Full wwPDB EM Validation Report (i)

Aug 8, 2026 – 07:45 am BST

PDB ID	:	9SDQ / pdb_00009sdq
EMDB ID	:	EMD-54790
Title	:	Cryo-EM structure of the Arabidopsis thaliana 40S ribosomal subunit (Head)
Authors	:	Sudeep, K.; 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	:	3.20 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 (i) 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 (1)) were used in the production of this report:

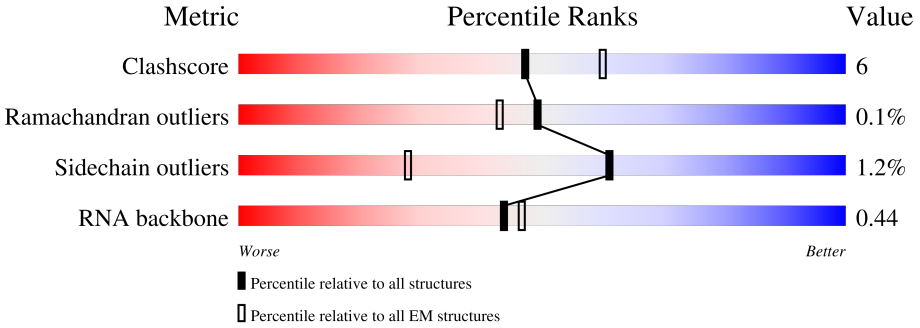
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal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

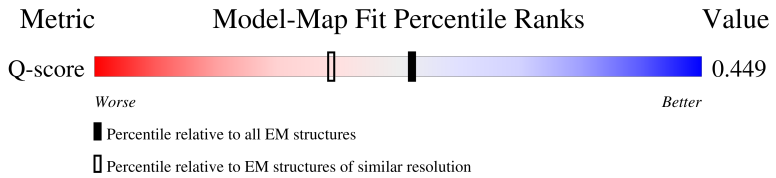
1 Overall quality at a glance (i)

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)	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	15020 (2.70 - 3.70)

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	498	53% 35% 11%
2	BD	250	9% 75% 9% 16%
3	BF	207	77% 12% 11%

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Mol	Chain	Length	Quality of chain
4	BP	152	68% 9% 24%
5	BQ	146	76% 19%
6	BS	152	77% 12% 11%
7	BT	142	84% 12%
8	BU	124	71% 10% 19%
9	Bc	64	72% 19% 8%
10	d	56	11% 75% 14% 11%
11	e	108	64% 6% 31%
12	BK	179	6% 41% 9% 49%
13	BR	141	39% 57%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 38198 atoms, of which 16736 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 RNA (500-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	2	497	15949	4734	5356	1862	3500	497	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS3z.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	BD	210	3370	1041	1730	300	291	8	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS7z.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	BF	185	2968	914	1510	274	264	6	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS19x.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	BP	116	1932	602	997	170	158	5	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS9z.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	BQ	140	2296	714	1174	212	191	5	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein uS13z/uS13y/uS13x.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	BS	136	2265	694	1154	220	192	5	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein eS19x.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	BT	136	2161	673	1097	202	186	3	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein uS10z/uS10x.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	BU	100	1648	499	857	148	141	3	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein eS28x.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	Bc	59	955	286	489	93	85	2	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS14z/uS14y/uS14x.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	d	50	808	253	402	83	65	5	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein eS25y.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	e	75	1228	373	631	111	109	4	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein eS10x.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	BK	92	1561	512	788	125	132	4	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein eS17w.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	BR	60	1052	319	551	96	84	2	0	0

- Molecule 14 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
14	2	3	3	3	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	2	1	1	1	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

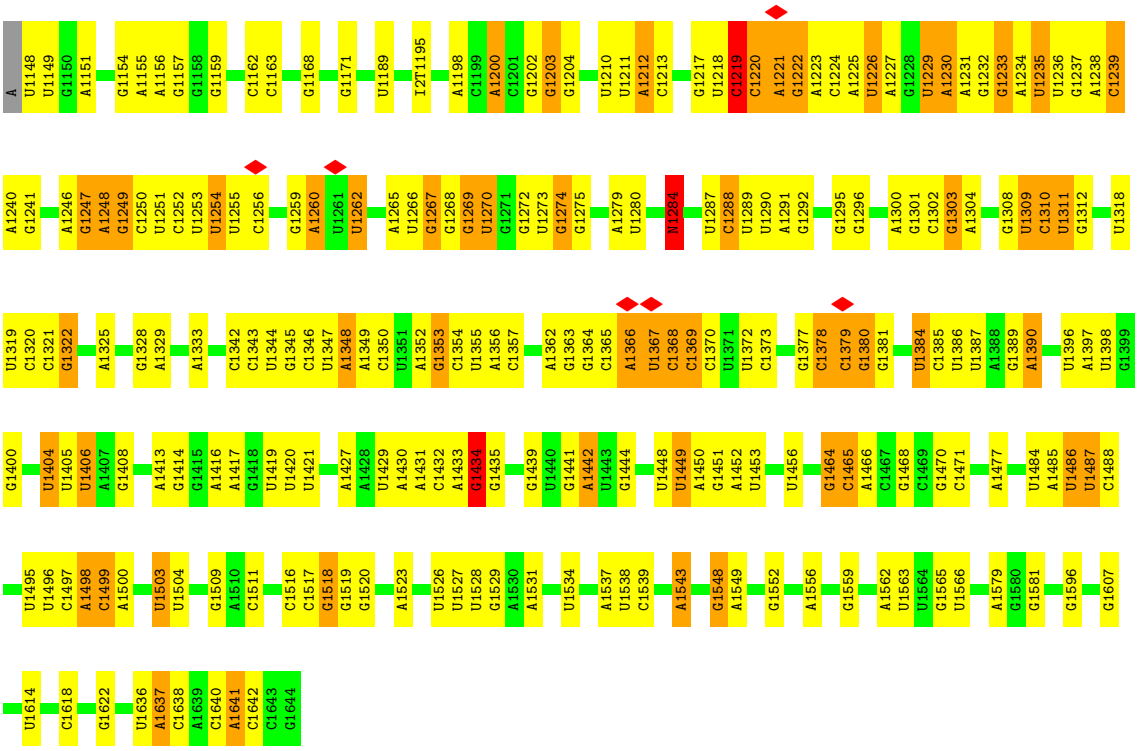
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	d	1	1	1	0

