



Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 02:27 pm BST

PDB ID : 9SDP / pdb_00009sdp
EMDB ID : EMD-54789
Title : Cryo-EM structure of the Arabidopsis thaliana 40S ribosomal subunit
Authors : Karki, S.; Lu, X.; Paatero, A.O.; Ruonala, R.; Tranter, D.; Guryanov, S.;
Rehan, S.; Hellmann, E.; Haakonsson, A.; Butcher, S.J.; Huiskonen, J.T.;
Kajander, T.; Helariutta, Y.; Paavilainen, V.O.
Deposited on : 2025-08-14
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

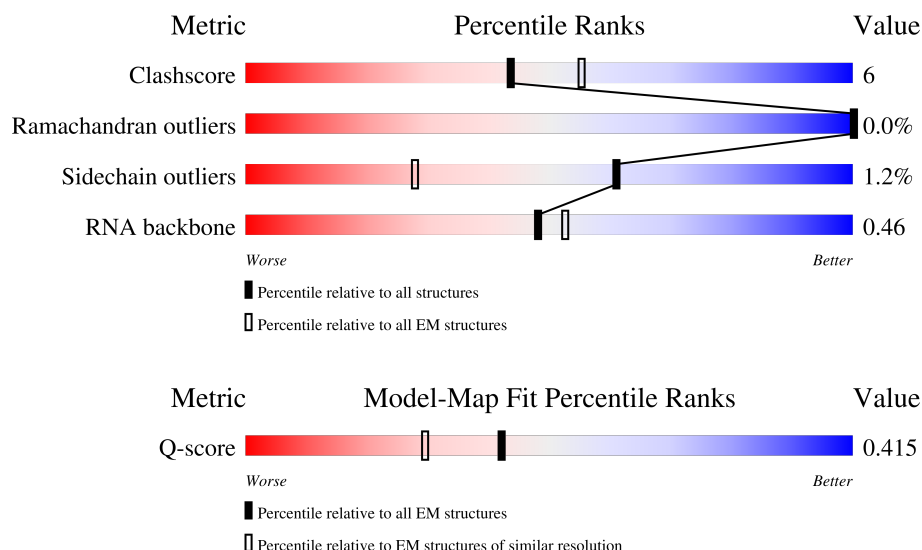
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.30 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	15087 (2.80 - 3.80)

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	9	1804	
2	BA	280	
3	BB	262	

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Mol	Chain	Length	Quality of chain
4	BC	276	
5	BE	261	
6	BG	249	
7	BH	191	
8	BI	222	
9	BJ	197	
10	BL	160	
11	BN	151	
12	cS	150	
13	BV	82	
14	BW	130	
15	BX	142	
16	BY	133	
17	BZ	130	
18	Bb	86	
19	Be	62	
20	Cn	25	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 44802 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	9	1081	Total	C	N	O	P	0	0
			23135	10353	4182	7519	1081		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	604	UY1	U	modified residue	GB X16077.1

- Molecule 2 is a protein called Small ribosomal subunit protein uS2y.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	189	Total	C	N	O	S	0	0
			1500	957	263	268	12		

- Molecule 3 is a protein called Small ribosomal subunit protein eS1z.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BB	208	Total	C	N	O	S	0	0
			1696	1075	312	301	8		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5w.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BC	216	Total	C	N	O	S	0	0
			1683	1088	298	290	7		

- Molecule 5 is a protein called Small ribosomal subunit protein eS4z.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BE	255	Total	C	N	O	S	0	0
			2058	1316	382	354	6		

- Molecule 6 is a protein called Small ribosomal subunit protein eS6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BG	199	Total	C	N	O	S	0	0
			1579	993	310	268	8		

- Molecule 7 is a protein called Small ribosomal subunit protein eS7z.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BH	176	Total	C	N	O	S	0	0
			1439	918	262	258	1		

- Molecule 8 is a protein called Small ribosomal subunit protein eS8z.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BI	183	Total	C	N	O	S	0	0
			1480	921	293	262	4		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4y.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BJ	171	Total	C	N	O	S	0	0
			1432	906	280	242	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS17z.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BL	138	Total	C	N	O	S	0	0
			1106	709	214	178	5		

- Molecule 11 is a protein called Small ribosomal subunit protein uS15y.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BN	149	Total	C	N	O	S	0	0
			1192	760	223	207	2		

- Molecule 12 is a protein called Small ribosomal subunit protein uS11x.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	cS	126	Total	C	N	O	S	0	0
			952	586	188	174	4		

- Molecule 13 is a protein called Small ribosomal subunit protein eS21z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BV	72	Total	C	N	O	S	0	0
			561	350	103	105	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8z/uS8w.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BW	129	Total	C	N	O	S	0	0
			1033	660	188	180	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS12y.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BX	138	Total	C	N	O	S	0	0
			1075	684	206	182	3		

- Molecule 16 is a protein called Small ribosomal subunit protein eS24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BY	110	Total	C	N	O	S	0	0
			917	587	176	152	2		

- Molecule 17 is a protein called Small ribosomal subunit protein eS26x.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BZ	97	Total	C	N	O	S	0	0
			783	482	165	130	6		

- Molecule 18 is a protein called Small ribosomal subunit protein eS27y.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Bb	85	Total	C	N	O	S	0	0
			660	411	120	122	7		

- Molecule 19 is a protein called Small ribosomal subunit protein eS30z/eS30y/eS30x.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	Be	39	Total	C	N	O	0	0
			292	175	70	47		

- Molecule 20 is a protein called Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Cn	22	Total	C	N	O	S	0	0
			211	130	55	23	3		

- Molecule 21 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	9	3	Total	K	0
			3	3	

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	9	14	Total	Mg	0
			14	14	

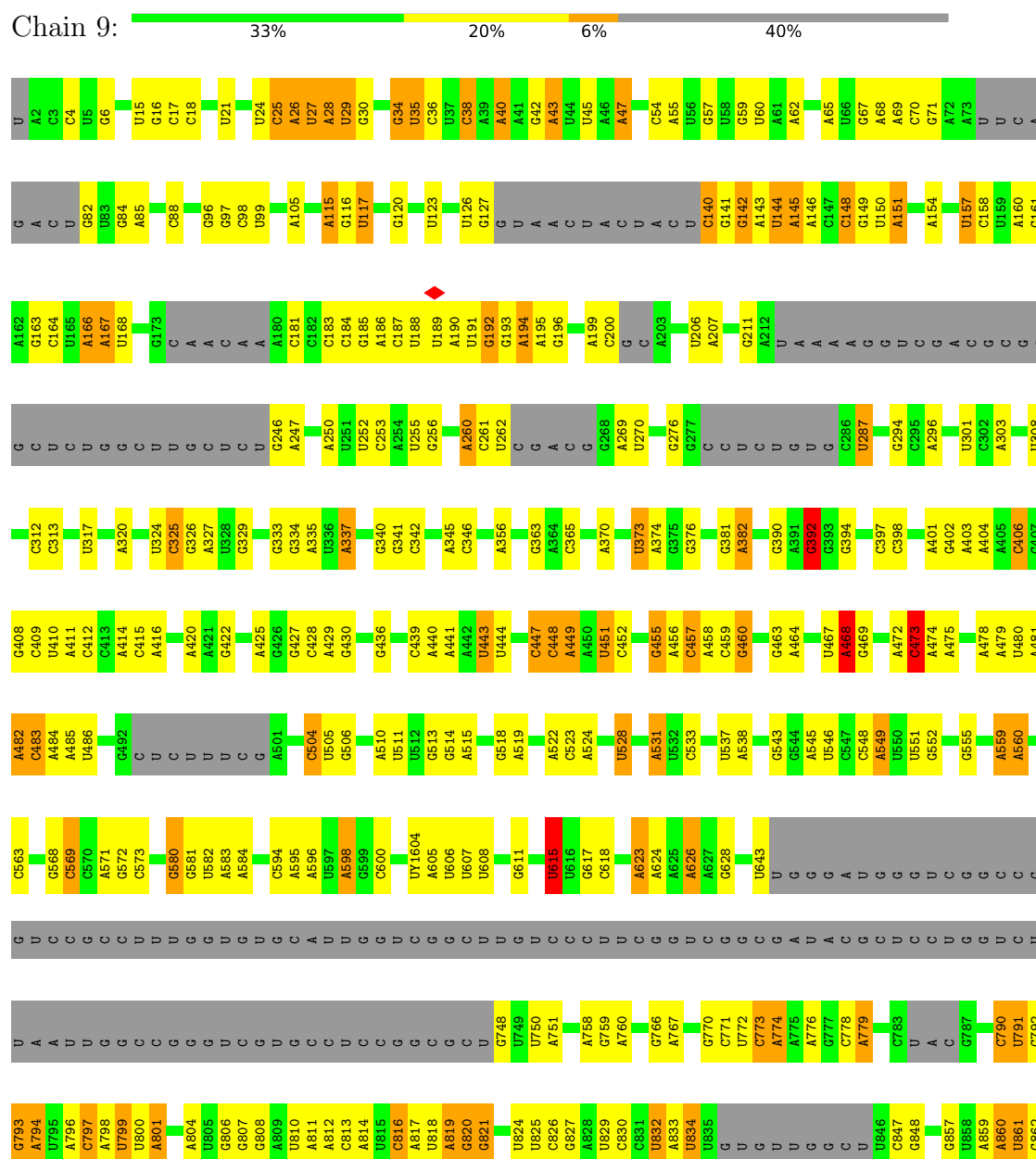
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

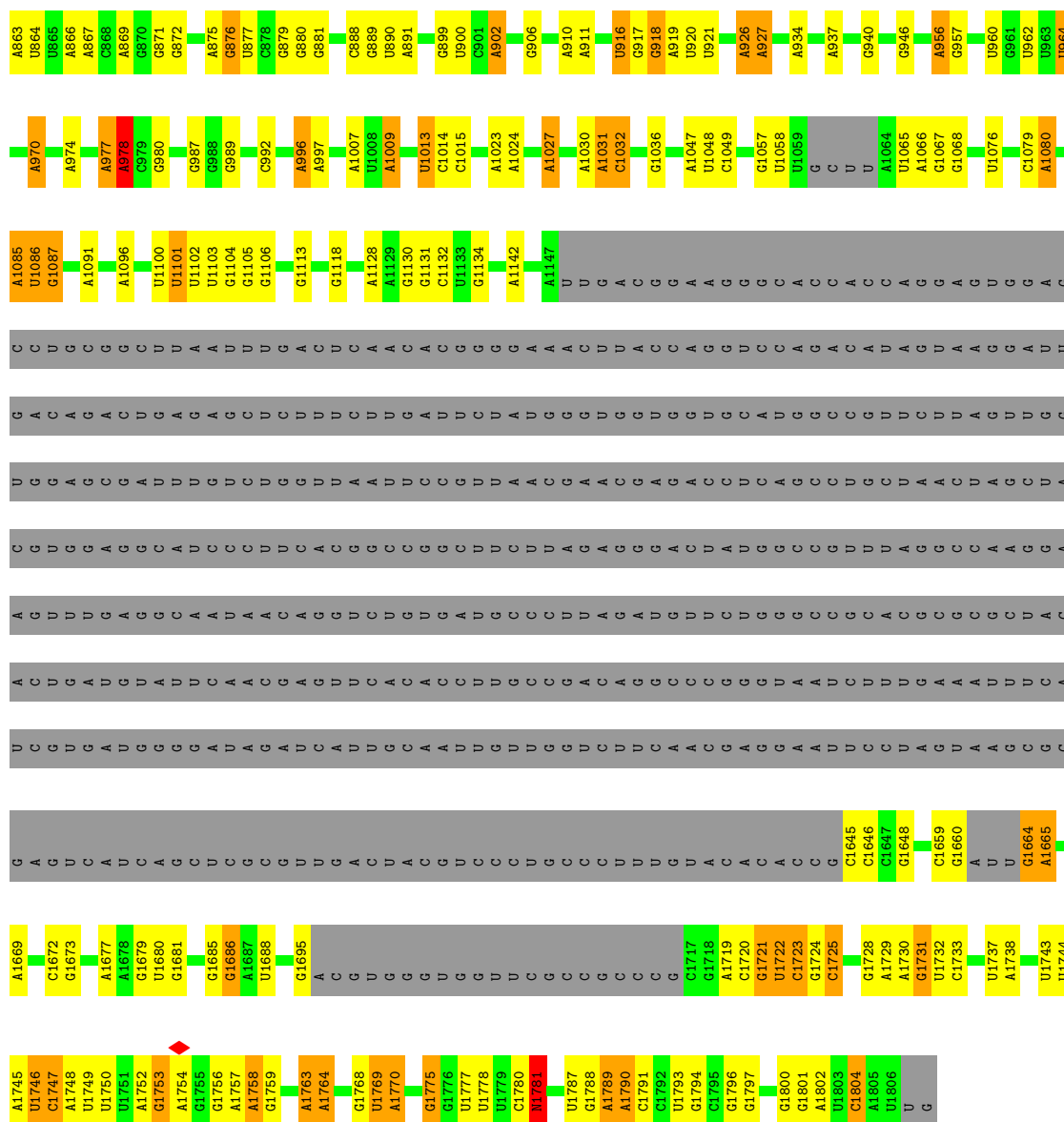
Mol	Chain	Residues	Atoms		AltConf
23	BZ	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

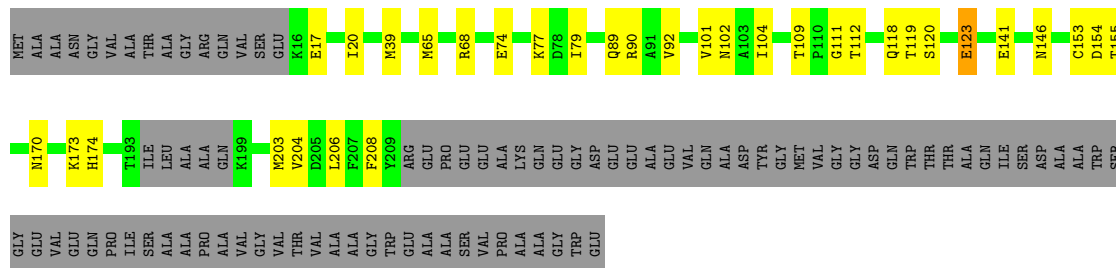
• Molecule 1: 18S RNA





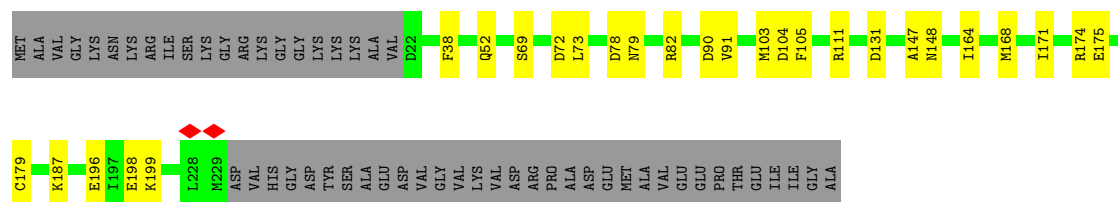
- Molecule 2: Small ribosomal subunit protein uS2y

Chain BA: 56% 11% 32%



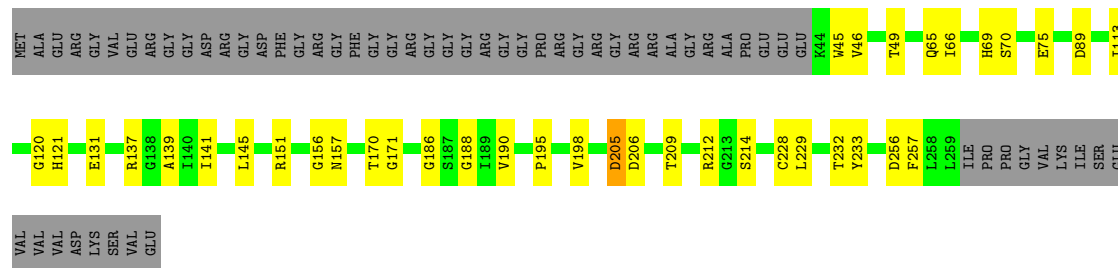
- Molecule 3: Small ribosomal subunit protein eS1z

Chain BB: 69% 10% 21%



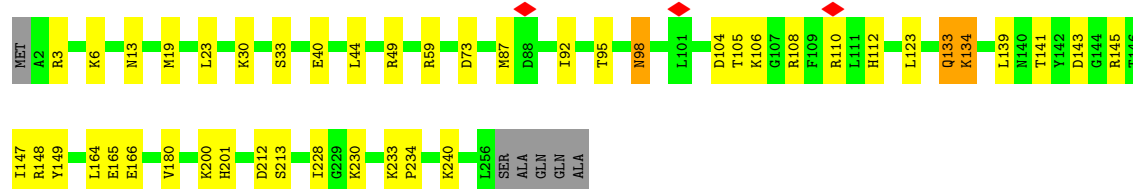
- Molecule 4: Small ribosomal subunit protein uS5w

Chain BC:



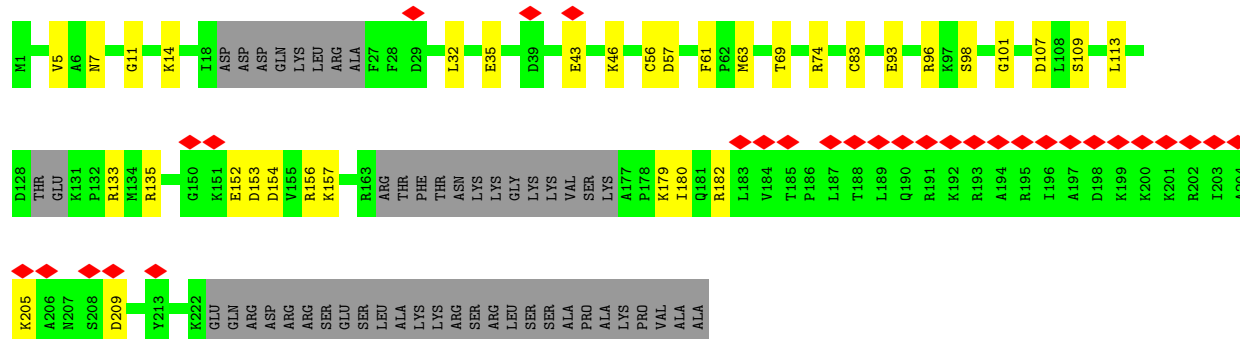
- Molecule 5: Small ribosomal subunit protein eS4z

