



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 04:31 PM EDT

PDB ID : 8FLA / pdb_00008fla
EMDB ID : EMD-29272
Title : Human nuclear pre-60S ribosomal subunit (State K1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.63 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:

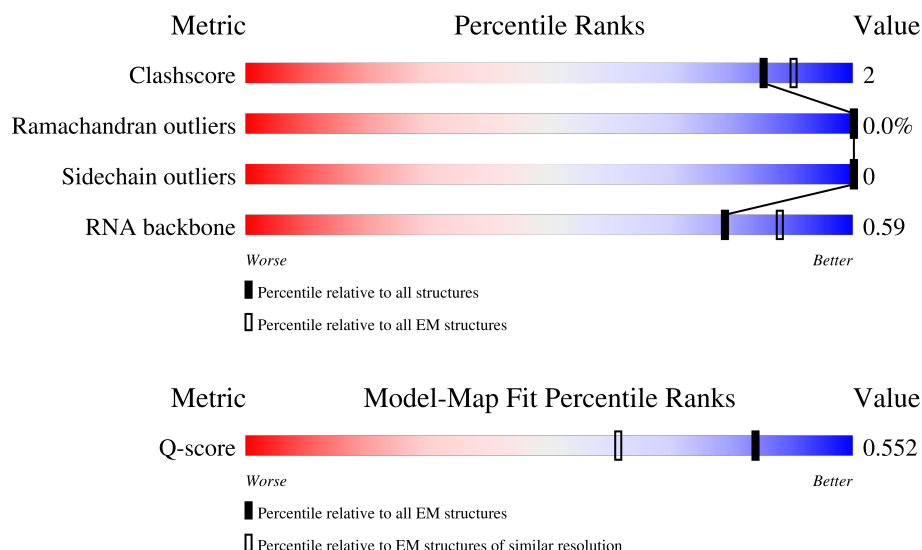
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.63 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.



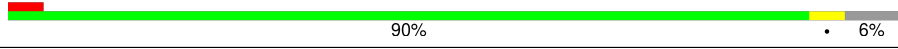
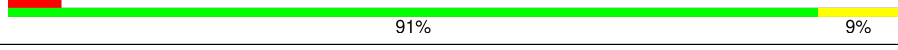
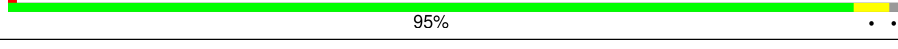
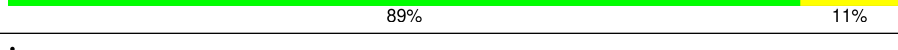
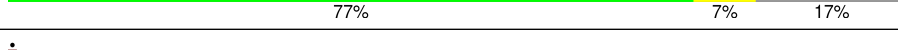
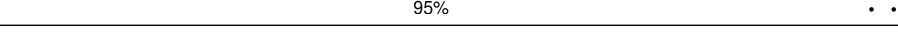
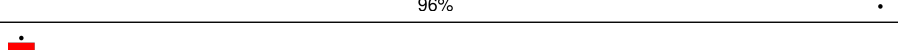
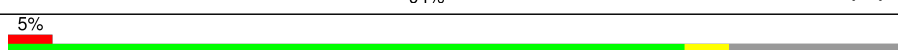
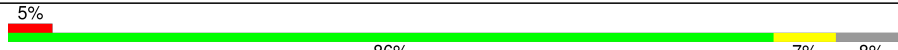
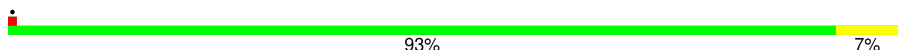
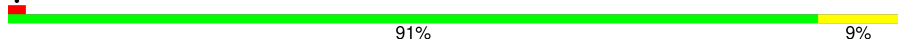
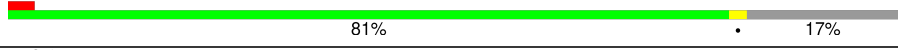
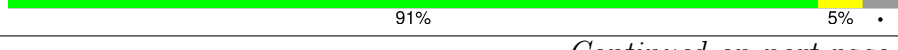
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8888 (2.13 - 3.13)

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	BA	165	
2	L1	157	
3	L2	1167	

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Mol	Chain	Length	Quality of chain
4	L3	5070	
5	L4	121	
6	L5	178	
7	L6	211	
8	L7	203	
9	L8	215	
10	L9	204	
11	LA	184	
12	LB	188	
13	LC	176	
14	LD	196	
15	LE	160	
16	LF	128	
17	LG	140	
18	LH	156	
19	LI	145	
20	LJ	136	
21	LK	148	
22	LL	137	
23	LM	159	
24	LN	403	
25	LO	115	
26	LP	125	
27	LQ	135	
28	LR	117	

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Mol	Chain	Length	Quality of chain
29	LS	123	
30	LT	110	
31	LU	105	
32	LV	106	
33	LW	97	
34	LX	92	
35	LY	70	
36	LZ	51	
37	NK	129	
38	NL	478	
39	NP	134	
40	NR	203	
41	SA	427	
42	SB	297	
43	SC	288	
44	SD	248	
45	SE	266	
46	SF	257	
47	SG	192	
48	SH	293	
49	SI	255	
50	SK	245	
51	SL	490	
52	SM	588	
53	SQ	239	

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Mol	Chain	Length	Quality of chain
54	SR	634	8% 90% 5% 5%
55	SV	163	78% 7% 15%
56	VB	99	11% 55% 41%

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 153309 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 L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	BA	91	Total	C	N	O	0	0
			449	267	91	91		

- 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 ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	72	Total	C	N	O	P	0	0
			1535	683	278	502	72		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L3	3420	Total	C	N	O	P	0	0
			73423	32721	13453	23829	3420		

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

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

- Molecule 6 is a protein called 60S ribosomal protein L11.

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

- Molecule 7 is a protein called 60S ribosomal protein L13.

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

- Molecule 8 is a protein called 60S ribosomal protein L13a.

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

- Molecule 9 is a protein called 60S ribosomal protein L14.

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

- Molecule 10 is a protein called 60S ribosomal protein L15.

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

- Molecule 11 is a protein called 60S ribosomal protein L17.

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

- Molecule 12 is a protein called 60S ribosomal protein L18.

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

- Molecule 13 is a protein called 60S ribosomal protein L18a.

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

- Molecule 14 is a protein called 60S ribosomal protein L19.

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

- Molecule 15 is a protein called 60S ribosomal protein L21.

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

- Molecule 16 is a protein called 60S ribosomal protein L22.

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

- Molecule 17 is a protein called 60S ribosomal protein L23.

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

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LH	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 19 is a protein called 60S ribosomal protein L26.

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

- Molecule 20 is a protein called 60S ribosomal protein L27.

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

- Molecule 21 is a protein called 60S ribosomal protein L27a.

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

- Molecule 22 is a protein called 60S ribosomal protein L28.

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

- Molecule 23 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LM	91	Total	C	N	O	S	0	0
			751	469	165	113	4		

- Molecule 24 is a protein called 60S ribosomal protein L3.

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

- Molecule 25 is a protein called 60S ribosomal protein L30.

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

- Molecule 26 is a protein called 60S ribosomal protein L31.

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

- Molecule 27 is a protein called 60S ribosomal protein L32.

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

- Molecule 28 is a protein called 60S ribosomal protein L34.

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

- Molecule 29 is a protein called 60S ribosomal protein L35.

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

- Molecule 30 is a protein called 60S ribosomal protein L35a.

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

- Molecule 31 is a protein called 60S ribosomal protein L36.

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

- Molecule 32 is a protein called 60S ribosomal protein L36a.

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

- Molecule 33 is a protein called 60S ribosomal protein L37.

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

- Molecule 34 is a protein called 60S ribosomal protein L37a.

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

- Molecule 35 is a protein called 60S ribosomal protein L38.

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

- Molecule 36 is a protein called 60S ribosomal protein L39.

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

- Molecule 37 is a protein called Protein LLP homolog.

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

- Molecule 38 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NL	323	Total	C	N	O	S	0	0
			2666	1658	531	475	2		

- Molecule 39 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NP	104	Total	C	N	O	S	0	0
			847	520	178	145	4		

- Molecule 40 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	NR	152	Total	C	N	O	P	S	1	0
			1299	809	249	235	1	5		

- Molecule 41 is a protein called 60S ribosomal protein L4.

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

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SB	275	Total	C	N	O	S	0	0
			2243	1419	406	404	14		

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SC	217	Total	C	N	O	S	0	0
			1747	1124	332	287	4		

- Molecule 44 is a protein called 60S ribosomal protein L7.

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

- Molecule 45 is a protein called 60S ribosomal protein L7a.

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

- Molecule 46 is a protein called 60S ribosomal protein L8.

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

- Molecule 47 is a protein called 60S ribosomal protein L9.

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

- Molecule 48 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SH	150	Total	C	N	O	S	0	0
			1120	716	198	203	3		

- Molecule 49 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SI	234	Total	C	N	O	S	1	0
			1937	1254	363	316	4		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 51 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SL	238	Total	C	N	O	S	0	0
			1917	1227	337	347	6		

- Molecule 52 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SM	399	Total	C	N	O	S	0	0
			3278	2120	576	571	11		

- Molecule 53 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	SQ	127	Total	C	N	O	0	0
			650	388	132	130		

- Molecule 54 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SR	601	Total	C	N	O	S	0	0
			4932	3105	899	902	26		

- Molecule 55 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 56 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	VB	58	Total	C	N	O	S	0	0
			455	285	95	74	1		

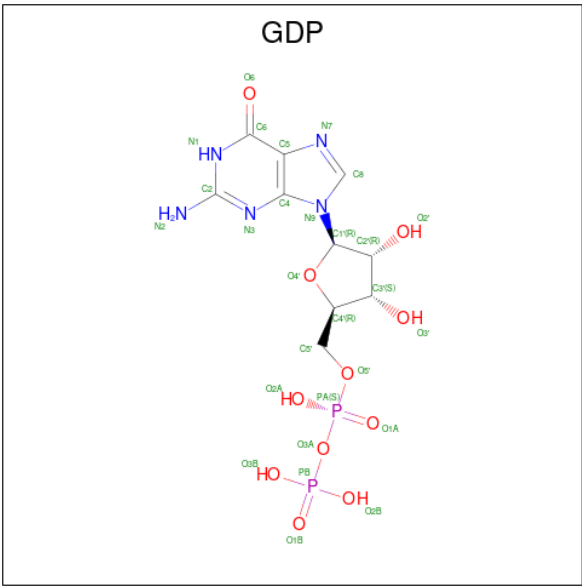
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	L1	3	Total	Mg	0
			3	3	
57	L3	74	Total	Mg	0
			74	74	
57	L4	3	Total	Mg	0
			3	3	
57	LG	1	Total	Mg	0
			1	1	
57	LN	1	Total	Mg	0
			1	1	
57	LQ	1	Total	Mg	0
			1	1	
57	LT	1	Total	Mg	0
			1	1	
57	LW	1	Total	Mg	0
			1	1	
57	SA	1	Total	Mg	0
			1	1	
57	SF	1	Total	Mg	0
			1	1	
57	SR	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
59	SR	1	Total	C	N	O	P	0
			28	10	5	11	2	

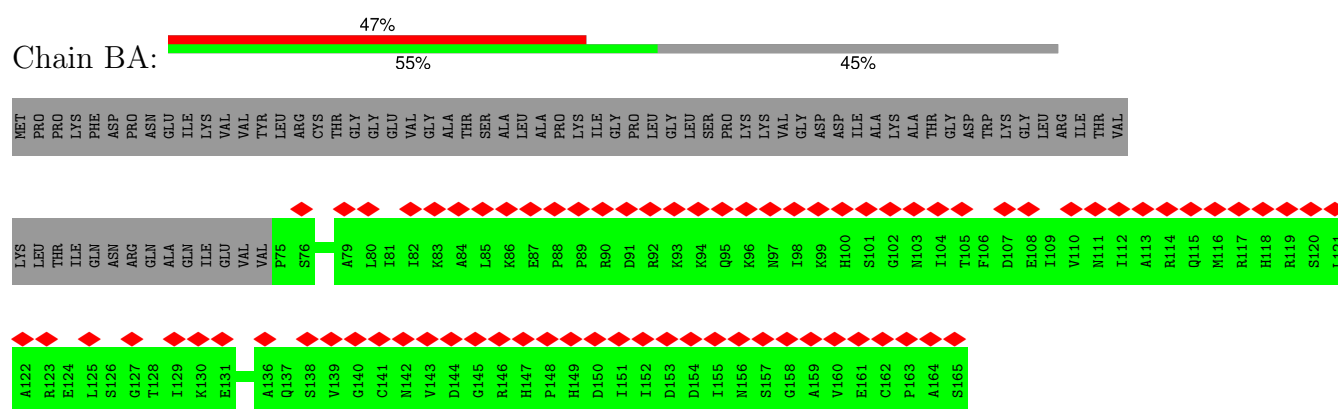
- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
60	SR	1	Total	K	0
			1	1	

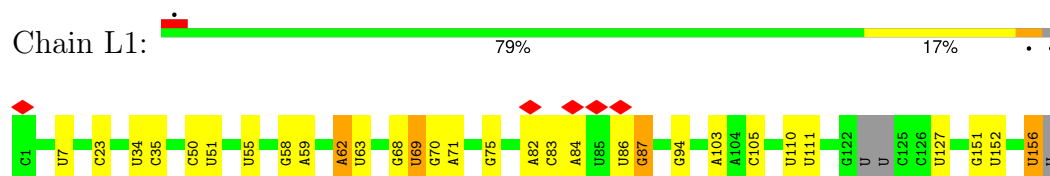
3 Residue-property plots [i](#)

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

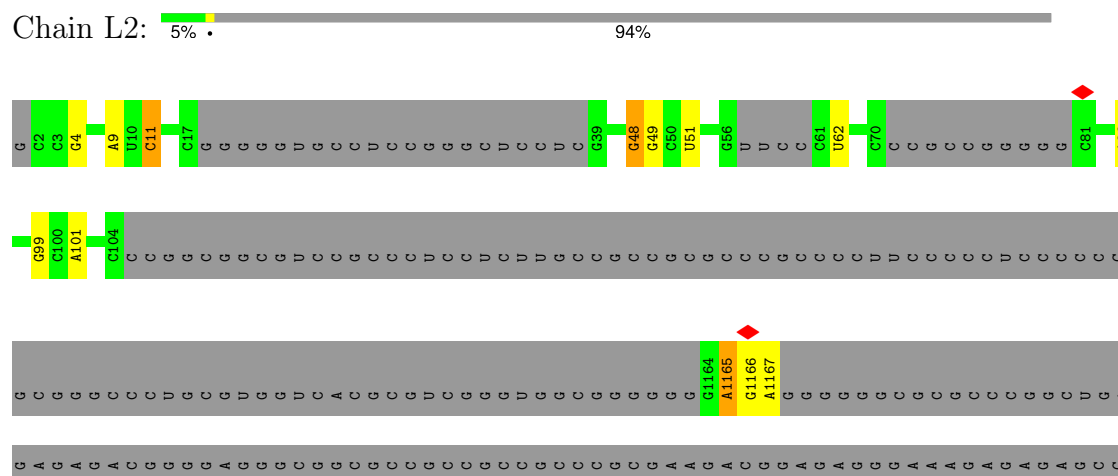
• Molecule 1: 60S ribosomal protein L12

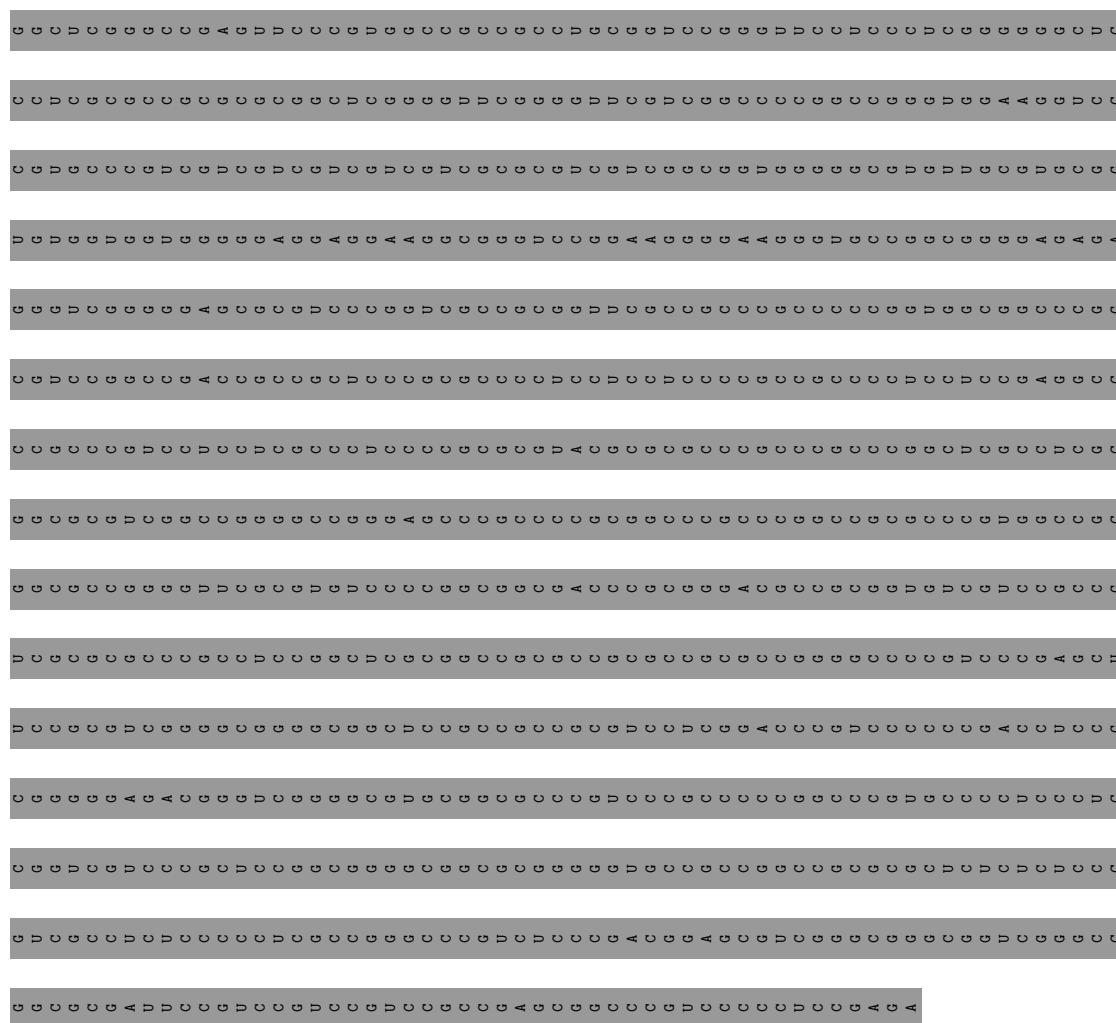


• Molecule 2: 5.8S rRNA

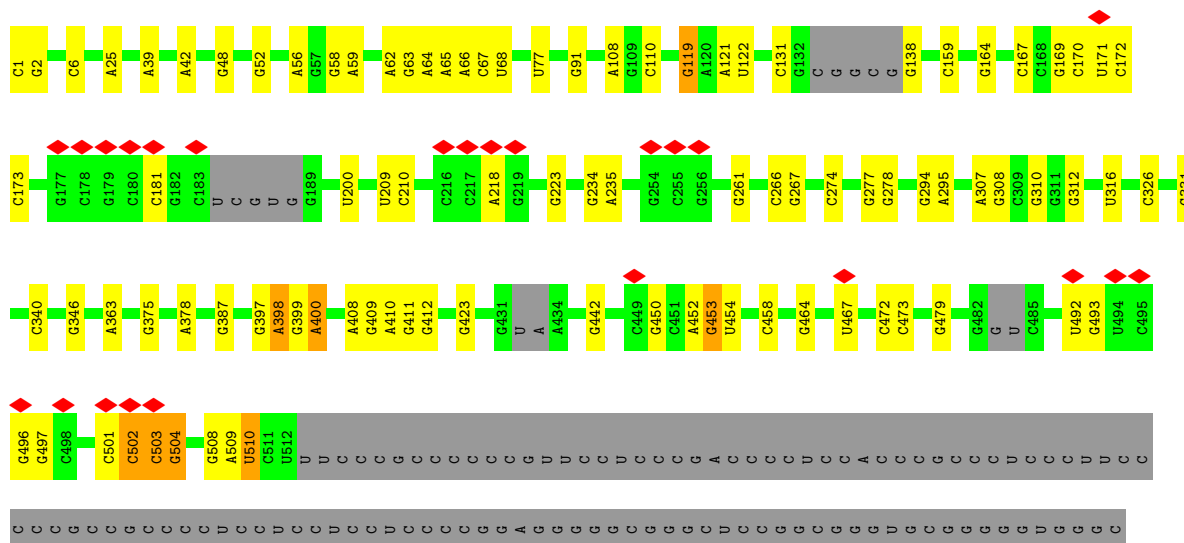


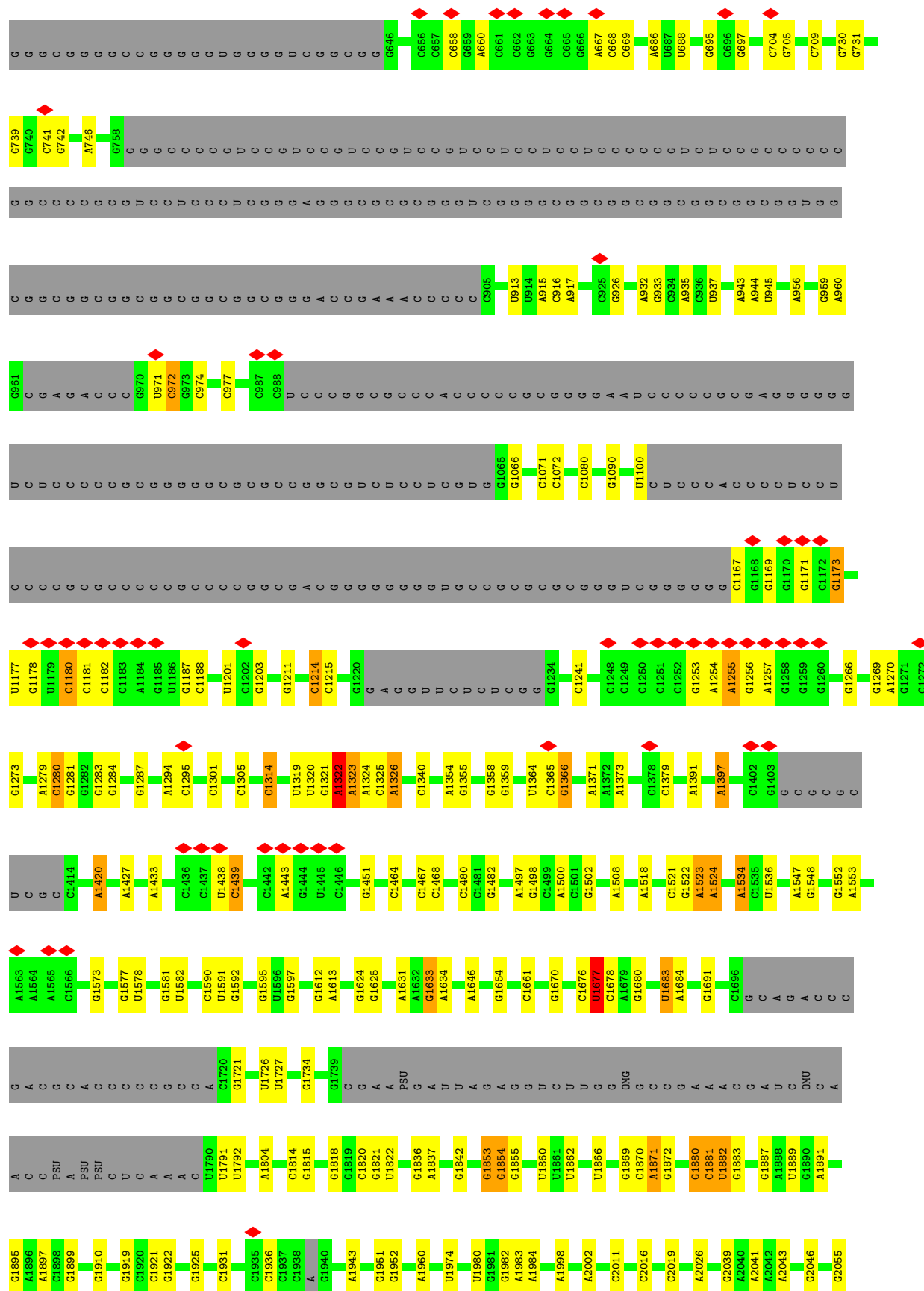
• Molecule 3: ITS2 rRNA

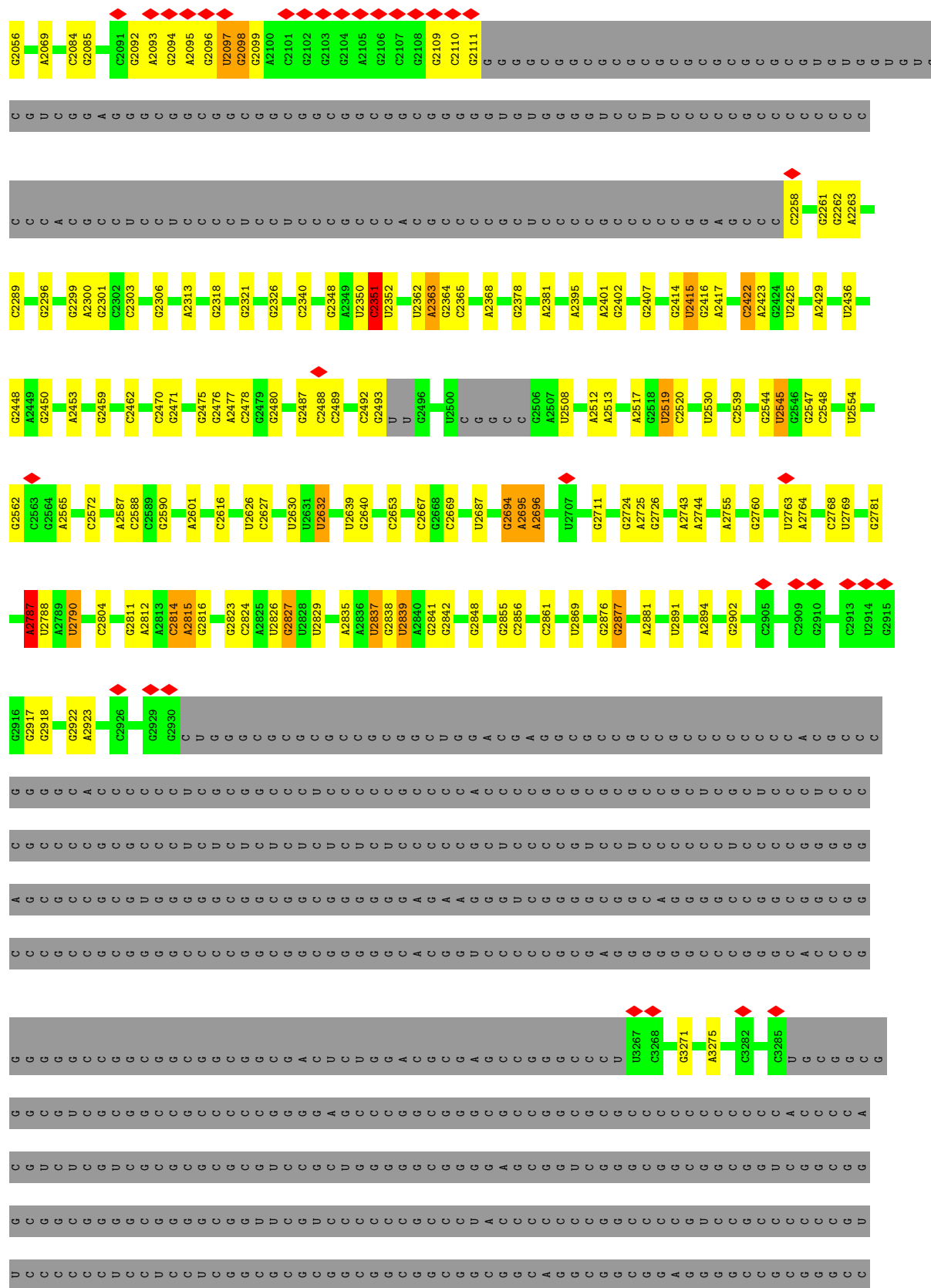




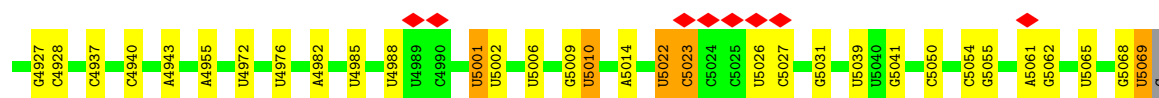
- Molecule 4: 28S rRNA



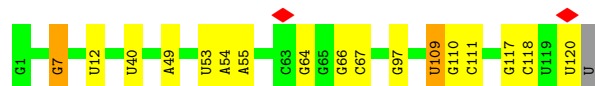
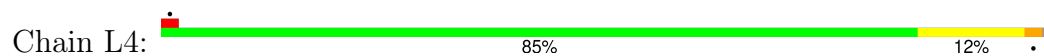