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.

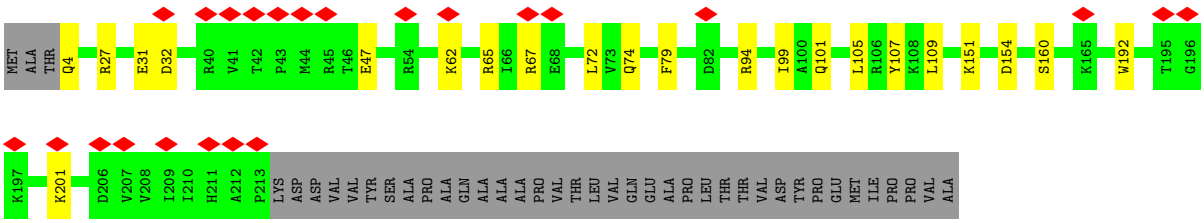
- Molecule 1: RNA (500-MER)

Chain 2:



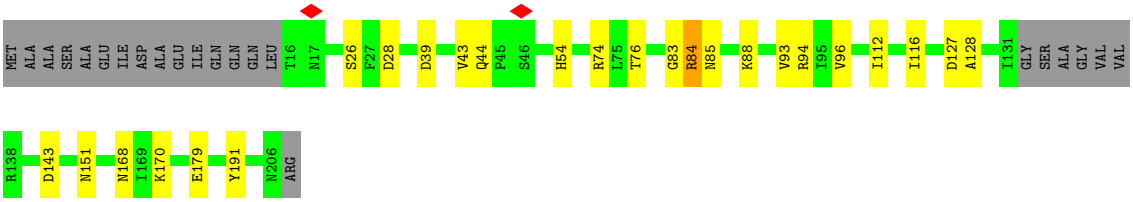
- Molecule 2: Small ribosomal subunit protein uS3z

Chain BD:



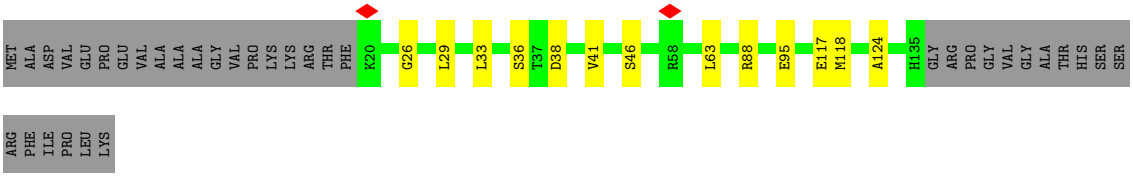
- Molecule 3: Small ribosomal subunit protein uS7z

Chain BF:



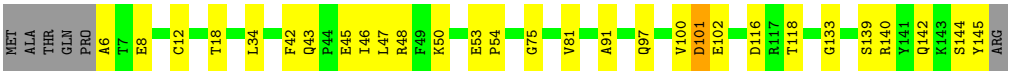
- Molecule 4: Small ribosomal subunit protein uS19x

Chain BP:



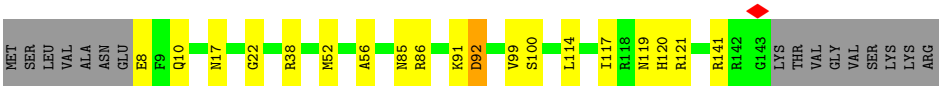
- Molecule 5: Small ribosomal subunit protein uS9z

Chain BQ:



- Molecule 6: Small ribosomal subunit protein uS13z/uS13y/uS13x

Chain BS:

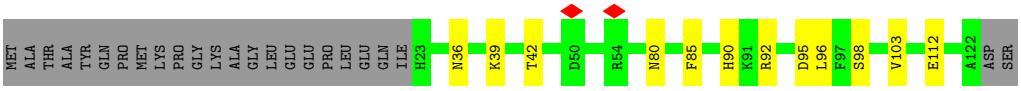


- Molecule 7: Small ribosomal subunit protein eS19x

Chain BT:

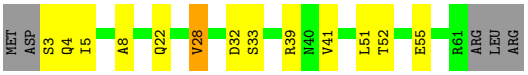
- Molecule 8: Small ribosomal subunit protein uS10z/uS10x

Chain BU:



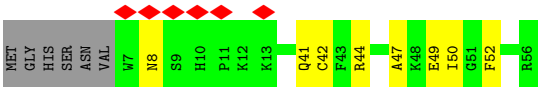
- Molecule 9: Small ribosomal subunit protein eS28x

Chain Bc:



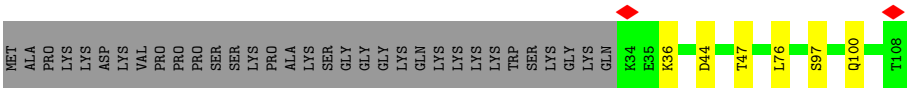
- Molecule 10: Small ribosomal subunit protein uS14z/uS14y/uS14x

Chain d:



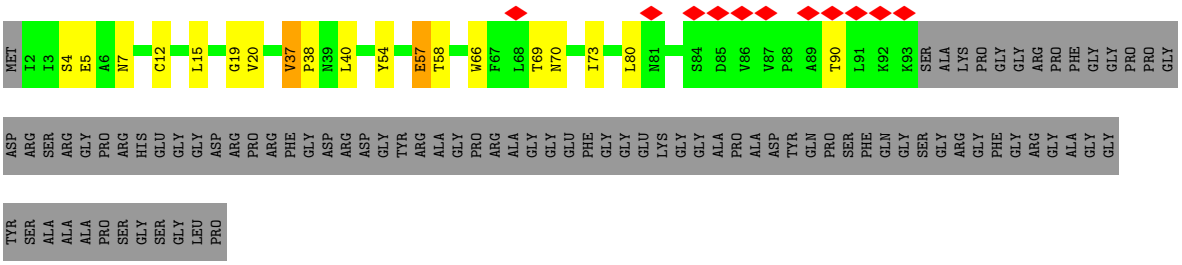
- Molecule 11: Small ribosomal subunit protein eS25y

Chain e:



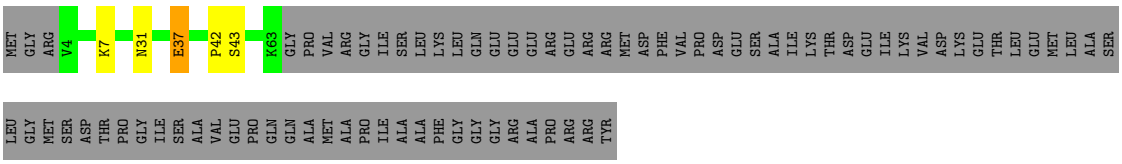
- Molecule 12: Small ribosomal subunit protein eS10x

Chain BK:



- Molecule 13: Small ribosomal subunit protein eS17w

Chain BR:



4 Experimental information (i)

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 ($e^-/Å^2$)	24.512	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	10500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, 4AC, MG, OMU, I2T, OMC, OMG, ZN