Chain BE:



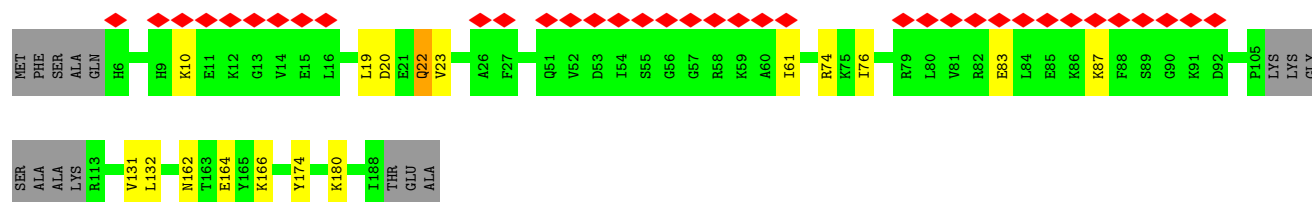
- Molecule 6: Small ribosomal subunit protein eS6y

Chain BG:

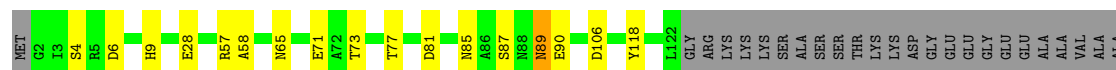


- Molecule 7: Small ribosomal subunit protein eS7z

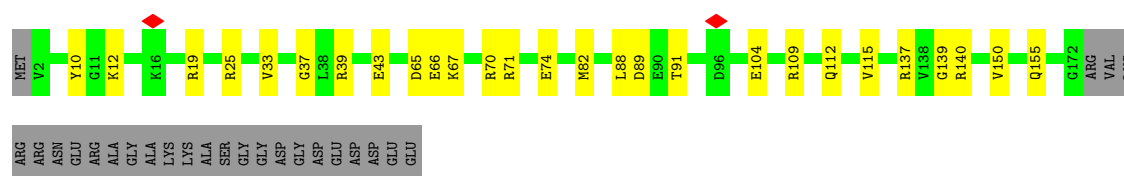
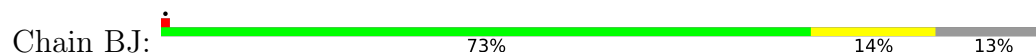
Chain BH:



- Molecule 8: Small ribosomal subunit protein eS8z



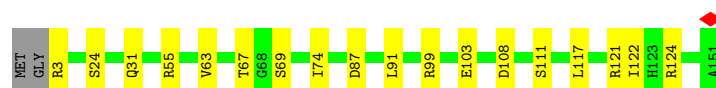
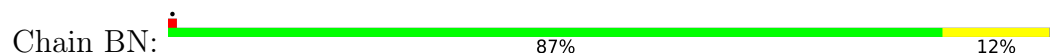
- Molecule 9: Small ribosomal subunit protein uS4y



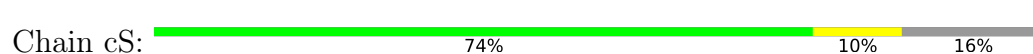
- Molecule 10: Small ribosomal subunit protein uS17z



- Molecule 11: Small ribosomal subunit protein uS15y

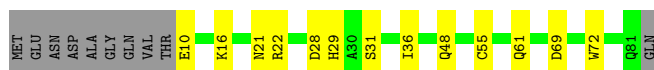


- Molecule 12: Small ribosomal subunit protein uS11x

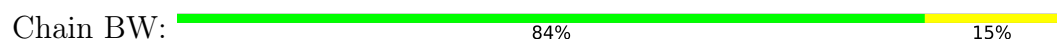




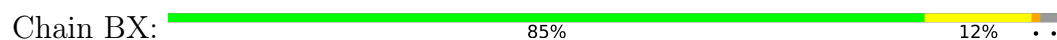
- Molecule 13: Small ribosomal subunit protein eS21z



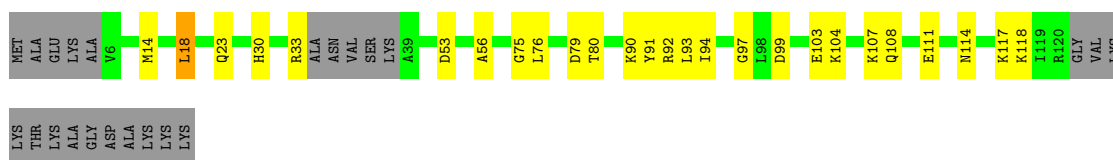
- Molecule 14: Small ribosomal subunit protein uS8z/uS8w



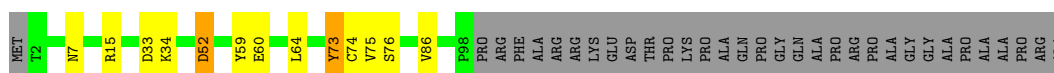
- Molecule 15: Small ribosomal subunit protein uS12y



- Molecule 16: Small ribosomal subunit protein eS24z



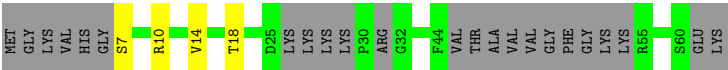
- Molecule 17: Small ribosomal subunit protein eS26x



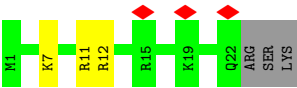
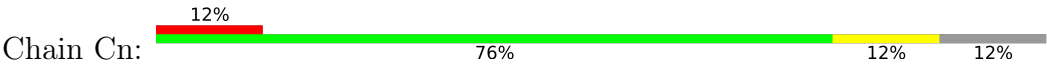
- Molecule 18: Small ribosomal subunit protein eS27y



- Molecule 19: Small ribosomal subunit protein eS30z/eS30y/eS30x



● Molecule 20: Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115070	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24.512	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.319	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	378.0, 378.0, 378.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MA6, 4AC, A2M, ZN, OMC, UY1, OMU, OMG, K

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	9	0.22	0/25437	0.29	0/39618
2	BA	0.19	0/1532	0.33	0/2070
3	BB	0.17	0/1724	0.31	0/2313
4	BC	0.21	0/1719	0.35	0/2319
5	BE	0.17	0/2100	0.32	0/2819
6	BG	0.16	0/1599	0.31	0/2127
7	BH	0.15	0/1461	0.27	0/1964
8	BI	0.16	0/1503	0.31	0/2008
9	BJ	0.18	0/1458	0.35	0/1954
10	BL	0.19	0/1132	0.35	0/1514
11	BN	0.18	0/1216	0.28	0/1632
12	cS	0.18	0/964	0.32	0/1293
13	BV	0.17	0/570	0.29	0/766
14	BW	0.24	0/1051	0.33	0/1406
15	BX	0.19	0/1092	0.35	0/1453
16	BY	0.16	0/931	0.31	0/1233
17	BZ	0.38	0/797	0.53	1/1069 (0.1%)
18	Bb	0.18	0/670	0.28	0/899
19	Be	0.14	0/294	0.23	0/387
20	Cn	0.27	0/212	0.47	0/269
All	All	0.21	0/47462	0.30	1/69113 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	BZ	73	TYR	CA-C-O	-5.01	116.18	121.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9	23135	0	11665	270	0
2	BA	1500	0	1507	21	0
3	BB	1696	0	1760	15	0
4	BC	1683	0	1782	28	0
5	BE	2058	0	2163	39	0
6	BG	1579	0	1694	22	0
7	BH	1439	0	1508	11	0
8	BI	1480	0	1527	23	0
9	BJ	1432	0	1485	17	0
10	BL	1106	0	1169	21	0
11	BN	1192	0	1276	13	0
12	cS	952	0	988	11	0
13	BV	561	0	557	10	0
14	BW	1033	0	1070	16	0
15	BX	1075	0	1146	16	0
16	BY	917	0	981	17	0
17	BZ	783	0	810	10	0
18	Bb	660	0	672	8	0
19	Be	292	0	288	2	0
20	Cn	211	0	258	2	0
21	9	3	0	0	0	0
22	9	14	0	0	0	0
23	BZ	1	0	0	0	0
All	All	44802	0	34306	501	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 6.

