1.23
1	L5	3637	PSU	C6-N1	2.39	1.40	1.36
1	L5	4423	PSU	O4-C4	-2.38	1.19	1.23
47	Pt	54	2MU	C2'-C1'	2.37	1.59	1.53
48	S2	572	PSU	C2-N1	2.36	1.39	1.36
48	S2	1056	PSU	C2-N1	2.36	1.39	1.36
1	L5	4531	PSU	C2-N1	2.35	1.39	1.36
1	L5	3920	PSU	C2-N1	2.35	1.39	1.36
72	SX	62	HY3	C5-N	2.35	1.57	1.49
48	S2	159	A2M	O3'-C3'	-2.34	1.37	1.43
1	L5	5001	PSU	O4-C4	-2.34	1.19	1.23
1	L5	4420	PSU	O4'-C1'	-2.33	1.40	1.43
1	L5	4293	PSU	C2-N1	2.33	1.39	1.36
48	S2	1842	4AC	O7-C7	-2.33	1.18	1.23
1	L5	4569	PSU	O4-C4	-2.32	1.19	1.23
1	L5	2422	OMC	C4-N3	-2.32	1.30	1.34
1	L5	1792	PSU	C2-N1	2.31	1.39	1.36
1	L5	4353	PSU	O4-C4	-2.31	1.19	1.23
1	L5	2824	OMC	C4-N3	-2.31	1.30	1.34
48	S2	36	PSU	O4-C4	-2.31	1.19	1.23
1	L5	3830	A2M	O3'-C3'	-2.31	1.37	1.43
48	S2	1136	PSU	O4-C4	-2.31	1.19	1.23
47	Pt	10	2MG	C4-N3	2.30	1.39	1.34
1	L5	4500	PSU	O4-C4	-2.29	1.19	1.23
48	S2	1337	4AC	O7-C7	-2.29	1.18	1.23
1	L5	2632	PSU	C2-N1	2.28	1.39	1.36
1	L5	1781	PSU	C2-N1	2.28	1.39	1.36
48	S2	1832	6MZ	C6-N1	-2.27	1.31	1.35
48	S2	517	OMC	C4-N3	-2.27	1.30	1.34
1	L5	3770	PSU	C2-N1	2.27	1.39	1.36
48	S2	1244	PSU	C2-N1	2.26	1.39	1.36
1	L5	3841	OMC	C4-N3	-2.25	1.30	1.34
1	L5	4500	PSU	C2-N1	2.25	1.39	1.36
1	L5	1677	PSU	O4-C4	-2.24	1.19	1.23
48	S2	1445	PSU	O4-C4	-2.24	1.19	1.23
1	L5	3718	A2M	O3'-C3'	-2.23	1.37	1.43
48	S2	1232	PSU	O4-C4	-2.23	1.19	1.23
1	L5	4523	A2M	O3'-C3'	-2.23	1.37	1.43
1	L5	1677	PSU	O4'-C1'	-2.23	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1056	PSU	O4-C4	-2.22	1.19	1.23
1	L5	4296	PSU	O4-C4	-2.22	1.19	1.23
1	L5	2839	PSU	C6-N1	2.22	1.39	1.36
1	L5	1326	A2M	C5-C4	2.22	1.43	1.39
1	L5	1524	A2M	O3'-C3'	-2.22	1.37	1.43
48	S2	966	PSU	C2-N1	2.21	1.39	1.36
1	L5	3818	UY1	O4'-C1'	-2.21	1.40	1.43
48	S2	468	A2M	O4'-C4'	-2.21	1.40	1.45
48	S2	1842	4AC	CM7-C7	2.21	1.55	1.50
1	L5	1534	A2M	O3'-C3'	-2.20	1.37	1.43
1	L5	2815	A2M	O5'-C5'	-2.20	1.37	1.44
48	S2	1081	PSU	C4-N3	2.20	1.43	1.38
48	S2	1239	PSU	O4'-C1'	-2.20	1.40	1.43
48	S2	512	A2M	O3'-C3'	-2.20	1.37	1.43
1	L5	1782	PSU	O4-C4	-2.19	1.19	1.23
48	S2	572	PSU	O4'-C1'	-2.19	1.40	1.43
1	L5	400	A2M	O4'-C4'	-2.19	1.40	1.45
48	S2	1832	6MZ	C8-N9	-2.19	1.33	1.37
1	L5	4493	PSU	C2-N1	2.18	1.39	1.36
1	L5	4431	PSU	C2-N1	2.18	1.39	1.36
1	L5	3695	PSU	O4-C4	-2.18	1.19	1.23
1	L5	3887	OMC	C4-N3	-2.17	1.30	1.34
48	S2	1851	MA6	C8-N9	-2.17	1.33	1.37
1	L5	3853	PSU	C6-N1	2.17	1.39	1.36
1	L5	3762	PSU	C2-N1	2.17	1.39	1.36
1	L5	3758	PSU	C2-N1	2.16	1.39	1.36
48	S2	93	PSU	C2-N1	2.15	1.39	1.36
48	S2	1239	PSU	O4-C4	-2.14	1.19	1.23
1	L5	1744	PSU	C2-N1	2.13	1.39	1.36
48	S2	1643	PSU	O4'-C1'	-2.13	1.40	1.43
1	L5	4220	6MZ	C8-N9	-2.13	1.33	1.37
1	L5	3792	OMG	O6-C6	-2.13	1.19	1.23
1	L5	4471	PSU	C2-N1	2.12	1.39	1.36
1	L5	4420	PSU	C2-N3	2.12	1.41	1.37
48	S2	918	PSU	O4'-C1'	-2.11	1.40	1.43
1	L5	3830	A2M	O4'-C4'	-2.11	1.40	1.45
48	S2	1177	PSU	C2-N1	2.11	1.39	1.36
48	S2	1337	4AC	CM7-C7	2.10	1.54	1.50
1	L5	4689	PSU	C2-N1	2.10	1.39	1.36
1	L5	1316	OMG	O6-C6	-2.10	1.19	1.23
48	S2	1703	OMC	C4-N3	-2.09	1.30	1.34
1	L5	1881	OMC	C4-N3	-2.09	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3841	OMC	O2-C2	-2.09	1.19	1.23
1	L5	1340	OMC	O2-C2	-2.09	1.19	1.23
1	L5	3724	A2M	O4'-C4'	-2.08	1.40	1.45
48	S2	1081	PSU	O4'-C1'	-2.08	1.41	1.43
48	S2	34	PSU	C4-N3	2.08	1.42	1.38
1	L5	1524	A2M	O4'-C4'	-2.08	1.40	1.45
1	L5	4530	UR3	C5-C4	2.08	1.49	1.43
48	S2	1692	PSU	O4-C4	-2.08	1.19	1.23
1	L5	4296	PSU	O4'-C1'	-2.08	1.41	1.43
47	Pt	55	PSU	O4'-C1'	-2.08	1.41	1.43
1	L5	4457	PSU	C6-N1	2.08	1.39	1.36
1	L5	3701	OMC	C4-N3	-2.07	1.30	1.34
1	L5	4361	PSU	C2-N1	2.07	1.39	1.36
48	S2	1842	4AC	C4-N4	2.06	1.43	1.39
1	L5	3925	OMU	O4-C4	-2.06	1.20	1.24
3	L8	14	OMU	O4-C4	-2.06	1.20	1.24
48	S2	1832	6MZ	O2'-C2'	2.06	1.48	1.43
48	S2	1832	6MZ	C4-N9	-2.05	1.33	1.37
48	S2	1391	OMC	C4-N3	-2.05	1.30	1.34
1	L5	1881	OMC	O2-C2	-2.05	1.19	1.23
47	Pt	13	PSU	O4'-C1'	-2.04	1.41	1.43
1	L5	3734	PSU	C2-N1	2.04	1.39	1.36
1	L5	4628	PSU	O4'-C1'	-2.04	1.41	1.43
48	S2	815	PSU	C6-N1	2.03	1.39	1.36
1	L5	4523	A2M	O4'-C4'	-2.03	1.40	1.45
1	L5	4530	UR3	O2-C2	-2.03	1.18	1.22
1	L5	4456	OMC	O2-C2	-2.03	1.19	1.23
1	L5	3785	A2M	O4'-C4'	-2.02	1.40	1.45
1	L5	1779	PSU	C2-N1	2.02	1.39	1.36
48	S2	1081	PSU	C2-N1	2.02	1.39	1.36
48	S2	1383	A2M	O3'-C3'	-2.02	1.38	1.43
48	S2	1832	6MZ	C5-C6	-2.02	1.37	1.41
1	L5	4569	PSU	O4'-C1'	-2.01	1.41	1.43
1	L5	4569	PSU	C4-N3	2.01	1.42	1.38
1	L5	4420	PSU	C6-N1	2.01	1.39	1.36
48	S2	406	PSU	C2-N1	2.01	1.39	1.36