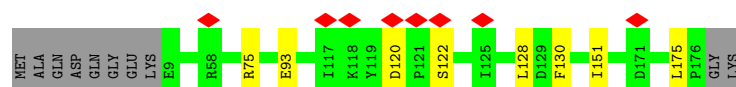




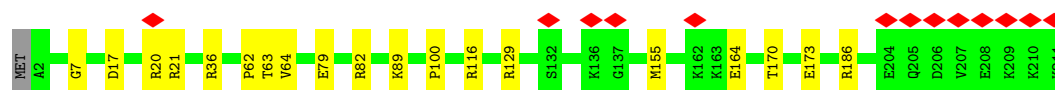
- Molecule 5: 5S rRNA



- Molecule 6: 60S ribosomal protein L11



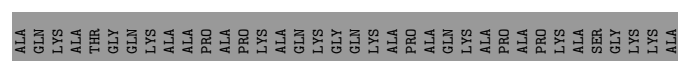
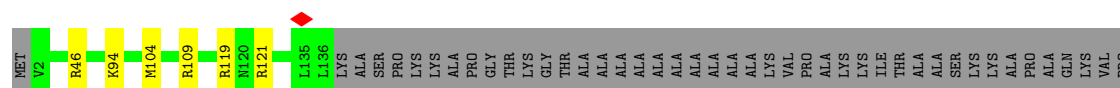
- Molecule 7: 60S ribosomal protein L13



- Molecule 8: 60S ribosomal protein L13a



- Molecule 9: 60S ribosomal protein L14

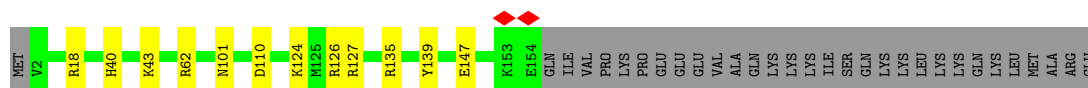
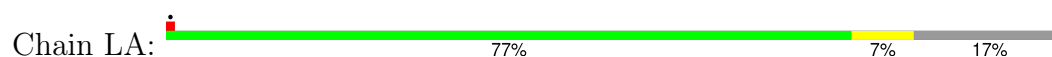


- Molecule 10: 60S ribosomal protein L15

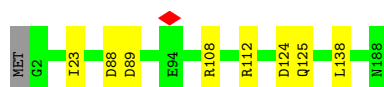




- Molecule 11: 60S ribosomal protein L17



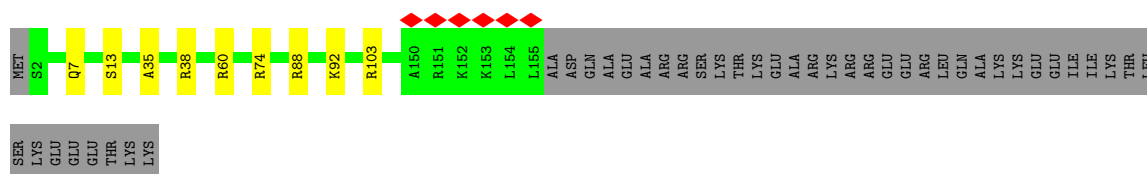
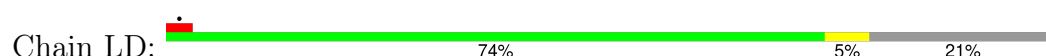
- Molecule 12: 60S ribosomal protein L18



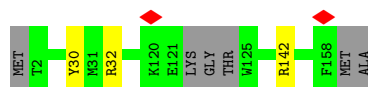
- Molecule 13: 60S ribosomal protein L18a



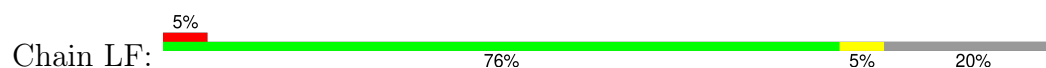
- Molecule 14: 60S ribosomal protein L19



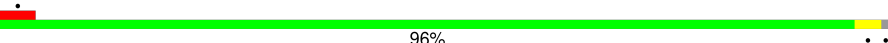
- Molecule 15: 60S ribosomal protein L21

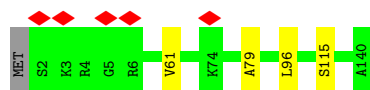


- Molecule 16: 60S ribosomal protein L22



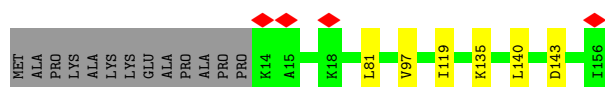
- Molecule 17: 60S ribosomal protein L23

Chain LG:  96%



- Molecule 18: 60S ribosomal protein L23a

Chain LH:  88%



- Molecule 19: 60S ribosomal protein L26

Chain LI:  5% 86% 7% 8%

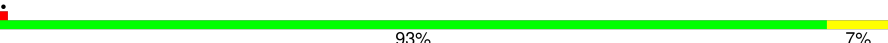


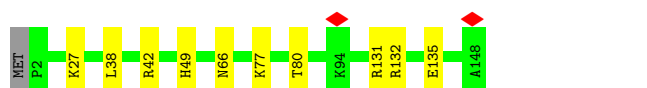
- Molecule 20: 60S ribosomal protein L27

Chain LJ:  88% 11%



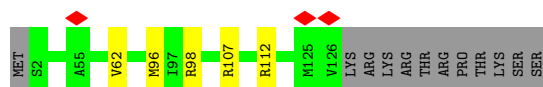
- Molecule 21: 60S ribosomal protein L27a

Chain LK:  93% 7%



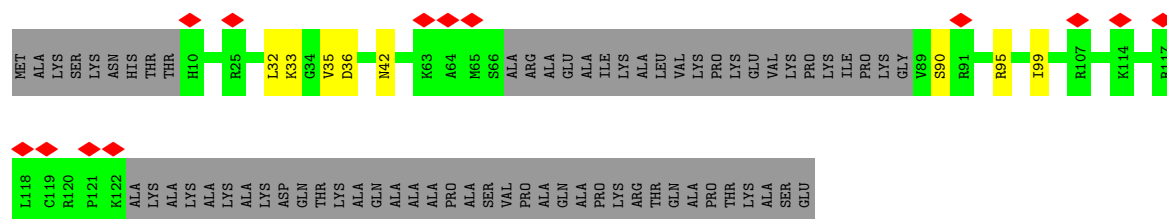
- Molecule 22: 60S ribosomal protein L28

Chain LL:  88% 9%

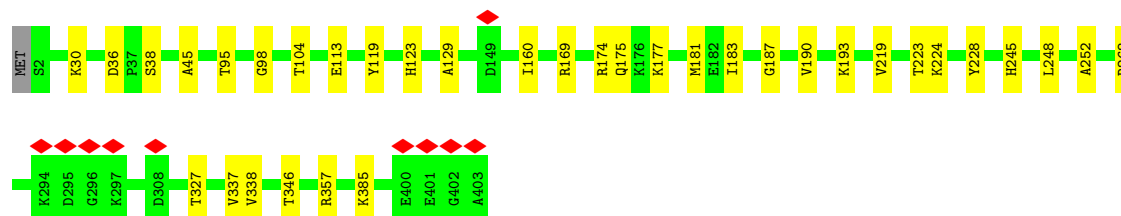


- Molecule 23: 60S ribosomal protein L29

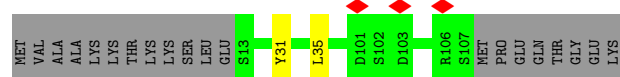
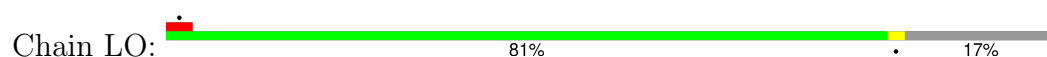
Chain LM:  8% 52% 5% 43%



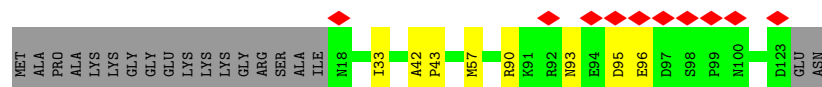
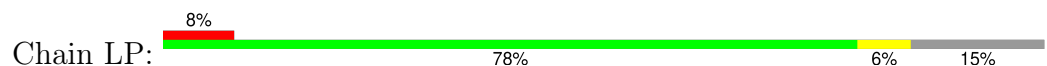
- Molecule 24: 60S ribosomal protein L3



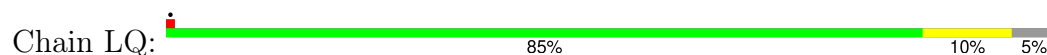
- Molecule 25: 60S ribosomal protein L30



- Molecule 26: 60S ribosomal protein L31



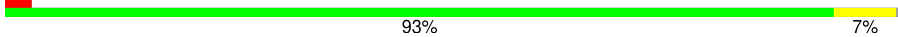
- Molecule 27: 60S ribosomal protein L32



- Molecule 28: 60S ribosomal protein L34

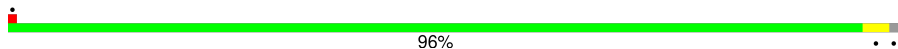


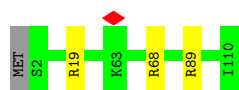
- Molecule 29: 60S ribosomal protein L35

Chain LS:  93% 7%

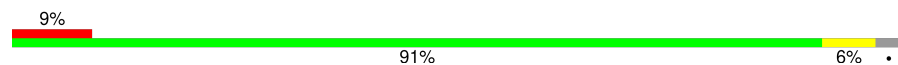


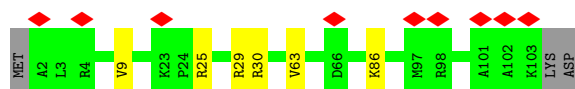
- Molecule 30: 60S ribosomal protein L35a

Chain LT:  96%

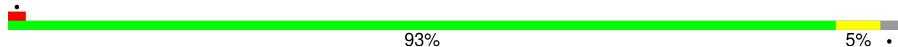


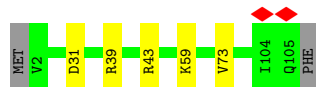
- Molecule 31: 60S ribosomal protein L36

Chain LU:  9% 91% 6%



- Molecule 32: 60S ribosomal protein L36a

Chain LV:  93% 5%

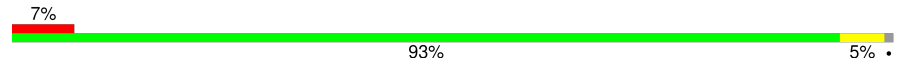


- Molecule 33: 60S ribosomal protein L37

Chain LW:  84% 5% 11%



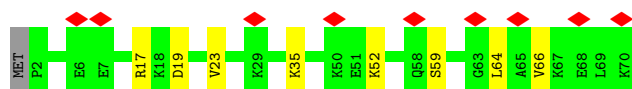
- Molecule 34: 60S ribosomal protein L37a

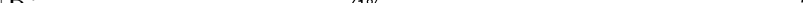
Chain LX:  7% 93% 5%



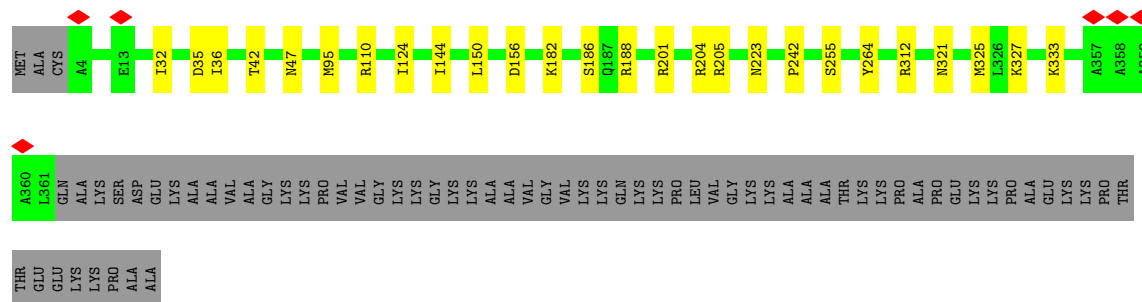
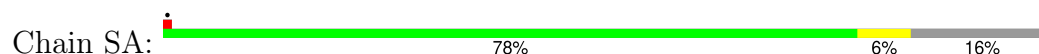
- Molecule 35: 60S ribosomal protein L38

Chain LY:  13% 87% 11%



- Chain NB: 

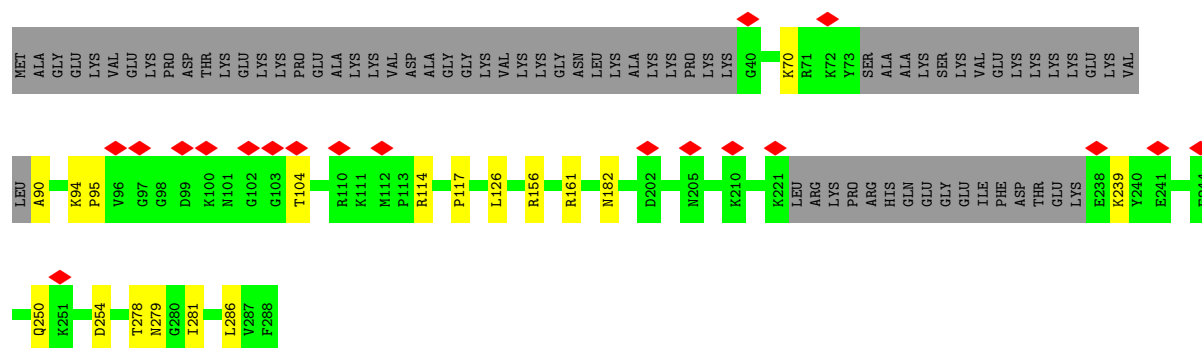
- Molecule 41: 60S ribosomal protein L4



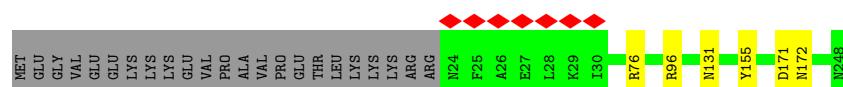
- Molecule 42: 60S ribosomal protein L5

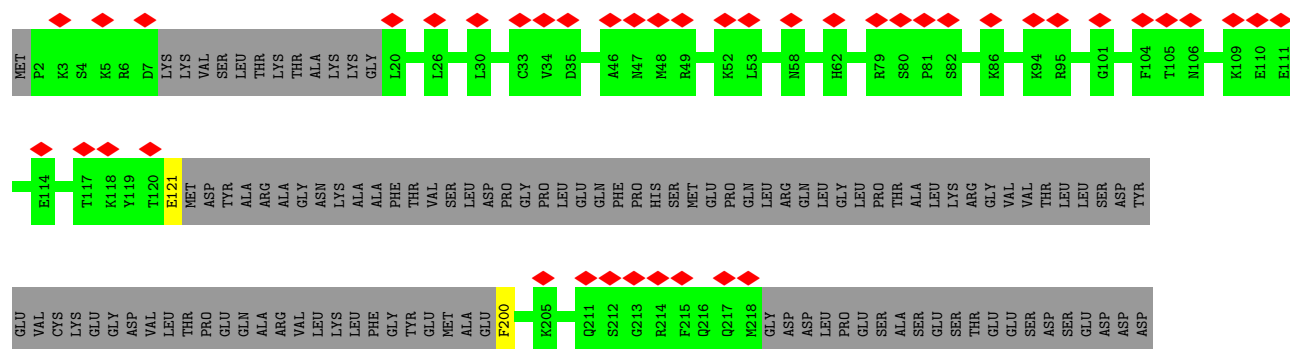


- Molecule 43: 60S ribosomal protein L6

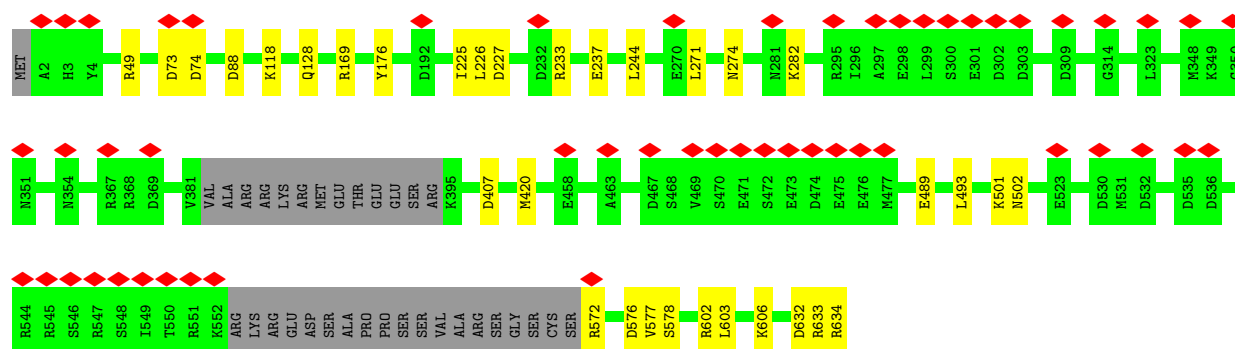
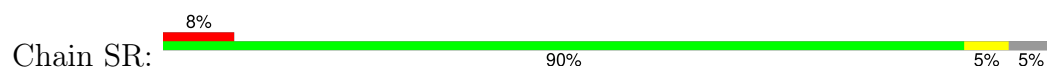


- Molecule 44: 60S ribosomal protein L7

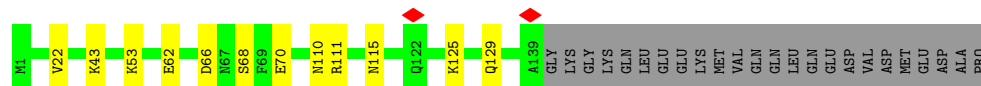
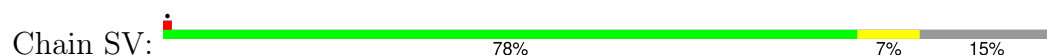




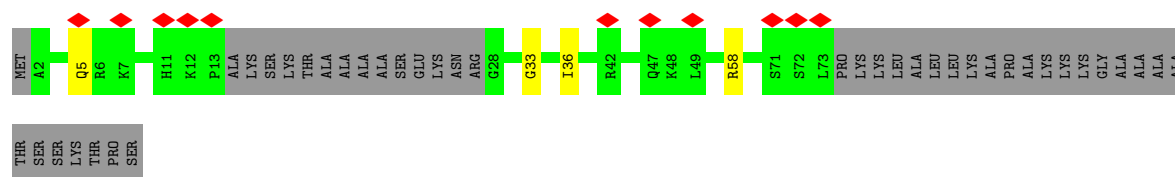
• Molecule 54: GTP-binding protein 4



• Molecule 55: Probable ribosome biogenesis protein RLP24



• Molecule 56: Leydig cell tumor 10 kDa protein homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64178	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	11.844	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.192	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, A2M, MG, 1MA, 6MZ, OMC, OMU, GDP, OMG, K, UR3, PSU, PTR, HIC

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	BA	0.09	0/448	0.23	0/622
2	L1	0.14	0/3589	0.24	0/5589
3	L2	0.11	0/1709	0.27	0/2653
4	L3	0.15	0/79642	0.25	0/124218
5	L4	0.17	0/2861	0.26	0/4459
6	L5	0.12	0/1372	0.27	0/1836
7	L6	0.12	0/1732	0.27	0/2315
8	L7	0.12	0/1682	0.26	0/2250
9	L8	0.12	0/1133	0.25	0/1516
10	L9	0.13	0/1746	0.27	0/2338
11	LA	0.15	0/1268	0.35	0/1701
12	LB	0.13	0/1536	0.30	0/2052
13	LC	0.13	0/1501	0.28	0/2013
14	LD	0.10	0/1305	0.23	0/1727
15	LE	0.14	0/1291	0.30	0/1724
16	LF	0.10	0/856	0.27	0/1149
17	LG	0.13	0/1048	0.29	0/1402
18	LH	0.12	0/1175	0.26	0/1572
19	LI	0.13	0/1132	0.27	0/1504
20	LJ	0.12	0/1130	0.25	0/1507
21	LK	0.12	0/1191	0.26	0/1591
22	LL	0.11	0/1017	0.28	0/1364
23	LM	0.14	0/763	0.29	0/1005
24	LN	0.13	0/3294	0.29	0/4406
25	LO	0.11	0/748	0.24	0/1004
26	LP	0.11	0/894	0.26	0/1204
27	LQ	0.12	0/1071	0.27	0/1429
28	LR	0.11	0/898	0.28	0/1197
29	LS	0.10	0/1023	0.22	0/1351
30	LT	0.12	0/895	0.27	0/1198
31	LU	0.11	0/843	0.25	0/1115
32	LV	0.14	0/864	0.29	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LW	0.13	0/720	0.32	0/952
34	LX	0.10	0/718	0.27	0/953
35	LY	0.11	0/575	0.27	0/761
36	LZ	0.12	0/454	0.25	0/599
37	NK	0.10	0/587	0.24	0/767
38	NL	0.11	0/2705	0.24	0/3624
39	NP	0.11	0/864	0.25	0/1154
40	NR	0.11	0/1306	0.27	0/1740
41	SA	0.12	0/2907	0.27	0/3905
42	SB	0.13	0/2287	0.27	0/3065
43	SC	0.12	0/1781	0.29	0/2388
44	SD	0.12	0/1905	0.27	0/2539
45	SE	0.14	0/1903	0.29	0/2559
46	SF	0.12	0/1914	0.30	0/2567
47	SG	0.13	0/1537	0.27	0/2066
48	SH	0.12	0/1147	0.26	0/1558
49	SI	0.13	0/1980	0.30	0/2656
50	SK	0.12	0/1877	0.28	0/2554
51	SL	0.11	0/1949	0.28	0/2621
52	SM	0.13	0/3357	0.27	0/4529
53	SQ	0.08	0/648	0.24	0/894
54	SR	0.11	0/5014	0.25	0/6727
55	SV	0.12	0/1207	0.27	0/1600
56	VB	0.10	0/459	0.23	0/605
All	All	0.14	0/161458	0.26	0/235534

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 [i](#)

