Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 09:28 pm BST

PDB ID	:	6SWD
EMDB ID	:	EMD-10323
Title	:	IC2 body model of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in P. abyssi
Authors	:	Coureux, P.-D.; Mechulam, Y.; Schmitt, E.
Deposited on	:	2019-09-20
Resolution	:	3.20 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:

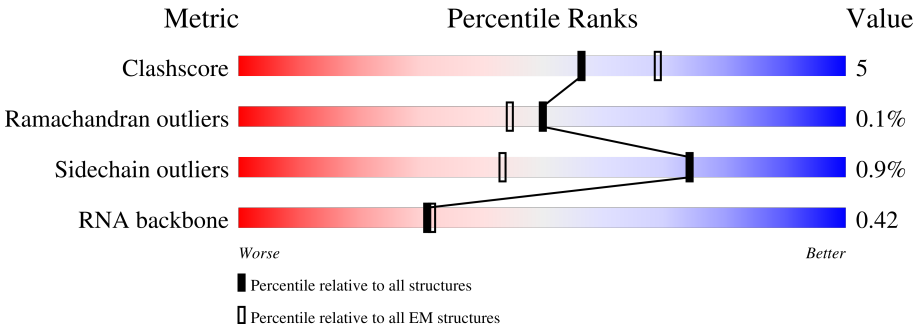
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.20 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	2	1044	67% 29% 5%
2	A	199	77% 18% 6%
3	B	202	9% 83% 14%
4	C	63	5% 90% 6%
5	D	180	83% 14%
6	E	243	88% 11%
7	F	236	9% 78% 18%

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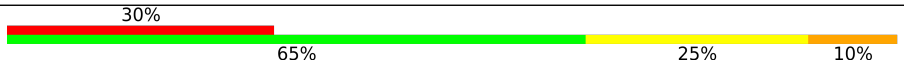
Mol	Chain	Length	Quality of chain
8	G	125	
9	I	130	
10	J	127	
11	M	137	
12	N	147	
13	Q	158	
14	R	113	
15	V	99	
16	W	65	
17	0	36	
18	5	20	
19	6	113	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 41548 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1044	22543	10048	4165	7286	1044	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	188	1533	995	268	266	4	0	0

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	196	1571	1017	269	281	4	0	0

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	61	482	304	85	85	8	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	175	1470	924	284	258	4	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	242	1983	1281	358	339	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 9 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 10 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	126	Total	C	N	O	0	0
			996	617	206	173		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	128	Total	C	N	O	S	0	0
			964	597	192	173	2		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 13 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	152	Total	C	N	O	S	0	0
			1262	804	240	214	4		

- Molecule 14 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	109	Total	C	N	O	S	0	0
			900	572	174	151	3		

- Molecule 15 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 16 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	63	Total	C	N	O	S	0	0
			481	303	93	80	5		

- Molecule 17 is a protein called 30S ribosomal protein aL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 18 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 19 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	2	24	Total	Mg	0
			24	24	
20	5	1	Total	Mg	0
			1	1	

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
21	C	2	Total Zn 2 2	0
21	F	1	Total Zn 1 1	0
21	R	1	Total Zn 1 1	0
21	W	1	Total Zn 1 1	0

- Molecule 22 is water.

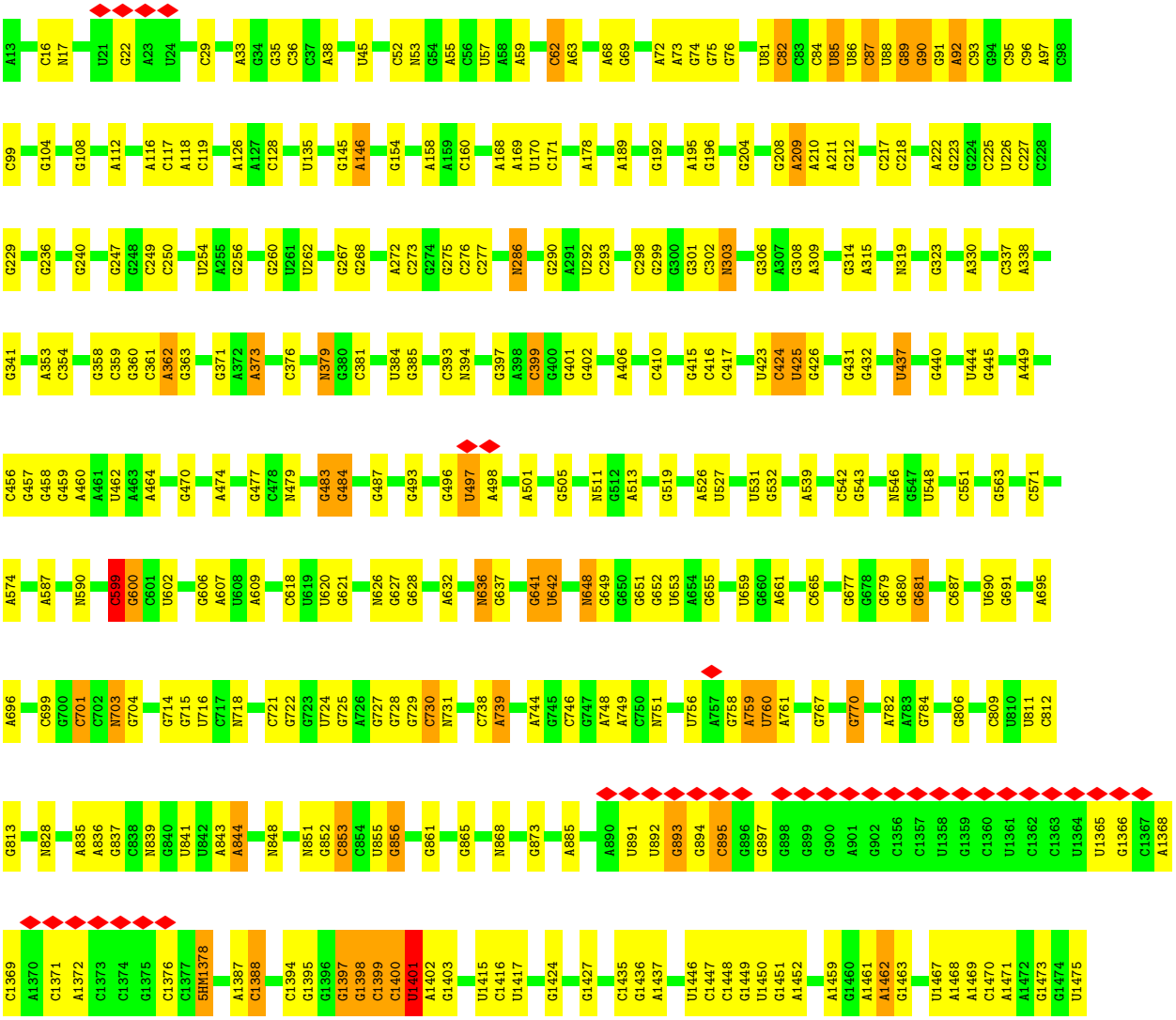
Mol	Chain	Residues	Atoms	AltConf
22	2	24	Total O 24 24	0
22	F	1	Total O 1 1	0
22	Q	1	Total O 1 1	0

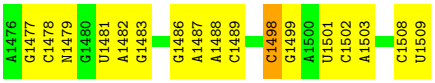
3 Residue-property plots (i)

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.

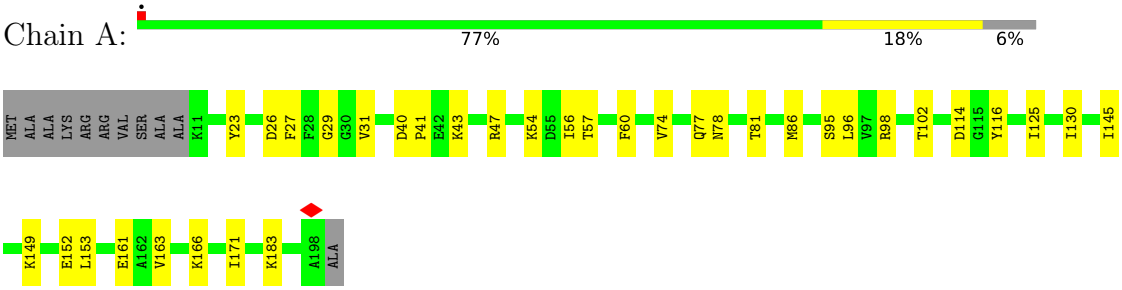
- Molecule 1: 16S ribosomal RNA

Chain 2:

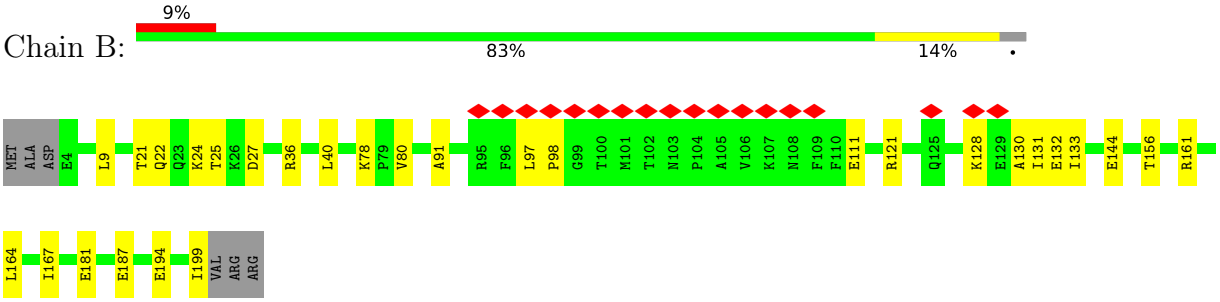




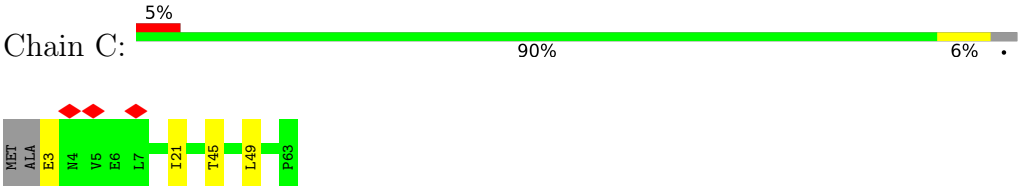
• Molecule 2: 30S ribosomal protein S3Ae



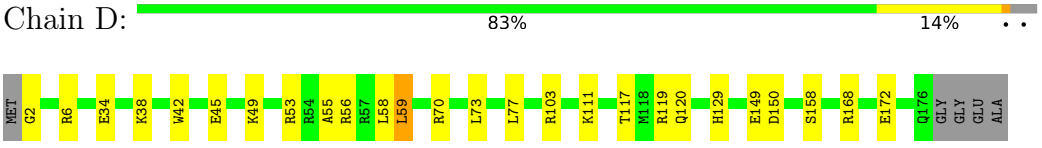
• Molecule 3: 30S ribosomal protein S2



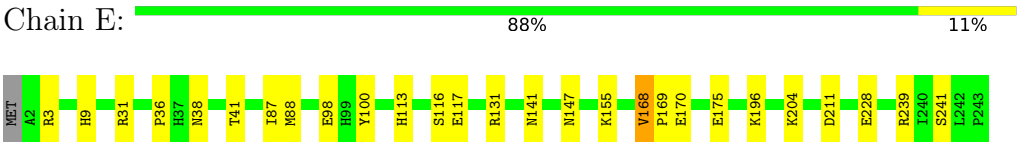
• Molecule 4: Zn-ribbon RNA-binding protein involved in translation



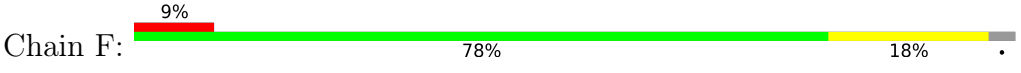
• Molecule 5: 30S ribosomal protein S4

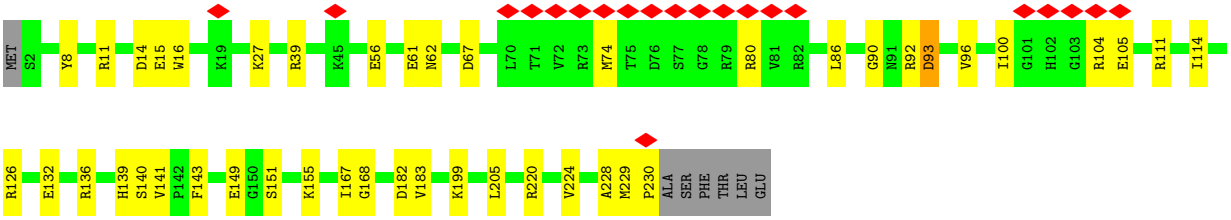


• Molecule 6: 30S ribosomal protein S4e

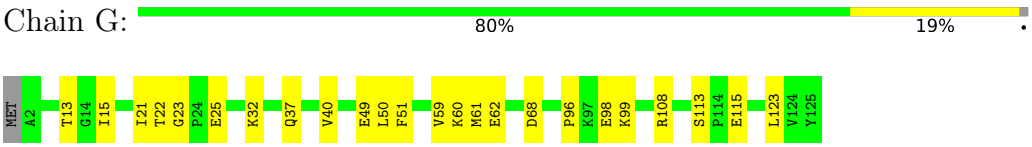


• Molecule 7: 30S ribosomal protein S5

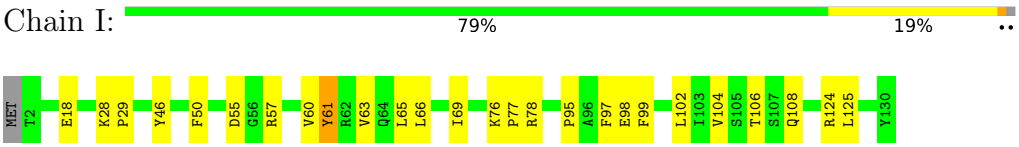




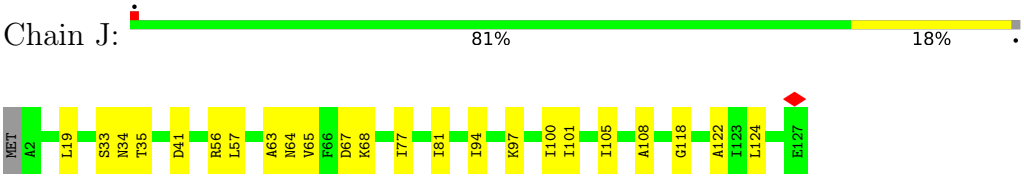
• Molecule 8: 30S ribosomal protein S6e



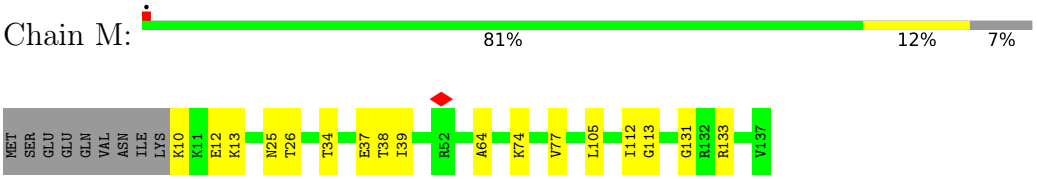
• Molecule 9: 30S ribosomal protein S8



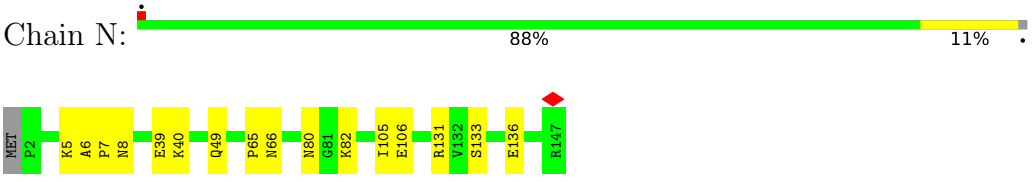
• Molecule 10: 30S ribosomal protein S8e