All (501) 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)
5:BE:165:GLU:OE1	5:BE:166:GLU:HG3	1.50	1.08
1:9:276:G:H1	1:9:287:U:H3	1.16	0.93
1:9:1672:C:N3	1:9:1743:U:O4	2.02	0.92
9:BJ:39:ARG:NH1	9:BJ:43:GLU:OE2	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:1105:G:O4'	14:BW:8:ASN:ND2	2.06	0.89
9:BJ:66:GLU:OE1	9:BJ:71:ARG:NH2	2.07	0.87
1:9:325:C:O2	1:9:327:A:N6	2.09	0.86
5:BE:165:GLU:CD	5:BE:166:GLU:HG3	2.02	0.84
1:9:821:G:O6	1:9:859:A:N1	2.10	0.83
1:9:808:G:OP2	1:9:808:G:N2	2.10	0.83
1:9:1646:C:O2	1:9:1770:A:N6	2.12	0.82
1:9:1721:G:O2'	1:9:1722:U:O4'	1.97	0.82
9:BJ:140:ARG:O	9:BJ:140:ARG:NE	2.14	0.81
1:9:181:C:N4	1:9:200:C:O2	2.14	0.80
1:9:154:A:N6	1:9:422:G:O6	2.14	0.80
1:9:820:G:O2'	1:9:821:G:OP2	1.98	0.80
1:9:143:A:O2'	1:9:144:U:O5'	2.00	0.80
1:9:1763:A:O2'	1:9:1764:A:O4'	1.98	0.80
1:9:1086:U:O2'	1:9:1087:G:O5'	2.01	0.78
2:BA:111:GLY:N	2:BA:141:GLU:OE2	2.16	0.78
3:BB:104:ASP:OD1	3:BB:105:PHE:N	2.18	0.76
12:cS:120:ARG:NH1	17:BZ:52:ASP:OD2	2.19	0.76
1:9:54:C:OP1	16:BY:114:ASN:ND2	2.20	0.74
1:9:1659:C:N4	1:9:1660:G:O6	2.21	0.74
10:BL:70:GLU:OE1	10:BL:70:GLU:N	2.19	0.74
5:BE:104:ASP:OD1	5:BE:105:THR:N	2.21	0.74
1:9:869:A:OP1	14:BW:28:ARG:NH2	2.21	0.73
1:9:26:A:O2'	1:9:27:U:OP1	2.06	0.73
10:BL:69:ARG:O	10:BL:69:ARG:NH1	2.21	0.73
1:9:996:A:O2'	1:9:1793:U:O2	2.06	0.73
14:BW:98:GLN:OE1	14:BW:98:GLN:N	2.21	0.72
1:9:1804:C:O2	17:BZ:7:ASN:ND2	2.22	0.72
5:BE:73:ASP:OD2	5:BE:145:ARG:NH2	2.23	0.71
8:BI:211:LYS:O	8:BI:214:GLN:NE2	2.22	0.71
1:9:24:U:OP1	9:BJ:12:LYS:NZ	2.23	0.70
1:9:779:A:OP2	1:9:793:G:N2	2.24	0.70
1:9:392:OMG:OP1	1:9:427:G:O2'	2.08	0.70
19:Be:7:SER:OG	19:Be:10:ARG:NH2	2.25	0.69
1:9:406:C:OP1	5:BE:3:ARG:NH1	2.25	0.69
1:9:373:U:N3	1:9:376:G:N7	2.40	0.69
7:BH:131:VAL:HG12	7:BH:131:VAL:O	1.93	0.69
11:BN:108:ASP:OD2	11:BN:111:SER:OG	2.08	0.69
4:BC:120:GLY:O	4:BC:121:HIS:ND1	2.26	0.68
13:BV:48:GLN:N	13:BV:48:GLN:OE1	2.26	0.68
16:BY:104:LYS:NZ	16:BY:108:GLN:OE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:cS:45:ASP:OD1	12:cS:47:SER:N	2.26	0.68
1:9:1763:A:O2'	1:9:1764:A:O5'	2.12	0.68
13:BV:16:LYS:NZ	13:BV:21:ASN:O	2.27	0.68
1:9:832:U:O2	1:9:848:G:O6	2.12	0.68
1:9:65:A:O2'	1:9:67:G:OP2	2.11	0.68
1:9:964:U:OP2	11:BN:55:ARG:NH1	2.26	0.67
1:9:559:A:O2'	1:9:560:A:O5'	2.11	0.67
8:BI:170:ASP:OD1	8:BI:171:SER:N	2.27	0.67
1:9:449:A:OP2	5:BE:59:ARG:NH1	2.29	0.66
2:BA:90:ARG:NH1	2:BA:206:LEU:O	2.29	0.66
1:9:1686:G:N2	1:9:1728:G:O2'	2.29	0.66
11:BN:31:GLN:N	11:BN:31:GLN:OE1	2.27	0.66
1:9:1031:A:O2'	1:9:1032:C:OP1	2.11	0.66
5:BE:212:ASP:OD1	5:BE:213:SER:N	2.29	0.65
15:BX:72:GLN:OE1	15:BX:73:LEU:N	2.29	0.65
1:9:528:U:N3	1:9:531:A:OP2	2.29	0.65
1:9:335:A:OP1	8:BI:57:ARG:NH1	2.30	0.65
15:BX:35:GLU:OE1	15:BX:35:GLU:N	2.28	0.65
4:BC:205:ASP:N	4:BC:205:ASP:OD1	2.30	0.64
1:9:834:U:O4	1:9:847:C:N3	2.30	0.64
1:9:778:C:O2'	1:9:792:G:N2	2.31	0.64
1:9:569:C:O2	15:BX:63:SER:OG	2.17	0.63
1:9:926:A:O2'	1:9:927:A:OP1	2.14	0.63
1:9:758:A:N6	1:9:797:C:O2	2.31	0.63
2:BA:74:GLU:OE1	2:BA:74:GLU:N	2.31	0.62
1:9:791:U:OP1	5:BE:240:LYS:NZ	2.33	0.62
4:BC:131:GLU:OE1	4:BC:131:GLU:N	2.33	0.61
6:BG:179:LYS:NZ	6:BG:180:ILE:O	2.30	0.61
1:9:143:A:HO2'	1:9:144:U:H6	1.47	0.61
10:BL:155:SER:OG	10:BL:156:LYS:N	2.32	0.61
1:9:451:U:OP1	5:BE:49:ARG:NH1	2.34	0.61
17:BZ:60:GLU:N	17:BZ:60:GLU:OE1	2.33	0.61
1:9:150:U:H3'	1:9:151:A:H5''	1.81	0.61
16:BY:103:GLU:OE1	16:BY:103:GLU:N	2.33	0.61
5:BE:40:GLU:OE1	5:BE:40:GLU:N	2.35	0.60
9:BJ:137:ARG:NH1	9:BJ:139:GLY:O	2.34	0.60
5:BE:6:LYS:O	5:BE:30:LYS:NZ	2.31	0.60
16:BY:79:ASP:OD1	16:BY:80:THR:N	2.34	0.60
1:9:340:G:O2'	10:BL:155:SER:O	2.17	0.59
14:BW:23:ARG:NH2	18:Bb:5:ASN:O	2.35	0.59
15:BX:101:ILE:HD11	15:BX:119:PHE:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:185:G:OP1	8:BI:159:LYS:NZ	2.36	0.59
4:BC:256:ASP:OD1	4:BC:257:PHE:N	2.35	0.59
4:BC:190:VAL:O	4:BC:209:THR:OG1	2.19	0.59
1:9:906:G:OP2	12:cS:37:ASN:ND2	2.33	0.59
1:9:1796:G:C4	1:9:1797:G:C8	2.90	0.59
1:9:105:A:N3	1:9:312:C:N4	2.51	0.59
1:9:1660:G:H22	1:9:1753:G:H2'	1.67	0.59
18:Bb:42:CYS:SG	18:Bb:60:ASN:ND2	2.76	0.59
15:BX:94:GLU:N	15:BX:94:GLU:OE1	2.36	0.58
3:BB:78:ASP:OD1	3:BB:79:ASN:ND2	2.37	0.58
1:9:1732:U:H2'	1:9:1733:C:H6	1.69	0.58
10:BL:56:ARG:NH2	10:BL:76:TYR:O	2.37	0.58
4:BC:171:GLY:N	4:BC:228:CYS:SG	2.77	0.58
1:9:16:G:H2'	1:9:17:C:C6	2.39	0.57
8:BI:28:GLU:OE1	8:BI:28:GLU:N	2.37	0.57
2:BA:203:MET:SD	2:BA:204:VAL:N	2.78	0.57
19:Be:14:VAL:O	19:Be:18:THR:OG1	2.21	0.57
1:9:256:G:OP1	5:BE:134:LYS:N	2.37	0.57
4:BC:156:GLY:O	4:BC:157:ASN:OD1	2.23	0.57
1:9:127:G:O6	1:9:296:A:N6	2.38	0.56
1:9:888:C:H2'	1:9:889:G:H8	1.69	0.56
4:BC:49:THR:OG1	4:BC:75:GLU:OE2	2.12	0.56
3:BB:198:GLU:OE1	3:BB:199:LYS:N	2.37	0.56
5:BE:165:GLU:OE1	5:BE:166:GLU:CG	2.40	0.56
8:BI:81:ASP:OD1	8:BI:81:ASP:N	2.38	0.56
1:9:334:G:OP2	8:BI:189:ARG:NH1	2.38	0.56
8:BI:9:HIS:O	8:BI:9:HIS:ND1	2.38	0.56
9:BJ:82:MET:HG3	9:BJ:88:LEU:HD22	1.88	0.56
1:9:70:C:N4	1:9:71:G:O6	2.39	0.55
1:9:26:A:HO2'	1:9:27:U:P	2.29	0.55
1:9:187:C:H2'	1:9:188:U:C6	2.41	0.55
1:9:329:G:N3	10:BL:104:GLN:NE2	2.55	0.55
5:BE:23:LEU:HD23	5:BE:23:LEU:H	1.71	0.55
1:9:940:G:N7	17:BZ:15:ARG:NH1	2.55	0.55
9:BJ:104:GLU:N	9:BJ:104:GLU:OE1	2.38	0.55
6:BG:43:GLU:O	6:BG:46:LYS:NZ	2.40	0.54
10:BL:77:VAL:HG22	10:BL:77:VAL:O	2.07	0.54
1:9:1769:U:O2'	1:9:1770:A:OP2	2.16	0.54
1:9:881:G:O6	1:9:956:A:N6	2.40	0.54
1:9:875:A:HO2'	1:9:876:G:H8	1.52	0.54
1:9:916:U:O2	1:9:918:G:N1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:39:MET:CE	2:BA:153:CYS:HB2	2.38	0.54
1:9:559:A:O2'	1:9:560:A:O4'	2.24	0.54
1:9:970:A:OP2	11:BN:124:ARG:NH2	2.40	0.54
5:BE:233:LYS:NZ	5:BE:234:PRO:O	2.41	0.54
1:9:301:U:O2	5:BE:33:SER:OG	2.22	0.54
4:BC:214:SER:O	4:BC:214:SER:OG	2.23	0.54
4:BC:229:LEU:O	4:BC:232:THR:HG22	2.07	0.54
1:9:443:U:H3	1:9:468:A2M:H62	1.54	0.54
6:BG:7:ASN:O	6:BG:11:GLY:N	2.34	0.54
16:BY:30:HIS:NE2	16:BY:33:ARG:O	2.41	0.54
2:BA:154:ASP:OD1	2:BA:155:THR:N	2.39	0.53
9:BJ:19:ARG:O	9:BJ:25:ARG:NH2	2.41	0.53
2:BA:123:GLU:N	2:BA:123:GLU:OE1	2.41	0.53
5:BE:87:MET:HE1	5:BE:123:LEU:H	1.72	0.53
6:BG:57:ASP:OD1	6:BG:61:PHE:N	2.42	0.53
8:BI:85:ASN:OD1	8:BI:87:SER:N	2.41	0.53
4:BC:89:ASP:OD1	4:BC:89:ASP:N	2.41	0.53
6:BG:152:GLU:OE1	6:BG:152:GLU:N	2.42	0.53
1:9:1730:A:C2	1:9:1731:G:H1'	2.43	0.52
1:9:1752:A:H2'	1:9:1753:G:N9	2.24	0.52
3:BB:90:ASP:OD1	3:BB:91:VAL:N	2.41	0.52
3:BB:164:ILE:O	3:BB:168:MET:HG3	2.10	0.52
5:BE:98:ASN:OD1	5:BE:98:ASN:N	2.43	0.52
9:BJ:109:ARG:NH1	9:BJ:155:GLN:OE1	2.39	0.52
15:BX:46:ALA:O	15:BX:100:LEU:HD12	2.09	0.52
2:BA:90:ARG:NH1	2:BA:208:PHE:O	2.42	0.52
1:9:474:A:C2	1:9:475:A:C8	2.97	0.52
1:9:513:G:H2'	1:9:514:G:H8	1.74	0.52
10:BL:112:ASP:OD1	10:BL:112:ASP:N	2.41	0.52
10:BL:124:GLU:OE1	15:BX:11:ARG:CZ	2.58	0.52
9:BJ:65:ASP:OD1	9:BJ:66:GLU:N	2.43	0.52
1:9:605:A:C4	1:9:606:U:C5	2.98	0.52
1:9:126:U:OP1	5:BE:148:ARG:NH2	2.37	0.52
1:9:447:C:O2'	1:9:449:A:N7	2.38	0.52
1:9:1731:G:C2	1:9:1732:U:C6	2.98	0.52
3:BB:82:ARG:NH1	3:BB:103:MET:SD	2.82	0.52
2:BA:65:MET:HE2	13:BV:72:TRP:CD1	2.46	0.51
2:BA:173:LYS:HG3	2:BA:174:HIS:H	1.75	0.51
4:BC:75:GLU:OE1	4:BC:75:GLU:N	2.37	0.51
1:9:1102:U:OP1	4:BC:170:THR:OG1	2.19	0.51
2:BA:77:LYS:O	2:BA:102:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:160:A:OP1	6:BG:83:CYS:N	2.38	0.51
1:9:819:A:C8	1:9:821:G:H1'	2.45	0.51
10:BL:51:GLY:N	10:BL:55:ASN:OD1	2.43	0.51
1:9:1130:G:C2	1:9:1131:G:C8	2.99	0.51
6:BG:153:ASP:OD1	6:BG:154:ASP:N	2.44	0.51
1:9:335:A:OP2	8:BI:192:GLN:NE2	2.40	0.51
9:BJ:89:ASP:OD2	9:BJ:91:THR:OG1	2.18	0.51
17:BZ:33:ASP:OD1	17:BZ:34:LYS:N	2.44	0.50
1:9:96:G:O2'	1:9:464:A:O2'	2.22	0.50
1:9:97:G:H21	1:9:430:G:H5'	1.76	0.50
1:9:439:C:H2'	1:9:440:A:O4'	2.11	0.50
1:9:1067:G:H2'	1:9:1068:G:H8	1.76	0.50
4:BC:65:GLN:N	4:BC:65:GLN:OE1	2.45	0.50
1:9:185:G:C2	1:9:196:G:C6	2.99	0.50
1:9:115:A:N6	1:9:250:A:N7	2.60	0.50
1:9:876:G:H2'	1:9:877:U:O4'	2.10	0.50
16:BY:91:TYR:OH	16:BY:92:ARG:NH2	2.44	0.50
20:Cn:7:LYS:O	20:Cn:11:ARG:HG2	2.11	0.50
2:BA:68:ARG:HD2	13:BV:36:ILE:HD11	1.94	0.49
13:BV:61:GLN:OE1	14:BW:20:ARG:NH2	2.42	0.49
1:9:146:A:N6	1:9:164:C:N3	2.59	0.49
1:9:146:A:N1	6:BG:135:ARG:NH1	2.60	0.49
1:9:188:U:O2	1:9:193:G:N2	2.45	0.49
1:9:595:A:H2'	1:9:596:A:C8	2.47	0.49
1:9:790:C:H42	5:BE:112:HIS:CE1	2.30	0.49
7:BH:10:LYS:NZ	7:BH:20:ASP:OD2	2.45	0.49
1:9:934:A:N3	3:BB:111:ARG:NH2	2.60	0.49
1:9:1723:C:C2	1:9:1724:G:C8	3.00	0.49
11:BN:67:THR:HG23	11:BN:69:SER:H	1.76	0.49
1:9:47:A:C2	1:9:429:A:N1	2.80	0.49
5:BE:143:ASP:N	5:BE:143:ASP:OD1	2.45	0.49
10:BL:103:MET:SD	10:BL:106:THR:OG1	2.71	0.49
1:9:467:U:H2'	1:9:468:A2M:O4'	2.12	0.49
1:9:157:U:OP2	16:BY:118:LYS:NZ	2.37	0.49
1:9:260:A:N3	8:BI:65:ASN:ND2	2.60	0.49
1:9:1648:G:O2'	1:9:1789:MA6:O2'	2.27	0.49
1:9:1794:G:OP1	12:cS:149:ARG:NH2	2.46	0.49
1:9:504:C:C2	1:9:505:U:C5	3.01	0.49
1:9:1007:A:H1'	1:9:1009:A:N7	2.27	0.49
9:BJ:109:ARG:NH2	9:BJ:150:VAL:O	2.43	0.49
12:cS:30:VAL:HB	12:cS:92:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:1105:G:O3'	14:BW:76:SER:OG	2.31	0.49
14:BW:92:ARG:HG3	14:BW:93:LEU:HD12	1.94	0.49
1:9:117:U:O2'	1:9:337:A:N3	2.39	0.48
1:9:345:A:H2'	1:9:346:C:H6	1.78	0.48
1:9:151:A:H4'	1:9:151:A:OP1	2.12	0.48
1:9:401:A:H2'	1:9:402:G:O4'	2.12	0.48
1:9:1672:C:C4	1:9:1743:U:O4	2.65	0.48
3:BB:171:ILE:HG21	3:BB:196:GLU:OE1	2.14	0.48
1:9:794:A:OP1	5:BE:108:ARG:NH1	2.47	0.48
10:BL:109:VAL:HG12	10:BL:130:ILE:O	2.13	0.48
1:9:185:G:N1	1:9:194:A:N7	2.62	0.48
1:9:559:A:H4'	1:9:560:A:OP1	2.14	0.48
8:BI:4:SER:OG	8:BI:6:ASP:OD1	2.30	0.48
11:BN:87:ASP:OD1	11:BN:87:ASP:N	2.42	0.48
11:BN:91:LEU:HB3	11:BN:122:ILE:HD11	1.95	0.48
5:BE:104:ASP:OD2	5:BE:110:ARG:NH2	2.45	0.48
1:9:611:G:H21	1:9:618:C:H5''	1.79	0.48
1:9:1746:U:O2'	1:9:1747:C:OP1	2.31	0.47
16:BY:18:LEU:H	16:BY:18:LEU:HD22	1.79	0.47
2:BA:89:GLN:O	2:BA:92:VAL:HG12	2.14	0.47
4:BC:113:ILE:HG22	4:BC:139:ALA:HB1	1.96	0.47
1:9:772:U:H2'	1:9:773:C:H5''	1.95	0.47
1:9:1085:A:O3'	1:9:1086:U:H2'	2.13	0.47
1:9:1781:4AC:H5	1:9:1781:4AC:O7	2.14	0.47
4:BC:89:ASP:HB2	4:BC:113:ILE:HD11	1.96	0.47
6:BG:35:GLU:OE1	6:BG:35:GLU:N	2.48	0.47
1:9:750:U:H2'	1:9:751:A:O4'	2.15	0.47
5:BE:133:GLN:OE1	5:BE:134:LYS:N	2.47	0.47
1:9:549:A:C6	1:9:598:A:C8	3.02	0.47
1:9:1732:U:H2'	1:9:1733:C:C6	2.47	0.47
2:BA:170:ASN:OD1	2:BA:170:ASN:N	2.47	0.47
2:BA:203:MET:SD	2:BA:204:VAL:HG12	2.55	0.47
5:BE:95:THR:O	5:BE:95:THR:HG22	2.15	0.47
8:BI:156:LEU:HD12	8:BI:156:LEU:H	1.78	0.47
13:BV:22:ARG:NH1	13:BV:55:CYS:SG	2.76	0.47
1:9:1067:G:H2'	1:9:1068:G:C8	2.50	0.47
4:BC:151:ARG:NE	13:BV:10:GLU:OE1	2.41	0.47
4:BC:188:GLY:N	4:BC:206:ASP:OD1	2.48	0.47
1:9:879:G:HO2'	1:9:940:G:HO2'	1.58	0.47
1:9:860:A:O2'	1:9:861:U:O3'	2.33	0.46
1:9:1101:U:O4	4:BC:212:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BG:69:THR:O	6:BG:101:GLY:HA3	2.15	0.46
9:BJ:33:VAL:O	9:BJ:37:GLY:N	2.48	0.46
14:BW:32:LYS:O	14:BW:35:ILE:HG22	2.15	0.46
1:9:411:A:H2'	1:9:412:C:H6	1.81	0.46
1:9:816:C:N3	1:9:862:G:O2'	2.43	0.46
16:BY:99:ASP:OD1	16:BY:99:ASP:N	2.48	0.46
1:9:1721:G:H2'	1:9:1722:U:C6	2.50	0.46
1:9:1744:U:H2'	1:9:1745:A:C8	2.50	0.46
8:BI:89:ASN:OD1	8:BI:89:ASN:N	2.47	0.46
1:9:143:A:O2'	1:9:144:U:P	2.73	0.46
1:9:261:C:H2'	1:9:262:U:C6	2.50	0.46
4:BC:186:GLY:N	4:BC:206:ASP:OD2	2.48	0.46
5:BE:139:LEU:HD21	5:BE:147:ILE:HB	1.97	0.46
10:BL:108:ILE:HD11	10:BL:129:ASN:HB3	1.97	0.46
11:BN:67:THR:HG21	11:BN:74:ILE:HD11	1.97	0.46
16:BY:53:ASP:OD2	16:BY:56:ALA:HB2	2.16	0.46
1:9:15:U:H2'	1:9:16:G:O4'	2.15	0.46
1:9:810:U:O2'	14:BW:78:ARG:NH1	2.46	0.46
1:9:920:U:C2	1:9:921:U:C6	3.04	0.46
1:9:206:U:O4	1:9:207:A:N6	2.48	0.46
1:9:872:G:OP1	11:BN:121:ARG:NH1	2.48	0.46
1:9:1660:G:O6	1:9:1753:G:N2	2.49	0.46
2:BA:79:ILE:HB	2:BA:101:VAL:HG13	1.98	0.46
1:9:615:OMU:OP1	15:BX:17:ARG:NH1	2.38	0.46
1:9:573:C:O2	1:9:573:C:O4'	2.34	0.46
1:9:1067:G:C2	1:9:1068:G:N7	2.84	0.46
12:cS:38:ASP:OD1	12:cS:38:ASP:N	2.49	0.46
1:9:960:U:OP1	1:9:1076:U:O2'	2.34	0.46
4:BC:195:PRO:HA	4:BC:198:VAL:HG12	1.98	0.46
14:BW:36:LYS:HA	14:BW:39:ILE:HG22	1.98	0.46
1:9:98:C:H2'	1:9:99:U:C6	2.51	0.45
1:9:773:C:O2'	1:9:774:A:OP1	2.25	0.45
1:9:71:G:N1	1:9:82:G:C6	2.84	0.45
1:9:804:A:H4'	5:BE:201:HIS:CE1	2.51	0.45
1:9:799:U:C6	1:9:801:A:N6	2.84	0.45
2:BA:146:ASN:ND2	13:BV:29:HIS:O	2.49	0.45
17:BZ:86:VAL:HG13	17:BZ:86:VAL:O	2.16	0.45
7:BH:131:VAL:O	7:BH:131:VAL:CG1	2.63	0.45
1:9:919:A:C4	1:9:920:U:C6	3.05	0.45
1:9:26:A:O2'	1:9:27:U:P	2.73	0.45
1:9:902:A:H4'	12:cS:59:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:1732:U:C2	1:9:1733:C:C5	3.04	0.45
1:9:826:C:H3'	1:9:827:G:H21	1.82	0.45
1:9:1013:OMU:HM23	1:9:1013:OMU:H1'	1.74	0.45
1:9:1680:U:C2	1:9:1681:G:C8	3.04	0.45
1:9:1775:G:OP1	1:9:1778:U:H4'	2.17	0.45
5:BE:73:ASP:C	5:BE:164:LEU:HD11	2.42	0.45
8:BI:156:LEU:O	8:BI:160:ILE:HG12	2.17	0.45
1:9:875:A:C2	1:9:876:G:C6	3.05	0.45
8:BI:206:LEU:O	8:BI:210:MET:HG2	2.17	0.45
1:9:607:U:O2'	1:9:608:U:H5'	2.17	0.44
1:9:977:A:H2'	1:9:978:A2M:H8	1.99	0.44
1:9:410:U:H2'	1:9:411:A:H8	1.81	0.44
4:BC:66:ILE:O	4:BC:70:SER:N	2.50	0.44
17:BZ:64:LEU:N	17:BZ:64:LEU:HD12	2.32	0.44
1:9:25:C:N4	9:BJ:10:TYR:O	2.50	0.44
1:9:211:G:N2	1:9:255:U:C4	2.85	0.44
1:9:605:A:C5	1:9:606:U:C5	3.05	0.44
1:9:1057:G:H2'	1:9:1058:U:O4'	2.17	0.44
11:BN:63:VAL:O	11:BN:67:THR:HG22	2.18	0.44
14:BW:76:SER:HB3	14:BW:77:PRO:HD3	2.00	0.44
1:9:181:C:H42	1:9:200:C:H1'	1.82	0.44
1:9:392:OMG:N3	1:9:392:OMG:H2'	2.31	0.44
1:9:455:G:N1	1:9:460:G:C6	2.85	0.44
1:9:1725:C:O2	1:9:1725:C:H2'	2.18	0.44
1:9:485:A:H2'	1:9:486:U:C6	2.52	0.44
1:9:821:G:O6	1:9:859:A:C6	2.69	0.44
1:9:1685:G:C2	1:9:1731:G:O6	2.70	0.44
1:9:1780:C:H2'	1:9:1781:4AC:H6	1.99	0.44
1:9:34:G:H2'	1:9:35:U:H5''	1.99	0.44
1:9:606:U:O2	1:9:607:U:C5	2.70	0.44
1:9:1118:G:O2'	1:9:1134:G:O6	2.34	0.44
8:BI:58:ALA:HB2	8:BI:194:GLY:HA2	1.99	0.44
16:BY:90:LYS:HE2	16:BY:94:ILE:HD11	1.99	0.44
18:Bb:17:GLU:OE1	18:Bb:18:LYS:N	2.51	0.44
1:9:626:A:O2'	1:9:1036:G:OP2	2.26	0.44
1:9:748:G:O6	1:9:814:A:N6	2.51	0.44
1:9:1768:G:H1'	1:9:1789:MA6:H2	1.99	0.44
1:9:890:U:C2	1:9:891:A:C8	3.06	0.44
3:BB:174:ARG:NH1	3:BB:175:GLU:OE1	2.51	0.44
6:BG:156:ARG:HE	6:BG:157:LYS:H	1.64	0.44
8:BI:71:GLU:OE1	8:BI:73:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:70:ARG:NH2	9:BJ:74:GLU:OE2	2.51	0.44
1:9:181:C:N4	1:9:199:A:N1	2.66	0.44
1:9:824:U:H2'	1:9:825:U:C6	2.53	0.44
1:9:832:U:O2	1:9:848:G:C6	2.70	0.44
4:BC:137:ARG:O	4:BC:141:ILE:HG12	2.18	0.44
8:BI:118:TYR:O	8:BI:164:GLN:NE2	2.51	0.44
8:BI:160:ILE:O	8:BI:164:GLN:HG2	2.18	0.44
1:9:1737:U:H2'	1:9:1738:A:O4'	2.18	0.43
3:BB:38:PHE:CD2	3:BB:73:LEU:HD23	2.53	0.43
15:BX:57:GLU:N	15:BX:57:GLU:OE1	2.51	0.43
1:9:67:G:O6	1:9:84:G:O2'	2.34	0.43
1:9:615:OMU:HM23	1:9:615:OMU:H1'	1.69	0.43
1:9:888:C:H2'	1:9:889:G:C8	2.52	0.43
3:BB:72:ASP:OD1	17:BZ:59:TYR:OH	2.36	0.43
7:BH:83:GLU:O	7:BH:87:LYS:HG2	2.17	0.43
9:BJ:88:LEU:H	9:BJ:88:LEU:HD23	1.83	0.43
10:BL:156:LYS:HG2	10:BL:157:THR:HG23	2.00	0.43
1:9:409:C:H4'	6:BG:93:GLU:OE2	2.19	0.43
1:9:766:G:H22	1:9:767:A:H62	1.66	0.43
3:BB:69:SER:OG	12:cS:127:ARG:NH1	2.51	0.43
16:BY:23:GLN:NE2	16:BY:75:GLY:O	2.51	0.43
1:9:164:C:OP1	6:BG:133:ARG:NH1	2.52	0.43
1:9:1673:G:C6	1:9:1743:U:C4	3.07	0.43
1:9:448:C:N4	1:9:463:G:OP2	2.40	0.43
1:9:594:C:H2'	1:9:595:A:H8	1.84	0.43
3:BB:179:CYS:SG	3:BB:187:LYS:NZ	2.90	0.43
10:BL:147:ILE:CG2	10:BL:164:LYS:HB3	2.49	0.43
15:BX:45:HIS:HB3	15:BX:100:LEU:HD11	2.01	0.43
1:9:414:A:O2'	1:9:415:C:H5'	2.18	0.43
1:9:1066:A:C2	1:9:1067:G:N7	2.86	0.43
2:BA:119:THR:HG23	2:BA:120:SER:N	2.33	0.43
5:BE:200:LYS:HG3	5:BE:201:HIS:H	1.83	0.43
15:BX:60:GLN:N	15:BX:61:PRO:CD	2.81	0.43
1:9:120:G:H1'	1:9:401:A:C6	2.53	0.43
1:9:145:A:C5	1:9:146:A:C8	3.07	0.43
1:9:1048:U:H2'	1:9:1049:C:C6	2.53	0.43
7:BH:19:LEU:HA	7:BH:22:GLN:OE1	2.19	0.43
8:BI:77:THR:HB	8:BI:106:ASP:OD1	2.19	0.43
14:BW:7:LEU:HA	14:BW:34:ILE:HD11	2.00	0.43
1:9:166:A:HO2'	1:9:167:A:P	2.40	0.43
1:9:571:A:H62	1:9:580:G:H21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BB:52:GLN:OE1	3:BB:52:GLN:N	2.52	0.43
1:9:43:A:C4	1:9:382:A:C6	3.07	0.43
1:9:1664:G:H1'	1:9:1665:A:C8	2.53	0.43
1:9:187:C:H2'	1:9:188:U:O4'	2.19	0.42
1:9:568:G:N1	1:9:584:A:OP2	2.48	0.42
8:BI:207:GLU:OE1	8:BI:208:PHE:N	2.52	0.42
10:BL:124:GLU:OE1	15:BX:11:ARG:NH2	2.51	0.42
5:BE:180:VAL:HG23	5:BE:228:ILE:O	2.18	0.42
1:9:1679:G:OP1	6:BG:96:ARG:NH2	2.52	0.42
2:BA:17:GLU:HA	2:BA:20:ILE:HD13	2.01	0.42
7:BH:20:ASP:HA	7:BH:23:VAL:HG22	2.01	0.42
1:9:793:G:OP1	5:BE:106:LYS:NZ	2.43	0.42
1:9:1745:A:H2'	1:9:1746:U:O4'	2.19	0.42
17:BZ:64:LEU:HD12	17:BZ:64:LEU:H	1.85	0.42
1:9:183:C:C2	1:9:184:C:C5	3.08	0.42
7:BH:76:ILE:HG13	7:BH:76:ILE:O	2.19	0.42
1:9:29:U:H2'	1:9:30:G:H8	1.84	0.42
1:9:334:G:C6	1:9:335:A:C6	3.08	0.42
1:9:1086:U:O2'	1:9:1087:G:P	2.78	0.42
2:BA:109:THR:O	2:BA:112:THR:OG1	2.30	0.42
6:BG:5:VAL:HA	6:BG:113:LEU:O	2.20	0.42
6:BG:205:LYS:O	6:BG:205:LYS:HD3	2.19	0.42
1:9:902:A:H4'	12:cS:59:MET:CE	2.50	0.42
1:9:962:U:OP2	18:Bb:22:LYS:NZ	2.47	0.42
1:9:1066:A:H3'	1:9:1067:G:H8	1.84	0.42
1:9:1748:A:C6	1:9:1749:U:O4	2.73	0.42
4:BC:113:ILE:HG21	4:BC:139:ALA:C	2.44	0.42
1:9:55:A:H1'	1:9:430:G:N2	2.35	0.42
1:9:1106:G:OP1	14:BW:76:SER:OG	2.31	0.42
1:9:35:U:C4	1:9:478:A:C2	3.08	0.42
1:9:411:A:C2	1:9:412:C:C5	3.08	0.42
1:9:980:G:N7	1:9:1027:A:N6	2.68	0.42
1:9:1103:U:OP1	14:BW:71:LYS:NZ	2.53	0.42
1:9:308:U:O2	10:BL:92:ARG:NE	2.42	0.41
1:9:468:A2M:H5''	1:9:468:A2M:H8	2.02	0.41
1:9:1793:U:H2'	1:9:1794:G:H8	1.85	0.41
4:BC:69:HIS:O	4:BC:70:SER:OG	2.32	0.41
5:BE:19:MET:HE2	5:BE:108:ARG:NH1	2.35	0.41
18:Bb:43:PHE:O	18:Bb:43:PHE:CG	2.73	0.41
1:9:140:OMC:OP2	6:BG:182:ARG:NH2	2.53	0.41
1:9:551:U:C4	1:9:552:G:N7	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:1065:U:H3'	1:9:1066:A:C2	2.55	0.41
14:BW:114:GLU:OE1	14:BW:115:GLU:N	2.53	0.41
1:9:183:C:H2'	1:9:184:C:H6	1.85	0.41
1:9:559:A:O2'	1:9:560:A:P	2.78	0.41
1:9:804:A:H4'	5:BE:201:HIS:HE1	1.85	0.41
1:9:806:G:N1	1:9:807:G:C5	2.88	0.41
1:9:811:A:H2'	1:9:812:A:O4'	2.19	0.41
1:9:1672:C:N3	1:9:1743:U:C4	2.84	0.41
1:9:1763:A:H2'	1:9:1764:A:C8	2.55	0.41
1:9:1787:U:O4	20:Cn:12:ARG:NH1	2.50	0.41
12:cS:55:ILE:CD1	12:cS:79:ASP:HB2	2.50	0.41
15:BX:35:GLU:OE2	15:BX:36:TRP:NE1	2.53	0.41
15:BX:73:LEU:HD23	15:BX:73:LEU:HA	1.89	0.41
1:9:55:A:C4	1:9:430:G:C2	3.08	0.41
4:BC:45:TRP:O	4:BC:46:VAL:C	2.63	0.41
1:9:17:C:C2	1:9:18:C:C5	3.08	0.41
1:9:308:U:O4'	10:BL:150:GLN:NE2	2.54	0.41
1:9:987:G:O6	1:9:1023:A:N6	2.54	0.41
4:BC:157:ASN:O	4:BC:157:ASN:CG	2.64	0.41
6:BG:74:ARG:HA	6:BG:98:SER:HA	2.02	0.41
1:9:345:A:C4	1:9:346:C:C5	3.09	0.41
1:9:767:A:C5	1:9:794:A:N7	2.88	0.41
3:BB:147:ALA:O	3:BB:148:ASN:HB3	2.21	0.41
6:BG:32:LEU:HD11	6:BG:63:MET:HE3	2.03	0.41
6:BG:56:CYS:O	6:BG:109:SER:N	2.53	0.41
7:BH:174:TYR:HE1	7:BH:180:LYS:HG3	1.85	0.41
13:BV:28:ASP:OD1	13:BV:31:SER:N	2.53	0.41
1:9:88:C:O2'	1:9:167:A:N1	2.49	0.41
1:9:192:G:H2'	1:9:193:G:C8	2.56	0.41
1:9:482:A:C2'	1:9:483:C:H5'	2.51	0.41
1:9:148:C:H1'	1:9:163:G:N2	2.35	0.41
1:9:505:U:H2'	1:9:506:G:C8	2.55	0.41
1:9:766:G:N2	1:9:767:A:H62	2.18	0.41
1:9:875:A:O2'	1:9:876:G:H8	2.01	0.41
10:BL:98:CYS:SG	10:BL:101:ALA:HB2	2.61	0.41
10:BL:98:CYS:SG	10:BL:99:HIS:N	2.93	0.41
14:BW:28:ARG:HB3	14:BW:29:PRO:HD3	2.03	0.41
15:BX:17:ARG:NE	15:BX:17:ARG:HA	2.35	0.41
16:BY:93:LEU:O	16:BY:97:GLY:N	2.54	0.41
1:9:21:U:O2	1:9:21:U:O4'	2.39	0.41
1:9:40:A:C5	1:9:473:OMC:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:141:G:C2	1:9:142:G:C5	3.08	0.41
1:9:474:A:N3	1:9:474:A:H2'	2.36	0.41
1:9:820:G:HO2'	1:9:821:G:P	2.33	0.41
1:9:824:U:C2	1:9:857:G:C2	3.09	0.41
1:9:1131:G:C5	1:9:1132:C:C5	3.09	0.41
1:9:1695:G:C6	1:9:1721:G:O6	2.74	0.41
5:BE:141:THR:OG1	5:BE:143:ASP:OD1	2.23	0.41
16:BY:107:LYS:O	16:BY:111:GLU:HG2	2.20	0.41
1:9:899:G:N2	12:cS:51:THR:HG21	2.36	0.41
1:9:1086:U:O2'	1:9:1087:G:H8	2.04	0.41
5:BE:92:ILE:HD11	16:BY:18:LEU:HD21	2.02	0.41
7:BH:164:GLU:OE1	7:BH:164:GLU:N	2.54	0.41
9:BJ:112:GLN:O	9:BJ:115:VAL:HG12	2.21	0.41
15:BX:56:ILE:HG22	15:BX:57:GLU:N	2.35	0.41
1:9:871:G:OP2	11:BN:3:ARG:NH2	2.54	0.40
1:9:1079:C:H2'	1:9:1080:A:O4'	2.21	0.40
1:9:1086:U:O2'	1:9:1087:G:C8	2.74	0.40
1:9:1756:G:H2'	1:9:1757:A:C8	2.56	0.40
11:BN:24:SER:OG	18:Bb:86:ASP:O	2.35	0.40
1:9:57:G:OP1	16:BY:117:LYS:NZ	2.38	0.40
1:9:194:A:H2'	1:9:195:A:C8	2.56	0.40
1:9:617:G:H4'	1:9:618:C:OP1	2.22	0.40
1:9:899:G:H2'	1:9:900:U:C6	2.57	0.40
2:BA:104:ILE:O	2:BA:104:ILE:HG13	2.21	0.40
4:BC:233:TYR:CZ	13:BV:10:GLU:OE2	2.74	0.40
7:BH:74:ARG:HG2	7:BH:132:LEU:HD21	2.03	0.40
7:BH:162:ASN:O	7:BH:166:LYS:NZ	2.54	0.40
11:BN:99:ARG:O	11:BN:103:GLU:HG2	2.21	0.40
17:BZ:74:CYS:O	17:BZ:75:VAL:C	2.64	0.40
18:Bb:42:CYS:O	18:Bb:43:PHE:HB3	2.20	0.40
1:9:397:C:H2'	1:9:398:C:C6	2.57	0.40
1:9:455:G:C2	1:9:457:C:O2	2.74	0.40
1:9:910:A:H2'	1:9:911:A:C8	2.57	0.40
5:BE:200:LYS:HD2	5:BE:200:LYS:HA	1.94	0.40
8:BI:207:GLU:HA	8:BI:210:MET:HG2	2.04	0.40
10:BL:148:ILE:HG22	10:BL:162:VAL:HA	2.04	0.40
18:Bb:44:ASN:OD1	18:Bb:60:ASN:ND2	2.46	0.40
1:9:1745:A:H2'	1:9:1746:U:C6	2.57	0.40
5:BE:133:GLN:OE1	5:BE:134:LYS:HB3	2.21	0.40
5:BE:139:LEU:H	5:BE:139:LEU:HD23	1.87	0.40
5:BE:149:TYR:HD2	6:BG:209:ASP:OD1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BY:14:MET:HE2	16:BY:23:GLN:CB	2.52	0.40
1:9:40:A:C2	1:9:473:OMC:C6	3.10	0.40
1:9:98:C:H2'	1:9:99:U:H6	1.86	0.40
1:9:333:G:H2'	1:9:334:G:H8	1.87	0.40
6:BG:107:ASP:OD1	6:BG:107:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BA	185/280 (66%)	181 (98%)	4 (2%)	0	100	100
3	BB	206/262 (79%)	194 (94%)	12 (6%)	0	100	100
4	BC	214/276 (78%)	204 (95%)	10 (5%)	0	100	100
5	BE	253/261 (97%)	236 (93%)	17 (7%)	0	100	100
6	BG	191/249 (77%)	182 (95%)	8 (4%)	1 (0%)	24	55
7	BH	172/191 (90%)	170 (99%)	2 (1%)	0	100	100
8	BI	179/222 (81%)	175 (98%)	4 (2%)	0	100	100
9	BJ	169/197 (86%)	160 (95%)	9 (5%)	0	100	100
10	BL	136/160 (85%)	133 (98%)	3 (2%)	0	100	100
11	BN	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
12	cS	124/150 (83%)	116 (94%)	8 (6%)	0	100	100
13	BV	70/82 (85%)	70 (100%)	0	0	100	100
14	BW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
15	BX	136/142 (96%)	130 (96%)	6 (4%)	0	100	100
16	BY	106/133 (80%)	103 (97%)	3 (3%)	0	100	100
17	BZ	95/130 (73%)	91 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Bb	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
19	Be	32/62 (52%)	32 (100%)	0	0	100	100
20	Cn	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
All	All	2645/3189 (83%)	2544 (96%)	100 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	BG	14	LYS