All (765) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1850	MA6	N1-C6-N6	-8.62	106.35	116.86
48	S2	1851	MA6	N1-C6-N6	-8.39	106.64	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1832	6MZ	C9-N6-C6	-7.92	115.51	122.85
1	L5	4531	PSU	C6-C5-C4	6.51	122.57	118.17
48	S2	1639	G7M	C1'-N9-C4	-6.40	107.59	126.49
48	S2	1850	MA6	N1-C2-N3	-6.33	118.99	128.58
1	L5	3818	UY1	C4-N3-C2	-5.96	118.16	126.37
1	L5	4530	UR3	C4-N3-C2	-5.96	119.78	124.58
48	S2	1851	MA6	N1-C2-N3	-5.88	119.69	128.58
1	L5	4220	6MZ	C5-C4-N3	-5.76	118.78	126.72
48	S2	1832	6MZ	N1-C2-N3	-5.73	119.90	128.58
1	L5	3818	UY1	C6-C5-C4	5.53	121.91	118.17
1	L5	3818	UY1	N1-C2-N3	5.46	120.93	115.17
47	Pt	54	2MU	C6-C5-C4	5.46	122.52	118.02
48	S2	1850	MA6	C5-C4-N3	-5.45	119.22	126.72
1	L5	4220	6MZ	N1-C2-N3	-5.30	120.56	128.58
48	S2	1639	G7M	C1'-N9-C8	5.30	144.62	126.74
1	L5	4220	6MZ	C9-N6-C6	5.28	127.74	122.85
48	S2	1851	MA6	C5-C6-N6	5.23	133.61	125.33
48	S2	866	PSU	C6-C5-C4	5.21	121.69	118.17
48	S2	1639	G7M	C5-C4-N3	-5.19	118.35	128.15
48	S2	1850	MA6	C5-C6-N6	5.16	133.50	125.33
1	L5	4220	6MZ	C4-C5-C6	5.16	121.07	116.78
48	S2	1326	UY1	C4-N3-C2	-5.06	119.40	126.37
48	S2	1851	MA6	C5-C4-N3	-5.06	119.75	126.72
1	L5	3851	PSU	C6-C5-C4	5.03	121.57	118.17
48	S2	1326	UY1	N1-C2-N3	5.00	120.44	115.17
1	L5	5001	PSU	C6-C5-C4	4.93	121.50	118.17
48	S2	1832	6MZ	C5-C4-N3	-4.91	119.95	126.72
48	S2	1056	PSU	C6-C5-C4	4.86	121.45	118.17
48	S2	1639	G7M	C2-N3-C4	4.84	120.63	112.30
48	S2	1326	UY1	C6-C5-C4	4.78	121.40	118.17
1	L5	4431	PSU	C6-C5-C4	4.77	121.39	118.17
48	S2	801	PSU	C6-C5-C4	4.76	121.39	118.17
1	L5	3884	PSU	C6-C5-C4	4.75	121.38	118.17
1	L5	3729	PSU	C6-C5-C4	4.68	121.33	118.17
1	L5	4442	PSU	C6-C5-C4	4.65	121.31	118.17
47	Pt	55	PSU	C6-C5-C4	4.60	121.28	118.17
1	L5	4296	PSU	C6-C5-C4	4.60	121.28	118.17
48	S2	572	PSU	C6-C5-C4	4.57	121.26	118.17
48	S2	1851	MA6	N9-C8-N7	-4.56	107.47	113.94
48	S2	1136	PSU	C6-C5-C4	4.55	121.25	118.17
48	S2	1239	PSU	C6-C5-C4	4.48	121.20	118.17
47	Pt	10	2MG	CM2-N2-C2	-4.46	114.06	123.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	109	PSU	C6-C5-C4	4.46	121.18	118.17
48	S2	1238	PSU	C6-C5-C4	4.46	121.18	118.17
48	S2	1367	PSU	C6-C5-C4	4.45	121.18	118.17
48	S2	573	PSU	C6-C5-C4	4.44	121.17	118.17
1	L5	4500	PSU	C6-C5-C4	4.43	121.16	118.17
1	L5	3715	PSU	C6-C5-C4	4.42	121.16	118.17
48	S2	918	PSU	C6-C5-C4	4.40	121.14	118.17
48	S2	1445	PSU	C6-C5-C4	4.34	121.11	118.17
1	L5	3734	PSU	C6-C5-C4	4.33	121.10	118.17
48	S2	1832	6MZ	N9-C8-N7	-4.31	107.82	113.94
1	L5	1860	PSU	C6-C5-C4	4.28	121.06	118.17
48	S2	36	PSU	C6-C5-C4	4.24	121.04	118.17
1	L5	4220	6MZ	N3-C4-N9	4.23	134.36	127.17
1	L5	2839	PSU	C6-C5-C4	4.20	121.01	118.17
48	S2	651	PSU	C6-C5-C4	4.19	121.00	118.17
1	L5	4530	UR3	C6-N1-C2	-4.19	118.38	121.80
47	Pt	13	PSU	C6-C5-C4	4.16	120.98	118.17
48	S2	105	PSU	C6-C5-C4	4.15	120.97	118.17
48	S2	1244	PSU	C6-C5-C4	4.13	120.96	118.17
48	S2	1851	MA6	C4-C5-C6	4.12	120.17	115.91
1	L5	3768	PSU	C6-C5-C4	4.08	120.93	118.17
1	L5	4353	PSU	C6-C5-C4	4.07	120.92	118.17
48	S2	1850	MA6	N9-C8-N7	-4.05	108.19	113.94
1	L5	4673	PSU	C6-C5-C4	4.02	120.89	118.17
48	S2	1639	G7M	N9-C4-N3	4.02	134.00	125.95
1	L5	4579	PSU	C6-C5-C4	4.02	120.89	118.17
48	S2	1383	A2M	C3'-C2'-C1'	-4.02	95.12	102.81
48	S2	1347	PSU	C6-C5-C4	4.01	120.88	118.17
48	S2	1832	6MZ	C5-C6-N1	4.01	122.46	118.15
47	Pt	10	2MG	N1-C2-N2	-4.00	112.47	116.56
1	L5	3920	PSU	C6-C5-C4	4.00	120.88	118.17
1	L5	4220	6MZ	N9-C8-N7	-4.00	108.26	113.94
48	S2	686	PSU	C6-C5-C4	3.97	120.85	118.17
48	S2	1232	PSU	C6-C5-C4	3.97	120.85	118.17
3	L8	69	PSU	C6-C5-C4	3.95	120.84	118.17
48	S2	1639	G7M	C5-C6-N1	3.94	119.99	111.84
48	S2	649	PSU	C6-C5-C4	3.92	120.82	118.17
1	L5	1862	PSU	C6-C5-C4	3.88	120.79	118.17
1	L5	1534	A2M	C3'-C2'-C1'	-3.87	95.39	102.81
47	Pt	20	H2U	C5-C4-N3	-3.87	112.57	116.69
48	S2	1850	MA6	C2-N3-C4	3.86	121.27	111.83
1	L5	4420	PSU	C6-C5-C4	3.85	120.77	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1779	PSU	C6-C5-C4	3.85	120.77	118.17
1	L5	4689	PSU	C6-C5-C4	3.84	120.77	118.17
1	L5	4628	PSU	C6-C5-C4	3.83	120.76	118.17
48	S2	1643	PSU	C6-C5-C4	3.83	120.76	118.17
48	S2	815	PSU	C6-C5-C4	3.82	120.75	118.17
1	L5	4447	5MC	C5-C6-N1	-3.81	119.17	123.31
1	L5	1781	PSU	C6-C5-C4	3.80	120.74	118.17
48	S2	93	PSU	C6-C5-C4	3.80	120.74	118.17
1	L5	3782	5MC	C5-C6-N1	-3.80	119.19	123.31
48	S2	296	PSU	C6-C5-C4	3.80	120.73	118.17
48	S2	966	PSU	C6-C5-C4	3.79	120.73	118.17
48	S2	1177	PSU	C6-C5-C4	3.78	120.72	118.17
48	S2	1851	MA6	C4-N9-C1'	-3.77	117.82	126.63
48	S2	1850	MA6	C4-C5-C6	3.77	119.81	115.91
1	L5	3764	PSU	O4-C4-N3	-3.76	113.03	120.11
1	L5	4423	PSU	C6-C5-C4	3.76	120.71	118.17
1	L5	4403	PSU	C6-C5-C4	3.75	120.70	118.17
1	L5	5010	PSU	C6-C5-C4	3.74	120.70	118.17
48	S2	166	A2M	O3'-C3'-C2'	3.71	121.58	111.19
48	S2	1243	PSU	C6-C5-C4	3.71	120.68	118.17
48	S2	166	A2M	C3'-C2'-C1'	-3.71	95.71	102.81
1	L5	4521	PSU	C6-C5-C4	3.70	120.67	118.17
1	L5	3758	PSU	C6-C5-C4	3.68	120.66	118.17
48	S2	34	PSU	C6-C5-C4	3.67	120.65	118.17
47	Pt	54	2MU	C4-N3-C2	-3.65	122.56	127.34
1	L5	1744	PSU	C6-C5-C4	3.61	120.61	118.17
48	S2	1832	6MZ	C2-N3-C4	3.60	120.62	111.83
48	S2	1850	MA6	C2-N1-C6	3.59	120.60	111.83
1	L5	3760	A2M	C3'-C2'-C1'	-3.58	95.95	102.81
3	L8	55	PSU	C6-C5-C4	3.58	120.59	118.17
1	L5	1536	PSU	O4-C4-N3	-3.58	113.39	120.11
1	L5	3770	PSU	C6-C5-C4	3.58	120.59	118.17
48	S2	1625	PSU	C6-C5-C4	3.57	120.58	118.17
1	L5	1677	PSU	C4-N3-C2	-3.56	121.47	126.37
48	S2	814	PSU	C6-C5-C4	3.55	120.57	118.17
1	L5	4471	PSU	C6-C5-C4	3.55	120.57	118.17
1	L5	4552	PSU	C6-C5-C4	3.53	120.56	118.17
47	Pt	54	2MU	C5-C6-N1	-3.53	119.48	123.31
1	L5	4299	PSU	C6-C5-C4	3.53	120.56	118.17
1	L5	1782	PSU	C6-C5-C4	3.53	120.55	118.17
1	L5	4498	OMU	C4-N3-C2	-3.50	122.26	126.61
48	S2	105	PSU	C4-N3-C2	-3.48	121.57	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1851	MA6	C2-N1-C6	3.48	120.33	111.83
1	L5	4293	PSU	C6-C5-C4	3.48	120.52	118.17
1	L5	3851	PSU	C4-N3-C2	-3.47	121.59	126.37
48	S2	1851	MA6	C2-N3-C4	3.47	120.30	111.83
48	S2	822	PSU	C6-C5-C4	3.46	120.51	118.17
48	S2	218	PSU	C6-C5-C4	3.45	120.50	118.17
1	L5	4361	PSU	C4-N3-C2	-3.45	121.61	126.37
48	S2	1326	UY1	C6-N1-C2	-3.45	119.49	122.69
48	S2	159	A2M	O3'-C3'-C2'	3.44	120.82	111.19
1	L5	2843	PSU	C6-C5-C4	3.44	120.50	118.17
1	L5	1744	PSU	C4-N3-C2	-3.43	121.65	126.37
1	L5	4576	PSU	C6-C5-C4	3.42	120.48	118.17
1	L5	1782	PSU	C4-N3-C2	-3.42	121.66	126.37
1	L5	3818	UY1	O2-C2-N1	-3.41	119.27	122.79
1	L5	3853	PSU	O4-C4-N3	-3.41	113.71	120.11
48	S2	609	PSU	C6-C5-C4	3.40	120.47	118.17
1	L5	4628	PSU	C4-N3-C2	-3.39	121.69	126.37
48	S2	1243	PSU	C4-N3-C2	-3.39	121.70	126.37
1	L5	4471	PSU	C4-N3-C2	-3.39	121.71	126.37
48	S2	1639	G7M	C2-N1-C6	-3.39	118.97	125.11
48	S2	159	A2M	O4'-C1'-C2'	3.38	112.41	106.59
48	S2	863	PSU	C4-N3-C2	-3.37	121.73	126.37
1	L5	4493	PSU	C6-C5-C4	3.36	120.44	118.17
48	S2	801	PSU	C4-N3-C2	-3.36	121.74	126.37
1	L5	1792	PSU	O4-C4-N3	-3.36	113.80	120.11
1	L5	4447	5MC	C1'-N1-C6	3.36	126.68	121.15
1	L5	1536	PSU	C4-N3-C2	-3.35	121.76	126.37
1	L5	4227	OMU	O4-C4-N3	-3.35	114.42	119.27
1	L5	5001	PSU	C4-N3-C2	-3.34	121.77	126.37
1	L5	4569	PSU	C6-C5-C4	3.34	120.43	118.17
1	L5	1677	PSU	O4-C4-N3	-3.33	113.85	120.11
48	S2	1232	PSU	C4-N3-C2	-3.32	121.79	126.37
1	L5	4531	PSU	C4-N3-C2	-3.32	121.80	126.37
1	L5	4220	6MZ	C2-N3-C4	3.32	119.93	111.83
1	L5	3715	PSU	C4-N3-C2	-3.31	121.81	126.37
48	S2	1850	MA6	N3-C4-N9	3.31	132.80	127.17
1	L5	4312	PSU	C4-N3-C2	-3.30	121.82	126.37
1	L5	4972	PSU	C6-C5-C4	3.30	120.40	118.17
1	L5	3770	PSU	C4-N3-C2	-3.29	121.83	126.37
1	L5	2508	PSU	C6-C5-C4	3.29	120.40	118.17
1	L5	1683	PSU	C4-N3-C2	-3.29	121.84	126.37
1	L5	3844	PSU	C6-C5-C4	3.29	120.39	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1136	PSU	C4-N3-C2	-3.29	121.84	126.37
1	L5	2632	PSU	C6-C5-C4	3.28	120.39	118.17
1	L5	4296	PSU	C4-N3-C2	-3.28	121.86	126.37
1	L5	3768	PSU	C4-N3-C2	-3.27	121.86	126.37
48	S2	686	PSU	C4-N3-C2	-3.27	121.86	126.37
48	S2	1850	MA6	C4-N9-C1'	-3.27	118.98	126.63
48	S2	468	A2M	C3'-C2'-C1'	-3.27	96.55	102.81
1	L5	4530	UR3	C5-C4-N3	3.27	119.34	115.04
1	L5	4532	PSU	O4-C4-N3	-3.26	113.99	120.11
48	S2	1625	PSU	C4-N3-C2	-3.26	121.88	126.37
48	S2	1851	MA6	N3-C4-N9	3.24	132.68	127.17
48	S2	1692	PSU	C4-N3-C2	-3.24	121.91	126.37
48	S2	1004	PSU	C6-C5-C4	3.24	120.36	118.17
1	L5	4442	PSU	C4-N3-C2	-3.23	121.92	126.37
1	L5	1683	PSU	O4-C4-N3	-3.23	114.04	120.11
48	S2	1804	OMU	O4-C4-N3	-3.22	114.60	119.27
48	S2	1851	MA6	C5-N7-C8	3.22	108.51	103.45
1	L5	4293	PSU	C4-N3-C2	-3.22	121.94	126.37
1	L5	2843	PSU	O4-C4-N3	-3.22	114.06	120.11
48	S2	109	PSU	C4-N3-C2	-3.22	121.94	126.37
48	S2	1081	PSU	C4-N3-C2	-3.21	121.94	126.37
1	L5	4579	PSU	C4-N3-C2	-3.21	121.95	126.37
1	L5	4431	PSU	C4-N3-C2	-3.21	121.95	126.37
1	L5	3695	PSU	C6-C5-C4	3.20	120.33	118.17
48	S2	609	PSU	C4-N3-C2	-3.20	121.96	126.37
48	S2	572	PSU	C4-N3-C2	-3.20	121.96	126.37
1	L5	4500	PSU	C4-N3-C2	-3.20	121.96	126.37
48	S2	159	A2M	C4-N9-C1'	-3.20	119.15	126.63
1	L5	3764	PSU	C4-N3-C2	-3.19	121.97	126.37
1	L5	1860	PSU	C4-N3-C2	-3.19	121.98	126.37
1	L5	4293	PSU	O4-C4-N3	-3.19	114.12	120.11
1	L5	1779	PSU	C4-N3-C2	-3.18	121.99	126.37
48	S2	406	PSU	C6-C5-C4	3.18	120.32	118.17
48	S2	34	PSU	C4-N3-C2	-3.17	122.00	126.37
1	L5	4620	OMU	O4-C4-N3	-3.17	114.68	119.27
1	L5	3729	PSU	C4-N3-C2	-3.17	122.01	126.37
48	S2	1056	PSU	C4-N3-C2	-3.17	122.01	126.37
48	S2	1239	PSU	C4-N3-C2	-3.16	122.01	126.37
1	L5	1582	PSU	O4-C4-N3	-3.16	114.18	120.11
48	S2	1174	PSU	C4-N3-C2	-3.16	122.02	126.37
1	L5	3639	PSU	C6-C5-C4	3.15	120.30	118.17
1	L5	3851	PSU	N1-C2-N3	3.15	118.49	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	406	PSU	O4-C4-N3	-3.15	114.19	120.11
48	S2	1692	PSU	O4-C4-N3	-3.14	114.21	120.11
1	L5	2632	PSU	O4-C4-N3	-3.14	114.21	120.11
1	L5	4403	PSU	O4-C4-N3	-3.14	114.22	120.11
48	S2	119	PSU	C4-N3-C2	-3.14	122.05	126.37
1	L5	4353	PSU	C4-N3-C2	-3.13	122.05	126.37
48	S2	1445	PSU	C4-N3-C2	-3.13	122.06	126.37
1	L5	4972	PSU	C4-N3-C2	-3.13	122.06	126.37
48	S2	815	PSU	O4-C4-N3	-3.13	114.24	120.11
1	L5	4442	PSU	N1-C2-N3	3.12	118.46	115.17
1	L5	3718	A2M	C3'-C2'-C1'	-3.12	96.83	102.81
1	L5	4579	PSU	N1-C2-N3	3.12	118.46	115.17
47	Pt	13	PSU	C4-N3-C2	-3.11	122.08	126.37
1	L5	3920	PSU	C4-N3-C2	-3.11	122.08	126.37
48	S2	1832	6MZ	N3-C4-N9	3.11	132.45	127.17
47	Pt	49	5MC	C5-C6-N1	-3.10	119.95	123.31
48	S2	105	PSU	O4-C4-N3	-3.10	114.29	120.11
1	L5	4403	PSU	C4-N3-C2	-3.09	122.11	126.37
48	S2	918	PSU	C4-N3-C2	-3.09	122.11	126.37
48	S2	218	PSU	O4-C4-N3	-3.09	114.31	120.11
1	L5	4312	PSU	C6-C5-C4	3.09	120.26	118.17
48	S2	1383	A2M	O3'-C3'-C2'	3.08	119.82	111.19
47	Pt	54	2MU	C2'-C1'-N1	-3.08	108.39	114.24
1	L5	4521	PSU	O4-C4-N3	-3.08	114.32	120.11
1	L5	4576	PSU	O4-C4-N3	-3.08	114.32	120.11
1	L5	2632	PSU	C4-N3-C2	-3.08	122.12	126.37
1	L5	4571	A2M	C3'-C2'-C1'	-3.08	96.91	102.81
1	L5	2508	PSU	O4-C4-N3	-3.08	114.33	120.11
1	L5	4523	A2M	C2'-C1'-N9	-3.07	108.69	113.75
1	L5	4500	PSU	N1-C2-N3	3.07	118.41	115.17
48	S2	1850	MA6	C5-N7-C8	3.07	108.28	103.45
1	L5	3844	PSU	C4-N3-C2	-3.07	122.14	126.37
48	S2	651	PSU	C4-N3-C2	-3.07	122.15	126.37
1	L5	3853	PSU	C4-N3-C2	-3.06	122.15	126.37
48	S2	681	PSU	C4-N3-C2	-3.06	122.15	126.37
48	S2	1244	PSU	C4-N3-C2	-3.06	122.15	126.37
1	L5	1792	PSU	C6-C5-C4	3.06	120.24	118.17
48	S2	296	PSU	C4-N3-C2	-3.06	122.16	126.37
1	L5	3925	OMU	C4-N3-C2	-3.06	122.82	126.61
48	S2	681	PSU	C6-C5-C4	3.06	120.24	118.17
1	L5	4353	PSU	O4-C4-N3	-3.06	114.36	120.11
48	S2	814	PSU	C4-N3-C2	-3.05	122.17	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4636	PSU	O4-C4-N3	-3.05	114.38	120.11
48	S2	119	PSU	C6-C5-C4	3.05	120.23	118.17
48	S2	1238	PSU	C4-N3-C2	-3.05	122.17	126.37
1	L5	4493	PSU	C4-N3-C2	-3.04	122.18	126.37
1	L5	2363	A2M	C3'-C2'-C1'	-3.04	96.99	102.81
1	L5	3830	A2M	C3'-C2'-C1'	-3.04	96.99	102.81
48	S2	573	PSU	C4-N3-C2	-3.04	122.19	126.37
48	S2	1639	G7M	O6-C6-C5	-3.03	121.25	128.01
3	L8	55	PSU	O4-C4-N3	-3.03	114.42	120.11
1	L5	4457	PSU	C4-N3-C2	-3.03	122.20	126.37
48	S2	1678	A2M	C2'-C1'-N9	3.03	118.73	113.75
1	L5	4972	PSU	O4-C4-N3	-3.02	114.44	120.11
1	L5	4493	PSU	O4-C4-N3	-3.01	114.44	120.11
1	L5	1792	PSU	C4-N3-C2	-3.01	122.22	126.37
48	S2	815	PSU	C4-N3-C2	-3.01	122.22	126.37
1	L5	1862	PSU	N1-C2-N3	3.01	118.34	115.17
1	L5	1524	A2M	O4'-C1'-C2'	3.00	111.75	106.59
48	S2	1174	PSU	C6-C5-C4	3.00	120.20	118.17
48	S2	119	PSU	O4-C4-N3	-3.00	114.48	120.11
48	S2	93	PSU	C4-N3-C2	-3.00	122.24	126.37
1	L5	4628	PSU	N1-C2-N3	3.00	118.33	115.17
48	S2	116	OMU	C4-N3-C2	-2.98	122.91	126.61
48	S2	1243	PSU	O4-C4-N3	-2.98	114.51	120.11
1	L5	1862	PSU	C4-N3-C2	-2.98	122.27	126.37
1	L5	4628	PSU	O4-C4-N3	-2.98	114.52	120.11
1	L5	4361	PSU	N1-C2-N3	2.97	118.30	115.17
1	L5	1677	PSU	C6-C5-C4	2.97	120.18	118.17
48	S2	1288	OMU	C4-N3-C2	-2.97	122.92	126.61
3	L8	14	OMU	O4-C4-N3	-2.97	114.97	119.27
1	L5	4552	PSU	C4-N3-C2	-2.97	122.28	126.37
3	L8	55	PSU	C4-N3-C2	-2.96	122.29	126.37
1	L5	4423	PSU	C4-N3-C2	-2.96	122.29	126.37
48	S2	1326	UY1	O2-C2-N1	-2.96	119.73	122.79
1	L5	3734	PSU	C4-N3-C2	-2.96	122.29	126.37
48	S2	866	PSU	C4-N3-C2	-2.96	122.29	126.37
1	L5	4471	PSU	O4-C4-N3	-2.96	114.54	120.11
48	S2	814	PSU	O4-C4-N3	-2.96	114.54	120.11
48	S2	1177	PSU	C4-N3-C2	-2.96	122.29	126.37
1	L5	3770	PSU	O4-C4-N3	-2.96	114.55	120.11
48	S2	159	A2M	C3'-C2'-C1'	-2.95	97.16	102.81
1	L5	2787	A2M	O3'-C3'-C2'	2.95	119.44	111.19
1	L5	1862	PSU	O4-C4-N3	-2.95	114.58	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3724	A2M	C4-N9-C1'	-2.94	119.76	126.63
3	L8	69	PSU	C4-N3-C2	-2.94	122.32	126.37
1	L5	3723	A2M	C3'-C2'-C1'	-2.94	97.18	102.81
48	S2	863	PSU	O4-C4-N3	-2.94	114.59	120.11
1	L5	3724	A2M	C3'-C2'-C1'	-2.93	97.19	102.81
1	L5	5010	PSU	O4-C4-N3	-2.92	114.62	120.11
1	L5	3920	PSU	N1-C2-N3	2.92	118.25	115.17
47	Pt	55	PSU	C4-N3-C2	-2.92	122.35	126.37
1	L5	4521	PSU	N1-C2-N3	2.92	118.24	115.17
48	S2	1347	PSU	O4-C4-N3	-2.92	114.63	120.11
48	S2	1347	PSU	C4-N3-C2	-2.91	122.36	126.37
1	L5	4361	PSU	O4-C4-N3	-2.91	114.64	120.11
1	L5	4220	6MZ	C5-N7-C8	2.91	108.03	103.45
48	S2	1367	PSU	C4-N3-C2	-2.91	122.36	126.37
1	L5	3724	A2M	C1'-N9-C8	2.91	133.55	127.09
48	S2	1850	MA6	C1'-N9-C8	2.91	133.55	127.09
1	L5	4579	PSU	O4-C4-N3	-2.91	114.65	120.11
1	L5	2363	A2M	C4-N9-C1'	-2.90	119.85	126.63
1	L5	1744	PSU	N1-C2-N3	2.90	118.23	115.17
1	L5	3782	5MC	CM5-C5-C6	-2.90	118.93	122.85
1	L5	3637	PSU	O4-C4-N3	-2.90	114.66	120.11
48	S2	93	PSU	O4-C4-N3	-2.90	114.67	120.11
48	S2	1851	MA6	C1'-N9-C8	2.89	133.52	127.09
1	L5	3818	UY1	C6-N1-C2	-2.89	120.00	122.69
1	L5	4532	PSU	C4-N3-C2	-2.89	122.39	126.37
48	S2	1337	4AC	C6-C5-C4	2.89	120.48	117.00
48	S2	627	OMU	CM2-O2'-C2'	-2.88	107.07	114.47
1	L5	1781	PSU	C4-N3-C2	-2.88	122.40	126.37
1	L5	4306	OMU	C4-N3-C2	-2.87	123.05	126.61
48	S2	27	A2M	C4-N9-C1'	-2.87	119.92	126.63
1	L5	398	A2M	C3'-C2'-C1'	-2.87	97.32	102.81
1	L5	5010	PSU	C4-N3-C2	-2.86	122.42	126.37
1	L5	3758	PSU	C4-N3-C2	-2.86	122.43	126.37
48	S2	590	A2M	O3'-C3'-C2'	2.86	119.19	111.19
48	S2	649	PSU	C4-N3-C2	-2.85	122.44	126.37
48	S2	1643	PSU	C4-N3-C2	-2.84	122.45	126.37
48	S2	159	A2M	C1'-N9-C8	2.84	133.41	127.09
1	L5	3762	PSU	C4-N3-C2	-2.84	122.45	126.37
1	L5	3830	A2M	O3'-C3'-C2'	2.84	119.14	111.19
48	S2	1248	B8N	C4-N3-C2	-2.84	122.12	125.62
3	L8	69	PSU	O4-C4-N3	-2.84	114.77	120.11
1	L5	1536	PSU	C6-C5-C4	2.83	120.08	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3729	PSU	O4-C4-N3	-2.83	114.79	120.11
48	S2	1004	PSU	O4-C4-N3	-2.83	114.79	120.11
1	L5	3785	A2M	O4'-C1'-N9	2.83	113.52	108.09
1	L5	3695	PSU	C4-N3-C2	-2.82	122.48	126.37
48	S2	651	PSU	O4-C4-N3	-2.82	114.82	120.11
1	L5	4620	OMU	O4-C4-C5	2.82	130.02	125.16
48	S2	649	PSU	O4-C4-N3	-2.81	114.82	120.11
48	S2	1625	PSU	O4-C4-N3	-2.81	114.83	120.11
1	L5	2508	PSU	C4-N3-C2	-2.81	122.50	126.37
1	L5	4420	PSU	C4-N3-C2	-2.81	122.50	126.37
1	L5	1536	PSU	N1-C2-N3	2.80	118.12	115.17
48	S2	109	PSU	N1-C2-N3	2.80	118.12	115.17
1	L5	4306	OMU	O4-C4-N3	-2.80	115.22	119.27
48	S2	27	A2M	C1'-N9-C8	2.79	133.28	127.09
1	L5	4571	A2M	C2'-C1'-N9	2.79	118.34	113.75
1	L5	4521	PSU	C4-N3-C2	-2.78	122.54	126.37
1	L5	3768	PSU	O4-C4-N3	-2.78	114.88	120.11
1	L5	4500	PSU	O4-C4-N3	-2.78	114.88	120.11
1	L5	400	A2M	C3'-C2'-C1'	-2.78	97.49	102.81
48	S2	1639	G7M	CN7-N7-C5	2.77	130.26	126.80
1	L5	4471	PSU	N1-C2-N3	2.77	118.09	115.17
1	L5	4220	6MZ	C1'-N9-C8	-2.77	120.95	127.09
3	L8	14	OMU	C4-N3-C2	-2.77	123.18	126.61
48	S2	468	A2M	O3'-C3'-C2'	2.77	118.93	111.19
48	S2	918	PSU	O4-C4-N3	-2.77	114.91	120.11
48	S2	1004	PSU	C4-N3-C2	-2.76	122.56	126.37
48	S2	590	A2M	C2'-C1'-N9	2.76	118.30	113.75
1	L5	4442	PSU	O4-C4-N3	-2.76	114.92	120.11
1	L5	3760	A2M	C4-N9-C1'	-2.76	120.18	126.63
48	S2	1442	OMU	C4-N3-C2	-2.76	123.19	126.61
1	L5	3715	PSU	O4-C4-N3	-2.75	114.95	120.11
48	S2	1832	6MZ	C5-N7-C8	2.74	107.76	103.45
48	S2	1081	PSU	C6-C5-C4	2.74	120.02	118.17
48	S2	1367	PSU	O4-C4-N3	-2.73	114.98	120.11
1	L5	4531	PSU	N1-C2-N3	2.73	118.05	115.17
48	S2	609	PSU	O4-C4-N3	-2.73	114.99	120.11
48	S2	627	OMU	C4-N3-C2	-2.73	123.23	126.61
48	S2	1174	PSU	O4-C4-N3	-2.72	114.99	120.11
1	L5	4361	PSU	C6-C5-C4	2.72	120.01	118.17
48	S2	651	PSU	N1-C2-N3	2.72	118.04	115.17
48	S2	296	PSU	O4-C4-N3	-2.72	115.01	120.11
1	L5	4423	PSU	O4-C4-N3	-2.72	115.01	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4353	PSU	N1-C2-N3	2.72	118.03	115.17
1	L5	3723	A2M	C4-N9-C1'	-2.71	120.29	126.63
1	L5	3723	A2M	C2'-C1'-N9	2.71	118.21	113.75
1	L5	1582	PSU	C6-C5-C4	2.71	120.00	118.17
48	S2	863	PSU	C6-C5-C4	2.70	120.00	118.17
48	S2	627	OMU	O4-C4-N3	-2.70	115.35	119.27
1	L5	1860	PSU	O4-C4-N3	-2.70	115.03	120.11
1	L5	398	A2M	O3'-C3'-C2'	2.70	118.75	111.19
1	L5	3785	A2M	C3'-C2'-C1'	-2.70	97.64	102.81
48	S2	966	PSU	C4-N3-C2	-2.70	122.66	126.37
47	Pt	54	2MU	O4-C4-C5	2.69	128.00	124.92
1	L5	4447	5MC	C1'-N1-C2	-2.69	112.50	118.44
1	L5	5001	PSU	N1-C2-N3	2.68	118.00	115.17
1	L5	4636	PSU	C6-C5-C4	2.68	119.98	118.17
48	S2	1851	MA6	C4-N9-C8	2.67	108.54	105.74
48	S2	822	PSU	C4-N3-C2	-2.67	122.69	126.37
48	S2	218	PSU	C4-N3-C2	-2.67	122.69	126.37
1	L5	2837	OMU	O4-C4-N3	-2.66	115.41	119.27
1	L5	3770	PSU	N1-C2-N3	2.66	117.97	115.17
1	L5	3639	PSU	C4-N3-C2	-2.66	122.70	126.37
1	L5	1782	PSU	O4-C4-N3	-2.66	115.11	120.11
1	L5	3844	PSU	O4-C4-N3	-2.66	115.11	120.11
1	L5	3762	PSU	O4-C4-N3	-2.66	115.12	120.11
48	S2	172	OMU	C4-N3-C2	-2.65	123.32	126.61
1	L5	2415	OMU	O4-C4-N3	-2.65	115.43	119.27
1	L5	4220	6MZ	C3'-C2'-C1'	2.65	106.48	101.46
48	S2	649	PSU	N1-C2-N3	2.65	117.96	115.17
48	S2	512	A2M	C4-N9-C1'	-2.65	120.43	126.63
48	S2	1643	PSU	O4-C4-N3	-2.65	115.13	120.11
1	L5	4576	PSU	C4-N3-C2	-2.65	122.72	126.37
48	S2	1832	6MZ	C5'-C4'-C3'	-2.65	105.68	115.21
48	S2	1136	PSU	N1-C2-N3	2.65	117.96	115.17
1	L5	1522	OMG	C2'-C1'-N9	-2.65	109.22	114.24
1	L5	4569	PSU	C4-N3-C2	-2.64	122.73	126.37
1	L5	2415	OMU	C4-N3-C2	-2.64	123.33	126.61
48	S2	1804	OMU	N3-C2-N1	2.64	118.33	114.89
1	L5	3844	PSU	N1-C2-N3	2.64	117.95	115.17
1	L5	1860	PSU	N1-C2-N3	2.64	117.95	115.17
48	S2	512	A2M	C3'-C2'-C1'	-2.64	97.75	102.81