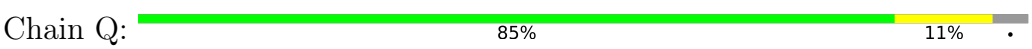
• Molecule 11: 30S ribosomal protein S11

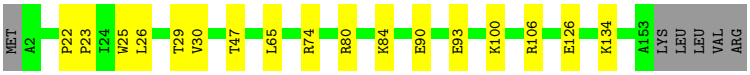


• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S15



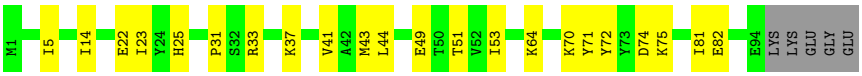


• Molecule 14: 30S ribosomal protein S17

Chain R:

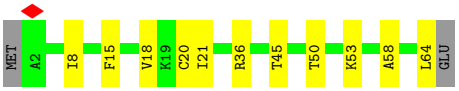
• Molecule 15: 30S ribosomal protein S24e

Chain V:



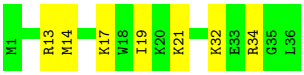
• Molecule 16: 30S ribosomal protein S27e

Chain W:



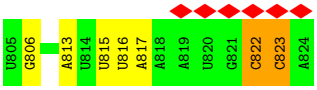
• Molecule 17: 30S ribosomal protein aL41

Chain 0:



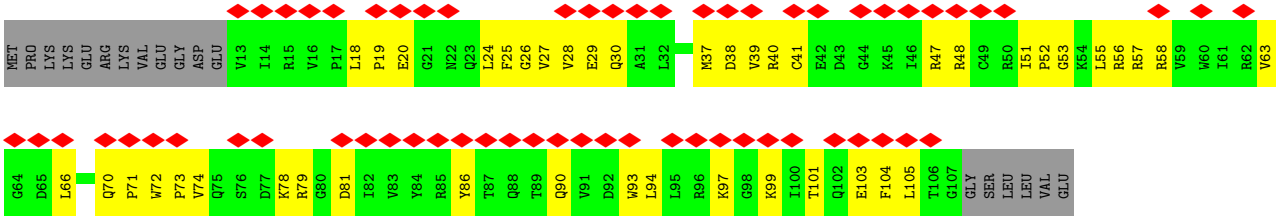
• Molecule 18: mRNA

Chain 5:



• Molecule 19: Translation initiation factor 1A

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142000	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 ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	379.32, 379.32, 379.32	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, 4AC, OMC, 5HM, MA6, ZN, LHH, 6MZ, UR3, MG

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	2	1.27	1/24391 (0.0%)	1.10	38/38014 (0.1%)
2	A	0.55	0/1559	0.56	0/2090
3	B	0.53	0/1602	0.55	0/2165
4	C	0.57	0/496	0.60	0/673
5	D	0.62	0/1494	0.58	0/2003
6	E	0.65	0/2032	0.60	0/2742
7	F	0.62	0/1838	0.62	0/2478
8	G	0.42	0/993	0.55	0/1329
9	I	0.71	0/1055	0.61	1/1415 (0.1%)
10	J	0.52	0/1005	0.56	0/1339
11	M	0.51	0/982	0.58	0/1322
12	N	0.62	0/1165	0.59	0/1547
13	Q	0.55	0/1290	0.55	0/1734
14	R	0.68	0/923	0.57	0/1247
15	V	0.66	0/808	0.55	0/1086
16	W	0.43	0/488	0.53	0/659
17	0	0.68	0/349	0.65	0/451
18	5	0.74	0/481	0.93	0/748
19	6	0.31	0/793	0.53	0/1072
All	All	1.02	1/43744 (0.0%)	0.93	39/64114 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	399	C	N1-C6	-5.44	1.33	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	393	C	C2-N1-C1'	6.82	126.30	118.80
1	2	293	C	C6-N1-C2	-6.49	117.70	120.30
1	2	759	A	O4'-C1'-N9	6.48	113.38	108.20
1	2	1470	C	O5'-P-OP1	-6.15	100.17	105.70
1	2	641	G	N1-C6-O6	-6.01	116.29	119.90
1	2	641	G	C5-C6-O6	5.96	132.18	128.60
1	2	721	C	C2-N1-C1'	5.94	125.34	118.80
1	2	171	C	C2-N1-C1'	5.91	125.30	118.80
1	2	844	A	C8-N9-C4	-5.71	103.52	105.80
1	2	87	C	C2-N1-C1'	5.71	125.08	118.80
1	2	852	G	N1-C6-O6	-5.70	116.48	119.90
1	2	393	C	C6-N1-C1'	-5.63	114.04	120.80
1	2	837	G	N3-C4-N9	5.60	129.36	126.00
1	2	87	C	N1-C2-O2	5.59	122.25	118.90
1	2	714	G	N1-C2-N2	5.57	121.21	116.20
1	2	314	G	N3-C4-N9	5.55	129.33	126.00
1	2	701	C	C2-N1-C1'	5.54	124.89	118.80
1	2	599	C	O4'-C1'-N1	5.52	112.62	108.20
1	2	302	C	C2-N1-C1'	5.52	124.87	118.80
1	2	1401	U	C2-N1-C1'	5.49	124.29	117.70
1	2	853	C	C6-N1-C2	-5.49	118.11	120.30
1	2	746	C	C6-N1-C2	-5.45	118.12	120.30
1	2	714	G	N3-C2-N2	-5.42	116.10	119.90
1	2	602	U	N3-C2-O2	-5.38	118.43	122.20
9	I	102	LEU	CA-CB-CG	5.34	127.58	115.30
1	2	856	G	N1-C6-O6	-5.32	116.71	119.90
1	2	1489	C	C6-N1-C2	-5.31	118.17	120.30
1	2	618	C	C2-N1-C1'	5.31	124.64	118.80
1	2	1388	C	C2-N1-C1'	5.30	124.63	118.80
1	2	35	G	N3-C4-N9	5.26	129.16	126.00
1	2	119	C	C6-N1-C2	-5.21	118.22	120.30
1	2	505	G	N3-C4-N9	5.14	129.08	126.00
1	2	727	G	N1-C6-O6	-5.13	116.83	119.90
1	2	770	G	C8-N9-C4	-5.09	104.36	106.40
1	2	171	C	C6-N1-C2	-5.08	118.27	120.30
1	2	1388	C	C6-N1-C2	-5.07	118.27	120.30
1	2	437	U	N3-C2-O2	-5.06	118.66	122.20
1	2	1498	C	C6-N1-C2	-5.05	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	458	G	N3-C4-N9	5.04	129.02	126.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	N	5	LYS	Peptide

