



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 03:05 AM EDT

PDB ID : 8FLF / pdb_00008ff
EMDB ID : EMD-29277
Title : Human nuclear pre-60S ribosomal subunit (State L3)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.65 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:

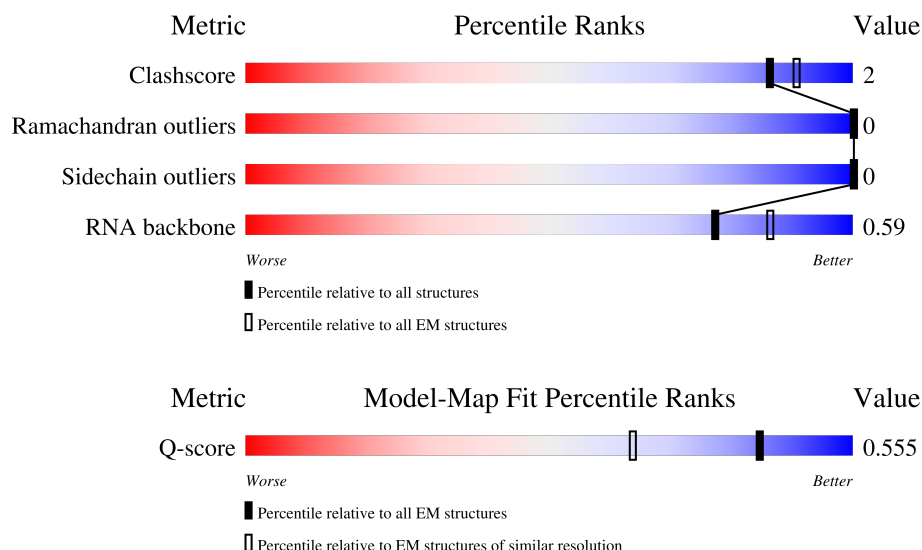
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.65 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.



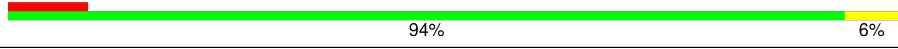
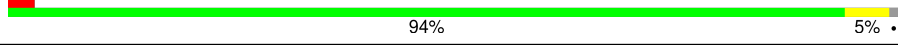
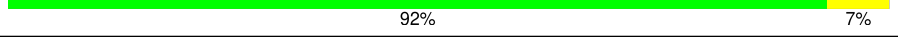
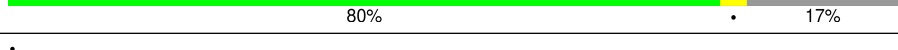
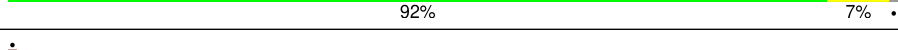
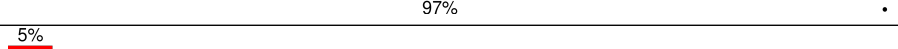
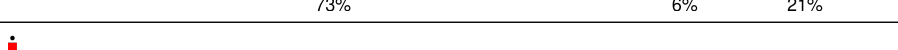
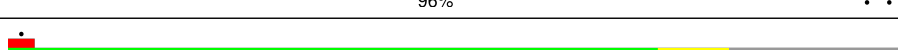
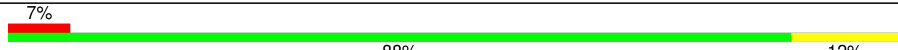
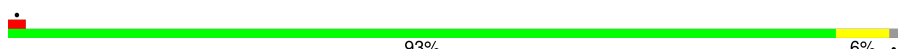
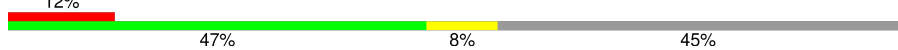
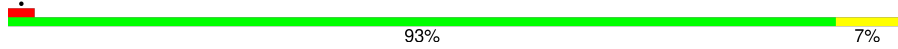
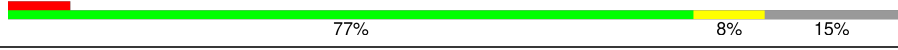
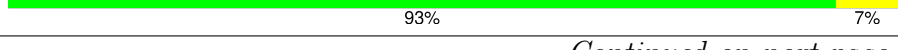
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9050 (2.15 - 3.15)

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	BE	214	
2	L1	157	
3	L3	5070	

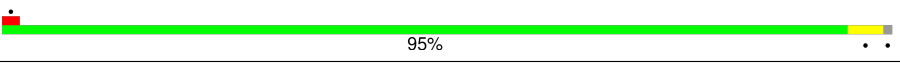
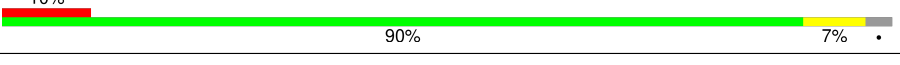
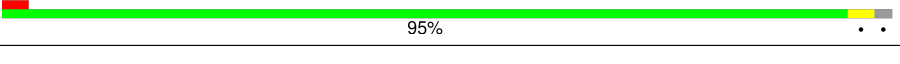
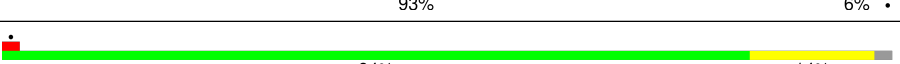
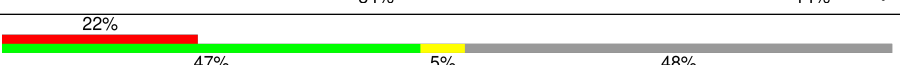
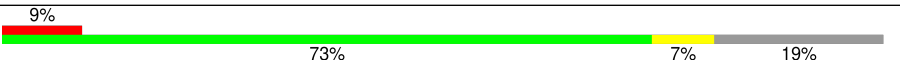
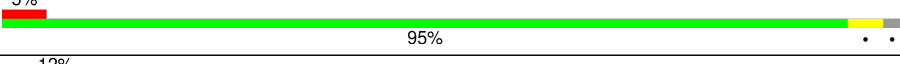
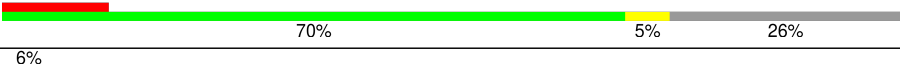
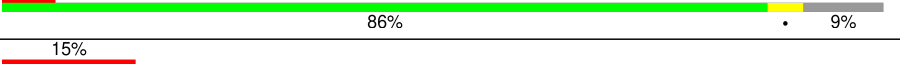
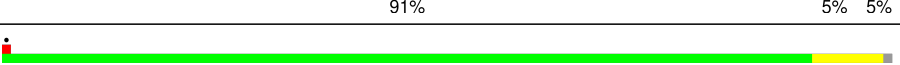
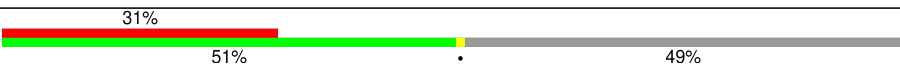
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Mol	Chain	Length	Quality of chain
4	L4	121	
5	L5	178	
6	L6	211	
7	L7	203	
8	L8	215	
9	L9	204	
10	LA	184	
11	LB	188	
12	LC	176	
13	LD	196	
14	LE	160	
15	LF	128	
16	LG	140	
17	LH	156	
18	LI	145	
19	LJ	136	
20	LK	148	
21	LL	137	
22	LM	159	
23	LN	403	
24	LO	115	
25	LP	125	
26	LQ	135	
27	LR	117	
28	LS	123	

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Mol	Chain	Length	Quality of chain
29	LT	110	
30	LU	105	
31	LV	106	
32	LW	97	
33	LX	92	
34	LY	70	
35	LZ	51	
36	NK	129	
37	NP	134	
38	SA	427	
39	SB	297	
40	SC	288	
41	SD	248	
42	SE	266	
43	SF	257	
44	SG	192	
45	SK	245	
46	SQ	239	
47	SR	634	
48	SV	163	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 134730 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BE	160	Total	C	N	O	S	0	0
			1295	827	242	218	8		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	154	Total	C	N	O	P	0	0
			3278	1463	581	1080	154		

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	3325	Total	C	N	O	P	0	0
			71370	31811	13073	23161	3325		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L4	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	168	Total	C	N	O	S	0	0
			1349	853	251	239	6		

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 7 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 8 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 9 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L9	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 10 is a protein called 60S ribosomal protein L17.

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

- Molecule 11 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LB	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 12 is a protein called 60S ribosomal protein L18a.

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

- Molecule 13 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LD	154	Total	C	N	O	S	0	0
			1289	805	277	198	9		

- Molecule 14 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LE	154	Total	C	N	O	S	0	0
			1264	803	246	210	5		

- Molecule 15 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LF	103	Total	C	N	O	S	0	0
			842	538	148	154	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

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

- Molecule 17 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LH	124	Total	C	N	O	S	0	0
			1020	651	194	174	1		

- Molecule 18 is a protein called 60S ribosomal protein L26.

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

- Molecule 19 is a protein called 60S ribosomal protein L27.

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

- Molecule 20 is a protein called 60S ribosomal protein L27a.

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

- Molecule 21 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LL	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LM	88	Total	C	N	O	S	0	0
			723	451	157	112	3		

- Molecule 23 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LN	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 24 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LO	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 25 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LP	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 26 is a protein called 60S ribosomal protein L32.

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

- Molecule 27 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LR	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 28 is a protein called 60S ribosomal protein L35.

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

- Molecule 29 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LT	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 30 is a protein called 60S ribosomal protein L36.

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

- Molecule 31 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LV	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 32 is a protein called 60S ribosomal protein L37.

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

- Molecule 33 is a protein called 60S ribosomal protein L37a.

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

- Molecule 34 is a protein called 60S ribosomal protein L38.

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

- Molecule 35 is a protein called 60S ribosomal protein L39.

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

- Molecule 36 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NK	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 37 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NP	108	Total	C	N	O	S	0	0
			876	537	182	153	4		

- Molecule 38 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 39 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SB	292	Total	C	N	O	S	0	0
			2376	1499	433	430	14		

- Molecule 40 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SC	214	Total	C	N	O	S	0	0
			1715	1103	325	283	4		

- Molecule 41 is a protein called 60S ribosomal protein L7.

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

- Molecule 42 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SE	231	Total	C	N	O	S	1	0
			1869	1191	361	313	4		

- Molecule 43 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SF	245	Total	C	N	O	S	0	0
			1876	1177	383	310	6		

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

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

- Molecule 45 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SK	226	Total	C	N	O	S	0	0
			1721	1070	296	343	12		

- Molecule 46 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	SQ	123	Total	C	N	O	0	0
			610	364	123	123		

- Molecule 47 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SR	243	Total	C	N	O	S	0	0
			2002	1238	377	375	12		

- Molecule 48 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SV	139	Total	C	N	O	S	0	0
			1184	754	229	191	10		

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	L1	5	Total 5	Mg 5	0
49	L3	71	Total 71	Mg 71	0
49	L4	3	Total 3	Mg 3	0
49	LG	1	Total 1	Mg 1	0
49	LM	1	Total 1	Mg 1	0
49	LN	1	Total 1	Mg 1	0
49	LQ	1	Total 1	Mg 1	0
49	LT	1	Total 1	Mg 1	0
49	LW	1	Total 1	Mg 1	0
49	SA	1	Total 1	Mg 1	0
49	SF	1	Total 1	Mg 1	0

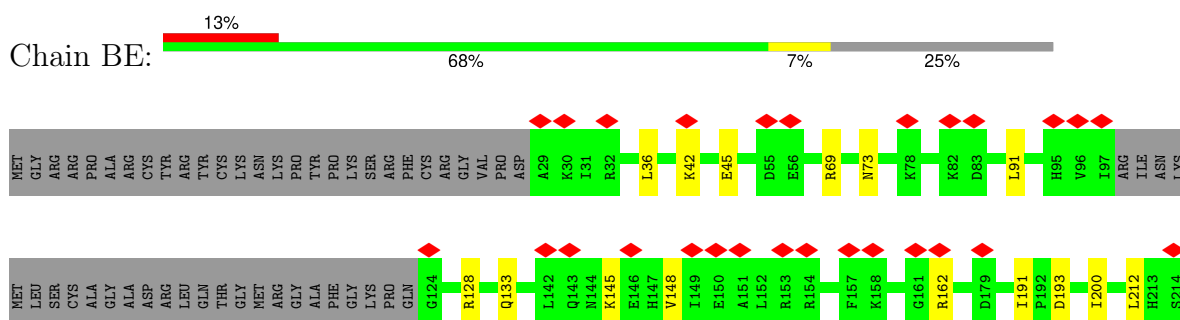
- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
50	LR	1	Total 1	Zn 1	0
50	LV	1	Total 1	Zn 1	0
50	LW	1	Total 1	Zn 1	0
50	LX	1	Total 1	Zn 1	0
50	NP	1	Total 1	Zn 1	0
50	SV	1	Total 1	Zn 1	0

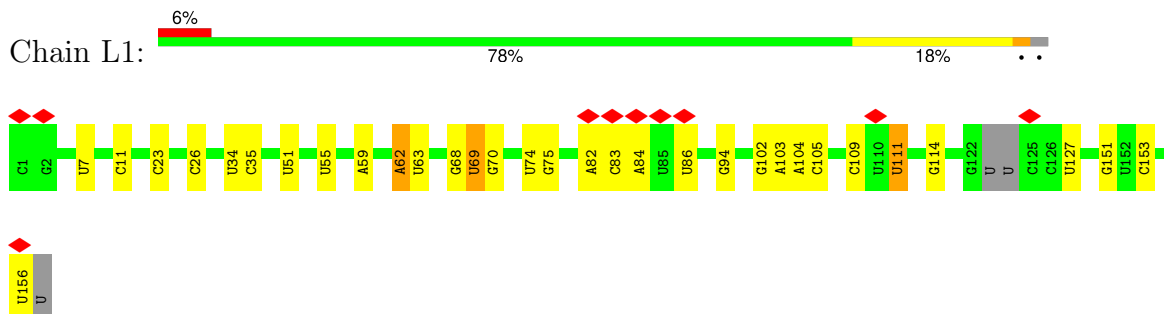
3 Residue-property plots

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

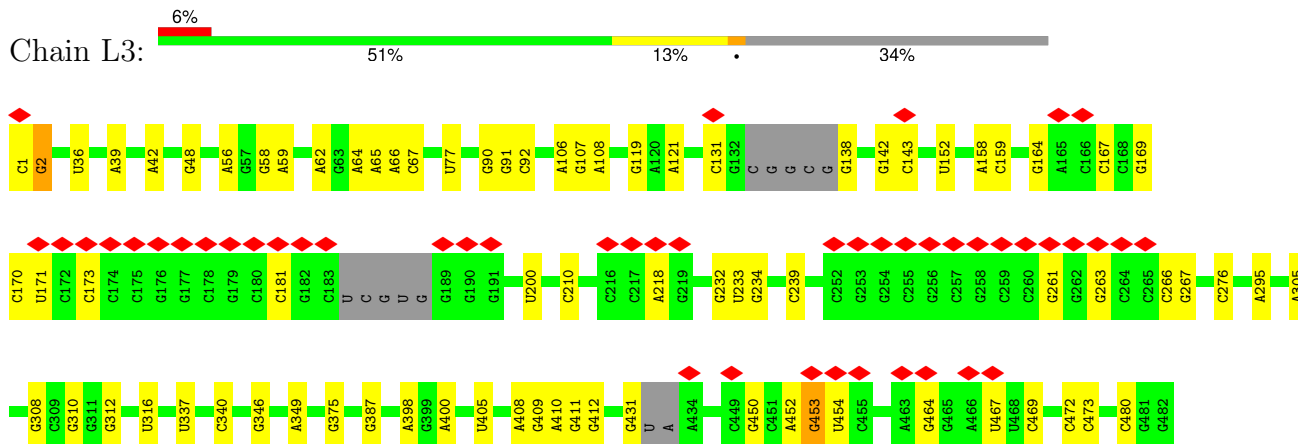
• Molecule 1: 60S ribosomal protein L10

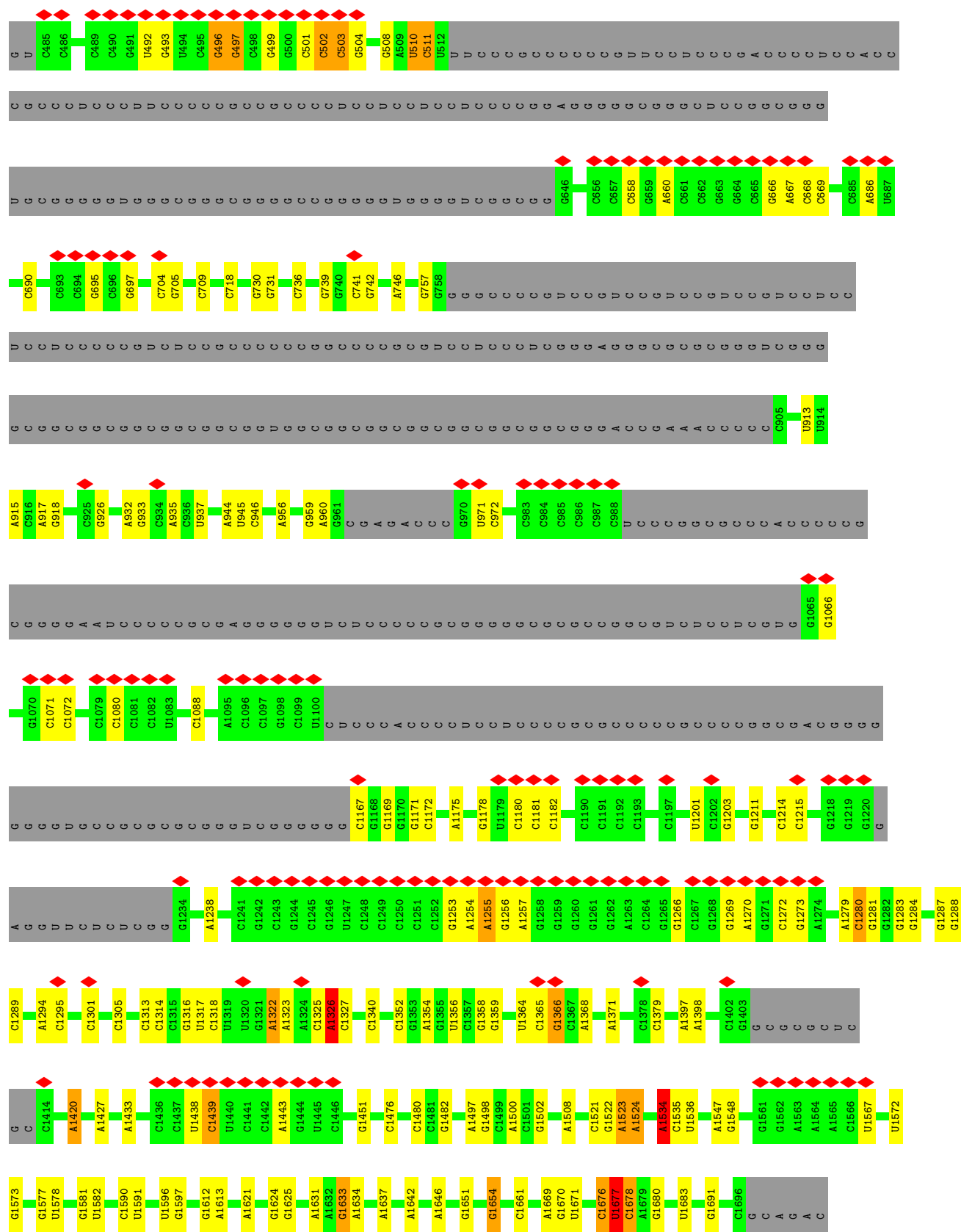


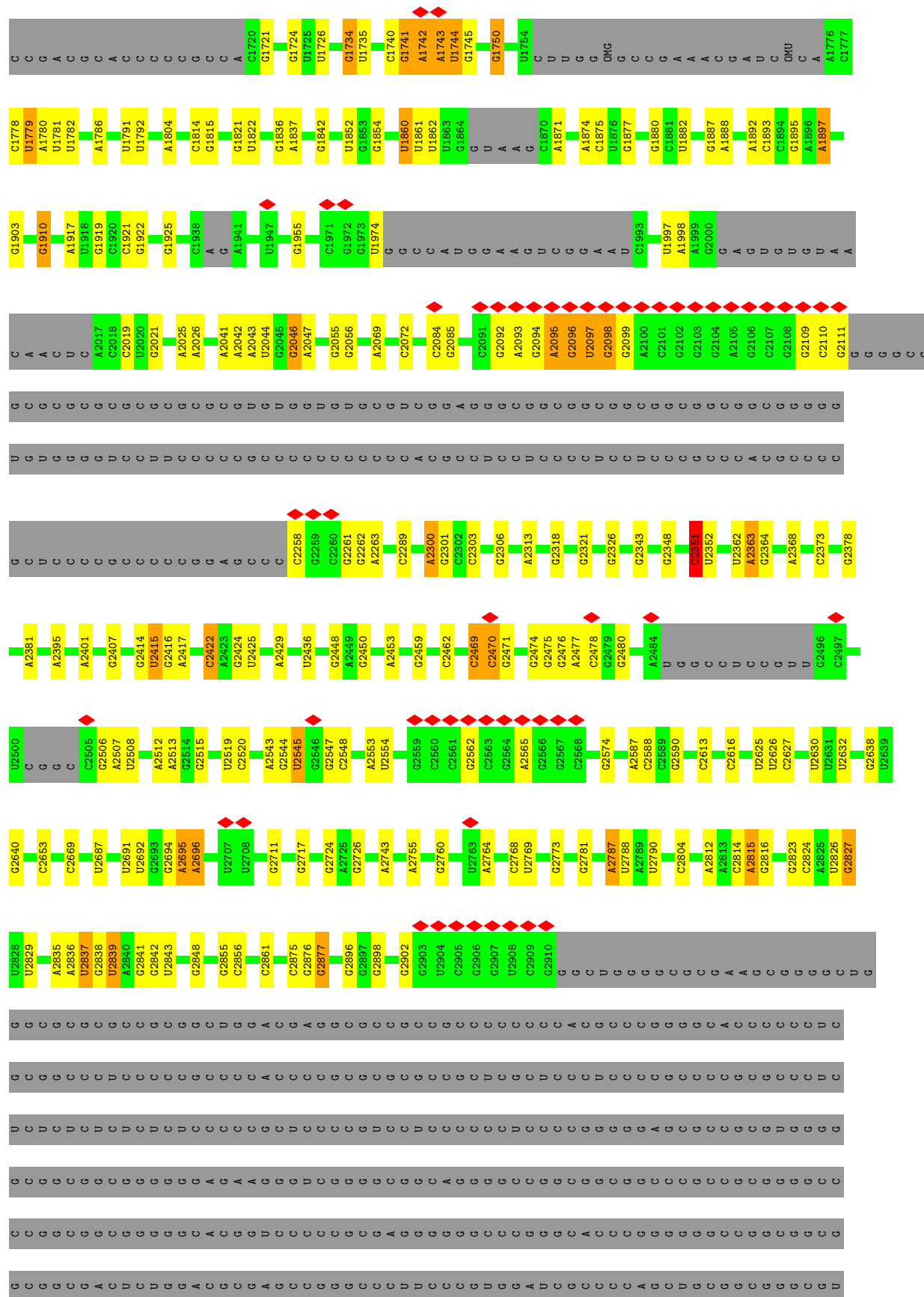
• Molecule 2: 5.8S rRNA

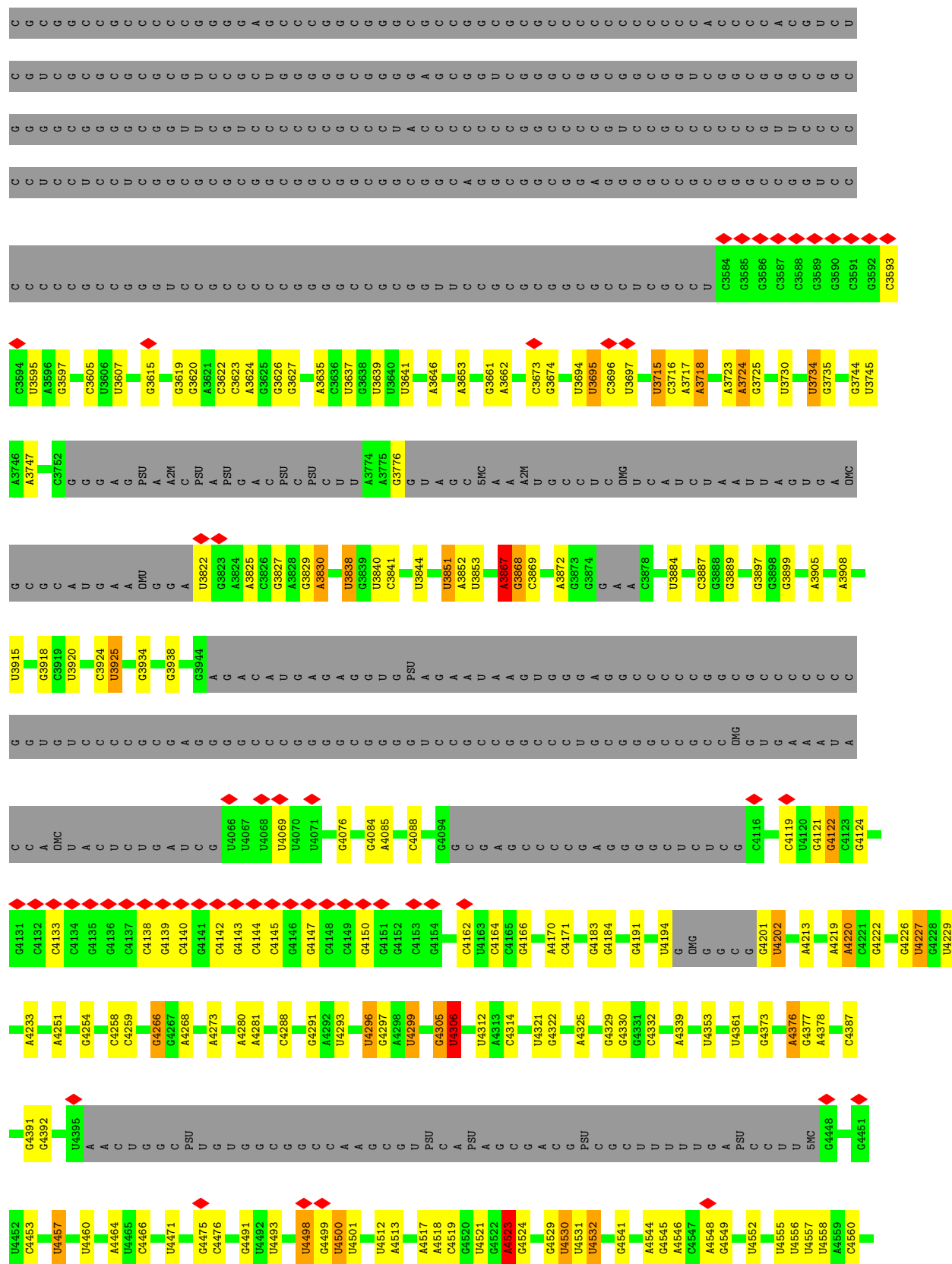


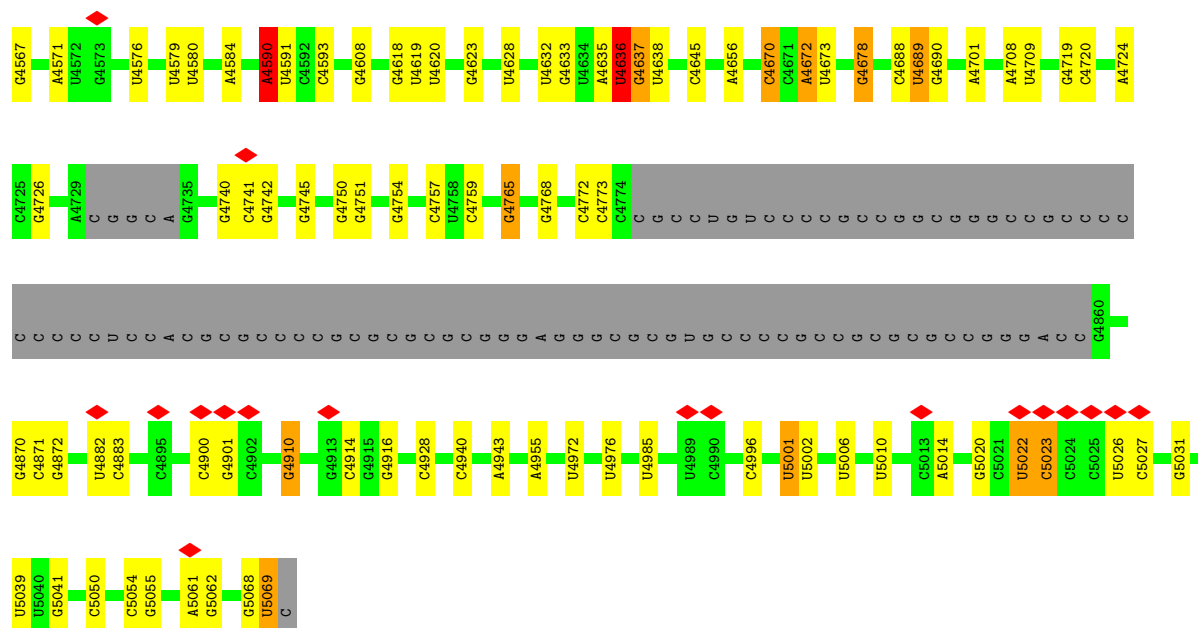
• Molecule 3: 28S rRNA



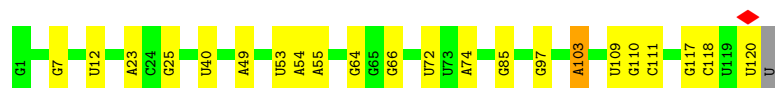
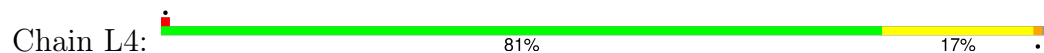