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	BA	449	0	207	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L1	3278	0	1665	14	0
3	L2	1535	0	789	6	0
4	L3	73423	0	37192	313	0
5	L4	2561	0	1295	7	0
6	L5	1349	0	1383	5	0
7	L6	1701	0	1818	15	0
8	L7	1650	0	1794	8	0
9	L8	1111	0	1174	7	0
10	L9	1701	0	1749	19	0
11	LA	1242	0	1269	11	0
12	LB	1512	0	1628	6	0
13	LC	1461	0	1502	5	0
14	LD	1289	0	1429	8	0
15	LE	1264	0	1328	4	0
16	LF	842	0	864	3	0
17	LG	1034	0	1097	4	0
18	LH	1156	0	1268	5	0
19	LI	1115	0	1205	6	0
20	LJ	1107	0	1182	8	0
21	LK	1162	0	1213	8	0
22	LL	1002	0	1068	5	0
23	LM	751	0	820	7	0
24	LN	3239	0	3377	25	0
25	LO	738	0	774	1	0
26	LP	879	0	924	5	0
27	LQ	1053	0	1147	10	0
28	LR	888	0	977	4	0
29	LS	1015	0	1148	7	0
30	LT	876	0	912	3	0
31	LU	832	0	917	6	0
32	LV	851	0	920	5	0
33	LW	705	0	737	5	0
34	LX	708	0	756	5	0
35	LY	569	0	637	7	0
36	LZ	444	0	483	5	0
37	NK	581	0	656	4	0
38	NL	2666	0	2774	15	0
39	NP	847	0	854	4	0
40	NR	1299	0	1318	3	0
41	SA	2853	0	3028	21	0
42	SB	2243	0	2268	7	0
43	SC	1747	0	1897	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	SD	1870	0	1996	5	0
45	SE	1869	0	2014	16	0
46	SF	1876	0	1970	12	0
47	SG	1518	0	1601	7	0
48	SH	1120	0	988	1	0
49	SI	1937	0	2070	12	0
50	SK	1852	0	1828	13	0
51	SL	1917	0	2018	6	0
52	SM	3278	0	3332	17	0
53	SQ	650	0	308	1	0
54	SR	4932	0	5071	25	0
55	SV	1184	0	1248	9	0
56	VB	455	0	504	4	0
57	L1	3	0	0	0	0
57	L3	74	0	0	0	0
57	L4	3	0	0	0	0
57	LG	1	0	0	0	0
57	LN	1	0	0	0	0
57	LQ	1	0	0	0	0
57	LT	1	0	0	0	0
57	LW	1	0	0	0	0
57	SA	1	0	0	0	0
57	SF	1	0	0	0	0
57	SR	1	0	0	0	0
58	LR	1	0	0	0	0
58	LV	1	0	0	0	0
58	LW	1	0	0	0	0
58	LX	1	0	0	0	0
58	NP	1	0	0	0	0
58	SV	1	0	0	0	0
59	SR	28	0	12	0	0
60	SR	1	0	0	0	0
All	All	153309	0	116403	564	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 (564) 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)
4:L3:2520:C:O2	4:L3:2640:G:N2	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:1480:C:O2'	4:L3:1482:G:OP2	1.97	0.82
4:L3:2262:G:OP2	22:LL:98:ARG:NH1	2.14	0.80
49:SI:252:ARG:NH1	52:SM:270:GLU:OE1	2.15	0.80
2:L1:51:U:OP2	36:LZ:21:ARG:NH2	2.16	0.79
4:L3:2601:A:OP1	28:LR:40:LYS:NZ	2.15	0.79
5:L4:40:U:O2	6:L5:75:ARG:NH1	2.16	0.78
4:L3:62:A:N3	4:L3:77:U:O2'	2.16	0.78
4:L3:695:G:O2'	4:L3:697:G:OP2	2.02	0.78
4:L3:1177:U:OP2	4:L3:1180:C:N4	2.17	0.78
4:L3:1283:G:O6	41:SA:312:ARG:NH1	2.16	0.78
2:L1:75:OMG:OP2	19:LI:74:TYR:OH	2.00	0.77
4:L3:295:A:OP2	32:LV:39:ARG:NH1	2.16	0.77
2:L1:62:A:OP1	29:LS:52:LYS:NZ	2.17	0.77
4:L3:4927:G:OP2	4:L3:4927:G:N2	2.15	0.77
4:L3:502:C:O2'	4:L3:503:C:OP1	2.02	0.77
4:L3:4156:G:OP2	4:L3:4157:A:O2'	2.03	0.76
4:L3:308:G:OP2	4:L3:308:G:N2	2.15	0.76
2:L1:87:G:OP1	29:LS:5:LYS:NZ	2.17	0.76
4:L3:1397:A:O2'	4:L3:1467:C:O2'	2.02	0.76
4:L3:2263:A:OP1	22:LL:107:ARG:NH2	2.18	0.76
4:L3:1280:C:O2'	41:SA:321:ASN:OD1	2.03	0.75
4:L3:3641:U:OP2	4:L3:3646:A:N6	2.18	0.75
4:L3:4305:G:O2'	4:L3:4306:OMU:O5'	2.03	0.75
4:L3:2318:G:N2	4:L3:2321:G:OP2	2.19	0.75
4:L3:1214:C:N4	23:LM:90:SER:O	2.20	0.74
4:L3:1397:A:HO2'	4:L3:1467:C:HO2'	1.34	0.74
4:L3:1931:C:N4	4:L3:2039:G:OP2	2.21	0.74
4:L3:1883:G:OP1	27:LQ:47:ARG:NH2	2.21	0.74
47:SG:41:ILE:HG21	47:SG:73:ILE:HD11	1.70	0.74
4:L3:4768:G:OP1	8:L7:168:TYR:OH	2.05	0.74
4:L3:4435:U:OP2	4:L3:4436:U:O2'	2.05	0.74
4:L3:1508:A:OP1	41:SA:110:ARG:NH2	2.21	0.73
4:L3:1853:G:O2'	4:L3:1854:G:OP2	2.04	0.73
3:L2:1165:A:O2'	3:L2:1167:A:OP1	2.06	0.73
3:L2:1167:A:O3'	4:L3:1:C:OP2	2.06	0.73
4:L3:119:G:O4'	45:SE:132:ARG:NH1	2.21	0.73
4:L3:4088:C:OP1	46:SF:37:ARG:NH2	2.21	0.72
17:LG:115:SER:OG	50:SK:145:GLN:OE1	2.07	0.72
4:L3:2326:G:OP1	27:LQ:108:ARG:NH2	2.22	0.72
7:L6:79:GLU:OE1	7:L6:82:ARG:NH2	2.22	0.72
4:L3:442:G:OP1	30:LT:68:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L9:73:ARG:HB3	10:L9:89:VAL:HG23	1.72	0.72
7:L6:129:ARG:NH1	29:LS:116:LEU:O	2.24	0.71
45:SE:90:GLN:NE2	49:SI:62:GLU:OE2	2.23	0.71
4:L3:2848:G:O2'	4:L3:3838:U:O4	2.04	0.71
4:L3:3620:G:OP1	4:L3:3622:C:N4	2.23	0.71
38:NL:456:ARG:NH2	52:SM:213:THR:O	2.25	0.70
38:NL:190:ARG:NH2	52:SM:117:ASP:OD1	2.24	0.70
52:SM:265:TYR:OH	52:SM:358:LYS:O	2.07	0.69
8:L7:182:GLU:OE2	9:L8:119:ARG:NH2	2.25	0.69
4:L3:4449:A:OP1	54:SR:118:LYS:NZ	2.24	0.69
4:L3:67:C:OP2	4:L3:312:G:N2	2.22	0.69
4:L3:1633:G:O6	4:L3:3918:G:O2'	2.11	0.69
50:SK:99:GLU:OE1	50:SK:125:THR:OG1	2.06	0.69
4:L3:937:U:OP1	9:L8:46:ARG:NH1	2.26	0.69
46:SF:142:GLU:O	46:SF:143:THR:OG1	2.11	0.69
4:L3:235:A:OP1	41:SA:201:ARG:NH2	2.25	0.69
4:L3:1889:U:OP1	30:LT:19:ARG:NH2	2.26	0.68
55:SV:125:LYS:O	55:SV:129:GLN:NE2	2.27	0.68
2:L1:156:U:OP2	45:SE:89:ARG:NH2	2.25	0.68
4:L3:4620:OMU:OP2	4:L3:4670:C:N4	2.23	0.68
4:L3:4765:G:OP1	47:SG:23:ARG:NE	2.26	0.68
44:SD:171:ASP:OD1	44:SD:172:ASN:N	2.26	0.68
4:L3:4124:G:N2	45:SE:43:GLN:O	2.27	0.68
51:SL:66:LEU:HD11	51:SL:251:LEU:HD21	1.75	0.68
4:L3:1322:1MA:O2'	4:L3:1323:A:O4'	2.12	0.67
4:L3:1090:G:OP1	15:LE:142:ARG:NH1	2.27	0.67
27:LQ:114:ARG:NH1	27:LQ:117:GLN:OE1	2.28	0.67
4:L3:974:C:O2	41:SA:327:LYS:NZ	2.25	0.66
3:L2:48:G:O2'	49:SI:79:ARG:NH1	2.28	0.66
4:L3:2545:U:O2'	4:L3:2547:G:N7	2.26	0.66
15:LE:32:ARG:O	42:SB:41:LYS:NZ	2.23	0.66
53:SQ:121:GLU:O	53:SQ:200:PHE:N	2.27	0.66
4:L3:4717:A:OP2	24:LN:30:LYS:NZ	2.27	0.66
4:L3:5002:U:OP2	24:LN:385:LYS:NZ	2.28	0.66
4:L3:408:A:O2'	4:L3:411:G:OP2	2.12	0.66
4:L3:1814:C:O2'	23:LM:42:ASN:OD1	2.06	0.66
11:LA:124:LYS:O	54:SR:602:ARG:NH1	2.28	0.66
4:L3:3715:PSU:H2'	4:L3:3716:C:O4'	1.95	0.66
7:L6:100:PRO:O	31:LU:25:ARG:NH2	2.27	0.65
4:L3:2588:C:OP1	4:L3:2768:C:O2'	2.11	0.65
4:L3:4626:A:OP2	24:LN:224:LYS:NZ	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L6:62:PRO:O	7:L6:63:THR:OG1	2.14	0.65
4:L3:1071:C:O2	43:SC:70:LYS:NZ	2.25	0.65
8:L7:189:ILE:HD11	9:L8:119:ARG:HG2	1.78	0.65
4:L3:1646:A:O2'	33:LW:49:TRP:O	2.14	0.64
24:LN:95:THR:OG1	24:LN:98:GLY:O	2.10	0.64
51:SL:82:LEU:HD12	51:SL:203:LEU:HD11	1.80	0.64
4:L3:2876:OMG:HM22	4:L3:2877:G:H5'	1.80	0.64
4:L3:4637:OMG:H2'	4:L3:4638:U:C6	2.33	0.64
20:LJ:9:LYS:NZ	20:LJ:83:THR:O	2.23	0.63
49:SI:105:ILE:HD13	49:SI:116:ILE:HD13	1.80	0.63
4:L3:1881:C:O2'	4:L3:1882:U:OP2	2.16	0.63
4:L3:1548:G:O2'	4:L3:2812:A:N3	2.28	0.63
4:L3:2407:G:N2	4:L3:2407:G:OP2	2.31	0.63
4:L3:2841:G:OP1	39:NP:10:HIS:NE2	2.30	0.63
10:L9:32:GLN:O	45:SE:59:ARG:NH2	2.31	0.63
4:L3:1518:A:OP1	21:LK:27:LYS:NZ	2.28	0.63
4:L3:5001:PSU:H2'	4:L3:5002:U:O4'	1.98	0.63
4:L3:63:G:OP2	10:L9:169:ARG:NH2	2.31	0.62
24:LN:357:ARG:NE	54:SR:407:ASP:OD1	2.29	0.62
6:L5:120:ASP:OD2	6:L5:122:SER:OG	2.08	0.62
4:L3:4500:PSU:H2'	4:L3:4501:U:C6	2.34	0.62
4:L3:1187:G:OP2	4:L3:1187:G:N2	2.23	0.62
4:L3:3717:A:OP2	4:L3:3735:G:N2	2.28	0.62
4:L3:4688:C:O2'	47:SG:155:SER:OG	2.06	0.62
24:LN:160:ILE:HD11	24:LN:190:VAL:HG13	1.81	0.62
46:SF:117:GLU:O	46:SF:162:ASN:ND2	2.33	0.62
4:L3:1943:A:C2	56:VB:36:ILE:HD12	2.35	0.62
43:SC:161:ARG:O	43:SC:182:ASN:ND2	2.32	0.62
4:L3:3776:G:OP2	4:L3:3776:G:N2	2.26	0.61
4:L3:1314:C:O2'	27:LQ:24:GLN:NE2	2.33	0.61
4:L3:2414:G:O2'	4:L3:2415:OMU:H5''	2.01	0.61
5:L4:7:G:OP1	42:SB:33:ARG:NH1	2.32	0.61
4:L3:4940:C:OP1	43:SC:156:ARG:NH2	2.32	0.61
4:L3:4220:6MZ:OP2	4:L3:4220:6MZ:H8	2.00	0.61
4:L3:267:G:OP1	29:LS:109:ARG:NH2	2.33	0.61
4:L3:400:A2M:HM'3	11:LA:101:ASN:HD22	1.66	0.61
4:L3:2626:U:OP2	54:SR:501:LYS:NZ	2.33	0.61
4:L3:4299:PSU:OP1	23:LM:33:LYS:NZ	2.33	0.61
21:LK:38:LEU:O	21:LK:42:ARG:NH1	2.34	0.60
34:LX:26:VAL:HG21	46:SF:180:LEU:HD11	1.82	0.60
23:LM:95:ARG:O	23:LM:99:ILE:HD12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SM:367:ASP:OD2	52:SM:369:THR:OG1	2.18	0.60
4:L3:4670:C:O2'	4:L3:4672:A:OP2	2.20	0.60
4:L3:2363:A2M:H2'	4:L3:2364:OMG:O4'	2.01	0.60
4:L3:4928:C:O4'	9:L8:121:ARG:NH1	2.34	0.60
56:VB:5:GLN:OE1	56:VB:5:GLN:N	2.34	0.60
4:L3:2923:A:O2'	35:LY:52:LYS:NZ	2.34	0.60
4:L3:375:G:OP2	33:LW:52:LYS:NZ	2.35	0.59
4:L3:2258:C:N3	43:SC:90:ALA:N	2.51	0.59
4:L3:3861:A:O2'	11:LA:135:ARG:NH2	2.35	0.59
43:SC:281:ILE:CG2	43:SC:286:LEU:HD11	2.32	0.59
4:L3:5039:U:O2'	55:SV:115:ASN:OD1	2.21	0.59
4:L3:5065:U:OP1	11:LA:43:LYS:NZ	2.34	0.59
52:SM:33:ASP:OD1	52:SM:36:ARG:NH2	2.36	0.59
45:SE:136:LEU:HD22	45:SE:202:VAL:CG1	2.33	0.59
4:L3:1438:U:O2'	4:L3:1439:C:OP1	2.21	0.58
38:NL:452:GLU:OE1	52:SM:63:THR:OG1	2.21	0.58
54:SR:176:TYR:CE1	54:SR:271:LEU:HD22	2.38	0.58
4:L3:2781:G:O2'	36:LZ:3:SER:O	2.21	0.58
4:L3:2922:G:O2'	4:L3:3275:A:N6	2.37	0.58
4:L3:4529:G:O2'	4:L3:4530:UR3:H5'	2.04	0.58
8:L7:202:LEU:O	8:L7:202:LEU:HD23	2.03	0.58
4:L3:4524:G:C2	24:LN:252:ALA:HB1	2.37	0.58
4:L3:453:G:O2'	4:L3:705:G:OP1	2.13	0.58
4:L3:2725:A:N6	14:LD:88:ARG:O	2.36	0.58
4:L3:1521:C:O2'	4:L3:1522:OMG:H5'	2.04	0.57
4:L3:294:G:OP2	32:LV:43:ARG:NH1	2.33	0.57
4:L3:3681:G:OP2	46:SF:128:ARG:NH2	2.37	0.57
4:L3:4536:OMC:HM22	4:L3:4537:C:O4'	2.04	0.57
4:L3:4633:G:O2'	4:L3:4635:A:OP2	2.19	0.57
11:LA:127:ARG:O	11:LA:139:TYR:N	2.37	0.57
4:L3:4371:G:OP1	32:LV:59:LYS:NZ	2.38	0.57
51:SL:82:LEU:CD1	51:SL:203:LEU:HD11	2.34	0.57
54:SR:420:MET:HE2	54:SR:420:MET:N	2.20	0.57
4:L3:3700:C:O2'	4:L3:3774:A:N3	2.36	0.56
4:L3:4724:A:O2'	24:LN:104:THR:HG22	2.05	0.56
4:L3:5068:G:N2	4:L3:5069:U:O4	2.38	0.56
26:LP:33:ILE:HG22	26:LP:33:ILE:O	2.05	0.56
4:L3:1433:A:N6	4:L3:1451:G:O2'	2.39	0.56
5:L4:12:U:O3'	5:L4:109:U:O2'	2.19	0.56
2:L1:50:C:HO2'	54:SR:578:SER:HG	1.52	0.56
4:L3:2296:G:O2'	41:SA:242:PRO:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LP:57:MET:SD	26:LP:90:ARG:NH1	2.79	0.56
4:L3:3938:G:N2	4:L3:4171:C:OP2	2.38	0.56
4:L3:4678:G:OP2	37:NK:14:ARG:NH1	2.38	0.56
4:L3:4541:G:N2	4:L3:4544:A:OP2	2.30	0.56
4:L3:1573:G:OP1	14:LD:92:LYS:NZ	2.36	0.56
4:L3:2695:A:OP1	35:LY:35:LYS:NZ	2.38	0.56
4:L3:4075:U:OP1	45:SE:249:ARG:NH2	2.39	0.56
4:L3:1980:U:O2'	4:L3:1982:G:N7	2.34	0.55
54:SR:73:ASP:OD1	54:SR:74:ASP:N	2.38	0.55
8:L7:190:ASP:OD1	8:L7:191:LYS:N	2.40	0.55
46:SF:133:TYR:HB3	46:SF:168:VAL:HG12	1.88	0.55
4:L3:4860:G:OP1	8:L7:169:ARG:NH1	2.40	0.55
4:L3:2835:A:O2'	24:LN:228:TYR:O	2.24	0.55
22:LL:112:ARG:NH1	43:SC:117:PRO:O	2.38	0.55
2:L1:69:PSU:H2'	2:L1:70:G:O4'	2.07	0.55
4:L3:4546:A:N7	46:SF:215:ASN:ND2	2.53	0.55
41:SA:35:ASP:OD1	41:SA:36:ILE:N	2.38	0.55
3:L2:99:G:N2	48:SH:129:GLU:OE1	2.40	0.55
4:L3:2306:G:OP1	27:LQ:128:ARG:NH1	2.39	0.55
2:L1:71:A:N6	2:L1:83:C:O4'	2.39	0.55
24:LN:223:THR:HG22	24:LN:338:VAL:HG13	1.89	0.55
4:L3:66:A:O2'	4:L3:326:C:O2	2.25	0.55
4:L3:331:G:OP1	10:L9:166:SER:OG	2.23	0.55
14:LD:13:SER:OG	14:LD:38:ARG:NH1	2.40	0.55
4:L3:267:G:N7	38:NL:147:ARG:NH1	2.55	0.54
43:SC:250:GLN:NE2	43:SC:254:ASP:OD2	2.39	0.54
4:L3:1677:PSU:H4'	4:L3:1680:G:C2	2.42	0.54
4:L3:4515:G:OP1	54:SR:49:ARG:NH1	2.40	0.54
38:NL:452:GLU:OE2	52:SM:63:THR:HG23	2.08	0.54
24:LN:187:GLY:O	24:LN:193:LYS:NZ	2.41	0.54
4:L3:1670:G:OP2	4:L3:1670:G:N2	2.32	0.54
4:L3:4305:G:HO2'	4:L3:4306:OMU:P	2.29	0.54
24:LN:36:ASP:OD1	24:LN:38:SER:OG	2.17	0.54
4:L3:68:U:OP1	10:L9:178:HIS:ND1	2.31	0.53
29:LS:35:LYS:O	54:SR:572:ARG:NH1	2.40	0.53
55:SV:70:GLU:N	55:SV:70:GLU:OE1	2.41	0.53
4:L3:3924:C:O2'	4:L3:3925:OMU:H5''	2.08	0.53
52:SM:370:ASP:OD2	52:SM:372:ARG:NH2	2.40	0.53
6:L5:93:GLU:OE2	6:L5:175:LEU:HD22	2.08	0.53
18:LH:119:ILE:HD12	18:LH:140:LEU:HD22	1.90	0.53
22:LL:62:VAL:HG11	22:LL:96:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:2876:OMG:C8	34:LX:16:THR:HG22	2.43	0.53
4:L3:5009:G:O2'	4:L3:5010:PSU:H5''	2.09	0.53
4:L3:5022:U:O2'	4:L3:5023:C:OP2	2.24	0.53
4:L3:4910:G:N2	8:L7:106:ASP:O	2.42	0.52
7:L6:7:GLY:O	21:LK:49:HIS:NE2	2.38	0.52
10:L9:115:VAL:HG22	10:L9:134:LEU:CD2	2.40	0.52
4:L3:4376:A:O2'	21:LK:42:ARG:NH1	2.43	0.52
7:L6:170:THR:OG1	7:L6:173:GLU:OE2	2.23	0.52
4:L3:277:G:OP2	31:LU:29:ARG:NH1	2.40	0.52
4:L3:1173:G:N2	4:L3:1188:C:N3	2.58	0.52
4:L3:1366:G:N2	4:L3:1371:A:OP2	2.42	0.52
4:L3:1931:C:N4	4:L3:2041:A:OP1	2.42	0.52
4:L3:4457:PSU:O4	24:LN:252:ALA:HB3	2.09	0.52
27:LQ:4:LEU:O	27:LQ:121:ARG:NH2	2.43	0.52
7:L6:63:THR:HG21	21:LK:66:ASN:HB3	1.92	0.52
38:NL:128:VAL:O	45:SE:150:LYS:NZ	2.33	0.52
11:LA:18:ARG:NH1	11:LA:147:GLU:OE1	2.42	0.52
21:LK:77:LYS:O	21:LK:80:THR:OG1	2.27	0.52
4:L3:730:G:OP2	44:SD:76:ARG:NE	2.43	0.51
4:L3:2639:U:O2'	4:L3:2694:G:O6	2.20	0.51
13:LC:173:ASN:ND2	13:LC:175:PHE:O	2.43	0.51
50:SK:121:LEU:O	50:SK:139:ARG:NH1	2.41	0.51
4:L3:2601:A:N6	4:L3:2744:A:OP2	2.40	0.51
20:LJ:68:ILE:O	20:LJ:115:LYS:NZ	2.37	0.51
4:L3:688:U:OP1	43:SC:94:LYS:NZ	2.43	0.51
4:L3:2436:U:OP2	18:LH:135:LYS:NZ	2.42	0.51
49:SI:148:THR:OG1	49:SI:243:ARG:NE	2.40	0.51
4:L3:3718:A2M:H2	4:L3:3934:G:O4'	2.09	0.51
15:LE:30:TYR:O	42:SB:41:LYS:NZ	2.34	0.51
4:L3:1255:A:OP1	4:L3:1257:A:N6	2.44	0.51
4:L3:1952:G:OP1	13:LC:139:ARG:NE	2.43	0.51
4:L3:1818:G:O2'	4:L3:1820:C:OP2	2.26	0.51
4:L3:2562:G:O2'	4:L3:2565:A:N6	2.44	0.51
4:L3:4296:PSU:H2'	4:L3:4297:G:O4'	2.11	0.51
4:L3:4691:A:OP1	47:SG:75:SER:OG	2.23	0.51
4:L3:2351:OMC:HM22	4:L3:2352:U:H5'	1.92	0.51
4:L3:2350:U:O5'	4:L3:2351:OMC:H5'	2.10	0.51
6:L5:128:LEU:HD22	6:L5:130:PHE:CE1	2.46	0.51
12:LB:88:ASP:OD1	12:LB:89:ASP:N	2.43	0.51
4:L3:2351:OMC:HM23	41:SA:95:MET:HG3	1.93	0.51
4:L3:3908:A:O2'	4:L3:4531:U:OP1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SE:57:TRP:O	45:SE:62:ARG:NH1	2.44	0.51
10:L9:193:ARG:O	10:L9:197:THR:HG23	2.10	0.51
46:SF:36:GLU:OE1	46:SF:163:ARG:NH1	2.41	0.51
4:L3:1683:PSU:H2'	4:L3:1684:A:C8	2.46	0.50
28:LR:44:SER:OG	28:LR:46:CYS:SG	2.56	0.50
4:L3:2303:C:OP1	27:LQ:107:ASN:ND2	2.42	0.50
4:L3:4985:U:O2	24:LN:174:ARG:NH1	2.43	0.50
4:L3:3868:G:O2'	4:L3:3869:OMC:H5''	2.11	0.50
10:L9:103:GLU:OE1	10:L9:165:THR:HG21	2.12	0.50
4:L3:1279:A:O2'	4:L3:1281:G:N7	2.38	0.50
4:L3:2407:G:O6	36:LZ:2:SER:N	2.44	0.50
4:L3:2415:OMU:HM22	4:L3:2415:OMU:C2	2.41	0.50
5:L4:117:G:OP1	42:SB:253:TYR:OH	2.18	0.50
2:L1:7:U:O2'	4:L3:1305:C:OP1	2.29	0.49
4:L3:52:G:OP2	33:LW:48:ASN:ND2	2.45	0.49
4:L3:3723:A:H2'	4:L3:3724:A2M:H8	1.94	0.49
24:LN:219:VAL:HG11	24:LN:337:VAL:HG13	1.94	0.49
45:SE:58:PRO:HD2	45:SE:61:ILE:HD12	1.93	0.49
38:NL:430:THR:O	38:NL:430:THR:HG22	2.11	0.49
51:SL:165:LEU:HB3	51:SL:169:ILE:HD12	1.93	0.49
4:L3:3734:PSU:H2'	4:L3:3735:G:O4'	2.13	0.49
17:LG:96:LEU:HD11	55:SV:22:VAL:CG2	2.43	0.49
17:LG:96:LEU:HD11	55:SV:22:VAL:HG23	1.95	0.49
41:SA:144:ILE:HG22	41:SA:144:ILE:O	2.12	0.49
4:L3:4587:G:OP1	8:L7:61:ARG:NH1	2.46	0.49
4:L3:1983:A:O2'	4:L3:2011:C:OP1	2.29	0.49
4:L3:2415:OMU:HM23	4:L3:2416:G:H8	1.76	0.49
2:L1:68:G:O2'	2:L1:69:PSU:H5''	2.12	0.49
4:L3:223:G:N3	41:SA:223:ASN:ND2	2.59	0.49
4:L3:1420:A:O2'	4:L3:1500:A:O2'	2.19	0.48
34:LX:69:TRP:NE1	46:SF:173:GLY:O	2.45	0.48
37:NK:95:ILE:HD12	37:NK:95:ILE:H	1.78	0.48
33:LW:14:LYS:NZ	36:LZ:51:LEU:OXT	2.44	0.48
14:LD:7:GLN:N	14:LD:7:GLN:OE1	2.46	0.48
35:LY:23:VAL:HG23	35:LY:64:LEU:HD21	1.94	0.48
52:SM:55:ASN:OD1	52:SM:62:ARG:NH1	2.46	0.48
4:L3:363:A:N7	4:L3:378:A:N6	2.62	0.48
4:L3:2869:U:O2'	4:L3:2881:A:N7	2.38	0.48
26:LP:95:ASP:OD1	26:LP:96:GLU:N	2.46	0.48
51:SL:248:VAL:O	51:SL:266:SER:OG	2.24	0.48
4:L3:1523:A:O2'	4:L3:1524:A2M:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:1895:G:OP1	44:SD:96:ARG:NH2	2.46	0.48
4:L3:2724:G:O2'	4:L3:2726:G:OP2	2.26	0.48
38:NL:227:ARG:O	38:NL:230:THR:HG22	2.14	0.48
4:L3:2459:G:N2	4:L3:2462:C:OP2	2.43	0.48
18:LH:143:ASP:N	18:LH:143:ASP:OD1	2.45	0.48
50:SK:242:ASP:OD1	54:SR:169:ARG:NE	2.47	0.48
4:L3:110:C:OP1	7:L6:89:LYS:NZ	2.46	0.48
4:L3:1577:G:C2	4:L3:3637:PSU:H1'	2.49	0.48
55:SV:66:ASP:OD2	55:SV:68:SER:OG	2.25	0.48
4:L3:508:G:O2'	4:L3:510:U:OP2	2.29	0.48
10:L9:117:ASN:OD1	10:L9:118:SER:N	2.44	0.48
50:SK:21:ASN:ND2	50:SK:112:ASP:OD2	2.46	0.48
4:L3:1595:G:N2	54:SR:634:ARG:OXT	2.37	0.48
4:L3:4288:C:O2'	4:L3:4321:U:OP1	2.30	0.48
54:SR:226:LEU:O	54:SR:233:ARG:NH2	2.47	0.48
55:SV:110:ASN:OD1	55:SV:111:ARG:N	2.47	0.48
4:L3:278:G:OP2	31:LU:30:ARG:NH2	2.47	0.48
4:L3:5022:U:HO2'	4:L3:5023:C:P	2.37	0.48
47:SG:87:GLY:O	47:SG:186:THR:OG1	2.23	0.48
4:L3:1464:C:H5''	23:LM:32:LEU:HD12	1.96	0.47
5:L4:12:U:OP2	5:L4:67:C:O2'	2.29	0.47
4:L3:2572:C:O2'	20:LJ:112:ARG:NH2	2.44	0.47
52:SM:170:HIS:HB3	52:SM:283:LEU:HD11	1.96	0.47
55:SV:53:LYS:NZ	55:SV:62:GLU:OE2	2.35	0.47
4:L3:121:A:OP1	45:SE:110:LYS:NZ	2.39	0.47
4:L3:2340:C:H4'	41:SA:42:THR:HG23	1.95	0.47
4:L3:2590:G:O2'	4:L3:2755:A:N6	2.45	0.47
4:L3:2838:G:O2'	4:L3:2839:PSU:H5''	2.14	0.47
4:L3:3886:G:H2'	4:L3:3887:OMC:H5'	1.96	0.47
12:LB:124:ASP:OD1	12:LB:125:GLN:N	2.47	0.47
4:L3:3718:A2M:HM'3	4:L3:3718:A2M:H1'	1.68	0.47
4:L3:4392:OMG:HM23	4:L3:4392:OMG:H1'	1.66	0.47
10:L9:143:ARG:NH1	29:LS:95:LEU:HD23	2.30	0.47
4:L3:4493:PSU:O2'	4:L3:4494:OMG:H5'	2.15	0.47
47:SG:12:ILE:HG12	47:SG:18:ILE:HD12	1.95	0.47
5:L4:118:C:H41	42:SB:258:LYS:NZ	2.13	0.47
20:LJ:70:SER:O	20:LJ:111:ARG:NH1	2.48	0.47
29:LS:33:VAL:O	29:LS:37:THR:HG22	2.15	0.47
4:L3:4352:U:O2'	4:L3:4353:PSU:H5''	2.14	0.47
40:NR:150:LEU:HA	40:NR:153:LEU:HD13	1.97	0.47
4:L3:131:C:N4	4:L3:138:G:O6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:2299:G:OP1	41:SA:182:LYS:NZ	2.40	0.47
4:L3:423:G:OP1	11:LA:62:ARG:NH1	2.47	0.47
4:L3:458:C:OP2	43:SC:114:ARG:NH1	2.48	0.47
4:L3:2804:OMC:HM23	4:L3:2804:OMC:H1'	1.71	0.47
7:L6:116:ARG:NH2	7:L6:155:MET:O	2.43	0.47
24:LN:248:LEU:HD23	24:LN:248:LEU:H	1.80	0.47
41:SA:144:ILE:HG21	41:SA:150:LEU:HD11	1.97	0.47
4:L3:2811:G:N2	4:L3:2814:C:OP2	2.45	0.46
4:L3:3928:A:OP1	10:L9:90:ASN:ND2	2.44	0.46
35:LY:66:VAL:HG13	35:LY:66:VAL:O	2.15	0.46
49:SI:106:ASP:OD1	49:SI:106:ASP:N	2.48	0.46
4:L3:935:A:O2'	9:L8:46:ARG:NH1	2.48	0.46
10:L9:26:ARG:NH2	45:SE:165:GLU:OE1	2.44	0.46
4:L3:1591:U:OP2	4:L3:2856:C:O2'	2.31	0.46
18:LH:119:ILE:HD12	18:LH:140:LEU:CD2	2.46	0.46
4:L3:1872:G:O2'	4:L3:4219:A:N3	2.42	0.46
4:L3:2616:C:OP1	14:LD:60:ARG:NH1	2.48	0.46
4:L3:3830:A2M:HM'3	4:L3:3830:A2M:H1'	1.64	0.46
40:NR:62:LEU:HD12	40:NR:69:TYR:OH	2.15	0.46
4:L3:2378:G:N2	4:L3:2381:A:OP2	2.47	0.46
17:LG:61:VAL:N	17:LG:79:ALA:O	2.47	0.46
24:LN:175:GLN:NE2	24:LN:177:LYS:O	2.49	0.46
4:L3:1364:U:OP2	7:L6:36:ARG:NH2	2.44	0.46
4:L3:3718:A2M:H2	4:L3:3934:G:C1'	2.46	0.46
13:LC:95:ARG:NH1	13:LC:112:ASP:OD2	2.48	0.46
43:SC:95:PRO:HA	43:SC:104:THR:HG22	1.98	0.46
43:SC:278:THR:HG22	43:SC:279:ASN:H	1.81	0.46
4:L3:1998:A:N3	4:L3:2019:C:O2'	2.45	0.46
26:LP:93:ASN:ND2	26:LP:93:ASN:O	2.49	0.46
34:LX:26:VAL:HG22	46:SF:178:PRO:HD2	1.98	0.46
38:NL:225:PRO:HD2	38:NL:228:LEU:HD12	1.98	0.46
39:NP:26:PRO:O	55:SV:43:LYS:NZ	2.30	0.46
4:L3:4623:OMG:HM23	4:L3:4623:OMG:H1'	1.64	0.45
2:L1:127:U:O2	52:SM:13:SER:OG	2.26	0.45
4:L3:3654:G:O2'	4:L3:3693:U:OP1	2.32	0.45
4:L3:4620:OMU:HM23	4:L3:4620:OMU:H1'	1.82	0.45
4:L3:4635:A:H3'	4:L3:4636:PSU:H4'	1.99	0.45
4:L3:307:A:N3	4:L3:310:G:O2'	2.45	0.45
4:L3:2787:A2M:HM'3	4:L3:2790:U:OP2	2.17	0.45
4:L3:4937:C:N3	43:SC:239:LYS:NZ	2.61	0.45
34:LX:8:VAL:O	34:LX:11:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:3899:OMG:HM23	4:L3:3899:OMG:H1'	1.67	0.45
4:L3:4457:PSU:H1'	24:LN:252:ALA:HB3	1.97	0.45
4:L3:1321:G:O2'	4:L3:1322:1MA:H5'	2.17	0.45
4:L3:2415:OMU:HM23	4:L3:2416:G:C8	2.51	0.45
4:L3:2891:U:OP2	14:LD:74:ARG:NH1	2.49	0.45
12:LB:89:ASP:O	12:LB:112:ARG:NH1	2.50	0.45
27:LQ:84:GLU:O	27:LQ:87:VAL:HG22	2.17	0.45
35:LY:59:SER:O	35:LY:59:SER:OG	2.34	0.45
54:SR:233:ARG:NE	54:SR:237:GLU:OE2	2.48	0.45
54:SR:244:LEU:O	54:SR:282:LYS:NZ	2.37	0.45
4:L3:3627:OMG:HM23	4:L3:3627:OMG:H1'	1.64	0.45
4:L3:3744:OMG:HM23	4:L3:3744:OMG:H1'	1.62	0.45
49:SI:101:ARG:NH1	49:SI:122:LYS:O	2.49	0.45
50:SK:174:SER:O	50:SK:178:GLN:N	2.46	0.45
51:SL:71:TRP:N	51:SL:247:SER:O	2.45	0.45
42:SB:62:CYS:HB3	42:SB:105:LEU:HD22	1.99	0.45
4:L3:2402:G:O2'	28:LR:10:ARG:O	2.35	0.45
4:L3:3705:G:H21	46:SF:224:THR:HG21	1.82	0.45
4:L3:3729:U:O2'	4:L3:3730:PSU:H5''	2.17	0.45
4:L3:4228:OMG:H5''	4:L3:4229:U:O4'	2.17	0.45
15:LE:30:TYR:HB2	42:SB:38:ILE:HD12	1.99	0.45
49:SI:135:GLN:OE1	49:SI:135:GLN:N	2.48	0.45
3:L2:4:G:HO2'	49:SI:69:TRP:CD1	2.35	0.45
4:L3:2368:A:N6	4:L3:2827:G:O2'	2.50	0.45
52:SM:172:ILE:O	52:SM:176:ARG:N	2.50	0.45
54:SR:632:ASP:OD1	54:SR:633:ARG:N	2.49	0.45
4:L3:1468:C:OP1	21:LK:132:ARG:NH2	2.44	0.44
4:L3:4578:G:O2'	4:L3:4579:PSU:H5''	2.17	0.44
38:NL:217:THR:O	38:NL:217:THR:HG22	2.16	0.44
2:L1:75:OMG:HM23	2:L1:75:OMG:H1'	1.47	0.44
4:L3:2422:OMC:H2'	4:L3:2423:A:C8	2.52	0.44
52:SM:265:TYR:HB3	52:SM:362:ILE:HD11	2.00	0.44
4:L3:2837:OMU:HM23	4:L3:2837:OMU:H1'	1.57	0.44
4:L3:4456:OMC:HM23	4:L3:4456:OMC:H1'	1.58	0.44
12:LB:23:ILE:HD11	41:SA:32:ILE:O	2.18	0.44
41:SA:156:ASP:OD2	41:SA:255:SER:OG	2.36	0.44
4:L3:62:A:OP1	10:L9:172:ARG:NH1	2.51	0.44
4:L3:3896:C:O2'	24:LN:268:ARG:NH1	2.51	0.44
4:L3:4343:U:O2'	32:LV:31:ASP:OD1	2.34	0.44
7:L6:164:GLU:N	7:L6:164:GLU:OE1	2.51	0.44
20:LJ:76:ASN:OD1	20:LJ:77:TYR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LK:131:ARG:NH1	21:LK:135:GLU:OE2	2.50	0.44
45:SE:103:ARG:NH2	45:SE:192:ARG:O	2.51	0.44
4:L3:1340:OMC:HM23	4:L3:1340:OMC:H1'	1.54	0.44
4:L3:1590:C:O2'	39:NP:5:ARG:NH2	2.51	0.44
4:L3:1951:G:O2'	13:LC:95:ARG:NH2	2.50	0.44
4:L3:3724:A2M:H2'	4:L3:3725:G:C8	2.53	0.44
54:SR:489:GLU:O	54:SR:493:LEU:HD23	2.18	0.44
4:L3:2422:OMC:H1'	4:L3:2422:OMC:HM23	1.42	0.44
4:L3:4371:G:O2'	4:L3:4372:U:OP2	2.22	0.44
20:LJ:30:ASP:O	20:LJ:39:SER:OG	2.20	0.44
24:LN:181:MET:HE1	24:LN:346:THR:HG23	2.00	0.44
50:SK:103:ALA:O	50:SK:107:VAL:HG23	2.17	0.44
4:L3:2823:G:O2'	4:L3:2824:OMC:H5''	2.18	0.43
4:L3:4311:A:O2'	4:L3:4312:PSU:H5''	2.17	0.43
50:SK:49:VAL:HG12	50:SK:50:HIS:O	2.18	0.43
4:L3:2363:A2M:H1'	4:L3:2363:A2M:HM'3	1.58	0.43
4:L3:2815:A2M:HM'3	4:L3:2815:A2M:H1'	1.81	0.43
4:L3:4155:C:OP2	38:NL:464:LYS:NZ	2.40	0.43
19:LI:34:LEU:HD12	19:LI:44:VAL:HG23	2.00	0.43
54:SR:576:ASP:OD1	54:SR:577:VAL:N	2.51	0.43
4:L3:2815:A2M:H2'	4:L3:2816:G:C8	2.53	0.43
16:LF:57:GLY:O	16:LF:60:VAL:HG23	2.18	0.43
4:L3:2326:G:H5''	27:LQ:127:ALA:HB2	2.00	0.43
4:L3:2415:OMU:O5'	4:L3:2415:OMU:H6	2.18	0.43
4:L3:4637:OMG:HM23	4:L3:4637:OMG:H1'	1.67	0.43
10:L9:165:THR:HG23	10:L9:168:GLY:H	1.83	0.43
31:LU:63:VAL:HG12	31:LU:63:VAL:O	2.19	0.43
43:SC:278:THR:HG22	43:SC:279:ASN:N	2.32	0.43
4:L3:1427:A:C2	12:LB:138:LEU:HD23	2.53	0.43
4:L3:4620:OMU:H6	4:L3:4620:OMU:O5'	2.19	0.43
14:LD:7:GLN:NE2	14:LD:35:ALA:O	2.50	0.43
24:LN:113:GLU:OE2	24:LN:169:ARG:N	2.51	0.43
24:LN:119:TYR:OH	24:LN:129:ALA:N	2.51	0.43
4:L3:2517:A:N3	4:L3:2539:C:O2'	2.50	0.43
4:L3:3841:OMC:H1'	4:L3:3841:OMC:HM23	1.49	0.43
10:L9:115:VAL:HA	10:L9:134:LEU:HD23	2.01	0.43
11:LA:40:HIS:NE2	11:LA:110:ASP:O	2.49	0.43
16:LF:25:CYS:O	16:LF:29:VAL:HG12	2.18	0.43
19:LI:67:ILE:O	19:LI:84:ARG:NH2	2.52	0.43
50:SK:101:LEU:HB3	50:SK:107:VAL:HG21	2.00	0.43
2:L1:58:G:O6	33:LW:63:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4139:G:H21	4:L3:4140:C:N4	2.17	0.43
4:L3:4405:G:O2'	56:VB:33:GLY:O	2.34	0.43
13:LC:15:ARG:HB3	13:LC:27:LEU:HD23	2.00	0.43
16:LF:47:ILE:HD12	16:LF:63:ILE:HD11	2.00	0.43
50:SK:77:THR:HG22	50:SK:80:GLU:CD	2.44	0.43
4:L3:2097:U:O3'	4:L3:2098:G:H4'	2.18	0.43
4:L3:4678:G:N7	37:NK:11:ARG:NH2	2.66	0.43
9:L8:104:MET:HE3	9:L8:109:ARG:HG2	2.00	0.43
4:L3:346:G:OP1	19:LI:8:THR:HG23	2.19	0.42
4:L3:709:C:OP1	30:LT:89:ARG:NH2	2.50	0.42
4:L3:4305:G:H4'	4:L3:4306:OMU:OP1	2.19	0.42
47:SG:128:MET:SD	47:SG:146:LEU:HD21	2.59	0.42
54:SR:227:ASP:OD1	54:SR:274:ASN:ND2	2.49	0.42
2:L1:152:U:OP1	4:L3:4162:C:N4	2.51	0.42
4:L3:399:G:H21	11:LA:101:ASN:HD21	1.67	0.42
4:L3:3717:A:H2'	4:L3:3718:A2M:H8	2.01	0.42
4:L3:4571:A2M:HM'3	4:L3:4571:A2M:H1'	1.59	0.42
35:LY:17:ARG:NH2	35:LY:19:ASP:OD2	2.49	0.42
4:L3:4570:G:H2'	4:L3:4571:A2M:H8	2.00	0.42
4:L3:1391:A:N3	4:L3:4364:G:O2'	2.49	0.42
4:L3:4252:C:OP2	4:L3:4253:A:O2'	2.24	0.42
38:NL:160:GLU:C	38:NL:161:LEU:HD22	2.44	0.42
52:SM:332:PHE:HD2	52:SM:377:ILE:HD11	1.84	0.42
4:L3:1899:G:O2'	27:LQ:57:ASN:OD1	2.35	0.42
40:NR:90:GLU:OE1	40:NR:91:GLN:NE2	2.53	0.42
4:L3:2519:U:O2'	4:L3:2530:U:O2	2.35	0.42
23:LM:99:ILE:HD12	23:LM:99:ILE:H	1.85	0.42
4:L3:503:C:O2'	4:L3:504:G:O5'	2.32	0.42
4:L3:2667:C:OP2	14:LD:103:ARG:NH1	2.52	0.42
4:L3:2763:U:O2	38:NL:387:ARG:NH2	2.47	0.42
4:L3:4162:C:O2'	45:SE:69:ILE:HD11	2.20	0.42
4:L3:4590:A2M:HM'3	4:L3:4590:A2M:H1'	1.77	0.42
4:L3:4593:C:OP2	37:NK:2:ALA:N	2.53	0.42
38:NL:429:ARG:NH1	49:SI:183:GLU:OE1	2.53	0.42
49:SI:123:LYS:O	49:SI:126:SER:OG	2.35	0.42
4:L3:2630:U:H2'	4:L3:2632:PSU:H1'	2.01	0.42
4:L3:4530:UR3:H6	4:L3:4530:UR3:O5'	2.20	0.42
4:L3:1373:A:OP1	41:SA:47:ASN:ND2	2.49	0.42
4:L3:4618:OMG:HM23	4:L3:4618:OMG:H1'	1.65	0.42
38:NL:254:HIS:CE1	38:NL:258:LEU:HD11	2.55	0.42
4:L3:4745:G:H22	4:L3:4955:A:H2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4872:G:OP2	9:L8:94:LYS:NZ	2.44	0.41
4:L3:4988:U:OP2	24:LN:123:HIS:ND1	2.52	0.41
4:L3:2861:OMC:HM23	4:L3:2861:OMC:H1'	1.44	0.41
52:SM:362:ILE:HG22	52:SM:363:GLY:N	2.35	0.41
54:SR:225:ILE:HG13	54:SR:271:LEU:HD21	2.02	0.41
4:L3:122:U:O4	45:SE:107:LYS:NZ	2.52	0.41
4:L3:1727:U:OP1	44:SD:131:ASN:ND2	2.52	0.41
10:L9:51:LEU:HD22	10:L9:117:ASN:ND2	2.35	0.41
24:LN:45:ALA:HB3	24:LN:183:ILE:HG23	2.02	0.41
28:LR:59:VAL:HG22	28:LR:60:ARG:H	1.85	0.41
41:SA:124:ILE:HG21	41:SA:264:TYR:OH	2.20	0.41
4:L3:400:A2M:HM'3	4:L3:400:A2M:H1'	1.65	0.41
4:L3:972:C:C6	43:SC:126:LEU:HD13	2.55	0.41
4:L3:2562:G:N2	4:L3:2565:A:OP2	2.50	0.41
5:L4:55:A:O2'	6:L5:151:ILE:O	2.24	0.41
10:L9:43:THR:HG23	10:L9:44:ARG:HG3	2.03	0.41
11:LA:126:ARG:HD2	54:SR:603:LEU:O	2.19	0.41
41:SA:204:ARG:NH1	41:SA:205:ARG:O	2.52	0.41
4:L3:397:G:H2'	4:L3:398:A2M:H5'	2.02	0.41
7:L6:21:ARG:HB2	10:L9:197:THR:HG22	2.03	0.41
39:NP:29:ASP:OD1	39:NP:30:GLU:N	2.53	0.41
54:SR:128:GLN:OE1	56:VB:58:ARG:NE	2.54	0.41
4:L3:2362:U:H2'	4:L3:2363:A2M:H8	2.03	0.41
4:L3:2448:G:O2'	46:SF:21:LYS:NZ	2.39	0.41
4:L3:3852:A:N7	4:L3:3853:PSU:N1	2.69	0.41
7:L6:17:ASP:OD2	7:L6:20:ARG:NE	2.42	0.41
7:L6:186:ARG:HG2	31:LU:9:VAL:HG21	2.01	0.41
18:LH:81:LEU:HD12	18:LH:97:VAL:CG1	2.50	0.41
20:LJ:21:ARG:NH1	20:LJ:47:ASP:OD1	2.54	0.41
45:SE:164:ILE:O	45:SE:168:VAL:HG13	2.21	0.41
52:SM:274:GLU:CB	52:SM:362:ILE:HD12	2.51	0.41
4:L3:1355:G:OP1	12:LB:108:ARG:NH1	2.47	0.41
4:L3:4455:G:O2'	4:L3:4456:OMC:H5''	2.20	0.41
19:LI:109:LEU:HD22	19:LI:115:ARG:NH1	2.36	0.41
54:SR:176:TYR:CD1	54:SR:271:LEU:HD22	2.55	0.41
3:L2:9:A:N3	3:L2:11:C:O2'	2.53	0.41
4:L3:2815:A2M:H2'	4:L3:2816:G:H8	1.85	0.41
4:L3:3619:G:H22	4:L3:3624:A:H1'	1.86	0.41
4:L3:4478:G:N2	4:L3:4608:G:O2'	2.54	0.41
19:LI:51:LYS:NZ	19:LI:71:VAL:O	2.50	0.41
20:LJ:22:LYS:NZ	20:LJ:132:GLN:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:2043:A:N1	4:L3:4515:G:O2'	2.45	0.41
4:L3:2364:OMG:O2'	4:L3:2365:OMC:H5''	2.20	0.41
4:L3:4569:U:OP1	4:L3:4982:A:O2'	2.33	0.41
7:L6:63:THR:HG22	7:L6:64:VAL:N	2.35	0.41
49:SI:182:ILE:HD11	49:SI:194:LEU:HD13	2.02	0.41
50:SK:56:CYS:HB2	50:SK:62:MET:HE1	2.03	0.41
4:L3:1577:G:O2'	4:L3:1612:G:H4'	2.21	0.40
4:L3:4646:U:O2'	54:SR:502:ASN:OD1	2.24	0.40
24:LN:327:THR:HG22	24:LN:327:THR:O	2.20	0.40
41:SA:325:MET:HE1	44:SD:155:TYR:CE1	2.57	0.40
50:SK:199:VAL:HG23	50:SK:204:ALA:HB2	2.04	0.40
4:L3:400:A2M:HM'3	11:LA:101:ASN:ND2	2.35	0.40
4:L3:1880:G:OP1	4:L3:1882:U:O2'	2.20	0.40
4:L3:2696:A:H62	35:LY:35:LYS:NZ	2.19	0.40
4:L3:4619:U:H2'	4:L3:4620:OMU:H6	2.03	0.40
22:LL:62:VAL:HG11	22:LL:96:MET:CE	2.51	0.40
32:LV:73:VAL:O	32:LV:73:VAL:HG12	2.21	0.40
36:LZ:46:ARG:NH1	54:SR:606:LYS:O	2.54	0.40
4:L3:307:A:OP1	31:LU:86:LYS:NZ	2.54	0.40
4:L3:977:C:O5'	41:SA:333:LYS:NZ	2.55	0.40
4:L3:1870:C:H2'	4:L3:1871:A2M:H8	2.04	0.40
4:L3:4494:OMG:H8	4:L3:4494:OMG:O5'	2.05	0.40
4:L3:4498:OMU:HM23	4:L3:4498:OMU:H1'	1.57	0.40
23:LM:35:VAL:HG12	23:LM:36:ASP:N	2.37	0.40
25:LO:31:TYR:CZ	25:LO:35:LEU:HD11	2.57	0.40
4:L3:1552:G:O2'	4:L3:1553:A:OP2	2.36	0.40
10:L9:103:GLU:OE2	10:L9:118:SER:OG	2.27	0.40
26:LP:42:ALA:HB3	26:LP:43:PRO:HD3	2.03	0.40
41:SA:186:SER:O	41:SA:188:ARG:NH1	2.49	0.40
50:SK:155:SER:OG	50:SK:156:ASN:N	2.53	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	BA	89/165 (54%)	89 (100%)	0	0	100	100
6	L5	166/178 (93%)	165 (99%)	1 (1%)	0	100	100
7	L6	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
8	L7	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
9	L8	133/215 (62%)	132 (99%)	1 (1%)	0	100	100
10	L9	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
11	LA	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
12	LB	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
13	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
14	LD	152/196 (78%)	151 (99%)	1 (1%)	0	100	100
15	LE	150/160 (94%)	144 (96%)	6 (4%)	0	100	100
16	LF	101/128 (79%)	100 (99%)	1 (1%)	0	100	100
17	LG	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
18	LH	141/156 (90%)	141 (100%)	0	0	100	100
19	LI	132/145 (91%)	132 (100%)	0	0	100	100
20	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
21	LK	145/148 (98%)	144 (99%)	1 (1%)	0	100	100
22	LL	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
23	LM	87/159 (55%)	86 (99%)	1 (1%)	0	100	100
24	LN	399/403 (99%)	394 (99%)	5 (1%)	0	100	100
25	LO	93/115 (81%)	93 (100%)	0	0	100	100
26	LP	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
27	LQ	126/135 (93%)	126 (100%)	0	0	100	100
28	LR	110/117 (94%)	110 (100%)	0	0	100	100
29	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
30	LT	107/110 (97%)	107 (100%)	0	0	100	100
31	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
32	LV	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
33	LW	84/97 (87%)	84 (100%)	0	0	100	100
34	LX	89/92 (97%)	86 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	LY	67/70 (96%)	67 (100%)	0	0	100	100
36	LZ	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
37	NK	63/129 (49%)	63 (100%)	0	0	100	100
38	NL	317/478 (66%)	316 (100%)	1 (0%)	0	100	100
39	NP	100/134 (75%)	98 (98%)	2 (2%)	0	100	100
40	NR	150/203 (74%)	146 (97%)	4 (3%)	0	100	100
41	SA	356/427 (83%)	351 (99%)	5 (1%)	0	100	100
42	SB	273/297 (92%)	270 (99%)	3 (1%)	0	100	100
43	SC	211/288 (73%)	206 (98%)	5 (2%)	0	100	100
44	SD	223/248 (90%)	218 (98%)	5 (2%)	0	100	100
45	SE	228/266 (86%)	225 (99%)	3 (1%)	0	100	100
46	SF	243/257 (95%)	236 (97%)	7 (3%)	0	100	100
47	SG	188/192 (98%)	188 (100%)	0	0	100	100
48	SH	148/293 (50%)	145 (98%)	3 (2%)	0	100	100
49	SI	231/255 (91%)	228 (99%)	3 (1%)	0	100	100
50	SK	242/245 (99%)	237 (98%)	5 (2%)	0	100	100
51	SL	236/490 (48%)	231 (98%)	5 (2%)	0	100	100
52	SM	393/588 (67%)	389 (99%)	4 (1%)	0	100	100
53	SQ	121/239 (51%)	120 (99%)	1 (1%)	0	100	100
54	SR	595/634 (94%)	588 (99%)	6 (1%)	1 (0%)	43	58
55	SV	137/163 (84%)	137 (100%)	0	0	100	100
56	VB	54/99 (54%)	54 (100%)	0	0	100	100
All	All	8865/10803 (82%)	8755 (99%)	109 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
54	SR	88	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	L5	142/149 (95%)	142 (100%)	0	100	100
7	L6	176/177 (99%)	176 (100%)	0	100	100
8	L7	173/174 (99%)	173 (100%)	0	100	100
9	L8	115/161 (71%)	115 (100%)	0	100	100
10	L9	171/172 (99%)	171 (100%)	0	100	100
11	LA	134/163 (82%)	134 (100%)	0	100	100
12	LB	164/165 (99%)	164 (100%)	0	100	100
13	LC	157/157 (100%)	157 (100%)	0	100	100
14	LD	138/175 (79%)	138 (100%)	0	100	100
15	LE	136/140 (97%)	136 (100%)	0	100	100
16	LF	93/115 (81%)	93 (100%)	0	100	100
17	LG	106/107 (99%)	106 (100%)	0	100	100
18	LH	124/133 (93%)	124 (100%)	0	100	100
19	LI	124/135 (92%)	124 (100%)	0	100	100
20	LJ	117/118 (99%)	117 (100%)	0	100	100
21	LK	120/121 (99%)	120 (100%)	0	100	100
22	LL	109/121 (90%)	109 (100%)	0	100	100
23	LM	77/126 (61%)	77 (100%)	0	100	100
24	LN	347/348 (100%)	347 (100%)	0	100	100
25	LO	80/97 (82%)	80 (100%)	0	100	100
26	LP	97/110 (88%)	97 (100%)	0	100	100
27	LQ	114/121 (94%)	114 (100%)	0	100	100
28	LR	96/100 (96%)	96 (100%)	0	100	100
29	LS	109/110 (99%)	109 (100%)	0	100	100
30	LT	88/89 (99%)	88 (100%)	0	100	100
31	LU	86/89 (97%)	86 (100%)	0	100	100
32	LV	92/94 (98%)	92 (100%)	0	100	100
33	LW	73/80 (91%)	73 (100%)	0	100	100
34	LX	74/75 (99%)	74 (100%)	0	100	100
35	LY	64/65 (98%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	LZ	47/48 (98%)	47 (100%)	0	100	100
37	NK	61/115 (53%)	61 (100%)	0	100	100
38	NL	280/402 (70%)	280 (100%)	0	100	100
39	NP	88/114 (77%)	88 (100%)	0	100	100
40	NR	140/183 (76%)	140 (100%)	0	100	100
41	SA	298/348 (86%)	298 (100%)	0	100	100
42	SB	234/250 (94%)	234 (100%)	0	100	100
43	SC	192/252 (76%)	192 (100%)	0	100	100
44	SD	194/215 (90%)	194 (100%)	0	100	100
45	SE	198/223 (89%)	198 (100%)	0	100	100
46	SF	188/199 (94%)	188 (100%)	0	100	100
47	SG	169/171 (99%)	169 (100%)	0	100	100
48	SH	102/274 (37%)	102 (100%)	0	100	100
49	SI	210/228 (92%)	210 (100%)	0	100	100
50	SK	212/213 (100%)	212 (100%)	0	100	100
51	SL	221/437 (51%)	221 (100%)	0	100	100
52	SM	354/509 (70%)	354 (100%)	0	100	100
53	SQ	6/214 (3%)	6 (100%)	0	100	100
54	SR	545/574 (95%)	545 (100%)	0	100	100
55	SV	128/149 (86%)	128 (100%)	0	100	100
56	VB	48/76 (63%)	48 (100%)	0	100	100
All	All	7611/9181 (83%)	7611 (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 (61) such sidechains are listed below:

Mol	Chain	Res	Type
6	L5	104	ASN
9	L8	34	ASN
9	L8	48	GLN
10	L9	86	HIS
10	L9	109	HIS
11	LA	10	ASN

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Mol	Chain	Res	Type
11	LA	56	GLN
11	LA	97	ASN
11	LA	101	ASN
12	LB	162	HIS
14	LD	141	HIS
15	LE	66	ASN
16	LF	41	GLN
17	LG	27	ASN
18	LH	33	HIS
19	LI	18	HIS
19	LI	20	ASN
19	LI	43	ASN
19	LI	127	GLN
20	LJ	127	ASN
21	LK	19	HIS
21	LK	28	HIS
22	LL	23	GLN
22	LL	36	ASN
24	LN	138	GLN
24	LN	208	ASN
24	LN	322	HIS
25	LO	15	ASN
25	LO	72	HIS
26	LP	30	HIS
26	LP	121	ASN
27	LQ	52	GLN
30	LT	99	HIS
31	LU	26	HIS
32	LV	102	GLN
38	NL	124	ASN
38	NL	216	GLN
38	NL	267	GLN
39	NP	13	HIS
39	NP	91	GLN
39	NP	99	GLN
41	SA	43	ASN
41	SA	112	HIS
41	SA	198	ASN
41	SA	203	GLN
41	SA	310	HIS
43	SC	190	HIS
45	SE	149	ASN

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Mol	Chain	Res	Type
45	SE	153	GLN
45	SE	208	ASN
46	SF	22	HIS
46	SF	139	HIS
47	SG	39	ASN
48	SH	119	HIS
50	SK	68	HIS
52	SM	209	HIS
54	SR	157	HIS
54	SR	209	HIS
54	SR	218	GLN
54	SR	246	HIS
55	SV	132	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	17 (11%)	0
3	L2	67/1167 (5%)	9 (13%)	0
4	L3	3391/5070 (66%)	408 (12%)	8 (0%)
5	L4	119/121 (98%)	10 (8%)	1 (0%)
All	All	3729/6515 (57%)	444 (11%)	9 (0%)

All (444) 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	84	A
2	L1	86	U
2	L1	87	G
2	L1	94	G
2	L1	103	A
2	L1	105	C
2	L1	110	U
2	L1	111	U

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Mol	Chain	Res	Type
2	L1	151	G
2	L1	156	U
3	L2	11	C
3	L2	48	G
3	L2	49	G
3	L2	51	U
3	L2	62	U
3	L2	96	A
3	L2	101	A
3	L2	1165	A
3	L2	1166	G
4	L3	2	G
4	L3	6	C
4	L3	25	A
4	L3	39	A
4	L3	42	A
4	L3	48	G
4	L3	56	A
4	L3	58	G
4	L3	59	A
4	L3	64	A
4	L3	65	A
4	L3	91	G
4	L3	108	A
4	L3	119	G
4	L3	159	C
4	L3	164	G
4	L3	167	C
4	L3	169	G
4	L3	170	C
4	L3	171	U
4	L3	172	C
4	L3	173	C
4	L3	181	C
4	L3	200	U
4	L3	209	U
4	L3	210	C
4	L3	218	A
4	L3	234	G
4	L3	261	G
4	L3	266	C
4	L3	274	C

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Mol	Chain	Res	Type
4	L3	316	U
4	L3	340	C
4	L3	387	G
4	L3	409	G
4	L3	410	A
4	L3	412	G
4	L3	450	G
4	L3	452	A
4	L3	453	G
4	L3	454	U
4	L3	464	G
4	L3	467	U
4	L3	472	C
4	L3	473	C
4	L3	479	G
4	L3	492	U
4	L3	493	G
4	L3	496	G
4	L3	497	G
4	L3	501	C
4	L3	502	C
4	L3	503	C
4	L3	504	G
4	L3	509	A
4	L3	510	U
4	L3	658	C
4	L3	660	A
4	L3	667	A
4	L3	668	C
4	L3	669	C
4	L3	686	A
4	L3	704	C
4	L3	731	G
4	L3	739	G
4	L3	741	C
4	L3	742	G
4	L3	746	A
4	L3	913	U
4	L3	915	A
4	L3	916	C
4	L3	917	A
4	L3	926	G

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Mol	Chain	Res	Type
4	L3	932	A
4	L3	933	G
4	L3	943	A
4	L3	944	A
4	L3	945	U
4	L3	956	A
4	L3	959	G
4	L3	960	A
4	L3	971	U
4	L3	972	C
4	L3	1066	G
4	L3	1072	C
4	L3	1080	C
4	L3	1100	U
4	L3	1167	C
4	L3	1169	G
4	L3	1171	G
4	L3	1173	G
4	L3	1178	G
4	L3	1180	C
4	L3	1181	C
4	L3	1182	C
4	L3	1201	U
4	L3	1203	G
4	L3	1211	G
4	L3	1214	C
4	L3	1215	C
4	L3	1241	C
4	L3	1253	G
4	L3	1254	A
4	L3	1255	A
4	L3	1256	G
4	L3	1266	G
4	L3	1269	G
4	L3	1270	A
4	L3	1273	G
4	L3	1280	C
4	L3	1284	G
4	L3	1287	G
4	L3	1294	A
4	L3	1295	C
4	L3	1301	C

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Mol	Chain	Res	Type
4	L3	1314	C
4	L3	1319	U
4	L3	1320	U
4	L3	1322	1MA
4	L3	1323	A
4	L3	1325	C
4	L3	1326	A2M
4	L3	1354	A
4	L3	1358	G
4	L3	1359	G
4	L3	1365	C
4	L3	1366	G
4	L3	1379	C
4	L3	1397	A
4	L3	1420	A
4	L3	1439	C
4	L3	1443	A
4	L3	1497	A
4	L3	1498	G
4	L3	1502	G
4	L3	1523	A
4	L3	1534	A2M
4	L3	1547	A
4	L3	1578	U
4	L3	1581	G
4	L3	1592	G
4	L3	1597	G
4	L3	1613	A
4	L3	1624	G
4	L3	1625	OMG
4	L3	1631	A
4	L3	1633	G
4	L3	1634	A
4	L3	1654	G
4	L3	1661	C
4	L3	1676	C
4	L3	1677	PSU
4	L3	1678	C
4	L3	1691	G
4	L3	1721	G
4	L3	1726	U
4	L3	1734	G

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Mol	Chain	Res	Type
4	L3	1791	U
4	L3	1804	A
4	L3	1815	G
4	L3	1821	G
4	L3	1822	U
4	L3	1836	G
4	L3	1837	A
4	L3	1842	G
4	L3	1854	G
4	L3	1855	G
4	L3	1866	U
4	L3	1869	G
4	L3	1880	G
4	L3	1881	C
4	L3	1882	U
4	L3	1887	G
4	L3	1891	A
4	L3	1897	A
4	L3	1910	G
4	L3	1919	G
4	L3	1921	C
4	L3	1922	G
4	L3	1925	G
4	L3	1936	C
4	L3	1960	A
4	L3	1974	U
4	L3	1984	A
4	L3	2002	A
4	L3	2016	C
4	L3	2026	A
4	L3	2046	G
4	L3	2055	G
4	L3	2056	G
4	L3	2069	A
4	L3	2084	C
4	L3	2085	G
4	L3	2092	G
4	L3	2093	A
4	L3	2094	G
4	L3	2095	A
4	L3	2096	G
4	L3	2097	U