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	2	22543	0	11390	101	0
2	A	1533	0	1627	25	0
3	B	1571	0	1630	17	0
4	C	482	0	462	4	0
5	D	1470	0	1542	21	0
6	E	1983	0	2060	16	0
7	F	1808	0	1879	30	0
8	G	977	0	1037	13	0
9	I	1034	0	1069	20	0
10	J	996	0	1076	17	0
11	M	964	0	994	10	0
12	N	1148	0	1248	8	0
13	Q	1262	0	1331	13	0
14	R	900	0	921	11	0
15	V	790	0	806	17	0
16	W	481	0	512	9	0
17	0	343	0	407	5	0
18	5	430	0	215	3	0
19	6	777	0	806	38	0
20	2	24	0	0	0	0
20	5	1	0	0	0	0
21	C	2	0	0	0	0
21	F	1	0	0	0	0
21	R	1	0	0	0	0
21	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	2	24	0	0	0	0
22	F	1	0	0	0	0
22	Q	1	0	0	0	0
All	All	41548	0	31012	337	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 5.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:168:VAL:HG23	6:E:169:PRO:HD3	1.51	0.90
2:A:47:ARG:HB3	11:M:34:THR:HG21	1.55	0.88
2:A:47:ARG:NH2	11:M:37:GLU:OE1	2.10	0.84
1:2:303:4AC:O2'	5:D:6:ARG:NH1	2.14	0.80
1:2:651:G:H21	11:M:38:THR:HG21	1.45	0.80
1:2:1462:A:N6	19:6:55:LEU:O	2.15	0.79
1:2:445:G:OP2	15:V:33:ARG:NH1	2.15	0.78
1:2:563:G:H21	9:I:124:ARG:HH21	1.31	0.78
7:F:16:TRP:O	7:F:27:LYS:NZ	2.18	0.77
2:A:145:ILE:HD11	2:A:171:ILE:HG12	1.65	0.76
7:F:61:GLU:O	7:F:92:ARG:NH2	2.19	0.73
2:A:23:TYR:O	2:A:81:THR:OG1	2.07	0.73
19:6:28:VAL:HA	19:6:39:VAL:HA	1.70	0.73
2:A:41:PRO:HB3	2:A:74:VAL:HG11	1.69	0.72
13:Q:106:ARG:NH2	13:Q:126:GLU:OE2	2.24	0.71
12:N:65:PRO:O	12:N:66:ASN:ND2	2.24	0.71
19:6:97:LYS:HG3	19:6:99:LYS:HG2	1.72	0.70
9:I:28:LYS:HB3	9:I:29:PRO:HD3	1.74	0.70
19:6:78:LYS:O	19:6:79:ARG:NH1	2.24	0.70
12:N:6:ALA:HB3	12:N:7:PRO:HD3	1.73	0.70
3:B:36:ARG:HH21	3:B:40:LEU:HD22	1.57	0.69
15:V:22:GLU:OE1	15:V:64:LYS:NZ	2.25	0.69
15:V:72:TYR:OH	15:V:82:GLU:OE2	2.07	0.69
19:6:24:LEU:HD13	19:6:71:PRO:HG3	1.73	0.69
7:F:56:GLU:O	7:F:62:ASN:ND2	2.25	0.69
1:2:483:G:H2'	1:2:497:U:H5	1.58	0.68
4:C:3:GLU:HB2	7:F:230:PRO:HD2	1.76	0.68
1:2:563:G:N2	9:I:124:ARG:HH21	1.91	0.67
19:6:47:ARG:HA	19:6:78:LYS:HA	1.77	0.67
1:2:424:C:H4'	1:2:425:U:H5	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:167:ILE:HG12	7:F:168:GLY:H	1.60	0.67
19:6:40:ARG:NH1	19:6:41:CYS:O	2.28	0.67
1:2:323:G:N7	6:E:3:ARG:NH1	2.42	0.66
5:D:103:ARG:NH1	5:D:149:GLU:OE2	2.28	0.66
6:E:98:GLU:OE1	6:E:100:TYR:OH	2.07	0.65
1:2:1397:G:H1	1:2:1446:U:H3	1.45	0.65
7:F:220:ARG:NH1	9:I:98:GLU:OE1	2.32	0.63
10:J:57:LEU:HB2	10:J:118:GLY:HA2	1.80	0.63
1:2:89:G:H2'	1:2:90:G:C8	2.35	0.62
9:I:106:THR:HG23	9:I:108:GLN:H	1.64	0.62
1:2:91:G:H2'	1:2:92:A:C8	2.36	0.61
3:B:78:LYS:NZ	3:B:194:GLU:O	2.33	0.61
19:6:51:ILE:HD11	19:6:55:LEU:HB2	1.81	0.61
3:B:156:THR:HG21	3:B:167:ILE:HG13	1.82	0.60
9:I:50:PHE:HB3	9:I:63:VAL:HG22	1.82	0.60
7:F:140:SER:OG	7:F:141:VAL:N	2.34	0.60
1:2:703:4AC:H5	1:2:703:4AC:O7	2.01	0.60
1:2:806:G:OP1	16:W:53:LYS:NZ	2.34	0.60
4:C:3:GLU:HB2	7:F:229:MET:HA	1.84	0.60
1:2:636:4AC:CM7	1:2:703:4AC:HM73	2.32	0.59
5:D:168:ARG:NH1	5:D:172:GLU:OE2	2.34	0.59
8:G:13:THR:HG23	8:G:15:ILE:HG12	1.83	0.59
1:2:306:G:N2	1:2:309:A:OP2	2.25	0.59
8:G:21:ILE:HD12	8:G:25:GLU:HB3	1.84	0.59
16:W:20:CYS:SG	16:W:21:ILE:N	2.76	0.59
8:G:98:GLU:HG3	8:G:99:LYS:H	1.68	0.58
9:I:76:LYS:O	9:I:78:ARG:N	2.36	0.58
12:N:49:GLN:HG2	12:N:106:GLU:HG2	1.85	0.58
18:5:822:C:O2'	18:5:823:C:O4'	2.20	0.58
1:2:1483:G:O6	17:0:21:LYS:NZ	2.36	0.58
7:F:149:GLU:HG2	7:F:199:LYS:HB2	1.86	0.57
1:2:1399:C:H2'	1:2:1400:C:H6	1.70	0.57
7:F:14:ASP:OD1	7:F:15:GLU:N	2.38	0.57
1:2:648:4AC:O2	1:2:677:G:N2	2.39	0.56
3:B:111:GLU:HG3	3:B:133:ILE:HD11	1.87	0.56
13:Q:74:ARG:NH1	13:Q:80:ARG:HD3	2.21	0.56
9:I:18:GLU:HB3	9:I:65:LEU:HD13	1.87	0.56
6:E:131:ARG:NH1	6:E:141:ASN:OD1	2.39	0.56
8:G:40:VAL:HG23	8:G:60:LYS:HA	1.88	0.56
9:I:104:VAL:HG22	9:I:125:LEU:HD23	1.88	0.55
6:E:175:GLU:OE2	6:E:239:ARG:NH2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:32:LYS:O	17:0:34:ARG:N	2.39	0.55
1:2:1481:U:O4	17:0:17:LYS:NZ	2.40	0.55
19:6:57:ARG:HG3	19:6:58:ARG:N	2.21	0.55
1:2:1462:A:H5'	19:6:56:ARG:HE	1.71	0.55
5:D:56:ARG:HB3	7:F:132:GLU:HG2	1.89	0.55
1:2:91:G:H2'	1:2:92:A:H8	1.71	0.55
1:2:484:G:O2'	1:2:496:G:N2	2.40	0.55
19:6:72:TRP:CD1	19:6:73:PRO:HD2	2.41	0.55
1:2:417:C:OP1	5:D:117:THR:HG21	2.06	0.55
1:2:636:4AC:HM73	1:2:703:4AC:HM73	1.89	0.55
11:M:64:ALA:HB1	11:M:105:LEU:HD13	1.89	0.55
3:B:25:THR:HG22	3:B:27:ASP:H	1.71	0.54
1:2:1446:U:H2'	1:2:1447:C:H6	1.73	0.54
19:6:51:ILE:HD12	19:6:52:PRO:HD2	1.90	0.54
1:2:303:4AC:HO2'	5:D:6:ARG:HH12	1.53	0.54
10:J:65:VAL:HG11	10:J:105:ILE:HD11	1.89	0.54
1:2:85:U:H2'	1:2:86:U:O4'	2.07	0.54
1:2:724:U:H2'	1:2:725:G:O4'	2.06	0.54
18:5:822:C:H2'	18:5:823:C:C6	2.43	0.54
16:W:50:THR:O	16:W:50:THR:OG1	2.22	0.53
7:F:151:SER:O	7:F:151:SER:OG	2.24	0.53
3:B:21:THR:HG22	3:B:22:GLN:H	1.73	0.53
1:2:301:G:O6	5:D:2:GLY:N	2.42	0.53
11:M:39:ILE:HG23	11:M:74:LYS:HD2	1.91	0.53
19:6:70:GLN:O	19:6:81:ASP:N	2.42	0.53
1:2:359:C:O2'	1:2:360:G:H5'	2.09	0.52
1:2:424:C:O2'	1:2:425:U:OP2	2.27	0.52
1:2:1462:A:H2	19:6:51:ILE:HG21	1.74	0.52
14:R:20:LYS:HD3	14:R:94:LEU:HD12	1.91	0.52
14:R:41:ASP:OD1	14:R:41:ASP:N	2.37	0.52
1:2:483:G:H2'	1:2:497:U:C5	2.42	0.52
1:2:75:G:H2'	1:2:76:G:C8	2.44	0.52
8:G:113:SER:OG	8:G:115:GLU:OE1	2.24	0.52
7:F:104:ARG:HG3	7:F:105:GLU:HG3	1.92	0.52
1:2:1402:A:H2'	1:2:1403:G:C8	2.44	0.52
2:A:77:GLN:O	2:A:78:ASN:ND2	2.42	0.52
14:R:55:HIS:HB2	14:R:66:ARG:HD2	1.91	0.52
1:2:1365:U:H2'	1:2:1366:G:C8	2.45	0.52
14:R:84:ASP:HB3	14:R:108:ARG:O	2.09	0.52
1:2:145:G:H2'	1:2:146:A:C8	2.45	0.52
5:D:73:LEU:O	5:D:77:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:204:G:O2'	10:J:64:ASN:OD1	2.10	0.52
7:F:93:ASP:O	7:F:126:ARG:NH2	2.42	0.52
5:D:150:ASP:OD1	5:D:150:ASP:N	2.43	0.51
1:2:84:C:H2'	1:2:85:U:O4'	2.10	0.51
6:E:204:LYS:NZ	6:E:211:ASP:OD2	2.43	0.51
2:A:54:LYS:HE2	2:A:60:PHE:HA	1.92	0.51
6:E:87:ILE:HG22	6:E:88:MET:HG2	1.92	0.51
1:2:1450:U:H2'	1:2:1451:G:H5'	1.90	0.51
14:R:84:ASP:N	14:R:84:ASP:OD1	2.43	0.51
1:2:62:C:N4	1:2:362:A:OP2	2.42	0.51
5:D:59:LEU:HD22	7:F:132:GLU:O	2.11	0.51
9:I:76:LYS:HB3	9:I:77:PRO:HD3	1.91	0.51
1:2:1416:C:H2'	1:2:1417:U:H6	1.75	0.51
12:N:80:ASN:HB3	12:N:82:LYS:HG2	1.92	0.51
15:V:43:MET:HG2	15:V:44:LEU:HD12	1.92	0.50
19:6:72:TRP:O	19:6:79:ARG:HD2	2.09	0.50
1:2:247:G:OP1	14:R:66:ARG:NH1	2.45	0.50
13:Q:29:THR:HG22	13:Q:30:VAL:H	1.77	0.50
15:V:37:LYS:O	15:V:41:VAL:HG13	2.11	0.50
1:2:424:C:H4'	1:2:425:U:C5	2.46	0.50
5:D:58:LEU:HD13	5:D:70:ARG:HA	1.93	0.50
19:6:39:VAL:HG13	19:6:47:ARG:HB2	1.92	0.50
5:D:42:TRP:HA	5:D:45:GLU:HG3	1.94	0.50
9:I:95:PRO:HD2	9:I:99:PHE:HB3	1.94	0.50
13:Q:25:TRP:CG	16:W:64:LEU:HD12	2.47	0.50
2:A:26:ASP:OD1	2:A:27:PHE:N	2.44	0.49
7:F:167:ILE:HG12	7:F:168:GLY:N	2.27	0.49
2:A:152:GLU:OE1	2:A:152:GLU:N	2.43	0.49
9:I:60:VAL:HG22	9:I:61:TYR:N	2.27	0.49
15:V:49:GLU:N	15:V:49:GLU:OE1	2.45	0.49
3:B:128:LYS:HA	3:B:131:ILE:HD12	1.93	0.49
1:2:1402:A:H2'	1:2:1403:G:H8	1.77	0.49
2:A:145:ILE:HD11	2:A:171:ILE:CG1	2.41	0.49
1:2:648:4AC:O7	1:2:648:4AC:H5	2.11	0.49
3:B:80:VAL:HG12	3:B:91:ALA:HB1	1.95	0.49
3:B:128:LYS:O	3:B:132:GLU:HG3	2.13	0.49
1:2:22:G:H1'	7:F:74:MET:SD	2.53	0.49
1:2:894:G:H2'	1:2:895:C:O4'	2.13	0.49
19:6:72:TRP:CG	19:6:73:PRO:HD2	2.48	0.49
15:V:23:ILE:HD13	15:V:31:PRO:HG2	1.94	0.49
19:6:74:VAL:O	19:6:79:ARG:NE	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:10:LYS:HD2	11:M:12:GLU:HB3	1.95	0.48
13:Q:90:GLU:OE1	13:Q:90:GLU:N	2.45	0.48
3:B:121:ARG:NH2	3:B:144:GLU:OE2	2.47	0.48
6:E:9:HIS:O	6:E:31:ARG:NH1	2.42	0.48
7:F:224:VAL:HG21	7:F:228:ALA:HB2	1.95	0.48
14:R:110:GLU:CD	14:R:110:GLU:H	2.17	0.48
15:V:25:HIS:O	15:V:25:HIS:ND1	2.46	0.48
7:F:8:TYR:HD1	7:F:11:ARG:HH21	1.62	0.48
1:2:1462:A:N3	1:2:1462:A:H2'	2.29	0.48
1:2:267:G:H5'	10:J:97:LYS:HB3	1.95	0.48
11:M:13:LYS:O	11:M:77:VAL:HG12	2.14	0.48
1:2:496:G:N2	19:6:53:GLY:O	2.47	0.48
3:B:24:LYS:O	3:B:25:THR:OG1	2.28	0.48
2:A:86:MET:HG3	2:A:163:VAL:HG12	1.96	0.47
9:I:97:PHE:O	9:I:98:GLU:HG3	2.14	0.47
1:2:1378:5HM:H11	1:2:1378:5HM:O5'	2.14	0.47
1:2:1448:C:H2'	1:2:1449:G:C8	2.49	0.47
19:6:74:VAL:HB	19:6:79:ARG:HE	1.80	0.47
17:0:13:ARG:NH1	17:0:14:MET:O	2.46	0.47
1:2:379:4AC:O7	1:2:379:4AC:H5	2.15	0.47
1:2:189:A:O3'	6:E:155:LYS:NZ	2.43	0.47
1:2:1416:C:H2'	1:2:1417:U:C6	2.49	0.47
13:Q:23:PRO:HD2	13:Q:26:LEU:HD12	1.97	0.47
14:R:105:VAL:HG21	14:R:108:ARG:HH11	1.79	0.47
1:2:75:G:O2'	1:2:168:A:N3	2.46	0.47
9:I:46:TYR:HD1	9:I:69:ILE:HG22	1.80	0.47
15:V:72:TYR:HE2	15:V:81:ILE:HD11	1.80	0.47
1:2:410:C:O2'	1:2:587:A:N3	2.44	0.46
9:I:76:LYS:HD2	9:I:76:LYS:HA	1.70	0.46
6:E:38:ASN:OD1	6:E:38:ASN:N	2.44	0.46
8:G:22:THR:OG1	8:G:23:GLY:N	2.48	0.46
1:2:835:A:H5'	7:F:151:SER:HB2	1.98	0.46
1:2:1462:A:C6	19:6:56:ARG:HA	2.50	0.46
6:E:169:PRO:HG2	6:E:170:GLU:OE2	2.16	0.46
13:Q:22:PRO:HA	13:Q:65:LEU:HD13	1.98	0.46
1:2:208:G:O2'	1:2:209:A:H5"	2.15	0.46
19:6:97:LYS:HE2	19:6:99:LYS:HZ3	1.80	0.46
10:J:33:SER:HB3	10:J:56:ARG:HD2	1.97	0.46
1:2:92:A:H2'	1:2:93:C:C6	2.51	0.46
1:2:192:G:N1	1:2:195:A:OP2	2.48	0.46
1:2:1502:C:H2'	1:2:1503:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:164:LEU:HD23	3:B:164:LEU:HA	1.75	0.46
5:D:34:GLU:OE1	5:D:119:ARG:NH2	2.45	0.46
10:J:34:ASN:HB3	10:J:94:ILE:HD12	1.98	0.46
5:D:49:LYS:O	5:D:53:ARG:HG3	2.16	0.45
13:Q:25:TRP:CD1	16:W:64:LEU:HD12	2.51	0.45
14:R:30:HIS:O	14:R:30:HIS:ND1	2.49	0.45
16:W:15:PHE:O	16:W:64:LEU:HB2	2.17	0.45
1:2:738:C:H2'	1:2:739:A:H5"	1.98	0.45
10:J:67:ASP:CG	10:J:68:LYS:H	2.20	0.45
19:6:48:ARG:HD2	19:6:78:LYS:HD3	1.98	0.45
1:2:89:G:H2'	1:2:90:G:H8	1.76	0.45
1:2:680:G:H2'	1:2:681:G:C8	2.52	0.45
6:E:116:SER:OG	6:E:117:GLU:N	2.50	0.45
8:G:68:ASP:CG	8:G:108:ARG:HH21	2.18	0.45
12:N:8:ASN:O	12:N:8:ASN:ND2	2.50	0.45
8:G:68:ASP:OD1	8:G:108:ARG:NE	2.50	0.45
1:2:81:U:H2'	1:2:82:C:C6	2.52	0.45
8:G:32:LYS:HA	8:G:32:LYS:HD3	1.84	0.45
5:D:103:ARG:HA	5:D:103:ARG:HD3	1.84	0.44
7:F:86:LEU:HD12	7:F:100:ILE:HG12	1.99	0.44
1:2:759:A:H4'	1:2:760:U:H5"	1.98	0.44
7:F:111:ARG:HE	7:F:111:ARG:HB2	1.64	0.44
9:I:55:ASP:HB3	16:W:8:ILE:HG12	1.98	0.44
19:6:37:MET:O	19:6:48:ARG:HA	2.18	0.44
7:F:93:ASP:O	7:F:126:ARG:CZ	2.65	0.44
17:0:13:ARG:NH2	17:0:19:ILE:HD12	2.33	0.44
13:Q:47:THR:HG22	13:Q:93:GLU:OE2	2.17	0.44
1:2:548:U:OP1	13:Q:134:LYS:NZ	2.51	0.44
15:V:51:THR:HG22	15:V:71:TYR:HD1	1.82	0.44
19:6:30:GLN:O	19:6:38:ASP:HB2	2.18	0.44
19:6:90:GLN:HA	19:6:93:TRP:HB3	1.98	0.44
2:A:96:LEU:HB3	2:A:125:ILE:HD13	1.99	0.44
4:C:3:GLU:N	7:F:229:MET:HG2	2.33	0.44
1:2:636:4AC:HM71	1:2:703:4AC:HM73	1.99	0.44
8:G:49:GLU:C	8:G:51:PHE:H	2.22	0.44
19:6:18:LEU:N	19:6:20:GLU:OE2	2.51	0.44
1:2:444:U:H2'	1:2:445:G:O4'	2.18	0.43
2:A:40:ASP:OD1	2:A:40:ASP:N	2.52	0.43
2:A:183:LYS:HD2	2:A:183:LYS:HA	1.82	0.43
1:2:599:C:H4'	1:2:600:G:O5'	2.18	0.43
8:G:40:VAL:HG21	8:G:59:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:641:G:H2'	1:2:642:U:C6	2.53	0.43
9:I:60:VAL:HG22	9:I:61:TYR:H	1.83	0.43
11:M:112:ILE:HG22	11:M:113:GLY:O	2.19	0.43
1:2:637:G:C2	1:2:704:G:C2	3.06	0.43
3:B:187:GLU:HG2	3:B:187:GLU:O	2.18	0.43
13:Q:100:LYS:HE3	13:Q:100:LYS:HB3	1.83	0.43
5:D:111:LYS:HD2	5:D:111:LYS:HA	1.76	0.43
10:J:33:SER:CB	10:J:56:ARG:HD2	2.49	0.43
12:N:39:GLU:O	12:N:40:LYS:HG2	2.18	0.43
3:B:9:LEU:HD23	3:B:9:LEU:HA	1.87	0.43
19:6:104:PHE:O	19:6:105:LEU:HD23	2.18	0.43
6:E:196:LYS:HE2	6:E:196:LYS:HB2	1.85	0.43
1:2:416:C:O2'	5:D:120:GLN:HG3	2.19	0.43
1:2:526:A:H4'	1:2:527:U:H5"	2.00	0.43
1:2:651:G:OP1	2:A:43:LYS:NZ	2.50	0.43
7:F:205:LEU:HD23	7:F:205:LEU:HA	1.82	0.43
9:I:57:ARG:HG3	9:I:57:ARG:O	2.19	0.43
13:Q:29:THR:HG22	13:Q:30:VAL:N	2.34	0.43
10:J:33:SER:O	10:J:33:SER:OG	2.35	0.43
10:J:124:LEU:HD12	10:J:124:LEU:HA	1.90	0.43
1:2:1394:C:N4	1:2:1395:G:O6	2.52	0.42
7:F:62:ASN:HB3	7:F:90:GLY:O	2.18	0.42
11:M:131:GLY:O	11:M:133:ARG:N	2.51	0.42
19:6:29:GLU:O	19:6:63:VAL:HG21	2.19	0.42
10:J:19:LEU:HD23	10:J:19:LEU:HA	1.82	0.42
10:J:108:ALA:HB1	10:J:122:ALA:HB1	1.99	0.42
1:2:1397:G:C2'	1:2:1398:G:H5'	2.50	0.42
11:M:25:ASN:OD1	11:M:26:THR:N	2.40	0.42
1:2:729:G:H2'	1:2:730:C:C6	2.55	0.42
1:2:756:U:H2'	1:2:758:G:OP2	2.20	0.42
6:E:228:GLU:H	6:E:228:GLU:HG3	1.60	0.42
14:R:79:ASN:OD1	14:R:79:ASN:N	2.53	0.42
1:2:68:A:H4'	1:2:69:G:O5'	2.19	0.42
10:J:81:ILE:O	10:J:100:ILE:HB	2.19	0.42
19:6:101:THR:HG23	19:6:103:GLU:HG2	2.01	0.42
1:2:286:4AC:O7	1:2:286:4AC:H5	2.19	0.42
9:I:69:ILE:HG21	9:I:69:ILE:HD13	1.80	0.42
15:V:14:ILE:HG23	15:V:81:ILE:HD12	2.00	0.42
19:6:93:TRP:HE3	19:6:94:LEU:HD12	1.84	0.42
1:2:606:G:O2'	1:2:607:A:H5'	2.19	0.42
1:2:1400:C:H2'	1:2:1401:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:18:VAL:CG2	16:W:58:ALA:HB3	2.50	0.42
1:2:659:U:O2'	1:2:661:A:N7	2.41	0.42
5:D:55:ALA:O	5:D:59:LEU:HB2	2.19	0.42
19:6:19:PRO:HG3	19:6:25:PHE:CE2	2.55	0.42
2:A:56:ILE:O	2:A:57:THR:OG1	2.30	0.42
8:G:37:GLN:H	8:G:62:GLU:HB2	1.85	0.42
1:2:627:G:H2'	1:2:628:G:C8	2.55	0.41
5:D:38:LYS:HA	5:D:38:LYS:HD2	1.92	0.41
6:E:113:HIS:NE2	6:E:241:SER:O	2.53	0.41
7:F:155:LYS:HB2	7:F:155:LYS:HE3	1.75	0.41
19:6:27:VAL:HG12	19:6:66:LEU:HA	2.01	0.41
1:2:303:4AC:HO2'	5:D:6:ARG:NH1	2.15	0.41
1:2:303:4AC:H5	1:2:303:4AC:O7	2.20	0.41
4:C:21:ILE:O	7:F:39:ARG:HD3	2.19	0.41
7:F:139:HIS:ND1	7:F:182:ASP:OD2	2.54	0.41
13:Q:84:LYS:HB2	13:Q:84:LYS:HE3	1.87	0.41
1:2:135:U:O2	6:E:147:ASN:ND2	2.53	0.41
1:2:272:A:H2'	1:2:273:C:C5	2.56	0.41
2:A:153:LEU:HD23	2:A:153:LEU:HA	1.75	0.41
2:A:98:ARG:NH1	2:A:98:ARG:HA	2.35	0.41
14:R:70:ILE:HD11	14:R:88:ILE:CD1	2.50	0.41
3:B:161:ARG:CZ	3:B:199:ILE:HD11	2.51	0.41
5:D:129:HIS:ND1	5:D:158:SER:OG	2.48	0.41
7:F:114:ILE:HD13	7:F:114:ILE:HA	1.85	0.41
15:V:74:ASP:OD1	15:V:75:LYS:N	2.53	0.41
18:5:822:C:H2'	18:5:823:C:N1	2.35	0.41
19:6:66:LEU:O	19:6:86:TYR:HB2	2.21	0.41
1:2:96:C:H2'	1:2:97:A:C8	2.55	0.41
1:2:892:U:H2'	1:2:893:G:O4'	2.21	0.41
1:2:1446:U:H2'	1:2:1447:C:C6	2.53	0.41
2:A:114:ASP:N	2:A:114:ASP:OD1	2.53	0.41
3:B:130:ALA:O	3:B:133:ILE:HG22	2.20	0.41
15:V:5:ILE:HG21	15:V:44:LEU:HD11	2.02	0.41
1:2:1399:C:H2'	1:2:1400:C:C6	2.51	0.41
10:J:35:THR:O	10:J:94:ILE:HA	2.21	0.41
10:J:41:ASP:OD1	10:J:41:ASP:N	2.32	0.41
10:J:63:ALA:HB2	10:J:77:ILE:CG2	2.50	0.41
10:J:101:ILE:HA	10:J:101:ILE:HD13	1.78	0.41
12:N:133:SER:OG	12:N:136:GLU:HG2	2.21	0.41
15:V:70:LYS:HE3	15:V:70:LYS:HB2	1.90	0.41
2:A:114:ASP:HB2	2:A:116:TYR:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:161:GLU:HB2	2:A:166:LYS:HB3	2.03	0.41
8:G:61:MET:HB3	8:G:123:LEU:HD23	2.01	0.41
15:V:33:ARG:NH2	15:V:53:ILE:O	2.54	0.41
15:V:37:LYS:HE3	15:V:51:THR:OG1	2.21	0.41
1:2:695:A:H2'	1:2:696:A:C8	2.56	0.40
1:2:1501:U:H2'	1:2:1502:C:C6	2.57	0.40
9:I:65:LEU:O	9:I:66:LEU:HD23	2.22	0.40
2:A:102:THR:HG21	2:A:130:ILE:HG12	2.03	0.40
19:6:26:GLY:HA2	19:6:39:VAL:HG21	2.03	0.40
19:6:93:TRP:CE3	19:6:94:LEU:HD12	2.56	0.40
1:2:703:4AC:O5'	1:2:703:4AC:H6	2.21	0.40
1:2:1462:A:OP1	19:6:56:ARG:NE	2.55	0.40
2:A:95:SER:O	2:A:95:SER:OG	2.38	0.40
3:B:97:LEU:HA	3:B:98:PRO:HD3	1.95	0.40
12:N:105:ILE:HD13	12:N:105:ILE:HA	1.85	0.40
15:V:72:TYR:CE2	15:V:81:ILE:HD11	2.57	0.40
2:A:29:GLY:O	2:A:31:VAL:HG22	2.21	0.40
2:A:149:LYS:HA	2:A:149:LYS:HD3	1.82	0.40
16:W:36:ARG:HH11	16:W:45:THR:HG21	1.87	0.40
19:6:57:ARG:NE	19:6:58:ARG:HG3	2.37	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	A	186/199 (94%)	170 (91%)	16 (9%)	0	100	100
3	B	194/202 (96%)	181 (93%)	13 (7%)	0	100	100
4	C	59/63 (94%)	51 (86%)	8 (14%)	0	100	100
5	D	173/180 (96%)	163 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	E	240/243 (99%)	216 (90%)	23 (10%)	1 (0%)	30 64
7	F	227/236 (96%)	202 (89%)	25 (11%)	0	100 100
8	G	122/125 (98%)	102 (84%)	19 (16%)	1 (1%)	16 51
9	I	127/130 (98%)	117 (92%)	10 (8%)	0	100 100
10	J	124/127 (98%)	113 (91%)	11 (9%)	0	100 100
11	M	126/137 (92%)	110 (87%)	16 (13%)	0	100 100
12	N	144/147 (98%)	124 (86%)	20 (14%)	0	100 100
13	Q	150/158 (95%)	140 (93%)	10 (7%)	0	100 100
14	R	107/113 (95%)	91 (85%)	16 (15%)	0	100 100
15	V	92/99 (93%)	82 (89%)	10 (11%)	0	100 100
16	W	61/65 (94%)	49 (80%)	12 (20%)	0	100 100
17	0	34/36 (94%)	27 (79%)	7 (21%)	0	100 100
19	6	93/113 (82%)	79 (85%)	14 (15%)	0	100 100
All	All	2259/2373 (95%)	2017 (89%)	240 (11%)	2 (0%)	50 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	36	PRO
8	G	96	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	161/167 (96%)	161 (100%)	0	100 100
3	B	168/173 (97%)	167 (99%)	1 (1%)	84 92
4	C	54/55 (98%)	52 (96%)	2 (4%)	29 62
5	D	158/160 (99%)	157 (99%)	1 (1%)	84 92
6	E	213/214 (100%)	211 (99%)	2 (1%)	75 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	F	192/198 (97%)	185 (96%)	7 (4%)	30 62
8	G	107/108 (99%)	106 (99%)	1 (1%)	75 89
9	I	106/107 (99%)	105 (99%)	1 (1%)	75 89
10	J	102/103 (99%)	102 (100%)	0	100 100
11	M	95/104 (91%)	95 (100%)	0	100 100
12	N	120/121 (99%)	119 (99%)	1 (1%)	79 90
13	Q	137/143 (96%)	137 (100%)	0	100 100
14	R	98/102 (96%)	97 (99%)	1 (1%)	73 87
15	V	86/90 (96%)	86 (100%)	0	100 100
16	W	54/56 (96%)	54 (100%)	0	100 100
17	0	34/34 (100%)	34 (100%)	0	100 100
19	6	83/99 (84%)	83 (100%)	0	100 100
All	All	1968/2034 (97%)	1951 (99%)	17 (1%)	74 89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	181	GLU
4	C	45	THR
4	C	49	LEU
5	D	59	LEU
6	E	41	THR
6	E	168	VAL
7	F	67	ASP
7	F	80	ARG
7	F	93	ASP
7	F	96	VAL
7	F	136	ARG
7	F	143	PHE
7	F	183	VAL
8	G	50	LEU
9	I	61	TYR
12	N	131	ARG
14	R	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	78	ASN
5	D	164	GLN
5	D	176	GLN
6	E	99	HIS
6	E	192	ASN
7	F	203	ASN
8	G	118	GLN
8	G	120	ASN
9	I	9	ASN
11	M	80	HIS
12	N	8	ASN
12	N	66	ASN
12	N	130	ASN
13	Q	85	HIS
13	Q	112	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1013/1044 (97%)	211 (20%)	3 (0%)
18	5	19/20 (95%)	7 (36%)	0
All	All	1032/1064 (96%)	218 (21%)	3 (0%)