1	L5	3768	PSU	N1-C2-N3	2.64	117.95	115.17
1	L5	2815	A2M	C5'-C4'-C3'	2.64	124.71	115.21
48	S2	121	OMU	C4-N3-C2	-2.63	123.34	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1081	PSU	O4-C4-N3	-2.63	115.17	120.11
1	L5	4673	PSU	O4-C4-N3	-2.63	115.18	120.11
48	S2	590	A2M	C3'-C2'-C1'	-2.62	97.78	102.81
1	L5	1779	PSU	O4-C4-N3	-2.62	115.18	120.11
48	S2	172	OMU	O4-C4-N3	-2.62	115.47	119.27
1	L5	2632	PSU	N1-C2-N3	2.62	117.93	115.17
1	L5	4673	PSU	C4-N3-C2	-2.62	122.77	126.37
48	S2	1239	PSU	O4-C4-N3	-2.61	115.20	120.11
1	L5	4498	OMU	O4-C4-N3	-2.61	115.49	119.27
48	S2	686	PSU	O4-C4-N3	-2.61	115.21	120.11
1	L5	1322	1MA	N1-C6-N6	2.61	126.26	119.71
48	S2	966	PSU	O4-C4-N3	-2.60	115.22	120.11
48	S2	27	A2M	C3'-C2'-C1'	-2.60	97.83	102.81
48	S2	512	A2M	C1'-N9-C8	2.60	132.87	127.09
1	L5	4312	PSU	O4-C4-N3	-2.60	115.23	120.11
48	S2	576	A2M	C4-N9-C1'	-2.59	120.57	126.63
1	L5	4532	PSU	C6-C5-C4	2.59	119.92	118.17
48	S2	681	PSU	O4-C4-N3	-2.59	115.25	120.11
48	S2	105	PSU	N1-C2-N3	2.58	117.89	115.17
48	S2	109	PSU	O4-C4-N3	-2.58	115.26	120.11
48	S2	428	OMU	O4-C4-N3	-2.58	115.54	119.27
1	L5	1782	PSU	N1-C2-N3	2.58	117.88	115.17
1	L5	1781	PSU	O4-C4-N3	-2.58	115.27	120.11
48	S2	34	PSU	O4-C4-N3	-2.58	115.27	120.11
1	L5	2363	A2M	C6-C5-C4	-2.57	113.66	117.18
48	S2	36	PSU	C4-N3-C2	-2.57	122.83	126.37
1	L5	3920	PSU	O4-C4-N3	-2.57	115.28	120.11
48	S2	1692	PSU	N1-C2-N3	2.57	117.88	115.17
1	L5	2843	PSU	C4-N3-C2	-2.57	122.83	126.37
48	S2	1244	PSU	O4-C4-N3	-2.56	115.30	120.11
1	L5	4306	OMU	N3-C2-N1	2.56	118.22	114.89
1	L5	3825	A2M	C3'-C2'-C1'	-2.56	97.91	102.81
1	L5	4312	PSU	O2-C2-N1	-2.55	120.16	122.79
1	L5	3785	A2M	O4'-C4'-C3'	2.55	110.21	105.15
48	S2	1678	A2M	C4-N9-C1'	-2.54	120.68	126.63
48	S2	34	PSU	N1-C2-N3	2.54	117.85	115.17
48	S2	484	A2M	C1'-N9-C8	2.54	132.73	127.09
48	S2	590	A2M	O4'-C1'-C2'	2.54	110.95	106.59
48	S2	1678	A2M	C3'-C2'-C1'	-2.53	97.96	102.81
1	L5	3758	PSU	O4-C4-N3	-2.53	115.36	120.11
1	L5	3723	A2M	O4'-C1'-C2'	2.53	110.94	106.59
48	S2	1136	PSU	O4-C4-N3	-2.52	115.37	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1871	A2M	C3'-C2'-C1'	-2.52	97.98	102.81
48	S2	354	OMU	C4-N3-C2	-2.52	123.48	126.61
1	L5	2363	A2M	C1'-N9-C8	2.52	132.68	127.09
48	S2	918	PSU	N1-C2-N3	2.52	117.82	115.17
48	S2	1804	OMU	C4-N3-C2	-2.52	123.49	126.61
1	L5	2815	A2M	O4'-C4'-C3'	2.51	110.14	105.15
48	S2	1056	PSU	N1-C2-N3	2.51	117.82	115.17
48	S2	1692	PSU	C6-C5-C4	2.51	119.87	118.17
1	L5	3760	A2M	O3'-C3'-C2'	2.51	118.22	111.19
1	L5	3851	PSU	O4-C4-N3	-2.51	115.39	120.11
48	S2	815	PSU	N1-C2-N3	2.51	117.82	115.17
1	L5	5001	PSU	O4-C4-N3	-2.51	115.39	120.11
1	L5	4431	PSU	N1-C2-N3	2.51	117.81	115.17
48	S2	166	A2M	C4-N9-C1'	-2.51	120.77	126.63
1	L5	1744	PSU	O4-C4-N3	-2.51	115.40	120.11
48	S2	1445	PSU	O4-C4-N3	-2.51	115.40	120.11
1	L5	3785	A2M	C4'-O4'-C1'	-2.51	103.94	109.47
48	S2	573	PSU	O4-C4-N3	-2.50	115.40	120.11
48	S2	801	PSU	O4-C4-N3	-2.50	115.40	120.11
48	S2	1031	A2M	C3'-C2'-C1'	-2.50	98.01	102.81
48	S2	1804	OMU	O4-C4-C5	2.50	129.48	125.16
48	S2	576	A2M	C3'-C2'-C1'	-2.50	98.02	102.81
1	L5	4590	A2M	C1'-N9-C8	2.50	132.64	127.09
48	S2	572	PSU	O4-C4-N3	-2.50	115.42	120.11
1	L5	4312	PSU	N1-C2-N3	2.49	117.80	115.17
48	S2	1442	OMU	O4-C4-N3	-2.49	115.66	119.27
1	L5	3899	OMG	C2'-C1'-N9	-2.49	109.51	114.24
1	L5	4420	PSU	O4-C4-N3	-2.49	115.43	120.11
48	S2	866	PSU	N1-C2-N3	2.49	117.79	115.17
48	S2	1288	OMU	O4-C4-N3	-2.49	115.67	119.27
3	L8	14	OMU	C6-C5-C4	2.48	122.70	119.53
1	L5	2837	OMU	O4-C4-C5	2.48	129.44	125.16
48	S2	918	PSU	O4'-C1'-C2'	2.47	108.57	105.15
48	S2	822	PSU	O4-C4-N3	-2.47	115.47	120.11
48	S2	1177	PSU	O4-C4-N3	-2.47	115.47	120.11
48	S2	172	OMU	C6-C5-C4	2.47	122.69	119.53
1	L5	1326	A2M	C3'-C2'-C1'	-2.47	98.08	102.81
48	S2	296	PSU	N1-C2-N3	2.46	117.76	115.17
48	S2	428	OMU	C4-N3-C2	-2.46	123.56	126.61
1	L5	3853	PSU	N1-C2-N3	2.46	117.76	115.17
1	L5	4689	PSU	C4-N3-C2	-2.46	122.99	126.37
3	L8	14	OMU	N3-C2-N1	2.45	118.09	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1871	A2M	C2'-C1'-N9	-2.45	109.72	113.75
1	L5	3627	OMG	C2'-C1'-N9	-2.45	109.59	114.24
1	L5	2787	A2M	C3'-C2'-C1'	-2.45	98.12	102.81
48	S2	1367	PSU	N1-C2-N3	2.44	117.75	115.17
1	L5	4296	PSU	O4-C4-N3	-2.44	115.52	120.11
1	L5	1536	PSU	C5-C6-N1	-2.44	118.75	122.14
48	S2	1232	PSU	O4-C4-N3	-2.44	115.53	120.11
48	S2	1238	PSU	O4-C4-N3	-2.44	115.53	120.11
48	S2	1625	PSU	N1-C2-N3	2.44	117.73	115.17
48	S2	1842	4AC	O2-C2-N3	-2.43	118.50	122.33
1	L5	3723	A2M	C1'-N9-C8	2.43	132.49	127.09
48	S2	1347	PSU	N1-C2-N3	2.43	117.73	115.17
1	L5	2815	A2M	C4-N9-C1'	-2.42	120.97	126.63
48	S2	1243	PSU	N1-C2-N3	2.42	117.72	115.17
48	S2	1232	PSU	N1-C2-N3	2.42	117.72	115.17
48	S2	406	PSU	C4-N3-C2	-2.42	123.04	126.37
48	S2	406	PSU	N1-C2-N3	2.42	117.72	115.17
1	L5	4457	PSU	O4-C4-N3	-2.42	115.57	120.11
1	L5	3637	PSU	C6-C5-C4	2.42	119.81	118.17
48	S2	172	OMU	CM2-O2'-C2'	-2.41	108.28	114.47
1	L5	4571	A2M	O4'-C1'-C2'	2.41	110.74	106.59
1	L5	3734	PSU	O4-C4-N3	-2.41	115.59	120.11
48	S2	866	PSU	O4-C4-N3	-2.41	115.59	120.11
48	S2	166	A2M	C1'-N9-C8	2.40	132.43	127.09
1	L5	4299	PSU	O4-C4-N3	-2.40	115.60	120.11
3	L8	55	PSU	N1-C2-N3	2.40	117.70	115.17
48	S2	668	A2M	C4-N9-C1'	-2.40	121.02	126.63
1	L5	2815	A2M	C1'-N9-C8	2.40	132.42	127.09
1	L5	5010	PSU	N1-C2-N3	2.39	117.69	115.17
72	SX	62	HY3	O-C-CA	-2.39	118.53	124.86
1	L5	4403	PSU	N1-C2-N3	2.39	117.69	115.17
47	Pt	55	PSU	O4-C4-N3	-2.39	115.62	120.11
1	L5	1677	PSU	N1-C2-N3	2.39	117.69	115.17
1	L5	3884	PSU	O4-C4-N3	-2.39	115.62	120.11
1	L5	1582	PSU	C4-N3-C2	-2.39	123.08	126.37
48	S2	354	OMU	O4-C4-N3	-2.39	115.82	119.27
48	S2	484	A2M	C4-N9-C1'	-2.38	121.06	126.63
1	L5	2363	A2M	O4'-C1'-C2'	2.38	110.68	106.59
48	S2	1383	A2M	C1'-N9-C8	2.38	132.37	127.09
1	L5	3925	OMU	C6-C5-C4	2.38	122.57	119.53
48	S2	668	A2M	C6-C5-C4	-2.38	113.93	117.18
48	S2	863	PSU	N1-C2-N3	2.37	117.67	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2415	OMU	C6-C5-C4	2.37	122.56	119.53
1	L5	4227	OMU	C4-N3-C2	-2.37	123.67	126.61
48	S2	1678	A2M	C6-C5-C4	-2.37	113.94	117.18
1	L5	4442	PSU	O4'-C1'-C2'	2.36	108.42	105.15
1	L5	2839	PSU	O4-C4-N3	-2.36	115.68	120.11
1	L5	1326	A2M	C1'-N9-C8	2.36	132.33	127.09
1	L5	3715	PSU	N1-C2-N3	2.36	117.65	115.17
1	L5	4590	A2M	C4-N9-C1'	-2.36	121.12	126.63
48	S2	119	PSU	N1-C2-N3	2.35	117.65	115.17
48	S2	218	PSU	N1-C2-N3	2.35	117.64	115.17
48	S2	1442	OMU	CM2-O2'-C2'	-2.35	108.45	114.47
47	Pt	10	2MG	N1-C2-N3	2.34	127.62	123.68
1	L5	4431	PSU	O4-C4-N3	-2.34	115.71	120.11
1	L5	3724	A2M	O3'-C3'-C2'	2.34	117.74	111.19
1	L5	4689	PSU	O4-C4-N3	-2.34	115.71	120.11
48	S2	573	PSU	N1-C2-N3	2.34	117.64	115.17
1	L5	4296	PSU	N1-C2-N3	2.34	117.63	115.17
1	L5	3785	A2M	C2'-C1'-N9	-2.34	109.91	113.75
1	L5	1779	PSU	N1-C2-N3	2.34	117.63	115.17
48	S2	1851	MA6	C4-C5-N7	-2.34	107.91	110.58
1	L5	3884	PSU	N1-C2-N3	2.34	117.63	115.17
1	L5	3695	PSU	N1-C2-N3	2.33	117.63	115.17
48	S2	1244	PSU	N1-C2-N3	2.33	117.63	115.17
1	L5	3853	PSU	C6-C5-C4	2.33	119.75	118.17
1	L5	3785	A2M	C2-N1-C6	-2.33	114.90	118.73
48	S2	468	A2M	C4-N9-C1'	-2.33	121.19	126.63
48	S2	1288	OMU	C6-C5-C4	2.33	122.51	119.53
1	L5	2401	A2M	O3'-C3'-C2'	2.33	117.70	111.19
1	L5	1871	A2M	C4-N9-C1'	-2.32	121.20	126.63
48	S2	1239	PSU	N1-C2-N3	2.32	117.62	115.17
3	L8	69	PSU	N1-C2-N3	2.32	117.62	115.17
1	L5	3760	A2M	C1'-N9-C8	2.32	132.25	127.09
1	L5	4552	PSU	O4-C4-N3	-2.32	115.75	120.11
1	L5	4493	PSU	N1-C2-N3	2.32	117.61	115.17
1	L5	3760	A2M	C5'-C4'-C3'	-2.32	106.86	115.21
48	S2	1177	PSU	N1-C2-N3	2.32	117.61	115.17
48	S2	354	OMU	C6-C5-C4	2.32	122.49	119.53
48	S2	576	A2M	C1'-N9-C8	2.31	132.22	127.09
48	S2	1248	B8N	C31-N3-C4	2.31	120.44	117.18
48	S2	1678	A2M	O4'-C1'-C2'	2.31	110.56	106.59
1	L5	4299	PSU	C4-N3-C2	-2.30	123.20	126.37
1	L5	4569	PSU	O4-C4-N3	-2.30	115.79	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3762	PSU	C6-C5-C4	2.30	119.72	118.17
1	L5	2508	PSU	N1-C2-N3	2.30	117.59	115.17
1	L5	1781	PSU	N1-C2-N3	2.30	117.59	115.17
1	L5	4423	PSU	N1-C2-N3	2.30	117.59	115.17
48	S2	576	A2M	O3'-C3'-C2'	2.29	117.60	111.19
1	L5	4196	OMG	CM2-O2'-C2'	2.29	120.36	114.47
47	Pt	54	2MU	O2'-C2'-C1'	2.29	113.33	108.99
47	Pt	13	PSU	N1-C2-N3	2.29	117.58	115.17
1	L5	3729	PSU	N1-C2-N3	2.28	117.57	115.17
48	S2	1238	PSU	N1-C2-N3	2.28	117.57	115.17
1	L5	4972	PSU	N1-C2-N3	2.28	117.57	115.17
1	L5	2837	OMU	N3-C2-N1	2.28	117.86	114.89
1	L5	3760	A2M	O3'-C3'-C4'	-2.28	104.54	111.08
47	Pt	54	2MU	O4-C4-N3	-2.27	115.84	120.11
1	L5	3925	OMU	O4-C4-N3	-2.27	115.98	119.27
1	L5	2415	OMU	N3-C2-N1	2.27	117.85	114.89
47	Pt	13	PSU	O4-C4-N3	-2.27	115.85	120.11
1	L5	3825	A2M	O4'-C1'-C2'	2.27	110.49	106.59
48	S2	468	A2M	O4'-C1'-C2'	2.27	110.49	106.59
1	L5	3884	PSU	C4-N3-C2	-2.26	123.25	126.37
48	S2	1174	PSU	N1-C2-N3	2.26	117.55	115.17
48	S2	1056	PSU	O4-C4-N3	-2.26	115.87	120.11
48	S2	27	A2M	C6-C5-C4	-2.26	114.09	117.18
1	L5	3639	PSU	N1-C2-N3	2.26	117.55	115.17
48	S2	512	A2M	C6-C5-C4	-2.25	114.11	117.18
1	L5	3695	PSU	O4-C4-N3	-2.25	115.89	120.11
48	S2	801	PSU	N1-C2-N3	2.24	117.53	115.17
1	L5	3639	PSU	O4-C4-N3	-2.24	115.90	120.11
1	L5	3637	PSU	N1-C2-N3	2.24	117.53	115.17
48	S2	428	OMU	CM2-O2'-C2'	-2.23	108.75	114.47
48	S2	172	OMU	O4-C4-C5	2.23	129.01	125.16
1	L5	4576	PSU	N1-C2-N3	2.23	117.52	115.17
1	L5	3760	A2M	O4'-C1'-C2'	2.23	110.42	106.59
48	S2	354	OMU	N3-C2-N1	2.22	117.78	114.89
48	S2	966	PSU	N1-C2-N3	2.22	117.51	115.17
1	L5	1871	A2M	O3'-C3'-C2'	2.22	117.40	111.19
1	L5	3758	PSU	N1-C2-N3	2.22	117.51	115.17
48	S2	468	A2M	C1'-N9-C8	2.22	132.02	127.09
1	L5	3762	PSU	N1-C2-N3	2.21	117.50	115.17
1	L5	4220	6MZ	C4-N9-C8	2.21	108.06	105.74
1	L5	4523	A2M	C3'-C2'-C1'	-2.21	98.57	102.81
1	L5	4457	PSU	N1-C2-N3	2.21	117.50	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L8	14	OMU	O4-C4-C5	2.21	128.97	125.16
48	S2	468	A2M	C6-C5-C4	-2.21	114.16	117.18
1	L5	4498	OMU	N3-C2-N1	2.21	117.77	114.89
48	S2	822	PSU	O4'-C1'-C2'	2.21	108.20	105.15
48	S2	1832	6MZ	C4-N9-C8	2.21	108.05	105.74
1	L5	4532	PSU	N1-C2-N3	2.20	117.49	115.17
48	S2	159	A2M	C6-C5-C4	-2.20	114.17	117.18
48	S2	1004	PSU	N1-C2-N3	2.20	117.49	115.17
1	L5	4457	PSU	C6-C5-C4	2.20	119.66	118.17
1	L5	2839	PSU	C4-N3-C2	-2.20	123.34	126.37
48	S2	172	OMU	N3-C2-N1	2.20	117.75	114.89
48	S2	1031	A2M	C1'-N9-C8	2.20	131.97	127.09
1	L5	1677	PSU	O4'-C1'-C2'	2.20	108.19	105.15
1	L5	3867	A2M	C6-C5-C4	-2.19	114.18	117.18
1	L5	3718	A2M	O4'-C1'-C2'	2.19	110.36	106.59
48	S2	1081	PSU	N1-C2-N3	2.19	117.48	115.17
1	L5	3925	OMU	N3-C2-N1	2.19	117.75	114.89
48	S2	1442	OMU	N3-C2-N1	2.19	117.75	114.89
48	S2	1031	A2M	C6-C5-C4	-2.19	114.19	117.18
48	S2	1445	PSU	N1-C2-N3	2.19	117.47	115.17
1	L5	4293	PSU	N1-C2-N3	2.19	117.47	115.17
48	S2	668	A2M	C1'-N9-C8	2.19	131.95	127.09
48	S2	1850	MA6	C4-C5-N7	-2.18	108.08	110.58
48	S2	572	PSU	N1-C2-N3	2.18	117.47	115.17
1	L5	4420	PSU	O4'-C1'-C2'	2.18	108.17	105.15
48	S2	1678	A2M	C1'-N9-C8	2.18	131.94	127.09
1	L5	1792	PSU	N1-C2-N3	2.17	117.46	115.17
1	L5	3818	UY1	C5-C6-N1	-2.17	119.12	122.14
48	S2	627	OMU	O4-C4-C5	2.17	128.91	125.16
48	S2	1643	PSU	N1-C2-N3	2.17	117.46	115.17
1	L5	3760	A2M	C2-N1-C6	-2.16	115.18	118.73
1	L5	2415	OMU	O4-C4-C5	2.16	128.89	125.16
1	L5	4227	OMU	O2-C2-N3	-2.16	117.50	121.49
1	L5	1871	A2M	C1'-N9-C8	2.16	131.89	127.09
48	S2	1383	A2M	C4-N9-C1'	-2.16	121.59	126.63
48	S2	428	OMU	O4-C4-C5	2.16	128.88	125.16
48	S2	686	PSU	N1-C2-N3	2.15	117.44	115.17
1	L5	1582	PSU	N1-C2-N3	2.15	117.44	115.17
1	L5	3920	PSU	C5-C6-N1	-2.15	119.16	122.14
48	S2	99	A2M	C3'-C2'-C1'	-2.14	98.70	102.81
1	L5	4306	OMU	O4-C4-C5	2.14	128.85	125.16
48	S2	1288	OMU	CM2-O2'-C2'	-2.14	108.98	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	572	PSU	O4'-C1'-C2'	2.14	108.11	105.15
1	L5	3760	A2M	C4'-O4'-C1'	-2.14	104.75	109.47
1	L5	4620	OMU	C6-C5-C4	2.13	122.26	119.53
48	S2	1832	6MZ	O4'-C1'-C2'	-2.13	102.05	106.62
1	L5	2837	OMU	C6-C5-C4	2.13	122.26	119.53
3	L8	69	PSU	O4'-C1'-C2'	2.13	108.10	105.15
1	L5	3718	A2M	C1'-N9-C8	2.13	131.81	127.09
48	S2	1383	A2M	C6-C5-C4	-2.13	114.28	117.18
1	L5	3825	A2M	C2-N1-C6	-2.13	115.24	118.73
1	L5	3785	A2M	C4-N9-C1'	-2.12	121.67	126.63
47	Pt	55	PSU	N1-C2-N3	2.12	117.41	115.17
1	L5	1871	A2M	C6-C5-C4	-2.12	114.28	117.18
1	L5	400	A2M	C1'-N9-C8	2.12	131.80	127.09
1	L5	1326	A2M	C2-N1-C6	-2.12	115.25	118.73
1	L5	1683	PSU	N1-C2-N3	2.12	117.40	115.17
1	L5	3785	A2M	O4'-C1'-C2'	2.12	110.23	106.59
1	L5	4673	PSU	N1-C2-N3	2.12	117.40	115.17
48	S2	1056	PSU	O4'-C1'-C2'	2.11	108.08	105.15
1	L5	3637	PSU	C6-N1-C2	-2.11	120.74	122.69
48	S2	668	A2M	O4'-C1'-C2'	2.11	110.22	106.59
1	L5	3734	PSU	N1-C2-N3	2.11	117.39	115.17
1	L5	3760	A2M	C5-C6-N1	2.11	122.86	117.51
1	L5	3830	A2M	C1'-N9-C8	2.10	131.77	127.09
1	L5	2401	A2M	C6-C5-C4	-2.10	114.31	117.18
47	Pt	10	2MG	C6-C5-C4	2.10	121.98	118.83
1	L5	4530	UR3	C3U-N3-C2	2.10	120.98	117.33
1	L5	4636	PSU	C4-N3-C2	-2.09	123.49	126.37
1	L5	2815	A2M	C6-C5-C4	-2.09	114.32	117.18
1	L5	3867	A2M	C4-N9-C1'	-2.09	121.74	126.63
1	L5	4498	OMU	C6-C5-C4	2.09	122.20	119.53
48	S2	428	OMU	C6-C5-C4	2.09	122.20	119.53
1	L5	1316	OMG	C2'-C1'-N9	-2.09	110.27	114.24
48	S2	576	A2M	O4'-C1'-C2'	2.09	110.18	106.59
48	S2	116	OMU	N3-C2-N1	2.08	117.60	114.89
1	L5	4220	6MZ	C6-C5-N7	-2.08	130.16	132.43
1	L5	3785	A2M	C5-C6-N1	2.08	122.80	117.51
48	S2	1031	A2M	C4-N9-C1'	-2.08	121.77	126.63
1	L5	4623	OMG	C2'-C1'-N9	-2.08	110.30	114.24
1	L5	4227	OMU	O4-C4-C5	2.07	128.74	125.16
1	L5	400	A2M	O4'-C1'-C2'	2.07	110.16	106.59
1	L5	4571	A2M	C1'-N9-C8	2.07	131.70	127.09
48	S2	121	OMU	O4-C4-N3	-2.07	116.27	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1288	OMU	N3-C2-N1	2.07	117.59	114.89
1	L5	3841	OMC	C4-N3-C2	2.07	123.53	120.26
1	L5	4306	OMU	C6-C5-C4	2.07	122.18	119.53
48	S2	1442	OMU	C6-C5-C4	2.06	122.17	119.53
1	L5	3867	A2M	C1'-N9-C8	2.06	131.67	127.09
1	L5	4523	A2M	C4-N9-C1'	-2.06	121.81	126.63
48	S2	1832	6MZ	C4-C5-C6	2.06	118.49	116.78
48	S2	27	A2M	C5-C6-N1	2.06	122.74	117.51
48	S2	627	OMU	N3-C2-N1	2.06	117.57	114.89
48	S2	27	A2M	O4'-C1'-C2'	2.06	110.13	106.59
1	L5	4590	A2M	C3'-C2'-C1'	-2.06	98.87	102.81
1	L5	3723	A2M	C2-N1-C6	-2.06	115.35	118.73
1	L5	1536	PSU	O2-C2-N3	-2.06	118.21	121.86
1	L5	2839	PSU	N1-C2-N3	2.06	117.33	115.17
48	S2	1678	A2M	O3'-C3'-C4'	-2.06	105.18	111.08
1	L5	2843	PSU	N1-C2-N3	2.05	117.33	115.17
1	L5	3723	A2M	C5-C6-N1	2.05	122.72	117.51
48	S2	1383	A2M	C5-C6-N1	2.05	122.72	117.51
48	S2	93	PSU	N1-C2-N3	2.05	117.32	115.17
48	S2	468	A2M	C5-C6-N1	2.05	122.70	117.51
1	L5	4571	A2M	C4-N9-C1'	-2.04	121.85	126.63
1	L5	4571	A2M	C2-N1-C6	-2.04	115.37	118.73
1	L5	2839	PSU	C6-N1-C2	-2.04	120.80	122.69
1	L5	3718	A2M	C2-N1-C6	-2.04	115.38	118.73
1	L5	4552	PSU	N1-C2-N3	2.04	117.32	115.17
1	L5	2837	OMU	C2'-C1'-N1	-2.04	110.37	114.24
1	L5	3724	A2M	O4'-C1'-C2'	2.03	110.09	106.59
1	L5	3734	PSU	O4'-C1'-C2'	2.03	107.96	105.15
48	S2	428	OMU	N3-C2-N1	2.03	117.53	114.89
48	S2	576	A2M	C6-C5-C4	-2.03	114.41	117.18
48	S2	1804	OMU	C6-C5-C4	2.02	122.12	119.53
48	S2	354	OMU	C2'-C1'-N1	-2.02	110.40	114.24
48	S2	484	A2M	C6-C5-C4	-2.02	114.42	117.18
48	S2	1442	OMU	O4-C4-C5	2.02	128.65	125.16
1	L5	1524	A2M	C6-C5-C4	-2.02	114.42	117.18
48	S2	822	PSU	N1-C2-N3	2.02	117.29	115.17
48	S2	354	OMU	O4-C4-C5	2.02	128.64	125.16
1	L5	3718	A2M	O3'-C3'-C2'	2.01	116.82	111.19
1	L5	4620	OMU	N3-C2-N1	2.01	117.51	114.89
48	S2	1337	4AC	C5-C6-N1	-2.01	118.57	121.84
1	L5	398	A2M	C5-C6-N1	2.01	122.61	117.51
48	S2	484	A2M	C5-C6-N1	2.01	122.61	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	36	PSU	O4-C4-N3	-2.01	116.34	120.11
1	L5	398	A2M	C2-N1-C6	-2.00	115.44	118.73
1	L5	3830	A2M	C4-N9-C1'	-2.00	121.95	126.63
48	S2	590	A2M	C5-C6-N1	2.00	122.60	117.51
48	S2	609	PSU	N1-C2-N3	2.00	117.28	115.17
48	S2	484	A2M	O4'-C1'-C2'	2.00	110.03	106.59
1	L5	4636	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L8	14	OMU	C1'-C2'-O2'-CM2
30	Lb	5	MLZ	N-CA-CB-CG
1	L5	1677	PSU	C2'-C1'-C5-C4
1	L5	1677	PSU	O4'-C1'-C5-C4
1	L5	1677	PSU	C2'-C1'-C5-C6
1	L5	2364	OMG	C1'-C2'-O2'-CM2
1	L5	2424	OMG	C1'-C2'-O2'-CM2
1	L5	2804	OMC	C1'-C2'-O2'-CM2
1	L5	3723	A2M	C1'-C2'-O2'-CM'
1	L5	3764	PSU	O4'-C1'-C5-C4
1	L5	3764	PSU	O4'-C1'-C5-C6
1	L5	3792	OMG	C1'-C2'-O2'-CM2
1	L5	4196	OMG	C1'-C2'-O2'-CM2
1	L5	4536	OMC	C1'-C2'-O2'-CM2
1	L5	4590	A2M	C4'-C5'-O5'-P
47	Pt	54	2MU	C1'-C2'-O2'-C6'
48	S2	159	A2M	C1'-C2'-O2'-CM'
48	S2	462	OMC	C1'-C2'-O2'-CM2
48	S2	601	OMG	C1'-C2'-O2'-CM2
48	S2	867	OMG	C1'-C2'-O2'-CM2
48	S2	1243	PSU	O4'-C4'-C5'-O5'
48	S2	1326	UY1	C2'-C1'-C5-C4
48	S2	1490	OMG	C1'-C2'-O2'-CM2
48	S2	1678	A2M	C1'-C2'-O2'-CM'
48	S2	1804	OMU	C1'-C2'-O2'-CM2
1	L5	4420	PSU	C3'-C4'-C5'-O5'
1	L5	4636	PSU	C3'-C4'-C5'-O5'
48	S2	644	OMG	O4'-C4'-C5'-O5'
48	S2	1243	PSU	C3'-C4'-C5'-O5'
48	S2	1851	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
48	S2	1248	B8N	N34-C33-C34-O36
48	S2	428	OMU	C2'-C1'-N1-C6
1	L5	4420	PSU	O4'-C4'-C5'-O5'
1	L5	4636	PSU	O4'-C4'-C5'-O5'
48	S2	590	A2M	O4'-C4'-C5'-O5'
1	L5	3701	OMC	C2'-C1'-N1-C6
1	L5	3701	OMC	C2'-C1'-N1-C2
1	L5	1625	OMG	C3'-C2'-O2'-CM2
1	L5	2422	OMC	C3'-C4'-C5'-O5'
47	Pt	20	H2U	C3'-C4'-C5'-O5'
48	S2	590	A2M	C3'-C4'-C5'-O5'
48	S2	1490	OMG	O4'-C4'-C5'-O5'
48	S2	1851	MA6	C3'-C4'-C5'-O5'
1	L5	3760	A2M	C2'-C1'-N9-C8
48	S2	428	OMU	C2'-C1'-N1-C2
48	S2	644	OMG	C3'-C4'-C5'-O5'
1	L5	2422	OMC	O4'-C4'-C5'-O5'
1	L5	2815	A2M	C3'-C4'-C5'-O5'
1	L5	3785	A2M	O4'-C4'-C5'-O5'
1	L5	2787	A2M	C2'-C1'-N9-C8
1	L5	4500	PSU	C4'-C5'-O5'-P
48	S2	668	A2M	O4'-C4'-C5'-O5'
48	S2	668	A2M	C3'-C4'-C5'-O5'
48	S2	1248	B8N	N34-C33-C34-O35
1	L5	3785	A2M	C3'-C4'-C5'-O5'
48	S2	576	A2M	C1'-C2'-O2'-CM'
1	L5	4447	5MC	C2'-C1'-N1-C6
48	S2	1248	B8N	C4'-C5'-O5'-P
30	Lb	5	MLZ	C-CA-CB-CG
48	S2	428	OMU	O4'-C1'-N1-C2
48	S2	172	OMU	C3'-C2'-O2'-CM2
48	S2	428	OMU	C3'-C2'-O2'-CM2
1	L5	4447	5MC	O4'-C1'-N1-C6
1	L5	3760	A2M	C4'-C5'-O5'-P
1	L5	3760	A2M	C2'-C1'-N9-C4
48	S2	428	OMU	O4'-C1'-N1-C6
1	L5	1326	A2M	C4'-C5'-O5'-P
47	Pt	20	H2U	C4'-C5'-O5'-P
1	L5	3701	OMC	O4'-C1'-N1-C6
1	L5	2365	OMC	C3'-C2'-O2'-CM2
1	L5	2401	A2M	C3'-C2'-O2'-CM'
1	L5	1534	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	L5	2815	A2M	C4'-C5'-O5'-P
1	L5	3818	UY1	C4'-C5'-O5'-P
48	S2	1243	PSU	C4'-C5'-O5'-P
48	S2	1326	UY1	O4'-C1'-C5-C4
1	L5	2787	A2M	C2'-C1'-N9-C4
1	L5	3701	OMC	O4'-C1'-N1-C2
48	S2	1447	OMG	C3'-C4'-C5'-O5'
1	L5	1322	1MA	C2'-C1'-N9-C8
48	S2	644	OMG	C4'-C5'-O5'-P
47	Pt	20	H2U	O4'-C4'-C5'-O5'
1	L5	1326	A2M	C3'-C2'-O2'-CM'
1	L5	1524	A2M	C3'-C2'-O2'-CM'
1	L5	3760	A2M	C3'-C2'-O2'-CM'
1	L5	1322	1MA	C2'-C1'-N9-C4
48	S2	1490	OMG	C4'-C5'-O5'-P
1	L5	4447	5MC	O4'-C1'-N1-C2
48	S2	99	A2M	C4'-C5'-O5'-P
1	L5	4637	OMG	C1'-C2'-O2'-CM2
1	L5	3818	UY1	O4'-C1'-C5-C6
1	L5	4531	PSU	O4'-C1'-C5-C6
48	S2	1851	MA6	C4'-C5'-O5'-P
1	L5	3887	OMC	C3'-C4'-C5'-O5'
1	L5	3944	OMG	C3'-C4'-C5'-O5'
47	Pt	13	PSU	O4'-C4'-C5'-O5'
1	L5	3844	PSU	C4'-C5'-O5'-P
48	S2	1248	B8N	C32-C33-C34-O36
1	L5	3851	PSU	C3'-C4'-C5'-O5'
1	L5	2787	A2M	O4'-C1'-N9-C8
48	S2	590	A2M	O4'-C1'-N9-C8
1	L5	2351	OMC	C2'-C1'-N1-C2
1	L5	4447	5MC	C2'-C1'-N1-C2
48	S2	1490	OMG	C3'-C4'-C5'-O5'
48	S2	1081	PSU	C4'-C5'-O5'-P
48	S2	1248	B8N	C32-C33-C34-O35