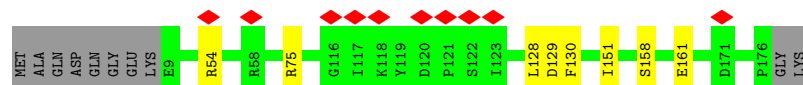
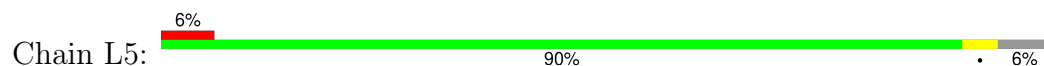




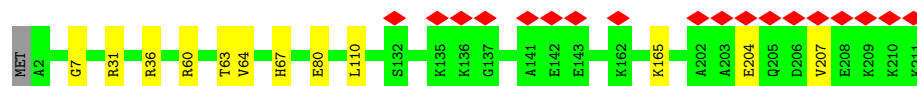
- Molecule 4: 5S rRNA



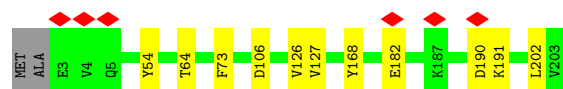
- Molecule 5: 60S ribosomal protein L11



- Molecule 6: 60S ribosomal protein L13

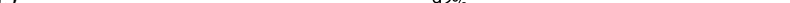


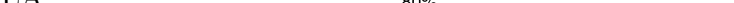
- Molecule 7: 60S ribosomal protein L13a



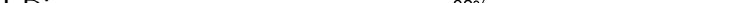
- Molecule 8: 60S ribosomal protein L14

[illegible]

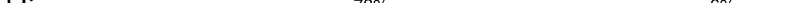
- Chain L9:  92% 7%

- Chain LA:  80% 17%

MET V2 R3 E9 M94 D110 K124 R127 M140 I146 K153 E154 GLN ILE VAL PRO LYS PRO GLU GLU GLU VAL ALA GLN LYS LYS LYS ILE ILE SER GLN LYS LYS LEU LYS LYS GLN LYS LEU MET ALA ARG ITH

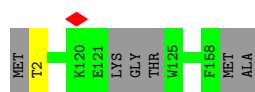
- Chain LB: 

- Chain LC: 97%

- Chain LD: 

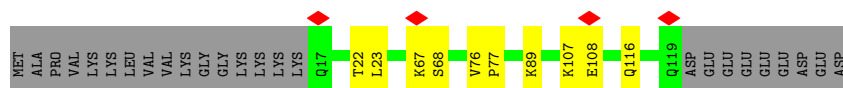
- WORLDWIDE
PDB
PROTEIN DATA BANK

Chain LE:  96%

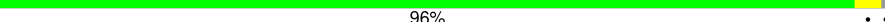


- Molecule 15: 60S ribosomal protein L22

Chain LF:  73% 8% 20%



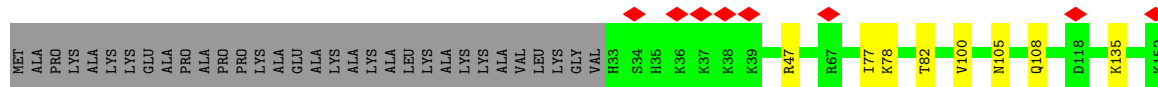
- Molecule 16: 60S ribosomal protein L23

Chain LG:  96%



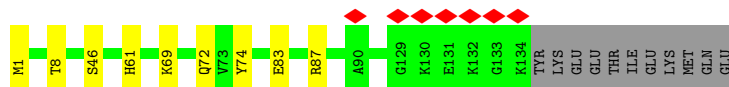
- Molecule 17: 60S ribosomal protein L23a

Chain LH:  6% 74% 5% 21%



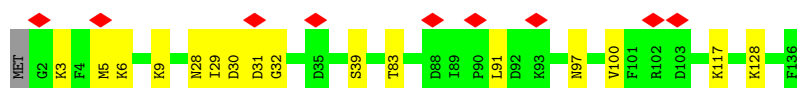
- Molecule 18: 60S ribosomal protein L26

Chain LI:  5% 86% 6% 8%



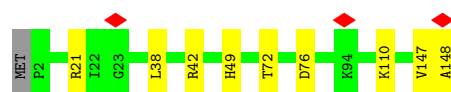
- Molecule 19: 60S ribosomal protein L27

Chain LJ:  7% 88% 12%

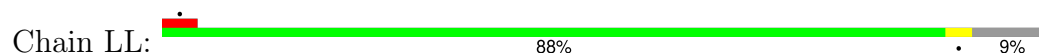


- Molecule 20: 60S ribosomal protein L27a

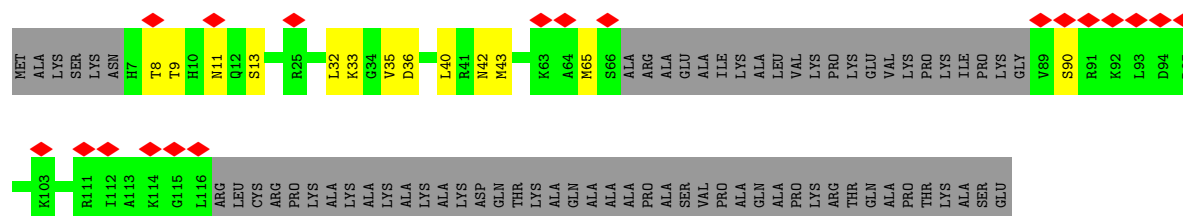
Chain LK:  93% 6%



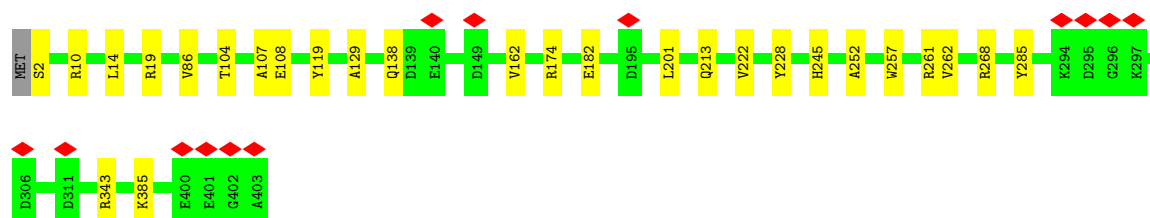
- Molecule 21: 60S ribosomal protein L28



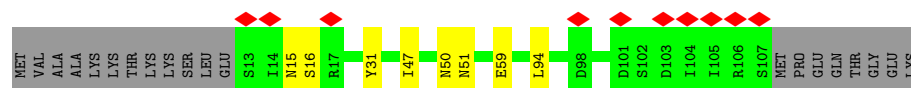
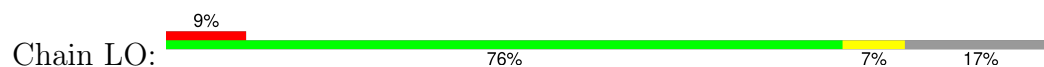
- Molecule 22: 60S ribosomal protein L29



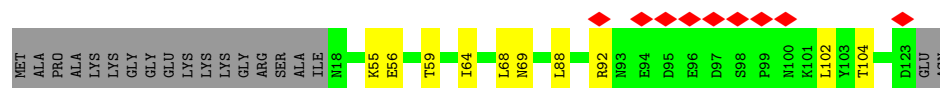
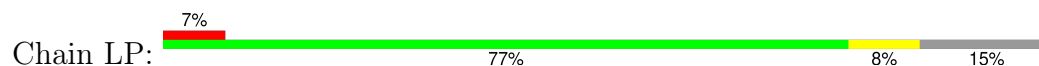
- Molecule 23: 60S ribosomal protein L3



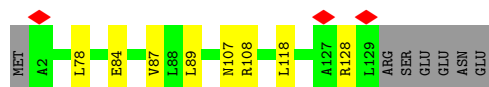
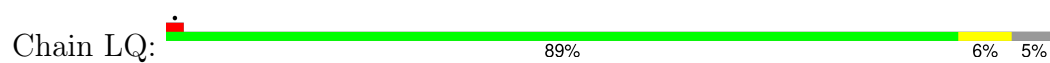
- Molecule 24: 60S ribosomal protein L30



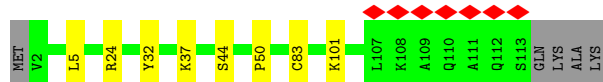
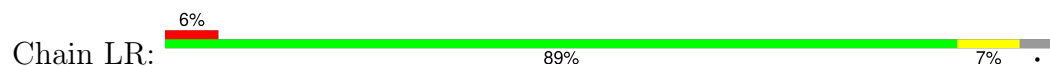
- Molecule 25: 60S ribosomal protein L31



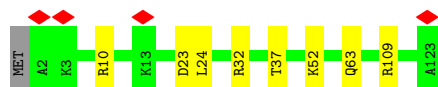
- Molecule 26: 60S ribosomal protein L32



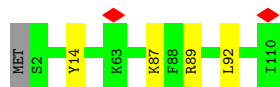
- Molecule 27: 60S ribosomal protein L34



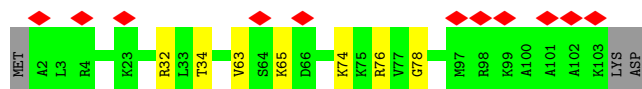
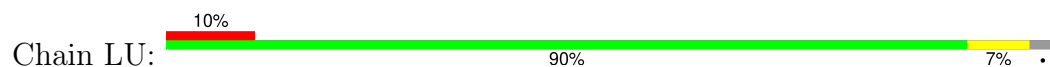
- Molecule 28: 60S ribosomal protein L35



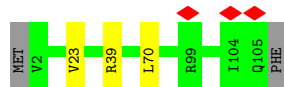
- Molecule 29: 60S ribosomal protein L35a



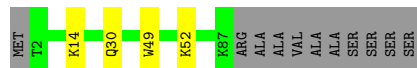
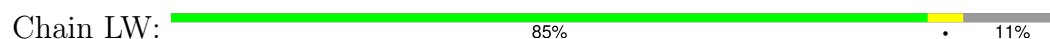
- Molecule 30: 60S ribosomal protein L36



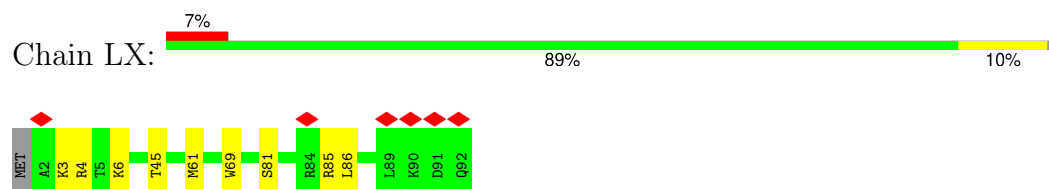
- Molecule 31: 60S ribosomal protein L36a



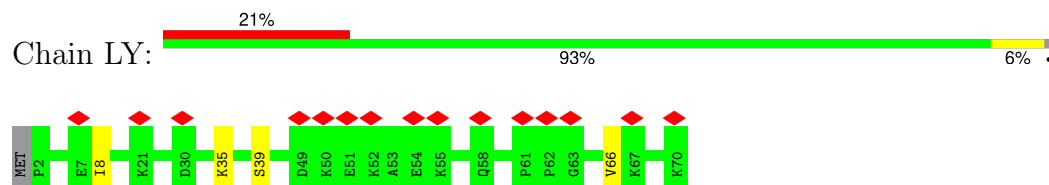
- Molecule 32: 60S ribosomal protein L37



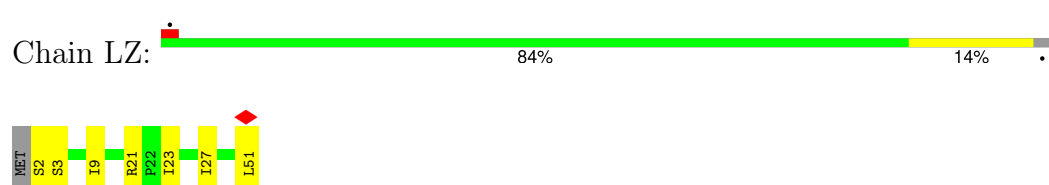
- Molecule 33: 60S ribosomal protein L37a



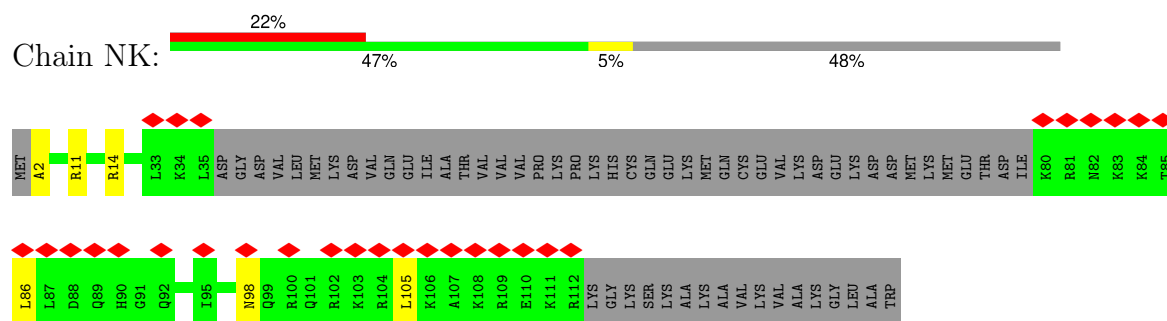
- Molecule 34: 60S ribosomal protein L38



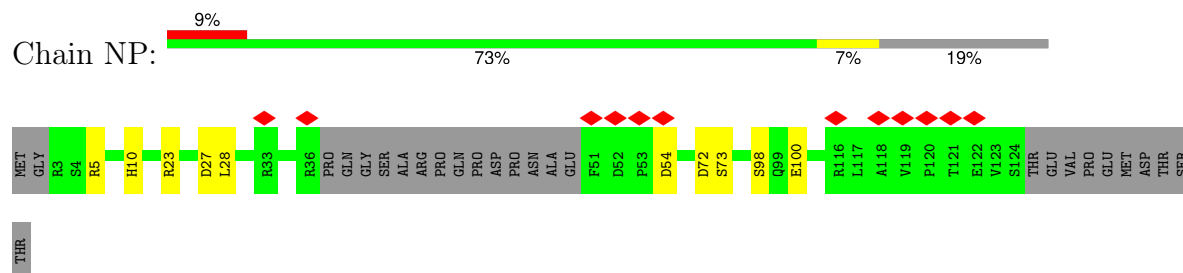
- Molecule 35: 60S ribosomal protein L39



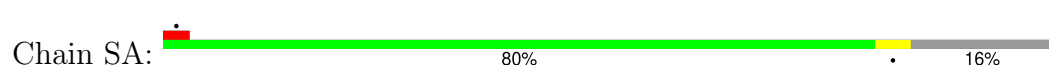
- Molecule 36: Protein LLP homolog



- Molecule 37: Zinc finger protein 593



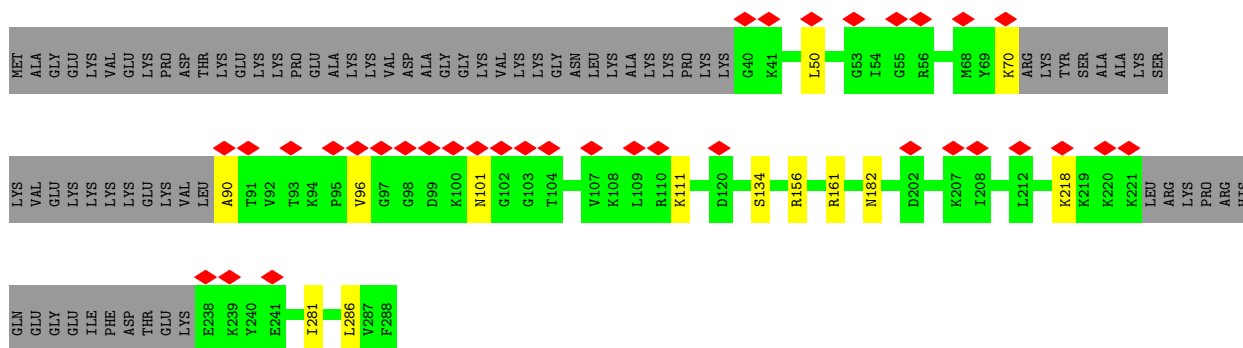
- Molecule 38: 60S ribosomal protein L4



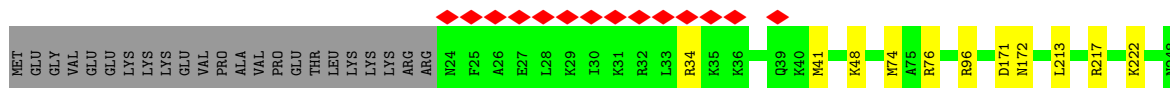
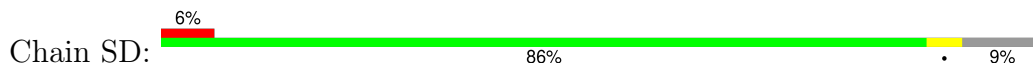
- Molecule 39: 60S ribosomal protein L5



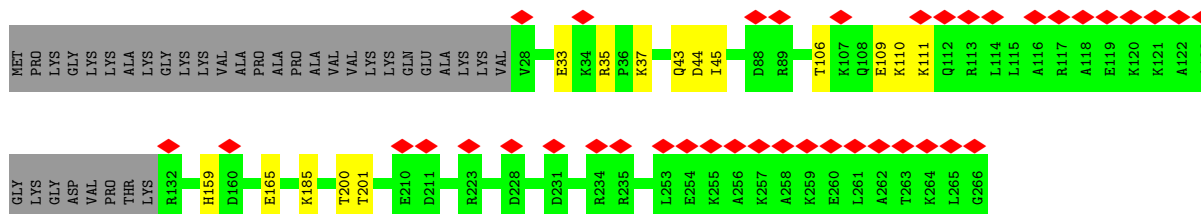
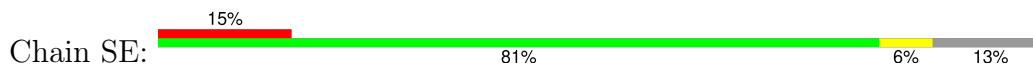
- Molecule 40: 60S ribosomal protein L6



- Molecule 41: 60S ribosomal protein L7

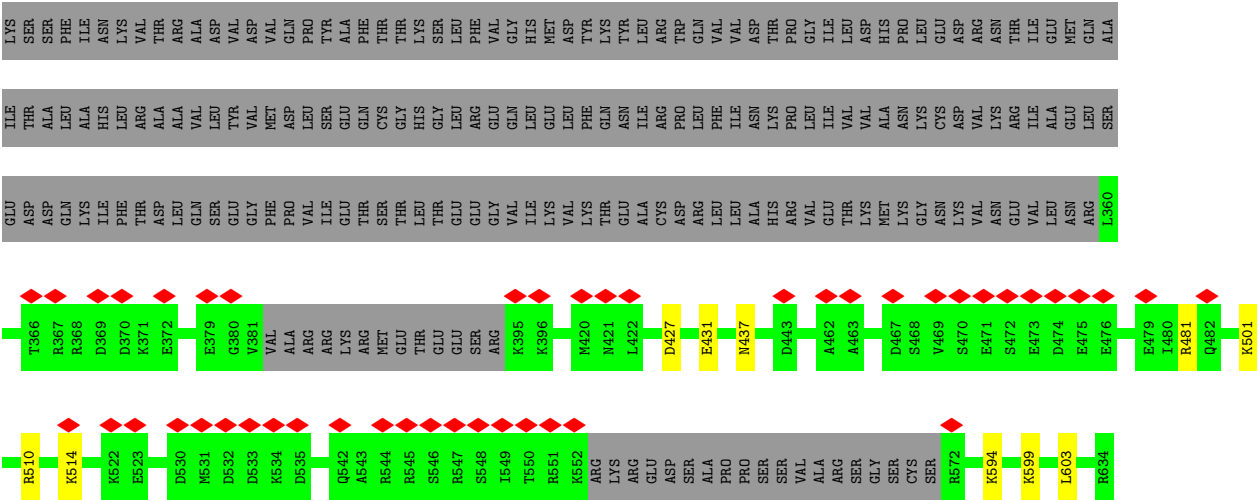


- Molecule 42: 60S ribosomal protein L7a

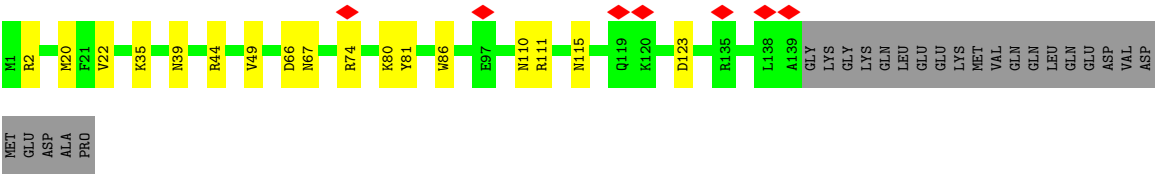


- Molecule 43: 60S ribosomal protein L8





● Molecule 48: Probable ribosome biogenesis protein RLP24



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33770	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.729	Depositor
Minimum map value	-1.531	Depositor
Average map value	0.052	Depositor
Map value standard deviation	0.180	Depositor
Recommended contour level	0.95	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 6MZ, HIC, OMU, UR3, OMG, 1MA, MG, PSU, OMC, A2M

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	BE	0.12	0/1323	0.30	0/1767
2	L1	0.15	0/3589	0.24	0/5589
3	L3	0.18	0/77299	0.27	0/120555
4	L4	0.23	0/2861	0.28	0/4459
5	L5	0.14	0/1372	0.30	0/1836
6	L6	0.14	0/1732	0.29	0/2315
7	L7	0.16	0/1682	0.29	0/2250
8	L8	0.15	0/1133	0.27	0/1516
9	L9	0.14	0/1746	0.27	0/2338
10	LA	0.14	0/1268	0.30	0/1701
11	LB	0.15	0/1536	0.31	0/2052
12	LC	0.18	0/1501	0.30	0/2013
13	LD	0.12	0/1305	0.25	0/1727
14	LE	0.18	0/1291	0.34	0/1724
15	LF	0.12	0/856	0.31	0/1149
16	LG	0.14	0/1048	0.32	0/1402
17	LH	0.11	0/1039	0.28	0/1394
18	LI	0.13	0/1132	0.28	0/1504
19	LJ	0.13	0/1130	0.27	0/1507
20	LK	0.15	0/1191	0.28	0/1591
21	LL	0.12	0/1017	0.26	0/1364
22	LM	0.14	0/735	0.31	0/970
23	LN	0.14	0/3294	0.30	0/4406
24	LO	0.11	0/748	0.24	0/1004
25	LP	0.14	0/894	0.28	0/1204
26	LQ	0.14	0/1071	0.28	0/1429
27	LR	0.14	0/898	0.33	0/1197
28	LS	0.11	0/1023	0.24	0/1351
29	LT	0.14	0/895	0.30	0/1198
30	LU	0.12	0/843	0.27	0/1115
31	LV	0.17	0/864	0.31	0/1140
32	LW	0.15	0/720	0.32	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LX	0.14	0/718	0.34	0/953
34	LY	0.11	0/575	0.27	0/761
35	LZ	0.14	0/454	0.27	0/599
36	NK	0.12	0/587	0.25	0/767
37	NP	0.12	0/893	0.27	0/1194
38	SA	0.14	0/2907	0.28	0/3905
39	SB	0.17	0/2421	0.30	0/3241
40	SC	0.12	0/1748	0.29	0/2345
41	SD	0.14	0/1905	0.28	0/2539
42	SE	0.13	0/1903	0.30	0/2559
43	SF	0.14	0/1914	0.32	0/2567
44	SG	0.15	0/1537	0.27	0/2066
45	SK	0.14	0/1745	0.31	0/2374
46	SQ	0.07	0/608	0.24	0/845
47	SR	0.11	0/2026	0.28	0/2690
48	SV	0.17	0/1207	0.31	0/1600
All	All	0.16	0/142184	0.28	0/208724

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	BE	1295	0	1331	10	0
2	L1	3278	0	1665	11	0
3	L3	71370	0	36162	287	0
4	L4	2561	0	1295	9	0
5	L5	1349	0	1383	6	0
6	L6	1701	0	1818	8	0
7	L7	1650	0	1794	8	0
8	L8	1111	0	1174	8	0
9	L9	1701	0	1749	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	LA	1242	0	1269	4	0
11	LB	1512	0	1628	10	0
12	LC	1461	0	1502	4	0
13	LD	1289	0	1429	10	0
14	LE	1264	0	1328	1	0
15	LF	842	0	864	7	0
16	LG	1034	0	1097	6	0
17	LH	1020	0	1098	6	0
18	LI	1115	0	1205	8	0
19	LJ	1107	0	1182	9	0
20	LK	1162	0	1213	7	0
21	LL	1002	0	1068	4	0
22	LM	723	0	779	11	0
23	LN	3239	0	3377	20	0
24	LO	738	0	774	4	0
25	LP	879	0	924	6	0
26	LQ	1053	0	1147	6	0
27	LR	888	0	977	7	0
28	LS	1015	0	1148	6	0
29	LT	876	0	912	3	0
30	LU	832	0	917	5	0
31	LV	851	0	920	3	0
32	LW	705	0	737	4	0
33	LX	708	0	756	10	0
34	LY	569	0	637	5	0
35	LZ	444	0	483	6	0
36	NK	581	0	656	5	0
37	NP	876	0	881	7	0
38	SA	2853	0	3028	12	0
39	SB	2376	0	2403	7	0
40	SC	1715	0	1862	10	0
41	SD	1870	0	1996	10	0
42	SE	1869	0	2014	12	0
43	SF	1876	0	1970	12	0
44	SG	1518	0	1601	10	0
45	SK	1721	0	1695	14	0
46	SQ	610	0	257	1	0
47	SR	2002	0	2072	9	0
48	SV	1184	0	1248	14	0
49	L1	5	0	0	0	0
49	L3	71	0	0	0	0
49	L4	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	LG	1	0	0	0	0
49	LM	1	0	0	0	0
49	LN	1	0	0	0	0
49	LQ	1	0	0	0	0
49	LT	1	0	0	0	0
49	LW	1	0	0	0	0
49	SA	1	0	0	0	0
49	SF	1	0	0	0	0
50	LR	1	0	0	0	0
50	LV	1	0	0	0	0
50	LW	1	0	0	0	0
50	LX	1	0	0	0	0
50	NP	1	0	0	0	0
50	SV	1	0	0	0	0
All	All	134730	0	99425	482	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 2.