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	0.23	0/11679	0.31	1/18194 (0.0%)
2	BD	0.16	0/1664	0.28	0/2236
3	BF	0.19	0/1478	0.30	0/1992
4	BP	0.18	0/953	0.26	0/1274
5	BQ	0.18	0/1142	0.29	0/1528
6	BS	0.21	0/1127	0.31	0/1506
7	BT	0.20	0/1086	0.27	0/1459
8	BU	0.18	0/801	0.27	0/1079
9	Bc	0.17	0/469	0.25	0/626
10	d	0.19	0/416	0.26	0/552
11	e	0.17	0/603	0.26	0/806
12	BK	0.14	0/794	0.29	0/1071
13	BR	0.17	0/507	0.27	0/673
All	All	0.21	0/22719	0.30	1/32996 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1637	A	C4'-C3'-O3'	5.13	117.10	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	10593	5356	5338	126	0
2	BD	1640	1730	1730	16	0
3	BF	1458	1510	1510	13	0
4	BP	935	997	997	11	0
5	BQ	1122	1174	1174	22	0
6	BS	1111	1154	1154	15	0
7	BT	1064	1097	1097	12	0
8	BU	791	857	857	9	0
9	Bc	466	489	489	7	0
10	d	406	402	402	7	0
11	e	597	631	631	4	0
12	BK	773	788	788	12	0
13	BR	501	551	551	3	0
14	2	3	0	0	0	0
15	2	1	0	0	0	0
16	d	1	0	0	0	0
All	All	21462	16736	16718	224	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 (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1464:G:O2'	1:2:1465:C:OP1	1.88	0.90
1:2:1308:G:OP2	1:2:1309:U:O2'	1.90	0.89
1:2:1537:A:OP2	11:e:97:SER:OG	1.92	0.87
3:BF:74:ARG:NH2	3:BF:151:ASN:OD1	2.08	0.87
1:2:1233:G:N2	1:2:1259:G:O2'	2.09	0.86
1:2:1239:C:N4	1:2:1254:U:O2	2.12	0.82
1:2:1222:G:N2	1:2:1450:A:OP2	2.13	0.82
1:2:1284:4AC:OP1	10:d:44:ARG:NH2	2.14	0.80
3:BF:83:GLY:O	3:BF:85:ASN:N	2.14	0.80
1:2:1220:C:O2	1:2:1452:A:N6	2.14	0.79
11:e:44:ASP:OD1	11:e:47:THR:OG1	1.99	0.79
1:2:1404:U:O2'	1:2:1406:U:OP2	2.01	0.78
6:BS:8:GLU:N	6:BS:8:GLU:OE1	2.17	0.78
1:2:1235:U:O2'	1:2:1262:U:O2'	2.02	0.76
13:BR:37:GLU:N	13:BR:37:GLU:OE1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BF:127:ASP:OD1	3:BF:128:ALA:N	2.20	0.73
10:d:49:GLU:OE1	10:d:49:GLU:N	2.21	0.73
3:BF:54:HIS:O	5:BQ:50:LYS:NZ	2.21	0.73
1:2:1556:A:OP2	4:BP:46:SER:OG	2.03	0.72
2:BD:74:GLN:NE2	2:BD:79:PHE:O	2.22	0.72
4:BP:36:SER:OG	4:BP:38:ASP:OD1	2.07	0.72
1:2:1362:A:O2'	7:BT:133:ASP:OD2	2.09	0.70
4:BP:95:GLU:OE1	4:BP:95:GLU:N	2.23	0.70
1:2:1439:G:N2	10:d:42:CYS:SG	2.65	0.70
1:2:1202:G:OP1	1:2:1203:G:O2'	2.05	0.69
6:BS:119:ASN:OD1	6:BS:120:HIS:N	2.28	0.67
1:2:1504:U:O4	1:2:1517:C:N3	2.27	0.67
7:BT:117:ASP:OD1	7:BT:118:THR:N	2.28	0.67
1:2:1288:C:H42	1:2:1429:U:H3	1.44	0.66
4:BP:117:GLU:N	4:BP:117:GLU:OE1	2.28	0.66
5:BQ:97:GLN:NE2	5:BQ:102:GLU:OE1	2.28	0.65
1:2:1238:A:OP2	1:2:1249:G:O2'	2.07	0.65
12:BK:15:LEU:O	12:BK:19:GLY:N	2.27	0.64
3:BF:26:SER:OG	3:BF:28:ASP:OD1	2.11	0.64
1:2:1503:U:HO2'	1:2:1526:U:HO2'	1.47	0.62
8:BU:36:ASN:ND2	8:BU:112:GLU:OE2	2.32	0.61
1:2:1272:G:O2'	1:2:1274:G:OP1	2.17	0.61
1:2:1552:G:OP1	6:BS:121:ARG:NH2	2.33	0.61
1:2:1509:G:N7	7:BT:102:ARG:NH2	2.49	0.61
8:BU:95:ASP:OD1	8:BU:96:LEU:N	2.33	0.61
7:BT:43:LEU:H	7:BT:43:LEU:HD23	1.66	0.61
1:2:1227:A:N6	1:2:1265:A:N1	2.48	0.60
2:BD:105:LEU:HD23	2:BD:109:LEU:HD23	1.84	0.60
7:BT:115:ASP:OD1	7:BT:116:LEU:N	2.34	0.60
9:Bc:32:ASP:OD1	9:Bc:33:SER:N	2.34	0.60
6:BS:99:VAL:O	6:BS:100:SER:OG	2.20	0.60
1:2:1353:G:O2'	1:2:1385:C:N3	2.33	0.59
2:BD:192:TRP:NE1	2:BD:201:LYS:O	2.34	0.59
1:2:1222:G:C1'	1:2:1269:G:H22	2.16	0.59
1:2:1430:A:OP2	2:BD:151:LYS:NZ	2.36	0.58
7:BT:31:LEU:HB3	7:BT:35:THR:HG21	1.85	0.58
1:2:1471:C:OP1	5:BQ:142:GLN:NE2	2.37	0.58
4:BP:118:MET:CG	6:BS:117:ILE:HD11	2.34	0.57
5:BQ:133:GLY:O	5:BQ:140:ARG:NH2	2.36	0.57
1:2:1511:C:OP1	7:BT:97:SER:OG	2.20	0.57
3:BF:44:GLN:OE1	3:BF:44:GLN:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1222:G:O4'	1:2:1269:G:N2	2.32	0.57
5:BQ:6:ALA:N	5:BQ:8:GLU:OE1	2.39	0.56
1:2:1333:A:OP2	2:BD:160:SER:OG	2.24	0.56
6:BS:92:ASP:N	6:BS:92:ASP:OD1	2.36	0.56
1:2:1225:A:N6	1:2:1267:G:O6	2.39	0.56
1:2:1210:U:OP2	1:2:1211:U:O2'	2.20	0.55
3:BF:76:THR:HG22	3:BF:96:VAL:HG21	1.87	0.55