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	
2	BA	161/221 (73%)	159 (99%)	2 (1%)	63	75
3	BB	185/226 (82%)	184 (100%)	1 (0%)	81	83
4	BC	185/225 (82%)	183 (99%)	2 (1%)	65	76
5	BE	224/228 (98%)	218 (97%)	6 (3%)	39	63
6	BG	170/213 (80%)	170 (100%)	0	100	100
7	BH	159/169 (94%)	157 (99%)	2 (1%)	61	74
8	BI	156/183 (85%)	154 (99%)	2 (1%)	61	74
9	BJ	153/172 (89%)	152 (99%)	1 (1%)	76	80
10	BL	119/135 (88%)	118 (99%)	1 (1%)	73	79
11	BN	132/133 (99%)	131 (99%)	1 (1%)	73	79
12	cS	99/120 (82%)	97 (98%)	2 (2%)	48	68
13	BV	59/67 (88%)	58 (98%)	1 (2%)	53	71
14	BW	111/112 (99%)	111 (100%)	0	100	100
15	BX	110/114 (96%)	108 (98%)	2 (2%)	51	70
16	BY	98/114 (86%)	96 (98%)	2 (2%)	48	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	BZ	86/108 (80%)	83 (96%)	3 (4%)	32	58
18	Bb	77/78 (99%)	77 (100%)	0	100	100
19	Be	27/49 (55%)	27 (100%)	0	100	100
20	Cn	21/24 (88%)	21 (100%)	0	100	100
All	All	2332/2691 (87%)	2304 (99%)	28 (1%)	61	75

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BA	118	GLN
2	BA	123	GLU
3	BB	131	ASP
4	BC	145	LEU
4	BC	205	ASP
5	BE	13	ASN
5	BE	44	LEU
5	BE	98	ASN
5	BE	133	GLN
5	BE	134	LYS
5	BE	230	LYS
7	BH	22	GLN
7	BH	61	ILE
8	BI	89	ASN
8	BI	90	GLU
9	BJ	67	LYS
10	BL	112	ASP
11	BN	117	LEU
12	cS	96	LEU
12	cS	137	ASP
13	BV	69	ASP
15	BX	71	VAL
15	BX	101	ILE
16	BY	18	LEU
16	BY	76	LEU
17	BZ	52	ASP
17	BZ	73	TYR
17	BZ	76	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	BA	82	GLN
2	BA	146	ASN
3	BB	42	ASN
5	BE	17	HIS
6	BG	87	HIS
7	BH	64	ASN
9	BJ	135	HIS
9	BJ	141	GLN
10	BL	34	GLN
10	BL	99	HIS
13	BV	42	ASN
17	BZ	7	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	9	1066/1804 (59%)	249 (23%)	13 (1%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	9	4	C
1	9	6	G
1	9	25	C
1	9	26	A
1	9	27	U
1	9	28	A2M
1	9	29	U
1	9	34	G
1	9	35	U
1	9	36	C
1	9	38	OMC
1	9	40	A
1	9	42	G
1	9	43	A
1	9	45	U
1	9	47	A
1	9	59	G
1	9	60	U
1	9	62	A
1	9	68	A
1	9	69	A