All (482) 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)
6:L6:60:ARG:NH2	6:L6:67:HIS:O	2.05	0.89
42:SE:106:THR:OG1	42:SE:109:GLU:OE1	1.92	0.86
4:L4:40:U:O2	5:L5:75:ARG:NH1	2.09	0.86
3:L3:2520:C:O2	3:L3:2640:G:N2	2.09	0.85
2:L1:51:U:OP2	35:LZ:21:ARG:NH2	2.09	0.85
3:L3:4220:6MZ:OP2	14:LE:2:THR:OG1	1.94	0.85
3:L3:3867:A2M:H8	3:L3:3867:A2M:H5''	1.57	0.84
3:L3:1480:C:O2'	3:L3:1482:G:OP2	1.96	0.83
3:L3:1317:U:OP1	20:LK:21:ARG:NH2	2.12	0.82
4:L4:72:U:O2	4:L4:103:A:N6	2.13	0.81
3:L3:4517:A:OP2	23:LN:2:SER:OG	1.98	0.80
3:L3:1572:U:O4	33:LX:4:ARG:NH2	2.16	0.78
3:L3:2300:A:N6	38:SA:178:ASN:OD1	2.17	0.78
3:L3:2448:G:O2'	43:Sf:21:LYS:NZ	2.17	0.78
3:L3:2773:G:OP1	34:LY:39:SER:OG	2.02	0.78
2:L1:62:A:OP1	28:LS:52:LYS:NZ	2.18	0.77
3:L3:1214:C:N4	22:LM:90:SER:O	2.18	0.77
3:L3:2545:U:O2'	3:L3:2547:G:N7	2.16	0.77
3:L3:1280:C:O2'	38:SA:321:ASN:OD1	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:152:U:OP2	9:L9:49:ARG:NH1	2.19	0.76
3:L3:5068:G:N2	3:L3:5069:U:O4	2.19	0.76
4:L4:12:U:O3'	4:L4:109:U:O2'	2.04	0.76
3:L3:308:G:OP2	3:L3:308:G:N2	2.17	0.75
3:L3:143:C:OP1	42:SE:111:LYS:NZ	2.20	0.75
3:L3:4688:C:O2'	44:SG:155:SER:OG	2.04	0.75
7:L7:182:GLU:OE2	8:L8:119:ARG:NH2	2.20	0.74
3:L3:1289:C:OP1	40:SC:218:LYS:NZ	2.20	0.74
3:L3:2263:A:OP1	21:LL:107:ARG:NH2	2.19	0.74
3:L3:4124:G:N2	42:SE:43:GLN:O	2.20	0.74
3:L3:62:A:N3	3:L3:77:U:O2'	2.20	0.74
3:L3:295:A:OP2	31:LV:39:ARG:NH1	2.22	0.73
3:L3:937:U:OP1	8:L8:46:ARG:NH1	2.21	0.73
39:SB:184:ASP:OD2	39:SB:187:SER:OG	2.05	0.73
3:L3:4985:U:O2	23:LN:174:ARG:NH1	2.22	0.73
3:L3:3776:G:N2	3:L3:3776:G:OP2	2.20	0.72
45:SK:79:GLN:NE2	47:SR:431:GLU:OE1	2.21	0.72
3:L3:2318:G:N2	3:L3:2321:G:OP2	2.16	0.72
33:LX:86:LEU:HD21	43:SF:108:PRO:HG2	1.71	0.72
3:L3:3747:A:N7	43:SF:245:ARG:NH2	2.36	0.72
26:LQ:84:GLU:O	26:LQ:87:VAL:HG12	1.88	0.71
3:L3:276:C:OP2	30:LU:34:THR:HG21	1.91	0.71
13:LD:52:ARG:NH1	13:LD:53:LYS:O	2.22	0.71
3:L3:408:A:O2'	3:L3:411:G:OP2	2.08	0.70
3:L3:2695:A:OP1	34:LY:35:LYS:NZ	2.24	0.70
37:NP:72:ASP:OD1	37:NP:73:SER:N	2.24	0.70
3:L3:2848:G:O2'	3:L3:3838:U:O4	2.05	0.70
3:L3:502:C:O2'	3:L3:503:C:OP1	2.05	0.70
9:L9:44:ARG:NH2	9:L9:120:TRP:O	2.25	0.69
44:SG:129:ARG:NH1	44:SG:156:ASN:OD1	2.25	0.69
3:L3:67:C:OP2	3:L3:312:G:N2	2.23	0.69
3:L3:1646:A:O2'	32:LW:49:TRP:O	2.09	0.69
3:L3:2875:C:O2'	33:LX:6:LYS:NZ	2.19	0.69
11:LB:122:THR:OG1	11:LB:124:ASP:OD1	2.06	0.69
22:LM:8:THR:O	22:LM:11:ASN:ND2	2.26	0.69
17:LH:78:LYS:O	28:LS:32:ARG:NE	2.24	0.69
16:LG:67:LYS:NZ	37:NP:54:ASP:OD2	2.25	0.69
3:L3:695:G:O2'	3:L3:697:G:OP2	2.10	0.68
3:L3:1364:U:OP2	6:L6:36:ARG:NH1	2.26	0.68
3:L3:2553:A:OP2	3:L3:2574:G:O2'	2.08	0.68
4:L4:55:A:O2'	5:L5:151:ILE:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:1998:A:N3	3:L3:2019:C:O2'	2.27	0.68
25:LP:59:THR:HG1	25:LP:104:THR:HG1	1.42	0.68
3:L3:2625:U:OP2	47:SR:510:ARG:NH2	2.27	0.67
3:L3:4314:C:O2'	22:LM:36:ASP:OD1	2.11	0.67
23:LN:108:GLU:OE2	23:LN:138:GLN:NE2	2.28	0.67
19:LJ:3:LYS:O	19:LJ:6:LYS:NZ	2.27	0.67
3:L3:1071:C:O2	40:SC:70:LYS:NZ	2.28	0.67
3:L3:2724:G:O2'	3:L3:2726:G:OP2	2.13	0.66
9:L9:11:TRP:NE1	42:SE:165:GLU:OE1	2.29	0.66
3:L3:2841:G:OP1	37:NP:10:HIS:NE2	2.23	0.66
47:SR:437:ASN:OD1	48:SV:2:ARG:NH1	2.29	0.66
3:L3:4623:OMG:OP1	23:LN:19:ARG:NH2	2.28	0.65
3:L3:4872:G:O6	8:L8:98:ARG:NH1	2.28	0.65
16:LG:96:LEU:HD11	48:SV:22:VAL:HG23	1.77	0.65
3:L3:1895:G:OP1	41:SD:96:ARG:NH2	2.30	0.65
4:L4:117:G:OP1	39:SB:253:TYR:OH	2.14	0.65
45:SK:99:GLU:OE1	45:SK:125:THR:OG1	2.15	0.65
3:L3:1325:C:H2'	3:L3:1326:A2M:H5'	1.78	0.64
3:L3:4460:U:OP1	23:LN:10:ARG:NH1	2.30	0.64
45:SK:88:LEU:O	48:SV:80:LYS:NZ	2.30	0.64
3:L3:121:A:OP1	42:SE:110:LYS:NZ	2.29	0.64
3:L3:453:G:O2'	3:L3:705:G:OP1	2.16	0.64
40:SC:161:ARG:O	40:SC:182:ASN:ND2	2.30	0.63
3:L3:2898:G:OP2	13:LD:135:LYS:NZ	2.23	0.63
20:LK:38:LEU:O	20:LK:42:ARG:NH1	2.32	0.63
3:L3:1743:A:O2'	3:L3:1744:PSU:H5''	1.98	0.63
3:L3:4765:G:OP1	44:SG:23:ARG:NE	2.31	0.63
42:SE:37:LYS:NZ	42:SE:44:ASP:OD2	2.30	0.62
3:L3:1255:A:OP1	3:L3:1257:A:N6	2.32	0.62
3:L3:4476:C:O2'	44:SG:173:ARG:NH2	2.32	0.62
7:L7:64:THR:OG1	23:LN:261:ARG:NH1	2.32	0.62
25:LP:55:LYS:NZ	25:LP:56:GLU:OE2	2.32	0.62
3:L3:2373:C:O4'	25:LP:69:ASN:ND2	2.33	0.62
3:L3:2258:C:N3	40:SC:90:ALA:N	2.48	0.62
3:L3:935:A:O2'	8:L8:46:ARG:NH1	2.33	0.62
3:L3:1368:A:C2	18:LI:1:MET:HE3	2.35	0.62
3:L3:4299:PSU:OP1	22:LM:33:LYS:NZ	2.28	0.62
3:L3:158:A:N1	3:L3:276:C:O2'	2.28	0.61
45:SK:103:ALA:O	45:SK:107:VAL:HG23	2.01	0.61
22:LM:32:LEU:HD13	22:LM:43:MET:HE1	1.82	0.61
19:LJ:31:ASP:OD1	19:LJ:32:GLY:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:3620:G:OP1	3:L3:3622:C:N4	2.34	0.60
44:SG:113:GLU:OE1	44:SG:115:ARG:NH2	2.34	0.60
3:L3:4088:C:OP1	43:SF:37:ARG:NH2	2.34	0.60
2:L1:109:C:O2'	2:L1:111:U:OP2	2.18	0.60
3:L3:2588:C:OP1	3:L3:2768:C:O2'	2.14	0.60
3:L3:375:G:OP2	32:LW:52:LYS:NZ	2.31	0.60
3:L3:4305:G:O2'	3:L3:4306:OMU:O5'	2.14	0.60
3:L3:4678:G:OP2	36:NK:14:ARG:NH1	2.35	0.60
11:LB:79:THR:CG2	11:LB:136:THR:HG22	2.31	0.60
1:BE:145:LYS:O	1:BE:148:VAL:HG12	2.02	0.60
3:L3:5039:U:O2'	48:SV:115:ASN:OD1	2.20	0.60
3:L3:1744:PSU:H2'	3:L3:1745:G:H8	1.67	0.59
3:L3:4213:A:H2'	22:LM:9:THR:HG21	1.83	0.59
3:L3:1326:A2M:H2'	3:L3:1327:C:H6	1.67	0.59
3:L3:1874:A:O2'	3:L3:4219:A:N3	2.29	0.59
3:L3:2696:A:H62	34:LY:35:LYS:HZ2	1.50	0.59
3:L3:1548:G:O2'	3:L3:2812:A:N3	2.33	0.59
3:L3:4910:G:N2	7:L7:106:ASP:O	2.35	0.59
9:L9:193:ARG:O	9:L9:197:THR:HG23	2.02	0.59
3:L3:1326:A2M:H2'	3:L3:1327:C:C6	2.37	0.59
7:L7:202:LEU:O	7:L7:202:LEU:HD23	2.03	0.59
3:L3:4928:C:O4'	8:L8:121:ARG:NH1	2.35	0.58
3:L3:2876:OMG:HM22	3:L3:2877:G:H5'	1.85	0.58
3:L3:1433:A:N6	3:L3:1451:G:O2'	2.36	0.58
3:L3:3605:C:OP2	13:LD:71:ARG:NH1	2.36	0.58
4:L4:7:G:OP1	39:SB:33:ARG:NH1	2.37	0.58
3:L3:508:G:O2'	3:L3:510:U:OP2	2.10	0.58
3:L3:3623:C:O2	13:LD:82:LYS:NZ	2.36	0.58
3:L3:3838:U:OP2	37:NP:23:ARG:NH2	2.37	0.57
42:SE:33:GLU:OE2	42:SE:35:ARG:NH2	2.36	0.57
3:L3:4457:PSU:H1'	23:LN:252:ALA:HB3	1.86	0.57
24:LO:31:TYR:OH	24:LO:59:GLU:OE2	2.19	0.57
31:LV:23:VAL:HG12	31:LV:70:LEU:HD23	1.86	0.57
3:L3:3908:A:O2'	3:L3:4531:U:OP1	2.21	0.57
15:LF:67:LYS:O	15:LF:68:SER:OG	2.21	0.57
47:SR:427:ASP:OD2	48:SV:81:TYR:OH	2.22	0.57
3:L3:480:C:OP1	21:LL:67:ARG:NH1	2.37	0.57
3:L3:1676:C:OP2	3:L3:1677:PSU:N1	2.35	0.57
3:L3:2414:G:O2'	3:L3:2415:OMU:H5''	2.05	0.57
3:L3:4678:G:N7	36:NK:11:ARG:NH2	2.52	0.57
3:L3:1366:G:N2	3:L3:1371:A:OP2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:26:C:O2'	38:SA:53:ALA:O	2.23	0.57
4:L4:23:A:N3	4:L4:118:C:O2'	2.27	0.57
3:L3:1508:A:OP1	38:SA:110:ARG:NH2	2.38	0.57
44:SG:128:MET:HA	44:SG:128:MET:HE2	1.87	0.57
27:LR:5:LEU:HD13	27:LR:32:TYR:CE1	2.40	0.56
3:L3:1567:U:OP1	33:LX:3:LYS:NZ	2.27	0.56
48:SV:35:LYS:O	48:SV:39:ASN:ND2	2.39	0.56
3:L3:1744:PSU:H2'	3:L3:1745:G:C8	2.40	0.56
1:BE:193:ASP:OD2	3:L3:1750:G:N2	2.38	0.55
3:L3:2042:A:O2'	3:L3:2043:A:O4'	2.17	0.55
2:L1:69:PSU:H2'	2:L1:70:G:O4'	2.06	0.55
3:L3:1734:G:N2	3:L3:1735:U:O4	2.33	0.55
3:L3:2717:G:OP1	15:LF:107:LYS:NZ	2.39	0.55
3:L3:4637:OMG:H2'	3:L3:4638:U:C6	2.41	0.55
9:L9:43:THR:OG1	9:L9:131:GLU:OE2	2.21	0.55
3:L3:3718:A2M:H2	3:L3:3934:G:O4'	2.07	0.55
11:LB:88:ASP:OD1	11:LB:89:ASP:N	2.40	0.55
3:L3:1279:A:O2'	38:SA:323:ARG:NH1	2.40	0.55
29:LT:14:TYR:OH	29:LT:92:LEU:O	2.22	0.55
3:L3:1591:U:OP2	3:L3:2856:C:O2'	2.22	0.55
33:LX:69:TRP:NE1	43:SF:173:GLY:O	2.40	0.55
40:SC:281:ILE:CG2	40:SC:286:LEU:HD11	2.37	0.55
3:L3:5001:PSU:H2'	3:L3:5002:U:O4'	2.07	0.54
23:LN:262:VAL:HG11	23:LN:268:ARG:HH21	1.73	0.54
6:L6:204:GLU:O	6:L6:207:VAL:HG22	2.08	0.54
3:L3:4726:G:OP2	36:NK:98:ASN:ND2	2.38	0.54
3:L3:2838:G:O2'	3:L3:2839:PSU:H5''	2.08	0.54
7:L7:190:ASP:OD1	7:L7:191:LYS:N	2.40	0.54
3:L3:267:G:OP1	28:LS:109:ARG:NH2	2.40	0.54
3:L3:1573:G:OP1	13:LD:92:LYS:NZ	2.40	0.54
3:L3:2262:G:OP2	21:LL:98:ARG:NH2	2.39	0.54
28:LS:10:ARG:NH2	28:LS:63:GLN:OE1	2.40	0.54
48:SV:44:ARG:NH1	48:SV:49:VAL:HG22	2.22	0.54
3:L3:2303:C:OP1	26:LQ:107:ASN:ND2	2.40	0.54
3:L3:4645:C:OP2	13:LD:62:ARG:NH1	2.41	0.54
3:L3:1903:G:OP1	29:LT:87:LYS:NZ	2.40	0.54
3:L3:2343:G:OP2	38:SA:109:ARG:NH2	2.41	0.54
2:L1:75:OMG:OP2	18:LI:74:TYR:OH	2.25	0.53
3:L3:496:G:O2'	3:L3:497:G:OP1	2.26	0.53
3:L3:1741:G:H3'	3:L3:1742:A:H5''	1.90	0.53
24:LO:50:ASN:OD1	24:LO:51:ASN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:690:C:OP1	40:SC:111:LYS:NZ	2.36	0.53
3:L3:4500:PSU:H2'	3:L3:4501:U:C6	2.42	0.53
3:L3:1438:U:O2'	3:L3:1439:C:OP1	2.22	0.53
9:L9:33:LEU:O	9:L9:65:ARG:NH2	2.41	0.53
3:L3:2416:G:O4'	47:SR:594:LYS:NZ	2.33	0.53
4:L4:85:G:OP1	41:SD:222:LYS:NZ	2.35	0.53
16:LG:96:LEU:HD11	48:SV:22:VAL:CG2	2.38	0.53
3:L3:1778:C:O2'	3:L3:1779:PSU:H5''	2.08	0.53
3:L3:1860:PSU:H2'	3:L3:1861:U:C6	2.43	0.53
3:L3:4296:PSU:H2'	3:L3:4297:G:O4'	2.09	0.53
3:L3:4226:G:O2'	3:L3:4227:OMU:H5''	2.08	0.53
9:L9:165:THR:HG23	9:L9:168:GLY:H	1.74	0.53
27:LR:44:SER:OG	27:LR:83:CYS:N	2.41	0.53
3:L3:3938:G:N2	3:L3:4171:C:OP2	2.41	0.53
3:L3:3641:U:OP2	3:L3:3646:A:N6	2.33	0.53
3:L3:3924:C:O2'	3:L3:3925:OMU:H5''	2.07	0.53
10:LA:124:LYS:HB3	10:LA:140:MET:HE3	1.91	0.52
45:SK:121:LEU:O	45:SK:139:ARG:NH1	2.42	0.52
3:L3:1427:A:C2	11:LB:138:LEU:HD23	2.45	0.52
12:LC:24:THR:HG23	12:LC:24:THR:O	2.09	0.52
17:LH:105:ASN:ND2	17:LH:108:GLN:OE1	2.42	0.52
3:L3:1283:G:O6	38:SA:312:ARG:NH2	2.43	0.52
3:L3:2626:U:OP2	47:SR:501:LYS:NZ	2.40	0.52
3:L3:4529:G:O2'	3:L3:4530:UR3:H5'	2.09	0.52
33:LX:86:LEU:HD23	33:LX:86:LEU:O	2.10	0.52
15:LF:108:GLU:N	15:LF:108:GLU:OE1	2.43	0.52
3:L3:709:C:OP1	29:LT:89:ARG:NH2	2.43	0.52
3:L3:4670:C:O2'	3:L3:4672:A:OP2	2.24	0.51
3:L3:1523:A:O2'	3:L3:1524:A2M:H5'	2.10	0.51
41:SD:171:ASP:OD1	41:SD:172:ASN:N	2.44	0.51
26:LQ:89:LEU:HD13	26:LQ:118:LEU:HD22	1.92	0.51
48:SV:66:ASP:OD1	48:SV:67:ASN:N	2.44	0.51
3:L3:2562:G:O2'	3:L3:2565:A:N6	2.44	0.51
3:L3:4259:C:OP2	5:L5:54:ARG:NH2	2.44	0.51
34:LY:8:ILE:HD12	34:LY:8:ILE:H	1.76	0.51
3:L3:1677:PSU:H4'	3:L3:1680:G:C2	2.46	0.51
3:L3:4280:A:N6	39:SB:28:THR:O	2.44	0.51
3:L3:1325:C:C2'	3:L3:1326:A2M:H5'	2.40	0.51
3:L3:3607:U:OP1	13:LD:88:ARG:NH1	2.43	0.50
3:L3:3661:G:N7	43:SF:152:SER:OG	2.44	0.50
3:L3:4523:A2M:H8	3:L3:4523:A2M:OP2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L9:103:GLU:OE1	9:L9:165:THR:HG21	2.11	0.50
37:NP:27:ASP:OD1	37:NP:28:LEU:N	2.40	0.50
3:L3:1279:A:O2'	3:L3:1281:G:N7	2.38	0.50
11:LB:99:LYS:NZ	11:LB:121:LEU:HD11	2.26	0.50
42:SE:44:ASP:OD1	42:SE:45:ILE:N	2.44	0.50
2:L1:11:C:O3'	10:LA:3:ARG:NH2	2.45	0.50
23:LN:222:VAL:O	23:LN:343:ARG:NH1	2.45	0.50
3:L3:239:C:OP1	18:LI:46:SER:OG	2.29	0.50
3:L3:4940:C:OP1	40:SC:156:ARG:NH2	2.45	0.50
19:LJ:30:ASP:O	19:LJ:39:SER:OG	2.12	0.49
33:LX:81:SER:OG	33:LX:85:ARG:NH1	2.31	0.49
1:BE:128:ARG:HH22	3:L3:1786:A:P	2.35	0.49
6:L6:7:GLY:O	20:LK:49:HIS:NE2	2.45	0.49
23:LN:86:VAL:HG13	23:LN:162:VAL:HG13	1.94	0.49
30:LU:63:VAL:HG23	30:LU:65:LYS:HG2	1.93	0.49
3:L3:36:U:OP1	3:L3:1651:G:N2	2.41	0.49
3:L3:1633:G:O6	3:L3:3918:G:O2'	2.29	0.49
42:SE:200:THR:HG22	42:SE:201:THR:HG23	1.94	0.49
3:L3:2351:OMC:HM23	38:SA:95:MET:HG3	1.94	0.49
3:L3:1088:C:O2	41:SD:74:MET:HE1	2.13	0.49
3:L3:4541:G:N2	3:L3:4544:A:OP2	2.38	0.49
3:L3:4633:G:O2'	3:L3:4635:A:OP2	2.28	0.49
3:L3:405:U:OP1	18:LI:87:ARG:NH2	2.45	0.49
3:L3:2562:G:N2	3:L3:2565:A:OP2	2.42	0.49
19:LJ:5:MET:O	19:LJ:28:ASN:ND2	2.42	0.49
27:LR:50:PRO:HG3	33:LX:61:MET:HE3	1.95	0.49
33:LX:45:THR:HG23	33:LX:45:THR:O	2.13	0.49
2:L1:68:G:O2'	2:L1:69:PSU:H5''	2.11	0.49
3:L3:337:U:OP1	6:L6:31:ARG:NH1	2.43	0.49
3:L3:1521:C:O2'	3:L3:1522:OMG:H5'	2.13	0.49
1:BE:162:ARG:NH2	12:LC:88:SER:OG	2.46	0.49
15:LF:116:GLN:O	47:SR:514:LYS:NZ	2.46	0.49
3:L3:1892:A:OP1	3:L3:1893:C:N4	2.35	0.48
2:L1:74:U:O4	18:LI:72:GLN:NE2	2.45	0.48
3:L3:5002:U:OP2	23:LN:385:LYS:NZ	2.46	0.48
3:L3:2843:U:O2'	3:L3:4632:U:OP1	2.31	0.48
3:L3:5022:U:O2'	3:L3:5023:C:OP2	2.30	0.48
45:SK:78:ASP:OD2	48:SV:74:ARG:NH1	2.46	0.48
38:SA:210:ILE:HD13	38:SA:230:LEU:HB2	1.95	0.48
3:L3:142:G:OP1	42:SE:111:LYS:NZ	2.42	0.48
3:L3:3734:PSU:H2'	3:L3:3735:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LA:94:MET:HE1	10:LA:146:ILE:HB	1.96	0.48
41:SD:41:MET:HE2	41:SD:41:MET:N	2.29	0.48
1:BE:191:ILE:HD12	1:BE:200:ILE:HD11	1.95	0.48
3:L3:1398:A:OP2	3:L3:1420:A:N6	2.45	0.48
3:L3:2861:OMC:H1'	3:L3:2861:OMC:HM23	1.41	0.48
3:L3:1814:C:O2'	22:LM:42:ASN:OD1	2.17	0.48
19:LJ:29:ILE:O	19:LJ:31:ASP:N	2.45	0.48
3:L3:4322:G:N2	3:L3:4325:A:OP2	2.43	0.48
3:L3:2469:C:O2'	3:L3:2470:C:OP1	2.26	0.47
3:L3:4724:A:O2'	23:LN:104:THR:HG22	2.14	0.47
42:SE:159:HIS:ND1	42:SE:185:LYS:HA	2.28	0.47
45:SK:150:SER:HA	45:SK:194:ALA:HB3	1.95	0.47
3:L3:3718:A2M:H2	3:L3:3934:G:C1'	2.44	0.47
3:L3:3724:A2M:H2'	3:L3:3725:G:C8	2.49	0.47
3:L3:2363:A2M:H2'	3:L3:2364:OMG:O4'	2.14	0.47
3:L3:4635:A:H3'	3:L3:4636:PSU:H4'	1.96	0.47
31:LV:23:VAL:HG12	31:LV:70:LEU:CD2	2.45	0.47
48:SV:110:ASN:OD1	48:SV:111:ARG:N	2.48	0.47
3:L3:2364:OMG:HM23	3:L3:2364:OMG:H1'	1.50	0.47
3:L3:2407:G:O6	35:LZ:2:SER:N	2.48	0.47
3:L3:3869:OMC:HM23	3:L3:3869:OMC:H1'	1.70	0.47
11:LB:154:LYS:NZ	11:LB:159:PRO:O	2.48	0.47
17:LH:77:ILE:HD13	17:LH:100:VAL:HG12	1.94	0.47
3:L3:2837:OMU:HM23	3:L3:2837:OMU:H1'	1.51	0.47
3:L3:4122:G:O6	27:LR:101:LYS:NZ	2.48	0.47
1:BE:36:LEU:HD11	1:BE:69:ARG:HG2	1.95	0.47
3:L3:2515:G:OP1	27:LR:37:LYS:NZ	2.48	0.47
33:LX:86:LEU:HD21	43:SF:108:PRO:CG	2.42	0.47
39:SB:64:ILE:HG13	39:SB:105:LEU:HD21	1.97	0.47
3:L3:1724:G:N2	22:LM:13:SER:O	2.43	0.46
3:L3:2424:OMG:HM23	3:L3:2424:OMG:H1'	1.65	0.46
22:LM:35:VAL:HB	22:LM:40:LEU:HD11	1.96	0.46
3:L3:1590:C:O2'	37:NP:5:ARG:NH2	2.48	0.46
32:LW:14:LYS:NZ	35:LZ:51:LEU:OXT	2.46	0.46
38:SA:204:ARG:NH1	38:SA:205:ARG:O	2.47	0.46
43:SF:5:ILE:HG22	43:SF:208:GLU:O	2.15	0.46
38:SA:254:GLU:OE2	38:SA:258:ARG:NH1	2.49	0.46
3:L3:90:G:OP2	3:L3:92:C:N4	2.46	0.46
3:L3:131:C:N4	3:L3:138:G:O6	2.49	0.46
3:L3:2351:OMC:HM22	3:L3:2352:U:H5'	1.97	0.46
3:L3:2378:G:N2	3:L3:2381:A:OP2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:SB:128:ASP:OD1	39:SB:129:GLU:N	2.47	0.46
46:SQ:121:GLU:O	46:SQ:200:PHE:N	2.40	0.46
3:L3:1534:A2M:HM'3	3:L3:1637:A:C2	2.50	0.46
3:L3:4580:U:O2'	23:LN:182:GLU:OE2	2.28	0.46
19:LJ:97:ASN:O	19:LJ:100:VAL:HG22	2.15	0.46
34:LY:66:VAL:HG13	34:LY:66:VAL:O	2.15	0.46
3:L3:2422:OMC:H1'	3:L3:2422:OMC:HM23	1.50	0.46
3:L3:2436:U:OP2	17:LH:135:LYS:NZ	2.47	0.46
20:LK:72:THR:HG22	20:LK:110:LYS:HB3	1.98	0.46
21:LL:20:ARG:NH1	26:LQ:78:LEU:O	2.45	0.46
24:LO:47:ILE:HD12	24:LO:94:LEU:HD11	1.98	0.46
1:BE:191:ILE:HD11	1:BE:212:LEU:HD22	1.98	0.46
2:L1:102:G:OP2	2:L1:104:A:O2'	2.25	0.46
3:L3:1:C:O2'	3:L3:2:G:OP1	2.30	0.46
3:L3:3717:A:H2'	3:L3:3718:A2M:H8	1.97	0.46
3:L3:2590:G:O2'	3:L3:2755:A:N6	2.48	0.45
3:L3:5022:U:HO2'	3:L3:5023:C:P	2.39	0.45
19:LJ:91:LEU:HD23	19:LJ:117:LYS:HD2	1.97	0.45
40:SC:50:LEU:HD23	40:SC:50:LEU:H	1.81	0.45
3:L3:2459:G:N2	3:L3:2462:C:OP2	2.45	0.45
3:L3:2815:A2M:H2'	3:L3:2816:G:C8	2.51	0.45
23:LN:10:ARG:NH1	23:LN:14:LEU:HD11	2.32	0.45
3:L3:431:G:N2	3:L3:3889:G:OP2	2.49	0.45
3:L3:3744:OMG:HM23	3:L3:3744:OMG:H1'	1.51	0.45
25:LP:92:ARG:HA	25:LP:102:LEU:HD23	1.99	0.45
25:LP:88:LEU:HD22	25:LP:104:THR:HG21	1.97	0.45
3:L3:718:C:OP1	41:SD:217:ARG:NH1	2.47	0.45
3:L3:3899:OMG:HM23	3:L3:3899:OMG:H1'	1.70	0.45
3:L3:1326:A2M:HM'3	3:L3:1326:A2M:H1'	1.56	0.45
3:L3:1340:OMC:HM23	3:L3:1340:OMC:H1'	1.51	0.45
3:L3:4288:C:O2'	3:L3:4321:U:OP1	2.34	0.45
3:L3:4305:G:HO2'	3:L3:4306:OMU:P	2.38	0.45
3:L3:2474:G:OP2	17:LH:47:ARG:NH1	2.50	0.45
3:L3:2824:OMC:HM23	3:L3:2824:OMC:H1'	1.58	0.45
30:LU:74:LYS:O	30:LU:78:GLY:N	2.47	0.45
3:L3:1288:G:OP1	40:SC:134:SER:OG	2.34	0.45
3:L3:1779:PSU:H2'	3:L3:1780:A:C8	2.52	0.45
23:LN:107:ALA:HB2	23:LN:201:LEU:HG	1.98	0.45
36:NK:86:LEU:HD12	36:NK:105:LEU:HD11	1.99	0.45
3:L3:2415:OMU:O5'	3:L3:2415:OMU:H6	2.17	0.45
3:L3:1534:A2M:HM'3	3:L3:1637:A:C4	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:1860:PSU:H2'	3:L3:1861:U:H6	1.81	0.44
3:L3:2616:C:OP1	13:LD:60:ARG:NH1	2.50	0.44
3:L3:3619:G:H22	3:L3:3624:A:H1'	1.82	0.44
11:LB:124:ASP:OD1	11:LB:125:GLN:N	2.50	0.44
3:L3:1352:C:O2'	3:L3:1356:U:OP1	2.35	0.44
3:L3:4637:OMG:H1'	3:L3:4637:OMG:HM23	1.50	0.44
3:L3:4768:G:OP1	7:L7:168:TYR:OH	2.34	0.44
4:L4:74:A:O2'	12:LC:53:LYS:NZ	2.45	0.44
3:L3:3744:OMG:H2'	3:L3:3745:U:O4'	2.17	0.44
3:L3:4201:G:O2'	3:L3:4202:U:OP2	2.27	0.44
1:BE:42:LYS:N	1:BE:45:GLU:OE1	2.50	0.44
3:L3:2046:G:O2'	3:L3:2047:A:N7	2.47	0.44
3:L3:2326:G:OP1	26:LQ:108:ARG:NH2	2.50	0.44
3:L3:2781:G:O2'	35:LZ:3:SER:O	2.36	0.44
7:L7:54:TYR:OH	7:L7:73:PHE:O	2.34	0.44
20:LK:76:ASP:OD1	20:LK:76:ASP:N	2.49	0.44
20:LK:147:VAL:HG22	20:LK:148:ALA:N	2.33	0.44
3:L3:232:G:O6	18:LI:61:HIS:N	2.44	0.44
3:L3:4593:C:OP2	36:NK:2:ALA:N	2.51	0.44
3:L3:2804:OMC:HM23	3:L3:2804:OMC:H1'	1.66	0.44
3:L3:4745:G:H22	3:L3:4955:A:H2	1.64	0.43
3:L3:4518:A:N7	23:LN:257:TRP:NE1	2.66	0.43
5:L5:128:LEU:HD22	5:L5:130:PHE:CE1	2.54	0.43
45:SK:199:VAL:HG23	45:SK:204:ALA:HB2	2.00	0.43
3:L3:2362:U:H2'	3:L3:2363:A2M:H8	2.00	0.43
22:LM:65:MET:HE2	22:LM:65:MET:N	2.33	0.43
37:NP:98:SER:OG	37:NP:100:GLU:OE1	2.28	0.43
3:L3:305:A:OP1	30:LU:76:ARG:NH1	2.51	0.43
3:L3:2368:A:N6	3:L3:2827:G:O2'	2.50	0.43
3:L3:4546:A:N7	43:SF:215:ASN:ND2	2.66	0.43
24:LO:15:ASN:OD1	24:LO:16:SER:N	2.52	0.43
3:L3:2823:G:O2'	3:L3:2824:OMC:H5''	2.19	0.43
3:L3:3841:OMC:HM23	3:L3:3841:OMC:H1'	1.56	0.43
7:L7:126:VAL:HG13	7:L7:127:VAL:HG23	2.00	0.43
25:LP:64:ILE:HG23	25:LP:68:LEU:HD23	2.00	0.43
45:SK:4:ARG:NH2	45:SK:210:THR:O	2.45	0.43
3:L3:2097:U:O3'	3:L3:2098:G:H4'	2.19	0.43
3:L3:3868:G:O2'	3:L3:3869:OMC:H5''	2.18	0.43
15:LF:22:THR:C	15:LF:23:LEU:HD12	2.44	0.43
3:L3:1534:A2M:HM'2	3:L3:1535:C:C6	2.54	0.43
3:L3:2072:C:O2'	41:SD:213:LEU:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LH:82:THR:HG21	28:LS:37:THR:HG22	2.00	0.43
43:SF:175:ILE:HG22	43:SF:175:ILE:O	2.19	0.43
11:LB:95:VAL:O	11:LB:95:VAL:HG13	2.19	0.43
19:LJ:9:LYS:NZ	19:LJ:83:THR:O	2.28	0.43
3:L3:511:C:O3'	6:L6:165:LYS:NZ	2.52	0.42
3:L3:1420:A:O2'	3:L3:1500:A:O2'	2.21	0.42
3:L3:2306:G:OP1	26:LQ:128:ARG:NH1	2.52	0.42
38:SA:209:ILE:HB	38:SA:229:LEU:HD13	2.00	0.42
3:L3:2095:A:HO2'	3:L3:2096:G:P	2.41	0.42
3:L3:2543:A:O2'	3:L3:2545:U:OP1	2.36	0.42
5:L5:128:LEU:HD23	5:L5:129:ASP:N	2.35	0.42
3:L3:1677:PSU:H4'	3:L3:1680:G:N1	2.33	0.42
6:L6:80:GLU:HG2	6:L6:110:LEU:HD12	2.01	0.42
3:L3:1654:G:N2	3:L3:1678:C:OP1	2.51	0.42
8:L8:36:ALA:HB2	8:L8:52:PHE:CE1	2.55	0.42
23:LN:119:TYR:OH	23:LN:129:ALA:N	2.52	0.42
45:SK:107:VAL:HG13	45:SK:118:HIS:HB2	2.01	0.42
13:LD:7:GLN:OE1	13:LD:7:GLN:N	2.47	0.42
44:SG:12:ILE:HG12	44:SG:18:ILE:HD12	2.02	0.42
45:SK:156:ASN:ND2	45:SK:201:ASP:OD2	2.51	0.42
45:SK:222:PHE:O	45:SK:224:LEU:N	2.51	0.42
3:L3:1897:A:O5'	11:LB:2:GLY:N	2.53	0.42
3:L3:3718:A2M:H1'	3:L3:3718:A2M:HM'3	1.65	0.42
6:L6:63:THR:HG22	6:L6:64:VAL:N	2.35	0.42
9:L9:124:ASP:OD1	9:L9:125:SER:N	2.51	0.42
27:LR:5:LEU:HD13	27:LR:32:TYR:HE1	1.80	0.42
3:L3:346:G:OP1	18:LI:8:THR:HG23	2.20	0.42
3:L3:3715:PSU:H2'	3:L3:3716:C:O4'	2.19	0.42
3:L3:4391:G:O2'	3:L3:4392:OMG:H5'	2.19	0.42
3:L3:4689:PSU:H2'	3:L3:4690:G:O4'	2.19	0.42
3:L3:2422:OMC:OP1	10:LA:127:ARG:NH2	2.44	0.42
3:L3:2896:G:OP1	13:LD:136:ARG:NH2	2.53	0.42
3:L3:3724:A2M:HM'3	3:L3:3724:A2M:H1'	1.68	0.42
3:L3:3827:G:O2'	3:L3:3829:G:OP2	2.33	0.42
44:SG:118:LEU:HD11	44:SG:167:VAL:HG22	2.00	0.42
1:BE:36:LEU:HD13	1:BE:73:ASN:HB2	2.02	0.42
3:L3:736:C:OP1	8:L8:74:ARG:NH2	2.51	0.42
3:L3:3723:A:H2'	3:L3:3724:A2M:H8	2.02	0.42
16:LG:96:LEU:HD13	48:SV:20:MET:SD	2.60	0.41
45:SK:163:PRO:HG3	45:SK:185:THR:HG22	2.01	0.41
3:L3:730:G:OP2	41:SD:76:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:2836:A:H1'	23:LN:228:TYR:CE2	2.55	0.41
5:L5:158:SER:N	5:L5:161:GLU:OE1	2.46	0.41
43:SF:142:GLU:O	43:SF:143:THR:OG1	2.32	0.41
3:L3:1910:G:O2'	3:L3:1917:A:N1	2.52	0.41
3:L3:2630:U:O4	15:LF:89:LYS:NZ	2.46	0.41
3:L3:4618:OMG:H5''	16:LG:15:ARG:HB2	2.03	0.41
28:LS:23:ASP:OD1	28:LS:24:LEU:N	2.53	0.41
8:L8:29:ASP:OD1	8:L8:30:VAL:N	2.52	0.41
44:SG:92:MET:HE1	44:SG:161:ILE:HD12	2.03	0.41
3:L3:4305:G:H4'	3:L3:4306:OMU:OP1	2.21	0.41
3:L3:4499:OMG:HM23	3:L3:4499:OMG:H1'	1.61	0.41
23:LN:213:GLN:NE2	23:LN:285:TYR:O	2.52	0.41
15:LF:76:VAL:HG13	15:LF:77:PRO:HD2	2.03	0.41
35:LZ:23:ILE:HD12	35:LZ:27:ILE:HD11	2.03	0.41
47:SR:481:ARG:NH1	48:SV:123:ASP:OD2	2.54	0.41
2:L1:7:U:O2'	3:L3:1305:C:OP1	2.39	0.41
3:L3:310:G:N7	30:LU:32:ARG:NH1	2.69	0.41
3:L3:1238:A:O3'	41:SD:48:LYS:NZ	2.53	0.41
3:L3:1621:A:OP2	32:LW:30:GLN:NE2	2.49	0.41
3:L3:3830:A2M:HM'3	3:L3:3830:A2M:H1'	1.67	0.41
3:L3:3851:PSU:H2'	3:L3:3852:A:O4'	2.21	0.41
16:LG:133:ALA:O	45:SK:106:ASN:ND2	2.49	0.41
18:LI:69:LYS:NZ	18:LI:83:GLU:OE2	2.42	0.41
40:SC:96:VAL:HG11	40:SC:101:ASN:O	2.21	0.41
47:SR:599:LYS:O	47:SR:603:LEU:HD13	2.21	0.41
1:BE:91:LEU:HD21	1:BE:133:GLN:OE1	2.21	0.41
3:L3:3744:OMG:H2'	3:L3:3745:U:C6	2.56	0.41
12:LC:45:TRP:HA	12:LC:48:VAL:HG12	2.03	0.41
19:LJ:128:LYS:NZ	42:SE:33:GLU:OE1	2.45	0.41
35:LZ:9:ILE:HG23	35:LZ:51:LEU:HD21	2.03	0.41
44:SG:118:LEU:HD21	44:SG:177:ASP:OD2	2.21	0.41
3:L3:3694:U:C2'	3:L3:3695:PSU:H5''	2.51	0.40
3:L3:4500:PSU:H2'	3:L3:4501:U:H6	1.82	0.40
3:L3:4618:OMG:HM22	3:L3:4619:U:O4'	2.21	0.40
3:L3:106:A:H2'	3:L3:107:G:O4'	2.21	0.40
3:L3:1669:A:N3	3:L3:1852:U:O2'	2.46	0.40
3:L3:1877:G:H1'	22:LM:8:THR:HG23	2.02	0.40
3:L3:3747:A:H62	43:SF:245:ARG:HH21	1.69	0.40
3:L3:1577:G:O2'	3:L3:1612:G:H4'	2.22	0.40
3:L3:3627:OMG:HM23	3:L3:3627:OMG:H1'	1.68	0.40
3:L3:4227:OMU:H1'	3:L3:4227:OMU:HM23	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:4376:A:O2'	20:LK:42:ARG:NH1	2.54	0.40
3:L3:4590:A2M:HM'2	3:L3:4591:U:H5'	2.04	0.40
39:SB:152:ARG:O	39:SB:157:ASN:ND2	2.54	0.40
3:L3:1316:OMG:HM22	3:L3:1316:OMG:H1'	1.56	0.40
3:L3:1427:A:H2	11:LB:138:LEU:HD23	1.83	0.40
3:L3:1439:C:OP2	41:SD:34:ARG:NH2	2.54	0.40
3:L3:2407:G:OP2	3:L3:2407:G:N2	2.52	0.40
3:L3:2613:C:OP1	27:LR:24:ARG:NH2	2.54	0.40
3:L3:2691:U:C2	3:L3:2692:U:C5	3.09	0.40
48:SV:81:TYR:CD1	48:SV:86:TRP:CZ3	3.09	0.40
3:L3:2835:A:O2'	23:LN:228:TYR:O	2.39	0.40
3:L3:4266:G:N3	3:L3:4266:G:H2'	2.37	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	
1	BE	156/214 (73%)	152 (97%)	4 (3%)	0	100	100
5	L5	166/178 (93%)	164 (99%)	2 (1%)	0	100	100
6	L6	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
7	L7	199/203 (98%)	199 (100%)	0	0	100	100
8	L8	133/215 (62%)	132 (99%)	1 (1%)	0	100	100
9	L9	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
10	LA	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
11	LB	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
12	LC	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
13	LD	152/196 (78%)	150 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	LE	150/160 (94%)	143 (95%)	7 (5%)	0	100	100
15	LF	101/128 (79%)	100 (99%)	1 (1%)	0	100	100
16	LG	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
17	LH	122/156 (78%)	121 (99%)	1 (1%)	0	100	100
18	LI	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
19	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
20	LK	145/148 (98%)	143 (99%)	2 (1%)	0	100	100
21	LL	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
22	LM	84/159 (53%)	82 (98%)	2 (2%)	0	100	100
23	LN	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
24	LO	93/115 (81%)	93 (100%)	0	0	100	100
25	LP	104/125 (83%)	104 (100%)	0	0	100	100
26	LQ	126/135 (93%)	126 (100%)	0	0	100	100
27	LR	110/117 (94%)	108 (98%)	2 (2%)	0	100	100
28	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
29	LT	107/110 (97%)	107 (100%)	0	0	100	100
30	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
31	LV	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
32	LW	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
33	LX	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
34	LY	67/70 (96%)	67 (100%)	0	0	100	100
35	LZ	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
36	NK	63/129 (49%)	63 (100%)	0	0	100	100
37	NP	104/134 (78%)	104 (100%)	0	0	100	100
38	SA	356/427 (83%)	349 (98%)	7 (2%)	0	100	100
39	SB	290/297 (98%)	286 (99%)	4 (1%)	0	100	100
40	SC	208/288 (72%)	199 (96%)	9 (4%)	0	100	100
41	SD	223/248 (90%)	219 (98%)	4 (2%)	0	100	100
42	SE	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
43	SF	243/257 (95%)	237 (98%)	6 (2%)	0	100	100
44	SG	188/192 (98%)	188 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	SK	224/245 (91%)	218 (97%)	6 (3%)	0	100	100
46	SQ	119/239 (50%)	118 (99%)	1 (1%)	0	100	100
47	SR	237/634 (37%)	237 (100%)	0	0	100	100
48	SV	137/163 (84%)	135 (98%)	2 (2%)	0	100	100
All	All	7021/8446 (83%)	6910 (98%)	111 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BE	137/181 (76%)	137 (100%)	0	100	100
5	L5	142/149 (95%)	142 (100%)	0	100	100
6	L6	176/177 (99%)	176 (100%)	0	100	100
7	L7	173/174 (99%)	173 (100%)	0	100	100
8	L8	115/161 (71%)	115 (100%)	0	100	100
9	L9	171/172 (99%)	171 (100%)	0	100	100
10	LA	134/163 (82%)	134 (100%)	0	100	100
11	LB	164/165 (99%)	164 (100%)	0	100	100
12	LC	157/157 (100%)	157 (100%)	0	100	100
13	LD	138/175 (79%)	138 (100%)	0	100	100
14	LE	136/140 (97%)	136 (100%)	0	100	100
15	LF	93/115 (81%)	93 (100%)	0	100	100
16	LG	106/107 (99%)	106 (100%)	0	100	100
17	LH	112/133 (84%)	112 (100%)	0	100	100
18	LI	124/135 (92%)	124 (100%)	0	100	100
19	LJ	117/118 (99%)	117 (100%)	0	100	100
20	LK	120/121 (99%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	LL	109/121 (90%)	109 (100%)	0	100	100
22	LM	74/126 (59%)	74 (100%)	0	100	100
23	LN	347/348 (100%)	347 (100%)	0	100	100
24	LO	80/97 (82%)	80 (100%)	0	100	100
25	LP	97/110 (88%)	97 (100%)	0	100	100
26	LQ	114/121 (94%)	114 (100%)	0	100	100
27	LR	96/100 (96%)	96 (100%)	0	100	100
28	LS	109/110 (99%)	109 (100%)	0	100	100
29	LT	88/89 (99%)	88 (100%)	0	100	100
30	LU	86/89 (97%)	86 (100%)	0	100	100
31	LV	92/94 (98%)	92 (100%)	0	100	100
32	LW	73/80 (91%)	73 (100%)	0	100	100
33	LX	74/75 (99%)	74 (100%)	0	100	100
34	LY	64/65 (98%)	64 (100%)	0	100	100
35	LZ	47/48 (98%)	47 (100%)	0	100	100
36	NK	61/115 (53%)	61 (100%)	0	100	100
37	NP	92/114 (81%)	92 (100%)	0	100	100
38	SA	298/348 (86%)	298 (100%)	0	100	100
39	SB	246/250 (98%)	246 (100%)	0	100	100
40	SC	189/252 (75%)	189 (100%)	0	100	100
41	SD	194/215 (90%)	194 (100%)	0	100	100
42	SE	198/223 (89%)	198 (100%)	0	100	100
43	SF	188/199 (94%)	188 (100%)	0	100	100
44	SG	169/171 (99%)	169 (100%)	0	100	100
45	SK	196/213 (92%)	196 (100%)	0	100	100
47	SR	218/574 (38%)	218 (100%)	0	100	100
48	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	6042/7039 (86%)	6042 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	BE	92	HIS
5	L5	104	ASN
6	L6	104	ASN
6	L6	111	GLN
7	L7	26	GLN
7	L7	42	ASN
7	L7	180	GLN
7	L7	184	ASN
8	L8	34	ASN
8	L8	69	HIS
9	L9	32	GLN
9	L9	86	HIS
9	L9	87	HIS
9	L9	109	HIS
14	LE	66	ASN
14	LE	144	ASN
16	LG	27	ASN
17	LH	107	HIS
18	LI	18	HIS
19	LJ	127	ASN
20	LK	19	HIS
20	LK	25	HIS
21	LL	100	ASN
23	LN	123	HIS
23	LN	258	HIS
25	LP	30	HIS
26	LQ	23	HIS
26	LQ	52	GLN
28	LS	98	HIS
29	LT	20	ASN
29	LT	99	HIS
31	LV	19	GLN
32	LW	13	ASN
33	LX	56	HIS
35	LZ	25	GLN
37	NP	13	HIS
37	NP	91	GLN
38	SA	38	ASN
38	SA	215	ASN
39	SB	202	GLN
39	SB	225	GLN
40	SC	43	HIS
40	SC	135	GLN