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Mol	Chain	Res	Type
4	L3	2098	G
4	L3	2099	G
4	L3	2109	G
4	L3	2110	C
4	L3	2111	G
4	L3	2261	G
4	L3	2289	C
4	L3	2300	A
4	L3	2301	G
4	L3	2313	A
4	L3	2348	G
4	L3	2351	OMC
4	L3	2395	A
4	L3	2417	A
4	L3	2422	OMC
4	L3	2425	U
4	L3	2429	A
4	L3	2450	G
4	L3	2453	A
4	L3	2470	C
4	L3	2471	G
4	L3	2475	G
4	L3	2476	G
4	L3	2477	A
4	L3	2478	C
4	L3	2480	G
4	L3	2487	G
4	L3	2488	C
4	L3	2489	C
4	L3	2492	C
4	L3	2493	G
4	L3	2512	A
4	L3	2513	A
4	L3	2519	U
4	L3	2544	G
4	L3	2545	U
4	L3	2548	C
4	L3	2554	U
4	L3	2587	A
4	L3	2627	C
4	L3	2653	C
4	L3	2669	C

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Mol	Chain	Res	Type
4	L3	2687	U
4	L3	2694	G
4	L3	2695	A
4	L3	2696	A
4	L3	2711	G
4	L3	2743	A
4	L3	2760	G
4	L3	2764	A
4	L3	2769	U
4	L3	2787	A2M
4	L3	2788	U
4	L3	2790	U
4	L3	2814	C
4	L3	2826	U
4	L3	2827	G
4	L3	2829	U
4	L3	2842	G
4	L3	2855	G
4	L3	2877	G
4	L3	2894	A
4	L3	2902	G
4	L3	2917	G
4	L3	2918	G
4	L3	3271	G
4	L3	3585	G
4	L3	3593	C
4	L3	3595	U
4	L3	3597	G
4	L3	3617	G
4	L3	3626	G
4	L3	3635	A
4	L3	3644	U
4	L3	3653	A
4	L3	3662	A
4	L3	3696	C
4	L3	3697	U
4	L3	3838	U
4	L3	3840	U
4	L3	3868	G
4	L3	3872	A
4	L3	3875	G
4	L3	3876	A

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Mol	Chain	Res	Type
4	L3	3877	A
4	L3	3887	OMC
4	L3	3897	G
4	L3	3905	A
4	L3	3915	U
4	L3	4069	U
4	L3	4076	G
4	L3	4084	G
4	L3	4085	A
4	L3	4119	C
4	L3	4122	G
4	L3	4127	A
4	L3	4133	C
4	L3	4139	G
4	L3	4140	C
4	L3	4142	C
4	L3	4143	G
4	L3	4144	C
4	L3	4145	C
4	L3	4147	G
4	L3	4150	G
4	L3	4154	G
4	L3	4162	C
4	L3	4163	U
4	L3	4170	A
4	L3	4183	G
4	L3	4184	G
4	L3	4191	G
4	L3	4202	U
4	L3	4220	6MZ
4	L3	4222	G
4	L3	4229	U
4	L3	4233	A
4	L3	4251	A
4	L3	4254	G
4	L3	4266	G
4	L3	4268	A
4	L3	4273	A
4	L3	4281	A
4	L3	4291	G
4	L3	4305	G
4	L3	4306	OMU

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Mol	Chain	Res	Type
4	L3	4329	G
4	L3	4330	G
4	L3	4332	C
4	L3	4339	A
4	L3	4373	G
4	L3	4376	A
4	L3	4377	G
4	L3	4378	A
4	L3	4387	C
4	L3	4415	A
4	L3	4418	G
4	L3	4437	U
4	L3	4438	U
4	L3	4439	U
4	L3	4453	C
4	L3	4464	A
4	L3	4466	C
4	L3	4475	G
4	L3	4498	OMU
4	L3	4512	U
4	L3	4513	A
4	L3	4518	A
4	L3	4519	C
4	L3	4523	A2M
4	L3	4524	G
4	L3	4532	PSU
4	L3	4545	G
4	L3	4548	A
4	L3	4549	G
4	L3	4556	U
4	L3	4558	U
4	L3	4560	C
4	L3	4567	G
4	L3	4584	A
4	L3	4590	A2M
4	L3	4608	G
4	L3	4618	OMG
4	L3	4636	PSU
4	L3	4637	OMG
4	L3	4656	A
4	L3	4670	C
4	L3	4672	A

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Mol	Chain	Res	Type
4	L3	4701	A
4	L3	4708	A
4	L3	4709	U
4	L3	4719	G
4	L3	4720	C
4	L3	4740	G
4	L3	4741	C
4	L3	4742	G
4	L3	4750	G
4	L3	4751	G
4	L3	4754	G
4	L3	4757	C
4	L3	4759	C
4	L3	4765	G
4	L3	4772	C
4	L3	4773	C
4	L3	4870	G
4	L3	4871	C
4	L3	4882	U
4	L3	4883	C
4	L3	4900	C
4	L3	4901	G
4	L3	4910	G
4	L3	4914	C
4	L3	4916	G
4	L3	4943	A
4	L3	4976	U
4	L3	5006	U
4	L3	5014	A
4	L3	5022	U
4	L3	5023	C
4	L3	5026	U
4	L3	5027	C
4	L3	5031	G
4	L3	5041	G
4	L3	5050	C
4	L3	5054	C
4	L3	5055	G
4	L3	5061	A
4	L3	5062	G
4	L3	5069	U
5	L4	7	G

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Mol	Chain	Res	Type
5	L4	49	A
5	L4	53	U
5	L4	54	A
5	L4	64	G
5	L4	66	G
5	L4	97	G
5	L4	110	G
5	L4	111	C
5	L4	120	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L3	496	G
4	L3	502	C
4	L3	503	C
4	L3	1322	1MA
4	L3	1324	A
4	L3	1853	G
4	L3	2095	A
4	L3	3616	U
5	L4	109	U

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

109 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	$\# Z > 2$
4	PSU	L3	3853	4	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
4	OMU	L3	3925	4	19,22,23	2.02	6 (31%)	25,31,34	1.83	5 (20%)
4	OMU	L3	4306	4	19,22,23	2.04	6 (31%)	25,31,34	1.86	4 (16%)
4	PSU	L3	4299	4	18,21,22	1.03	1 (5%)	21,30,33	2.02	5 (23%)
4	PSU	L3	3734	4	18,21,22	1.13	1 (5%)	21,30,33	1.96	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	HIC	LN	245	24	10,11,12	0.52	0	9,14,16	0.85	1 (11%)
4	PSU	L3	4579	4	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
4	PSU	L3	4521	4	18,21,22	1.08	1 (5%)	21,30,33	1.91	5 (23%)
4	PSU	L3	4628	4	18,21,22	1.06	1 (5%)	21,30,33	1.91	6 (28%)
4	PSU	L3	4361	4	18,21,22	1.05	1 (5%)	21,30,33	1.96	5 (23%)
4	A2M	L3	3825	4	22,25,26	0.84	0	30,36,39	2.09	7 (23%)
4	A2M	L3	400	4	22,25,26	0.86	0	30,36,39	2.07	7 (23%)
4	PSU	L3	1862	4	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
4	PSU	L3	4312	4	18,21,22	1.08	1 (5%)	21,30,33	1.97	5 (23%)
4	OMG	L3	4494	4	23,26,27	0.50	0	32,38,41	0.51	0
4	A2M	L3	4590	4	22,25,26	0.87	0	30,36,39	2.04	8 (26%)
4	PSU	L3	2632	4	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
4	PSU	L3	3851	4	18,21,22	1.14	1 (5%)	21,30,33	1.96	6 (28%)
4	OMU	L3	4498	4	19,22,23	2.11	7 (36%)	25,31,34	1.80	5 (20%)
4	PSU	L3	5010	4	18,21,22	1.11	1 (5%)	21,30,33	1.90	5 (23%)
4	A2M	L3	1524	4	22,25,26	0.88	0	30,36,39	2.11	8 (26%)
4	PSU	L3	4403	4	18,21,22	1.10	1 (5%)	21,30,33	1.96	6 (28%)
4	A2M	L3	2363	57,4	22,25,26	0.87	0	30,36,39	2.04	7 (23%)
4	OMC	L3	2861	4	19,22,23	0.51	0	25,31,34	0.68	0
4	PSU	L3	4532	4	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
4	A2M	L3	4571	4	22,25,26	0.85	0	30,36,39	2.03	7 (23%)
40	PTR	NR	127	40	15,16,17	1.26	1 (6%)	17,22,24	0.65	0
4	PSU	L3	3695	4	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
4	OMC	L3	3701	4	19,22,23	0.48	0	25,31,34	0.62	0
4	OMC	L3	1340	4	19,22,23	0.54	0	25,31,34	0.71	0
4	6MZ	L3	4220	4	22,25,26	1.14	2 (9%)	29,36,39	2.17	9 (31%)
4	A2M	L3	398	4	22,25,26	0.87	0	30,36,39	2.12	8 (26%)
4	PSU	L3	3637	4	18,21,22	1.09	1 (5%)	21,30,33	2.06	5 (23%)
4	OMC	L3	2365	4	19,22,23	0.52	0	25,31,34	0.65	0
4	OMC	L3	3841	4	19,22,23	0.51	0	25,31,34	0.66	0
4	PSU	L3	3730	4	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
4	PSU	L3	4293	4	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
4	OMG	L3	4228	4	23,26,27	0.51	0	32,38,41	0.57	0
4	OMC	L3	4536	4	19,22,23	0.51	0	25,31,34	0.66	0
4	A2M	L3	1534	57,4	22,25,26	0.84	0	30,36,39	2.13	9 (30%)
4	OMU	L3	2837	4	19,22,23	2.07	7 (36%)	25,31,34	1.82	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	L3	1326	4	22,25,26	0.87	0	30,36,39	2.07	7 (23%)
4	PSU	L3	4471	4	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L3	1536	4	18,21,22	1.11	1 (5%)	21,30,33	1.92	4 (19%)
4	OMC	L3	2351	57,4	19,22,23	0.55	0	25,31,34	0.80	1 (4%)
4	PSU	L3	3715	4	18,21,22	1.11	1 (5%)	21,30,33	1.94	6 (28%)
4	A2M	L3	3724	4	22,25,26	0.86	0	30,36,39	2.04	7 (23%)
4	PSU	L3	4972	4	18,21,22	1.08	1 (5%)	21,30,33	1.90	5 (23%)
4	OMG	L3	3627	4	23,26,27	0.48	0	32,38,41	0.58	0
4	PSU	L3	4636	4	18,21,22	1.10	1 (5%)	21,30,33	2.00	6 (28%)
4	A2M	L3	3867	4	22,25,26	0.85	0	30,36,39	2.10	8 (26%)
4	PSU	L3	2839	4	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
4	PSU	L3	4431	4	18,21,22	1.14	1 (5%)	21,30,33	1.93	5 (23%)
4	OMG	L3	1522	4	23,26,27	0.47	0	32,38,41	0.49	0
4	OMG	L3	4392	4	23,26,27	0.47	0	32,38,41	0.48	0
4	PSU	L3	5001	4	18,21,22	1.15	1 (5%)	21,30,33	1.95	5 (23%)
4	OMG	L3	4637	4	23,26,27	0.48	0	32,38,41	0.48	0
4	OMU	L3	4227	4	19,22,23	2.01	7 (36%)	25,31,34	1.81	4 (16%)
4	PSU	L3	2508	4	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
4	UR3	L3	4530	4	19,22,23	1.09	3 (15%)	26,32,35	1.51	2 (7%)
4	OMG	L3	4499	4	23,26,27	0.45	0	32,38,41	0.47	0
4	OMC	L3	2422	57,4	19,22,23	0.49	0	25,31,34	0.70	0
4	OMG	L3	1625	4	23,26,27	0.48	0	32,38,41	0.46	0
4	PSU	L3	3639	4	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
4	OMC	L3	4456	4	19,22,23	0.54	0	25,31,34	0.66	0
4	OMG	L3	4618	4	23,26,27	0.47	0	32,38,41	0.53	0
4	PSU	L3	4457	4	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
4	A2M	L3	4523	4	22,25,26	0.86	0	30,36,39	2.10	8 (26%)
4	OMC	L3	2824	4	19,22,23	0.52	0	25,31,34	0.62	0
4	PSU	L3	4493	4	18,21,22	1.08	1 (5%)	21,30,33	1.97	5 (23%)
4	PSU	L3	1683	4	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
4	OMG	L3	3899	4	23,26,27	0.47	0	32,38,41	0.55	0
4	PSU	L3	1582	4	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
4	OMG	L3	2364	4	23,26,27	0.48	0	32,38,41	0.45	0
2	PSU	L1	69	2	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
4	OMG	L3	1316	4	23,26,27	0.48	0	32,38,41	0.51	0
4	PSU	L3	4353	4	18,21,22	1.08	1 (5%)	21,30,33	2.04	6 (28%)
4	PSU	L3	4552	4	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMU	L3	4620	4	19,22,23	2.00	6 (31%)	25,31,34	1.66	4 (16%)
4	PSU	L3	4576	4	18,21,22	1.12	1 (5%)	21,30,33	1.94	6 (28%)
4	PSU	L3	3822	4	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
4	1MA	L3	1322	4	21,25,26	0.46	0	30,37,40	0.82	1 (3%)
4	A2M	L3	2787	4	22,25,26	0.86	0	30,36,39	2.11	7 (23%)
4	OMG	L3	3744	4	23,26,27	0.46	0	32,38,41	0.48	0
4	PSU	L3	4500	4	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
4	PSU	L3	3884	4	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
4	A2M	L3	3718	4	22,25,26	0.88	0	30,36,39	2.05	8 (26%)
4	PSU	L3	1677	4	18,21,22	1.02	1 (5%)	21,30,33	1.87	5 (23%)
4	A2M	L3	2401	4	22,25,26	0.85	0	30,36,39	2.13	8 (26%)
4	A2M	L3	2815	4	22,25,26	0.86	0	30,36,39	2.11	8 (26%)
4	PSU	L3	4673	4	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
4	PSU	L3	4689	4	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
4	OMU	L3	2415	4	19,22,23	2.06	7 (36%)	25,31,34	1.85	5 (20%)
4	OMC	L3	2804	4	19,22,23	0.51	0	25,31,34	0.67	0
4	OMG	L3	2424	4	23,26,27	0.47	0	32,38,41	0.45	0
4	PSU	L3	1860	4	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
4	OMC	L3	3887	4	19,22,23	0.52	0	25,31,34	0.66	0
4	A2M	L3	3830	4	22,25,26	0.86	0	30,36,39	2.10	8 (26%)
4	OMG	L3	4370	4	23,26,27	0.51	0	32,38,41	0.52	0
4	OMC	L3	3869	4	19,22,23	0.53	0	25,31,34	0.68	0
2	PSU	L1	55	2	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
4	PSU	L3	1792	4	18,21,22	1.08	1 (5%)	21,30,33	1.91	5 (23%)
4	A2M	L3	1871	4	22,25,26	0.84	0	30,36,39	2.19	8 (26%)
4	OMG	L3	2876	4	23,26,27	0.46	0	32,38,41	0.46	0
4	PSU	L3	3920	57,4	18,21,22	1.07	1 (5%)	21,30,33	1.93	5 (23%)
4	OMG	L3	4623	4	23,26,27	0.48	0	32,38,41	0.53	0
4	PSU	L3	4296	4	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
2	OMG	L1	75	2	23,26,27	0.47	0	32,38,41	0.49	0
4	PSU	L3	3844	4	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)

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
4	PSU	L3	3853	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	3925	4	-	1/9/27/28	0/2/2/2
4	OMU	L3	4306	4	-	4/9/27/28	0/2/2/2
4	PSU	L3	4299	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3734	4	-	0/7/25/26	0/2/2/2
24	HIC	LN	245	24	-	3/5/6/8	0/1/1/1
4	PSU	L3	4579	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4521	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4628	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4361	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3825	4	-	1/9/27/28	0/3/3/3
4	A2M	L3	400	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	1862	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4312	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4494	4	-	0/9/27/28	0/3/3/3
4	A2M	L3	4590	4	-	4/9/27/28	0/3/3/3
4	PSU	L3	2632	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3851	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4498	4	-	2/9/27/28	0/2/2/2
4	PSU	L3	5010	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	1524	4	-	3/9/27/28	0/3/3/3
4	PSU	L3	4403	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	2363	57,4	-	1/9/27/28	0/3/3/3
4	OMC	L3	2861	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	4532	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	4571	4	-	1/9/27/28	0/3/3/3
40	PTR	NR	127	40	-	2/10/11/13	0/1/1/1
4	PSU	L3	3695	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3701	4	-	6/9/27/28	0/2/2/2
4	OMC	L3	1340	4	-	1/9/27/28	0/2/2/2
4	6MZ	L3	4220	4	-	3/9/27/28	0/3/3/3
4	A2M	L3	398	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	3637	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	2365	4	-	0/9/27/28	0/2/2/2
4	OMC	L3	3841	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	3730	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4293	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4228	4	-	0/9/27/28	0/3/3/3
4	OMC	L3	4536	4	-	0/9/27/28	0/2/2/2
4	A2M	L3	1534	57,4	-	2/9/27/28	0/3/3/3
4	OMU	L3	2837	4	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A2M	L3	1326	4	-	3/9/27/28	0/3/3/3
4	PSU	L3	4471	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	1536	4	-	2/7/25/26	0/2/2/2
4	OMC	L3	2351	57,4	-	3/9/27/28	0/2/2/2
4	PSU	L3	3715	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3724	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4972	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3627	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4636	4	-	3/7/25/26	0/2/2/2
4	A2M	L3	3867	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	2839	4	-	1/7/25/26	0/2/2/2
4	PSU	L3	4431	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	1522	4	-	0/9/27/28	0/3/3/3
4	OMG	L3	4392	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	5001	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4637	4	-	3/9/27/28	0/3/3/3
4	OMU	L3	4227	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	2508	4	-	0/7/25/26	0/2/2/2
4	UR3	L3	4530	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4499	4	-	0/9/27/28	0/3/3/3
4	OMC	L3	2422	57,4	-	2/9/27/28	0/2/2/2
4	OMG	L3	1625	4	-	2/9/27/28	0/3/3/3
4	PSU	L3	3639	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	4456	4	-	1/9/27/28	0/2/2/2
4	OMG	L3	4618	4	-	3/9/27/28	0/3/3/3
4	PSU	L3	4457	4	-	1/7/25/26	0/2/2/2
4	A2M	L3	4523	4	-	2/9/27/28	0/3/3/3
4	OMC	L3	2824	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	4493	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	1683	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3899	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	1582	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	2364	4	-	2/9/27/28	0/3/3/3
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
4	OMG	L3	1316	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4353	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4552	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4620	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	4576	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3822	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1MA	L3	1322	4	-	0/7/25/26	0/3/3/3
4	A2M	L3	2787	4	-	5/9/27/28	0/3/3/3
4	OMG	L3	3744	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4500	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3884	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3718	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	1677	4	-	4/7/25/26	0/2/2/2
4	A2M	L3	2401	4	-	2/9/27/28	0/3/3/3
4	A2M	L3	2815	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4673	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4689	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	2415	4	-	1/9/27/28	0/2/2/2
4	OMC	L3	2804	4	-	1/9/27/28	0/2/2/2
4	OMG	L3	2424	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	1860	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3887	4	-	2/9/27/28	0/2/2/2
4	A2M	L3	3830	4	-	1/9/27/28	0/3/3/3
4	OMG	L3	4370	4	-	0/9/27/28	0/3/3/3
4	OMC	L3	3869	4	-	0/9/27/28	0/2/2/2
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
4	PSU	L3	1792	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	1871	4	-	1/9/27/28	0/3/3/3
4	OMG	L3	2876	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	3920	57,4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4623	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4296	4	-	0/7/25/26	0/2/2/2
2	OMG	L1	75	2	-	2/9/27/28	0/3/3/3
4	PSU	L3	3844	4	-	1/7/25/26	0/2/2/2

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	4498	OMU	C6-N1	4.85	1.49	1.38
4	L3	2837	OMU	C6-N1	4.76	1.49	1.38
4	L3	2415	OMU	C6-N1	4.73	1.49	1.38
4	L3	4306	OMU	C6-N1	4.71	1.49	1.38
4	L3	3925	OMU	C6-N1	4.66	1.49	1.38
4	L3	4620	OMU	C6-N1	4.65	1.49	1.38
4	L3	4227	OMU	C6-N1	4.63	1.49	1.38
40	NR	127	PTR	OH-CZ	-4.60	1.30	1.40
4	L3	4498	OMU	C2-N1	4.47	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	4306	OMU	C2-N1	4.31	1.45	1.38
4	L3	2837	OMU	C2-N1	4.27	1.45	1.38
4	L3	2415	OMU	C2-N1	4.24	1.45	1.38
4	L3	4620	OMU	C2-N1	4.16	1.45	1.38
4	L3	4498	OMU	C5-C4	4.16	1.52	1.43
4	L3	4227	OMU	C2-N1	4.14	1.44	1.38
4	L3	3925	OMU	C2-N1	4.09	1.44	1.38
4	L3	2837	OMU	C5-C4	4.09	1.52	1.43
4	L3	2415	OMU	C5-C4	4.06	1.52	1.43
4	L3	4220	6MZ	C6-N6	4.00	1.38	1.34
4	L3	3925	OMU	C5-C4	3.97	1.52	1.43
4	L3	4227	OMU	C5-C4	3.91	1.52	1.43
4	L3	4620	OMU	C5-C4	3.83	1.52	1.43
4	L3	4306	OMU	C5-C4	3.82	1.52	1.43
4	L3	4431	PSU	C6-C5	3.76	1.39	1.35
4	L3	3822	PSU	C6-C5	3.72	1.39	1.35
4	L3	2632	PSU	C6-C5	3.67	1.39	1.35
4	L3	5001	PSU	C6-C5	3.65	1.39	1.35
4	L3	3734	PSU	C6-C5	3.63	1.39	1.35
4	L3	2839	PSU	C6-C5	3.63	1.39	1.35
4	L3	1860	PSU	C6-C5	3.62	1.39	1.35
4	L3	3851	PSU	C6-C5	3.59	1.39	1.35
4	L3	3715	PSU	C6-C5	3.59	1.39	1.35
4	L3	5010	PSU	C6-C5	3.59	1.39	1.35
4	L3	4636	PSU	C6-C5	3.57	1.39	1.35
4	L3	1862	PSU	C6-C5	3.57	1.39	1.35
4	L3	4500	PSU	C6-C5	3.57	1.39	1.35
4	L3	4576	PSU	C6-C5	3.57	1.39	1.35
4	L3	3695	PSU	C6-C5	3.57	1.39	1.35
4	L3	1536	PSU	C6-C5	3.56	1.39	1.35
4	L3	2508	PSU	C6-C5	3.56	1.39	1.35
4	L3	3853	PSU	C6-C5	3.55	1.39	1.35
4	L3	3884	PSU	C6-C5	3.54	1.39	1.35
4	L3	4532	PSU	C6-C5	3.54	1.39	1.35
4	L3	4471	PSU	C6-C5	3.53	1.39	1.35
4	L3	4673	PSU	C6-C5	3.53	1.39	1.35
4	L3	4403	PSU	C6-C5	3.52	1.39	1.35
4	L3	4972	PSU	C6-C5	3.52	1.39	1.35
4	L3	1792	PSU	C6-C5	3.52	1.39	1.35
4	L3	1683	PSU	C6-C5	3.51	1.39	1.35
2	L1	69	PSU	C6-C5	3.51	1.39	1.35
4	L3	4457	PSU	C6-C5	3.50	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	3730	PSU	C6-C5	3.49	1.39	1.35
4	L3	4493	PSU	C6-C5	3.49	1.39	1.35
4	L3	3844	PSU	C6-C5	3.48	1.39	1.35
4	L3	3639	PSU	C6-C5	3.47	1.39	1.35
2	L1	55	PSU	C6-C5	3.46	1.39	1.35
4	L3	4521	PSU	C6-C5	3.45	1.39	1.35
4	L3	4552	PSU	C6-C5	3.45	1.39	1.35
4	L3	3637	PSU	C6-C5	3.44	1.39	1.35
4	L3	4353	PSU	C6-C5	3.42	1.39	1.35
4	L3	1582	PSU	C6-C5	3.41	1.39	1.35
4	L3	4689	PSU	C6-C5	3.39	1.39	1.35
4	L3	4312	PSU	C6-C5	3.39	1.39	1.35
4	L3	4579	PSU	C6-C5	3.37	1.39	1.35
4	L3	4296	PSU	C6-C5	3.37	1.39	1.35
4	L3	3920	PSU	C6-C5	3.32	1.39	1.35
4	L3	4628	PSU	C6-C5	3.27	1.38	1.35
4	L3	4361	PSU	C6-C5	3.25	1.38	1.35
4	L3	4293	PSU	C6-C5	3.24	1.38	1.35
4	L3	4299	PSU	C6-C5	3.15	1.38	1.35
4	L3	1677	PSU	C6-C5	3.01	1.38	1.35
4	L3	4306	OMU	O4-C4	-2.86	1.18	1.24
4	L3	4530	UR3	C2-N1	-2.83	1.34	1.38
4	L3	4620	OMU	O4-C4	-2.82	1.19	1.24
4	L3	4530	UR3	C4-N3	-2.79	1.35	1.40
4	L3	3925	OMU	O4-C4	-2.74	1.19	1.24
4	L3	4227	OMU	O4-C4	-2.73	1.19	1.24
4	L3	2415	OMU	O4-C4	-2.72	1.19	1.24
4	L3	2837	OMU	O4-C4	-2.71	1.19	1.24
4	L3	4498	OMU	O4-C4	-2.66	1.19	1.24
4	L3	4498	OMU	C2-N3	2.61	1.42	1.38
4	L3	2837	OMU	C2-N3	2.53	1.42	1.38
4	L3	2415	OMU	C2-N3	2.52	1.42	1.38
4	L3	3925	OMU	C2-N3	2.51	1.42	1.38
4	L3	4306	OMU	C2-N3	2.39	1.42	1.38
4	L3	4306	OMU	O2-C2	-2.39	1.18	1.23
4	L3	4227	OMU	C2-N3	2.37	1.42	1.38
4	L3	4620	OMU	C2-N3	2.26	1.41	1.38
4	L3	2415	OMU	O2-C2	-2.25	1.19	1.23
4	L3	4227	OMU	O2-C2	-2.25	1.19	1.23
4	L3	4620	OMU	O2-C2	-2.20	1.19	1.23
4	L3	3925	OMU	O2-C2	-2.20	1.19	1.23
4	L3	2837	OMU	O2-C2	-2.17	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	4498	OMU	C4-N3	2.16	1.42	1.38
4	L3	2837	OMU	C4-N3	2.14	1.42	1.38
4	L3	4530	UR3	C2-N3	-2.13	1.34	1.39
4	L3	4220	6MZ	C5-N7	-2.08	1.35	1.39
4	L3	4498	OMU	O2-C2	-2.08	1.19	1.23
4	L3	2415	OMU	C4-N3	2.07	1.42	1.38
4	L3	4227	OMU	C4-N3	2.02	1.42	1.38