There are no ring outliers.

51 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	2787	A2M	1	0
1	L5	2804	OMC	1	0
48	S2	116	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S2	1850	MA6	3	0
1	L5	2424	OMG	1	0
48	S2	121	OMU	1	0
1	L5	4457	PSU	1	0
48	S2	509	OMG	1	0
48	S2	1232	PSU	1	0
1	L5	1340	OMC	1	0
47	Pt	13	PSU	1	0
48	S2	484	A2M	1	0
1	L5	2351	OMC	3	0
1	L5	3762	PSU	1	0
1	L5	4536	OMC	1	0
48	S2	1832	6MZ	1	0
3	L8	14	OMU	1	0
48	S2	1692	PSU	1	0
48	S2	159	A2M	2	0
48	S2	1391	OMC	2	0
1	L5	4220	6MZ	2	0
1	L5	2364	OMG	1	0
1	L5	3718	A2M	3	0
47	Pt	20	H2U	1	0
1	L5	3867	A2M	1	0
1	L5	2876	OMG	1	0
48	S2	867	OMG	1	0
48	S2	1347	PSU	1	0
1	L5	3782	5MC	1	0
1	L5	4637	OMG	1	0
48	S2	468	A2M	1	0
1	L5	4456	OMC	1	0
48	S2	1842	4AC	1	0
1	L5	2415	OMU	2	0
1	L5	3944	OMG	1	0
48	S2	572	PSU	1	0
48	S2	354	OMU	1	0
1	L5	2815	A2M	2	0
48	S2	462	OMC	1	0
48	S2	27	A2M	1	0
48	S2	1804	OMU	1	0
48	S2	576	A2M	1	0
1	L5	4293	PSU	1	0
3	L8	75	OMG	1	0
5	LB	245	HIC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S2	166	A2M	1	0
48	S2	172	OMU	1	0
47	Pt	55	PSU	1	0
1	L5	2632	PSU	1	0
48	S2	99	A2M	1	0
1	L5	3792	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 573 ligands modelled in this entry, 549 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
85	SPD	L5	5600	-	9,9,9	0.30	0	8,8,8	0.73	0
84	PUT	L5	5621	-	5,5,5	0.18	0	4,4,4	0.28	0
84	PUT	L5	5614	-	5,5,5	0.12	0	4,4,4	0.24	0
85	SPD	L5	5603	-	9,9,9	0.25	0	8,8,8	0.24	0
85	SPD	L5	5607	-	9,9,9	0.29	0	8,8,8	0.70	0
85	SPD	S2	1902	-	9,9,9	0.26	0	8,8,8	0.34	0
87	TRS	L5	5618	-	7,7,7	0.47	0	9,9,9	0.63	0
85	SPD	L5	5608	-	9,9,9	0.25	0	8,8,8	0.24	0
85	SPD	L5	5606	-	9,9,9	0.26	0	8,8,8	0.61	0
84	PUT	L5	5616	-	5,5,5	0.11	0	4,4,4	0.27	0
84	PUT	L5	5611	-	5,5,5	0.09	0	4,4,4	0.18	0
84	PUT	L5	5612	-	5,5,5	0.18	0	4,4,4	0.17	0
84	PUT	L5	5613	-	5,5,5	0.20	0	4,4,4	0.18	0
85	SPD	L5	5604	-	9,9,9	0.28	0	8,8,8	0.64	0
85	SPD	L5	5602	-	9,9,9	0.29	0	8,8,8	0.96	0
84	PUT	L5	5615	-	5,5,5	0.15	0	4,4,4	0.21	0
85	SPD	L5	5609	-	9,9,9	0.26	0	8,8,8	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	SPD	L5	5605	-	9,9,9	0.31	0	8,8,8	0.43	0
85	SPD	L5	5610	-	9,9,9	0.29	0	8,8,8	0.41	0
85	SPD	L5	5620	-	9,9,9	0.22	0	8,8,8	0.49	0
85	SPD	L5	5601	-	9,9,9	0.31	0	8,8,8	0.68	0
86	A1B75	L5	5700	83	28,28,28	1.65	4 (14%)	30,37,37	1.39	5 (16%)
85	SPD	S2	1901	-	9,9,9	0.25	0	8,8,8	0.59	0
87	TRS	L5	5617	-	7,7,7	0.79	0	9,9,9	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	L5	5600	-	-	0/7/7/7	-
84	PUT	L5	5621	-	-	0/3/3/3	-
84	PUT	L5	5614	-	-	0/3/3/3	-
85	SPD	L5	5603	-	-	1/7/7/7	-
85	SPD	L5	5607	-	-	3/7/7/7	-
85	SPD	S2	1902	-	-	0/7/7/7	-
87	TRS	L5	5618	-	-	2/9/9/9	-
85	SPD	L5	5608	-	-	2/7/7/7	-
85	SPD	L5	5606	-	-	1/7/7/7	-
84	PUT	L5	5616	-	-	3/3/3/3	-
84	PUT	L5	5611	-	-	1/3/3/3	-
84	PUT	L5	5612	-	-	1/3/3/3	-
84	PUT	L5	5613	-	-	2/3/3/3	-
85	SPD	L5	5604	-	-	2/7/7/7	-
85	SPD	L5	5602	-	-	1/7/7/7	-
84	PUT	L5	5615	-	-	0/3/3/3	-
85	SPD	L5	5609	-	-	1/7/7/7	-
85	SPD	L5	5605	-	-	2/7/7/7	-
85	SPD	L5	5610	-	-	0/7/7/7	-
85	SPD	L5	5620	-	-	2/7/7/7	-
85	SPD	L5	5601	-	-	1/7/7/7	-
86	A1B75	L5	5700	83	-	1/16/36/36	0/3/3/3
85	SPD	S2	1901	-	-	2/7/7/7	-
87	TRS	L5	5617	-	-	3/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	L5	5700	A1B75	C3-N1	6.49	1.60	1.47
86	L5	5700	A1B75	O3-C5	-2.75	1.37	1.43
86	L5	5700	A1B75	C1-N2	2.60	1.39	1.34
86	L5	5700	A1B75	C4-N1	2.23	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	L5	5700	A1B75	C2-O2-C1	3.43	122.08	117.04
86	L5	5700	A1B75	O2-C1-O1	-3.26	119.76	124.55
86	L5	5700	A1B75	C4-C5-C2	2.62	106.68	103.32
86	L5	5700	A1B75	O2-C1-N2	2.37	114.87	111.01
86	L5	5700	A1B75	C7-C6-C3	2.14	117.03	113.40