All (218) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	C
1	2	29	C
1	2	33	A
1	2	36	C
1	2	38	A
1	2	45	U
1	2	52	C
1	2	55	A
1	2	57	U
1	2	59	A
1	2	62	C
1	2	63	A
1	2	72	A
1	2	73	A
1	2	74	G
1	2	82	C

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Mol	Chain	Res	Type
1	2	85	U
1	2	87	C
1	2	88	U
1	2	89	G
1	2	90	G
1	2	92	A
1	2	95	C
1	2	99	C
1	2	104	G
1	2	108	G
1	2	112	A
1	2	116	A
1	2	117	C
1	2	118	A
1	2	126	A
1	2	128	C
1	2	146	A
1	2	154	G
1	2	158	A
1	2	160	C
1	2	169	A
1	2	170	U
1	2	178	A
1	2	196	G
1	2	209	A
1	2	210	A
1	2	211	A
1	2	212	G
1	2	217	C
1	2	218	C
1	2	222	A
1	2	223	G
1	2	225	C
1	2	226	U
1	2	227	C
1	2	229	G
1	2	236	G
1	2	240	G
1	2	249	C
1	2	254	U
1	2	256	G
1	2	260	G

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Mol	Chain	Res	Type
1	2	262	U
1	2	268	G
1	2	275	G
1	2	276	C
1	2	277	C
1	2	290	G
1	2	292	U
1	2	298	C
1	2	299	G
1	2	308	G
1	2	315	A
1	2	330	A
1	2	337	C
1	2	338	A
1	2	341	G
1	2	353	A
1	2	354	C
1	2	358	G
1	2	361	C
1	2	362	A
1	2	363	G
1	2	371	G
1	2	373	A2M
1	2	376	C
1	2	381	C
1	2	384	U
1	2	385	G
1	2	397	G
1	2	399	C
1	2	401	G
1	2	402	G
1	2	406	A
1	2	415	G
1	2	423	U
1	2	424	C
1	2	425	U
1	2	426	G
1	2	431	G
1	2	432	G
1	2	437	U
1	2	440	G
1	2	449	A

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Mol	Chain	Res	Type
1	2	456	C
1	2	457	G
1	2	459	G
1	2	460	A
1	2	462	U
1	2	464	A
1	2	470	G
1	2	474	A
1	2	477	G
1	2	483	G
1	2	484	G
1	2	487	G
1	2	493	G
1	2	497	U
1	2	498	A
1	2	501	A
1	2	513	A
1	2	519	G
1	2	531	U
1	2	532	G
1	2	539	A
1	2	542	C
1	2	543	G
1	2	551	C
1	2	571	C
1	2	574	A
1	2	600	G
1	2	609	A
1	2	620	U
1	2	621	G
1	2	632	A
1	2	642	U
1	2	649	G
1	2	652	G
1	2	653	U
1	2	655	G
1	2	665	C
1	2	679	G
1	2	681	G
1	2	687	C
1	2	690	U
1	2	691	G

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Mol	Chain	Res	Type
1	2	699	C
1	2	701	C
1	2	715	G
1	2	716	U
1	2	722	G
1	2	728	G
1	2	730	C
1	2	739	A
1	2	744	A
1	2	748	A
1	2	749	A
1	2	760	U
1	2	761	A
1	2	767	G
1	2	770	G
1	2	782	A
1	2	784	G
1	2	809	C
1	2	811	U
1	2	812	C
1	2	813	G
1	2	836	A
1	2	841	U
1	2	843	A
1	2	844	A
1	2	853	C
1	2	855	U
1	2	856	G
1	2	861	G
1	2	865	G
1	2	873	G
1	2	885	A
1	2	891	U
1	2	893	G
1	2	895	C
1	2	897	G
1	2	1368	A
1	2	1369	C
1	2	1371	C
1	2	1372	A
1	2	1388	C
1	2	1397	G

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Mol	Chain	Res	Type
1	2	1398	G
1	2	1399	C
1	2	1400	C
1	2	1401	U
1	2	1415	U
1	2	1424	G
1	2	1427	G
1	2	1435	C
1	2	1436	G
1	2	1437	A
1	2	1452	A
1	2	1459	A
1	2	1461	A
1	2	1462	A
1	2	1463	G
1	2	1468	A
1	2	1471	A
1	2	1473	G
1	2	1475	U
1	2	1477	G
1	2	1478	C
1	2	1482	A
1	2	1486	G
1	2	1498	C
1	2	1499	G
1	2	1508	C
1	2	1509	U
18	5	806	G
18	5	813	A
18	5	815	U
18	5	816	U
18	5	817	A
18	5	822	C
18	5	823	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	87	C
1	2	599	C
1	2	1387	A