All (423) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4220	6MZ	C5-C4-N3	-5.76	118.78	126.72
4	L3	3825	A2M	C5-C4-N3	-5.67	118.92	126.72
4	L3	2815	A2M	C5-C4-N3	-5.66	118.93	126.72
4	L3	4571	A2M	C5-C4-N3	-5.61	119.00	126.72
4	L3	2363	A2M	C5-C4-N3	-5.61	119.00	126.72
4	L3	2787	A2M	C5-C4-N3	-5.59	119.01	126.72
4	L3	1534	A2M	C5-C4-N3	-5.57	119.05	126.72
4	L3	2401	A2M	C5-C4-N3	-5.56	119.06	126.72
4	L3	1326	A2M	C5-C4-N3	-5.52	119.11	126.72
4	L3	1524	A2M	C5-C4-N3	-5.52	119.11	126.72
4	L3	398	A2M	C5-C4-N3	-5.49	119.15	126.72
4	L3	3867	A2M	C5-C4-N3	-5.49	119.16	126.72
4	L3	4523	A2M	C5-C4-N3	-5.47	119.18	126.72
4	L3	400	A2M	C5-C4-N3	-5.47	119.18	126.72
4	L3	3830	A2M	C5-C4-N3	-5.47	119.18	126.72
4	L3	4306	OMU	C4-N3-C2	-5.45	119.85	126.61
4	L3	2837	OMU	C4-N3-C2	-5.44	119.85	126.61
4	L3	2415	OMU	C4-N3-C2	-5.44	119.86	126.61
4	L3	4227	OMU	C4-N3-C2	-5.43	119.87	126.61
4	L3	3925	OMU	C4-N3-C2	-5.42	119.89	126.61
4	L3	3724	A2M	C5-C4-N3	-5.41	119.27	126.72
4	L3	4498	OMU	C4-N3-C2	-5.40	119.91	126.61
4	L3	3718	A2M	C5-C4-N3	-5.37	119.33	126.72
4	L3	4530	UR3	C4-N3-C2	-5.36	120.26	124.58
4	L3	1871	A2M	C5-C4-N3	-5.32	119.39	126.72
4	L3	3637	PSU	N1-C2-N3	5.14	120.59	115.17
4	L3	4353	PSU	N1-C2-N3	5.12	120.57	115.17
4	L3	3637	PSU	C4-N3-C2	-5.11	119.33	126.37
4	L3	4353	PSU	C4-N3-C2	-5.06	119.40	126.37
4	L3	4299	PSU	C4-N3-C2	-5.04	119.42	126.37
4	L3	4299	PSU	N1-C2-N3	5.02	120.46	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4296	PSU	C4-N3-C2	-5.01	119.47	126.37
4	L3	4636	PSU	C4-N3-C2	-4.98	119.51	126.37
4	L3	1582	PSU	C4-N3-C2	-4.98	119.51	126.37
4	L3	4493	PSU	C4-N3-C2	-4.96	119.54	126.37
4	L3	4590	A2M	C5-C4-N3	-4.96	119.89	126.72
4	L3	4493	PSU	N1-C2-N3	4.94	120.38	115.17
4	L3	4296	PSU	N1-C2-N3	4.93	120.37	115.17
4	L3	4689	PSU	N1-C2-N3	4.92	120.36	115.17
4	L3	3851	PSU	C4-N3-C2	-4.91	119.60	126.37
4	L3	4532	PSU	C4-N3-C2	-4.91	119.61	126.37
4	L3	4312	PSU	N1-C2-N3	4.91	120.34	115.17
4	L3	4361	PSU	N1-C2-N3	4.91	120.34	115.17
4	L3	3695	PSU	C4-N3-C2	-4.90	119.62	126.37
4	L3	4403	PSU	C4-N3-C2	-4.89	119.63	126.37
4	L3	4636	PSU	N1-C2-N3	4.89	120.33	115.17
4	L3	4361	PSU	C4-N3-C2	-4.89	119.64	126.37
4	L3	4689	PSU	C4-N3-C2	-4.89	119.64	126.37
4	L3	4673	PSU	C4-N3-C2	-4.87	119.66	126.37
4	L3	4312	PSU	C4-N3-C2	-4.86	119.67	126.37
4	L3	5001	PSU	N1-C2-N3	4.86	120.30	115.17
4	L3	4552	PSU	C4-N3-C2	-4.86	119.68	126.37
4	L3	4500	PSU	C4-N3-C2	-4.86	119.68	126.37
4	L3	3844	PSU	N1-C2-N3	4.85	120.29	115.17
4	L3	1677	PSU	C4-N3-C2	-4.85	119.69	126.37
4	L3	2508	PSU	C4-N3-C2	-4.85	119.69	126.37
4	L3	4532	PSU	N1-C2-N3	4.85	120.29	115.17
4	L3	4471	PSU	N1-C2-N3	4.84	120.28	115.17
4	L3	1862	PSU	C4-N3-C2	-4.84	119.70	126.37
4	L3	1860	PSU	N1-C2-N3	4.84	120.27	115.17
4	L3	3734	PSU	N1-C2-N3	4.83	120.26	115.17
2	L1	55	PSU	C4-N3-C2	-4.83	119.72	126.37
4	L3	1862	PSU	N1-C2-N3	4.82	120.26	115.17
4	L3	1683	PSU	C4-N3-C2	-4.82	119.73	126.37
4	L3	3715	PSU	C4-N3-C2	-4.82	119.73	126.37
4	L3	4500	PSU	N1-C2-N3	4.82	120.25	115.17
4	L3	3639	PSU	C4-N3-C2	-4.82	119.74	126.37
4	L3	4673	PSU	N1-C2-N3	4.81	120.24	115.17
4	L3	4431	PSU	C4-N3-C2	-4.81	119.75	126.37
4	L3	3844	PSU	C4-N3-C2	-4.81	119.75	126.37
4	L3	3920	PSU	C4-N3-C2	-4.80	119.75	126.37
4	L3	3639	PSU	N1-C2-N3	4.80	120.23	115.17
4	L3	4403	PSU	N1-C2-N3	4.80	120.23	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2632	PSU	C4-N3-C2	-4.80	119.76	126.37
4	L3	3884	PSU	N1-C2-N3	4.80	120.23	115.17
4	L3	4576	PSU	N1-C2-N3	4.80	120.23	115.17
4	L3	1536	PSU	C4-N3-C2	-4.80	119.76	126.37
2	L1	69	PSU	C4-N3-C2	-4.80	119.76	126.37
4	L3	3734	PSU	C4-N3-C2	-4.80	119.77	126.37
4	L3	5001	PSU	C4-N3-C2	-4.79	119.77	126.37
4	L3	1860	PSU	C4-N3-C2	-4.79	119.78	126.37
4	L3	4521	PSU	C4-N3-C2	-4.78	119.78	126.37
4	L3	1792	PSU	N1-C2-N3	4.78	120.21	115.17
4	L3	1582	PSU	N1-C2-N3	4.78	120.21	115.17
4	L3	4457	PSU	N1-C2-N3	4.78	120.21	115.17
4	L3	4552	PSU	N1-C2-N3	4.78	120.21	115.17
4	L3	4457	PSU	C4-N3-C2	-4.77	119.80	126.37
4	L3	3695	PSU	N1-C2-N3	4.77	120.20	115.17
4	L3	3730	PSU	C4-N3-C2	-4.77	119.81	126.37
4	L3	5010	PSU	C4-N3-C2	-4.77	119.81	126.37
4	L3	3822	PSU	N1-C2-N3	4.77	120.19	115.17
4	L3	3715	PSU	N1-C2-N3	4.76	120.19	115.17
4	L3	3851	PSU	N1-C2-N3	4.76	120.19	115.17
4	L3	3730	PSU	N1-C2-N3	4.76	120.19	115.17
4	L3	2839	PSU	C4-N3-C2	-4.76	119.81	126.37
4	L3	2839	PSU	N1-C2-N3	4.76	120.19	115.17
4	L3	1792	PSU	C4-N3-C2	-4.76	119.82	126.37
4	L3	3822	PSU	C4-N3-C2	-4.75	119.83	126.37
4	L3	4521	PSU	N1-C2-N3	4.75	120.18	115.17
4	L3	4576	PSU	C4-N3-C2	-4.75	119.83	126.37
2	L1	55	PSU	N1-C2-N3	4.75	120.18	115.17
4	L3	4972	PSU	C4-N3-C2	-4.75	119.83	126.37
4	L3	1536	PSU	N1-C2-N3	4.74	120.17	115.17
4	L3	4471	PSU	C4-N3-C2	-4.73	119.85	126.37
4	L3	4972	PSU	N1-C2-N3	4.72	120.14	115.17
4	L3	1677	PSU	N1-C2-N3	4.71	120.14	115.17
4	L3	4431	PSU	N1-C2-N3	4.71	120.13	115.17
4	L3	3884	PSU	C4-N3-C2	-4.70	119.89	126.37
4	L3	4628	PSU	N1-C2-N3	4.70	120.13	115.17
4	L3	2363	A2M	N3-C4-N9	4.69	135.15	127.17
4	L3	2508	PSU	N1-C2-N3	4.69	120.11	115.17
4	L3	4579	PSU	C4-N3-C2	-4.69	119.91	126.37
4	L3	4579	PSU	N1-C2-N3	4.69	120.11	115.17
4	L3	5010	PSU	N1-C2-N3	4.69	120.11	115.17
4	L3	3825	A2M	N3-C4-N9	4.68	135.13	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4220	6MZ	N3-C4-N9	4.67	135.12	127.17
4	L3	4628	PSU	C4-N3-C2	-4.67	119.94	126.37
4	L3	3920	PSU	N1-C2-N3	4.67	120.09	115.17
2	L1	69	PSU	N1-C2-N3	4.66	120.08	115.17
4	L3	3853	PSU	N1-C2-N3	4.65	120.07	115.17
4	L3	1683	PSU	N1-C2-N3	4.64	120.06	115.17
4	L3	3853	PSU	C4-N3-C2	-4.64	119.98	126.37
4	L3	1534	A2M	N3-C4-N9	4.63	135.04	127.17
4	L3	2632	PSU	N1-C2-N3	4.60	120.02	115.17
4	L3	4571	A2M	N3-C4-N9	4.60	134.98	127.17
4	L3	4293	PSU	N1-C2-N3	4.59	120.00	115.17
4	L3	3867	A2M	N3-C4-N9	4.58	134.95	127.17
4	L3	4523	A2M	N3-C4-N9	4.57	134.93	127.17
4	L3	4620	OMU	C4-N3-C2	-4.56	120.95	126.61
4	L3	2815	A2M	N3-C4-N9	4.56	134.93	127.17
4	L3	2401	A2M	N3-C4-N9	4.56	134.92	127.17
4	L3	3830	A2M	N3-C4-N9	4.55	134.91	127.17
4	L3	2787	A2M	N3-C4-N9	4.55	134.91	127.17
4	L3	398	A2M	N3-C4-N9	4.54	134.88	127.17
4	L3	400	A2M	N3-C4-N9	4.53	134.87	127.17
4	L3	1524	A2M	N3-C4-N9	4.52	134.85	127.17
4	L3	1326	A2M	N3-C4-N9	4.51	134.84	127.17
4	L3	3724	A2M	N3-C4-N9	4.49	134.80	127.17
4	L3	3718	A2M	N3-C4-N9	4.44	134.72	127.17
4	L3	4293	PSU	C4-N3-C2	-4.43	120.26	126.37
4	L3	1871	A2M	N3-C4-N9	4.42	134.69	127.17
4	L3	4590	A2M	N3-C2-N1	-4.33	122.03	128.58
4	L3	4306	OMU	N3-C2-N1	4.23	120.39	114.89
4	L3	2415	OMU	N3-C2-N1	4.20	120.36	114.89
4	L3	1871	A2M	N3-C2-N1	-4.16	122.28	128.58
4	L3	3724	A2M	N3-C2-N1	-4.15	122.30	128.58
4	L3	4523	A2M	N3-C2-N1	-4.13	122.33	128.58
4	L3	400	A2M	N3-C2-N1	-4.12	122.34	128.58
4	L3	3830	A2M	N3-C2-N1	-4.12	122.34	128.58
4	L3	2363	A2M	N3-C2-N1	-4.12	122.35	128.58
4	L3	1524	A2M	N3-C2-N1	-4.12	122.35	128.58
4	L3	2401	A2M	N3-C2-N1	-4.11	122.37	128.58
4	L3	3925	OMU	N3-C2-N1	4.10	120.23	114.89
4	L3	3825	A2M	N3-C2-N1	-4.10	122.38	128.58
4	L3	3867	A2M	N3-C2-N1	-4.10	122.38	128.58
4	L3	398	A2M	N3-C2-N1	-4.09	122.39	128.58
4	L3	2837	OMU	N3-C2-N1	4.09	120.21	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2787	A2M	N3-C2-N1	-4.09	122.39	128.58
4	L3	2815	A2M	N3-C2-N1	-4.09	122.40	128.58
4	L3	1534	A2M	N3-C2-N1	-4.07	122.41	128.58
4	L3	4498	OMU	N3-C2-N1	4.07	120.19	114.89
4	L3	1326	A2M	N3-C2-N1	-4.06	122.44	128.58
4	L3	4571	A2M	N3-C2-N1	-4.03	122.49	128.58
4	L3	4220	6MZ	N1-C2-N3	-3.99	122.54	128.58
4	L3	4227	OMU	C5-C4-N3	3.92	120.30	114.80
4	L3	4590	A2M	N3-C4-N9	3.92	133.84	127.17
4	L3	3718	A2M	N3-C2-N1	-3.86	122.74	128.58
4	L3	4590	A2M	C5-N7-C8	3.82	109.46	103.45
4	L3	4220	6MZ	C5-N7-C8	3.82	109.45	103.45
4	L3	4227	OMU	N3-C2-N1	3.80	119.83	114.89
4	L3	2815	A2M	C5-N7-C8	3.79	109.41	103.45
4	L3	3830	A2M	C5-N7-C8	3.79	109.41	103.45
4	L3	3825	A2M	C5-N7-C8	3.79	109.41	103.45
4	L3	3867	A2M	C5-N7-C8	3.78	109.39	103.45
4	L3	2401	A2M	C5-N7-C8	3.77	109.38	103.45
4	L3	1871	A2M	C5-N7-C8	3.76	109.36	103.45
4	L3	398	A2M	C5-N7-C8	3.75	109.35	103.45
4	L3	1326	A2M	C5-N7-C8	3.75	109.34	103.45
4	L3	4523	A2M	C5-N7-C8	3.73	109.31	103.45
4	L3	4306	OMU	C5-C4-N3	3.72	120.01	114.80
4	L3	1524	A2M	C5-N7-C8	3.72	109.30	103.45
4	L3	2787	A2M	C5-N7-C8	3.72	109.29	103.45
4	L3	1534	A2M	C5-N7-C8	3.72	109.29	103.45
4	L3	3925	OMU	C5-C4-N3	3.72	120.00	114.80
4	L3	2837	OMU	C5-C4-N3	3.71	119.99	114.80
4	L3	4571	A2M	C5-N7-C8	3.69	109.26	103.45
4	L3	3825	A2M	C2-N3-C4	3.69	120.85	111.83
4	L3	4498	OMU	C5-C4-N3	3.69	119.97	114.80
4	L3	2815	A2M	C2-N3-C4	3.69	120.84	111.83
4	L3	2363	A2M	C5-N7-C8	3.68	109.24	103.45
4	L3	400	A2M	C5-N7-C8	3.67	109.21	103.45
4	L3	4220	6MZ	C2-N3-C4	3.66	120.77	111.83
4	L3	3718	A2M	C5-N7-C8	3.66	109.20	103.45
4	L3	1524	A2M	C2-N3-C4	3.65	120.75	111.83
4	L3	3724	A2M	C5-N7-C8	3.65	109.19	103.45
4	L3	2401	A2M	C2-N3-C4	3.65	120.75	111.83
4	L3	3867	A2M	C2-N3-C4	3.64	120.72	111.83
4	L3	2363	A2M	C2-N3-C4	3.64	120.71	111.83
4	L3	2415	OMU	C5-C4-N3	3.63	119.89	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2787	A2M	C2-N3-C4	3.62	120.66	111.83
4	L3	4523	A2M	C2-N3-C4	3.61	120.66	111.83
4	L3	1534	A2M	C2-N3-C4	3.61	120.65	111.83
4	L3	3830	A2M	C2-N3-C4	3.61	120.65	111.83
4	L3	1326	A2M	C2-N3-C4	3.61	120.64	111.83
4	L3	398	A2M	C2-N3-C4	3.60	120.63	111.83
4	L3	4571	A2M	C2-N3-C4	3.60	120.61	111.83
4	L3	4620	OMU	N3-C2-N1	3.59	119.57	114.89
4	L3	400	A2M	C2-N3-C4	3.58	120.58	111.83
4	L3	1871	A2M	C2-N3-C4	3.57	120.54	111.83
4	L3	3724	A2M	C2-N3-C4	3.55	120.49	111.83
4	L3	4590	A2M	C2-N3-C4	3.50	120.37	111.83
4	L3	3718	A2M	C2-N3-C4	3.46	120.29	111.83
4	L3	4620	OMU	C5-C4-N3	3.45	119.64	114.80
4	L3	4530	UR3	C5-C4-N3	3.32	119.42	115.04
4	L3	1871	A2M	C2'-C1'-N9	-3.28	108.36	113.75
4	L3	4590	A2M	C4-C5-N7	-3.20	106.92	110.58
4	L3	4227	OMU	O4-C4-C5	-3.18	119.68	125.16
4	L3	2815	A2M	C4-C5-N7	-3.09	107.05	110.58
4	L3	3925	OMU	O4-C4-C5	-3.08	119.84	125.16
4	L3	4220	6MZ	C4-C5-N7	-3.06	107.09	110.58
4	L3	1326	A2M	C4-C5-N7	-3.02	107.13	110.58
4	L3	3830	A2M	C4-C5-N7	-3.00	107.15	110.58
4	L3	1871	A2M	C4-C5-N7	-3.00	107.15	110.58
4	L3	2401	A2M	C4-C5-N7	-3.00	107.16	110.58
4	L3	4571	A2M	C4-C5-N7	-2.98	107.17	110.58
4	L3	2837	OMU	O4-C4-C5	-2.98	120.02	125.16
4	L3	3844	PSU	O2-C2-N1	-2.98	119.72	122.79
4	L3	4457	PSU	O2-C2-N1	-2.98	119.72	122.79
4	L3	1524	A2M	C4-C5-N7	-2.97	107.19	110.58
4	L3	398	A2M	C4-C5-N7	-2.97	107.19	110.58
4	L3	3639	PSU	O2-C2-N1	-2.96	119.73	122.79
4	L3	3825	A2M	C4-C5-N7	-2.96	107.20	110.58
4	L3	4628	PSU	O2-C2-N1	-2.96	119.74	122.79
4	L3	3822	PSU	O2-C2-N1	-2.96	119.74	122.79
4	L3	4500	PSU	O2-C2-N1	-2.96	119.74	122.79
4	L3	3867	A2M	C4-C5-N7	-2.95	107.20	110.58
4	L3	4306	OMU	O4-C4-C5	-2.93	120.10	125.16
4	L3	4361	PSU	O2-C2-N1	-2.93	119.77	122.79
4	L3	4353	PSU	O2-C2-N1	-2.93	119.77	122.79
4	L3	1536	PSU	O2-C2-N1	-2.93	119.77	122.79
4	L3	3730	PSU	O2-C2-N1	-2.93	119.77	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2787	A2M	C4-C5-N7	-2.93	107.24	110.58
4	L3	2839	PSU	O2-C2-N1	-2.92	119.77	122.79
4	L3	3724	A2M	C4-C5-N7	-2.92	107.25	110.58
4	L3	3830	A2M	N9-C8-N7	-2.92	109.80	113.94
4	L3	2415	OMU	O4-C4-C5	-2.91	120.14	125.16
4	L3	400	A2M	C4-C5-N7	-2.91	107.25	110.58
4	L3	4523	A2M	C4-C5-N7	-2.91	107.26	110.58
4	L3	3718	A2M	C4-C5-N7	-2.90	107.26	110.58
4	L3	4296	PSU	O2-C2-N1	-2.90	119.80	122.79
4	L3	1534	A2M	C4-C5-N7	-2.90	107.27	110.58
4	L3	4579	PSU	O2-C2-N1	-2.89	119.81	122.79
4	L3	4620	OMU	O4-C4-C5	-2.88	120.20	125.16
4	L3	2363	A2M	C4-C5-N7	-2.86	107.31	110.58
4	L3	4498	OMU	O4-C4-C5	-2.86	120.24	125.16
4	L3	3734	PSU	O2-C2-N1	-2.85	119.84	122.79
4	L3	3715	PSU	O2-C2-N1	-2.85	119.85	122.79
4	L3	4299	PSU	O2-C2-N1	-2.85	119.85	122.79
4	L3	1871	A2M	N9-C8-N7	-2.83	109.92	113.94
2	L1	55	PSU	O2-C2-N1	-2.83	119.87	122.79
4	L3	3867	A2M	N9-C8-N7	-2.82	109.94	113.94
4	L3	4636	PSU	O2-C2-N1	-2.82	119.88	122.79
4	L3	4590	A2M	N9-C8-N7	-2.81	109.94	113.94
4	L3	4431	PSU	O2-C2-N1	-2.81	119.89	122.79
4	L3	5001	PSU	O2-C2-N1	-2.81	119.89	122.79
4	L3	1677	PSU	O2-C2-N1	-2.80	119.90	122.79
4	L3	1683	PSU	O2-C2-N1	-2.80	119.90	122.79
4	L3	1862	PSU	O2-C2-N1	-2.79	119.91	122.79
4	L3	3637	PSU	C6-C5-C4	2.79	120.05	118.17
4	L3	3920	PSU	O2-C2-N1	-2.78	119.92	122.79
4	L3	3825	A2M	N9-C8-N7	-2.78	109.99	113.94
4	L3	3884	PSU	C6-N1-C2	-2.78	120.11	122.69
4	L3	1582	PSU	O2-C2-N1	-2.78	119.92	122.79
4	L3	3853	PSU	O2-C2-N1	-2.78	119.92	122.79
4	L3	4576	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L3	3884	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L3	4312	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L3	1860	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L3	2401	A2M	N9-C8-N7	-2.77	110.01	113.94
4	L3	4552	PSU	O2-C2-N1	-2.76	119.94	122.79
4	L3	4532	PSU	O2-C2-N1	-2.75	119.95	122.79
4	L3	5010	PSU	O2-C2-N1	-2.75	119.95	122.79
4	L3	4523	A2M	N9-C8-N7	-2.75	110.03	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4972	PSU	O2-C2-N1	-2.75	119.95	122.79
4	L3	3718	A2M	C2'-C1'-N9	-2.75	109.23	113.75
4	L3	1524	A2M	N9-C8-N7	-2.75	110.04	113.94
4	L3	4579	PSU	C6-N1-C2	-2.75	120.14	122.69
4	L3	4471	PSU	O2-C2-N1	-2.74	119.96	122.79
4	L3	398	A2M	N9-C8-N7	-2.72	110.07	113.94
4	L3	1326	A2M	N9-C8-N7	-2.72	110.07	113.94
4	L3	4403	PSU	O2-C2-N1	-2.72	119.99	122.79
4	L3	4493	PSU	O2-C2-N1	-2.71	119.99	122.79
4	L3	3851	PSU	O2-C2-N1	-2.71	119.99	122.79
4	L3	2815	A2M	N9-C8-N7	-2.71	110.09	113.94
4	L3	1534	A2M	N9-C8-N7	-2.68	110.13	113.94
2	L1	69	PSU	O2-C2-N1	-2.68	120.02	122.79
4	L3	2401	A2M	C2'-C1'-N9	-2.68	109.34	113.75
4	L3	3695	PSU	O2-C2-N1	-2.67	120.03	122.79
4	L3	3718	A2M	N9-C8-N7	-2.67	110.14	113.94
4	L3	3724	A2M	N9-C8-N7	-2.66	110.16	113.94
4	L3	4521	PSU	O2-C2-N1	-2.65	120.06	122.79
4	L3	4293	PSU	C6-N1-C2	-2.64	120.24	122.69
4	L3	1792	PSU	O2-C2-N1	-2.64	120.06	122.79
4	L3	5001	PSU	C6-N1-C2	-2.63	120.25	122.69
4	L3	4220	6MZ	C9-N6-C6	-2.63	120.42	122.85
4	L3	398	A2M	C2'-C1'-N9	-2.62	109.44	113.75
4	L3	400	A2M	N9-C8-N7	-2.60	110.24	113.94
4	L3	2508	PSU	O2-C2-N1	-2.60	120.11	122.79
4	L3	4628	PSU	C6-N1-C2	-2.60	120.28	122.69
4	L3	2787	A2M	N9-C8-N7	-2.60	110.25	113.94
4	L3	3822	PSU	C6-C5-C4	2.59	119.92	118.17
4	L3	4571	A2M	N9-C8-N7	-2.59	110.27	113.94
4	L3	4689	PSU	O2-C2-N1	-2.58	120.12	122.79
4	L3	4689	PSU	C6-N1-C2	-2.58	120.30	122.69
4	L3	4576	PSU	C6-N1-C2	-2.58	120.30	122.69
4	L3	2839	PSU	C6-N1-C2	-2.58	120.30	122.69
4	L3	4636	PSU	C6-C5-C4	2.57	119.91	118.17
4	L3	4353	PSU	C6-N1-C2	-2.56	120.31	122.69
4	L3	2363	A2M	N9-C8-N7	-2.56	110.30	113.94
4	L3	4220	6MZ	N9-C8-N7	-2.56	110.30	113.94
4	L3	3844	PSU	C6-N1-C2	-2.54	120.33	122.69
4	L3	4312	PSU	C6-N1-C2	-2.54	120.33	122.69
4	L3	4673	PSU	O2-C2-N1	-2.54	120.17	122.79
4	L3	4457	PSU	C6-N1-C2	-2.53	120.34	122.69
4	L3	3730	PSU	C6-N1-C2	-2.53	120.34	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	3734	PSU	C6-N1-C2	-2.52	120.35	122.69
4	L3	4293	PSU	O2-C2-N1	-2.51	120.20	122.79
4	L3	1860	PSU	C6-N1-C2	-2.51	120.37	122.69
4	L3	4532	PSU	C6-C5-C4	2.50	119.86	118.17
4	L3	4471	PSU	C6-N1-C2	-2.49	120.38	122.69
4	L3	3853	PSU	C6-N1-C2	-2.48	120.39	122.69
4	L3	3695	PSU	C6-C5-C4	2.48	119.85	118.17
4	L3	3637	PSU	O2-C2-N1	-2.48	120.23	122.79
4	L3	1536	PSU	C6-N1-C2	-2.47	120.40	122.69
4	L3	3844	PSU	C6-C5-C4	2.47	119.84	118.17
4	L3	3639	PSU	C6-N1-C2	-2.47	120.40	122.69
4	L3	4500	PSU	C6-N1-C2	-2.46	120.41	122.69
4	L3	4673	PSU	C6-N1-C2	-2.46	120.41	122.69
4	L3	2632	PSU	O2-C2-N1	-2.45	120.26	122.79
4	L3	4972	PSU	C6-N1-C2	-2.45	120.42	122.69
4	L3	1862	PSU	C6-N1-C2	-2.42	120.44	122.69
4	L3	4521	PSU	C6-N1-C2	-2.42	120.44	122.69
4	L3	4299	PSU	C6-N1-C2	-2.42	120.45	122.69
4	L3	4299	PSU	C6-C5-C4	2.41	119.80	118.17
4	L3	4361	PSU	C6-N1-C2	-2.41	120.46	122.69
4	L3	4552	PSU	C6-N1-C2	-2.40	120.46	122.69
4	L3	5010	PSU	C6-N1-C2	-2.40	120.47	122.69
4	L3	1677	PSU	C6-N1-C2	-2.39	120.47	122.69
4	L3	3822	PSU	C6-N1-C2	-2.39	120.47	122.69
4	L3	3715	PSU	C6-N1-C2	-2.38	120.48	122.69
4	L3	3920	PSU	C6-N1-C2	-2.38	120.49	122.69
4	L3	4493	PSU	C6-N1-C2	-2.38	120.49	122.69
2	L1	69	PSU	O4'-C1'-C2'	2.37	108.42	105.15
4	L3	3734	PSU	C6-C5-C4	2.36	119.77	118.17
4	L3	4431	PSU	C6-C5-C4	2.36	119.77	118.17
2	L1	55	PSU	C6-N1-C2	-2.36	120.50	122.69
4	L3	4403	PSU	C6-N1-C2	-2.35	120.51	122.69
4	L3	4403	PSU	C6-C5-C4	2.35	119.76	118.17
2	L1	55	PSU	C6-C5-C4	2.34	119.76	118.17
2	L1	69	PSU	C6-N1-C2	-2.34	120.52	122.69
4	L3	1524	A2M	C2'-C1'-N9	-2.34	109.90	113.75
4	L3	3637	PSU	C6-N1-C2	-2.34	120.52	122.69
4	L3	3639	PSU	C6-C5-C4	2.34	119.75	118.17
4	L3	3851	PSU	C6-N1-C2	-2.32	120.54	122.69
4	L3	4532	PSU	C6-N1-C2	-2.32	120.54	122.69
4	L3	4296	PSU	C6-C5-C4	2.31	119.73	118.17
4	L3	4296	PSU	C6-N1-C2	-2.31	120.55	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	3695	PSU	C6-N1-C2	-2.31	120.55	122.69
4	L3	4431	PSU	C6-N1-C2	-2.30	120.56	122.69
4	L3	1862	PSU	C6-C5-C4	2.29	119.72	118.17
4	L3	1792	PSU	C6-N1-C2	-2.29	120.57	122.69
4	L3	2415	OMU	O2-C2-N1	-2.29	119.82	122.80
4	L3	3925	OMU	O2-C2-N1	-2.28	119.82	122.80
4	L3	4673	PSU	C6-C5-C4	2.28	119.72	118.17
4	L3	1322	1MA	N1-C6-N6	2.26	125.38	119.71
4	L3	1792	PSU	C6-C5-C4	2.26	119.70	118.17
4	L3	1683	PSU	C6-C5-C4	2.25	119.69	118.17
4	L3	3851	PSU	O4'-C1'-C2'	2.23	108.23	105.15
4	L3	4523	A2M	C2'-C1'-N9	-2.23	110.08	113.75
4	L3	2508	PSU	C6-N1-C2	-2.23	120.62	122.69
4	L3	4471	PSU	C6-C5-C4	2.23	119.68	118.17
4	L3	2815	A2M	C2'-C1'-N9	-2.22	110.09	113.75
4	L3	3920	PSU	C6-C5-C4	2.22	119.67	118.17
4	L3	3730	PSU	C6-C5-C4	2.22	119.67	118.17
4	L3	4636	PSU	C6-N1-C2	-2.21	120.64	122.69
4	L3	4493	PSU	C6-C5-C4	2.21	119.67	118.17
4	L3	1860	PSU	C6-C5-C4	2.21	119.66	118.17
4	L3	2351	OMC	C1'-N1-C2	2.20	123.31	118.44
4	L3	1582	PSU	C6-C5-C4	2.20	119.66	118.17
4	L3	2632	PSU	C6-N1-C2	-2.20	120.65	122.69
4	L3	3851	PSU	C6-C5-C4	2.19	119.65	118.17
4	L3	3867	A2M	C2'-C1'-N9	-2.18	110.17	113.75
4	L3	4498	OMU	O2-C2-N1	-2.17	119.97	122.80
4	L3	4576	PSU	C6-C5-C4	2.17	119.64	118.17
4	L3	4689	PSU	C6-C5-C4	2.16	119.63	118.17
4	L3	1582	PSU	C6-N1-C2	-2.16	120.69	122.69
4	L3	1677	PSU	C6-C5-C4	2.15	119.62	118.17
4	L3	3715	PSU	O4'-C1'-C2'	2.14	108.11	105.15
4	L3	4552	PSU	C6-C5-C4	2.13	119.61	118.17
4	L3	5001	PSU	C6-C5-C4	2.13	119.61	118.17
4	L3	2837	OMU	O2-C2-N1	-2.13	120.03	122.80
4	L3	1683	PSU	C6-N1-C2	-2.13	120.72	122.69
4	L3	4361	PSU	C6-C5-C4	2.12	119.61	118.17
4	L3	4312	PSU	C6-C5-C4	2.12	119.60	118.17
4	L3	4353	PSU	C6-C5-C4	2.12	119.60	118.17
4	L3	4403	PSU	O4'-C1'-C2'	2.11	108.07	105.15
4	L3	2508	PSU	C6-C5-C4	2.11	119.59	118.17
4	L3	4353	PSU	O4'-C1'-C2'	2.10	108.06	105.15
4	L3	4590	A2M	C2-N1-C6	2.10	122.18	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	1534	A2M	O4'-C1'-C2'	-2.10	102.98	106.59
4	L3	4521	PSU	C6-C5-C4	2.09	119.58	118.17
4	L3	4576	PSU	O4'-C1'-C2'	2.07	108.01	105.15
4	L3	4628	PSU	C6-C5-C4	2.06	119.56	118.17
4	L3	4628	PSU	O4'-C1'-C2'	2.05	107.99	105.15
4	L3	3830	A2M	C2'-C1'-N9	-2.04	110.39	113.75
4	L3	3734	PSU	O4'-C1'-C2'	2.04	107.97	105.15
4	L3	1534	A2M	C3'-C2'-C1'	-2.03	98.92	102.81
4	L3	3715	PSU	C6-C5-C4	2.02	119.54	118.17
4	L3	4972	PSU	C6-C5-C4	2.02	119.54	118.17
4	L3	5010	PSU	C6-C5-C4	2.02	119.54	118.17
4	L3	4636	PSU	O4'-C1'-C2'	2.02	107.94	105.15
4	L3	4220	6MZ	C4-C5-C6	2.01	118.45	116.78
24	LN	245	HIC	NE2-CE1-ND1	-2.01	111.89	112.66