2:BD:72:LEU:HD22	12:BK:20:VAL:HG13	1.87	0.55
5:BQ:116:ASP:OD1	5:BQ:118:THR:N	2.40	0.55
1:2:1614:U:OP1	5:BQ:18:THR:HG22	2.07	0.55
2:BD:32:ASP:OD2	2:BD:65:ARG:NH1	2.40	0.55
8:BU:39:LYS:O	8:BU:42:THR:OG1	2.22	0.54
11:e:100:GLN:OE1	11:e:100:GLN:N	2.41	0.54
1:2:1247:G:O2'	1:2:1248:A:O5'	2.17	0.54
1:2:1464:G:HO2'	1:2:1465:C:P	2.23	0.54
2:BD:47:GLU:OE1	2:BD:47:GLU:N	2.41	0.53
12:BK:54:TYR:O	12:BK:69:THR:OG1	2.25	0.53
1:2:1543:A:OP1	11:e:36:LYS:NZ	2.42	0.53
1:2:1488:C:O2'	5:BQ:75:GLY:O	2.27	0.53
7:BT:34:TRP:HA	7:BT:37:ILE:HD13	1.91	0.53
1:2:1434:OMG:N3	1:2:1434:OMG:H2'	2.25	0.52
12:BK:5:GLU:OE1	12:BK:5:GLU:N	2.40	0.52
1:2:1218:U:H2'	1:2:1219:OMC:O4'	2.10	0.52
1:2:1221:A:H61	12:BK:40:LEU:HD13	1.75	0.52
1:2:1486:U:O2'	1:2:1487:U:P	2.68	0.52
1:2:1151:A:O2'	1:2:1642:C:OP2	2.26	0.52
1:2:1640:C:O2'	1:2:1641:A:OP1	2.26	0.51
1:2:1503:U:O2'	1:2:1526:U:O2'	2.19	0.51
1:2:1310:C:O2'	1:2:1311:U:O5'	2.29	0.51
1:2:1468:G:N7	6:BS:141:ARG:NH2	2.55	0.50
1:2:1534:U:OP1	3:BF:94:ARG:NH2	2.45	0.50
4:BP:38:ASP:O	4:BP:41:VAL:HG22	2.12	0.50
1:2:1498:A:H2'	1:2:1499:C:H2'	1.93	0.50
6:BS:10:GLN:OE1	6:BS:10:GLN:N	2.45	0.50
9:Bc:39:ARG:NH2	9:Bc:55:GLU:O	2.32	0.49
3:BF:179:GLU:OE2	3:BF:191:TYR:N	2.45	0.49
4:BP:118:MET:HG2	6:BS:117:ILE:HD11	1.94	0.49
5:BQ:43:GLN:OE1	5:BQ:43:GLN:N	2.41	0.49
1:2:1200:A:OP2	1:2:1470:G:N2	2.38	0.49
6:BS:22:GLY:HA2	6:BS:56:ALA:HB3	1.94	0.49
1:2:1265:A:H2'	1:2:1266:U:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1269:G:H2'	1:2:1270:U:C5	2.47	0.48
1:2:1442:A:OP2	2:BD:27:ARG:NH2	2.45	0.48
1:2:1548:G:O2'	1:2:1549:A:OP2	2.29	0.48
1:2:1229:U:H2'	1:2:1230:A:C4	2.48	0.48
3:BF:84:ARG:O	3:BF:88:LYS:NZ	2.45	0.48
1:2:1239:C:OP1	1:2:1249:G:N1	2.47	0.48
1:2:1311:U:H3	1:2:1322:G:H21	1.61	0.48
9:Bc:3:SER:OG	9:Bc:4:GLN:N	2.46	0.48
1:2:1488:C:N4	1:2:1531:A:OP2	2.46	0.48
1:2:1559:G:N1	1:2:1562:A:OP2	2.47	0.48
2:BD:62:LYS:O	2:BD:67:ARG:NH2	2.41	0.48
5:BQ:100:VAL:HG12	5:BQ:101:ASP:N	2.29	0.48
1:2:1284:4AC:H5	1:2:1284:4AC:O7	2.14	0.47
1:2:1289:U:O2	1:2:1289:U:H2'	2.15	0.47
1:2:1389:G:H2'	1:2:1390:A:O4'	2.14	0.47
1:2:1486:U:HO2'	1:2:1487:U:P	2.37	0.47
2:BD:4:GLN:N	2:BD:4:GLN:OE1	2.48	0.47
9:Bc:41:VAL:HG11	9:Bc:51:LEU:HD21	1.96	0.47
1:2:1288:C:N4	1:2:1429:U:H3	2.10	0.47
5:BQ:42:PHE:O	5:BQ:48:ARG:NH1	2.47	0.47
1:2:1168:G:O2'	1:2:1618:C:O2	2.32	0.46
1:2:1355:U:C2	1:2:1356:A:C8	3.03	0.46
5:BQ:133:GLY:O	5:BQ:140:ARG:NE	2.48	0.46
1:2:1364:G:H2'	1:2:1365:C:O4'	2.16	0.46
1:2:1345:G:C2	1:2:1346:C:C6	3.03	0.46
1:2:1416:A:H2'	1:2:1417:A:O4'	2.14	0.46
1:2:1517:C:H2'	1:2:1518:G:O4'	2.16	0.46
7:BT:36:ASP:OD1	7:BT:37:ILE:HD12	2.14	0.46
1:2:1224:C:N4	1:2:1225:A:H62	2.14	0.46
13:BR:42:PRO:O	13:BR:43:SER:OG	2.24	0.46
1:2:1226:U:H2'	1:2:1227:A:C8	2.51	0.46
6:BS:17:ASN:ND2	6:BS:17:ASN:O	2.49	0.46
1:2:1227:A:C6	1:2:1265:A:C2	3.04	0.46
1:2:1343:C:O2'	1:2:1345:G:N7	2.49	0.46
1:2:1221:A:N1	12:BK:40:LEU:HD22	2.31	0.46
10:d:41:GLN:OE1	10:d:41:GLN:N	2.42	0.46
1:2:1148:U:C2	1:2:1149:U:C5	3.04	0.45
9:Bc:8:ALA:HB1	9:Bc:28:VAL:HG22	1.98	0.45
12:BK:57:GLU:OE1	12:BK:66:TRP:NE1	2.49	0.45
2:BD:94:ARG:O	2:BD:101:GLN:NE2	2.41	0.45
1:2:1433:A:C2'	1:2:1434:OMG:OP2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BP:26:GLY:N	6:BS:91:LYS:O	2.50	0.45
2:BD:154:ASP:N	2:BD:154:ASP:OD1	2.50	0.45
1:2:1389:G:O5'	8:BU:92:ARG:NH2	2.50	0.45
12:BK:4:SER:OG	12:BK:7:ASN:OD1	2.31	0.45
1:2:1246:A:O2'	1:2:1248:A:OP1	2.33	0.44
1:2:1321:C:O2'	1:2:1406:U:O2	2.29	0.44
1:2:1484:U:O4	1:2:1485:A:N6	2.49	0.44
1:2:1363:G:H2'	1:2:1364:G:N9	2.32	0.44
1:2:1352:A:H2'	1:2:1353:G:O4'	2.16	0.44
5:BQ:45:GLU:OE2	5:BQ:48:ARG:NH1	2.50	0.44
5:BQ:34:LEU:C	5:BQ:34:LEU:HD23	2.43	0.44
5:BQ:53:GLU:HB2	5:BQ:54:PRO:HD3	1.99	0.44
5:BQ:116:ASP:OD1	5:BQ:118:THR:OG1	2.31	0.44
1:2:1225:A:H2'	1:2:1226:U:O4'	2.18	0.44