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5618	TRS	N-C-C2-O2
87	L5	5617	TRS	N-C-C3-O3
85	L5	5620	SPD	C3-C4-C5-N6
85	L5	5608	SPD	C3-C4-C5-N6
85	L5	5607	SPD	N6-C7-C8-C9
87	L5	5617	TRS	C2-C-C3-O3
85	L5	5605	SPD	C4-C5-N6-C7
85	L5	5603	SPD	C4-C5-N6-C7
85	L5	5607	SPD	C2-C3-C4-C5
84	L5	5613	PUT	C1-C2-C3-C4
84	L5	5616	PUT	C1-C2-C3-C4
85	S2	1901	SPD	C3-C4-C5-N6
85	L5	5620	SPD	C8-C7-N6-C5
85	L5	5609	SPD	N1-C2-C3-C4
86	L5	5700	A1B75	C14-C15-C16-N3
85	L5	5605	SPD	N1-C2-C3-C4
85	L5	5607	SPD	C4-C5-N6-C7
84	L5	5616	PUT	C2-C3-C4-N2
84	L5	5611	PUT	N1-C1-C2-C3
85	L5	5604	SPD	C2-C3-C4-C5
84	L5	5613	PUT	N1-C1-C2-C3
85	L5	5601	SPD	C4-C5-N6-C7
85	L5	5608	SPD	C8-C7-N6-C5
85	S2	1901	SPD	C4-C5-N6-C7