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

32 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	4AC	2	319	1	21,24,25	1.11	2 (9%)	29,34,37	1.25	3 (10%)
1	4AC	2	626	1	21,24,25	1.01	2 (9%)	29,34,37	1.26	4 (13%)
1	A2M	2	373	1	18,25,26	0.97	0	18,36,39	1.36	3 (16%)
1	4AC	2	636	1	21,24,25	1.12	2 (9%)	29,34,37	1.48	3 (10%)
1	4AC	2	546	1	21,24,25	1.02	2 (9%)	29,34,37	1.21	3 (10%)
1	4AC	2	53	1	21,24,25	1.06	2 (9%)	29,34,37	1.24	4 (13%)
1	UR3	2	1467	1	19,22,23	0.91	1 (5%)	26,32,35	1.37	2 (7%)
1	4AC	2	731	1	21,24,25	1.02	2 (9%)	29,34,37	1.18	3 (10%)
1	4AC	2	703	1	21,24,25	1.10	1 (4%)	29,34,37	1.78	5 (17%)
1	5HM	2	1378	1	19,23,24	2.89	7 (36%)	25,33,36	0.71	0
1	4AC	2	848	1	21,24,25	1.10	2 (9%)	29,34,37	1.27	2 (6%)
1	4AC	2	511	1	21,24,25	1.09	1 (4%)	29,34,37	1.31	3 (10%)
1	LHH	2	250	1	22,25,26	2.55	8 (36%)	29,35,38	1.24	2 (6%)
1	4AC	2	839	1	21,24,25	1.08	1 (4%)	29,34,37	1.28	3 (10%)
1	4AC	2	648	1	21,24,25	1.01	2 (9%)	29,34,37	1.40	4 (13%)
1	OMC	2	1376	1	19,22,23	0.82	0	26,31,34	0.94	1 (3%)
1	4AC	2	479	1	21,24,25	1.01	2 (9%)	29,34,37	1.44	4 (13%)
1	4AC	2	868	1	21,24,25	1.00	2 (9%)	29,34,37	1.28	3 (10%)
1	4AC	2	718	1	21,24,25	1.06	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	2	286	1	21,24,25	1.09	2 (9%)	29,34,37	1.36	4 (13%)
1	6MZ	2	1469	1,20	18,25,26	0.84	1 (5%)	16,36,39	2.24	3 (18%)
1	4AC	2	590	1	21,24,25	1.07	2 (9%)	29,34,37	1.43	4 (13%)
1	4AC	2	1479	1	21,24,25	1.13	2 (9%)	29,34,37	1.07	2 (6%)
1	MA6	2	1488	1	18,26,27	0.82	0	19,38,41	1.19	2 (10%)
1	4AC	2	394	1	21,24,25	1.03	2 (9%)	29,34,37	1.24	4 (13%)
1	4AC	2	379	1	21,24,25	1.06	2 (9%)	29,34,37	1.51	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	4AC	2	17	1	21,24,25	1.09	2 (9%)	29,34,37	1.28	4 (13%)
1	MA6	2	1487	1	18,26,27	0.86	0	19,38,41	1.19	2 (10%)
1	4AC	2	851	1	21,24,25	1.14	2 (9%)	29,34,37	1.40	2 (6%)
1	4AC	2	303	1	21,24,25	1.11	3 (14%)	29,34,37	1.30	4 (13%)
1	4AC	2	828	1	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	2	751	1	21,24,25	1.00	2 (9%)	29,34,37	1.16	3 (10%)

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	4AC	2	319	1	-	0/11/29/30	0/2/2/2
1	4AC	2	626	1	-	0/11/29/30	0/2/2/2
1	A2M	2	373	1	-	2/5/27/28	0/3/3/3
1	4AC	2	636	1	-	2/11/29/30	0/2/2/2
1	4AC	2	546	1	-	2/11/29/30	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	UR3	2	1467	1	-	1/7/25/26	0/2/2/2
1	4AC	2	731	1	-	0/11/29/30	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	5HM	2	1378	1	-	2/9/27/28	0/2/2/2
1	4AC	2	848	1	-	0/11/29/30	0/2/2/2
1	4AC	2	511	1	-	1/11/29/30	0/2/2/2
1	LHH	2	250	1	-	1/13/31/32	0/2/2/2
1	4AC	2	839	1	-	2/11/29/30	0/2/2/2
1	4AC	2	648	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
1	4AC	2	479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	868	1	-	1/11/29/30	0/2/2/2
1	4AC	2	718	1	-	2/11/29/30	0/2/2/2
1	4AC	2	286	1	-	2/11/29/30	0/2/2/2
1	6MZ	2	1469	1,20	-	0/5/27/28	0/3/3/3
1	4AC	2	590	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	0/7/29/30	0/3/3/3
1	4AC	2	394	1	-	2/11/29/30	0/2/2/2
1	4AC	2	379	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	17	1	-	2/11/29/30	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	4AC	2	851	1	-	0/11/29/30	0/2/2/2
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	4AC	2	828	1	-	0/11/29/30	0/2/2/2
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	250	LHH	C4-N4	6.38	1.49	1.39
1	2	1378	5HM	C4-N3	6.16	1.44	1.34
1	2	250	LHH	C7-N4	5.86	1.48	1.37
1	2	1378	5HM	C4-N4	5.29	1.47	1.34
1	2	1378	5HM	C2-N3	5.28	1.47	1.36
1	2	1378	5HM	C6-C5	4.94	1.48	1.34
1	2	250	LHH	O2-C2	-4.34	1.15	1.23
1	2	1378	5HM	C6-N1	3.80	1.44	1.38
1	2	250	LHH	C2-N1	-3.55	1.32	1.40
1	2	851	4AC	C4-N3	-3.51	1.26	1.32
1	2	319	4AC	C4-N3	-3.41	1.26	1.32
1	2	1378	5HM	O2-C2	-3.34	1.17	1.23
1	2	1479	4AC	C4-N3	-3.31	1.27	1.32
1	2	511	4AC	C4-N3	-3.28	1.27	1.32
1	2	590	4AC	C4-N3	-3.22	1.27	1.32
1	2	303	4AC	C4-N3	-3.21	1.27	1.32
1	2	848	4AC	C4-N3	-3.17	1.27	1.32
1	2	17	4AC	C4-N3	-3.14	1.27	1.32
1	2	839	4AC	C4-N3	-3.12	1.27	1.32
1	2	53	4AC	C4-N3	-3.12	1.27	1.32
1	2	731	4AC	C4-N3	-3.09	1.27	1.32
1	2	636	4AC	C4-N3	-3.09	1.27	1.32
1	2	286	4AC	C4-N3	-3.07	1.27	1.32
1	2	394	4AC	C4-N3	-3.06	1.27	1.32
1	2	703	4AC	C4-N3	-3.02	1.27	1.32
1	2	546	4AC	C4-N3	-2.98	1.27	1.32
1	2	626	4AC	C4-N3	-2.96	1.27	1.32
1	2	1378	5HM	C2-N1	2.92	1.46	1.40
1	2	751	4AC	C4-N3	-2.91	1.27	1.32
1	2	718	4AC	C4-N3	-2.90	1.27	1.32
1	2	379	4AC	C4-N3	-2.87	1.27	1.32
1	2	828	4AC	C4-N3	-2.85	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	250	LHH	C2-N3	-2.84	1.30	1.36
1	2	868	4AC	C4-N3	-2.83	1.27	1.32
1	2	648	4AC	C4-N3	-2.78	1.28	1.32
1	2	479	4AC	C4-N3	-2.77	1.28	1.32
1	2	250	LHH	C6-N1	-2.77	1.31	1.38
1	2	636	4AC	C4-N4	-2.51	1.36	1.39
1	2	250	LHH	C6-C5	2.47	1.40	1.35
1	2	590	4AC	C5-C4	2.41	1.46	1.40
1	2	848	4AC	C5-C4	2.35	1.45	1.40
1	2	718	4AC	C5-C4	2.33	1.45	1.40
1	2	731	4AC	C5-C4	2.25	1.45	1.40
1	2	648	4AC	C5-C4	2.23	1.45	1.40
1	2	394	4AC	C5-C4	2.23	1.45	1.40
1	2	479	4AC	C5-C4	2.23	1.45	1.40
1	2	851	4AC	C4-N4	-2.22	1.36	1.39
1	2	17	4AC	C5-C4	2.22	1.45	1.40
1	2	828	4AC	C5-C4	2.19	1.45	1.40
1	2	379	4AC	C5-C4	2.16	1.45	1.40
1	2	626	4AC	C5-C4	2.16	1.45	1.40
1	2	286	4AC	C5-C4	2.15	1.45	1.40
1	2	751	4AC	C5-C4	2.15	1.45	1.40
1	2	1469	6MZ	C5-C4	2.14	1.46	1.40
1	2	250	LHH	O7-C7	-2.13	1.18	1.23
1	2	303	4AC	C4-N4	-2.13	1.36	1.39
1	2	868	4AC	C5-C4	2.12	1.45	1.40
1	2	1479	4AC	C4-N4	-2.11	1.36	1.39
1	2	53	4AC	C5-C4	2.08	1.45	1.40
1	2	319	4AC	C5-C4	2.08	1.45	1.40
1	2	303	4AC	C5-C4	2.07	1.45	1.40
1	2	546	4AC	C5-C4	2.07	1.45	1.40
1	2	1467	UR3	C6-N1	-2.06	1.33	1.38

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1469	6MZ	C2-N1-C6	6.81	122.43	116.59
1	2	636	4AC	O7-C7-N4	5.50	130.71	121.82
1	2	703	4AC	O7-C7-N4	5.48	130.69	121.82
1	2	1467	UR3	C4-N3-C2	-5.06	119.80	124.56
1	2	851	4AC	O7-C7-N4	4.95	129.83	121.82
1	2	379	4AC	O7-C7-N4	4.86	129.69	121.82
1	2	590	4AC	O7-C7-N4	4.83	129.64	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	479	4AC	O7-C7-N4	4.60	129.27	121.82
1	2	848	4AC	O7-C7-N4	4.55	129.18	121.82
1	2	703	4AC	C5-C4-N4	-4.52	115.06	122.92
1	2	303	4AC	O7-C7-N4	4.52	129.14	121.82
1	2	286	4AC	O7-C7-N4	4.48	129.06	121.82
1	2	828	4AC	O7-C7-N4	4.48	129.06	121.82
1	2	839	4AC	O7-C7-N4	4.46	129.03	121.82
1	2	718	4AC	O7-C7-N4	4.46	129.03	121.82
1	2	703	4AC	N4-C4-N3	4.41	121.25	113.85
1	2	626	4AC	O7-C7-N4	4.29	128.76	121.82
1	2	394	4AC	O7-C7-N4	4.24	128.68	121.82
1	2	511	4AC	O7-C7-N4	4.19	128.60	121.82
1	2	17	4AC	O7-C7-N4	4.18	128.58	121.82
1	2	648	4AC	O7-C7-N4	4.18	128.58	121.82
1	2	53	4AC	O7-C7-N4	4.13	128.49	121.82
1	2	546	4AC	O7-C7-N4	4.11	128.48	121.82
1	2	319	4AC	O7-C7-N4	4.10	128.46	121.82
1	2	868	4AC	O7-C7-N4	4.08	128.42	121.82
1	2	636	4AC	CM7-C7-N4	-3.88	108.59	115.29
1	2	751	4AC	O7-C7-N4	3.76	127.90	121.82
1	2	1488	MA6	N3-C2-N1	-3.60	123.05	128.68
1	2	731	4AC	O7-C7-N4	3.58	127.61	121.82
1	2	379	4AC	C5-C4-N4	-3.52	116.80	122.92
1	2	1469	6MZ	N3-C2-N1	-3.46	123.27	128.68
1	2	1469	6MZ	C4-C5-N7	-3.45	105.80	109.40
1	2	648	4AC	N4-C4-N3	3.44	119.62	113.85
1	2	479	4AC	N4-C4-N3	3.42	119.58	113.85
1	2	1479	4AC	O7-C7-N4	3.38	127.29	121.82
1	2	379	4AC	N4-C4-N3	3.38	119.53	113.85
1	2	648	4AC	C5-C4-N4	-3.30	117.19	122.92
1	2	1487	MA6	C4-C5-N7	-3.22	106.05	109.40
1	2	1487	MA6	N3-C2-N1	-3.20	123.67	128.68
1	2	511	4AC	N4-C4-N3	2.97	118.84	113.85
1	2	479	4AC	C5-C4-N4	-2.92	117.84	122.92
1	2	286	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	2	626	4AC	CM7-C7-N4	-2.81	110.44	115.29
1	2	373	A2M	N3-C2-N1	-2.77	124.35	128.68
1	2	851	4AC	CM7-C7-N4	-2.77	110.51	115.29
1	2	373	A2M	C4-C5-N7	-2.75	106.54	109.40
1	2	731	4AC	O2-C2-N3	-2.73	117.89	122.33
1	2	17	4AC	O2-C2-N3	-2.72	117.90	122.33
1	2	751	4AC	N4-C4-N3	2.71	118.41	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	590	4AC	CM7-C7-N4	-2.70	110.62	115.29
1	2	718	4AC	CM7-C7-N4	-2.67	110.67	115.29
1	2	319	4AC	N4-C4-N3	2.65	118.30	113.85
1	2	828	4AC	CM7-C7-N4	-2.64	110.73	115.29
1	2	303	4AC	C5-C4-N4	-2.64	118.34	122.92
1	2	1376	OMC	O2-C2-N3	-2.64	118.05	122.33
1	2	286	4AC	C5-C4-N4	-2.63	118.36	122.92
1	2	868	4AC	N4-C4-N3	2.62	118.25	113.85
1	2	1467	UR3	C3U-N3-C4	2.62	121.63	117.89
1	2	286	4AC	N4-C4-N3	2.59	118.20	113.85
1	2	590	4AC	C1'-N1-C6	2.59	126.49	120.84
1	2	53	4AC	CM7-C7-N4	-2.54	110.89	115.29
1	2	848	4AC	CM7-C7-N4	-2.53	110.92	115.29
1	2	1488	MA6	C4-C5-N7	-2.53	106.77	109.40
1	2	303	4AC	N4-C4-N3	2.52	118.08	113.85
1	2	718	4AC	N4-C4-N3	2.52	118.08	113.85
1	2	546	4AC	N4-C4-N3	2.50	118.06	113.85
1	2	250	LHH	CM7-C7-N4	2.50	119.62	115.29
1	2	703	4AC	CM7-C7-N4	-2.49	110.99	115.29
1	2	394	4AC	CM7-C7-N4	-2.48	111.00	115.29
1	2	839	4AC	CM7-C7-N4	-2.47	111.02	115.29
1	2	636	4AC	C5-C4-N4	-2.46	118.64	122.92
1	2	17	4AC	CM7-C7-N4	-2.45	111.05	115.29
1	2	250	LHH	C5-C4-N3	-2.45	118.65	122.59
1	2	718	4AC	C5-C4-N4	-2.44	118.67	122.92
1	2	626	4AC	N4-C4-N3	2.44	117.95	113.85
1	2	319	4AC	C5-C4-N4	-2.41	118.72	122.92
1	2	828	4AC	N4-C4-N3	2.33	117.76	113.85
1	2	479	4AC	CM7-C7-N4	-2.32	111.27	115.29
1	2	511	4AC	C5-C4-N4	-2.31	118.91	122.92
1	2	53	4AC	N4-C4-N3	2.30	117.72	113.85
1	2	53	4AC	C5-C4-N4	-2.27	118.97	122.92
1	2	379	4AC	CM7-C7-N4	-2.24	111.42	115.29
1	2	394	4AC	N4-C4-N3	2.21	117.56	113.85
1	2	868	4AC	C5-C4-N4	-2.21	119.09	122.92
1	2	303	4AC	CM7-C7-N4	-2.20	111.49	115.29
1	2	626	4AC	C5-C4-N4	-2.19	119.11	122.92
1	2	839	4AC	N4-C4-N3	2.18	117.51	113.85
1	2	394	4AC	O2-C2-N3	-2.18	118.79	122.33
1	2	590	4AC	N4-C4-N3	2.15	117.46	113.85
1	2	648	4AC	CM7-C7-N4	-2.11	111.65	115.29
1	2	546	4AC	C5-C4-N4	-2.09	119.29	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	751	4AC	C5-C4-N4	-2.08	119.31	122.92
1	2	17	4AC	N4-C4-N3	2.07	117.33	113.85
1	2	1479	4AC	CM7-C7-N4	-2.07	111.71	115.29
1	2	731	4AC	CM7-C7-N4	-2.06	111.74	115.29
1	2	703	4AC	O7-C7-CM7	-2.02	118.31	122.06
1	2	373	A2M	O3'-C3'-C2'	2.01	116.89	111.17
1	2	828	4AC	C5-C4-N4	-2.01	119.43	122.92