1:2:1434:OMG:H4'	1:2:1434:OMG:OP1	2.18	0.44
3:BF:168:ASN:OD1	3:BF:170:LYS:N	2.35	0.44
1:2:1379:C:O2'	1:2:1380:G:H5"	2.18	0.44
1:2:1449:U:H5"	1:2:1450:A:H5'	1.99	0.44
8:BU:96:LEU:HD21	8:BU:98:SER:HB3	2.00	0.43
1:2:1363:G:OP1	7:BT:130:ARG:NH1	2.51	0.43
1:2:1301:G:N2	1:2:1304:A:OP2	2.35	0.43
1:2:1342:C:C6	1:2:1416:A:C2	3.06	0.43
8:BU:36:ASN:OD1	8:BU:36:ASN:N	2.52	0.43
1:2:1219:OMC:O2'	1:2:1220:C:OP1	2.37	0.43
4:BP:63:LEU:HD13	4:BP:63:LEU:C	2.44	0.43
8:BU:80:ASN:OD1	8:BU:80:ASN:N	2.52	0.43
1:2:1303:G:O2'	1:2:1304:A:O4'	2.30	0.43
1:2:1269:G:O2'	1:2:1270:U:O4'	2.37	0.43
3:BF:93:VAL:HG11	5:BQ:46:ILE:HD11	2.00	0.43
1:2:1353:G:H2'	1:2:1354:C:C6	2.54	0.43
1:2:1456:U:O3'	10:d:8:ASN:ND2	2.52	0.43
5:BQ:12:CYS:SG	5:BQ:91:ALA:N	2.92	0.43
5:BQ:139:SER:OG	5:BQ:140:ARG:N	2.52	0.42
9:Bc:5:ILE:HG23	9:Bc:52:THR:HG23	2.01	0.42
6:BS:114:LEU:HA	6:BS:117:ILE:HG22	2.02	0.42
1:2:1240:A:H2'	1:2:1241:G:O4'	2.19	0.42
2:BD:67:ARG:NH1	12:BK:90:THR:O	2.46	0.42
1:2:1345:G:C2	1:2:1346:C:C5	3.07	0.42
1:2:1252:C:H2'	1:2:1253:U:C6	2.54	0.42
1:2:1219:OMC:HM23	1:2:1219:OMC:H1'	1.92	0.42
1:2:1538:U:C4	1:2:1539:C:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1225:A:C6	1:2:1267:G:C6	3.08	0.42
5:BQ:144:SER:OG	5:BQ:145:TYR:N	2.53	0.42
1:2:1347:U:O2'	1:2:1348:A:H5'	2.20	0.42
1:2:1365:C:C2	1:2:1369:C:N4	2.88	0.42
1:2:1389:G:OP1	8:BU:90:HIS:ND1	2.46	0.42
12:BK:12:CYS:HB3	12:BK:80:LEU:HD11	2.00	0.42
2:BD:99:ILE:H	2:BD:99:ILE:HD12	1.85	0.42
6:BS:85:ASN:OD1	6:BS:86:ARG:N	2.53	0.42
12:BK:70:ASN:HA	12:BK:73:ILE:HD12	2.01	0.42
1:2:1231:A:O4'	1:2:1260:A:N6	2.53	0.41
1:2:1295:G:C8	1:2:1296:G:C8	3.08	0.41
5:BQ:100:VAL:HG12	5:BQ:101:ASP:H	1.84	0.41
1:2:1363:G:H2'	1:2:1364:G:C1'	2.50	0.41
7:BT:107:GLN:O	7:BT:110:THR:OG1	2.32	0.41
1:2:1212:A:H5"	1:2:1213:C:OP2	2.20	0.41
10:d:47:ALA:O	10:d:50:ILE:HG22	2.21	0.41
1:2:1386:U:H2'	1:2:1387:U:C6	2.56	0.41
1:2:1429:U:H2'	1:2:1430:A:C8	2.55	0.41
12:BK:37:VAL:HG22	12:BK:38:PRO:HD2	2.03	0.41
1:2:1233:G:H22	1:2:1259:G:C2'	2.33	0.41
1:2:1464:G:C2'	1:2:1465:C:OP1	2.68	0.41
8:BU:85:PHE:HB3	10:d:52:PHE:HB3	2.02	0.41
1:2:1640:C:HO2'	1:2:1641:A:P	2.43	0.41
6:BS:38:ARG:HD2	7:BT:46:LEU:HD21	2.02	0.41
1:2:1354:C:H2'	1:2:1355:U:C6	2.55	0.41
1:2:1366:A:H5'	1:2:1368:C:N4	2.36	0.41
1:2:1433:A:H2'	1:2:1434:OMG:OP2	2.21	0.41
1:2:1365:C:N4	1:2:1367:U:O3'	2.54	0.41
1:2:1413:A:H2'	1:2:1414:G:C8	2.55	0.41
1:2:1250:C:C2	1:2:1251:U:C6	3.10	0.41
1:2:1251:U:H2'	1:2:1252:C:H6	1.86	0.41
1:2:1320:C:H5'	13:BR:7:LYS:HG3	2.03	0.41
4:BP:88:ARG:O	4:BP:124:ALA:HB2	2.21	0.41
1:2:1365:C:N4	1:2:1367:U:H4'	2.36	0.40
1:2:1365:C:N3	1:2:1369:C:N4	2.69	0.40
1:2:1543:A:H2'	1:2:1543:A:N3	2.36	0.40
3:BF:112:ILE:O	3:BF:116:ILE:HG12	2.21	0.40
5:BQ:47:LEU:HD13	5:BQ:81:VAL:HG21	2.03	0.40
4:BP:29:LEU:HD23	4:BP:33:LEU:HD23	2.02	0.40
1:2:1279:A:C6	1:2:1444:G:C5	3.10	0.40
1:2:1377:G:C8	1:2:1378:C:H5	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1365:C:H3'	1:2:1367:U:OP2	2.21	0.40
2:BD:31:GLU:HA	2:BD:107:TYR:OH	2.22	0.40
1:2:1372:U:H2'	1:2:1373:C:C6	2.57	0.40
9:Bc:22:GLN:OE1	9:Bc:22:GLN:N	2.52	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	BD	208/250 (83%)	205 (99%)	3 (1%)	0	100	100
3	BF	181/207 (87%)	168 (93%)	12 (7%)	1 (1%)	21	56
4	BP	114/152 (75%)	109 (96%)	5 (4%)	0	100	100
5	BQ	138/146 (94%)	132 (96%)	6 (4%)	0	100	100
6	BS	134/152 (88%)	128 (96%)	6 (4%)	0	100	100
7	BT	134/142 (94%)	132 (98%)	2 (2%)	0	100	100
8	BU	98/124 (79%)	95 (97%)	3 (3%)	0	100	100
9	Bc	57/64 (89%)	57 (100%)	0	0	100	100
10	d	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	e	73/108 (68%)	71 (97%)	2 (3%)	0	100	100
12	BK	90/179 (50%)	90 (100%)	0	0	100	100
13	BR	58/141 (41%)	54 (93%)	4 (7%)	0	100	100
All	All	1333/1721 (78%)	1288 (97%)	44 (3%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	BF	84	ARG