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Mol	Chain	Res	Type
1	9	85	A
1	9	115	A
1	9	116	G
1	9	117	U
1	9	142	G
1	9	144	U
1	9	145	A
1	9	148	C
1	9	149	G
1	9	151	A
1	9	157	U
1	9	158	C
1	9	161	G
1	9	166	A
1	9	167	A
1	9	168	U
1	9	186	A
1	9	189	U
1	9	190	A
1	9	191	U
1	9	192	G
1	9	194	A
1	9	247	A
1	9	252	U
1	9	253	C
1	9	260	A
1	9	269	A
1	9	270	U
1	9	287	U
1	9	294	G
1	9	303	A
1	9	313	C
1	9	317	U
1	9	320	A
1	9	325	C
1	9	326	G
1	9	337	A
1	9	341	G
1	9	342	C
1	9	356	A
1	9	363	G
1	9	365	C

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Mol	Chain	Res	Type
1	9	370	A
1	9	373	U
1	9	374	A
1	9	381	G
1	9	382	A
1	9	390	G
1	9	392	OMG
1	9	394	G
1	9	403	A
1	9	404	A
1	9	406	C
1	9	408	G
1	9	416	A
1	9	420	A
1	9	425	A
1	9	428	C
1	9	436	G
1	9	441	A
1	9	443	U
1	9	444	U
1	9	447	C
1	9	448	C
1	9	449	A
1	9	451	U
1	9	452	C
1	9	455	G
1	9	456	A
1	9	457	C
1	9	458	A
1	9	459	C
1	9	460	G
1	9	468	A2M
1	9	469	G
1	9	472	A
1	9	473	OMC
1	9	479	A
1	9	480	U
1	9	481	A
1	9	482	A
1	9	483	C
1	9	484	A
1	9	504	C

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Mol	Chain	Res	Type
1	9	510	A
1	9	511	U
1	9	515	A
1	9	518	G
1	9	519	A
1	9	522	A
1	9	523	C
1	9	524	A
1	9	528	U
1	9	531	A
1	9	533	C
1	9	537	U
1	9	538	A
1	9	543	G
1	9	545	A
1	9	546	U
1	9	548	C
1	9	549	A
1	9	555	G
1	9	559	A
1	9	560	A
1	9	563	C
1	9	569	C
1	9	572	G
1	9	580	G
1	9	581	G
1	9	582	U
1	9	583	A
1	9	598	A
1	9	600	C
1	9	615	OMU
1	9	623	A2M
1	9	624	A
1	9	626	A
1	9	628	G
1	9	643	U
1	9	759	G
1	9	760	A
1	9	770	G
1	9	771	C
1	9	773	C
1	9	774	A

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Mol	Chain	Res	Type
1	9	776	A
1	9	779	A
1	9	790	C
1	9	791	U
1	9	793	G
1	9	794	A
1	9	796	A
1	9	797	C
1	9	798	A
1	9	799	U
1	9	800	U
1	9	801	A
1	9	813	C
1	9	816	C
1	9	817	A
1	9	818	U
1	9	819	A
1	9	821	G
1	9	829	U
1	9	830	C
1	9	832	U
1	9	833	A
1	9	834	U
1	9	860	A
1	9	861	U
1	9	863	A
1	9	864	U
1	9	866	A
1	9	867	A
1	9	876	G
1	9	880	G
1	9	902	A
1	9	916	U
1	9	917	G
1	9	918	G
1	9	927	A
1	9	937	A
1	9	946	G
1	9	957	G
1	9	964	U
1	9	970	A
1	9	974	A

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Mol	Chain	Res	Type
1	9	977	A
1	9	978	A2M
1	9	989	G
1	9	992	C
1	9	996	A
1	9	997	A
1	9	1009	A
1	9	1014	C
1	9	1015	C
1	9	1024	A
1	9	1027	A
1	9	1030	A
1	9	1031	A
1	9	1032	C
1	9	1047	A
1	9	1080	A
1	9	1085	A
1	9	1086	U
1	9	1087	G
1	9	1091	A
1	9	1096	A
1	9	1100	U
1	9	1101	U
1	9	1104	G
1	9	1113	G
1	9	1128	A
1	9	1142	A
1	9	1664	G
1	9	1665	A
1	9	1669	A
1	9	1677	A
1	9	1686	G
1	9	1688	U
1	9	1719	A
1	9	1720	C
1	9	1721	G
1	9	1722	U
1	9	1723	C
1	9	1725	C
1	9	1729	A
1	9	1731	G
1	9	1747	C

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Mol	Chain	Res	Type
1	9	1750	U
1	9	1753	G
1	9	1754	A
1	9	1758	A2M
1	9	1759	G
1	9	1763	A
1	9	1764	A
1	9	1770	A
1	9	1775	G
1	9	1777	U
1	9	1781	4AC
1	9	1788	G
1	9	1790	MA6
1	9	1791	C
1	9	1800	G
1	9	1801	G
1	9	1802	A
1	9	1804	C

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	9	26	A
1	9	68	A
1	9	166	A
1	9	324	U
1	9	559	A
1	9	773	C
1	9	798	A
1	9	820	G
1	9	926	A
1	9	956	A
1	9	1746	U
1	9	1763	A
1	9	1769	U

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	9	468	1	22,25,26	3.39	9 (40%)	31,36,39	2.84	10 (32%)
1	OMG	9	392	1	23,26,27	2.62	9 (39%)	33,38,41	2.03	11 (33%)
1	OMU	9	123	1	19,22,23	2.54	7 (36%)	26,31,34	2.20	5 (19%)
1	OMG	9	246	1	23,26,27	2.69	8 (34%)	33,38,41	2.20	11 (33%)
1	OMC	9	140	1	19,22,23	3.03	8 (42%)	26,31,34	0.61	0
1	OMU	9	615	1	19,22,23	2.67	6 (31%)	26,31,34	2.08	7 (26%)
1	OMU	9	1013	1	19,22,23	2.52	7 (36%)	26,31,34	2.31	8 (30%)
1	A2M	9	28	1	22,25,26	3.41	9 (40%)	31,36,39	2.63	10 (32%)
1	OMC	9	1645	1	19,22,23	2.95	8 (42%)	26,31,34	0.66	0
1	4AC	9	1781	1	21,24,25	3.55	9 (42%)	29,34,37	1.34	4 (13%)
1	UY1	9	604	1	19,22,23	4.09	8 (42%)	22,31,34	2.40	5 (22%)
1	OMC	9	38	1	19,22,23	2.98	8 (42%)	26,31,34	0.64	0
1	A2M	9	978	1	22,25,26	3.43	10 (45%)	31,36,39	2.62	10 (32%)
1	MA6	9	1789	1	23,26,27	1.32	3 (13%)	34,38,41	2.98	13 (38%)
1	A2M	9	1758	1	22,25,26	3.39	9 (40%)	31,36,39	2.60	10 (32%)
1	MA6	9	1790	1	23,26,27	1.31	3 (13%)	34,38,41	3.05	11 (32%)
1	OMC	9	473	1	19,22,23	2.99	8 (42%)	26,31,34	0.78	1 (3%)
1	A2M	9	623	1,22	22,25,26	3.38	10 (45%)	31,36,39	2.91	11 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	9	468	1	-	2/9/27/28	0/3/3/3
1	OMG	9	392	1	-	3/9/27/28	0/3/3/3
1	OMU	9	123	1	-	0/9/27/28	0/2/2/2
1	OMG	9	246	1	-	2/9/27/28	0/3/3/3
1	OMC	9	140	1	-	3/9/27/28	0/2/2/2
1	OMU	9	615	1	-	5/9/27/28	0/2/2/2
1	OMU	9	1013	1	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	9	28	1	-	3/9/27/28	0/3/3/3
1	OMC	9	1645	1	-	0/9/27/28	0/2/2/2
1	4AC	9	1781	1	-	2/11/29/30	0/2/2/2
1	UY1	9	604	1	-	2/9/27/28	0/2/2/2
1	OMC	9	38	1	-	2/9/27/28	0/2/2/2
1	A2M	9	978	1	-	2/9/27/28	0/3/3/3
1	MA6	9	1789	1	-	3/11/29/30	0/3/3/3
1	A2M	9	1758	1	-	2/9/27/28	0/3/3/3
1	MA6	9	1790	1	-	6/11/29/30	0/3/3/3
1	OMC	9	473	1	-	3/9/27/28	0/2/2/2
1	A2M	9	623	1,22	-	2/9/27/28	0/3/3/3

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9	604	UY1	C6-C5	10.62	1.47	1.35
1	9	604	UY1	C2-N1	9.24	1.49	1.36
1	9	978	A2M	C2'-C1'	-8.53	1.31	1.53
1	9	1758	A2M	C2'-C1'	-8.52	1.31	1.53
1	9	468	A2M	O4'-C1'	8.51	1.62	1.42
1	9	468	A2M	C2'-C1'	-8.50	1.31	1.53
1	9	623	A2M	C2'-C1'	-8.49	1.31	1.53
1	9	978	A2M	O4'-C1'	8.44	1.62	1.42
1	9	28	A2M	C2'-C1'	-8.43	1.31	1.53
1	9	28	A2M	O4'-C1'	8.42	1.61	1.42
1	9	1758	A2M	O4'-C1'	8.36	1.61	1.42
1	9	623	A2M	O4'-C1'	8.20	1.61	1.42
1	9	1781	4AC	C6-C5	7.41	1.52	1.35
1	9	1781	4AC	C4-N3	7.20	1.45	1.32
1	9	1781	4AC	C2-N3	6.92	1.50	1.36
1	9	246	OMG	C4-N3	6.87	1.50	1.34
1	9	392	OMG	C4-N3	6.55	1.49	1.34
1	9	623	A2M	O4'-C4'	-6.44	1.30	1.45
1	9	140	OMC	C2-N3	6.40	1.49	1.36
1	9	615	OMU	C2-N1	6.39	1.48	1.38
1	9	604	UY1	C2-N3	6.32	1.48	1.37
1	9	123	OMU	C2-N1	6.31	1.48	1.38
1	9	246	OMG	C2-N3	6.24	1.48	1.33
1	9	28	A2M	O4'-C4'	-6.22	1.31	1.45
1	9	38	OMC	C2-N3	6.19	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9	473	OMC	C2-N3	6.18	1.48	1.36
1	9	468	A2M	O4'-C4'	-6.17	1.31	1.45
1	9	1645	OMC	C2-N3	6.11	1.48	1.36
1	9	1758	A2M	O4'-C4'	-6.09	1.31	1.45
1	9	1013	OMU	C2-N1	6.08	1.48	1.38
1	9	392	OMG	C2-N3	6.07	1.47	1.33
1	9	978	A2M	O4'-C4'	-6.03	1.31	1.45
1	9	1781	4AC	C7-N4	6.01	1.48	1.37
1	9	38	OMC	C6-C5	5.99	1.49	1.35
1	9	140	OMC	C6-C5	5.95	1.48	1.35
1	9	1645	OMC	C6-C5	5.94	1.48	1.35
1	9	615	OMU	C6-C5	5.86	1.48	1.35
1	9	473	OMC	C6-C5	5.81	1.48	1.35
1	9	123	OMU	C6-C5	5.67	1.48	1.35
1	9	1013	OMU	C6-C5	5.61	1.48	1.35
1	9	246	OMG	C2-N2	5.46	1.47	1.34
1	9	140	OMC	C4-N3	5.45	1.45	1.34
1	9	473	OMC	C4-N3	5.38	1.45	1.34
1	9	615	OMU	C2-N3	5.31	1.47	1.38
1	9	392	OMG	C2-N2	5.27	1.46	1.34
1	9	1645	OMC	C4-N3	5.25	1.45	1.34
1	9	38	OMC	C4-N3	5.23	1.45	1.34
1	9	604	UY1	C6-N1	5.18	1.44	1.36
1	9	604	UY1	C1'-C5	-5.07	1.38	1.50
1	9	1781	4AC	C4-N4	5.05	1.47	1.39
1	9	1013	OMU	C2-N3	4.85	1.46	1.38
1	9	473	OMC	C2-N1	4.69	1.50	1.40
1	9	123	OMU	C2-N3	4.65	1.46	1.38
1	9	468	A2M	C6-N6	4.61	1.45	1.34
1	9	140	OMC	C4-N4	4.60	1.44	1.33
1	9	1645	OMC	C4-N4	4.53	1.44	1.33
1	9	38	OMC	C4-N4	4.49	1.44	1.33
1	9	140	OMC	C2-N1	4.48	1.49	1.40
1	9	473	OMC	C4-N4	4.44	1.44	1.33
1	9	1758	A2M	C6-N6	4.39	1.45	1.34
1	9	38	OMC	C2-N1	4.39	1.49	1.40
1	9	1781	4AC	C5-C4	4.37	1.50	1.40
1	9	623	A2M	C6-N6	4.28	1.44	1.34
1	9	28	A2M	C6-N6	4.25	1.44	1.34
1	9	978	A2M	C6-N6	4.23	1.44	1.34
1	9	1645	OMC	C2-N1	4.20	1.49	1.40
1	9	1781	4AC	C2-N1	3.85	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9	978	A2M	C5-C4	-3.63	1.32	1.39
1	9	392	OMG	C5-N7	-3.52	1.32	1.39
1	9	1789	MA6	C6-N6	3.49	1.47	1.36
1	9	28	A2M	C5-C4	-3.38	1.32	1.39
1	9	1790	MA6	C6-N6	3.34	1.46	1.36
1	9	1758	A2M	C5-C4	-3.30	1.32	1.39
1	9	140	OMC	C6-N1	3.29	1.45	1.38
1	9	623	A2M	O3'-C3'	-3.29	1.35	1.43
1	9	246	OMG	C5-N7	-3.26	1.32	1.39
1	9	246	OMG	C2-N1	3.24	1.45	1.37
1	9	1645	OMC	C6-N1	3.20	1.45	1.38
1	9	473	OMC	C6-N1	3.17	1.45	1.38
1	9	392	OMG	C2-N1	3.15	1.45	1.37
1	9	38	OMC	C6-N1	3.14	1.45	1.38
1	9	978	A2M	O3'-C3'	-3.14	1.35	1.43
1	9	28	A2M	O3'-C3'	-3.12	1.35	1.43
1	9	468	A2M	O3'-C3'	-3.09	1.35	1.43
1	9	978	A2M	C5-N7	-3.05	1.33	1.39
1	9	28	A2M	C5-N7	-3.01	1.33	1.39
1	9	1013	OMU	O4-C4	-2.97	1.18	1.24
1	9	623	A2M	C5-C4	-2.93	1.33	1.39
1	9	615	OMU	C4-N3	2.92	1.43	1.38
1	9	604	UY1	C4-N3	2.91	1.44	1.38
1	9	473	OMC	C5-C4	2.91	1.49	1.42
1	9	615	OMU	O4-C4	-2.88	1.18	1.24
1	9	1758	A2M	O3'-C3'	-2.87	1.36	1.43
1	9	1758	A2M	C5-N7	-2.87	1.33	1.39
1	9	123	OMU	O4-C4	-2.83	1.19	1.24
1	9	28	A2M	O2'-C2'	2.81	1.49	1.42
1	9	1645	OMC	O2-C2	-2.80	1.18	1.23
1	9	38	OMC	O2-C2	-2.80	1.18	1.23
1	9	468	A2M	O2'-C2'	2.79	1.49	1.42
1	9	1789	MA6	C5-C4	-2.77	1.33	1.39
1	9	140	OMC	C5-C4	2.76	1.49	1.42
1	9	246	OMG	O6-C6	-2.73	1.18	1.23
1	9	140	OMC	O2-C2	-2.73	1.18	1.23
1	9	38	OMC	C5-C4	2.73	1.49	1.42
1	9	1013	OMU	C4-N3	2.68	1.43	1.38
1	9	392	OMG	O6-C6	-2.68	1.18	1.23
1	9	473	OMC	O2-C2	-2.67	1.18	1.23
1	9	623	A2M	O2'-C2'	2.63	1.49	1.42
1	9	1645	OMC	C5-C4	2.63	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9	1758	A2M	O2'-C2'	2.62	1.49	1.42
1	9	1781	4AC	C6-N1	2.62	1.44	1.38
1	9	1790	MA6	C5-C4	-2.59	1.34	1.39
1	9	123	OMU	C4-N3	2.58	1.43	1.38
1	9	468	A2M	C5-C4	-2.58	1.34	1.39
1	9	623	A2M	C5-N7	-2.57	1.34	1.39
1	9	978	A2M	O2'-C2'	2.54	1.49	1.42
1	9	468	A2M	C5-N7	-2.53	1.34	1.39
1	9	246	OMG	C6-N1	2.49	1.43	1.38
1	9	246	OMG	C5-C6	2.49	1.53	1.44
1	9	1790	MA6	C5-N7	-2.47	1.34	1.39
1	9	615	OMU	O2-C2	-2.44	1.18	1.23
1	9	604	UY1	O2-C2	-2.44	1.18	1.23
1	9	604	UY1	O4-C4	-2.35	1.19	1.23
1	9	623	A2M	C8-N9	-2.33	1.33	1.37
1	9	123	OMU	O2-C2	-2.32	1.18	1.23
1	9	392	OMG	C5-C6	2.31	1.53	1.44
1	9	978	A2M	C8-N9	-2.30	1.33	1.37
1	9	123	OMU	C5-C4	2.23	1.48	1.43
1	9	468	A2M	C8-N9	-2.22	1.33	1.37
1	9	392	OMG	C4-N9	-2.18	1.32	1.38
1	9	1789	MA6	C5-N7	-2.16	1.34	1.39
1	9	1013	OMU	O2-C2	-2.15	1.19	1.23
1	9	392	OMG	C6-N1	2.08	1.42	1.38
1	9	623	A2M	O5'-C5'	-2.07	1.39	1.44
1	9	1013	OMU	C5-C4	2.07	1.48	1.43
1	9	28	A2M	C8-N9	-2.04	1.33	1.37
1	9	1758	A2M	O5'-C5'	-2.03	1.39	1.44
1	9	1781	4AC	O2-C2	-2.01	1.20	1.23
1	9	978	A2M	O5'-C5'	-2.00	1.39	1.44