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Mol	Chain	Res	Type
40	SC	136	HIS
40	SC	190	HIS
41	SD	116	GLN
41	SD	119	ASN
42	SE	43	GLN
42	SE	81	ASN
42	SE	82	GLN
42	SE	94	GLN
42	SE	153	GLN
43	SF	38	HIS
45	SK	68	HIS
45	SK	75	ASN
45	SK	156	ASN
47	SR	361	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	19 (12%)	0
3	L3	3295/5070 (64%)	408 (12%)	5 (0%)
4	L4	119/121 (98%)	11 (9%)	0
All	All	3566/5348 (66%)	438 (12%)	5 (0%)

All (438) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	23	C
2	L1	34	U
2	L1	35	C
2	L1	59	A
2	L1	62	A
2	L1	63	U
2	L1	82	A
2	L1	83	C
2	L1	84	A
2	L1	86	U
2	L1	94	G
2	L1	103	A
2	L1	105	C
2	L1	111	U
2	L1	114	G

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Mol	Chain	Res	Type
2	L1	127	U
2	L1	151	G
2	L1	153	C
2	L1	156	U
3	L3	2	G
3	L3	39	A
3	L3	42	A
3	L3	48	G
3	L3	56	A
3	L3	58	G
3	L3	59	A
3	L3	64	A
3	L3	65	A
3	L3	66	A
3	L3	91	G
3	L3	108	A
3	L3	119	G
3	L3	159	C
3	L3	164	G
3	L3	167	C
3	L3	169	G
3	L3	170	C
3	L3	171	U
3	L3	173	C
3	L3	181	C
3	L3	200	U
3	L3	210	C
3	L3	218	A
3	L3	233	U
3	L3	234	G
3	L3	261	G
3	L3	263	G
3	L3	266	C
3	L3	316	U
3	L3	340	C
3	L3	349	A
3	L3	387	G
3	L3	409	G
3	L3	410	A
3	L3	412	G
3	L3	450	G
3	L3	452	A

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Mol	Chain	Res	Type
3	L3	453	G
3	L3	454	U
3	L3	464	G
3	L3	467	U
3	L3	469	C
3	L3	472	C
3	L3	473	C
3	L3	492	U
3	L3	493	G
3	L3	496	G
3	L3	497	G
3	L3	499	G
3	L3	501	C
3	L3	502	C
3	L3	503	C
3	L3	504	G
3	L3	510	U
3	L3	511	C
3	L3	658	C
3	L3	660	A
3	L3	666	G
3	L3	667	A
3	L3	668	C
3	L3	669	C
3	L3	686	A
3	L3	704	C
3	L3	731	G
3	L3	739	G
3	L3	741	C
3	L3	742	G
3	L3	746	A
3	L3	757	G
3	L3	913	U
3	L3	915	A
3	L3	917	A
3	L3	918	G
3	L3	926	G
3	L3	932	A
3	L3	933	G
3	L3	944	A
3	L3	945	U
3	L3	946	C

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Mol	Chain	Res	Type
3	L3	956	A
3	L3	959	G
3	L3	960	A
3	L3	971	U
3	L3	972	C
3	L3	1066	G
3	L3	1072	C
3	L3	1080	C
3	L3	1167	C
3	L3	1169	G
3	L3	1171	G
3	L3	1172	C
3	L3	1175	A
3	L3	1178	G
3	L3	1180	C
3	L3	1181	C
3	L3	1182	C
3	L3	1201	U
3	L3	1203	G
3	L3	1211	G
3	L3	1215	C
3	L3	1253	G
3	L3	1254	A
3	L3	1255	A
3	L3	1256	G
3	L3	1266	G
3	L3	1269	G
3	L3	1270	A
3	L3	1272	C
3	L3	1273	G
3	L3	1280	C
3	L3	1284	G
3	L3	1287	G
3	L3	1294	A
3	L3	1295	C
3	L3	1301	C
3	L3	1313	C
3	L3	1314	C
3	L3	1318	C
3	L3	1322	1MA
3	L3	1323	A
3	L3	1326	A2M

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Mol	Chain	Res	Type
3	L3	1354	A
3	L3	1358	G
3	L3	1359	G
3	L3	1365	C
3	L3	1366	G
3	L3	1379	C
3	L3	1397	A
3	L3	1420	A
3	L3	1439	C
3	L3	1443	A
3	L3	1476	C
3	L3	1497	A
3	L3	1498	G
3	L3	1502	G
3	L3	1523	A
3	L3	1534	A2M
3	L3	1547	A
3	L3	1578	U
3	L3	1581	G
3	L3	1596	U
3	L3	1597	G
3	L3	1613	A
3	L3	1624	G
3	L3	1625	OMG
3	L3	1631	A
3	L3	1633	G
3	L3	1634	A
3	L3	1642	A
3	L3	1654	G
3	L3	1661	C
3	L3	1670	G
3	L3	1671	U
3	L3	1676	C
3	L3	1677	PSU
3	L3	1678	C
3	L3	1691	G
3	L3	1721	G
3	L3	1726	U
3	L3	1734	G
3	L3	1740	C
3	L3	1741	G
3	L3	1742	A

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Mol	Chain	Res	Type
3	L3	1743	A
3	L3	1750	G
3	L3	1791	U
3	L3	1804	A
3	L3	1815	G
3	L3	1821	G
3	L3	1822	U
3	L3	1836	G
3	L3	1837	A
3	L3	1842	G
3	L3	1854	G
3	L3	1875	C
3	L3	1880	G
3	L3	1882	U
3	L3	1887	G
3	L3	1888	A
3	L3	1897	A
3	L3	1910	G
3	L3	1919	G
3	L3	1921	C
3	L3	1922	G
3	L3	1925	G
3	L3	1955	G
3	L3	1974	U
3	L3	1997	U
3	L3	2021	G
3	L3	2025	A
3	L3	2026	A
3	L3	2041	A
3	L3	2044	U
3	L3	2046	G
3	L3	2055	G
3	L3	2056	G
3	L3	2069	A
3	L3	2084	C
3	L3	2085	G
3	L3	2092	G
3	L3	2093	A
3	L3	2094	G
3	L3	2095	A
3	L3	2096	G
3	L3	2097	U