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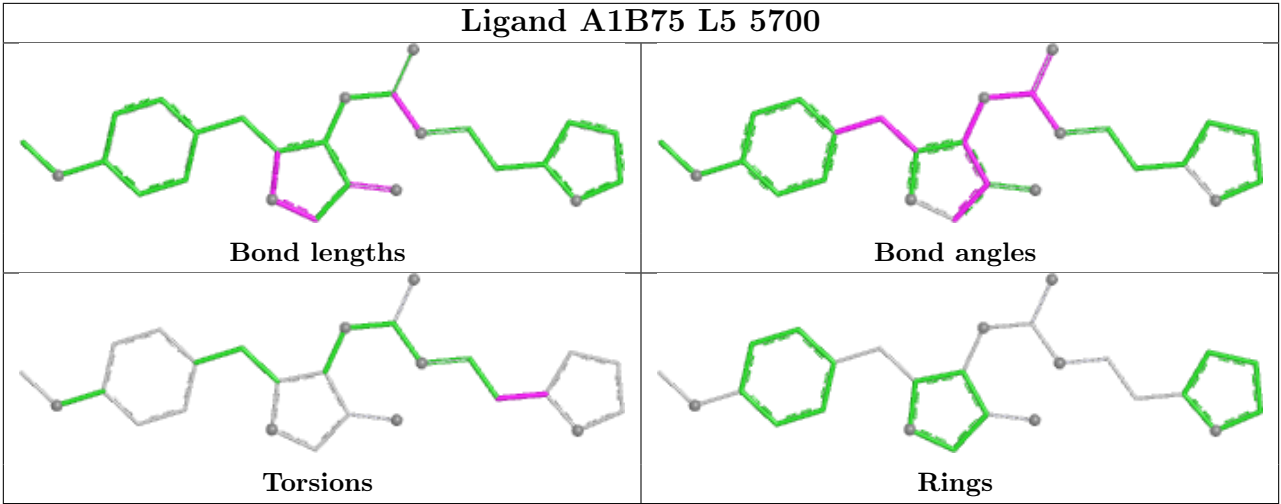
Mol	Chain	Res	Type	Atoms
87	L5	5618	TRS	C1-C-C2-O2
87	L5	5617	TRS	C1-C-C3-O3
85	L5	5606	SPD	C7-C8-C9-N10
84	L5	5612	PUT	C2-C3-C4-N2
84	L5	5616	PUT	N1-C1-C2-C3
85	L5	5602	SPD	C8-C7-N6-C5
85	L5	5604	SPD	C8-C7-N6-C5

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	L5	5621	PUT	1	0
85	L5	5607	SPD	1	0
87	L5	5618	TRS	1	0
84	L5	5616	PUT	3	0
84	L5	5615	PUT	1	0
85	L5	5610	SPD	1	0
86	L5	5700	A1B75	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
46	NC	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	NC	20:UNK	C	26:GLU	N	16.32

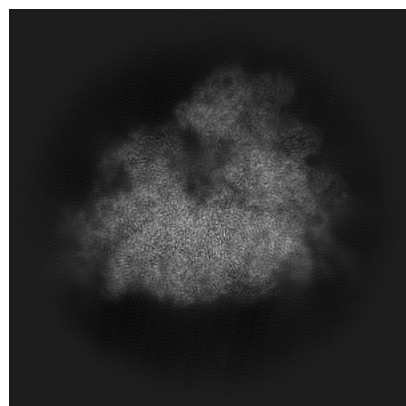
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70084. These allow visual inspection of the internal detail of the map and identification of artifacts.

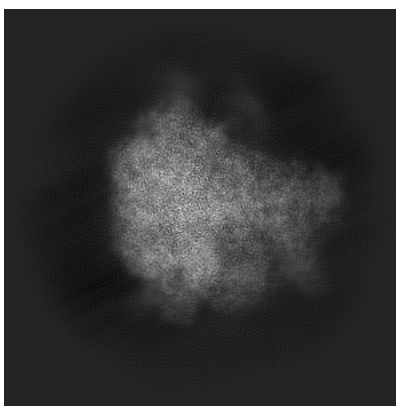
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

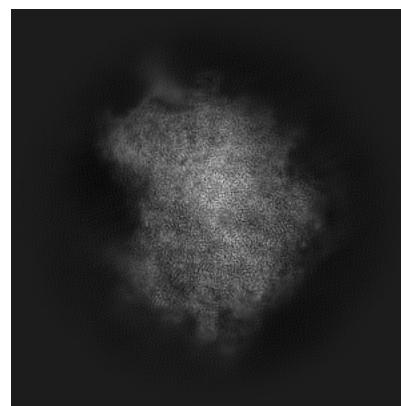
6.1.1 Primary map



X

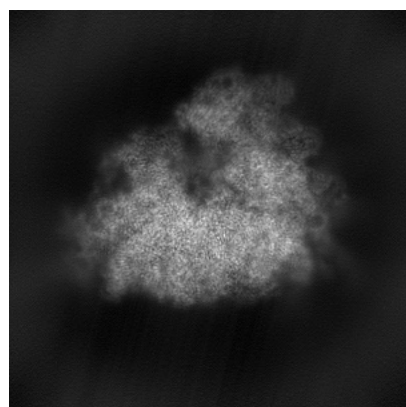


Y

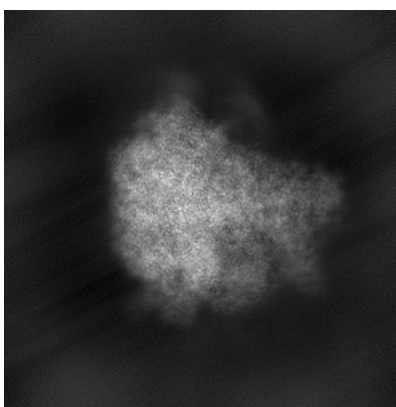


Z

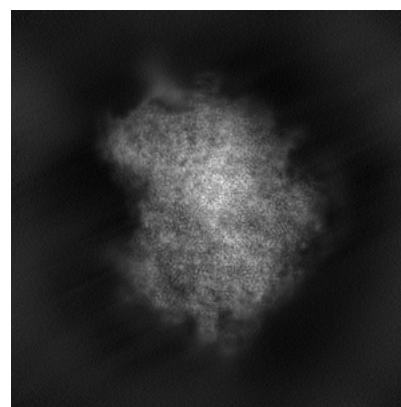
6.1.2 Raw map



X



Y

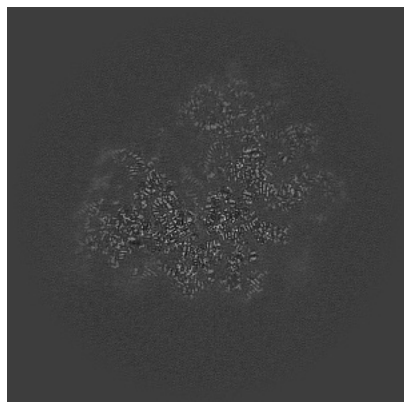


Z

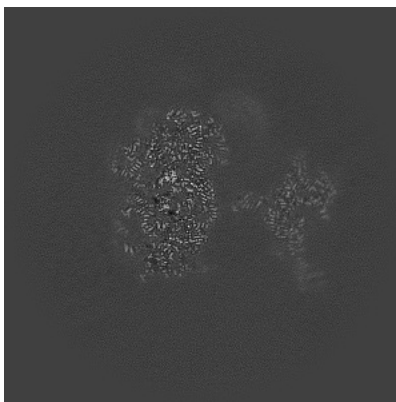
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

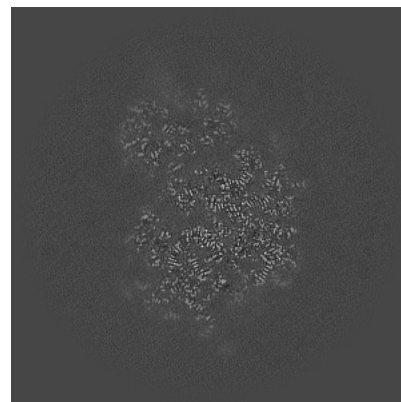
6.2.1 Primary map



X Index: 256

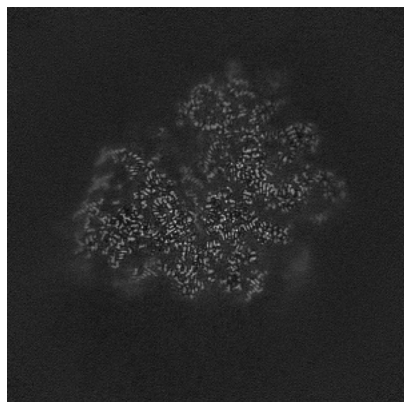


Y Index: 256

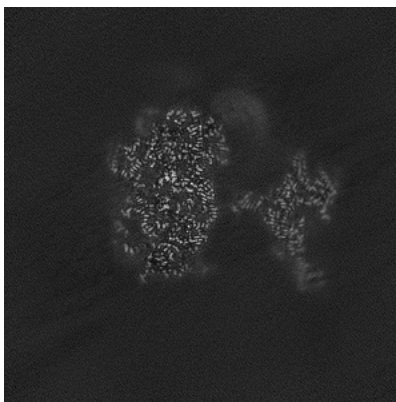


Z Index: 256

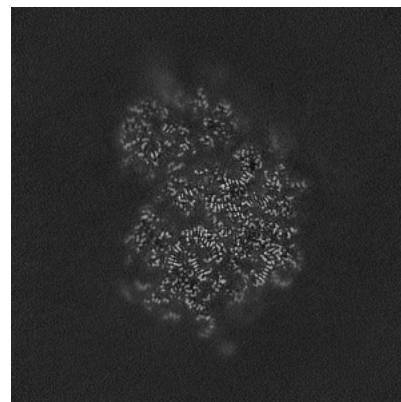
6.2.2 Raw map



X Index: 256



Y Index: 256

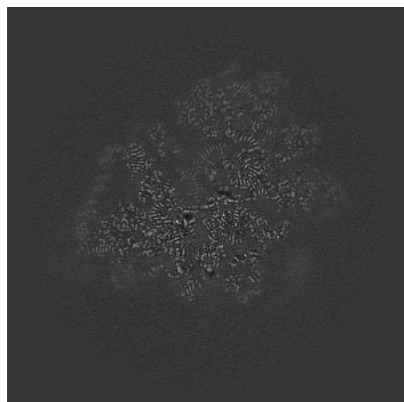


Z Index: 256

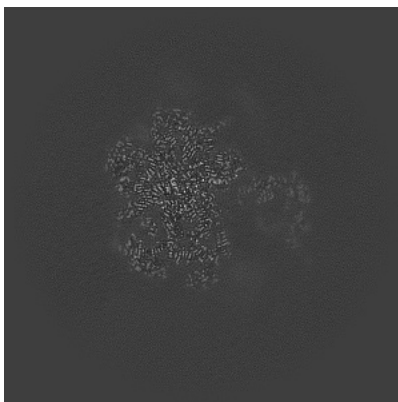
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

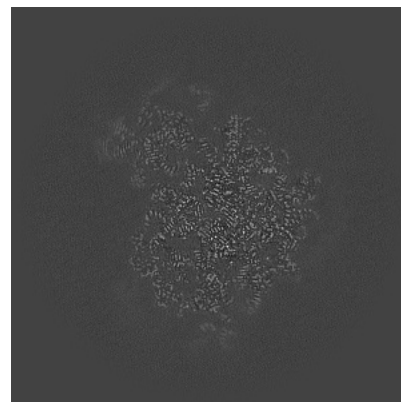
6.3.1 Primary map



X Index: 261

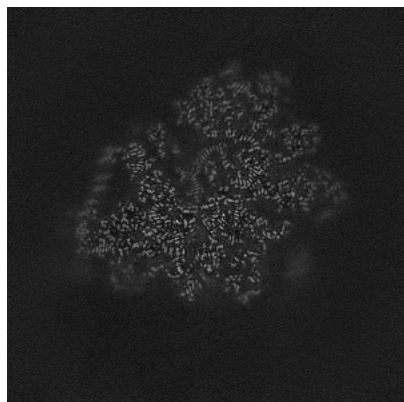


Y Index: 218

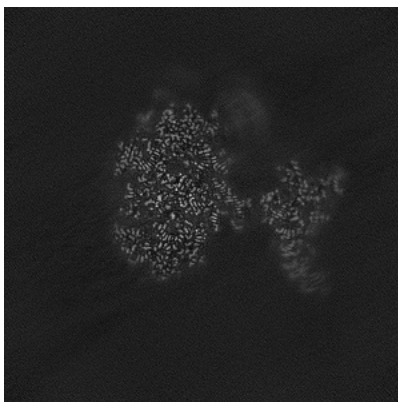


Z Index: 237

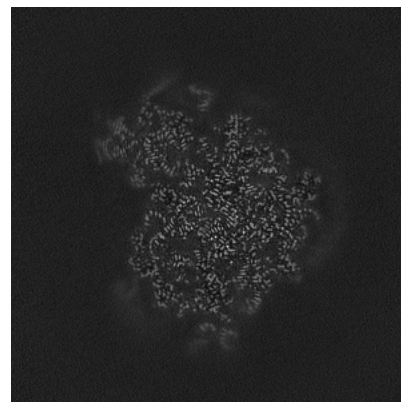
6.3.2 Raw map



X Index: 261



Y Index: 265

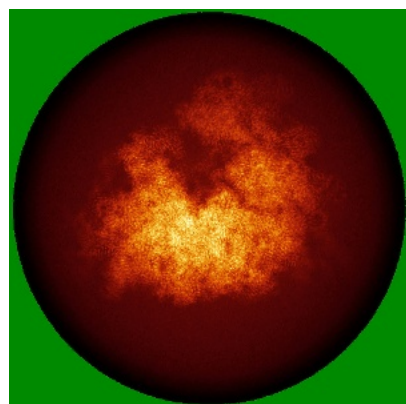


Z Index: 237

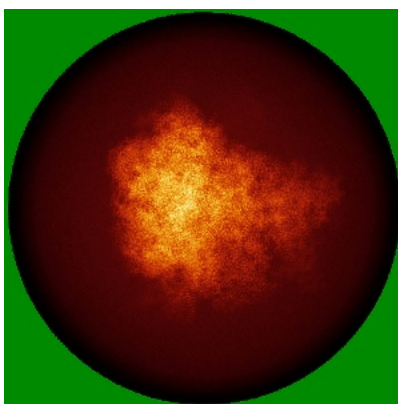
The images above show the largest variance slices of the map in three orthogonal directions.