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9	1790	MA6	N1-C6-N6	-11.52	104.49	117.08
1	9	1789	MA6	N1-C6-N6	-11.38	104.64	117.08
1	9	623	A2M	N6-C6-N1	-8.71	99.27	118.35
1	9	468	A2M	N6-C6-N1	-8.31	100.15	118.35
1	9	623	A2M	C5-C6-N6	7.52	139.80	123.43
1	9	468	A2M	C5-C6-N6	7.38	139.50	123.43
1	9	978	A2M	C5-C4-N3	-6.03	118.88	126.75
1	9	28	A2M	N6-C6-N1	-5.97	105.28	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9	1758	A2M	N6-C6-N1	-5.95	105.31	118.35
1	9	28	A2M	C5-C4-N3	-5.93	119.02	126.75
1	9	978	A2M	N6-C6-N1	-5.87	105.50	118.35
1	9	1758	A2M	C5-C4-N3	-5.86	119.11	126.75
1	9	123	OMU	C4-N3-C2	-5.85	118.86	126.58
1	9	1013	OMU	C4-N3-C2	-5.77	118.96	126.58
1	9	246	OMG	C5-C4-N3	-5.71	119.20	128.46
1	9	604	UY1	N1-C2-N3	5.64	121.52	115.13
1	9	392	OMG	C5-C4-N3	-5.63	119.32	128.46
1	9	1789	MA6	C5-C6-N6	5.61	135.07	125.30
1	9	604	UY1	O2-C2-N1	-5.60	116.62	122.79
1	9	615	OMU	C4-N3-C2	-5.58	119.22	126.58
1	9	1790	MA6	C5-C6-N6	5.57	135.01	125.30
1	9	28	A2M	N3-C2-N1	-5.53	119.95	128.60
1	9	1790	MA6	C5-C4-N3	-5.51	119.56	126.75
1	9	1758	A2M	N3-C2-N1	-5.48	120.03	128.60
1	9	1013	OMU	O4-C4-C5	-5.45	115.58	125.16
1	9	604	UY1	C4-N3-C2	-5.42	118.52	126.34
1	9	468	A2M	N3-C2-N1	-5.41	120.14	128.60
1	9	978	A2M	N3-C2-N1	-5.37	120.19	128.60
1	9	1789	MA6	N1-C2-N3	-5.31	120.30	128.60
1	9	28	A2M	C5-C6-N6	5.20	134.75	123.43
1	9	1758	A2M	C5-C6-N6	5.14	134.62	123.43
1	9	1790	MA6	N1-C2-N3	-5.06	120.69	128.60
1	9	978	A2M	C5-C6-N6	5.04	134.41	123.43
1	9	623	A2M	N3-C2-N1	-5.03	120.73	128.60
1	9	468	A2M	C5-C4-N3	-5.01	120.21	126.75
1	9	246	OMG	C2-N3-C4	5.00	121.21	112.30
1	9	123	OMU	O4-C4-C5	-4.89	116.55	125.16
1	9	623	A2M	C5-C4-N3	-4.85	120.42	126.75
1	9	123	OMU	N3-C2-N1	4.73	121.17	114.89
1	9	1013	OMU	N3-C2-N1	4.66	121.07	114.89
1	9	1789	MA6	N9-C8-N7	-4.65	107.55	113.91
1	9	392	OMG	C2-N3-C4	4.58	120.47	112.30
1	9	1789	MA6	C5-C4-N3	-4.56	120.80	126.75
1	9	1013	OMU	C5-C4-N3	4.54	121.64	114.84
1	9	615	OMU	O4-C4-C5	-4.41	117.40	125.16
1	9	123	OMU	C5-C4-N3	4.38	121.40	114.84
1	9	604	UY1	C6-N1-C2	-4.38	118.21	122.68
1	9	978	A2M	N9-C8-N7	-4.34	107.98	113.91
1	9	615	OMU	C5-C4-N3	4.26	121.21	114.84
1	9	615	OMU	N3-C2-N1	4.25	120.54	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9	1758	A2M	N9-C8-N7	-4.22	108.14	113.91
1	9	1790	MA6	N9-C8-N7	-4.21	108.16	113.91
1	9	28	A2M	N9-C8-N7	-4.16	108.22	113.91
1	9	623	A2M	N9-C8-N7	-3.97	108.48	113.91
1	9	1781	4AC	N4-C4-N3	3.93	120.46	113.85
1	9	1790	MA6	C4-C5-C6	3.87	120.21	115.88
1	9	246	OMG	C1'-N9-C4	-3.78	115.29	126.50
1	9	468	A2M	N9-C8-N7	-3.69	108.87	113.91
1	9	1758	A2M	C2-N3-C4	3.62	120.30	111.75
1	9	246	OMG	C1'-N9-C8	3.61	136.98	126.70
1	9	28	A2M	C2-N3-C4	3.61	120.28	111.75
1	9	978	A2M	C2-N3-C4	3.60	120.27	111.75
1	9	468	A2M	C2-N3-C4	3.58	120.22	111.75
1	9	978	A2M	N3-C4-N9	3.57	132.96	127.08
1	9	1790	MA6	N3-C4-N9	3.55	132.92	127.08
1	9	623	A2M	C2-N3-C4	3.50	120.01	111.75
1	9	1790	MA6	C2-N3-C4	3.41	119.80	111.75
1	9	28	A2M	N3-C4-N9	3.40	132.68	127.08
1	9	1758	A2M	N3-C4-N9	3.39	132.66	127.08
1	9	1789	MA6	C2-N1-C6	3.38	119.74	111.75
1	9	1789	MA6	C2-N3-C4	3.34	119.64	111.75
1	9	392	OMG	N9-C4-N3	3.32	132.60	125.94
1	9	246	OMG	C2-N1-C6	-3.31	119.07	125.10
1	9	1789	MA6	C5-N7-C8	3.24	108.11	103.51
1	9	246	OMG	N9-C4-N3	3.23	132.42	125.94
1	9	246	OMG	C5-C6-N1	3.17	121.25	113.19
1	9	1790	MA6	C2-N1-C6	3.17	119.25	111.75
1	9	392	OMG	C2-N1-C6	-3.12	119.42	125.10
1	9	246	OMG	O6-C6-C5	-3.11	118.34	126.60
1	9	978	A2M	C5-N7-C8	3.08	107.89	103.51
1	9	28	A2M	C5-N7-C8	3.05	107.84	103.51
1	9	978	A2M	C6-C5-C4	3.05	121.28	117.18
1	9	1790	MA6	C5-N7-C8	3.04	107.83	103.51
1	9	392	OMG	C1'-N9-C4	-3.04	117.48	126.50
1	9	123	OMU	O2-C2-N1	-3.03	118.75	122.79
1	9	1758	A2M	C5-N7-C8	3.02	107.80	103.51
1	9	1789	MA6	C4-C5-C6	3.01	119.25	115.88
1	9	392	OMG	O6-C6-C5	-2.97	118.72	126.60
1	9	392	OMG	C1'-N9-C8	2.96	135.13	126.70
1	9	468	A2M	C5-N7-C8	2.96	107.71	103.51
1	9	623	A2M	C5-N7-C8	2.96	107.71	103.51
1	9	1781	4AC	C5-C4-N3	-2.93	117.88	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9	1781	4AC	CM7-C7-N4	2.87	120.27	115.29
1	9	28	A2M	C6-C5-C4	2.86	121.03	117.18
1	9	392	OMG	C5-C6-N1	2.85	120.42	113.19
1	9	246	OMG	N9-C8-N7	-2.72	108.27	113.39
1	9	1758	A2M	C6-C5-C4	2.71	120.83	117.18
1	9	468	A2M	N3-C4-N9	2.67	131.47	127.08
1	9	1013	OMU	C1'-N1-C2	2.67	122.40	117.57
1	9	1013	OMU	O2-C2-N1	-2.58	119.36	122.79
1	9	623	A2M	C5-C4-N9	2.54	108.73	105.78
1	9	615	OMU	O2-C2-N1	-2.53	119.42	122.79
1	9	623	A2M	C4-C5-N7	-2.48	107.59	110.62
1	9	1789	MA6	C4-N9-C8	2.45	108.39	105.73
1	9	246	OMG	N2-C2-N1	2.44	121.91	116.71
1	9	615	OMU	C1'-N1-C2	2.42	121.95	117.57
1	9	1789	MA6	C4-C5-N7	-2.38	107.72	110.62
1	9	1013	OMU	O4-C4-N3	2.37	122.78	119.31
1	9	1789	MA6	N3-C4-N9	2.36	130.97	127.08
1	9	473	OMC	C2'-C1'-N1	-2.33	109.70	114.22
1	9	246	OMG	N1-C2-N3	-2.33	118.98	123.32
1	9	623	A2M	C3'-C2'-C1'	2.31	107.23	102.89
1	9	468	A2M	C4-C5-N7	-2.30	107.81	110.62
1	9	623	A2M	N3-C4-N9	2.28	130.84	127.08
1	9	392	OMG	N9-C8-N7	-2.27	109.11	113.39
1	9	392	OMG	N2-C2-N1	2.23	121.47	116.71
1	9	1781	4AC	C4-N3-C2	2.19	123.10	120.12
1	9	1790	MA6	C4-N9-C8	2.18	108.09	105.73
1	9	468	A2M	C5-C4-N9	2.17	108.31	105.78
1	9	28	A2M	C5-C4-N9	2.16	108.30	105.78
1	9	1789	MA6	C5-C4-N9	2.11	108.23	105.78
1	9	604	UY1	C5-C4-N3	2.10	121.34	116.58
1	9	1758	A2M	C5-C4-N9	2.10	108.22	105.78
1	9	1013	OMU	C6-N1-C2	-2.08	118.33	120.99
1	9	392	OMG	N1-C2-N3	-2.07	119.46	123.32
1	9	978	A2M	C5-C4-N9	2.04	108.15	105.78
1	9	615	OMU	CM2-O2'-C2'	2.02	119.82	114.52

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	9	28	A2M	C3'-C4'-C5'-O5'
1	9	38	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	9	38	OMC	O4'-C4'-C5'-O5'
1	9	246	OMG	O4'-C4'-C5'-O5'
1	9	246	OMG	C3'-C4'-C5'-O5'
1	9	392	OMG	O4'-C4'-C5'-O5'
1	9	392	OMG	C3'-C4'-C5'-O5'
1	9	468	A2M	O4'-C4'-C5'-O5'
1	9	468	A2M	C3'-C4'-C5'-O5'
1	9	473	OMC	O4'-C4'-C5'-O5'
1	9	615	OMU	C1'-C2'-O2'-CM2
1	9	615	OMU	O4'-C4'-C5'-O5'
1	9	978	A2M	O4'-C4'-C5'-O5'
1	9	978	A2M	C3'-C4'-C5'-O5'
1	9	1013	OMU	C1'-C2'-O2'-CM2
1	9	1758	A2M	O4'-C4'-C5'-O5'
1	9	1758	A2M	C3'-C4'-C5'-O5'
1	9	1781	4AC	O4'-C4'-C5'-O5'
1	9	1789	MA6	C5-C6-N6-C9
1	9	1790	MA6	C5-C6-N6-C9
1	9	1790	MA6	N1-C6-N6-C9
1	9	604	UY1	C2'-C1'-C5-C6
1	9	604	UY1	O4'-C1'-C5-C6
1	9	615	OMU	C3'-C4'-C5'-O5'
1	9	1790	MA6	C3'-C4'-C5'-O5'
1	9	140	OMC	C3'-C4'-C5'-O5'
1	9	140	OMC	O4'-C4'-C5'-O5'
1	9	473	OMC	C3'-C4'-C5'-O5'
1	9	1781	4AC	C3'-C4'-C5'-O5'
1	9	1789	MA6	N1-C6-N6-C9
1	9	28	A2M	O4'-C4'-C5'-O5'
1	9	1790	MA6	O4'-C4'-C5'-O5'
1	9	1789	MA6	C5-C6-N6-C10
1	9	623	A2M	C3'-C4'-C5'-O5'
1	9	140	OMC	C4'-C5'-O5'-P
1	9	1790	MA6	C4'-C5'-O5'-P
1	9	623	A2M	C4'-C5'-O5'-P
1	9	1790	MA6	C5-C6-N6-C10
1	9	392	OMG	C4'-C5'-O5'-P
1	9	28	A2M	C4'-C5'-O5'-P
1	9	615	OMU	C2'-C1'-N1-C6
1	9	615	OMU	C2'-C1'-N1-C2
1	9	473	OMC	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	9	468	A2M	3	0
1	9	392	OMG	2	0
1	9	140	OMC	1	0
1	9	615	OMU	2	0
1	9	1013	OMU	1	0
1	9	1781	4AC	2	0
1	9	978	A2M	1	0
1	9	1789	MA6	2	0
1	9	473	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

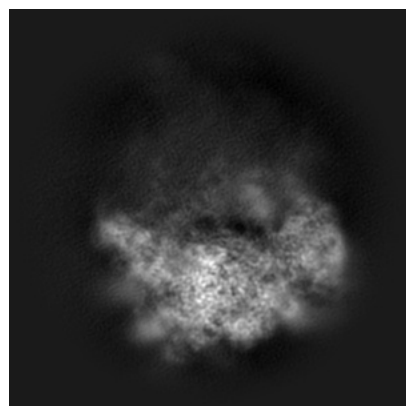
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54789. These allow visual inspection of the internal detail of the map and identification of artifacts.

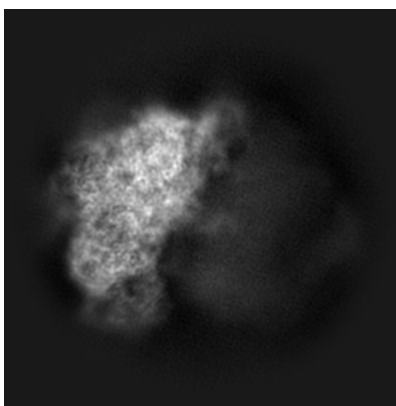
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

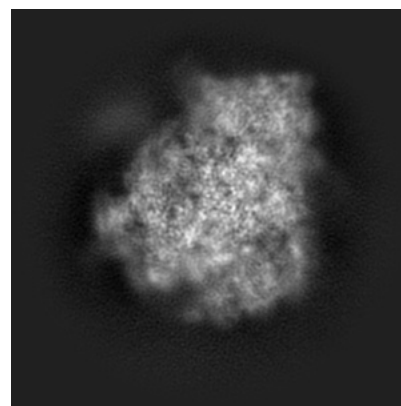
6.1.1 Primary map



X

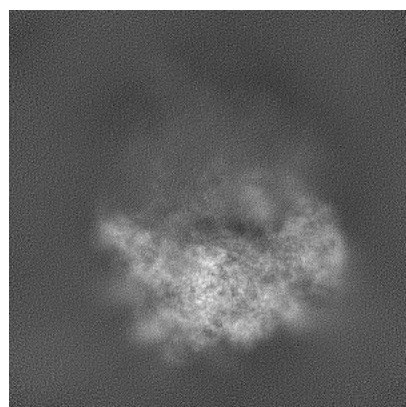


Y

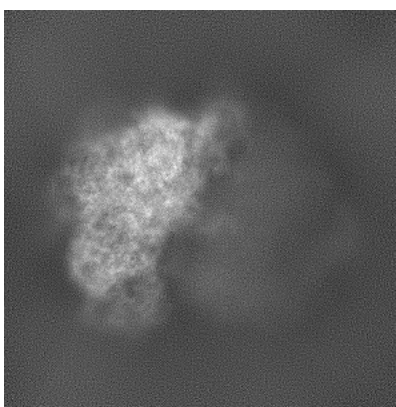


Z

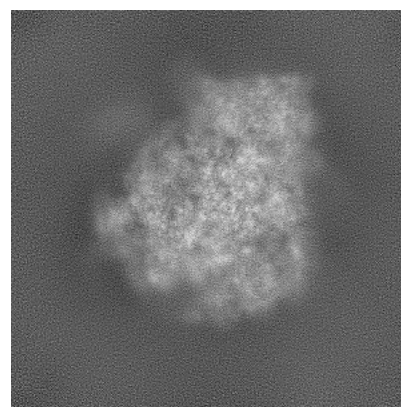
6.1.2 Raw map



X



Y

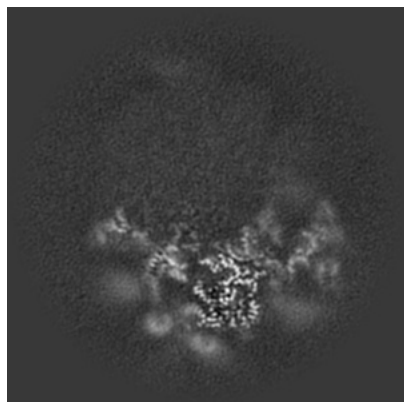


Z

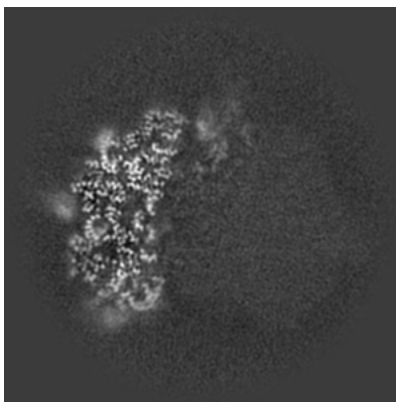
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