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Mol	Chain	Res	Type
3	L3	2098	G
3	L3	2099	G
3	L3	2109	G
3	L3	2110	C
3	L3	2111	G
3	L3	2261	G
3	L3	2289	C
3	L3	2300	A
3	L3	2301	G
3	L3	2313	A
3	L3	2348	G
3	L3	2351	OMC
3	L3	2395	A
3	L3	2417	A
3	L3	2422	OMC
3	L3	2425	U
3	L3	2429	A
3	L3	2450	G
3	L3	2453	A
3	L3	2470	C
3	L3	2471	G
3	L3	2475	G
3	L3	2476	G
3	L3	2477	A
3	L3	2478	C
3	L3	2480	G
3	L3	2506	G
3	L3	2507	A
3	L3	2512	A
3	L3	2513	A
3	L3	2519	U
3	L3	2544	G
3	L3	2545	U
3	L3	2548	C
3	L3	2554	U
3	L3	2587	A
3	L3	2627	C
3	L3	2638	G
3	L3	2653	C
3	L3	2669	C
3	L3	2687	U
3	L3	2694	G

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Mol	Chain	Res	Type
3	L3	2695	A
3	L3	2696	A
3	L3	2711	G
3	L3	2743	A
3	L3	2760	G
3	L3	2764	A
3	L3	2769	U
3	L3	2787	A2M
3	L3	2788	U
3	L3	2790	U
3	L3	2814	C
3	L3	2826	U
3	L3	2827	G
3	L3	2829	U
3	L3	2842	G
3	L3	2855	G
3	L3	2877	G
3	L3	2902	G
3	L3	3593	C
3	L3	3595	U
3	L3	3597	G
3	L3	3615	G
3	L3	3626	G
3	L3	3635	A
3	L3	3653	A
3	L3	3662	A
3	L3	3673	C
3	L3	3674	G
3	L3	3696	C
3	L3	3697	U
3	L3	3838	U
3	L3	3840	U
3	L3	3867	A2M
3	L3	3868	G
3	L3	3872	A
3	L3	3887	OMC
3	L3	3897	G
3	L3	3905	A
3	L3	3915	U
3	L3	4069	U
3	L3	4076	G
3	L3	4084	G

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Mol	Chain	Res	Type
3	L3	4085	A
3	L3	4119	C
3	L3	4121	G
3	L3	4122	G
3	L3	4133	C
3	L3	4138	C
3	L3	4139	G
3	L3	4140	C
3	L3	4142	C
3	L3	4143	G
3	L3	4144	C
3	L3	4145	C
3	L3	4147	G
3	L3	4150	G
3	L3	4162	C
3	L3	4164	C
3	L3	4166	G
3	L3	4170	A
3	L3	4183	G
3	L3	4184	G
3	L3	4191	G
3	L3	4194	U
3	L3	4202	U
3	L3	4222	G
3	L3	4229	U
3	L3	4233	A
3	L3	4251	A
3	L3	4254	G
3	L3	4258	C
3	L3	4266	G
3	L3	4268	A
3	L3	4273	A
3	L3	4281	A
3	L3	4291	G
3	L3	4305	G
3	L3	4306	OMU
3	L3	4329	G
3	L3	4330	G
3	L3	4332	C
3	L3	4339	A
3	L3	4373	G
3	L3	4376	A

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Mol	Chain	Res	Type
3	L3	4377	G
3	L3	4378	A
3	L3	4387	C
3	L3	4453	C
3	L3	4464	A
3	L3	4466	C
3	L3	4475	G
3	L3	4491	G
3	L3	4498	OMU
3	L3	4512	U
3	L3	4513	A
3	L3	4519	C
3	L3	4523	A2M
3	L3	4524	G
3	L3	4532	PSU
3	L3	4545	G
3	L3	4548	A
3	L3	4549	G
3	L3	4555	U
3	L3	4556	U
3	L3	4557	U
3	L3	4558	U
3	L3	4560	C
3	L3	4567	G
3	L3	4584	A
3	L3	4590	A2M
3	L3	4608	G
3	L3	4636	PSU
3	L3	4637	OMG
3	L3	4656	A
3	L3	4670	C
3	L3	4672	A
3	L3	4678	G
3	L3	4701	A
3	L3	4708	A
3	L3	4709	U
3	L3	4719	G
3	L3	4720	C
3	L3	4740	G
3	L3	4741	C
3	L3	4742	G
3	L3	4750	G

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Mol	Chain	Res	Type
3	L3	4751	G
3	L3	4754	G
3	L3	4757	C
3	L3	4759	C
3	L3	4765	G
3	L3	4772	C
3	L3	4773	C
3	L3	4870	G
3	L3	4871	C
3	L3	4882	U
3	L3	4883	C
3	L3	4900	C
3	L3	4901	G
3	L3	4910	G
3	L3	4914	C
3	L3	4916	G
3	L3	4943	A
3	L3	4976	U
3	L3	4996	C
3	L3	5006	U
3	L3	5014	A
3	L3	5020	G
3	L3	5022	U
3	L3	5023	C
3	L3	5026	U
3	L3	5027	C
3	L3	5031	G
3	L3	5041	G
3	L3	5050	C
3	L3	5054	C
3	L3	5055	G
3	L3	5061	A
3	L3	5062	G
3	L3	5069	U
4	L4	25	G
4	L4	49	A
4	L4	53	U
4	L4	54	A
4	L4	64	G
4	L4	66	G
4	L4	97	G
4	L4	103	A

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Mol	Chain	Res	Type
4	L4	110	G
4	L4	111	C
4	L4	120	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L3	496	G
3	L3	502	C
3	L3	503	C
3	L3	2095	A
3	L3	2469	C

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

110 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
3	PSU	L3	3734	3	18,21,22	1.14	1 (5%)	21,30,33	1.98	5 (23%)
3	PSU	L3	1781	3	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
3	OMC	L3	3887	3	19,22,23	0.52	0	25,31,34	0.66	0
3	A2M	L3	3718	3	22,25,26	0.91	1 (4%)	30,36,39	2.02	7 (23%)
3	UR3	L3	4530	3	19,22,23	1.09	3 (15%)	26,32,35	1.49	2 (7%)
3	PSU	L3	4361	3	18,21,22	1.10	1 (5%)	21,30,33	2.00	5 (23%)
3	A2M	L3	2815	3	22,25,26	0.87	0	30,36,39	2.09	8 (26%)
3	A2M	L3	3724	3	22,25,26	0.87	0	30,36,39	2.05	7 (23%)
3	OMG	L3	4618	3	23,26,27	0.49	0	32,38,41	0.55	0
3	PSU	L3	4353	3	18,21,22	1.07	1 (5%)	21,30,33	1.98	5 (23%)
3	PSU	L3	4576	3	18,21,22	1.10	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L3	4500	3	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L3	3695	3	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L3	2424	3	23,26,27	0.48	0	32,38,41	0.45	0
3	PSU	L3	4636	3	18,21,22	1.10	1 (5%)	21,30,33	2.00	5 (23%)
3	PSU	L3	4628	3	18,21,22	1.06	1 (5%)	21,30,33	1.90	5 (23%)
3	PSU	L3	4457	3	18,21,22	1.10	1 (5%)	21,30,33	1.98	6 (28%)
3	PSU	L3	4299	3	18,21,22	1.00	1 (5%)	21,30,33	1.97	5 (23%)
3	PSU	L3	1862	3	18,21,22	1.10	1 (5%)	21,30,33	1.92	6 (28%)
3	OMC	L3	2365	3	19,22,23	0.54	0	25,31,34	0.66	0
3	A2M	L3	1326	3	22,25,26	0.89	0	30,36,39	2.12	8 (26%)
3	PSU	L3	4972	3	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
3	OMU	L3	4620	3	19,22,23	2.01	6 (31%)	25,31,34	1.72	4 (16%)
3	PSU	L3	3822	3	18,21,22	1.17	1 (5%)	21,30,33	1.98	5 (23%)
3	OMG	L3	4499	3	23,26,27	0.43	0	32,38,41	0.47	0
3	PSU	L3	1744	3	18,21,22	1.11	1 (5%)	21,30,33	1.97	5 (23%)
3	PSU	L3	3730	3	18,21,22	1.08	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L3	4579	3	18,21,22	1.05	2 (11%)	21,30,33	1.90	4 (19%)
3	PSU	L3	3715	3	18,21,22	1.13	1 (5%)	21,30,33	1.94	6 (28%)
23	HIC	LN	245	23	10,11,12	1.51	1 (10%)	9,14,16	1.22	1 (11%)
3	PSU	L3	2632	3	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
3	OMC	L3	2824	3	19,22,23	0.52	0	25,31,34	0.64	0
3	PSU	L3	3853	3	18,21,22	1.09	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L3	2351	49,3	19,22,23	0.57	0	25,31,34	0.81	1 (4%)
3	OMC	L3	4536	3	19,22,23	0.53	0	25,31,34	0.64	0
3	OMU	L3	4306	3	19,22,23	2.02	6 (31%)	25,31,34	1.88	4 (16%)
3	PSU	L3	4532	3	18,21,22	1.08	1 (5%)	21,30,33	1.97	5 (23%)
3	OMG	L3	4370	3	23,26,27	0.53	0	32,38,41	0.59	0
3	PSU	L3	1677	3	18,21,22	1.04	1 (5%)	21,30,33	1.89	5 (23%)
3	A2M	L3	1524	3	22,25,26	0.87	0	30,36,39	2.12	8 (26%)
3	PSU	L3	3851	3	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
3	A2M	L3	2363	49,3	22,25,26	0.87	1 (4%)	30,36,39	2.01	7 (23%)
3	A2M	L3	3825	3	22,25,26	0.85	0	30,36,39	2.09	7 (23%)
3	OMG	L3	3899	3	23,26,27	0.49	0	32,38,41	0.55	0
3	PSU	L3	5010	3	18,21,22	1.10	1 (5%)	21,30,33	1.90	5 (23%)
3	OMG	L3	4392	3	23,26,27	0.48	0	32,38,41	0.48	0
3	PSU	L3	4296	3	18,21,22	1.10	2 (11%)	21,30,33	2.01	5 (23%)
3	1MA	L3	1322	3	21,25,26	0.41	0	30,37,40	0.76	1 (3%)
3	PSU	L3	3639	3	18,21,22	1.10	1 (5%)	21,30,33	1.93	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L3	3744	3	23,26,27	0.46	0	32,38,41	0.47	0
3	PSU	L3	1683	3	18,21,22	1.11	2 (11%)	21,30,33	2.06	5 (23%)
3	PSU	L3	4689	3	18,21,22	1.06	1 (5%)	21,30,33	2.06	5 (23%)
2	PSU	L1	55	2	18,21,22	1.11	1 (5%)	21,30,33	2.00	5 (23%)
3	OMG	L3	4228	3	23,26,27	0.53	0	32,38,41	0.57	0
2	OMG	L1	75	2	23,26,27	0.48	0	32,38,41	0.47	0
3	PSU	L3	4312	3	18,21,22	1.08	1 (5%)	21,30,33	2.00	5 (23%)
3	OMG	L3	1316	3	23,26,27	0.49	0	32,38,41	0.47	0
3	A2M	L3	1871	3	22,25,26	0.85	0	30,36,39	2.14	8 (26%)
3	OMC	L3	3701	3	19,22,23	0.49	0	25,31,34	0.59	0
3	PSU	L3	3884	3	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L3	1860	3	18,21,22	1.04	2 (11%)	21,30,33	1.87	5 (23%)
3	A2M	L3	4590	3	22,25,26	0.90	1 (4%)	30,36,39	2.04	7 (23%)
3	PSU	L3	3844	3	18,21,22	1.11	1 (5%)	21,30,33	1.97	5 (23%)
2	PSU	L1	69	2	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
3	OMG	L3	4623	3	23,26,27	0.49	0	32,38,41	0.54	0
3	PSU	L3	1792	3	18,21,22	1.06	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L3	1779	3	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
3	OMC	L3	1340	3	19,22,23	0.57	0	25,31,34	0.72	0
3	PSU	L3	4471	3	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
3	A2M	L3	398	3	22,25,26	0.86	0	30,36,39	2.12	8 (26%)
3	A2M	L3	4523	3	22,25,26	0.85	0	30,36,39	2.11	8 (26%)
3	OMC	L3	2861	3	19,22,23	0.52	0	25,31,34	0.63	0
3	PSU	L3	4521	3	18,21,22	1.07	1 (5%)	21,30,33	1.92	5 (23%)
3	OMC	L3	2804	3	19,22,23	0.52	0	25,31,34	0.64	0
3	PSU	L3	4493	3	18,21,22	1.11	1 (5%)	21,30,33	1.94	4 (19%)
3	PSU	L3	4293	3	18,21,22	1.03	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L3	5001	3	18,21,22	1.11	1 (5%)	21,30,33	1.96	5 (23%)
3	OMC	L3	4456	3	19,22,23	0.54	0	25,31,34	0.66	0
3	OMG	L3	2876	3	23,26,27	0.48	0	32,38,41	0.46	0
3	A2M	L3	3830	3	22,25,26	0.85	0	30,36,39	2.08	8 (26%)
3	A2M	L3	400	3	22,25,26	0.86	0	30,36,39	2.11	8 (26%)
3	PSU	L3	4552	3	18,21,22	1.06	1 (5%)	21,30,33	1.94	5 (23%)
3	OMU	L3	4498	3	19,22,23	2.11	7 (36%)	25,31,34	1.80	5 (20%)
3	6MZ	L3	4220	3	22,25,26	1.13	1 (4%)	29,36,39	2.16	9 (31%)
3	OMG	L3	1522	3	23,26,27	0.51	0	32,38,41	0.53	0
3	OMU	L3	3925	3	19,22,23	1.99	6 (31%)	25,31,34	1.88	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L3	3841	3	19,22,23	0.52	0	25,31,34	0.66	0
3	A2M	L3	2787	3	22,25,26	0.87	1 (4%)	30,36,39	2.10	7 (23%)
3	OMG	L3	3627	3	23,26,27	0.49	0	32,38,41	0.55	0
3	PSU	L3	1782	3	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L3	2508	3	18,21,22	1.06	1 (5%)	21,30,33	1.92	5 (23%)
3	PSU	L3	1536	3	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
3	A2M	L3	2401	3	22,25,26	0.87	0	30,36,39	2.13	8 (26%)
3	A2M	L3	4571	3	22,25,26	0.86	0	30,36,39	2.02	7 (23%)
3	PSU	L3	4673	3	18,21,22	1.10	2 (11%)	21,30,33	1.95	5 (23%)
3	OMG	L3	4637	3	23,26,27	0.49	0	32,38,41	0.49	0
3	PSU	L3	1582	3	18,21,22	1.06	1 (5%)	21,30,33	1.92	5 (23%)
3	PSU	L3	3637	3	18,21,22	1.09	1 (5%)	21,30,33	2.01	5 (23%)
3	PSU	L3	2839	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
3	OMC	L3	2422	49,3	19,22,23	0.52	0	25,31,34	0.71	0
3	OMU	L3	4227	3	19,22,23	2.02	6 (31%)	25,31,34	1.82	5 (20%)
3	OMG	L3	4494	3	23,26,27	0.52	0	32,38,41	0.48	0
3	A2M	L3	1534	49,3	22,25,26	0.88	1 (4%)	30,36,39	2.10	8 (26%)
3	OMG	L3	2364	3	23,26,27	0.48	0	32,38,41	0.50	0
3	PSU	L3	3920	49,3	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)
3	A2M	L3	3867	3	22,25,26	0.88	0	30,36,39	2.11	7 (23%)
3	OMU	L3	2837	3	19,22,23	2.04	7 (36%)	25,31,34	1.84	5 (20%)
3	OMG	L3	1625	3	23,26,27	0.48	0	32,38,41	0.46	0
3	OMU	L3	2415	3	19,22,23	2.03	6 (31%)	25,31,34	1.84	5 (20%)
3	OMC	L3	3869	3	19,22,23	0.55	0	25,31,34	0.68	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
3	PSU	L3	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1781	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	3887	3	-	2/9/27/28	0/2/2/2
3	A2M	L3	3718	3	-	1/9/27/28	0/3/3/3
3	UR3	L3	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4361	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2815	3	-	0/9/27/28	0/3/3/3
3	A2M	L3	3724	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L3	4618	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4500	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3695	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	2424	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4636	3	-	3/7/25/26	0/2/2/2
3	PSU	L3	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1862	3	-	2/7/25/26	0/2/2/2
3	OMC	L3	2365	3	-	0/9/27/28	0/2/2/2
3	A2M	L3	1326	3	-	3/9/27/28	0/3/3/3
3	PSU	L3	4972	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	3822	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4499	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	1744	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3730	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3715	3	-	0/7/25/26	0/2/2/2
23	HIC	LN	245	23	-	0/5/6/8	0/1/1/1
3	PSU	L3	2632	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2824	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	3853	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2351	49,3	-	2/9/27/28	0/2/2/2
3	OMC	L3	4536	3	-	1/9/27/28	0/2/2/2
3	OMU	L3	4306	3	-	4/9/27/28	0/2/2/2
3	PSU	L3	4532	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4370	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	1677	3	-	3/7/25/26	0/2/2/2
3	A2M	L3	1524	3	-	2/9/27/28	0/3/3/3
3	PSU	L3	3851	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2363	49,3	-	0/9/27/28	0/3/3/3
3	A2M	L3	3825	3	-	0/9/27/28	0/3/3/3
3	OMG	L3	3899	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	5010	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4392	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	4296	3	-	0/7/25/26	0/2/2/2
3	1MA	L3	1322	3	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	3639	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	3744	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	1683	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4689	3	-	0/7/25/26	0/2/2/2
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
3	OMG	L3	4228	3	-	0/9/27/28	0/3/3/3
2	OMG	L1	75	2	-	1/9/27/28	0/3/3/3
3	PSU	L3	4312	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	1316	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	1871	3	-	1/9/27/28	0/3/3/3
3	OMC	L3	3701	3	-	7/9/27/28	0/2/2/2
3	PSU	L3	3884	3	-	2/7/25/26	0/2/2/2
3	PSU	L3	1860	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	4590	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	3844	3	-	1/7/25/26	0/2/2/2
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
3	OMG	L3	4623	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	1792	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1779	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4471	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	398	3	-	0/9/27/28	0/3/3/3
3	A2M	L3	4523	3	-	2/9/27/28	0/3/3/3
3	OMC	L3	2861	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4521	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2804	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	4493	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	5001	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	4456	3	-	0/9/27/28	0/2/2/2
3	OMG	L3	2876	3	-	0/9/27/28	0/3/3/3
3	A2M	L3	3830	3	-	1/9/27/28	0/3/3/3
3	A2M	L3	400	3	-	0/9/27/28	0/3/3/3
3	PSU	L3	4552	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	4498	3	-	0/9/27/28	0/2/2/2
3	6MZ	L3	4220	3	-	0/9/27/28	0/3/3/3
3	OMG	L3	1522	3	-	0/9/27/28	0/3/3/3
3	OMU	L3	3925	3	-	1/9/27/28	0/2/2/2
3	OMC	L3	3841	3	-	1/9/27/28	0/2/2/2
3	A2M	L3	2787	3	-	5/9/27/28	0/3/3/3
3	OMG	L3	3627	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1536	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2401	3	-	2/9/27/28	0/3/3/3
3	A2M	L3	4571	3	-	2/9/27/28	0/3/3/3
3	PSU	L3	4673	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4637	3	-	3/9/27/28	0/3/3/3
3	PSU	L3	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3637	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	2839	3	-	2/7/25/26	0/2/2/2
3	OMC	L3	2422	49,3	-	1/9/27/28	0/2/2/2
3	OMU	L3	4227	3	-	1/9/27/28	0/2/2/2
3	OMG	L3	4494	3	-	0/9/27/28	0/3/3/3
3	A2M	L3	1534	49,3	-	0/9/27/28	0/3/3/3
3	OMG	L3	2364	3	-	1/9/27/28	0/3/3/3
3	PSU	L3	3920	49,3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3867	3	-	2/9/27/28	0/3/3/3
3	OMU	L3	2837	3	-	1/9/27/28	0/2/2/2
3	OMG	L3	1625	3	-	2/9/27/28	0/3/3/3
3	OMU	L3	2415	3	-	0/9/27/28	0/2/2/2
3	OMC	L3	3869	3	-	1/9/27/28	0/2/2/2

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	4498	OMU	C6-N1	4.87	1.49	1.38
3	L3	4620	OMU	C6-N1	4.71	1.49	1.38
3	L3	2415	OMU	C6-N1	4.69	1.49	1.38
3	L3	4227	OMU	C6-N1	4.65	1.49	1.38
3	L3	2837	OMU	C6-N1	4.64	1.49	1.38
3	L3	4306	OMU	C6-N1	4.60	1.49	1.38
3	L3	3925	OMU	C6-N1	4.57	1.49	1.38
3	L3	4306	OMU	C2-N1	4.38	1.45	1.38
3	L3	4498	OMU	C2-N1	4.34	1.45	1.38
3	L3	2415	OMU	C2-N1	4.19	1.45	1.38
3	L3	2837	OMU	C2-N1	4.19	1.45	1.38
3	L3	4498	OMU	C5-C4	4.14	1.52	1.43
3	L3	4227	OMU	C2-N1	4.08	1.44	1.38
3	L3	4620	OMU	C2-N1	4.05	1.44	1.38
3	L3	2837	OMU	C5-C4	4.02	1.52	1.43
3	L3	3925	OMU	C2-N1	4.00	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	2415	OMU	C5-C4	3.97	1.52	1.43
3	L3	4220	6MZ	C6-N6	3.97	1.38	1.34
3	L3	3925	OMU	C5-C4	3.93	1.52	1.43
3	L3	4227	OMU	C5-C4	3.93	1.52	1.43
3	L3	4620	OMU	C5-C4	3.90	1.52	1.43
3	L3	3822	PSU	C6-C5	3.86	1.39	1.35
3	L3	4306	OMU	C5-C4	3.76	1.51	1.43
3	L3	3734	PSU	C6-C5	3.70	1.39	1.35
3	L3	4500	PSU	C6-C5	3.68	1.39	1.35
3	L3	1744	PSU	C6-C5	3.68	1.39	1.35
3	L3	1782	PSU	C6-C5	3.62	1.39	1.35
3	L3	1779	PSU	C6-C5	3.60	1.39	1.35
3	L3	5010	PSU	C6-C5	3.60	1.39	1.35
3	L3	1781	PSU	C6-C5	3.59	1.39	1.35
3	L3	3715	PSU	C6-C5	3.59	1.39	1.35
3	L3	4576	PSU	C6-C5	3.57	1.39	1.35
3	L3	4493	PSU	C6-C5	3.56	1.39	1.35
3	L3	3853	PSU	C6-C5	3.54	1.39	1.35
2	L1	69	PSU	C6-C5	3.54	1.39	1.35
3	L3	3844	PSU	C6-C5	3.53	1.39	1.35
3	L3	3695	PSU	C6-C5	3.52	1.39	1.35
3	L3	3851	PSU	C6-C5	3.52	1.39	1.35
3	L3	2632	PSU	C6-C5	3.51	1.39	1.35
3	L3	1862	PSU	C6-C5	3.50	1.39	1.35
3	L3	5001	PSU	C6-C5	3.50	1.39	1.35
3	L3	4361	PSU	C6-C5	3.50	1.39	1.35
2	L1	55	PSU	C6-C5	3.50	1.39	1.35
3	L3	4636	PSU	C6-C5	3.49	1.39	1.35
3	L3	4972	PSU	C6-C5	3.49	1.39	1.35
3	L3	3639	PSU	C6-C5	3.46	1.39	1.35
3	L3	3637	PSU	C6-C5	3.46	1.39	1.35
3	L3	3884	PSU	C6-C5	3.45	1.39	1.35
3	L3	4457	PSU	C6-C5	3.45	1.39	1.35
3	L3	3730	PSU	C6-C5	3.44	1.39	1.35
3	L3	4673	PSU	C6-C5	3.44	1.39	1.35
3	L3	4471	PSU	C6-C5	3.43	1.39	1.35
3	L3	4532	PSU	C6-C5	3.43	1.39	1.35
3	L3	4312	PSU	C6-C5	3.42	1.39	1.35
3	L3	2839	PSU	C6-C5	3.41	1.39	1.35
3	L3	1582	PSU	C6-C5	3.40	1.39	1.35
3	L3	1536	PSU	C6-C5	3.40	1.39	1.35
3	L3	4296	PSU	C6-C5	3.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	4521	PSU	C6-C5	3.38	1.39	1.35
3	L3	4353	PSU	C6-C5	3.35	1.39	1.35
3	L3	3920	PSU	C6-C5	3.34	1.39	1.35
3	L3	2508	PSU	C6-C5	3.34	1.39	1.35
3	L3	1792	PSU	C6-C5	3.32	1.39	1.35
3	L3	4628	PSU	C6-C5	3.31	1.39	1.35
3	L3	4552	PSU	C6-C5	3.29	1.38	1.35
3	L3	1683	PSU	C6-C5	3.25	1.38	1.35
3	L3	1860	PSU	C6-C5	3.24	1.38	1.35
3	L3	4689	PSU	C6-C5	3.23	1.38	1.35
3	L3	4579	PSU	C6-C5	3.19	1.38	1.35
3	L3	4293	PSU	C6-C5	3.15	1.38	1.35
23	LN	245	HIC	CD2-CG	3.04	1.41	1.36
3	L3	4306	OMU	O4-C4	-2.98	1.18	1.24
3	L3	1677	PSU	C6-C5	2.91	1.38	1.35
3	L3	4620	OMU	O4-C4	-2.88	1.18	1.24
3	L3	4299	PSU	C6-C5	2.87	1.38	1.35
3	L3	4530	UR3	C2-N1	-2.84	1.34	1.38
3	L3	3925	OMU	O4-C4	-2.81	1.19	1.24
3	L3	4530	UR3	C4-N3	-2.78	1.35	1.40
3	L3	4227	OMU	O4-C4	-2.78	1.19	1.24
3	L3	2837	OMU	O4-C4	-2.76	1.19	1.24
3	L3	2415	OMU	O4-C4	-2.71	1.19	1.24
3	L3	4498	OMU	C2-N3	2.69	1.42	1.38
3	L3	4498	OMU	O4-C4	-2.68	1.19	1.24
3	L3	2837	OMU	C2-N3	2.51	1.42	1.38
3	L3	4306	OMU	O2-C2	-2.46	1.18	1.23
3	L3	4227	OMU	O2-C2	-2.44	1.18	1.23
3	L3	2415	OMU	C2-N3	2.39	1.42	1.38
3	L3	4227	OMU	C2-N3	2.39	1.42	1.38
3	L3	3925	OMU	C2-N3	2.32	1.42	1.38
3	L3	4498	OMU	C4-N3	2.29	1.42	1.38
3	L3	2415	OMU	O2-C2	-2.28	1.19	1.23
3	L3	4620	OMU	O2-C2	-2.28	1.19	1.23
3	L3	3925	OMU	O2-C2	-2.26	1.19	1.23
3	L3	4620	OMU	C2-N3	2.24	1.41	1.38
3	L3	4306	OMU	C2-N3	2.19	1.41	1.38
3	L3	4530	UR3	C2-N3	-2.11	1.34	1.39
3	L3	4498	OMU	O2-C2	-2.10	1.19	1.23
3	L3	2837	OMU	O2-C2	-2.08	1.19	1.23
3	L3	2787	A2M	C5-N7	-2.07	1.35	1.39
3	L3	3718	A2M	C5-N7	-2.07	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	1534	A2M	C5-N7	-2.06	1.35	1.39
3	L3	4673	PSU	C4-C5	-2.04	1.38	1.44
3	L3	4579	PSU	C4-C5	-2.04	1.38	1.44
3	L3	1683	PSU	C4-C5	-2.04	1.38	1.44
3	L3	2837	OMU	C4-N3	2.03	1.42	1.38
3	L3	2363	A2M	C5-N7	-2.02	1.35	1.39
3	L3	4296	PSU	C4-C5	-2.01	1.38	1.44
3	L3	1860	PSU	C4-C5	-2.01	1.38	1.44
3	L3	4590	A2M	C5-N7	-2.01	1.35	1.39