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	75	OMG	C1'-C2'-O2'-CM2
4	L3	398	A2M	C1'-C2'-O2'-CM'
4	L3	400	A2M	C1'-C2'-O2'-CM'
4	L3	1316	OMG	C1'-C2'-O2'-CM2
4	L3	1326	A2M	O4'-C4'-C5'-O5'
4	L3	1340	OMC	C1'-C2'-O2'-CM2
4	L3	2363	A2M	C1'-C2'-O2'-CM'
4	L3	2364	OMG	C1'-C2'-O2'-CM2
4	L3	2415	OMU	C1'-C2'-O2'-CM2
4	L3	2422	OMC	C1'-C2'-O2'-CM2
4	L3	2787	A2M	O4'-C4'-C5'-O5'
4	L3	2787	A2M	C3'-C4'-C5'-O5'
4	L3	2804	OMC	C1'-C2'-O2'-CM2
4	L3	2815	A2M	C1'-C2'-O2'-CM'
4	L3	2837	OMU	C1'-C2'-O2'-CM2
4	L3	2861	OMC	C1'-C2'-O2'-CM2
4	L3	3627	OMG	C1'-C2'-O2'-CM2
4	L3	3701	OMC	C2'-C1'-N1-C6
4	L3	3718	A2M	C1'-C2'-O2'-CM'
4	L3	3724	A2M	C1'-C2'-O2'-CM'
4	L3	3744	OMG	C1'-C2'-O2'-CM2
4	L3	3825	A2M	C1'-C2'-O2'-CM'
4	L3	3830	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
4	L3	3841	OMC	C1'-C2'-O2'-CM2
4	L3	3867	A2M	C1'-C2'-O2'-CM'
4	L3	3887	OMC	O4'-C4'-C5'-O5'
4	L3	3899	OMG	C1'-C2'-O2'-CM2
4	L3	3925	OMU	C1'-C2'-O2'-CM2
4	L3	4392	OMG	C1'-C2'-O2'-CM2
4	L3	4456	OMC	C1'-C2'-O2'-CM2
4	L3	4498	OMU	C1'-C2'-O2'-CM2
4	L3	4571	A2M	C1'-C2'-O2'-CM'
4	L3	4590	A2M	C3'-C4'-C5'-O5'
4	L3	4590	A2M	C1'-C2'-O2'-CM'
4	L3	4618	OMG	C1'-C2'-O2'-CM2
4	L3	4623	OMG	C1'-C2'-O2'-CM2
4	L3	4637	OMG	O4'-C4'-C5'-O5'
4	L3	4637	OMG	C1'-C2'-O2'-CM2
40	NR	127	PTR	O-C-CA-CB
4	L3	3701	OMC	C2'-C1'-N1-C2
4	L3	1326	A2M	C3'-C4'-C5'-O5'
4	L3	1677	PSU	C3'-C4'-C5'-O5'
4	L3	2401	A2M	O4'-C4'-C5'-O5'
4	L3	2401	A2M	C3'-C4'-C5'-O5'
4	L3	3887	OMC	C3'-C4'-C5'-O5'
4	L3	4220	6MZ	O4'-C4'-C5'-O5'
4	L3	4523	A2M	O4'-C4'-C5'-O5'
4	L3	4618	OMG	O4'-C4'-C5'-O5'
4	L3	1677	PSU	O4'-C4'-C5'-O5'
4	L3	4306	OMU	C3'-C4'-C5'-O5'
4	L3	4306	OMU	O4'-C4'-C5'-O5'
4	L3	4523	A2M	C3'-C4'-C5'-O5'
4	L3	4590	A2M	O4'-C4'-C5'-O5'
4	L3	4637	OMG	C3'-C4'-C5'-O5'
4	L3	3701	OMC	O4'-C4'-C5'-O5'
4	L3	4220	6MZ	C3'-C4'-C5'-O5'
4	L3	4618	OMG	C3'-C4'-C5'-O5'
4	L3	1625	OMG	C3'-C4'-C5'-O5'
4	L3	3701	OMC	C3'-C4'-C5'-O5'
4	L3	4590	A2M	C4'-C5'-O5'-P
24	LN	245	HIC	CA-CB-CG-ND1
4	L3	2787	A2M	C2'-C1'-N9-C8
4	L3	1534	A2M	C3'-C2'-O2'-CM'
24	LN	245	HIC	C-CA-CB-CG
4	L3	2351	OMC	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
4	L3	2364	OMG	C3'-C2'-O2'-CM2
4	L3	4306	OMU	C4'-C5'-O5'-P
4	L3	1536	PSU	O4'-C1'-C5-C4
4	L3	2839	PSU	O4'-C1'-C5-C4
4	L3	4457	PSU	O4'-C1'-C5-C4
4	L3	4636	PSU	O4'-C1'-C5-C4
4	L3	2787	A2M	C2'-C1'-N9-C4
4	L3	3701	OMC	O4'-C1'-N1-C6
4	L3	4220	6MZ	C4'-C5'-O5'-P
4	L3	1534	A2M	O4'-C4'-C5'-O5'
24	LN	245	HIC	CA-CB-CG-CD2
4	L3	1524	A2M	O4'-C1'-N9-C8
4	L3	3701	OMC	O4'-C1'-N1-C2
4	L3	1524	A2M	O4'-C1'-N9-C4
4	L3	3844	PSU	C4'-C5'-O5'-P
4	L3	4636	PSU	C4'-C5'-O5'-P
4	L3	2424	OMG	C1'-C2'-O2'-CM2
4	L3	1536	PSU	O4'-C1'-C5-C6
4	L3	1677	PSU	O4'-C1'-C5-C6
4	L3	2787	A2M	O4'-C1'-N9-C8
4	L3	1524	A2M	C3'-C2'-O2'-CM'
4	L3	1326	A2M	C4'-C5'-O5'-P
4	L3	2422	OMC	O4'-C4'-C5'-O5'
4	L3	2351	OMC	C2'-C1'-N1-C6
40	NR	127	PTR	CZ-OH-P-O1P
4	L3	1677	PSU	C2'-C1'-C5-C6
4	L3	4636	PSU	O4'-C4'-C5'-O5'
2	L1	75	OMG	C4'-C5'-O5'-P
4	L3	2876	OMG	C3'-C2'-O2'-CM2
4	L3	1625	OMG	O4'-C4'-C5'-O5'
4	L3	1871	A2M	C3'-C4'-C5'-O5'
4	L3	2351	OMC	C2'-C1'-N1-C2
4	L3	4306	OMU	C2'-C1'-N1-C2
4	L3	4498	OMU	C4'-C5'-O5'-P

There are no ring outliers.

67 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	3853	PSU	1	0
4	L3	3925	OMU	1	0
4	L3	4306	OMU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	4299	PSU	1	0
4	L3	3734	PSU	1	0
4	L3	4579	PSU	1	0
4	L3	400	A2M	3	0
4	L3	4312	PSU	1	0
4	L3	4494	OMG	2	0
4	L3	4590	A2M	1	0
4	L3	2632	PSU	1	0
4	L3	4498	OMU	1	0
4	L3	5010	PSU	1	0
4	L3	1524	A2M	1	0
4	L3	2363	A2M	3	0
4	L3	2861	OMC	1	0
4	L3	4571	A2M	2	0
4	L3	1340	OMC	1	0
4	L3	4220	6MZ	1	0
4	L3	398	A2M	1	0
4	L3	3637	PSU	1	0
4	L3	2365	OMC	1	0
4	L3	3841	OMC	1	0
4	L3	3730	PSU	1	0
4	L3	4228	OMG	1	0
4	L3	4536	OMC	1	0
4	L3	2837	OMU	1	0
4	L3	2351	OMC	3	0
4	L3	3715	PSU	1	0
4	L3	3724	A2M	2	0
4	L3	3627	OMG	1	0
4	L3	4636	PSU	1	0
4	L3	2839	PSU	1	0
4	L3	1522	OMG	1	0
4	L3	4392	OMG	1	0
4	L3	5001	PSU	1	0
4	L3	4637	OMG	2	0
4	L3	4530	UR3	2	0
4	L3	2422	OMC	2	0
4	L3	4456	OMC	2	0
4	L3	4618	OMG	1	0
4	L3	4457	PSU	2	0
4	L3	2824	OMC	1	0
4	L3	4493	PSU	1	0
4	L3	1683	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	3899	OMG	1	0
4	L3	2364	OMG	2	0
2	L1	69	PSU	2	0
4	L3	4353	PSU	1	0
4	L3	4620	OMU	4	0
4	L3	1322	1MA	2	0
4	L3	2787	A2M	1	0
4	L3	3744	OMG	1	0
4	L3	4500	PSU	1	0
4	L3	3718	A2M	4	0
4	L3	1677	PSU	1	0
4	L3	2815	A2M	3	0
4	L3	2415	OMU	5	0
4	L3	2804	OMC	1	0
4	L3	3887	OMC	1	0
4	L3	3830	A2M	1	0
4	L3	3869	OMC	1	0
4	L3	1871	A2M	1	0
4	L3	2876	OMG	2	0
4	L3	4623	OMG	1	0
4	L3	4296	PSU	1	0
2	L1	75	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 95 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	GDP	SR	1001	57,60	29,30,30	3.03	12 (41%)	45,47,47	2.70	17 (37%)

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
59	GDP	SR	1001	57,60	-	0/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	SR	1001	GDP	O6-C6	8.78	1.40	1.23
59	SR	1001	GDP	C5-N7	6.53	1.52	1.39
59	SR	1001	GDP	PA-O3A	5.18	1.65	1.59
59	SR	1001	GDP	C2-N2	4.83	1.45	1.34
59	SR	1001	GDP	C8-N9	-3.99	1.28	1.37
59	SR	1001	GDP	C4-N9	-3.84	1.28	1.38
59	SR	1001	GDP	C5-C4	3.78	1.49	1.38
59	SR	1001	GDP	C4-N3	2.82	1.40	1.34
59	SR	1001	GDP	PB-O2B	-2.29	1.46	1.54
59	SR	1001	GDP	O4'-C1'	2.28	1.47	1.42
59	SR	1001	GDP	PB-O3B	-2.28	1.46	1.54
59	SR	1001	GDP	C2'-C3'	-2.04	1.47	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	SR	1001	GDP	C8-N9-C4	7.85	120.73	106.03
59	SR	1001	GDP	C5-C4-N3	-6.75	117.65	128.39
59	SR	1001	GDP	N9-C4-N3	6.74	139.43	125.95
59	SR	1001	GDP	C2-N3-C4	5.37	121.54	112.30
59	SR	1001	GDP	C6-C5-N7	4.76	138.95	130.29
59	SR	1001	GDP	C4-C5-N7	-4.63	103.33	110.67
59	SR	1001	GDP	C3'-C2'-C1'	3.22	107.55	101.46
59	SR	1001	GDP	N9-C8-N7	-3.09	107.67	113.40
59	SR	1001	GDP	C2-N1-C6	-3.00	119.67	125.11
59	SR	1001	GDP	O2B-PB-O3A	2.95	114.53	104.64
59	SR	1001	GDP	O3B-PB-O3A	2.81	114.06	104.64
59	SR	1001	GDP	C2'-C3'-C4'	2.65	107.74	102.61
59	SR	1001	GDP	C5-C6-N1	2.60	119.87	113.25
59	SR	1001	GDP	C1'-N9-C4	-2.59	118.83	126.49
59	SR	1001	GDP	O6-C6-C5	-2.46	120.05	126.53
59	SR	1001	GDP	O2A-PA-O1A	-2.42	101.19	112.44
59	SR	1001	GDP	C1'-N9-C8	-2.23	120.41	126.73

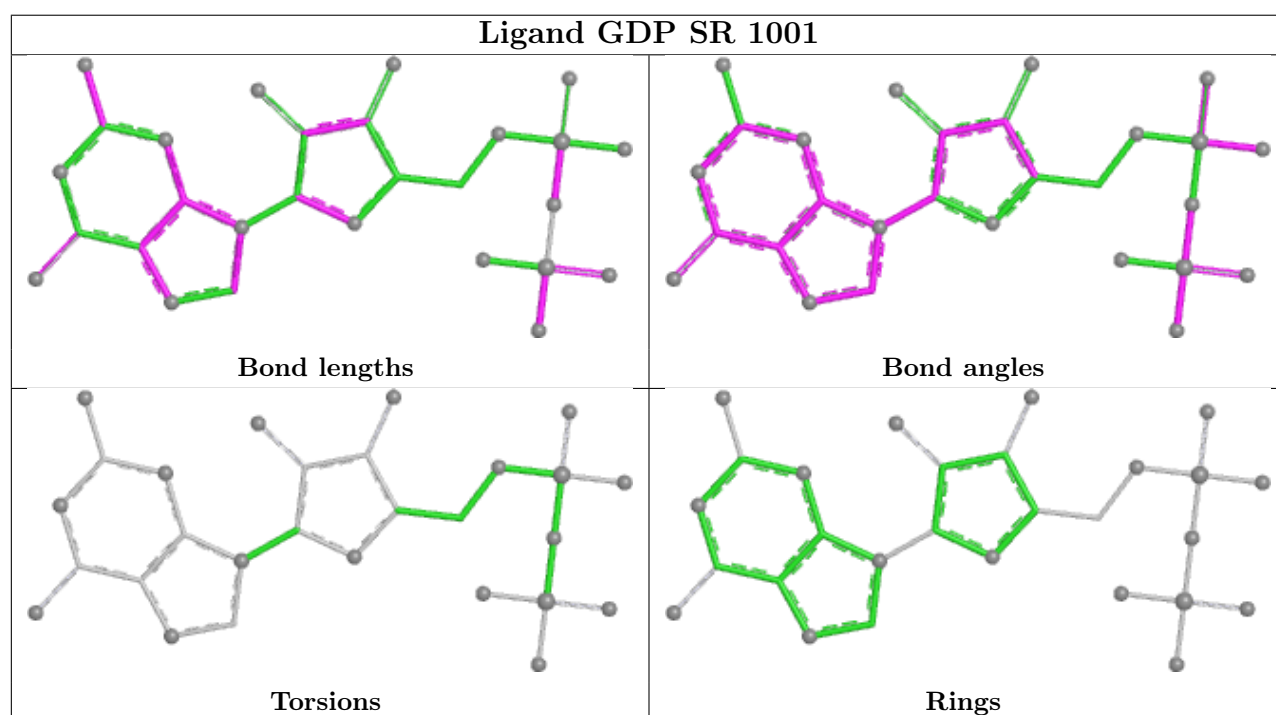
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

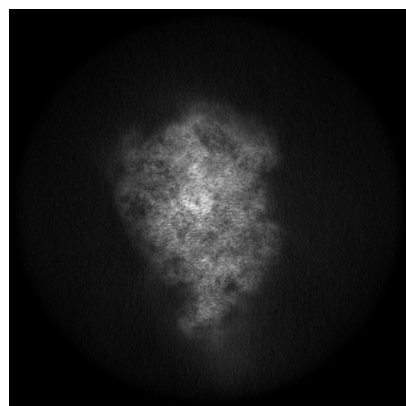
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29272. These allow visual inspection of the internal detail of the map and identification of artifacts.

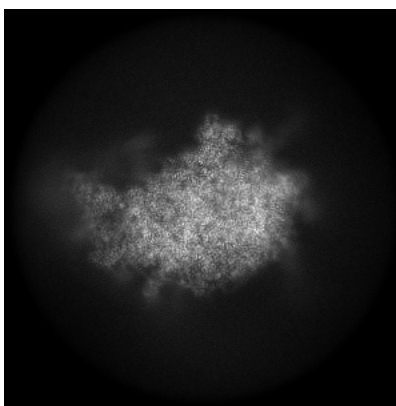
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

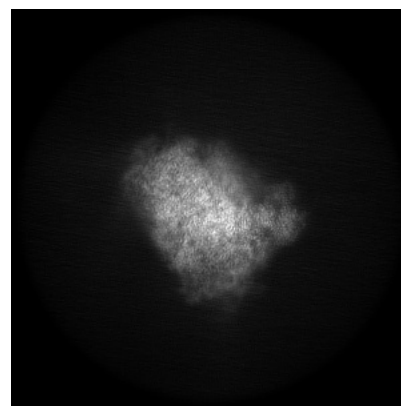
6.1.1 Primary map



X

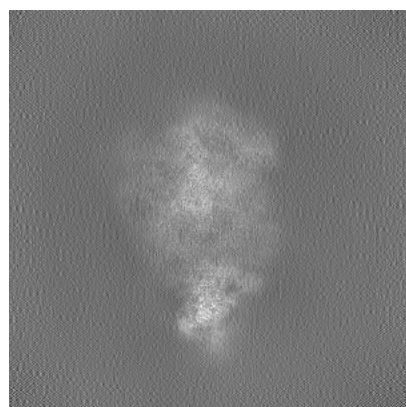


Y

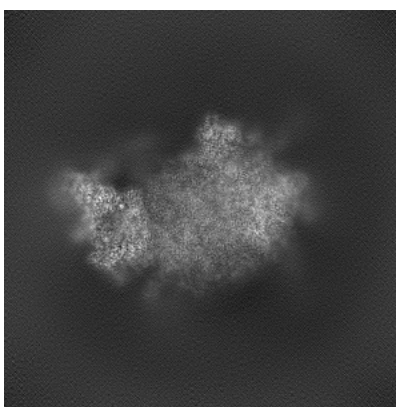


Z

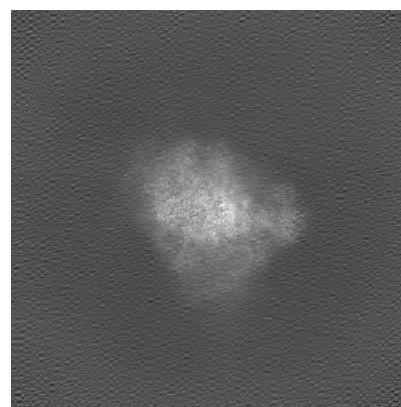
6.1.2 Raw map



X



Y

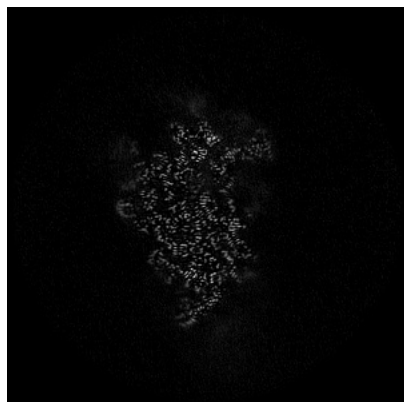


Z

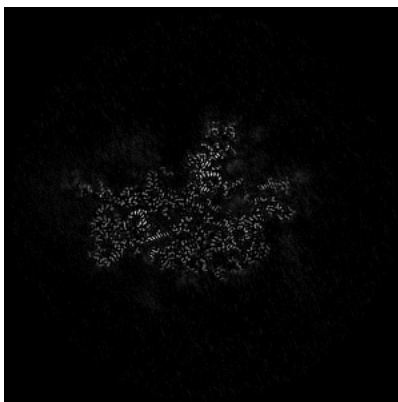
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

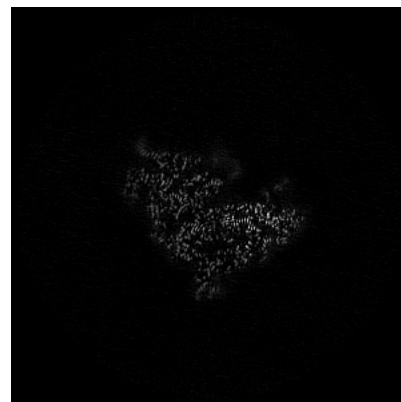
6.2.1 Primary map



X Index: 240

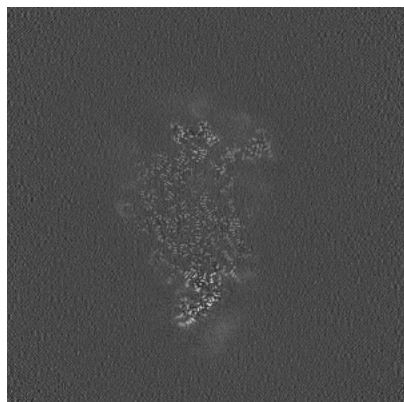


Y Index: 240

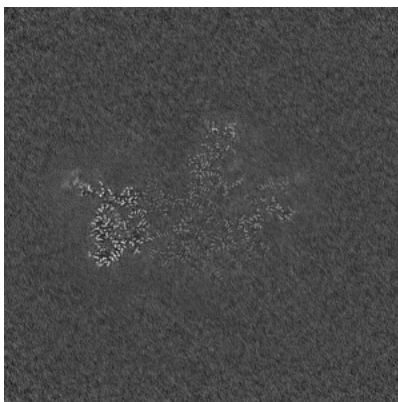


Z Index: 240

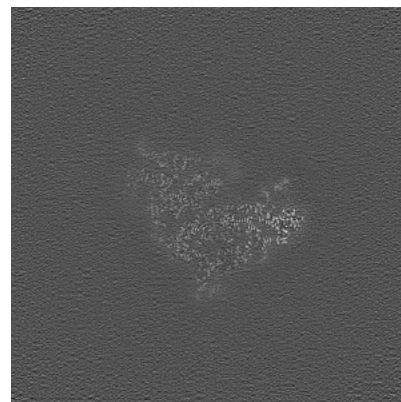
6.2.2 Raw map



X Index: 240



Y Index: 240

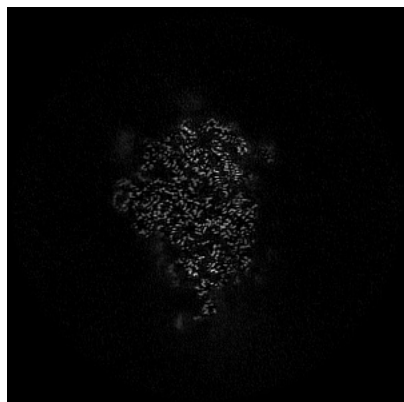


Z Index: 240

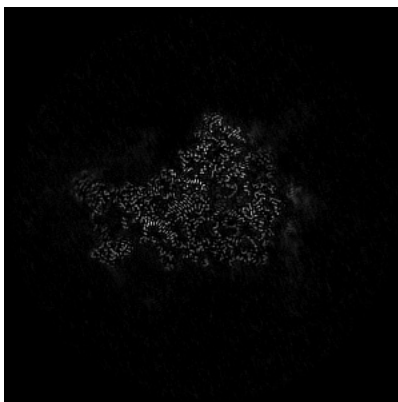
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

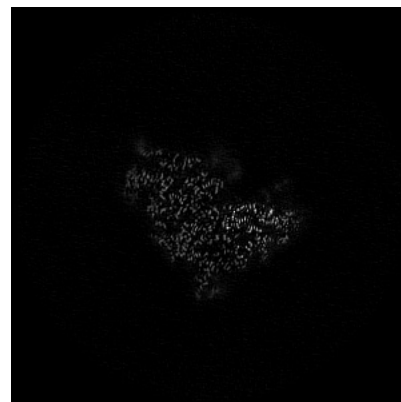
6.3.1 Primary map



X Index: 226

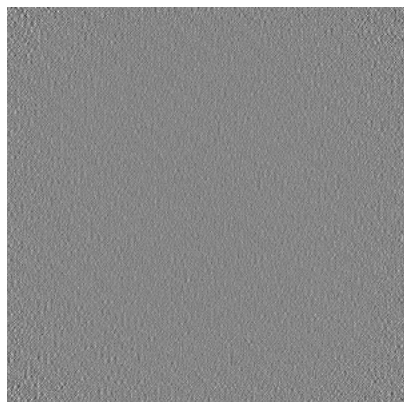


Y Index: 227

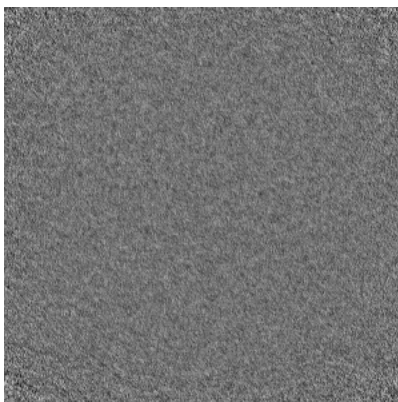


Z Index: 239

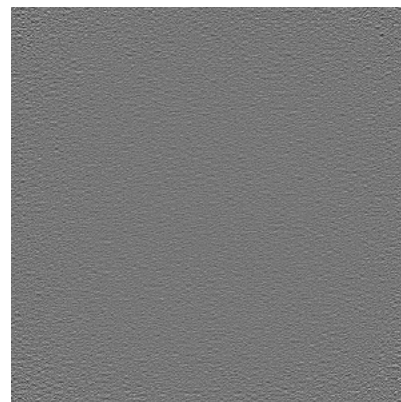
6.3.2 Raw map



X Index: 0



Y Index: 0

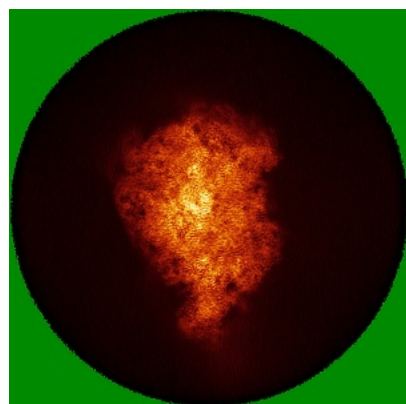


Z Index: 0

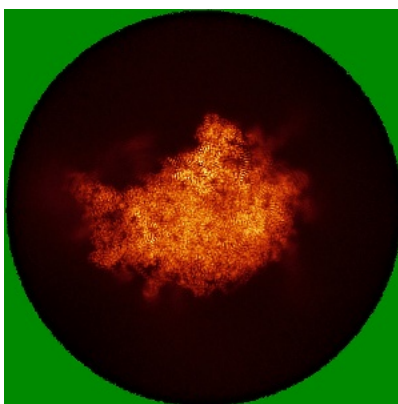
The images above show the largest variance slices of the map in three orthogonal directions.

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

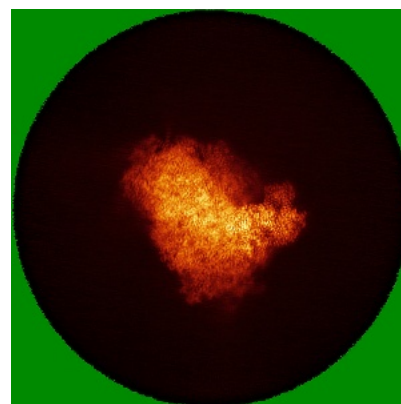
6.4.1 Primary map



X

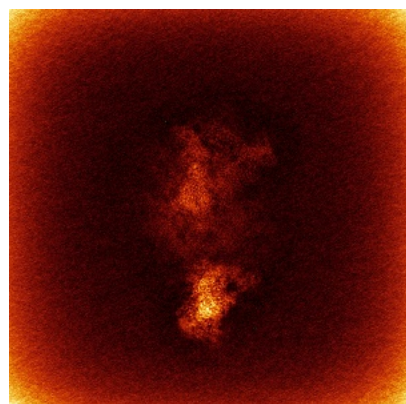


Y

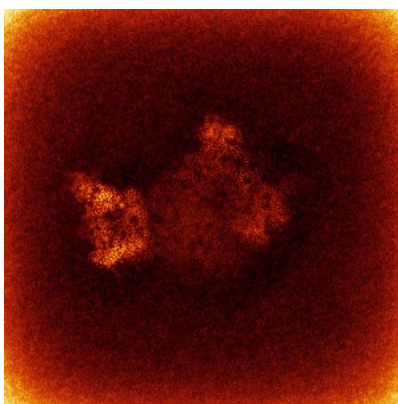


Z

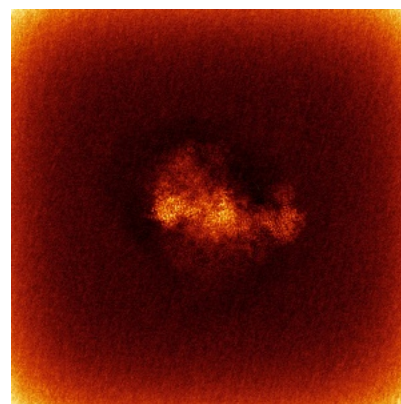
6.4.2 Raw map



X



Y



Z

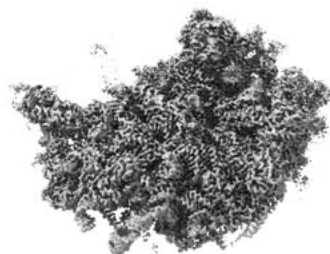
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



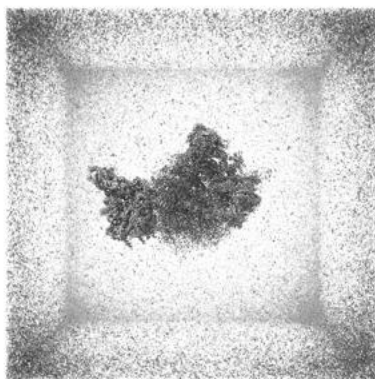
Z

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.