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	17	4AC	C3'-C4'-C5'-O5'
1	2	286	4AC	O4'-C4'-C5'-O5'
1	2	286	4AC	C3'-C4'-C5'-O5'
1	2	373	A2M	O4'-C4'-C5'-O5'
1	2	394	4AC	O4'-C4'-C5'-O5'
1	2	394	4AC	C3'-C4'-C5'-O5'
1	2	546	4AC	O4'-C4'-C5'-O5'
1	2	546	4AC	C3'-C4'-C5'-O5'
1	2	636	4AC	C3'-C4'-C5'-O5'
1	2	839	4AC	O4'-C4'-C5'-O5'
1	2	17	4AC	O4'-C4'-C5'-O5'
1	2	373	A2M	C3'-C4'-C5'-O5'
1	2	636	4AC	O4'-C4'-C5'-O5'
1	2	718	4AC	O4'-C4'-C5'-O5'
1	2	839	4AC	C3'-C4'-C5'-O5'
1	2	718	4AC	C3'-C4'-C5'-O5'
1	2	1376	OMC	C3'-C4'-C5'-O5'
1	2	1376	OMC	O4'-C4'-C5'-O5'
1	2	1378	5HM	C4-C5-CM5-OM5
1	2	1378	5HM	C6-C5-CM5-OM5
1	2	250	LHH	O4'-C4'-C5'-O5'
1	2	511	4AC	C3'-C4'-C5'-O5'
1	2	1467	UR3	O4'-C4'-C5'-O5'
1	2	868	4AC	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	636	4AC	3	0
1	2	703	4AC	5	0
1	2	1378	5HM	1	0
1	2	648	4AC	2	0
1	2	286	4AC	1	0
1	2	379	4AC	1	0
1	2	303	4AC	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 30 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	902:G	O3'	1356:C	P	14.11

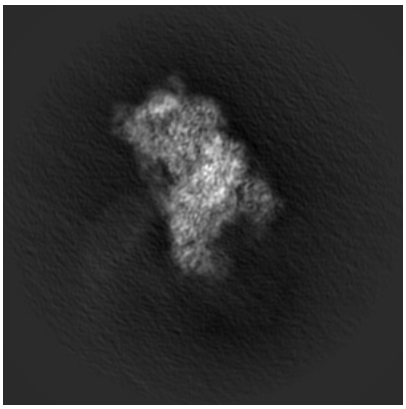
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10323. These allow visual inspection of the internal detail of the map and identification of artifacts.

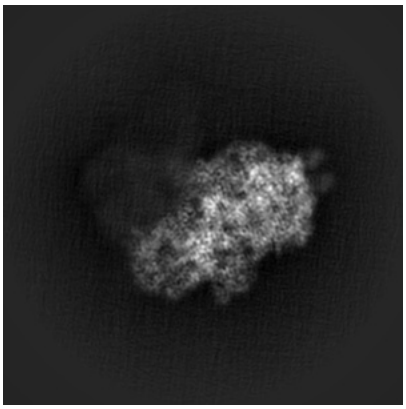
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

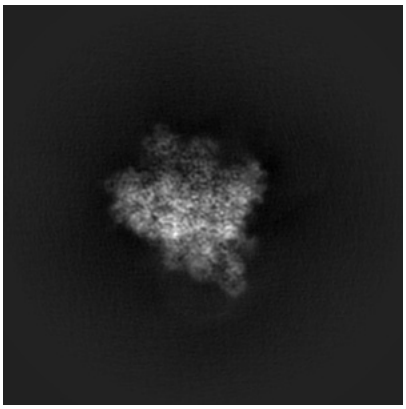
6.1.1 Primary map



X

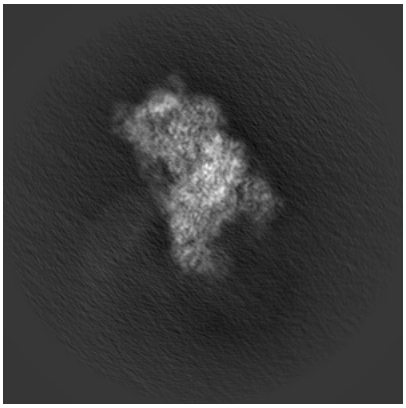


Y

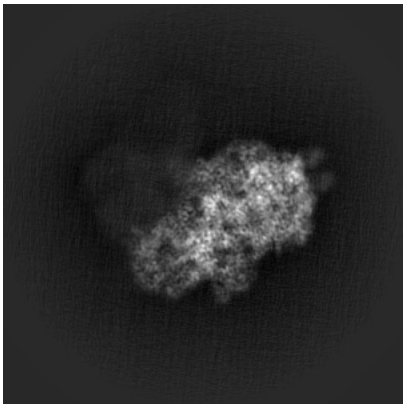


Z

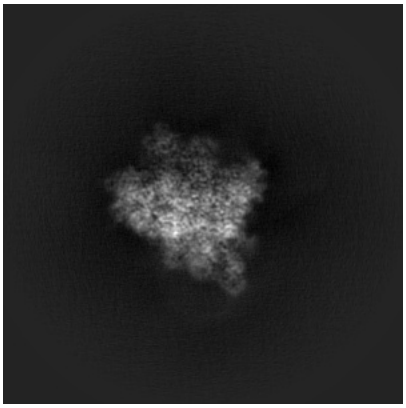
6.1.2 Raw map



X



Y

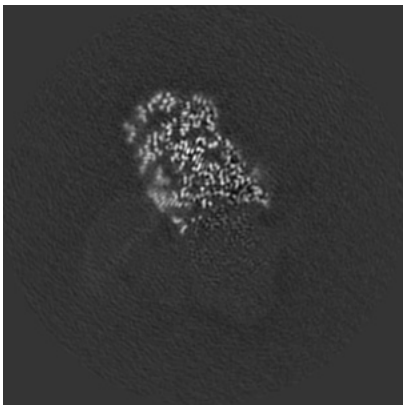


Z

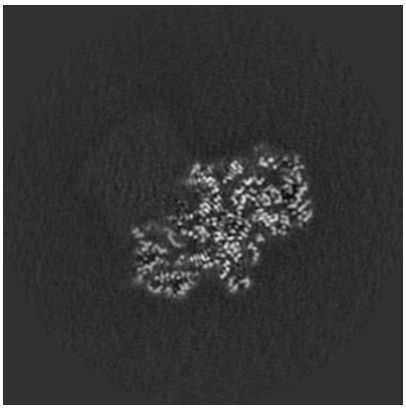
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

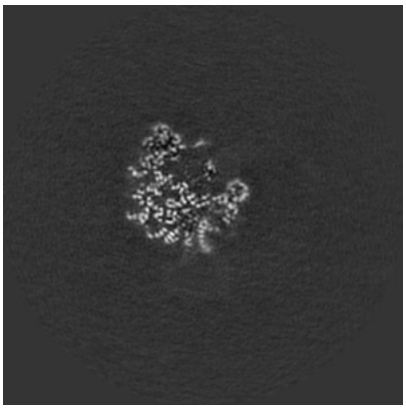
6.2.1 Primary map



X Index: 174

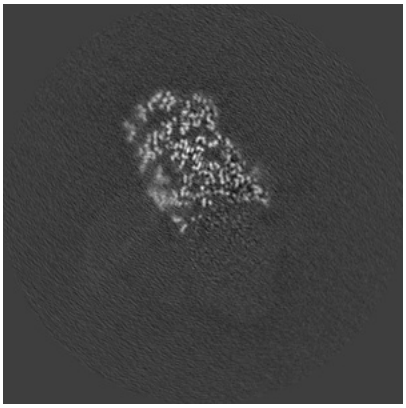


Y Index: 174

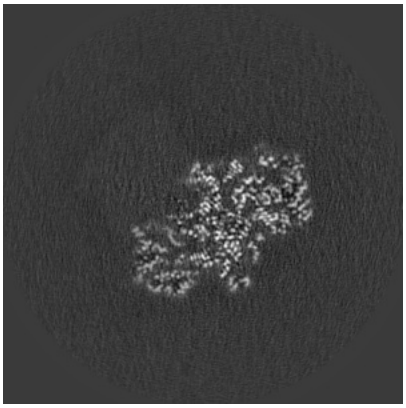


Z Index: 174

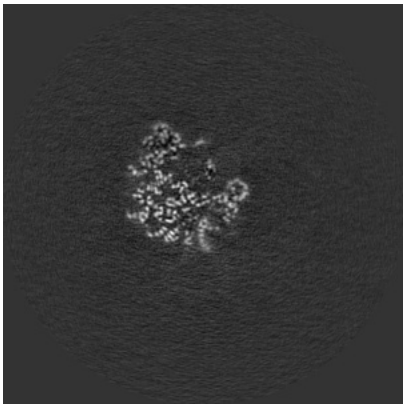
6.2.2 Raw map



X Index: 174



Y Index: 174

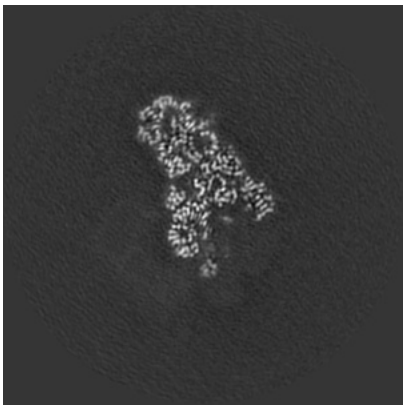


Z Index: 174

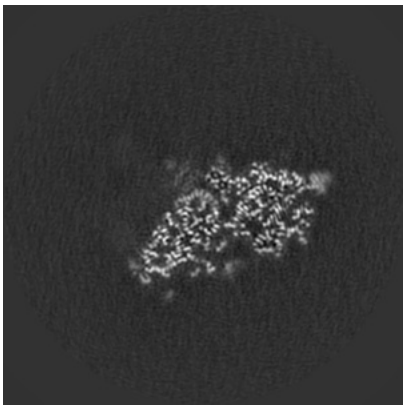
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

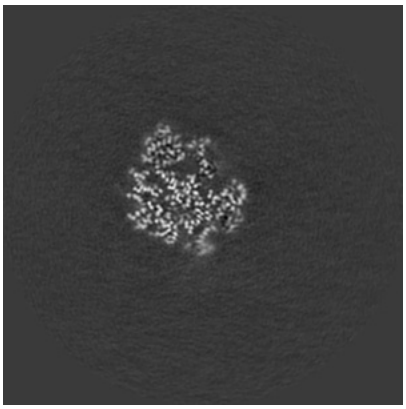
6.3.1 Primary map



X Index: 149

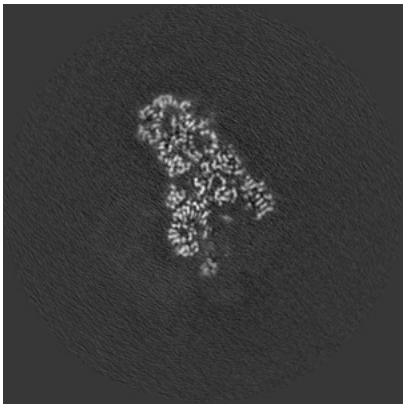


Y Index: 154

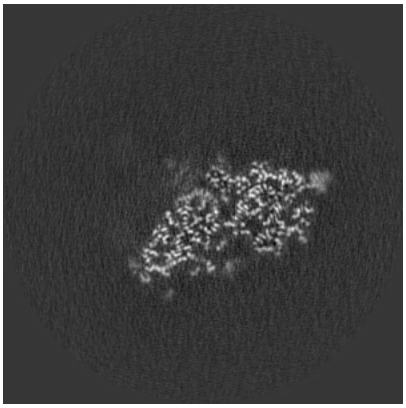


Z Index: 178

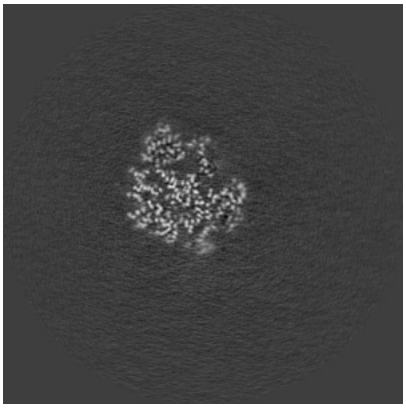
6.3.2 Raw map



X Index: 149



Y Index: 154

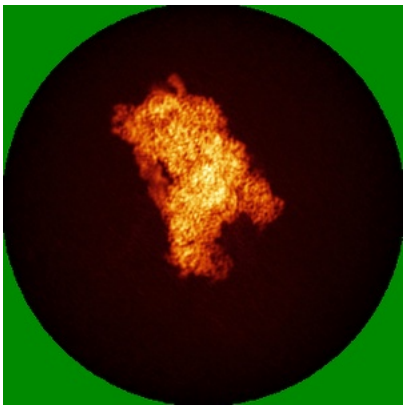


Z Index: 178

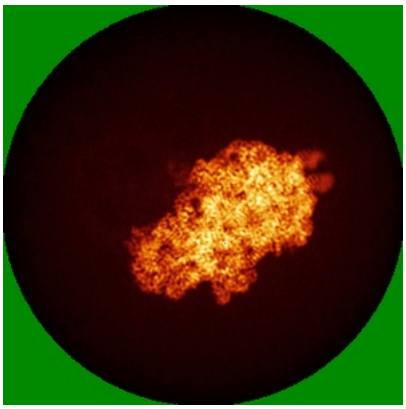
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