All (430) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	1326	A2M	C5-C4-N3	-5.74	118.82	126.72
3	L3	3825	A2M	C5-C4-N3	-5.68	118.89	126.72
3	L3	3925	OMU	C4-N3-C2	-5.67	119.58	126.61
3	L3	2815	A2M	C5-C4-N3	-5.65	118.94	126.72
3	L3	3718	A2M	C5-C4-N3	-5.61	118.99	126.72
3	L3	2787	A2M	C5-C4-N3	-5.55	119.08	126.72
3	L3	1534	A2M	C5-C4-N3	-5.55	119.08	126.72
3	L3	4523	A2M	C5-C4-N3	-5.53	119.10	126.72
3	L3	400	A2M	C5-C4-N3	-5.53	119.11	126.72
3	L3	2837	OMU	C4-N3-C2	-5.53	119.75	126.61
3	L3	2415	OMU	C4-N3-C2	-5.51	119.77	126.61
3	L3	4571	A2M	C5-C4-N3	-5.49	119.15	126.72
3	L3	2363	A2M	C5-C4-N3	-5.49	119.16	126.72
3	L3	2401	A2M	C5-C4-N3	-5.47	119.18	126.72
3	L3	3867	A2M	C5-C4-N3	-5.45	119.21	126.72
3	L3	4220	6MZ	C5-C4-N3	-5.45	119.21	126.72
3	L3	398	A2M	C5-C4-N3	-5.45	119.21	126.72
3	L3	4227	OMU	C4-N3-C2	-5.44	119.86	126.61
3	L3	4306	OMU	C4-N3-C2	-5.43	119.87	126.61
3	L3	1524	A2M	C5-C4-N3	-5.42	119.25	126.72
3	L3	3830	A2M	C5-C4-N3	-5.39	119.29	126.72
3	L3	1871	A2M	C5-C4-N3	-5.39	119.30	126.72
3	L3	4498	OMU	C4-N3-C2	-5.38	119.94	126.61
3	L3	4689	PSU	N1-C2-N3	5.34	120.80	115.17
3	L3	3724	A2M	C5-C4-N3	-5.33	119.38	126.72
3	L3	4530	UR3	C4-N3-C2	-5.29	120.32	124.58
3	L3	4590	A2M	C5-C4-N3	-5.16	119.61	126.72
3	L3	4312	PSU	N1-C2-N3	5.11	120.56	115.17
3	L3	4689	PSU	C4-N3-C2	-5.11	119.34	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	3637	PSU	N1-C2-N3	5.10	120.55	115.17
3	L3	4296	PSU	C4-N3-C2	-5.10	119.35	126.37
3	L3	1683	PSU	C4-N3-C2	-5.08	119.37	126.37
3	L3	1683	PSU	N1-C2-N3	5.07	120.51	115.17
3	L3	4493	PSU	C4-N3-C2	-5.05	119.42	126.37
3	L3	4636	PSU	C4-N3-C2	-5.03	119.44	126.37
3	L3	4361	PSU	N1-C2-N3	5.02	120.46	115.17
3	L3	3637	PSU	C4-N3-C2	-5.01	119.47	126.37
3	L3	1744	PSU	C4-N3-C2	-5.00	119.48	126.37
3	L3	4299	PSU	C4-N3-C2	-5.00	119.48	126.37
3	L3	4312	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L3	4457	PSU	N1-C2-N3	4.97	120.41	115.17
3	L3	4296	PSU	N1-C2-N3	4.96	120.40	115.17
3	L3	1792	PSU	C4-N3-C2	-4.96	119.54	126.37
3	L3	4353	PSU	N1-C2-N3	4.96	120.40	115.17
3	L3	4620	OMU	C4-N3-C2	-4.95	120.46	126.61
2	L1	55	PSU	C4-N3-C2	-4.95	119.55	126.37
3	L3	4636	PSU	N1-C2-N3	4.93	120.37	115.17
3	L3	4353	PSU	C4-N3-C2	-4.93	119.58	126.37
3	L3	3822	PSU	N1-C2-N3	4.93	120.36	115.17
3	L3	3844	PSU	N1-C2-N3	4.92	120.36	115.17
3	L3	4361	PSU	C4-N3-C2	-4.91	119.60	126.37
3	L3	4532	PSU	C4-N3-C2	-4.91	119.60	126.37
3	L3	3695	PSU	C4-N3-C2	-4.91	119.61	126.37
3	L3	1582	PSU	C4-N3-C2	-4.91	119.61	126.37
3	L3	3734	PSU	N1-C2-N3	4.91	120.34	115.17
3	L3	5001	PSU	N1-C2-N3	4.91	120.34	115.17
2	L1	55	PSU	N1-C2-N3	4.90	120.34	115.17
3	L3	1781	PSU	C4-N3-C2	-4.90	119.62	126.37
3	L3	4299	PSU	N1-C2-N3	4.89	120.33	115.17
3	L3	2508	PSU	C4-N3-C2	-4.89	119.63	126.37
3	L3	4532	PSU	N1-C2-N3	4.87	120.31	115.17
3	L3	3734	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L3	4576	PSU	N1-C2-N3	4.86	120.30	115.17
3	L3	4471	PSU	N1-C2-N3	4.86	120.30	115.17
3	L3	3695	PSU	N1-C2-N3	4.86	120.29	115.17
3	L3	3851	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L3	1677	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L3	2839	PSU	N1-C2-N3	4.85	120.28	115.17
3	L3	3730	PSU	C4-N3-C2	-4.85	119.70	126.37
3	L3	4521	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L3	5010	PSU	C4-N3-C2	-4.84	119.70	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4552	PSU	C4-N3-C2	-4.84	119.71	126.37
3	L3	4576	PSU	C4-N3-C2	-4.83	119.71	126.37
3	L3	3884	PSU	N1-C2-N3	4.83	120.26	115.17
3	L3	4493	PSU	N1-C2-N3	4.83	120.26	115.17
3	L3	4457	PSU	C4-N3-C2	-4.82	119.72	126.37
3	L3	4500	PSU	N1-C2-N3	4.82	120.26	115.17
3	L3	5001	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L3	1744	PSU	N1-C2-N3	4.82	120.25	115.17
3	L3	2839	PSU	C4-N3-C2	-4.81	119.74	126.37
3	L3	3639	PSU	C4-N3-C2	-4.81	119.74	126.37
3	L3	4552	PSU	N1-C2-N3	4.81	120.24	115.17
3	L3	1536	PSU	C4-N3-C2	-4.81	119.75	126.37
3	L3	1782	PSU	C4-N3-C2	-4.80	119.75	126.37
3	L3	4972	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	4673	PSU	C4-N3-C2	-4.80	119.76	126.37
3	L3	4972	PSU	C4-N3-C2	-4.80	119.76	126.37
3	L3	4673	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	3844	PSU	C4-N3-C2	-4.80	119.76	126.37
3	L3	4521	PSU	N1-C2-N3	4.80	120.23	115.17
3	L3	3715	PSU	C4-N3-C2	-4.80	119.77	126.37
3	L3	1782	PSU	N1-C2-N3	4.79	120.22	115.17
3	L3	3822	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L3	3730	PSU	N1-C2-N3	4.79	120.22	115.17
3	L3	4500	PSU	C4-N3-C2	-4.78	119.78	126.37
3	L3	1862	PSU	N1-C2-N3	4.78	120.21	115.17
3	L3	1779	PSU	C4-N3-C2	-4.78	119.79	126.37
3	L3	1779	PSU	N1-C2-N3	4.77	120.20	115.17
3	L3	3884	PSU	C4-N3-C2	-4.77	119.80	126.37
2	L1	69	PSU	C4-N3-C2	-4.76	119.81	126.37
3	L3	1781	PSU	N1-C2-N3	4.76	120.19	115.17
3	L3	1677	PSU	N1-C2-N3	4.76	120.19	115.17
3	L3	4471	PSU	C4-N3-C2	-4.76	119.82	126.37
3	L3	4293	PSU	C4-N3-C2	-4.76	119.82	126.37
3	L3	2632	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L3	1582	PSU	N1-C2-N3	4.74	120.17	115.17
3	L3	3851	PSU	N1-C2-N3	4.74	120.17	115.17
3	L3	3920	PSU	C4-N3-C2	-4.74	119.84	126.37
3	L3	1792	PSU	N1-C2-N3	4.74	120.17	115.17
3	L3	1536	PSU	N1-C2-N3	4.73	120.16	115.17
2	L1	69	PSU	N1-C2-N3	4.73	120.15	115.17
3	L3	3639	PSU	N1-C2-N3	4.72	120.15	115.17
3	L3	3715	PSU	N1-C2-N3	4.71	120.14	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	5010	PSU	N1-C2-N3	4.71	120.14	115.17
3	L3	3825	A2M	N3-C4-N9	4.71	135.18	127.17
3	L3	4293	PSU	N1-C2-N3	4.70	120.13	115.17
3	L3	4628	PSU	C4-N3-C2	-4.69	119.91	126.37
3	L3	4628	PSU	N1-C2-N3	4.68	120.11	115.17
3	L3	1862	PSU	C4-N3-C2	-4.68	119.92	126.37
3	L3	4579	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L3	2508	PSU	N1-C2-N3	4.66	120.08	115.17
3	L3	2632	PSU	N1-C2-N3	4.65	120.08	115.17
3	L3	3920	PSU	N1-C2-N3	4.65	120.07	115.17
3	L3	1860	PSU	C4-N3-C2	-4.65	119.97	126.37
3	L3	3718	A2M	N3-C4-N9	4.65	135.07	127.17
3	L3	4571	A2M	N3-C4-N9	4.63	135.04	127.17
3	L3	4579	PSU	N1-C2-N3	4.63	120.05	115.17
3	L3	4523	A2M	N3-C4-N9	4.59	134.98	127.17
3	L3	1860	PSU	N1-C2-N3	4.58	120.00	115.17
3	L3	400	A2M	N3-C4-N9	4.58	134.95	127.17
3	L3	2363	A2M	N3-C4-N9	4.57	134.94	127.17
3	L3	3853	PSU	N1-C2-N3	4.57	119.99	115.17
3	L3	3853	PSU	C4-N3-C2	-4.56	120.08	126.37
3	L3	1326	A2M	N3-C4-N9	4.55	134.91	127.17
3	L3	1534	A2M	N3-C4-N9	4.55	134.91	127.17
3	L3	2787	A2M	N3-C4-N9	4.54	134.88	127.17
3	L3	2815	A2M	N3-C4-N9	4.53	134.87	127.17
3	L3	398	A2M	N3-C4-N9	4.52	134.85	127.17
3	L3	3867	A2M	N3-C4-N9	4.50	134.82	127.17
3	L3	1871	A2M	N3-C4-N9	4.49	134.80	127.17
3	L3	2401	A2M	N3-C4-N9	4.48	134.78	127.17
3	L3	3830	A2M	N3-C4-N9	4.47	134.77	127.17
3	L3	3724	A2M	N3-C4-N9	4.46	134.75	127.17
3	L3	1524	A2M	N3-C4-N9	4.44	134.72	127.17
3	L3	4306	OMU	N3-C2-N1	4.40	120.62	114.89
3	L3	4220	6MZ	N3-C4-N9	4.26	134.42	127.17
3	L3	3724	A2M	N3-C2-N1	-4.22	122.20	128.58
3	L3	3830	A2M	N3-C2-N1	-4.21	122.20	128.58
3	L3	1524	A2M	N3-C2-N1	-4.18	122.26	128.58
3	L3	3925	OMU	N3-C2-N1	4.15	120.29	114.89
3	L3	1871	A2M	N3-C2-N1	-4.13	122.33	128.58
3	L3	3825	A2M	N3-C2-N1	-4.13	122.34	128.58
3	L3	400	A2M	N3-C2-N1	-4.12	122.34	128.58
3	L3	3867	A2M	N3-C2-N1	-4.12	122.35	128.58
3	L3	398	A2M	N3-C2-N1	-4.10	122.38	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4590	A2M	N3-C2-N1	-4.10	122.38	128.58
3	L3	2787	A2M	N3-C2-N1	-4.09	122.39	128.58
3	L3	2815	A2M	N3-C2-N1	-4.08	122.41	128.58
3	L3	4523	A2M	N3-C2-N1	-4.07	122.41	128.58
3	L3	2415	OMU	N3-C2-N1	4.06	120.18	114.89
3	L3	4590	A2M	N3-C4-N9	4.05	134.06	127.17
3	L3	2363	A2M	N3-C2-N1	-4.05	122.45	128.58
3	L3	4220	6MZ	N1-C2-N3	-4.04	122.47	128.58
3	L3	2401	A2M	N3-C2-N1	-4.03	122.48	128.58
3	L3	4571	A2M	N3-C2-N1	-4.01	122.51	128.58
3	L3	4498	OMU	N3-C2-N1	3.98	120.07	114.89
3	L3	1534	A2M	N3-C2-N1	-3.96	122.58	128.58
3	L3	4227	OMU	N3-C2-N1	3.96	120.05	114.89
3	L3	1326	A2M	N3-C2-N1	-3.90	122.67	128.58
3	L3	4220	6MZ	C5-N7-C8	3.90	109.58	103.45
3	L3	2837	OMU	N3-C2-N1	3.88	119.94	114.89
3	L3	3925	OMU	C5-C4-N3	3.87	120.22	114.80
3	L3	2837	OMU	C5-C4-N3	3.86	120.21	114.80
3	L3	4227	OMU	C5-C4-N3	3.86	120.20	114.80
3	L3	1534	A2M	C5-N7-C8	3.84	109.48	103.45
3	L3	2415	OMU	C5-C4-N3	3.81	120.14	114.80
3	L3	4590	A2M	C5-N7-C8	3.80	109.42	103.45
3	L3	4523	A2M	C5-N7-C8	3.79	109.40	103.45
3	L3	2401	A2M	C5-N7-C8	3.76	109.36	103.45
3	L3	2815	A2M	C5-N7-C8	3.75	109.35	103.45
3	L3	2787	A2M	C5-N7-C8	3.75	109.34	103.45
3	L3	3830	A2M	C5-N7-C8	3.75	109.34	103.45
3	L3	1326	A2M	C5-N7-C8	3.74	109.33	103.45
3	L3	3825	A2M	C5-N7-C8	3.74	109.33	103.45
3	L3	4620	OMU	N3-C2-N1	3.72	119.74	114.89
3	L3	1871	A2M	C5-N7-C8	3.72	109.29	103.45
3	L3	3718	A2M	N3-C2-N1	-3.71	122.96	128.58
3	L3	3825	A2M	C2-N3-C4	3.71	120.89	111.83
3	L3	4498	OMU	C5-C4-N3	3.71	119.99	114.80
3	L3	398	A2M	C5-N7-C8	3.70	109.27	103.45
3	L3	400	A2M	C5-N7-C8	3.70	109.26	103.45
3	L3	1524	A2M	C5-N7-C8	3.69	109.25	103.45
3	L3	3724	A2M	C5-N7-C8	3.69	109.25	103.45
3	L3	4620	OMU	C5-C4-N3	3.68	119.95	114.80
3	L3	4306	OMU	C5-C4-N3	3.67	119.94	114.80
3	L3	2815	A2M	C2-N3-C4	3.66	120.77	111.83
3	L3	4571	A2M	C5-N7-C8	3.66	109.20	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	2363	A2M	C5-N7-C8	3.65	109.19	103.45
3	L3	400	A2M	C2-N3-C4	3.63	120.69	111.83
3	L3	1326	A2M	C2-N3-C4	3.63	120.69	111.83
3	L3	4523	A2M	C2-N3-C4	3.60	120.64	111.83
3	L3	3867	A2M	C2-N3-C4	3.60	120.62	111.83
3	L3	2787	A2M	C2-N3-C4	3.60	120.62	111.83
3	L3	2401	A2M	C2-N3-C4	3.60	120.61	111.83
3	L3	4220	6MZ	C2-N3-C4	3.60	120.61	111.83
3	L3	1524	A2M	C2-N3-C4	3.59	120.60	111.83
3	L3	4571	A2M	C2-N3-C4	3.58	120.58	111.83
3	L3	3867	A2M	C5-N7-C8	3.58	109.08	103.45
3	L3	1871	A2M	C2-N3-C4	3.58	120.57	111.83
3	L3	3718	A2M	C5-N7-C8	3.58	109.07	103.45
3	L3	398	A2M	C2-N3-C4	3.57	120.56	111.83
3	L3	1534	A2M	C2-N3-C4	3.57	120.55	111.83
3	L3	3830	A2M	C2-N3-C4	3.57	120.55	111.83
3	L3	2363	A2M	C2-N3-C4	3.56	120.52	111.83
3	L3	3724	A2M	C2-N3-C4	3.52	120.42	111.83
3	L3	4590	A2M	C2-N3-C4	3.50	120.38	111.83
3	L3	3718	A2M	C2-N3-C4	3.45	120.25	111.83
3	L3	4220	6MZ	C4-C5-N7	-3.32	106.78	110.58
3	L3	4530	UR3	C5-C4-N3	3.28	119.36	115.04
3	L3	1326	A2M	C4-C5-N7	-3.18	106.95	110.58
3	L3	4590	A2M	C4-C5-N7	-3.18	106.95	110.58
3	L3	2837	OMU	O4-C4-C5	-3.12	119.78	125.16
3	L3	1534	A2M	C4-C5-N7	-3.11	107.03	110.58
3	L3	2401	A2M	C2'-C1'-N9	-3.08	108.69	113.75
3	L3	2815	A2M	C4-C5-N7	-3.05	107.09	110.58
3	L3	1683	PSU	O2-C2-N1	-3.04	119.65	122.79
3	L3	1536	PSU	O2-C2-N1	-3.04	119.65	122.79
3	L3	4227	OMU	O4-C4-C5	-3.03	119.94	125.16
3	L3	3822	PSU	O2-C2-N1	-3.01	119.69	122.79
3	L3	3925	OMU	O4-C4-C5	-3.00	119.98	125.16
3	L3	4579	PSU	O2-C2-N1	-2.99	119.70	122.79
3	L3	4457	PSU	O2-C2-N1	-2.98	119.71	122.79
2	L1	69	PSU	O2-C2-N1	-2.98	119.72	122.79
3	L3	2401	A2M	C4-C5-N7	-2.97	107.18	110.58
3	L3	2415	OMU	O4-C4-C5	-2.97	120.04	125.16
3	L3	4523	A2M	C4-C5-N7	-2.96	107.19	110.58
3	L3	1677	PSU	O2-C2-N1	-2.95	119.74	122.79
3	L3	4220	6MZ	C9-N6-C6	-2.95	120.12	122.85
3	L3	4498	OMU	O4-C4-C5	-2.95	120.08	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	3844	PSU	O2-C2-N1	-2.94	119.75	122.79
3	L3	3830	A2M	C4-C5-N7	-2.94	107.22	110.58
3	L3	398	A2M	C4-C5-N7	-2.93	107.23	110.58
3	L3	1524	A2M	C4-C5-N7	-2.93	107.23	110.58
3	L3	400	A2M	C4-C5-N7	-2.92	107.24	110.58
3	L3	4636	PSU	O2-C2-N1	-2.92	119.78	122.79
3	L3	1871	A2M	C2'-C1'-N9	-2.92	108.95	113.75
23	LN	245	HIC	NE2-CE1-ND1	-2.92	111.55	112.66
3	L3	1871	A2M	C4-C5-N7	-2.91	107.26	110.58
3	L3	3724	A2M	C4-C5-N7	-2.90	107.26	110.58
3	L3	3825	A2M	C4-C5-N7	-2.90	107.27	110.58
3	L3	2787	A2M	C4-C5-N7	-2.90	107.27	110.58
3	L3	4500	PSU	O2-C2-N1	-2.90	119.80	122.79
3	L3	3718	A2M	C4-C5-N7	-2.88	107.28	110.58
3	L3	3734	PSU	O2-C2-N1	-2.88	119.81	122.79
3	L3	5001	PSU	O2-C2-N1	-2.88	119.82	122.79
3	L3	4361	PSU	O2-C2-N1	-2.88	119.82	122.79
3	L3	3830	A2M	N9-C8-N7	-2.88	109.85	113.94
3	L3	4306	OMU	O4-C4-C5	-2.88	120.20	125.16
3	L3	4571	A2M	C4-C5-N7	-2.88	107.29	110.58
3	L3	4620	OMU	O4-C4-C5	-2.87	120.20	125.16
3	L3	4312	PSU	O2-C2-N1	-2.87	119.83	122.79
3	L3	2363	A2M	C4-C5-N7	-2.85	107.32	110.58
3	L3	3853	PSU	O2-C2-N1	-2.84	119.86	122.79
3	L3	3884	PSU	O2-C2-N1	-2.83	119.87	122.79
3	L3	1782	PSU	O2-C2-N1	-2.83	119.87	122.79
3	L3	4590	A2M	N9-C8-N7	-2.83	109.92	113.94
3	L3	2401	A2M	N9-C8-N7	-2.82	109.93	113.94
3	L3	1779	PSU	O2-C2-N1	-2.82	119.88	122.79
3	L3	2508	PSU	O2-C2-N1	-2.82	119.88	122.79
3	L3	4471	PSU	O2-C2-N1	-2.82	119.88	122.79
3	L3	4579	PSU	C6-N1-C2	-2.82	120.08	122.69
3	L3	2839	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L3	1871	A2M	N9-C8-N7	-2.81	109.96	113.94
3	L3	4299	PSU	O2-C2-N1	-2.80	119.91	122.79
3	L3	1860	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L3	3639	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L3	1862	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L3	4523	A2M	N9-C8-N7	-2.78	109.99	113.94
3	L3	4576	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L3	1524	A2M	N9-C8-N7	-2.77	110.01	113.94
3	L3	3867	A2M	C4-C5-N7	-2.76	107.43	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	3715	PSU	O2-C2-N1	-2.75	119.95	122.79
3	L3	4628	PSU	O2-C2-N1	-2.75	119.95	122.79
3	L3	3724	A2M	N9-C8-N7	-2.75	110.04	113.94
3	L3	4689	PSU	C6-N1-C2	-2.74	120.14	122.69
3	L3	4972	PSU	O2-C2-N1	-2.73	119.97	122.79
3	L3	1534	A2M	N9-C8-N7	-2.73	110.06	113.94
3	L3	4532	PSU	O2-C2-N1	-2.73	119.97	122.79
3	L3	3825	A2M	N9-C8-N7	-2.72	110.07	113.94
3	L3	3695	PSU	O2-C2-N1	-2.72	119.98	122.79
3	L3	400	A2M	N9-C8-N7	-2.71	110.08	113.94
3	L3	3851	PSU	O2-C2-N1	-2.71	119.99	122.79
3	L3	398	A2M	N9-C8-N7	-2.71	110.10	113.94
3	L3	1582	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L3	4353	PSU	O2-C2-N1	-2.69	120.01	122.79
3	L3	4293	PSU	O2-C2-N1	-2.69	120.01	122.79
2	L1	55	PSU	O2-C2-N1	-2.69	120.02	122.79
3	L3	3730	PSU	O2-C2-N1	-2.68	120.02	122.79
3	L3	4296	PSU	O2-C2-N1	-2.68	120.02	122.79
3	L3	3884	PSU	C6-N1-C2	-2.68	120.20	122.69
3	L3	4628	PSU	C6-N1-C2	-2.68	120.21	122.69
3	L3	4457	PSU	C6-N1-C2	-2.66	120.22	122.69
2	L1	55	PSU	C6-C5-C4	2.66	119.97	118.17
3	L3	4220	6MZ	N9-C8-N7	-2.66	110.17	113.94
3	L3	2787	A2M	N9-C8-N7	-2.65	110.18	113.94
3	L3	2815	A2M	N9-C8-N7	-2.65	110.18	113.94
3	L3	5001	PSU	C6-N1-C2	-2.64	120.25	122.69
3	L3	1860	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L3	3637	PSU	C6-C5-C4	2.62	119.94	118.17
3	L3	1524	A2M	C2'-C1'-N9	-2.62	109.44	113.75
3	L3	4571	A2M	N9-C8-N7	-2.62	110.22	113.94
3	L3	2363	A2M	N9-C8-N7	-2.61	110.23	113.94
3	L3	4673	PSU	C6-N1-C2	-2.60	120.28	122.69
3	L3	4361	PSU	C6-N1-C2	-2.60	120.28	122.69
3	L3	4471	PSU	C6-N1-C2	-2.60	120.28	122.69
3	L3	3867	A2M	N9-C8-N7	-2.59	110.26	113.94
3	L3	4689	PSU	O2-C2-N1	-2.59	120.12	122.79
3	L3	4673	PSU	O2-C2-N1	-2.58	120.12	122.79
3	L3	1326	A2M	N9-C8-N7	-2.58	110.27	113.94
3	L3	3920	PSU	O2-C2-N1	-2.58	120.13	122.79
3	L3	4521	PSU	O2-C2-N1	-2.56	120.14	122.79
3	L3	4312	PSU	C6-N1-C2	-2.56	120.32	122.69
3	L3	1862	PSU	C6-N1-C2	-2.56	120.32	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	2839	PSU	C6-N1-C2	-2.56	120.32	122.69
3	L3	1781	PSU	O2-C2-N1	-2.55	120.15	122.79
3	L3	2632	PSU	O2-C2-N1	-2.55	120.16	122.79
3	L3	3844	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L3	4523	A2M	C2'-C1'-N9	-2.54	109.57	113.75
3	L3	3695	PSU	C6-C5-C4	2.54	119.89	118.17
3	L3	3822	PSU	C6-C5-C4	2.53	119.88	118.17
3	L3	1683	PSU	C6-C5-C4	2.53	119.88	118.17
3	L3	5010	PSU	O2-C2-N1	-2.53	120.18	122.79
3	L3	4552	PSU	C6-N1-C2	-2.52	120.35	122.69
3	L3	1792	PSU	O2-C2-N1	-2.52	120.19	122.79
3	L3	3734	PSU	C6-N1-C2	-2.52	120.36	122.69
3	L3	4552	PSU	O2-C2-N1	-2.52	120.19	122.79
3	L3	4532	PSU	C6-C5-C4	2.51	119.87	118.17
3	L3	4220	6MZ	C6-C5-N7	2.51	135.17	132.43
3	L3	3822	PSU	C6-N1-C2	-2.51	120.37	122.69
3	L3	1779	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L3	3920	PSU	C6-N1-C2	-2.49	120.38	122.69
2	L1	69	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L3	4500	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L3	398	A2M	C2'-C1'-N9	-2.48	109.68	113.75
3	L3	4972	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L3	4636	PSU	C6-C5-C4	2.47	119.84	118.17
3	L3	1744	PSU	O2-C2-N1	-2.46	120.25	122.79
3	L3	400	A2M	C2'-C1'-N9	-2.45	109.71	113.75
3	L3	3853	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L3	1536	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L3	4576	PSU	C6-N1-C2	-2.42	120.44	122.69
3	L3	4521	PSU	C6-N1-C2	-2.42	120.44	122.69
3	L3	1782	PSU	C6-N1-C2	-2.41	120.45	122.69
3	L3	3730	PSU	C6-N1-C2	-2.41	120.45	122.69
3	L3	3637	PSU	C6-N1-C2	-2.41	120.45	122.69
3	L3	1677	PSU	C6-N1-C2	-2.40	120.46	122.69
3	L3	3844	PSU	C6-C5-C4	2.40	119.79	118.17
3	L3	4293	PSU	C6-N1-C2	-2.39	120.47	122.69
3	L3	3718	A2M	N9-C8-N7	-2.39	110.54	113.94
3	L3	3639	PSU	C6-N1-C2	-2.39	120.47	122.69
3	L3	3695	PSU	C6-N1-C2	-2.38	120.48	122.69
3	L3	1744	PSU	C6-C5-C4	2.38	119.78	118.17
3	L3	4353	PSU	C6-N1-C2	-2.37	120.49	122.69
3	L3	4296	PSU	C6-N1-C2	-2.36	120.50	122.69
3	L3	3715	PSU	C6-N1-C2	-2.36	120.50	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4471	PSU	C6-C5-C4	2.36	119.76	118.17
3	L3	2632	PSU	C6-N1-C2	-2.35	120.51	122.69
3	L3	3730	PSU	C6-C5-C4	2.34	119.75	118.17
3	L3	1677	PSU	C6-C5-C4	2.34	119.75	118.17
2	L1	55	PSU	C6-N1-C2	-2.33	120.53	122.69
3	L3	3734	PSU	C6-C5-C4	2.32	119.74	118.17
3	L3	1683	PSU	C6-N1-C2	-2.32	120.54	122.69
3	L3	3851	PSU	C6-N1-C2	-2.32	120.54	122.69
3	L3	4296	PSU	C6-C5-C4	2.30	119.73	118.17
2	L1	69	PSU	O4'-C1'-C2'	2.30	108.33	105.15
3	L3	4498	OMU	O2-C2-N1	-2.30	119.80	122.80
3	L3	4673	PSU	C6-C5-C4	2.30	119.72	118.17
3	L3	1781	PSU	C6-N1-C2	-2.29	120.56	122.69
3	L3	4532	PSU	C6-N1-C2	-2.29	120.56	122.69
3	L3	4636	PSU	C6-N1-C2	-2.28	120.58	122.69
3	L3	1782	PSU	C6-C5-C4	2.27	119.71	118.17
3	L3	4353	PSU	C6-C5-C4	2.26	119.70	118.17
3	L3	3925	OMU	O2-C2-N1	-2.25	119.86	122.80
3	L3	3715	PSU	O4'-C1'-C2'	2.25	108.27	105.15
3	L3	1322	1MA	N1-C6-N6	2.25	125.35	119.71
3	L3	4361	PSU	C6-C5-C4	2.24	119.68	118.17
3	L3	4576	PSU	C6-C5-C4	2.23	119.68	118.17
3	L3	1781	PSU	C6-C5-C4	2.23	119.68	118.17
3	L3	3637	PSU	O2-C2-N1	-2.22	120.49	122.79
3	L3	4493	PSU	O2-C2-N1	-2.22	120.50	122.79
3	L3	5010	PSU	C6-N1-C2	-2.22	120.63	122.69
3	L3	4500	PSU	C6-C5-C4	2.22	119.67	118.17
3	L3	2839	PSU	C6-C5-C4	2.22	119.67	118.17
3	L3	2351	OMC	C1'-N1-C2	2.21	123.32	118.44
3	L3	4299	PSU	C6-C5-C4	2.19	119.65	118.17
3	L3	4552	PSU	C6-C5-C4	2.18	119.65	118.17
3	L3	4457	PSU	C6-C5-C4	2.18	119.64	118.17
3	L3	1744	PSU	C6-N1-C2	-2.18	120.67	122.69
3	L3	3715	PSU	C6-C5-C4	2.17	119.64	118.17
3	L3	4493	PSU	C6-N1-C2	-2.15	120.69	122.69
3	L3	2415	OMU	O2-C2-N1	-2.14	120.02	122.80
3	L3	1582	PSU	C6-N1-C2	-2.13	120.72	122.69
3	L3	1792	PSU	C6-C5-C4	2.13	119.61	118.17
3	L3	5010	PSU	C6-C5-C4	2.13	119.61	118.17
3	L3	1779	PSU	C6-C5-C4	2.13	119.61	118.17
3	L3	4299	PSU	C6-N1-C2	-2.12	120.72	122.69
3	L3	1582	PSU	C6-C5-C4	2.12	119.61	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	1862	PSU	C6-C5-C4	2.12	119.60	118.17
3	L3	3639	PSU	C6-C5-C4	2.11	119.60	118.17
3	L3	4227	OMU	O2-C2-N1	-2.11	120.05	122.80
3	L3	2837	OMU	O2-C2-N1	-2.10	120.06	122.80
3	L3	1792	PSU	C6-N1-C2	-2.09	120.75	122.69
3	L3	4972	PSU	C6-C5-C4	2.09	119.58	118.17
3	L3	2815	A2M	C2'-C1'-N9	-2.09	110.32	113.75
3	L3	2508	PSU	C6-C5-C4	2.09	119.58	118.17
3	L3	2508	PSU	C6-N1-C2	-2.08	120.76	122.69
3	L3	3851	PSU	O4'-C1'-C2'	2.07	108.02	105.15
3	L3	5001	PSU	C6-C5-C4	2.05	119.56	118.17
3	L3	1536	PSU	C6-C5-C4	2.05	119.56	118.17
3	L3	4689	PSU	C6-C5-C4	2.05	119.56	118.17
3	L3	1326	A2M	C2'-C1'-N9	-2.05	110.38	113.75
3	L3	1862	PSU	O4'-C1'-C2'	2.04	107.98	105.15
3	L3	1534	A2M	C3'-C2'-C1'	-2.04	98.89	102.81
3	L3	4628	PSU	C6-C5-C4	2.04	119.55	118.17
3	L3	3830	A2M	C2'-C1'-N9	-2.03	110.41	113.75
3	L3	4521	PSU	C6-C5-C4	2.03	119.54	118.17
3	L3	4312	PSU	C6-C5-C4	2.01	119.53	118.17
3	L3	4457	PSU	O4'-C1'-C2'	2.01	107.93	105.15
3	L3	1860	PSU	O4'-C1'-C2'	2.01	107.93	105.15
3	L3	3639	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	75	OMG	C1'-C2'-O2'-CM2
3	L3	1316	OMG	C1'-C2'-O2'-CM2
3	L3	1326	A2M	C1'-C2'-O2'-CM'
3	L3	1340	OMC	C1'-C2'-O2'-CM2
3	L3	1871	A2M	C1'-C2'-O2'-CM'
3	L3	2364	OMG	C1'-C2'-O2'-CM2
3	L3	2422	OMC	C1'-C2'-O2'-CM2
3	L3	2424	OMG	C1'-C2'-O2'-CM2
3	L3	2804	OMC	C1'-C2'-O2'-CM2
3	L3	2824	OMC	C1'-C2'-O2'-CM2
3	L3	2837	OMU	C1'-C2'-O2'-CM2
3	L3	2861	OMC	C1'-C2'-O2'-CM2
3	L3	3627	OMG	C1'-C2'-O2'-CM2
3	L3	3701	OMC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
3	L3	3701	OMC	C2'-C1'-N1-C6
3	L3	3718	A2M	C1'-C2'-O2'-CM'
3	L3	3724	A2M	C1'-C2'-O2'-CM'
3	L3	3744	OMG	C1'-C2'-O2'-CM2
3	L3	3830	A2M	C1'-C2'-O2'-CM'
3	L3	3841	OMC	C1'-C2'-O2'-CM2
3	L3	3867	A2M	C3'-C4'-C5'-O5'
3	L3	3869	OMC	C1'-C2'-O2'-CM2
3	L3	3887	OMC	C3'-C4'-C5'-O5'
3	L3	3887	OMC	O4'-C4'-C5'-O5'
3	L3	3899	OMG	C1'-C2'-O2'-CM2
3	L3	3925	OMU	C1'-C2'-O2'-CM2
3	L3	4227	OMU	C1'-C2'-O2'-CM2
3	L3	4392	OMG	C1'-C2'-O2'-CM2
3	L3	4499	OMG	C1'-C2'-O2'-CM2
3	L3	4536	OMC	C1'-C2'-O2'-CM2
3	L3	4571	A2M	C1'-C2'-O2'-CM'
3	L3	4590	A2M	C4'-C5'-O5'-P
3	L3	4636	PSU	C2'-C1'-C5-C4
3	L3	4637	OMG	O4'-C4'-C5'-O5'
3	L3	4637	OMG	C1'-C2'-O2'-CM2
3	L3	2787	A2M	C3'-C4'-C5'-O5'
3	L3	1326	A2M	C3'-C4'-C5'-O5'
3	L3	1862	PSU	C3'-C4'-C5'-O5'
3	L3	1862	PSU	O4'-C4'-C5'-O5'
3	L3	2787	A2M	O4'-C4'-C5'-O5'
3	L3	3867	A2M	O4'-C4'-C5'-O5'
3	L3	4306	OMU	C3'-C4'-C5'-O5'
3	L3	4306	OMU	O4'-C4'-C5'-O5'
3	L3	4523	A2M	O4'-C4'-C5'-O5'
3	L3	4523	A2M	C3'-C4'-C5'-O5'
3	L3	1322	1MA	O4'-C4'-C5'-O5'
3	L3	1677	PSU	C3'-C4'-C5'-O5'
3	L3	1677	PSU	O4'-C4'-C5'-O5'
3	L3	2401	A2M	C3'-C4'-C5'-O5'
3	L3	4637	OMG	C3'-C4'-C5'-O5'
3	L3	1326	A2M	O4'-C4'-C5'-O5'
3	L3	3701	OMC	O4'-C4'-C5'-O5'
3	L3	3701	OMC	C3'-C4'-C5'-O5'
3	L3	2401	A2M	O4'-C4'-C5'-O5'
3	L3	1322	1MA	C3'-C4'-C5'-O5'
3	L3	2787	A2M	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
3	L3	1625	OMG	C3'-C4'-C5'-O5'
3	L3	4306	OMU	C4'-C5'-O5'-P
3	L3	1677	PSU	O4'-C1'-C5-C4
3	L3	2839	PSU	O4'-C1'-C5-C4
3	L3	3884	PSU	O4'-C1'-C5-C4
3	L3	4636	PSU	O4'-C1'-C5-C4
3	L3	2787	A2M	C2'-C1'-N9-C4
3	L3	1524	A2M	O4'-C1'-N9-C8
3	L3	3701	OMC	O4'-C1'-N1-C6
3	L3	3701	OMC	C4'-C5'-O5'-P
3	L3	3844	PSU	C4'-C5'-O5'-P
3	L3	4636	PSU	C4'-C5'-O5'-P
3	L3	4618	OMG	O4'-C4'-C5'-O5'
3	L3	1524	A2M	O4'-C1'-N9-C4
3	L3	2839	PSU	O4'-C1'-C5-C6
3	L3	3884	PSU	O4'-C1'-C5-C6
3	L3	2351	OMC	C2'-C1'-N1-C6
3	L3	2787	A2M	O4'-C1'-N9-C8
3	L3	4306	OMU	C2'-C1'-N1-C6
3	L3	3701	OMC	O4'-C1'-N1-C2
3	L3	2351	OMC	C2'-C1'-N1-C2
3	L3	4571	A2M	C3'-C2'-O2'-CM'
3	L3	1625	OMG	C4'-C5'-O5'-P