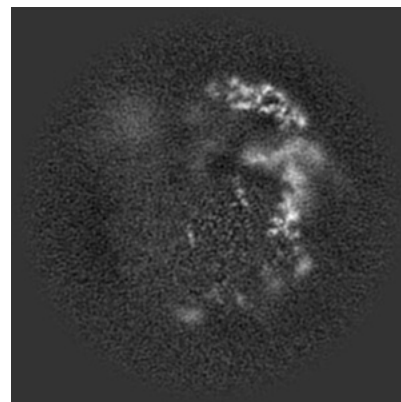
6.2.1 Primary map



X Index: 225

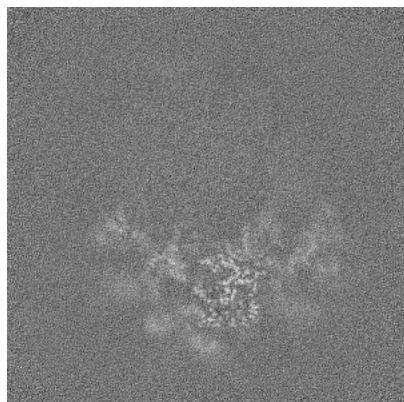


Y Index: 225

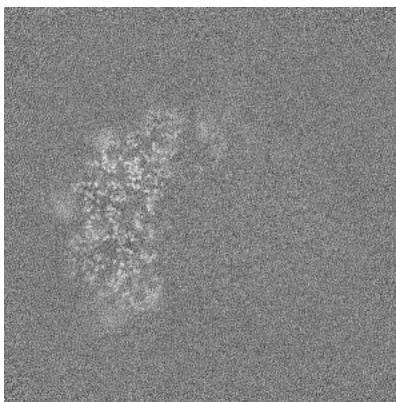


Z Index: 225

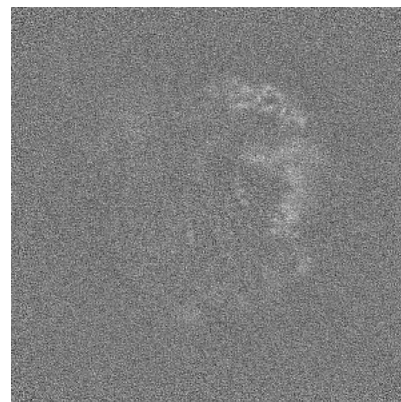
6.2.2 Raw map



X Index: 225



Y Index: 225

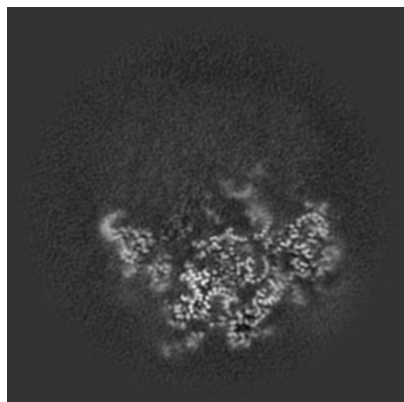


Z Index: 225

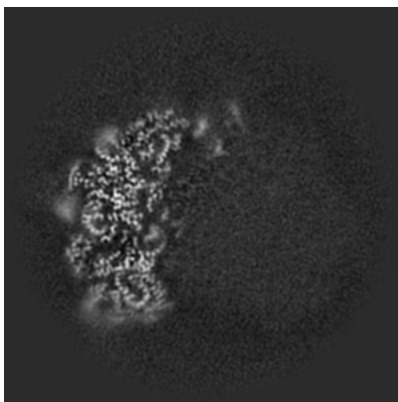
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

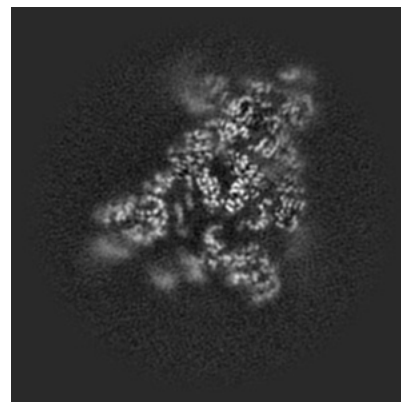
6.3.1 Primary map



X Index: 269

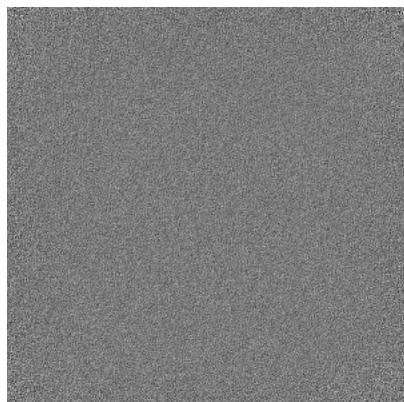


Y Index: 218

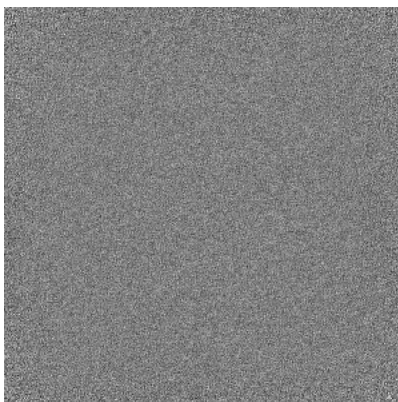


Z Index: 160

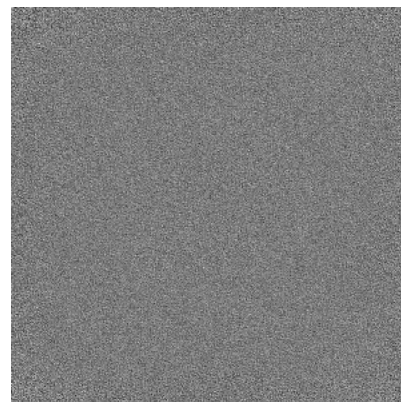
6.3.2 Raw map



X Index: 0



Y Index: 0

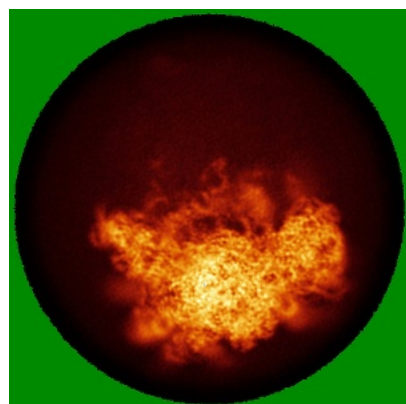


Z Index: 449

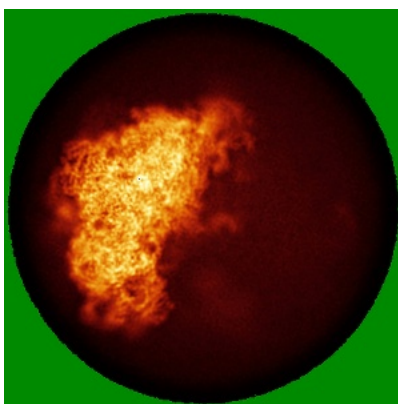
The images above show the largest variance slices of the map in three orthogonal directions.

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

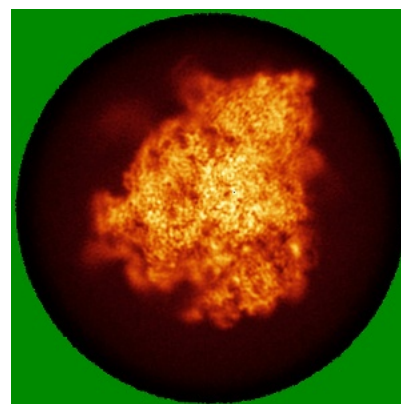
6.4.1 Primary map



X

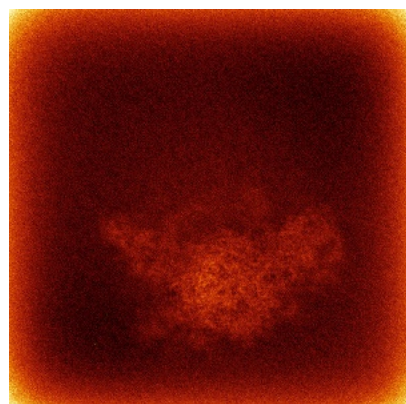


Y

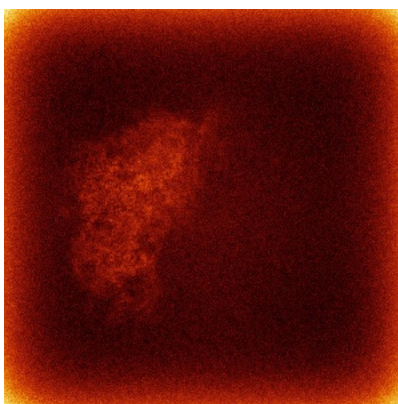


Z

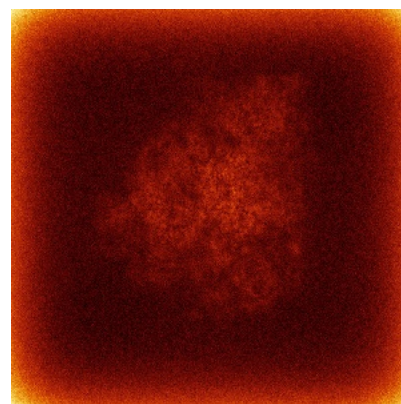
6.4.2 Raw map



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



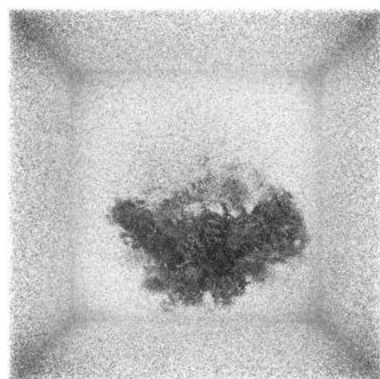
Y



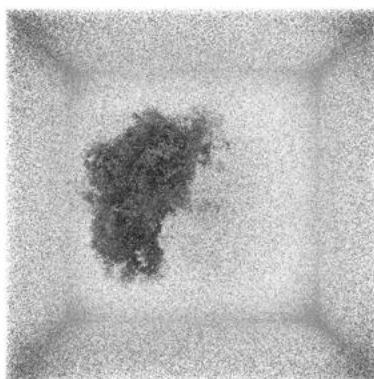
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

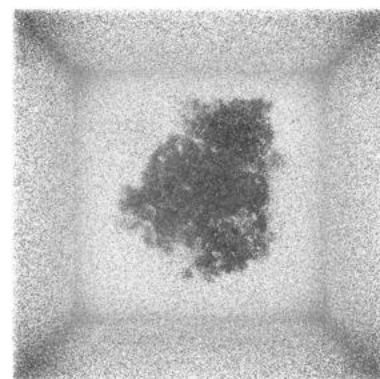
6.5.2 Raw map



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.

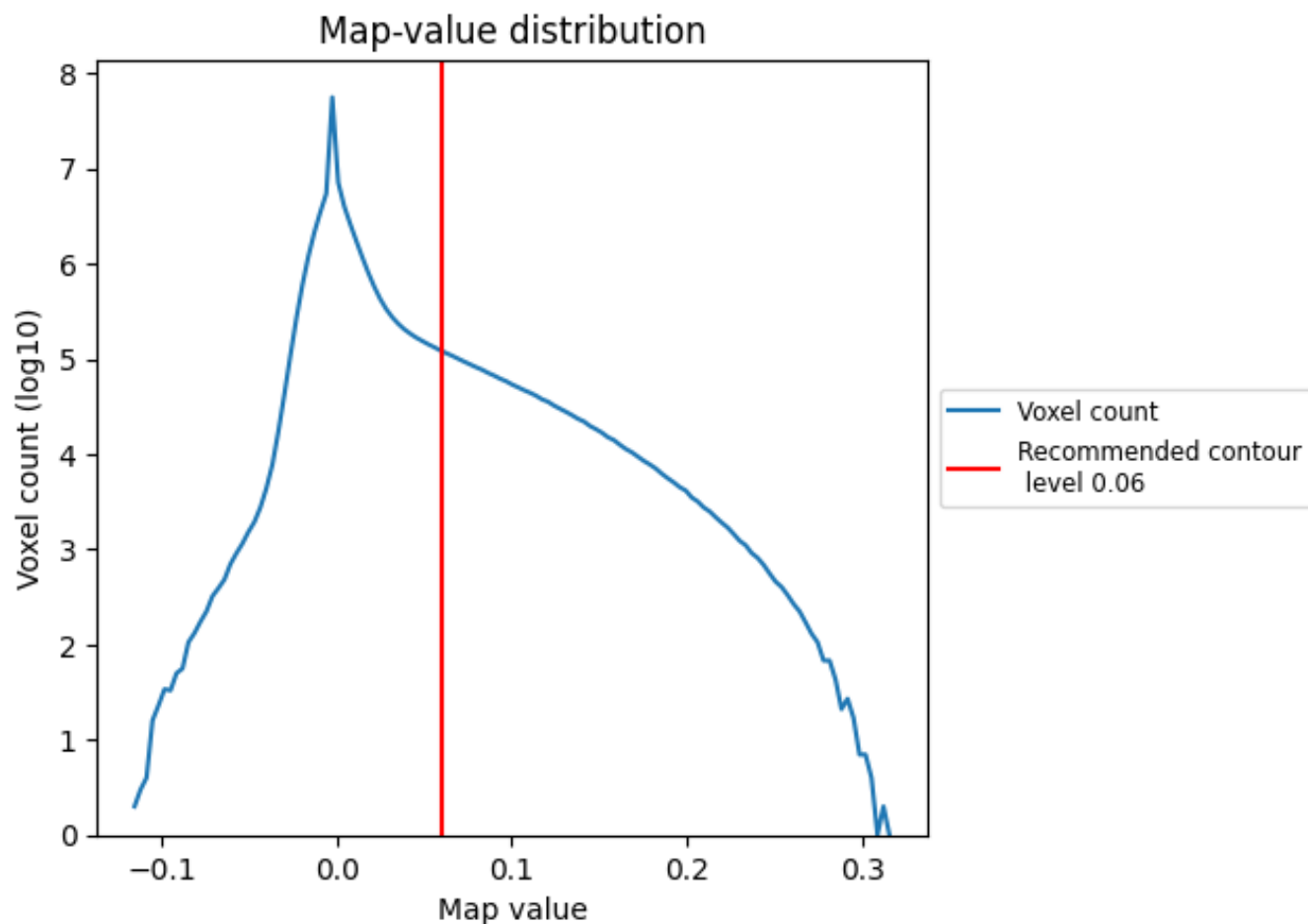
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

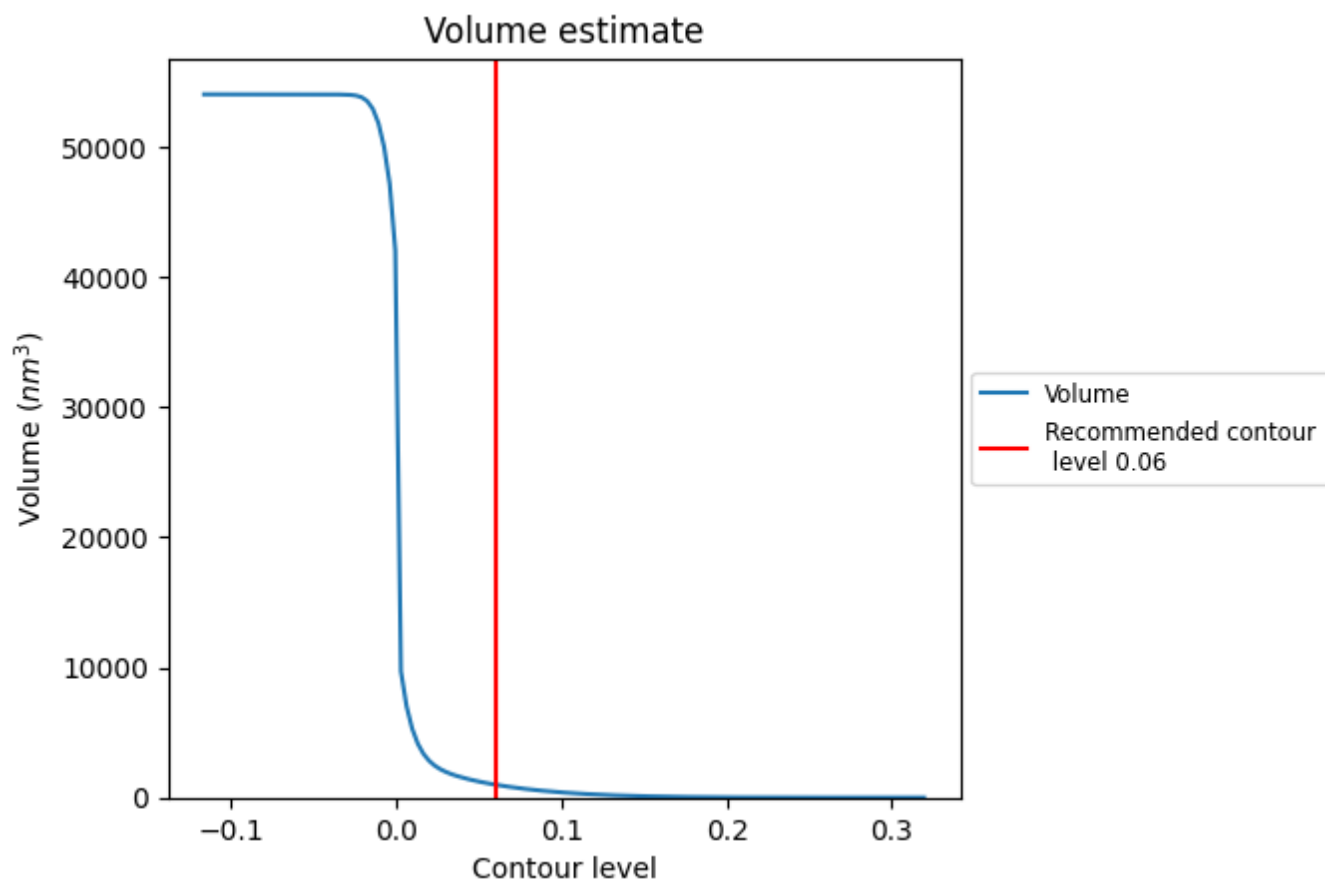
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