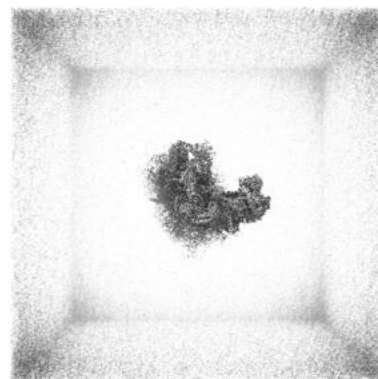
6.5.2 Raw map



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.

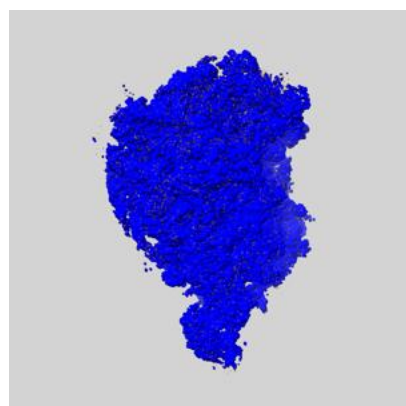
6.6 Mask visualisation [i](#)

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

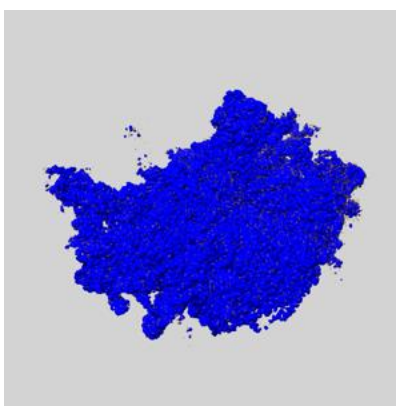
A mask typically either:

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

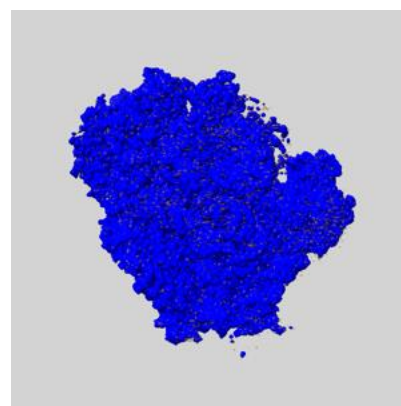
6.6.1 emd_29272_msk_1.map [i](#)



X



Y

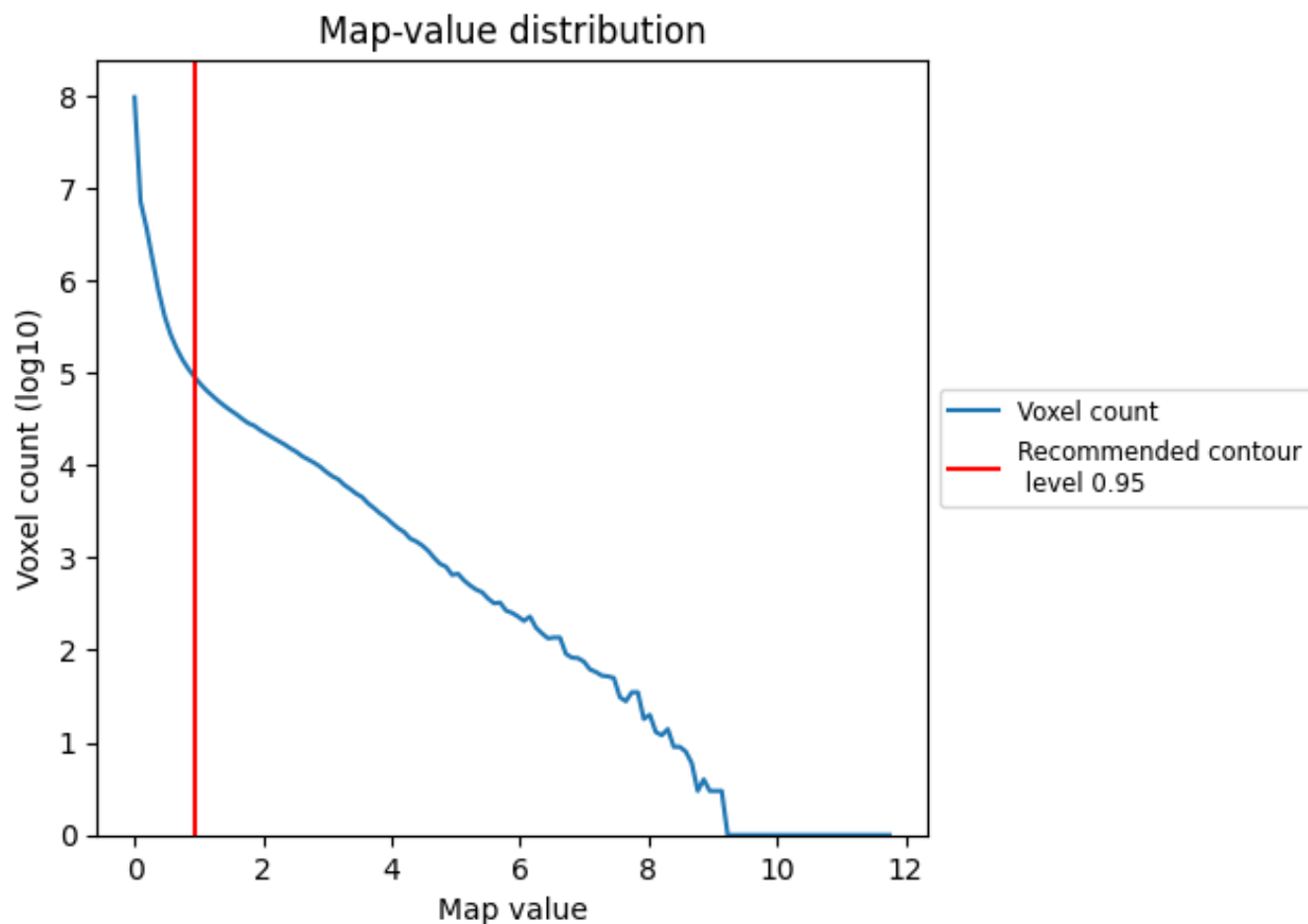


Z

7 Map analysis [i](#)

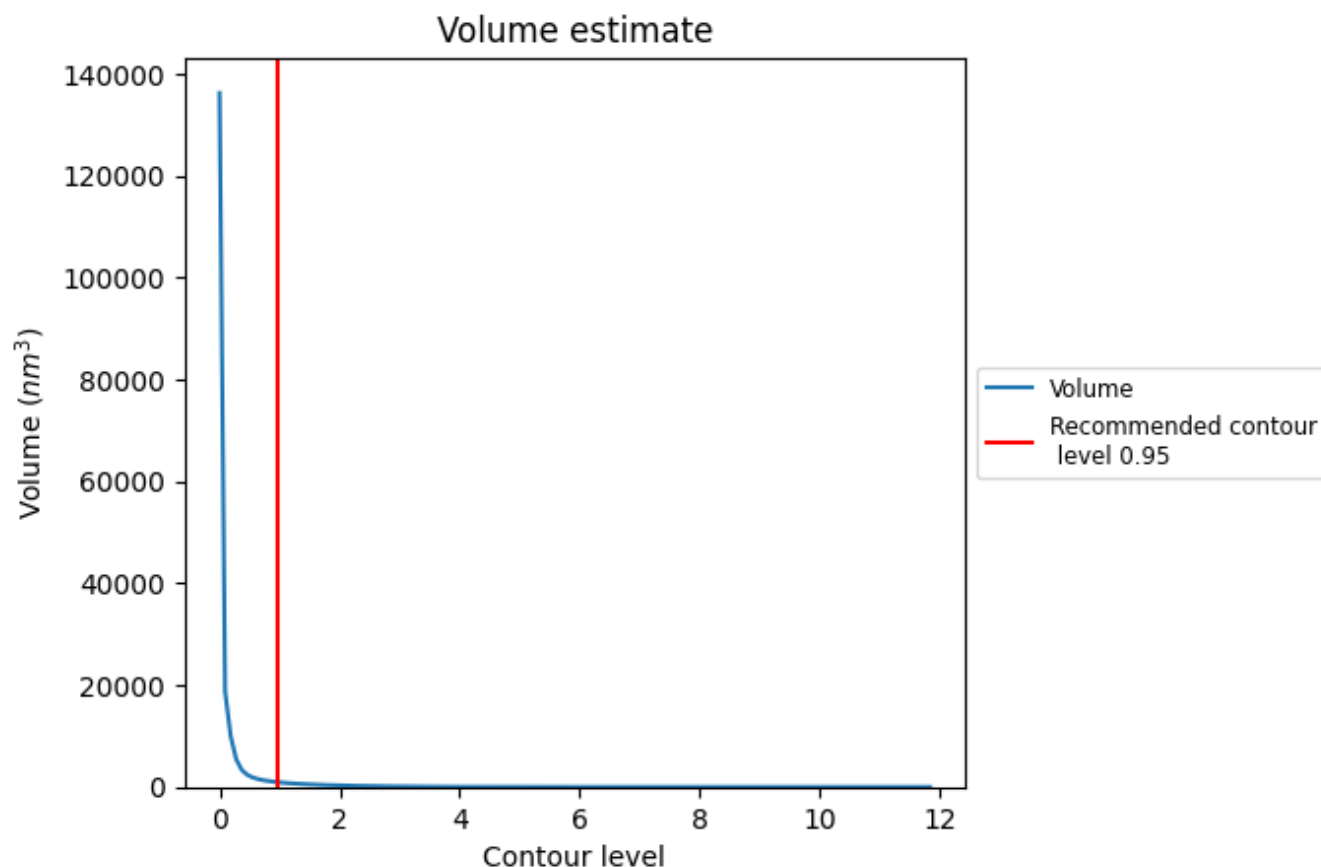
This section contains the results of statistical analysis of the map.

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.

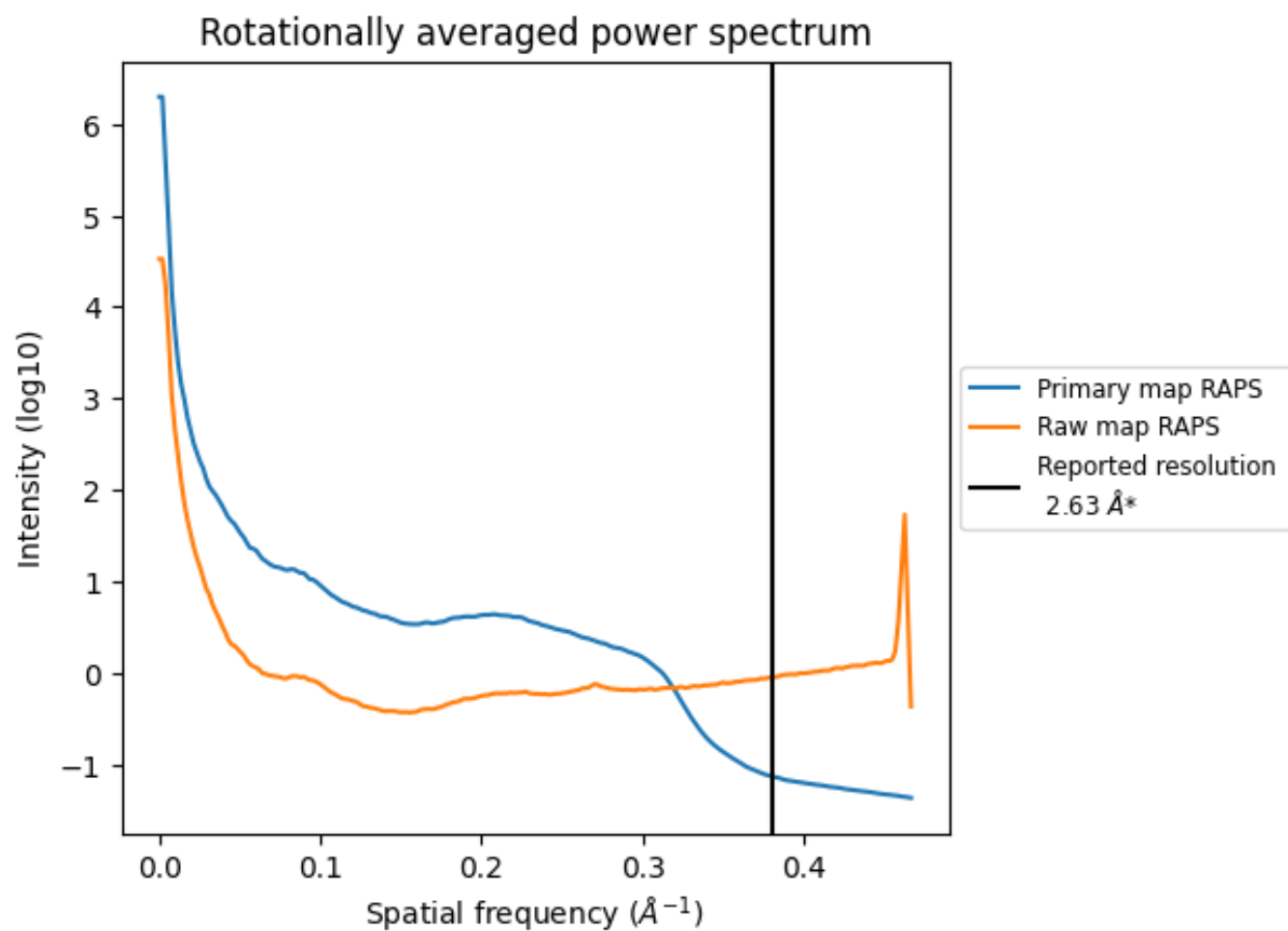
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 956 nm^3 ; this corresponds to an approximate mass of 864 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 ⓘ

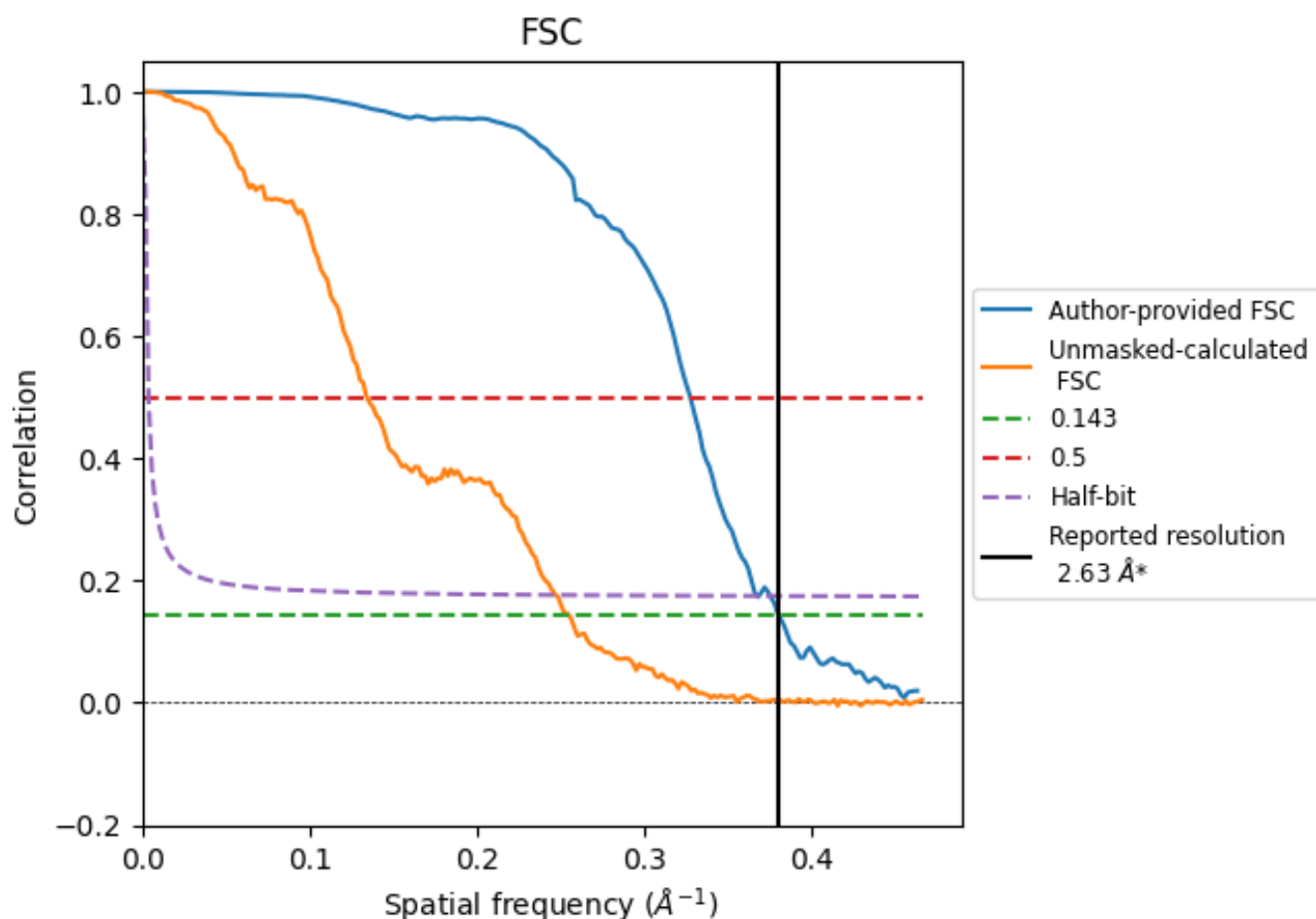


*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

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 0.380 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

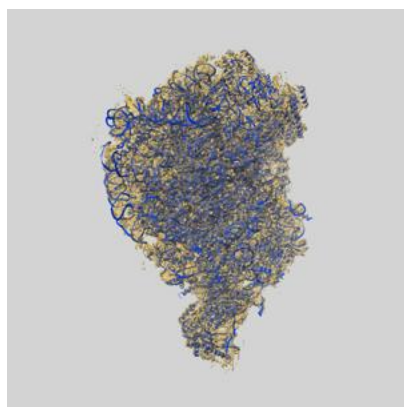
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.63	3.05	2.72
Unmasked-calculated*	3.92	7.45	4.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 2.63 by more than 10 %

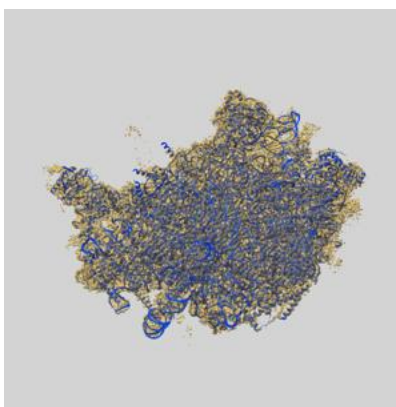
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29272 and PDB model 8FLA. Per-residue inclusion information can be found in section 3 on page 16.

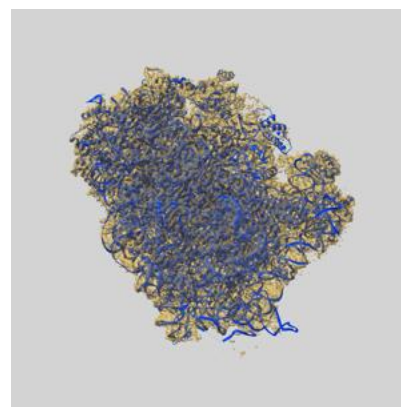
9.1 Map-model overlay [i](#)



X



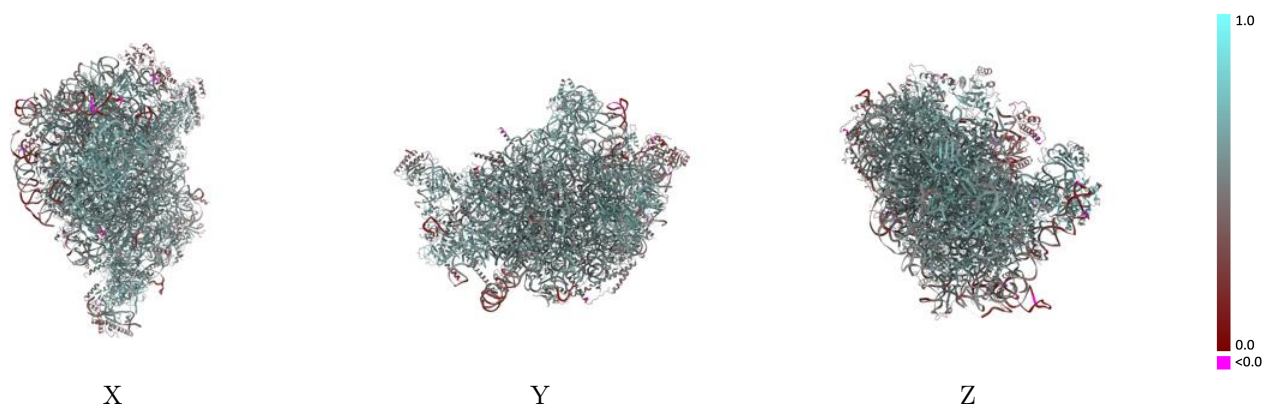
Y



Z

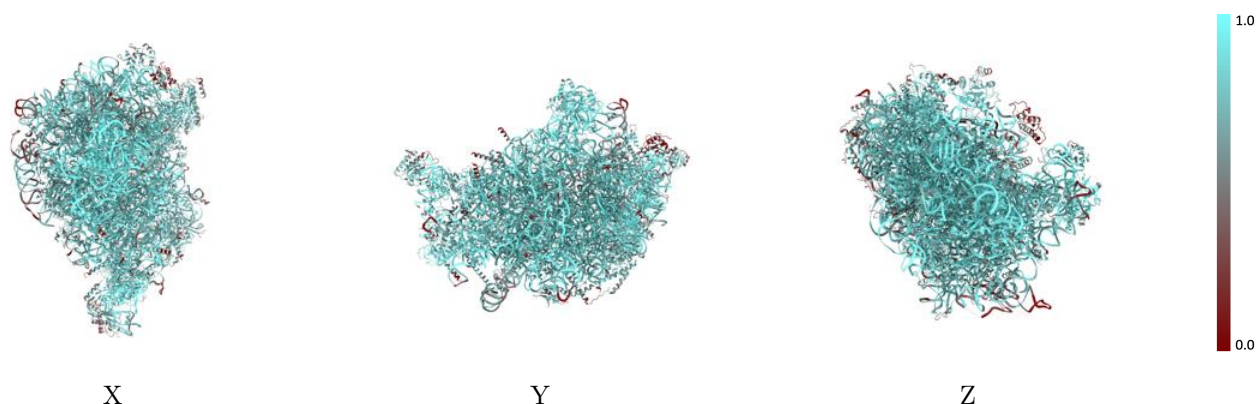
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



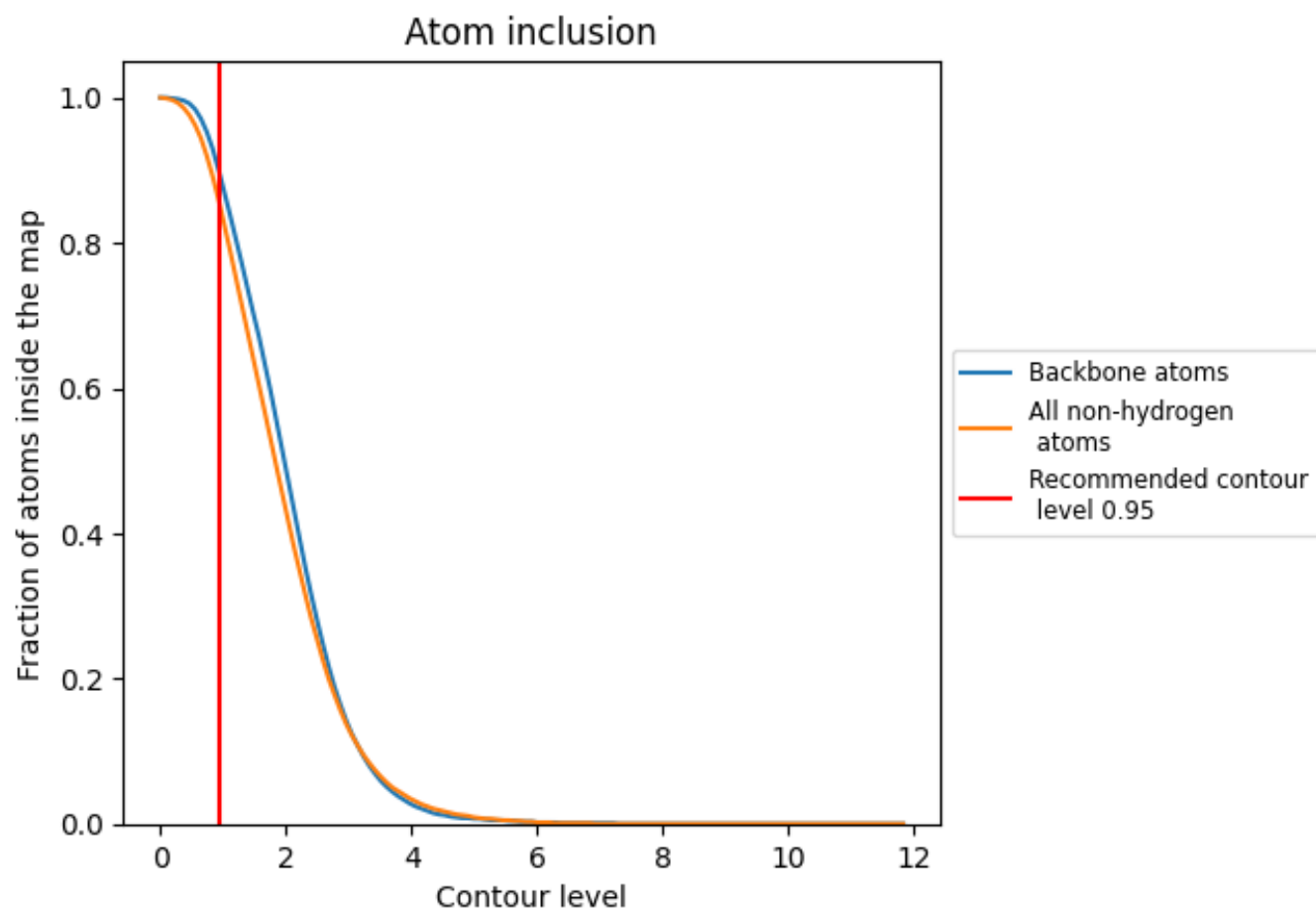
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 89% of all backbone atoms, 85% 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	 0.8510	 0.5520
BA	 0.2070	 0.2570
L1	 0.9320	 0.5860
L2	 0.8410	 0.5270
L3	 0.8860	 0.5380
L4	 0.9810	 0.6200
L5	 0.8050	 0.5560
L6	 0.7720	 0.5400
L7	 0.8920	 0.6090
L8	 0.8760	 0.5920
L9	 0.9210	 0.6170
LA	 0.8280	 0.5600
LB	 0.8620	 0.5920
LC	 0.9580	 0.6510
LD	 0.7840	 0.5500
LE	 0.8870	 0.5830
LF	 0.7180	 0.5170
LG	 0.8590	 0.5950
LH	 0.8260	 0.5860
LI	 0.7840	 0.5470
LJ	 0.8480	 0.5780
LK	 0.8800	 0.5970
LL	 0.8240	 0.5620
LM	 0.7260	 0.5290
LN	 0.8330	 0.5700
LO	 0.7180	 0.5330
LP	 0.7500	 0.5380
LQ	 0.8180	 0.5720
LR	 0.8320	 0.5700
LS	 0.7930	 0.5600
LT	 0.8740	 0.5860
LU	 0.7430	 0.5270
LV	 0.8860	 0.6070
LW	 0.8830	 0.5880
LX	 0.7560	 0.5480



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Chain	Atom inclusion	Q-score
LY	 0.6890	 0.5190
LZ	 0.8700	 0.5800
NK	 0.6170	 0.4650
NL	 0.7270	 0.5400
NP	 0.7520	 0.5340
NR	 0.7000	 0.5370
SA	 0.8400	 0.5750
SB	 0.8830	 0.5990
SC	 0.7310	 0.5300
SD	 0.8520	 0.5810
SE	 0.8570	 0.5890
SF	 0.8600	 0.5910
SG	 0.8860	 0.6050
SH	 0.7990	 0.5400
SI	 0.8230	 0.5730
SK	 0.8000	 0.5500
SL	 0.6310	 0.4720
SM	 0.8880	 0.6130
SQ	 0.5930	 0.3800
SR	 0.7390	 0.5290
SV	 0.7700	 0.5240
VB	 0.6160	 0.5440