There are no ring outliers.

57 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	3734	PSU	1	0
3	L3	3718	A2M	4	0
3	L3	4530	UR3	1	0
3	L3	2815	A2M	1	0
3	L3	3724	A2M	3	0
3	L3	4618	OMG	2	0
3	L3	4500	PSU	2	0
3	L3	3695	PSU	1	0
3	L3	2424	OMG	1	0
3	L3	4636	PSU	1	0
3	L3	4457	PSU	1	0
3	L3	4299	PSU	1	0
3	L3	1326	A2M	5	0
3	L3	4499	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	1744	PSU	3	0
3	L3	3715	PSU	1	0
3	L3	2824	OMC	2	0
3	L3	2351	OMC	2	0
3	L3	4306	OMU	3	0
3	L3	1677	PSU	3	0
3	L3	1524	A2M	1	0
3	L3	3851	PSU	1	0
3	L3	2363	A2M	2	0
3	L3	3899	OMG	1	0
3	L3	4392	OMG	1	0
3	L3	4296	PSU	1	0
3	L3	3744	OMG	3	0
3	L3	4689	PSU	1	0
2	L1	75	OMG	1	0
3	L3	1316	OMG	1	0
3	L3	1860	PSU	2	0
3	L3	4590	A2M	1	0
2	L1	69	PSU	2	0
3	L3	4623	OMG	1	0
3	L3	1779	PSU	2	0
3	L3	1340	OMC	1	0
3	L3	4523	A2M	1	0
3	L3	2861	OMC	1	0
3	L3	2804	OMC	1	0
3	L3	5001	PSU	1	0
3	L3	2876	OMG	1	0
3	L3	3830	A2M	1	0
3	L3	4220	6MZ	1	0
3	L3	1522	OMG	1	0
3	L3	3925	OMU	1	0
3	L3	3841	OMC	1	0
3	L3	3627	OMG	1	0
3	L3	4637	OMG	2	0
3	L3	2839	PSU	1	0
3	L3	2422	OMC	2	0
3	L3	4227	OMU	2	0
3	L3	1534	A2M	3	0
3	L3	2364	OMG	2	0
3	L3	3867	A2M	1	0
3	L3	2837	OMU	1	0
3	L3	2415	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	3869	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 93 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

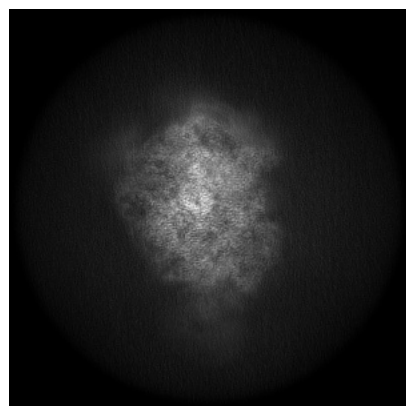
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29277. These allow visual inspection of the internal detail of the map and identification of artifacts.

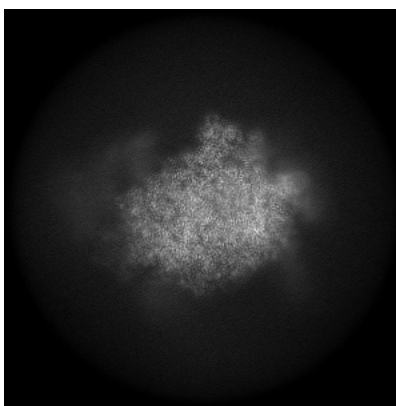
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

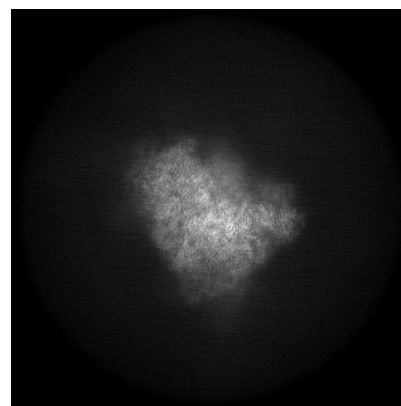
6.1.1 Primary map



X

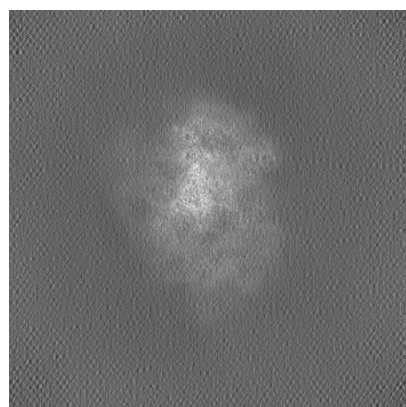


Y

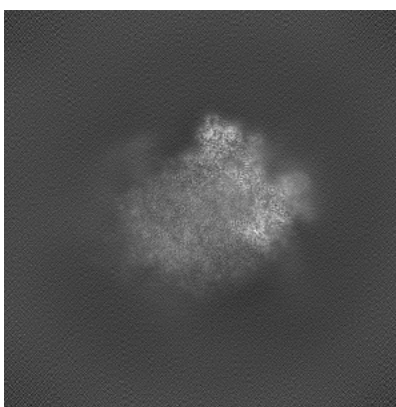


Z

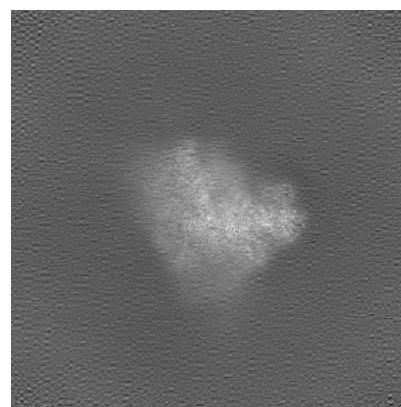
6.1.2 Raw map



X



Y

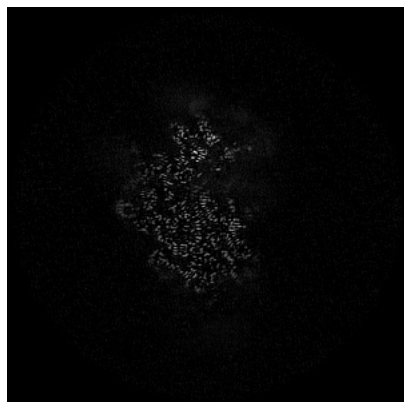


Z

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

6.2 Central slices [i](#)

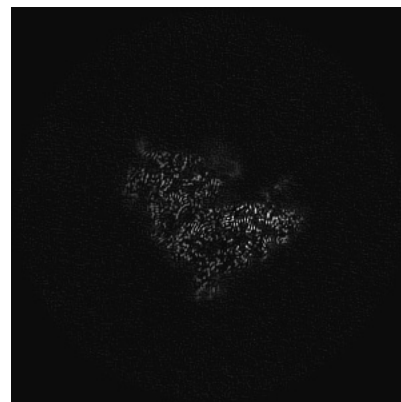
6.2.1 Primary map



X Index: 240

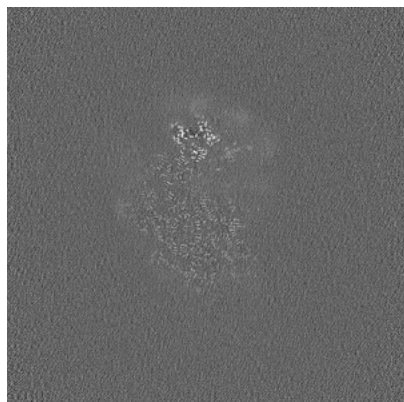


Y Index: 240

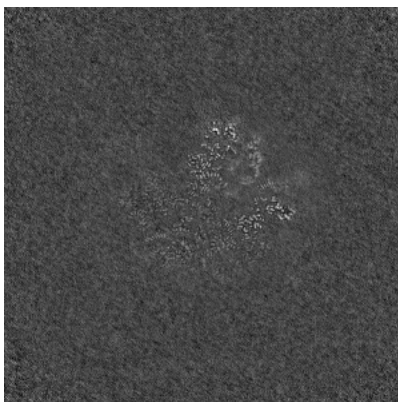


Z Index: 240

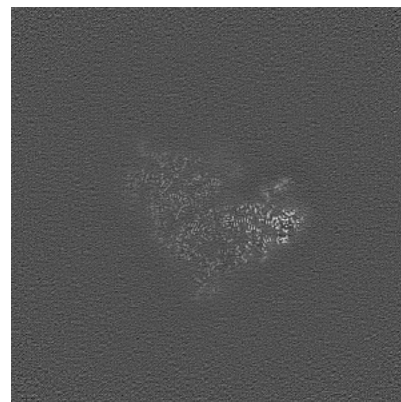
6.2.2 Raw map



X Index: 240



Y Index: 240

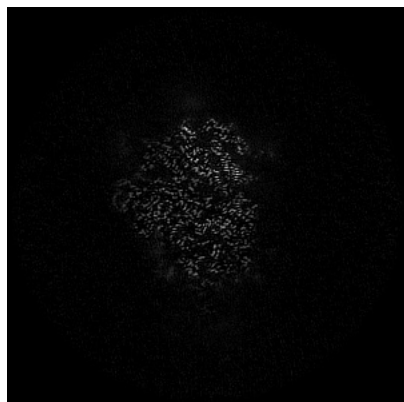


Z Index: 240

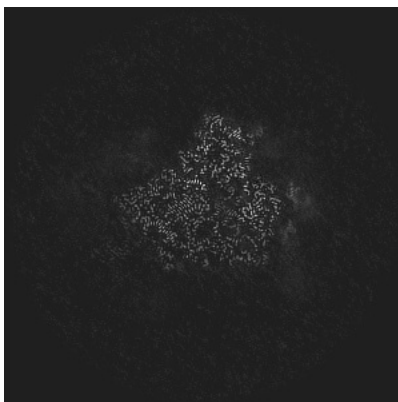
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

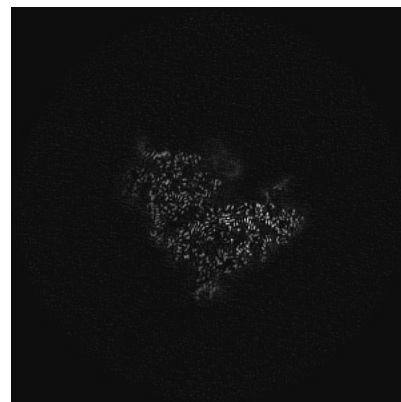
6.3.1 Primary map



X Index: 226

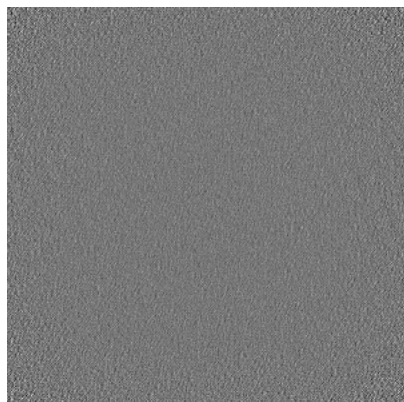


Y Index: 227

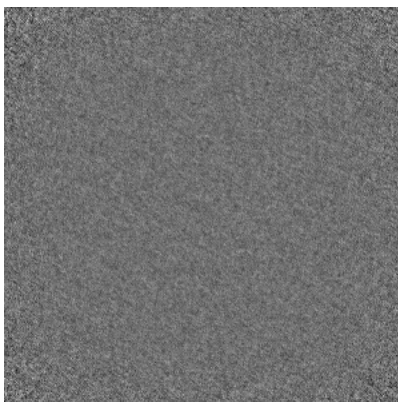


Z Index: 241

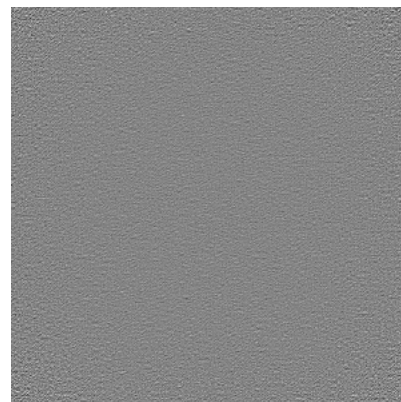
6.3.2 Raw map



X Index: 0



Y Index: 0

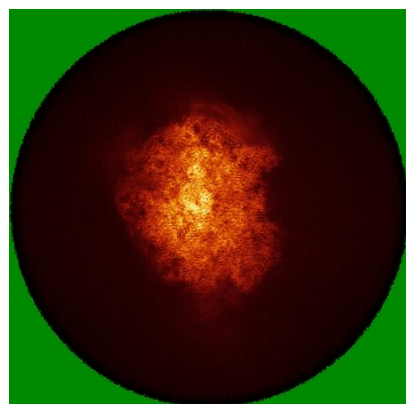


Z Index: 0

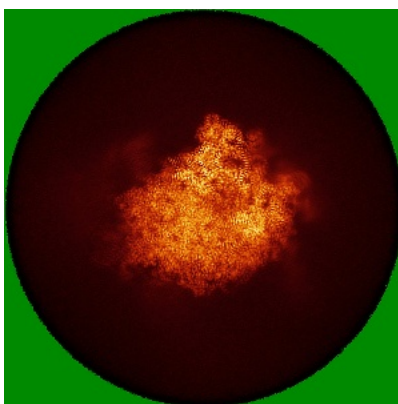
The images above show the largest variance slices of the map in three orthogonal directions.

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

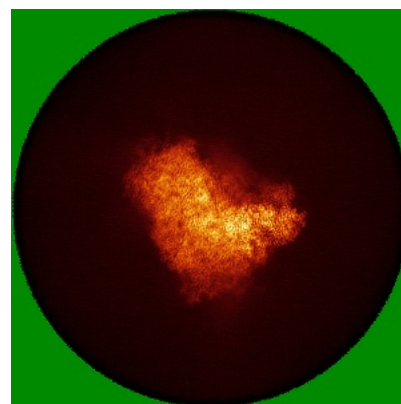
6.4.1 Primary map



X

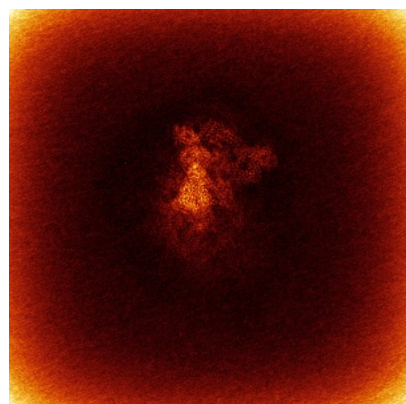


Y

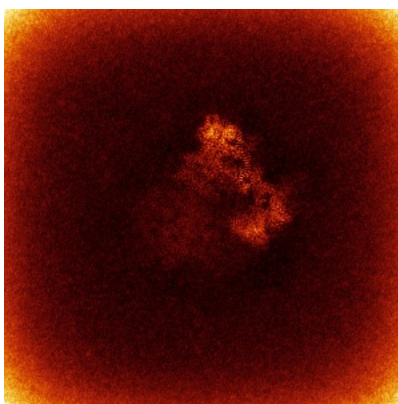


Z

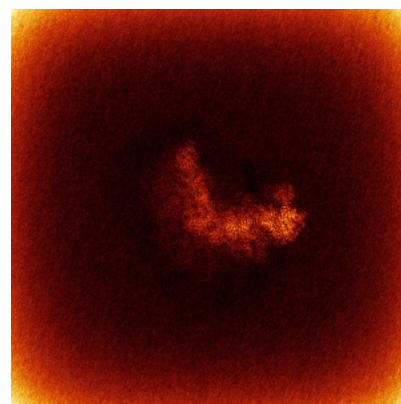
6.4.2 Raw map



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



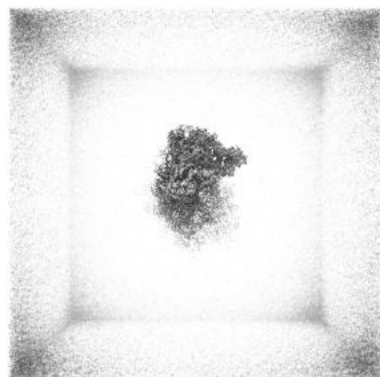
Y



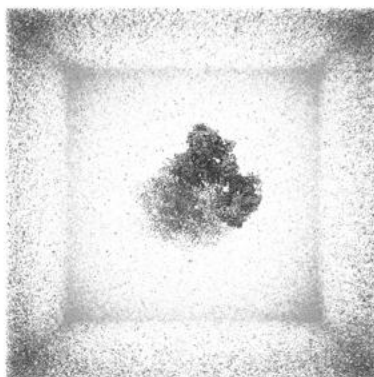
Z

The images above show the 3D surface view of the map at the recommended contour level 0.95. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

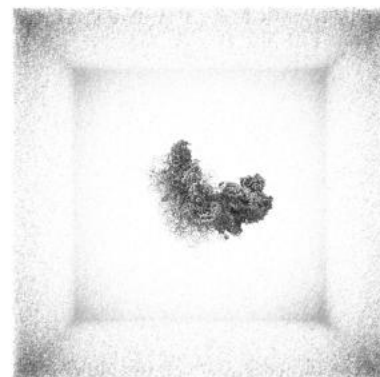
6.5.2 Raw map



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.