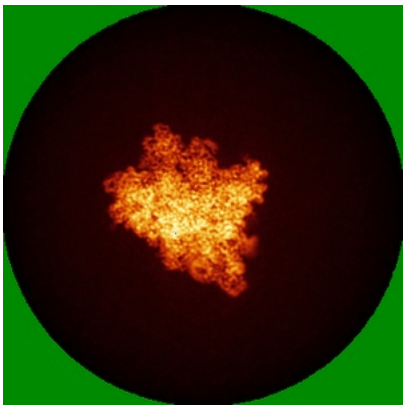
6.4.1 Primary map



X

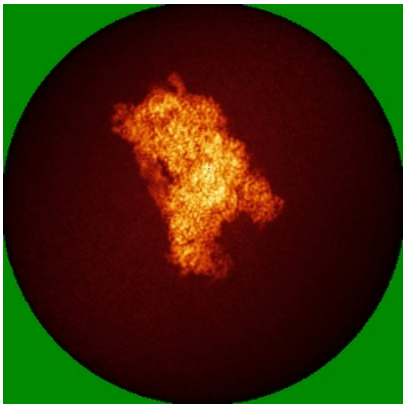


Y

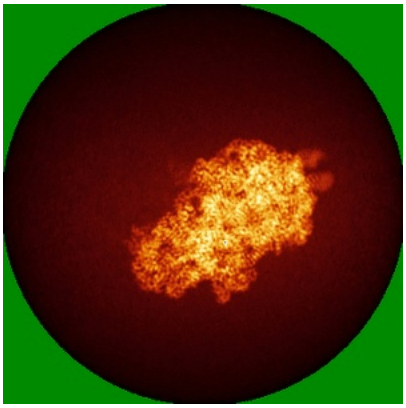


Z

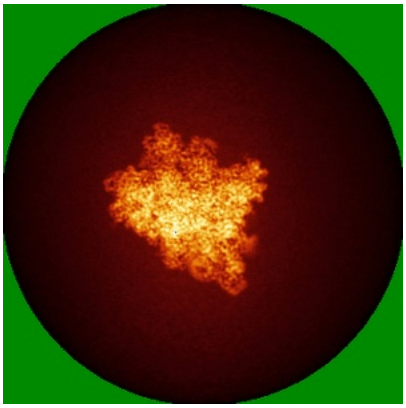
6.4.2 Raw map



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 0.006. 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.

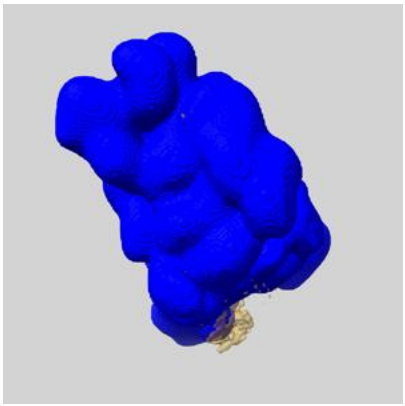
6.6 Mask visualisation (i)

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

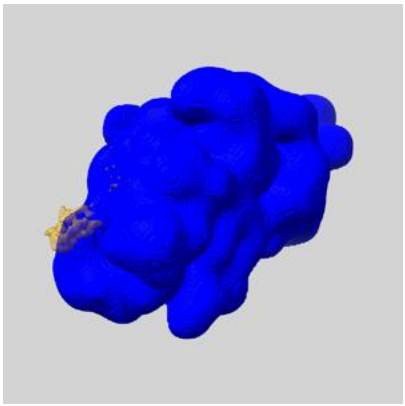
A mask typically either:

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

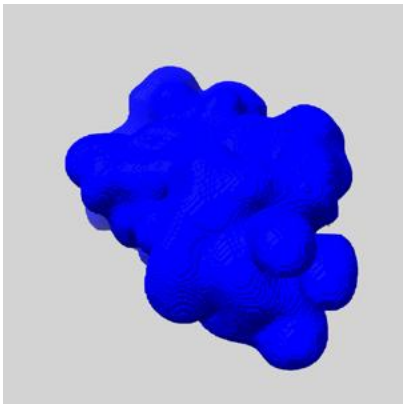
6.6.1 emd_10323_msk_1.map (i)



X



Y

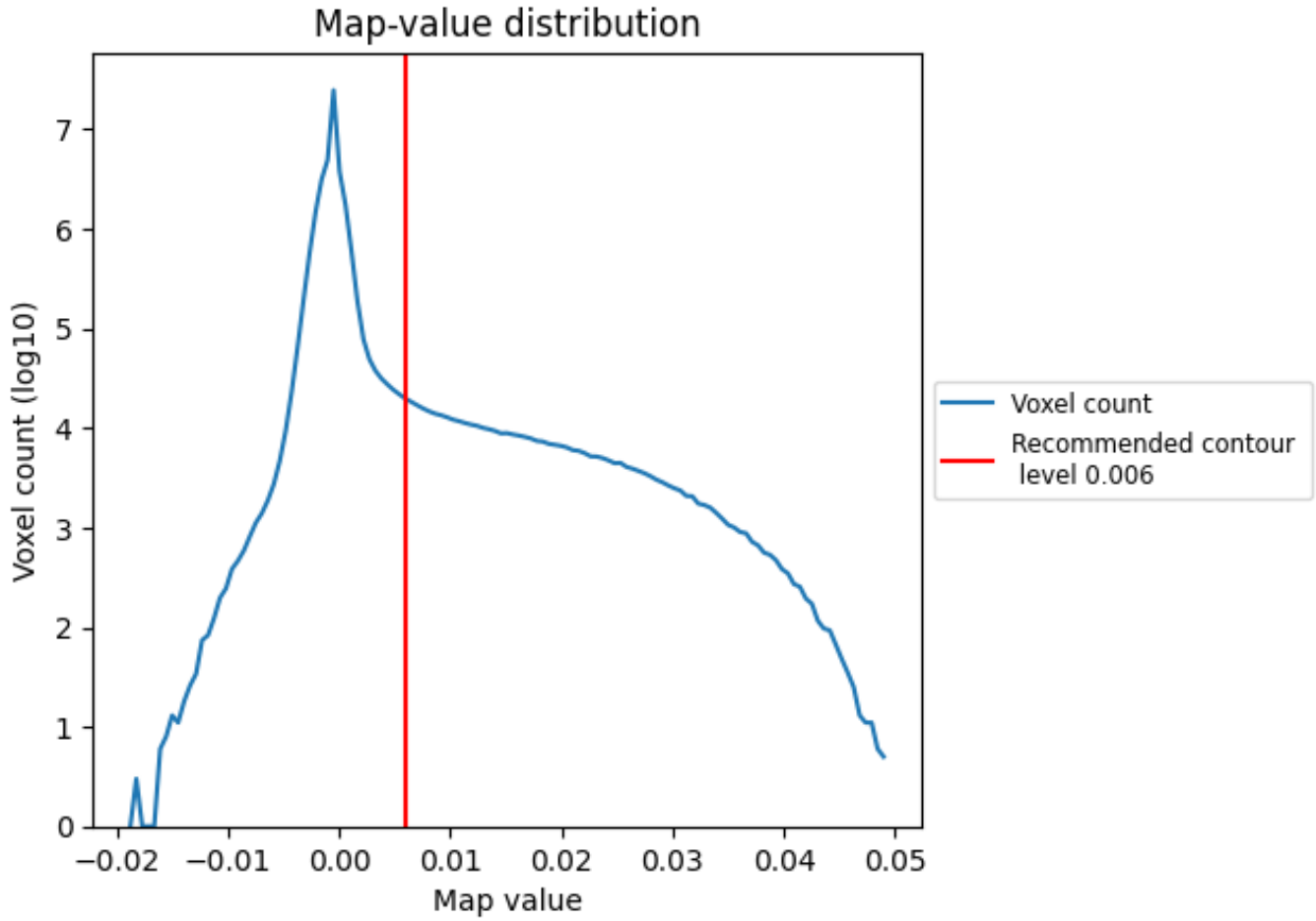


Z

7 Map analysis

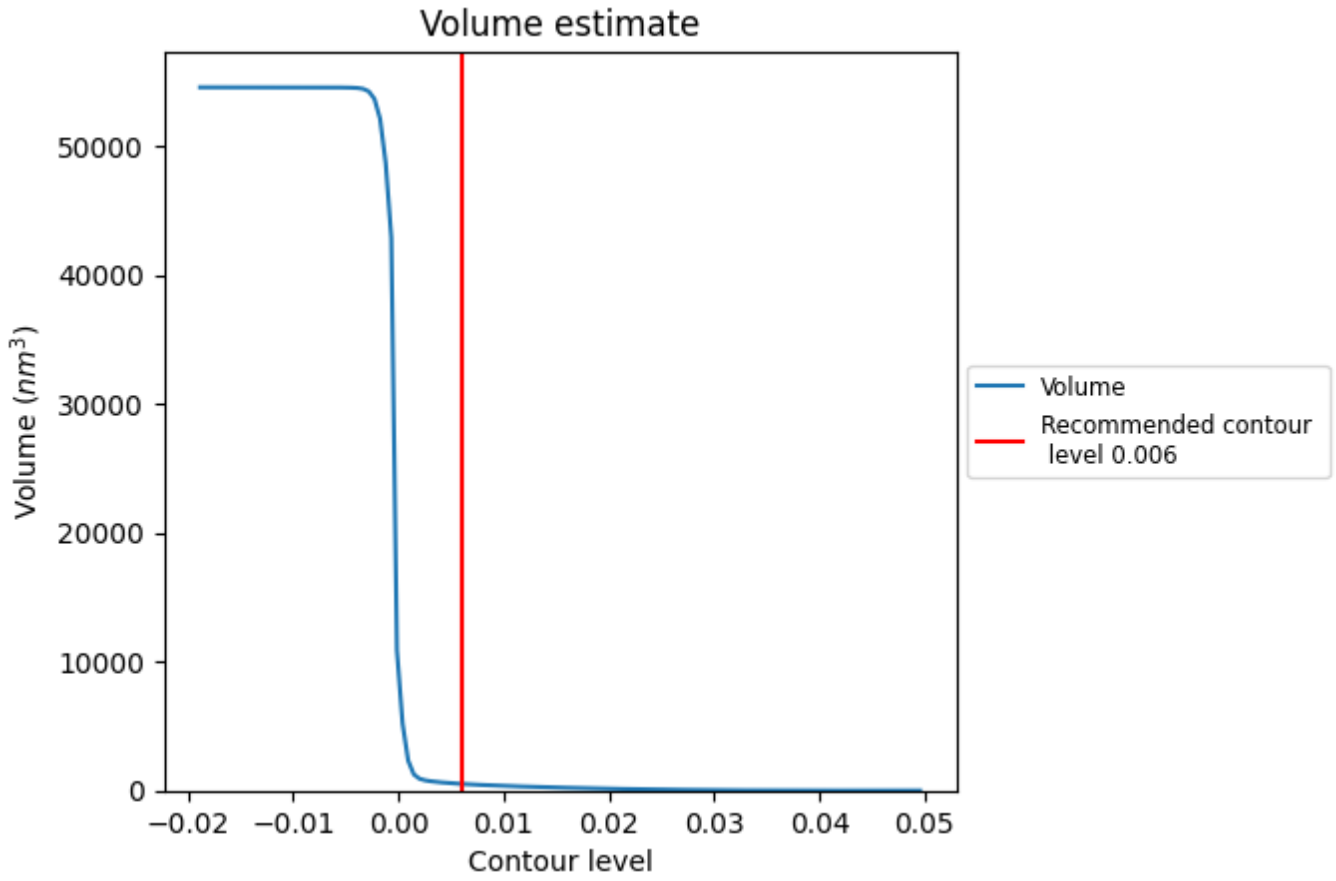
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

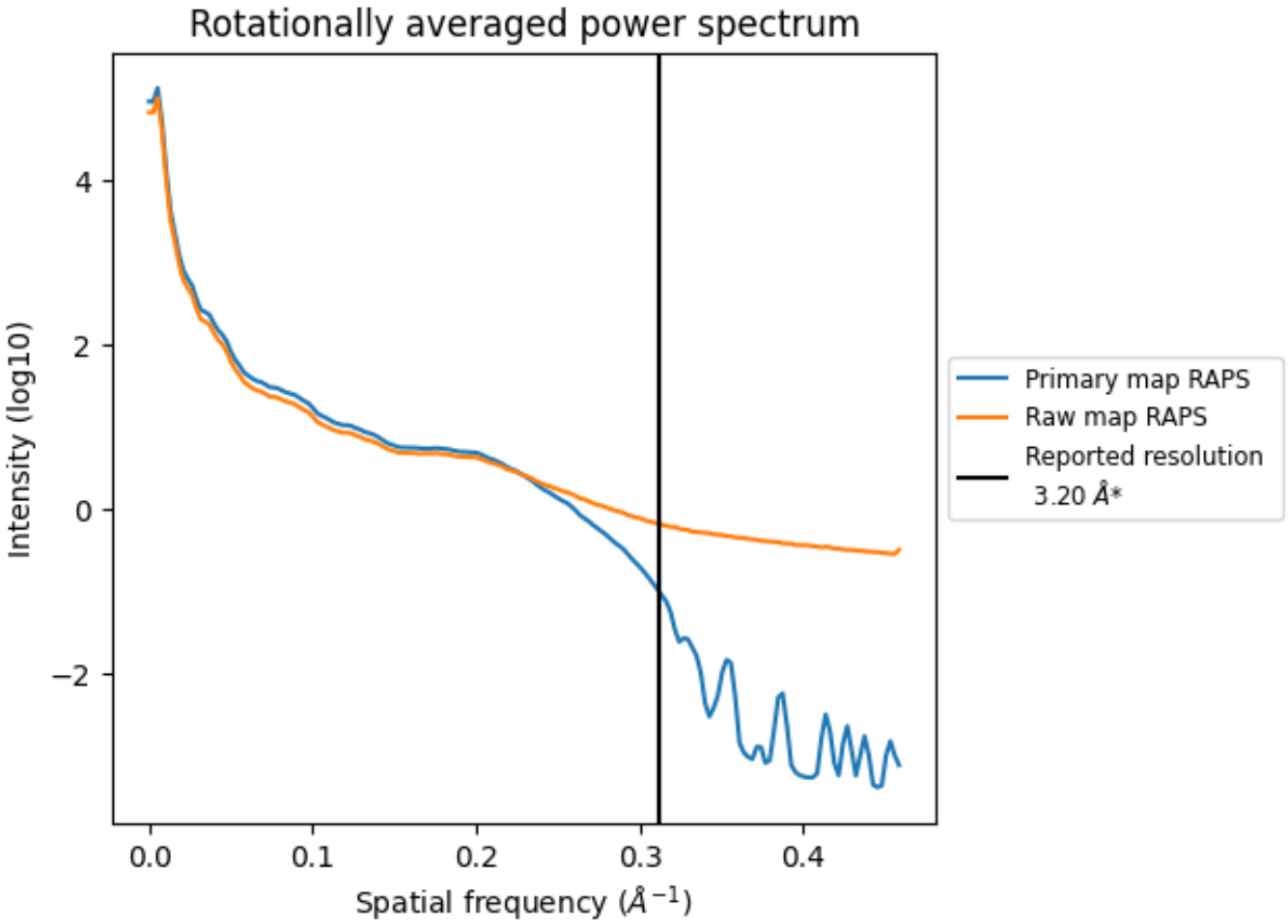
7.2 Volume estimate (i)