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

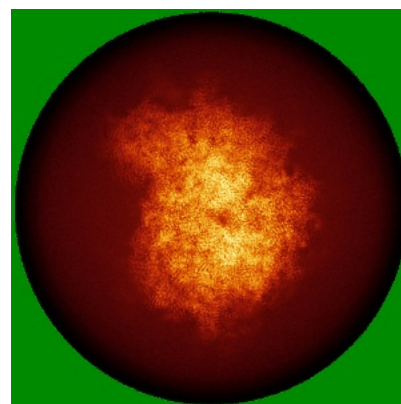
6.4.1 Primary map



X

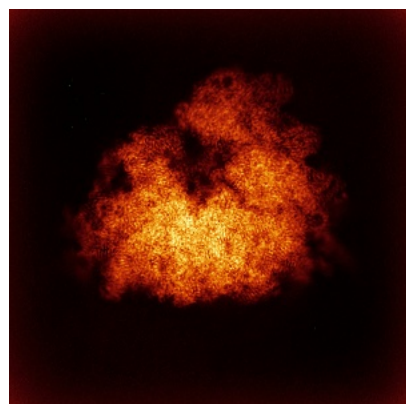


Y

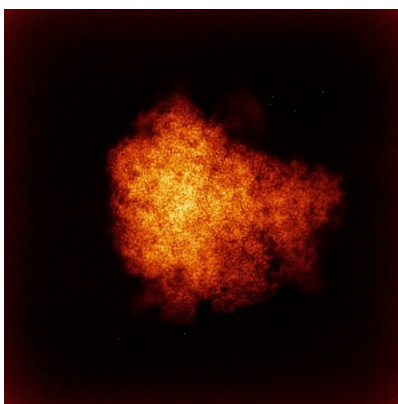


Z

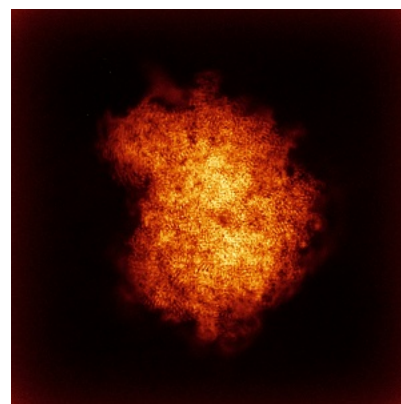
6.4.2 Raw map



X



Y

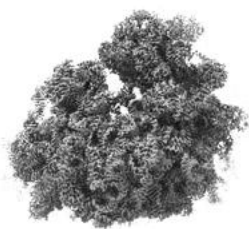


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

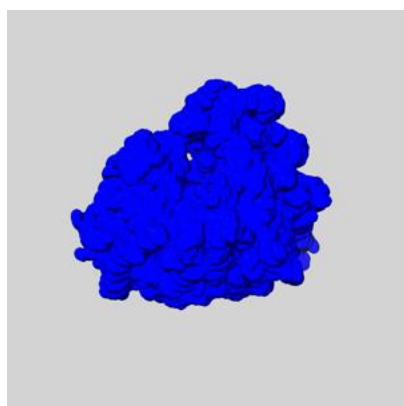
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

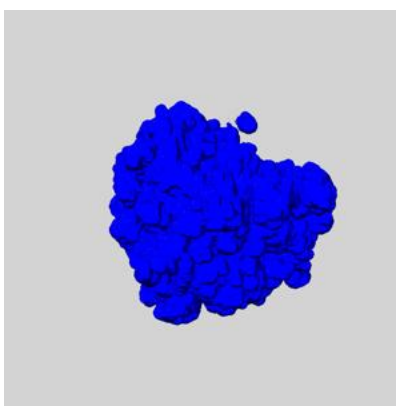
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

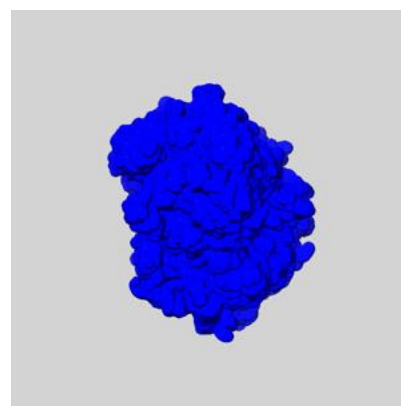
6.6.1 emd_70084_msk_1.map [i](#)



X



Y

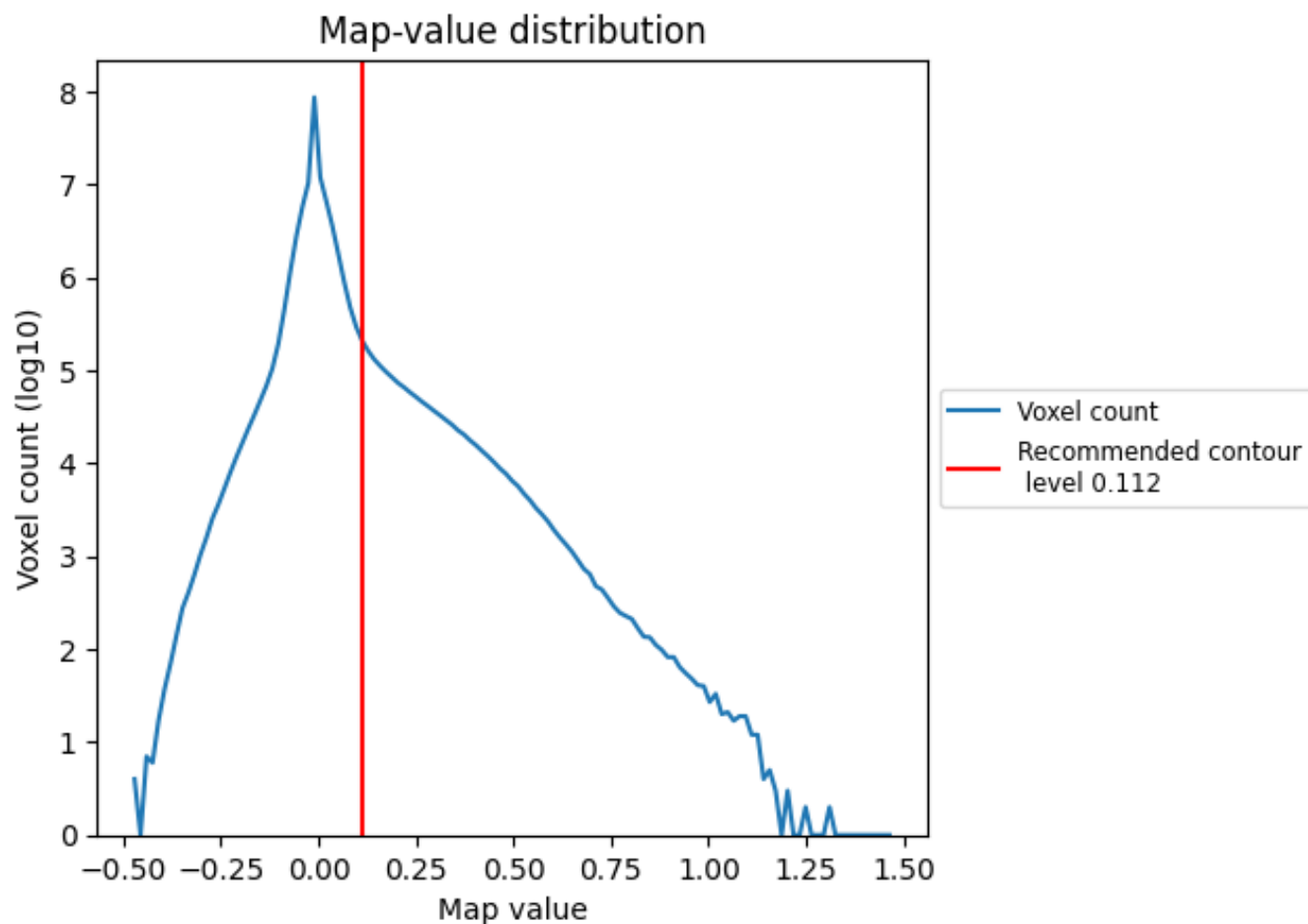


Z

7 Map analysis [i](#)

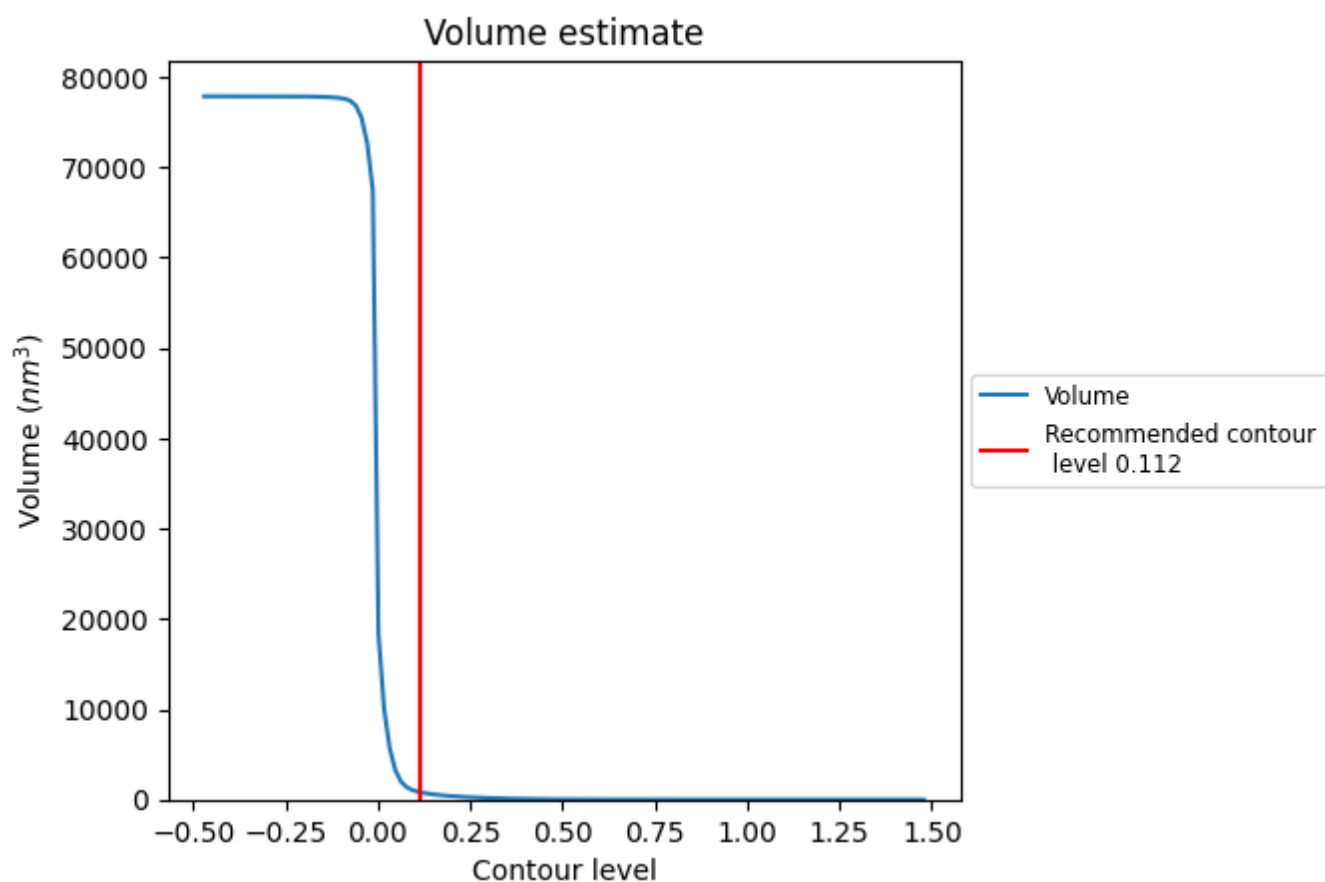
This section contains the results of statistical analysis of the map.

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.

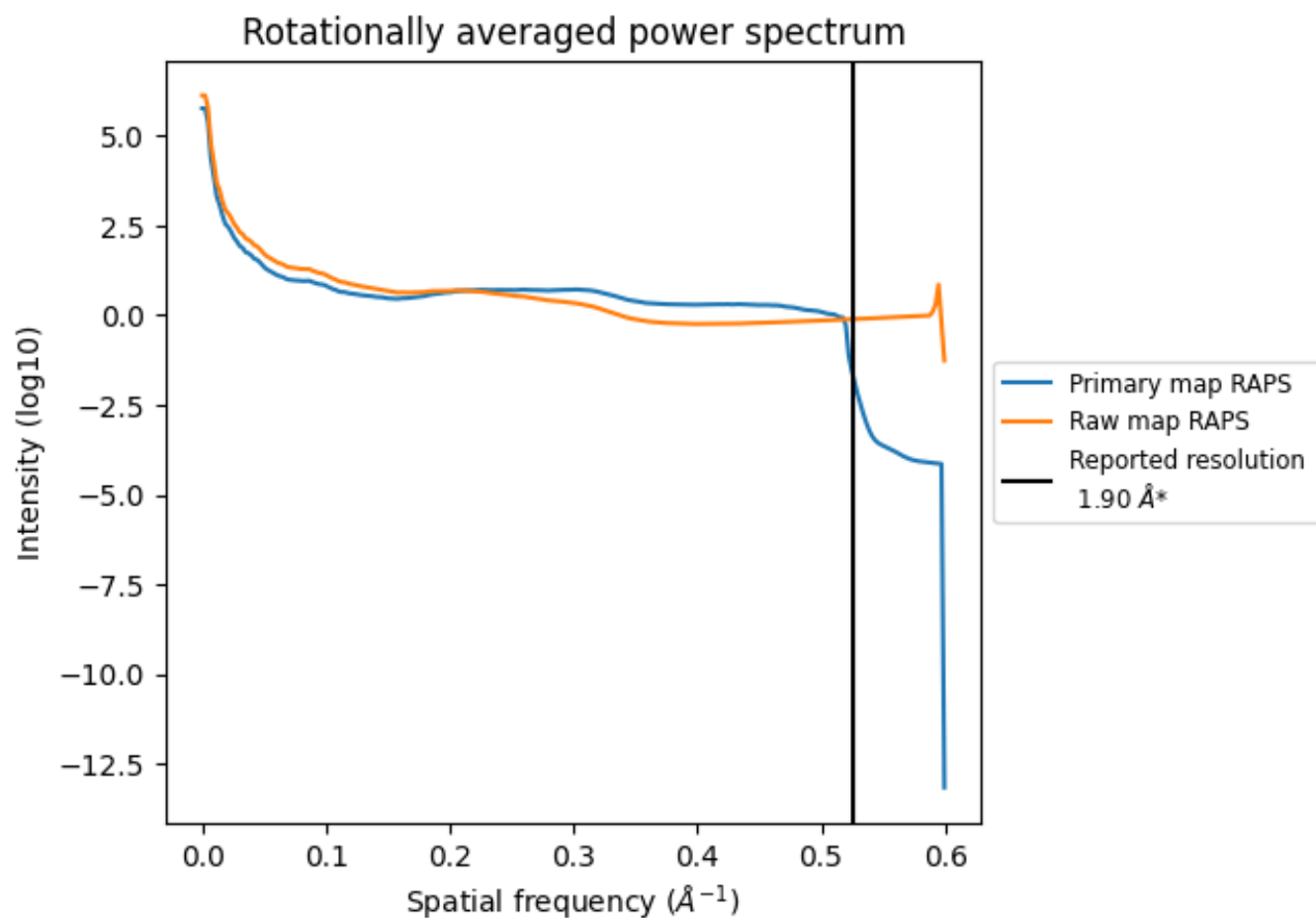
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 834 nm^3 ; this corresponds to an approximate mass of 753 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