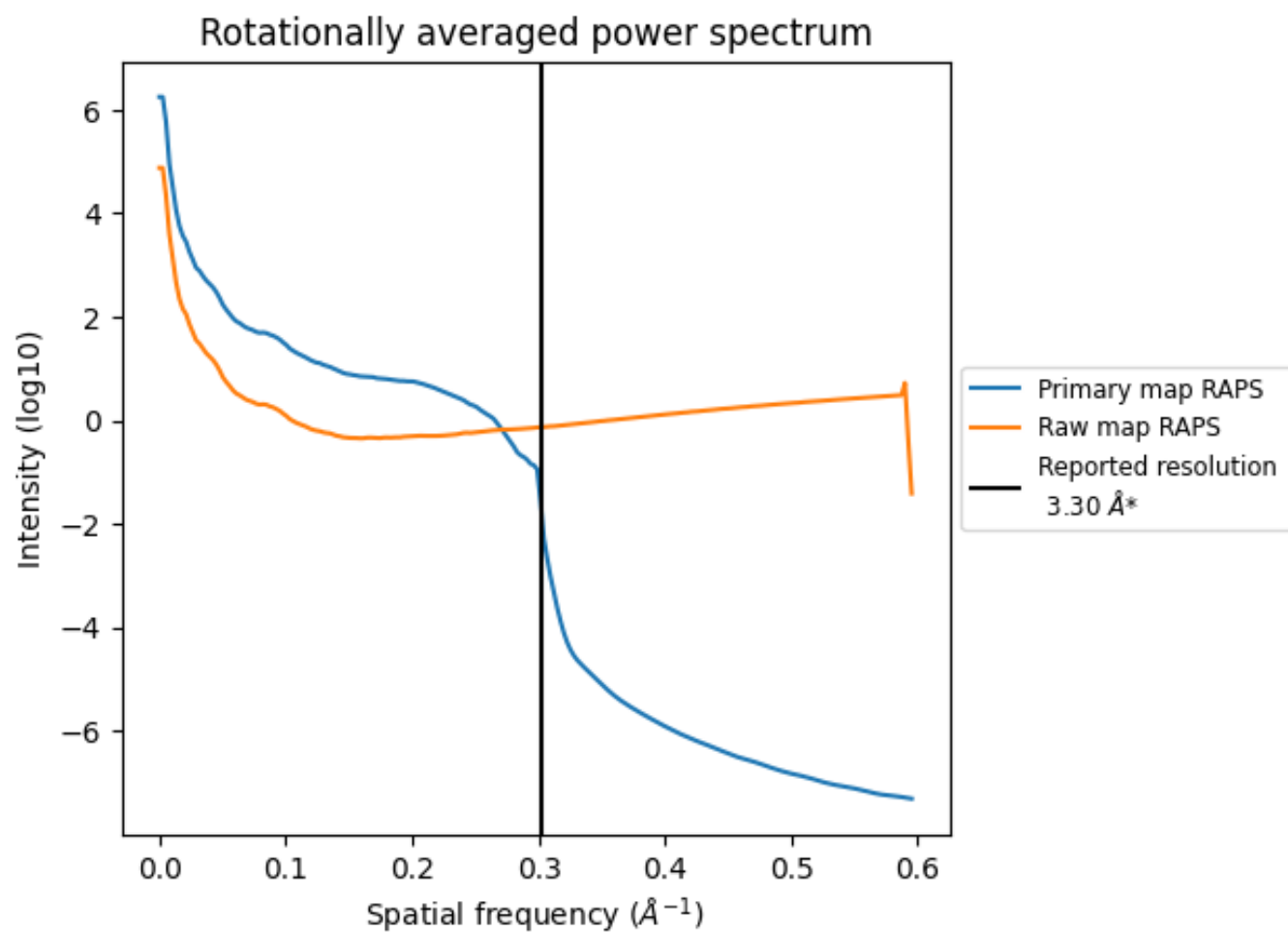
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 997 nm³; this corresponds to an approximate mass of 901 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

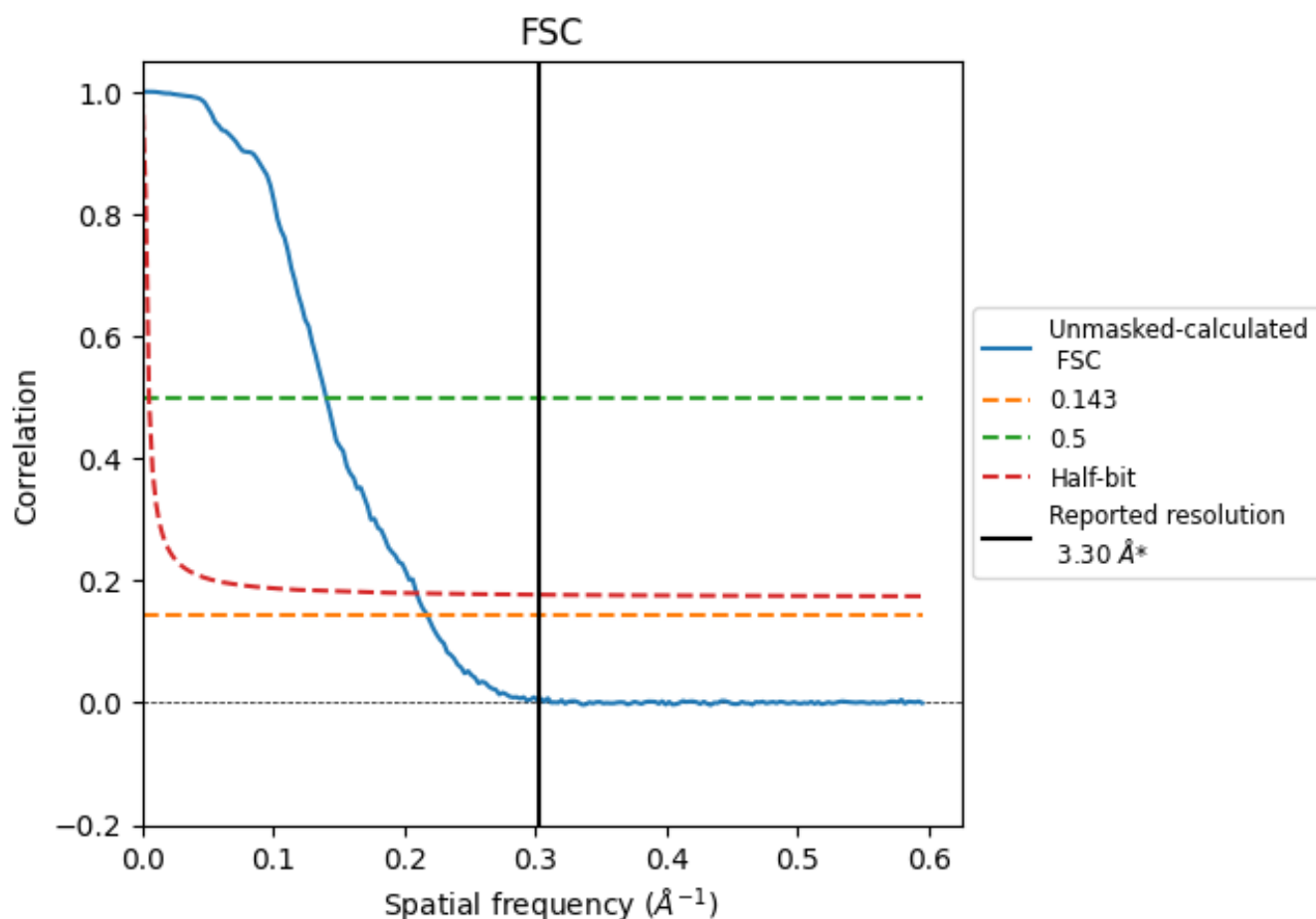


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

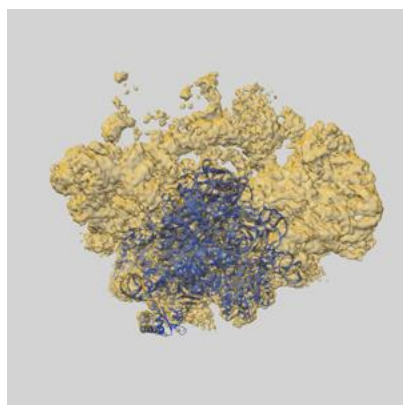
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.60	7.13	4.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.60 differs from the reported value 3.3 by more than 10 %

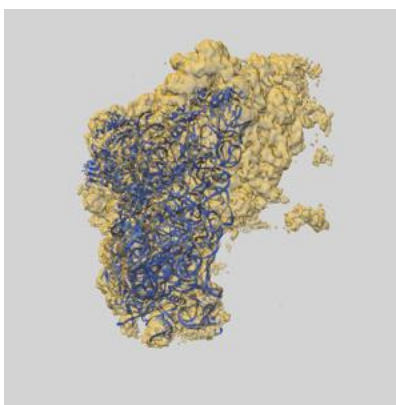
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54789 and PDB model 9SDP. Per-residue inclusion information can be found in section [3](#) on page [8](#).

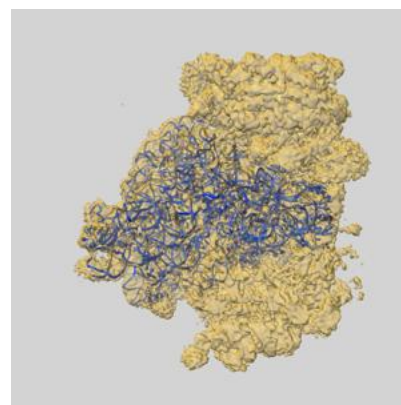
9.1 Map-model overlay [i](#)



X



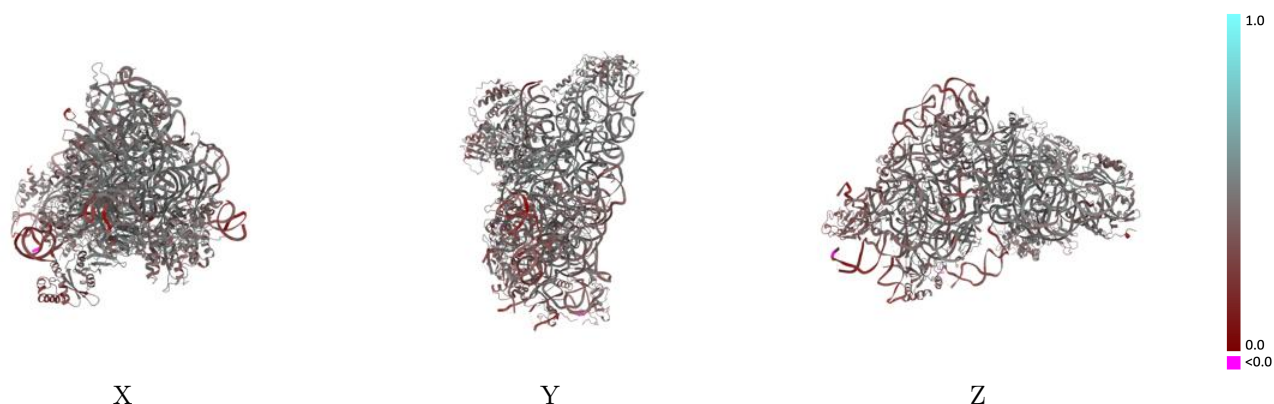
Y



Z

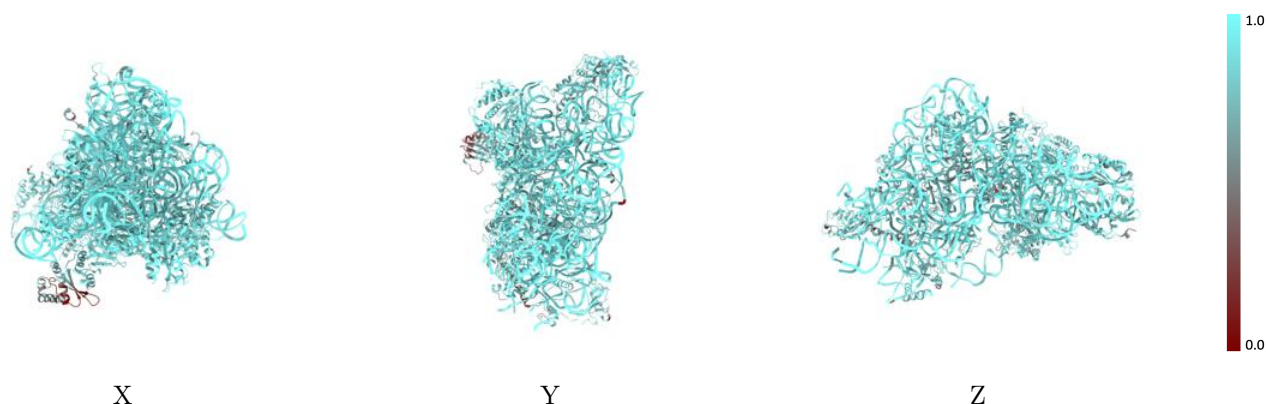
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



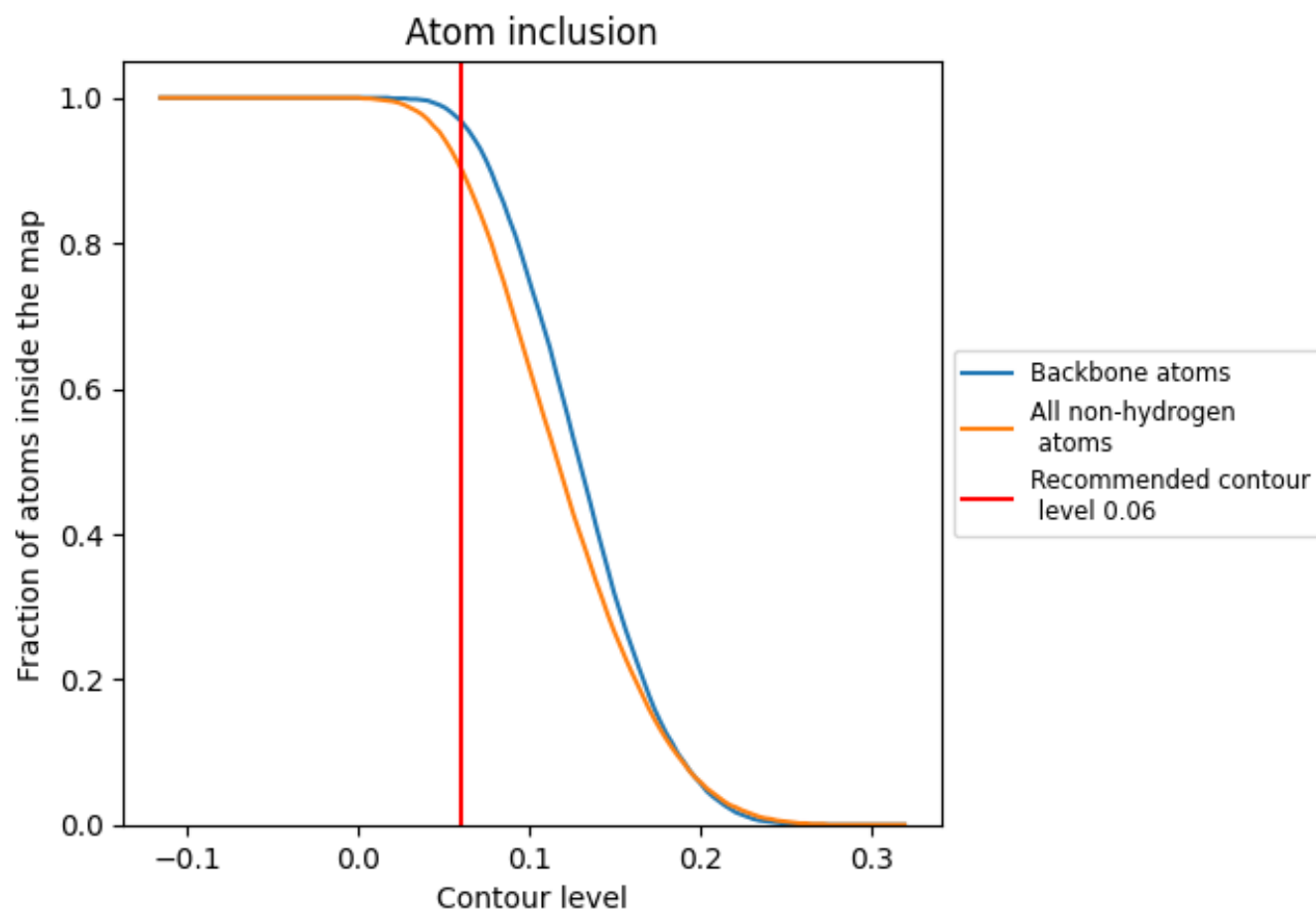
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.4150
9	 0.9560	 0.4030
BA	 0.9010	 0.4310
BB	 0.8530	 0.4480
BC	 0.8990	 0.4600
BE	 0.7980	 0.4220
BG	 0.7220	 0.3700
BH	 0.6420	 0.3730
BI	 0.8720	 0.4160
BJ	 0.8570	 0.3990
BL	 0.9040	 0.4630
BN	 0.8990	 0.4550
BV	 0.9110	 0.4610
BW	 0.9160	 0.4850
BX	 0.8710	 0.4350
BY	 0.8620	 0.3670
BZ	 0.8440	 0.4720
Bb	 0.9140	 0.4410
Be	 0.8600	 0.3720
Cn	 0.7320	 0.4540
cS	 0.8780	 0.4540