The volume at the recommended contour level is 519 nm^3; this corresponds to an approximate mass of 469 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)

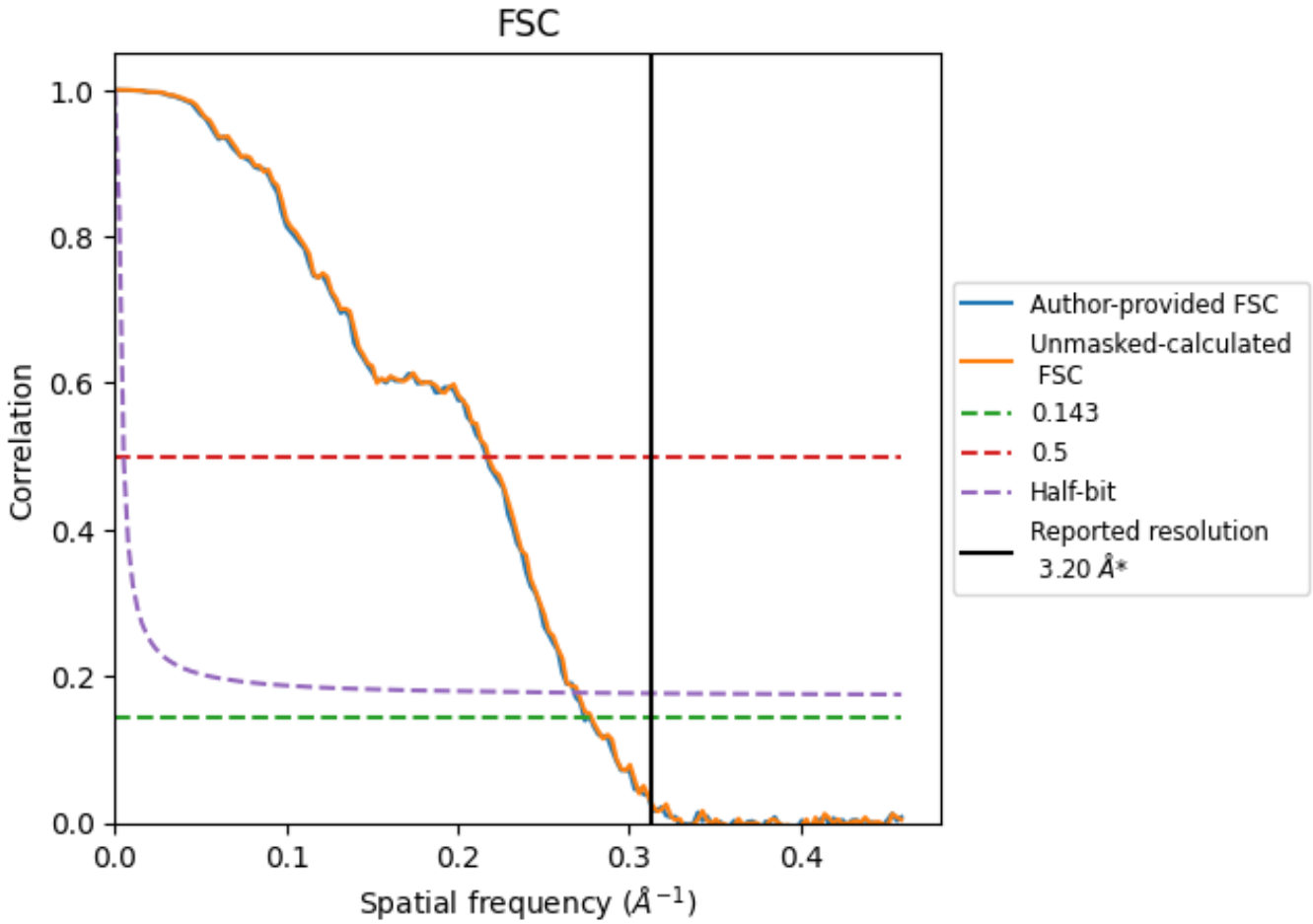


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.65	4.61	3.73
Unmasked-calculated*	3.60	4.59	3.70

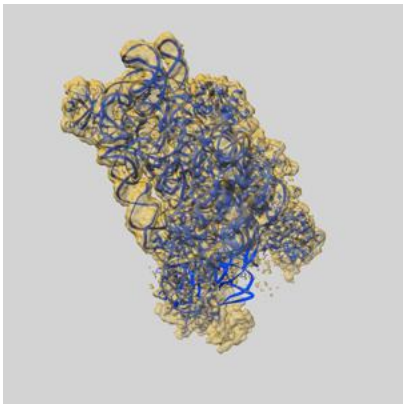
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.65 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 3.2 by more than 10 %

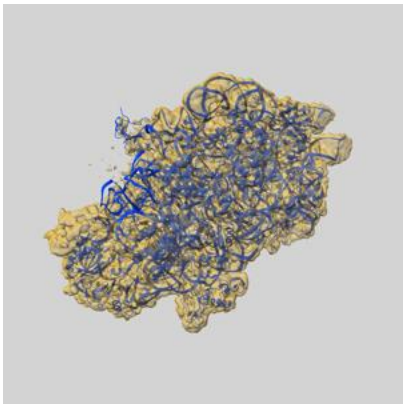
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10323 and PDB model 6SWD. Per-residue inclusion information can be found in section 3 on page 8.

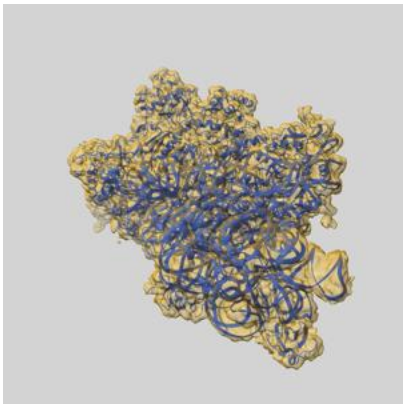
9.1 Map-model overlay



X



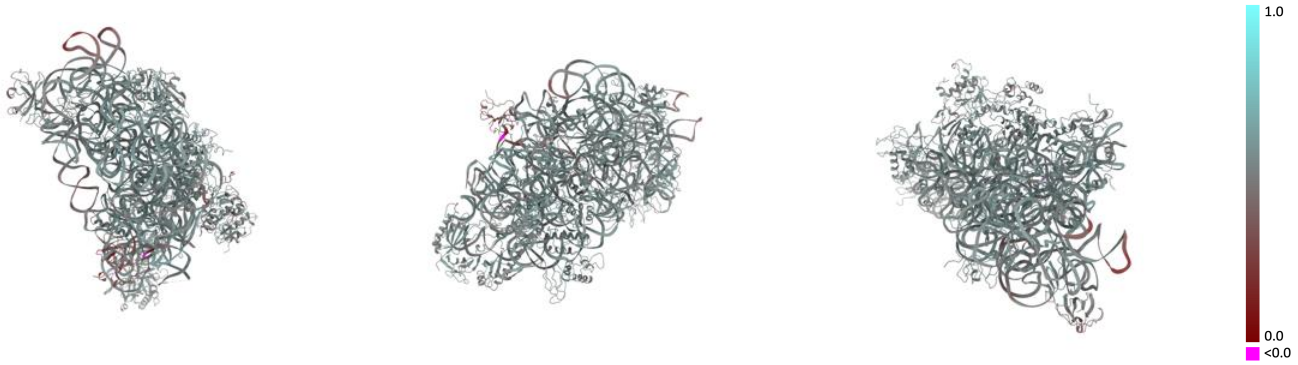
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

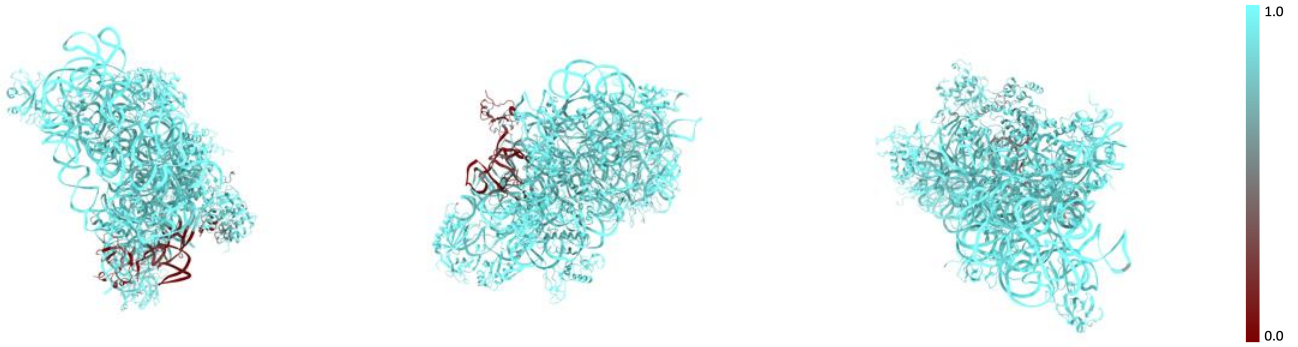
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

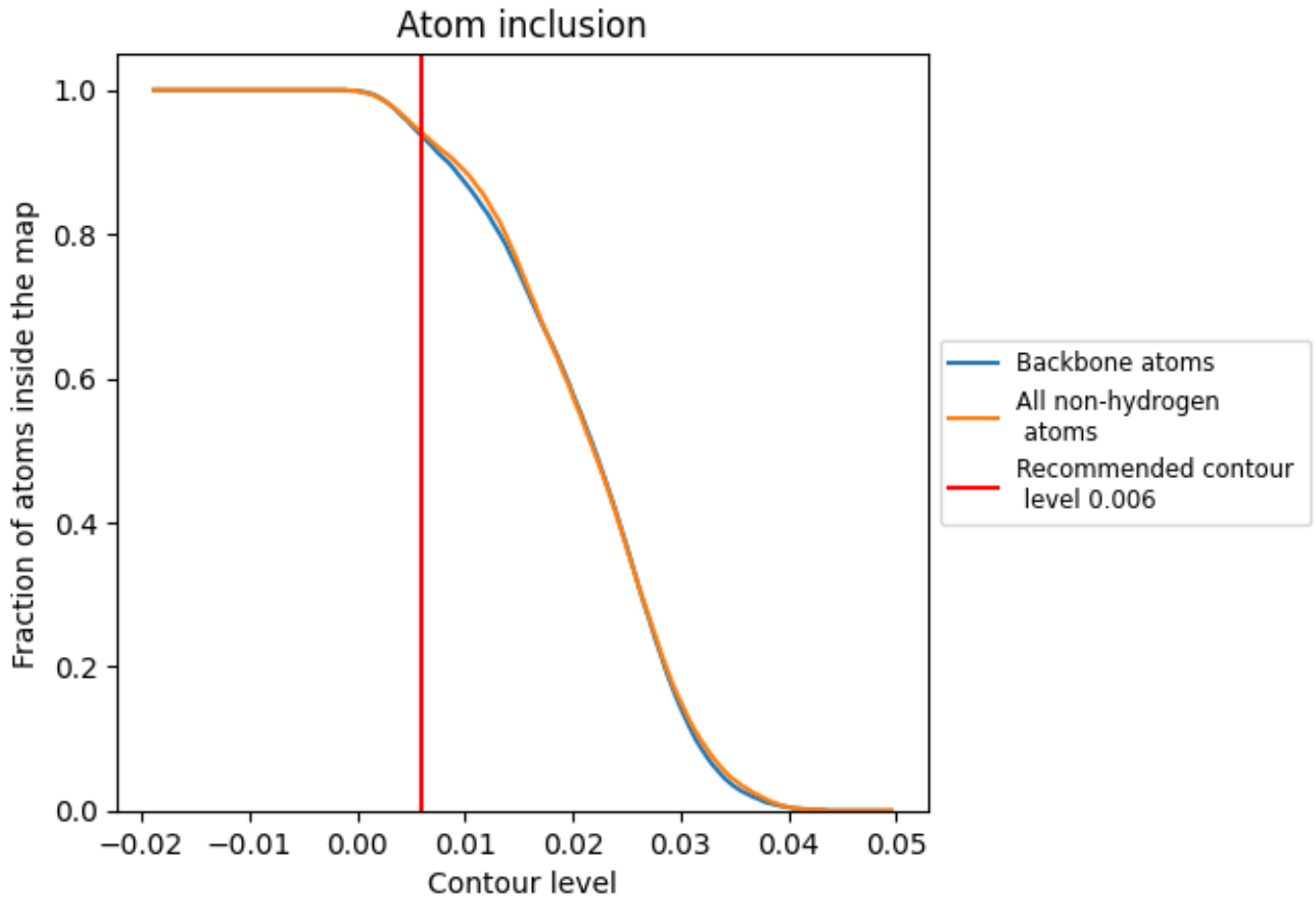
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.5260
0	0.9470	0.5410
2	0.9620	0.5310
5	0.6700	0.4290
6	0.3070	0.3220
A	0.9690	0.5240
B	0.8700	0.5220
C	0.9170	0.5140
D	0.9730	0.5430
E	0.9760	0.5410
F	0.8800	0.5310
G	0.9630	0.4920
I	0.9710	0.5480
J	0.9700	0.5350
M	0.9670	0.5290
N	0.9680	0.5380
Q	0.9720	0.5300
R	0.9710	0.5460
V	0.9730	0.5210
W	0.9620	0.5290