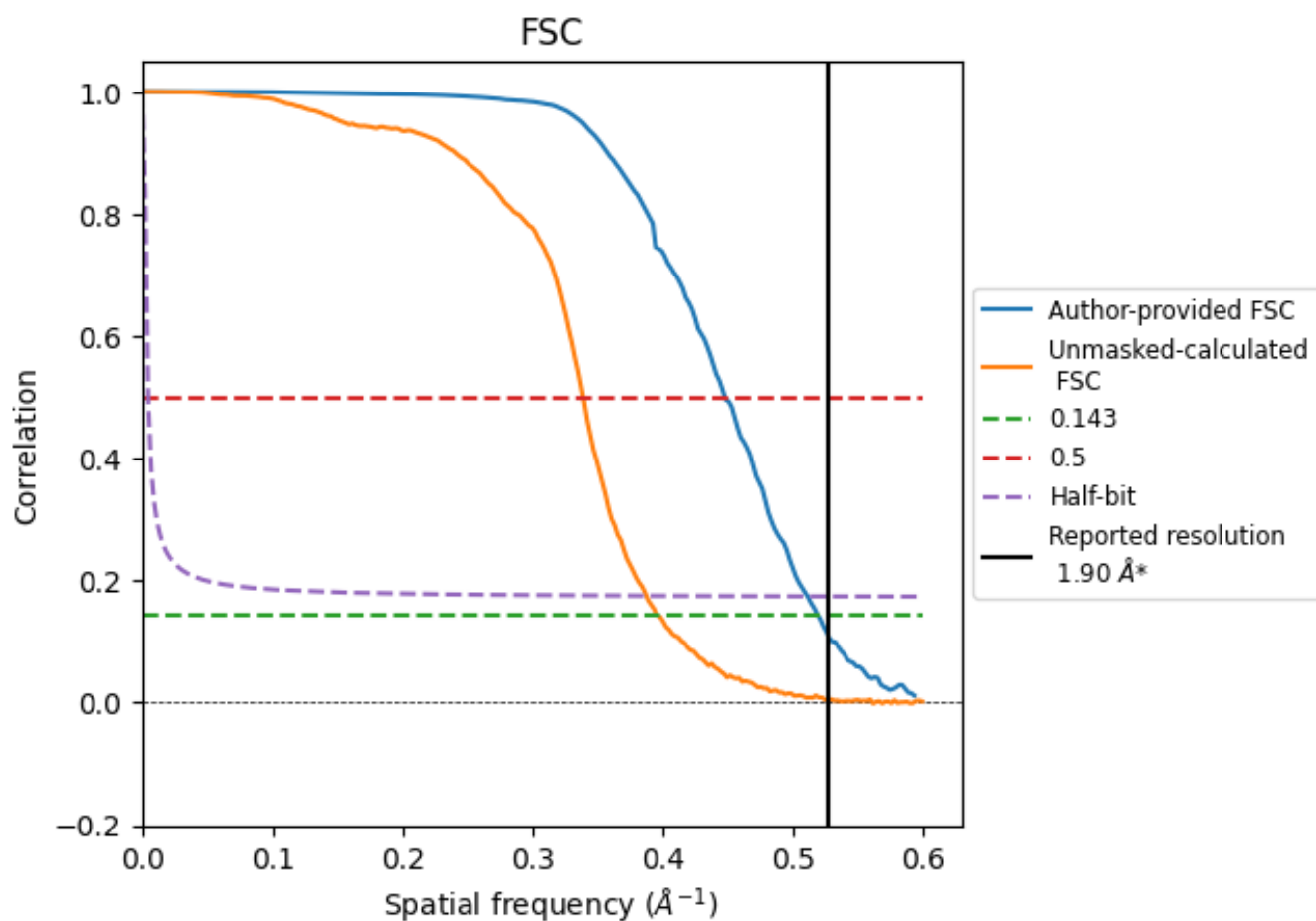


*Reported resolution corresponds to spatial frequency of 0.526 Å⁻¹

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 0.526 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

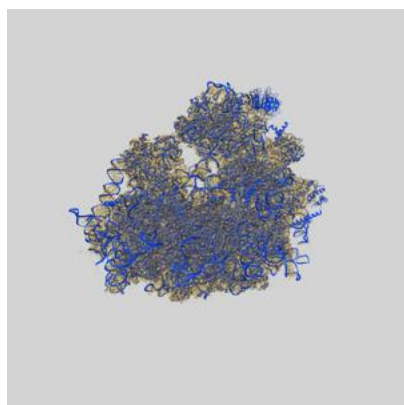
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.90	-	-
Author-provided FSC curve	1.93	2.23	1.96
Unmasked-calculated*	2.53	2.95	2.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.53 differs from the reported value 1.9 by more than 10 %

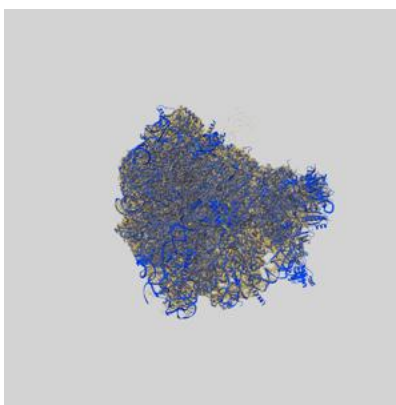
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70084 and PDB model 9O3W. Per-residue inclusion information can be found in [section 3](#) on [page 29](#).

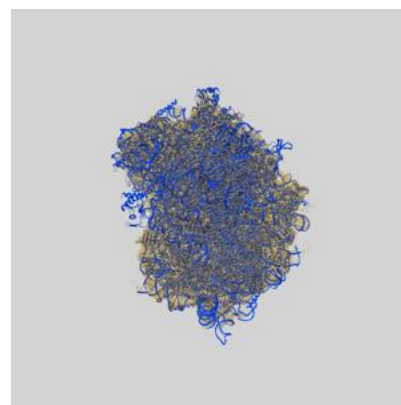
9.1 Map-model overlay [i](#)



X



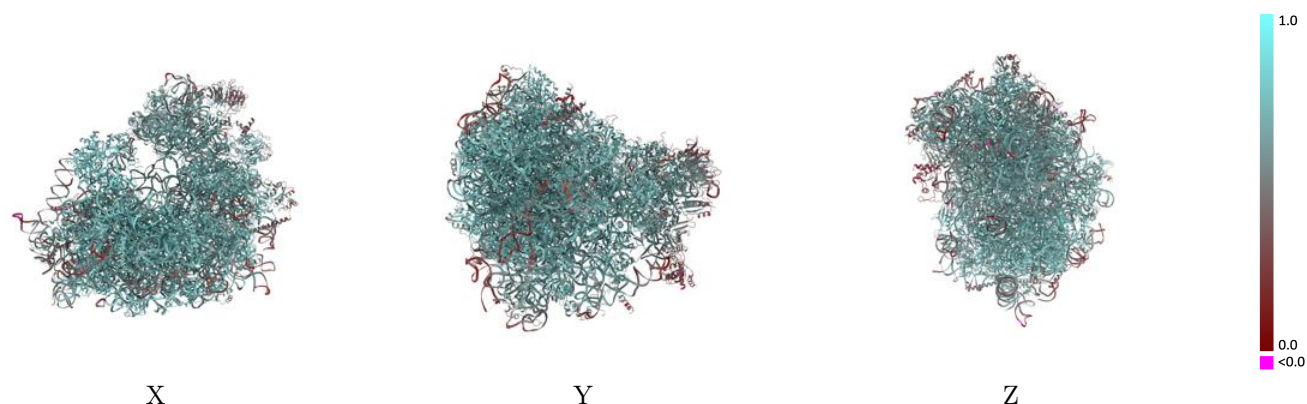
Y



Z

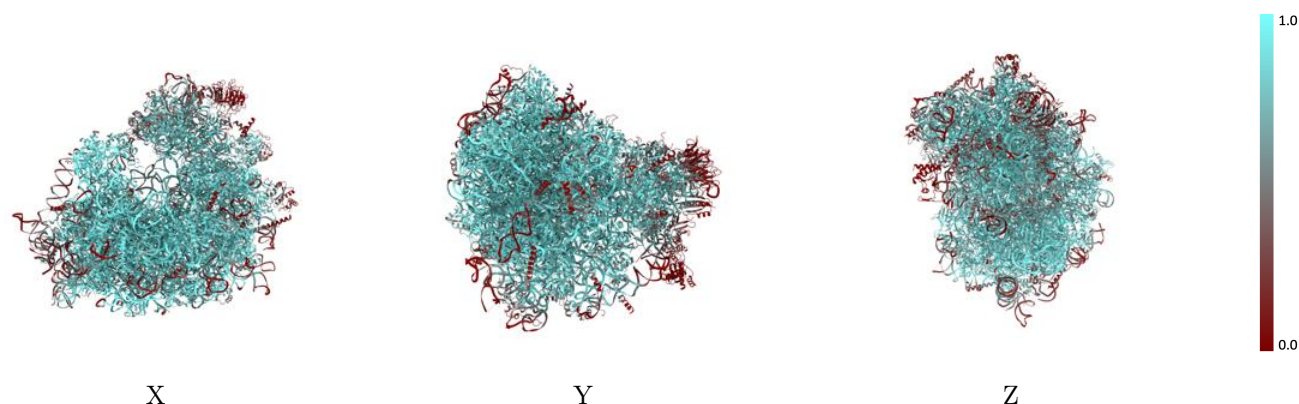
The images above show the 3D surface view of the map at the recommended contour level 0.112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



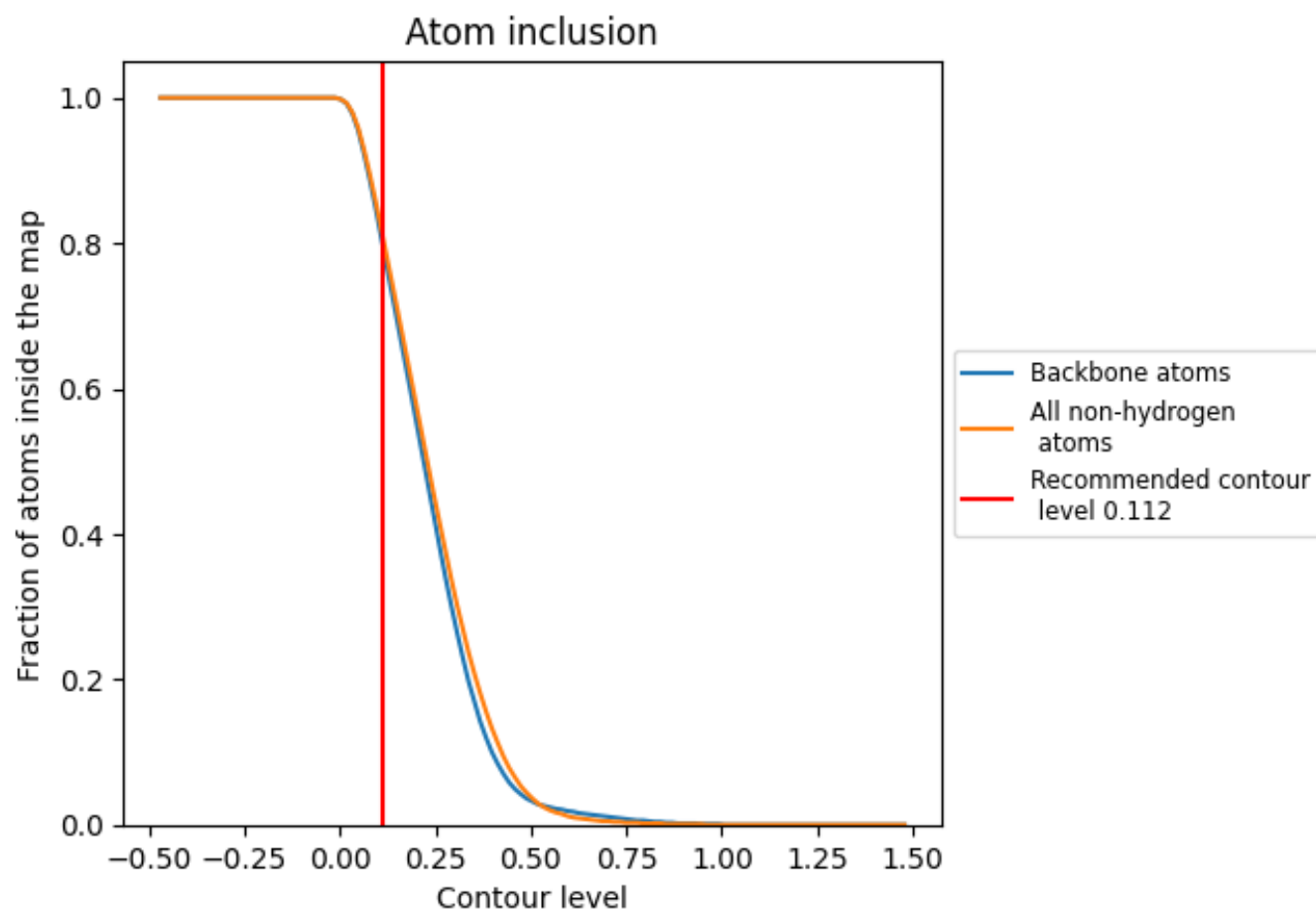
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.112).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 81% 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 (0.112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.6780
L5	 0.8520	 0.6900
L7	 0.9830	 0.7430
L8	 0.9050	 0.7100
LA	 0.9610	 0.7770
LB	 0.9100	 0.7510
LC	 0.9120	 0.7390
LD	 0.8570	 0.7120
LE	 0.7770	 0.6670
LF	 0.9140	 0.7530
LG	 0.7500	 0.6580
LH	 0.8760	 0.7170
LI	 0.8760	 0.7240
LJ	 0.8060	 0.6790
LL	 0.8590	 0.7120
LM	 0.8900	 0.7140
LN	 0.9830	 0.7820
LO	 0.9140	 0.7500
LP	 0.9280	 0.7570
LQ	 0.9570	 0.7670
LR	 0.8060	 0.6910
LS	 0.9500	 0.7630
LT	 0.8560	 0.7220
LU	 0.7220	 0.6350
LV	 0.9330	 0.7630
LW	 0.8520	 0.7140
LX	 0.8880	 0.7240
LY	 0.8600	 0.7100
LZ	 0.8740	 0.7130
La	 0.9440	 0.7640
Lb	 0.6690	 0.6440
Lc	 0.8750	 0.7170
Ld	 0.8600	 0.7270
Le	 0.9550	 0.7640
Lf	 0.9440	 0.7590



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Chain	Atom inclusion	Q-score
Lg	 0.8870	 0.7360
Lh	 0.8550	 0.7110
Li	 0.8420	 0.7100
Lj	 0.9730	 0.7730
Lk	 0.6910	 0.6390
Ll	 0.9320	 0.7420
Lm	 0.8900	 0.7340
Ln	 0.8860	 0.7430
Lo	 0.8820	 0.7450
Lp	 0.9170	 0.7600
Lr	 0.9150	 0.7320
NC	 0.3640	 0.4800
Pt	 0.7330	 0.6350
S2	 0.8300	 0.6590
SA	 0.7140	 0.6450
SB	 0.7980	 0.6760
SC	 0.7690	 0.6780
SD	 0.4760	 0.5530
SE	 0.7220	 0.6490
SF	 0.6950	 0.6380
SG	 0.4100	 0.5190
SH	 0.4200	 0.5270
SI	 0.7770	 0.6740
SJ	 0.6850	 0.6220
SK	 0.3250	 0.4850
SL	 0.8520	 0.7120
SM	 0.0030	 0.2580
SN	 0.8800	 0.7230
SO	 0.8680	 0.7130
SP	 0.4640	 0.5450
SQ	 0.6170	 0.6330
SR	 0.4650	 0.5620
SS	 0.6000	 0.6190
ST	 0.6140	 0.6180
SU	 0.4280	 0.5280
SV	 0.7020	 0.6590
SW	 0.9090	 0.7250
SX	 0.8810	 0.7190
SY	 0.5120	 0.5500
SZ	 0.4660	 0.5570
Sa	 0.8810	 0.7200
Sb	 0.7000	 0.6520

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Chain	Atom inclusion	Q-score
Sc	 0.5870	 0.5880
Sd	 0.7880	 0.6730
Se	 0.6130	 0.6020
Sf	 0.0180	 0.2740
Sg	 0.1770	 0.4600
mR	 0.3530	 0.5920