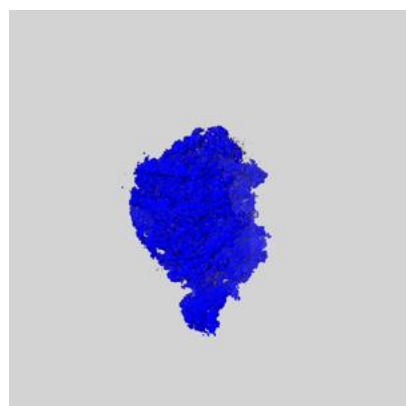
6.6 Mask visualisation [i](#)

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

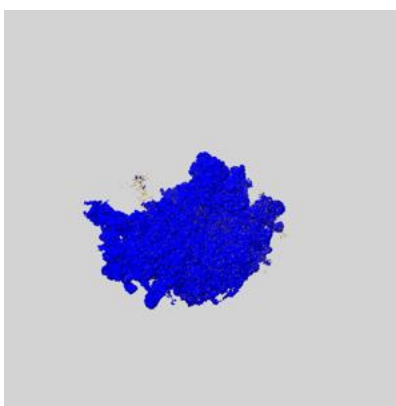
A mask typically either:

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

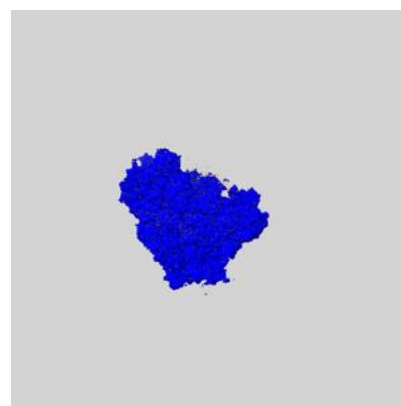
6.6.1 emd_29277_msk_1.map [i](#)



X



Y

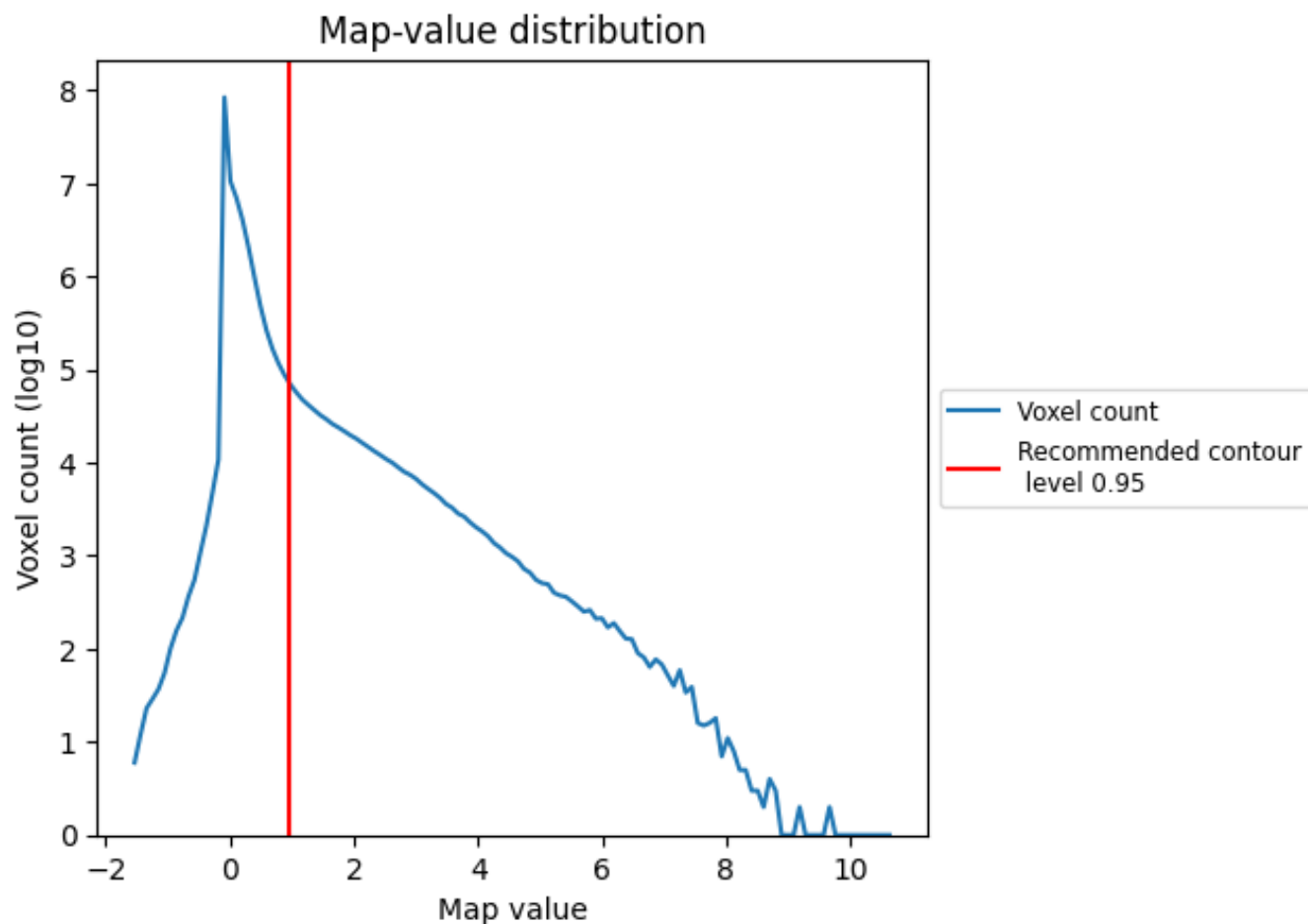


Z

7 Map analysis [i](#)

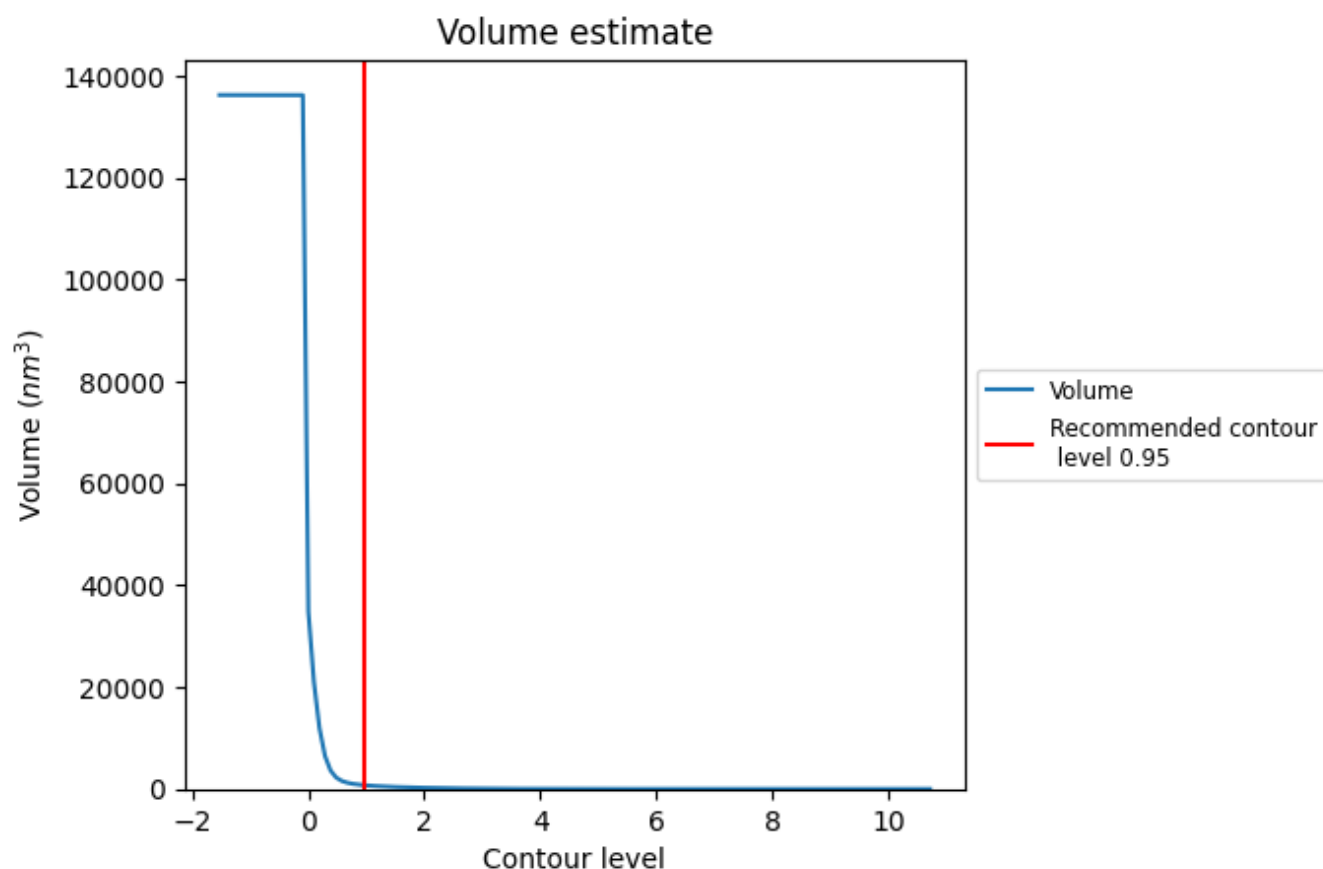
This section contains the results of statistical analysis of the map.

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.

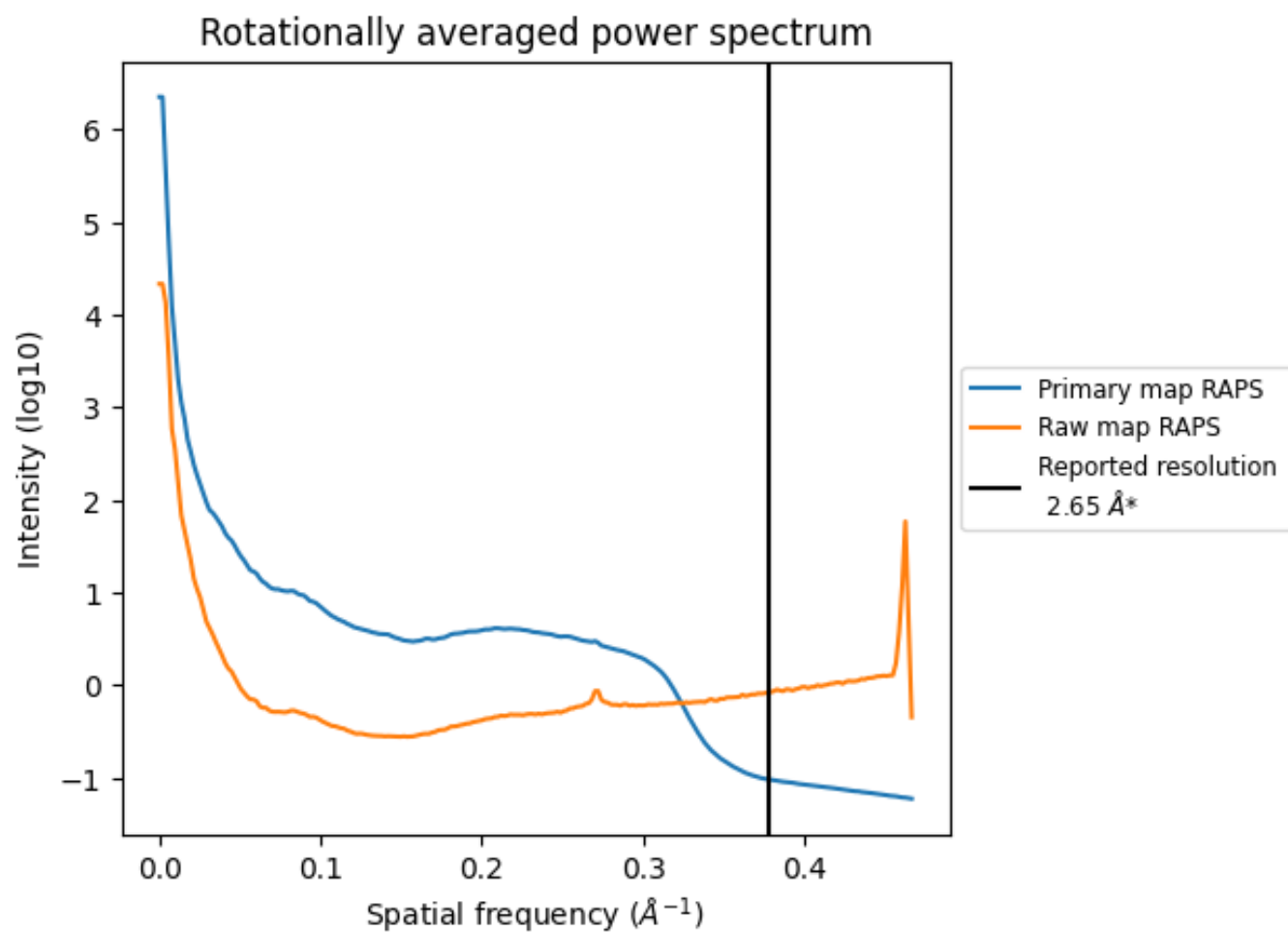
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 751 nm^3 ; this corresponds to an approximate mass of 678 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 ⓘ

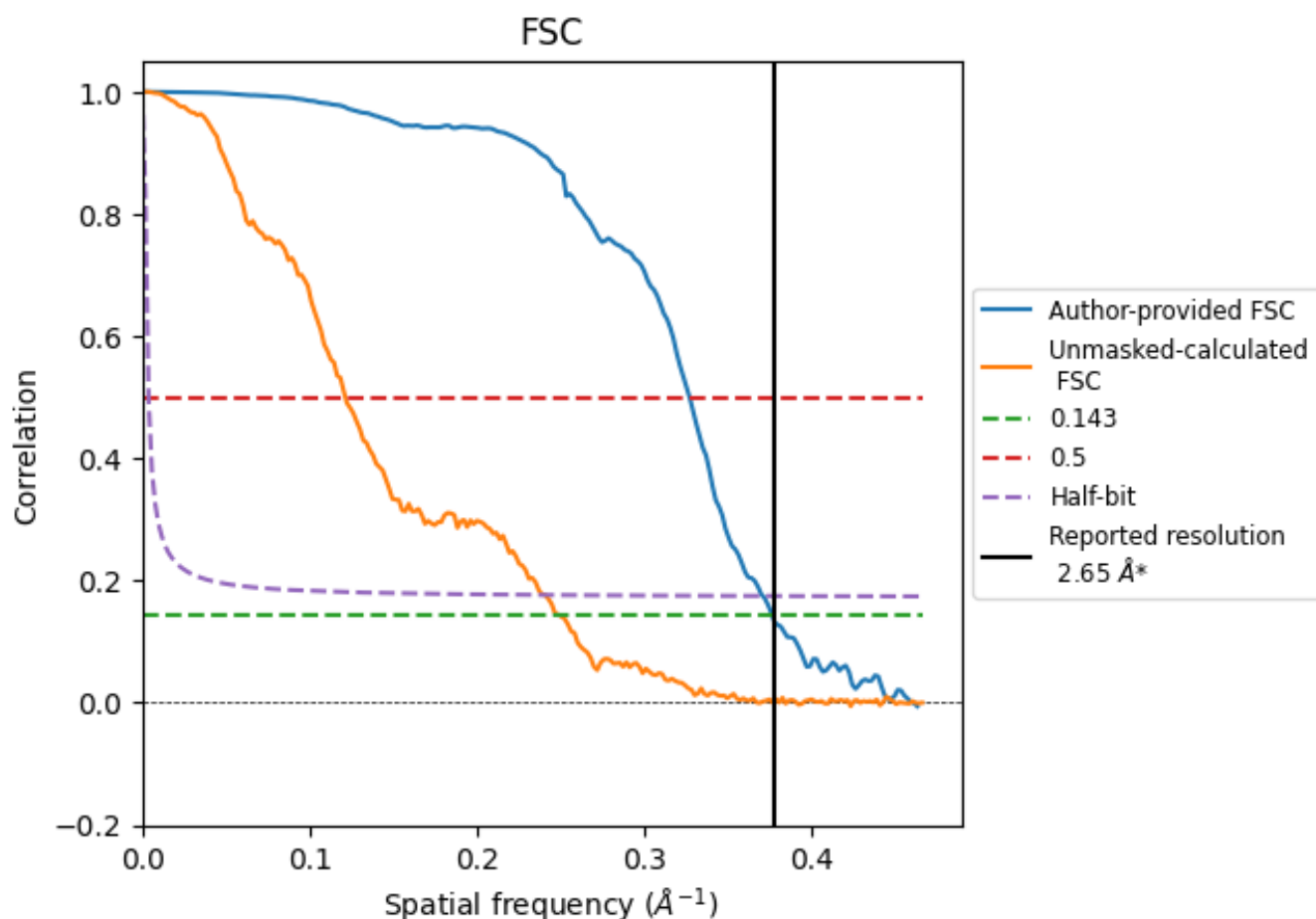


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

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 0.377 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

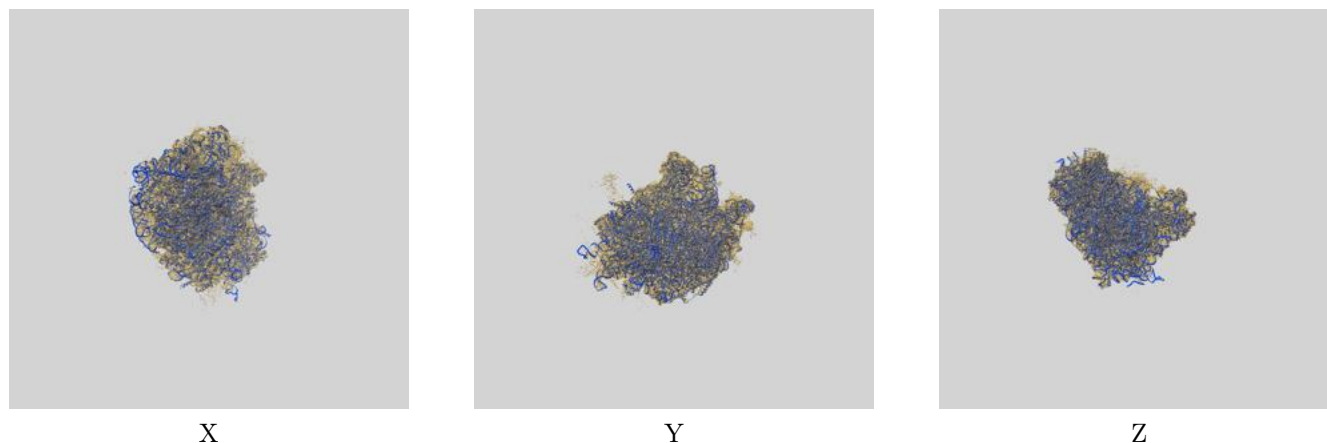
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	3.06	2.69
Unmasked-calculated*	4.01	8.23	4.15

*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 4.01 differs from the reported value 2.65 by more than 10 %

9 Map-model fit [i](#)

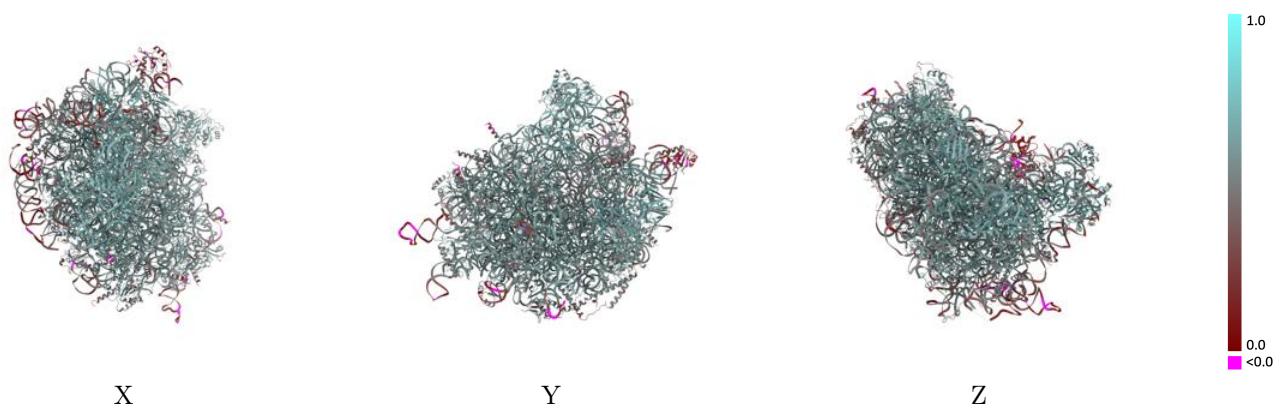
This section contains information regarding the fit between EMDB map EMD-29277 and PDB model 8FLF. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



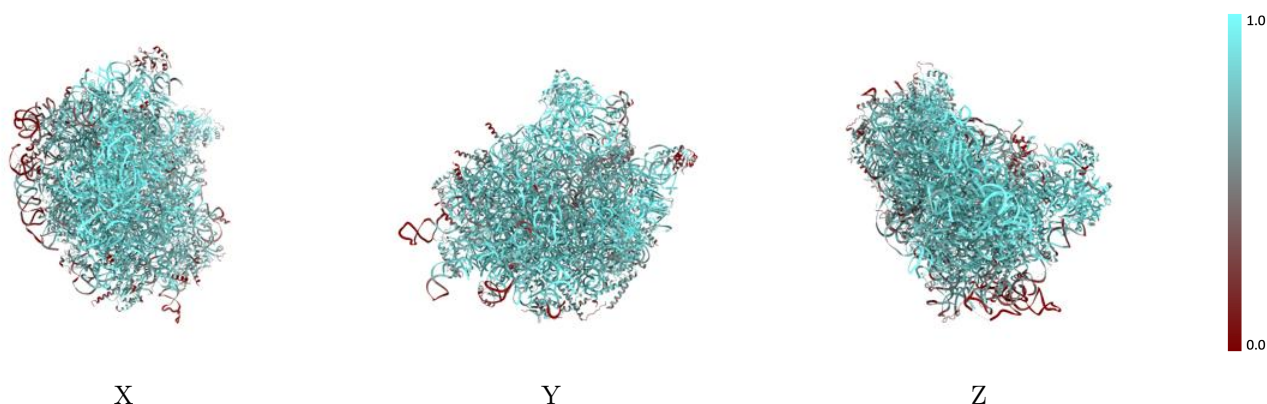
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



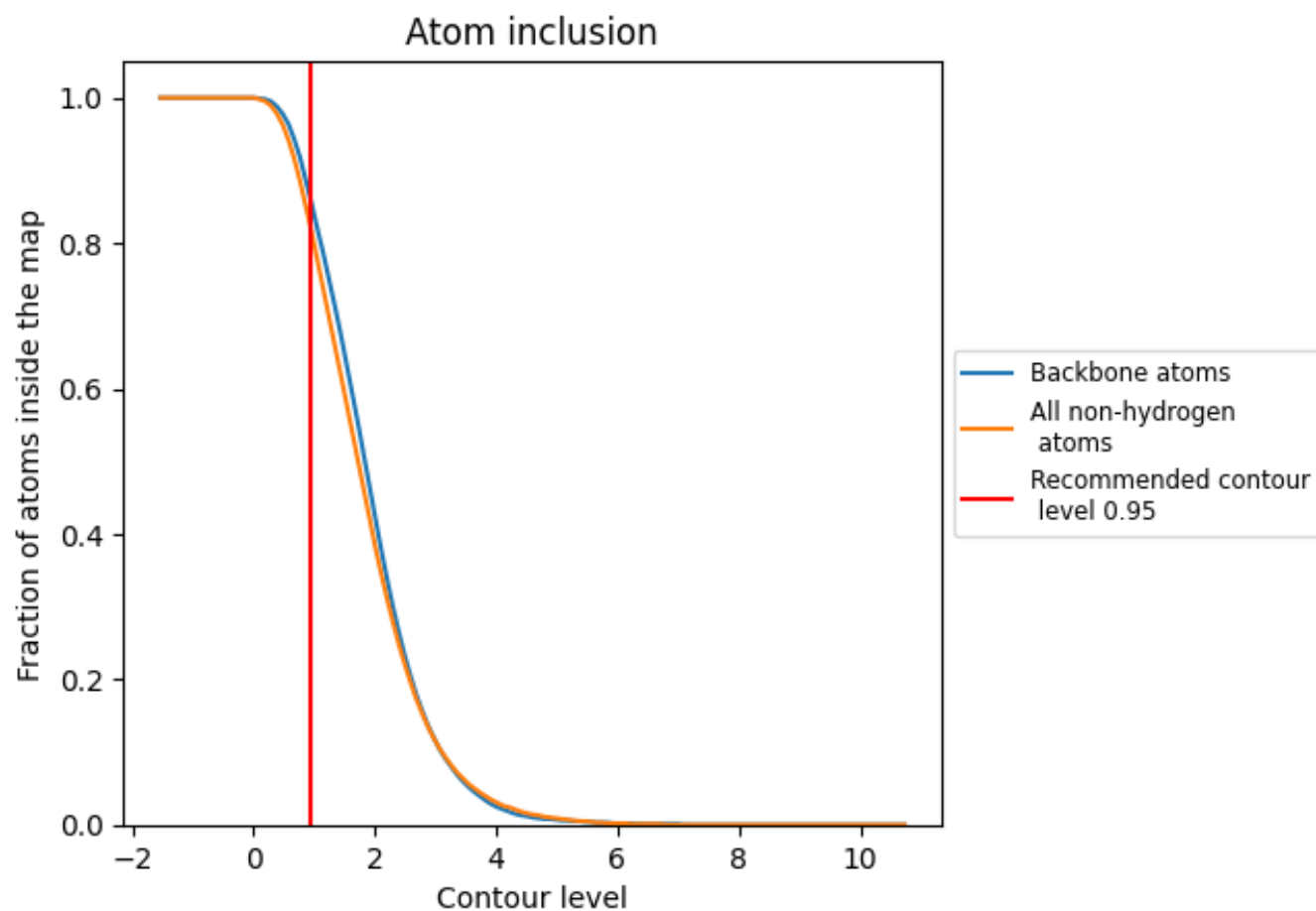
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.5550
BE	 0.6160	 0.4590
L1	 0.8800	 0.5740
L3	 0.8370	 0.5410
L4	 0.9890	 0.6320
L5	 0.7940	 0.5730
L6	 0.7470	 0.5480
L7	 0.8770	 0.6090
L8	 0.8820	 0.6090
L9	 0.8800	 0.6060
LA	 0.8120	 0.5840
LB	 0.8490	 0.6010
LC	 0.9590	 0.6490
LD	 0.7670	 0.5600
LE	 0.8970	 0.6110
LF	 0.6980	 0.5260
LG	 0.8580	 0.6070
LH	 0.7420	 0.5730
LI	 0.7620	 0.5620
LJ	 0.7200	 0.5380
LK	 0.8740	 0.6060
LL	 0.7900	 0.5670
LM	 0.6720	 0.5390
LN	 0.8240	 0.5880
LO	 0.6800	 0.5250
LP	 0.7520	 0.5550
LQ	 0.8080	 0.5880
LR	 0.7750	 0.5630
LS	 0.7260	 0.5450
LT	 0.8520	 0.5980
LU	 0.7080	 0.5360
LV	 0.8780	 0.6220
LW	 0.8690	 0.6010
LX	 0.7200	 0.5440
LY	 0.6160	 0.5090



Continued on next page...

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Chain	Atom inclusion	Q-score
LZ	 0.8700	 0.6020
NK	 0.5110	 0.4630
NP	 0.6930	 0.5560
SA	 0.8100	 0.5820
SB	 0.8750	 0.6080
SC	 0.6380	 0.5180
SD	 0.8260	 0.5850
SE	 0.6550	 0.5060
SF	 0.8210	 0.5930
SG	 0.8950	 0.6110
SK	 0.8200	 0.5820
SQ	 0.3750	 0.2460
SR	 0.6360	 0.5100
SV	 0.7500	 0.5490