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	BD	175/207 (84%)	175 (100%)	0	100	100
3	BF	159/174 (91%)	156 (98%)	3 (2%)	50	73
4	BP	102/129 (79%)	102 (100%)	0	100	100
5	BQ	118/123 (96%)	117 (99%)	1 (1%)	73	82
6	BS	118/132 (89%)	116 (98%)	2 (2%)	53	75
7	BT	110/112 (98%)	110 (100%)	0	100	100
8	BU	92/111 (83%)	91 (99%)	1 (1%)	65	79
9	Bc	52/57 (91%)	51 (98%)	1 (2%)	50	73
10	d	43/48 (90%)	43 (100%)	0	100	100
11	e	66/93 (71%)	65 (98%)	1 (2%)	57	76
12	BK	85/137 (62%)	82 (96%)	3 (4%)	32	64
13	BR	57/122 (47%)	55 (96%)	2 (4%)	32	64
All	All	1177/1445 (82%)	1163 (99%)	14 (1%)	61	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	BF	39	ASP
3	BF	43	VAL
3	BF	143	ASP
5	BQ	101	ASP
6	BS	52	MET
6	BS	92	ASP
8	BU	103	VAL
9	Bc	28	VAL
11	e	76	LEU
12	BK	37	VAL

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Mol	Chain	Res	Type
12	BK	57	GLU
12	BK	58	THR
13	BR	31	ASN
13	BR	37	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	BD	211	HIS
3	BF	85	ASN
5	BQ	73	ASN
5	BQ	103	GLN
6	BS	135	HIS
7	BT	13	HIS
7	BT	106	GLN
11	e	39	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	496/498 (99%)	133 (26%)	12 (2%)

All (133) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	1154	G
1	2	1155	A
1	2	1156	A
1	2	1157	G
1	2	1159	G
1	2	1162	C
1	2	1163	C
1	2	1171	G
1	2	1189	U
1	2	1198	A
1	2	1200	A
1	2	1203	G
1	2	1204	G
1	2	1212	A
1	2	1217	G

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Mol	Chain	Res	Type
1	2	1220	C
1	2	1221	A
1	2	1222	G
1	2	1223	A
1	2	1226	U
1	2	1229	U
1	2	1230	A
1	2	1232	G
1	2	1233	G
1	2	1234	A
1	2	1235	U
1	2	1236	U
1	2	1237	G
1	2	1239	C
1	2	1247	G
1	2	1248	A
1	2	1249	G
1	2	1255	U
1	2	1256	C
1	2	1260	A
1	2	1262	U
1	2	1267	G
1	2	1268	G
1	2	1269	G
1	2	1270	U
1	2	1273	U
1	2	1274	G
1	2	1280	U
1	2	1284	4AC
1	2	1287	U
1	2	1288	C
1	2	1290	U
1	2	1291	A
1	2	1292	G
1	2	1300	A
1	2	1302	C
1	2	1303	G
1	2	1309	U
1	2	1310	C
1	2	1311	U
1	2	1312	G
1	2	1318	U

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Mol	Chain	Res	Type
1	2	1319	U
1	2	1322	G
1	2	1325	A
1	2	1328	G
1	2	1329	A
1	2	1344	U
1	2	1348	A
1	2	1349	A
1	2	1350	C
1	2	1353	G
1	2	1357	C
1	2	1366	A
1	2	1367	U
1	2	1368	C
1	2	1370	C
1	2	1378	C
1	2	1379	C
1	2	1380	G
1	2	1381	G
1	2	1384	OMU
1	2	1390	A
1	2	1396	U
1	2	1397	A
1	2	1398	U
1	2	1400	G
1	2	1404	U
1	2	1405	U
1	2	1406	U
1	2	1408	G
1	2	1419	U
1	2	1420	U
1	2	1421	U
1	2	1427	A
1	2	1431	A
1	2	1432	C
1	2	1434	OMG
1	2	1435	G
1	2	1441	G
1	2	1442	A
1	2	1448	U
1	2	1449	U
1	2	1451	G

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Mol	Chain	Res	Type
1	2	1453	U
1	2	1465	C
1	2	1466	A
1	2	1477	A
1	2	1487	U
1	2	1495	U
1	2	1496	U
1	2	1497	C
1	2	1498	A
1	2	1499	C
1	2	1500	A
1	2	1503	U
1	2	1516	C
1	2	1518	G
1	2	1519	G
1	2	1520	G
1	2	1523	A
1	2	1527	U
1	2	1528	U
1	2	1529	G
1	2	1543	A
1	2	1548	G
1	2	1563	U
1	2	1565	G
1	2	1566	U
1	2	1579	A
1	2	1581	G
1	2	1596	G
1	2	1607	G
1	2	1622	G
1	2	1636	U
1	2	1637	A
1	2	1638	C
1	2	1641	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1219	OMC
1	2	1247	G
1	2	1254	U
1	2	1369	C

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Mol	Chain	Res	Type
1	2	1434	OMG
1	2	1464	G
1	2	1486	U
1	2	1495	U
1	2	1497	C
1	2	1527	U
1	2	1528	U
1	2	1637	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMC	2	1219	1	19,22,23	2.92	8 (42%)	26,31,34	0.70	0
1	OMG	2	1275	1	23,26,27	2.37	8 (34%)	33,38,41	1.97	9 (27%)
1	OMG	2	1434	1	23,26,27	2.35	7 (30%)	33,38,41	2.00	9 (27%)
1	4AC	2	1284	1	21,24,25	3.38	10 (47%)	29,34,37	1.33	5 (17%)
1	I2T	2	1195	1	24,29,30	3.06	8 (33%)	29,42,45	1.77	6 (20%)
1	OMU	2	1384	1	19,22,23	2.92	6 (31%)	26,31,34	1.77	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2	1219	1	-	0/9/27/28	0/2/2/2
1	OMG	2	1275	1	-	1/9/27/28	0/3/3/3
1	OMG	2	1434	1	-	2/9/27/28	0/3/3/3
1	4AC	2	1284	1	-	2/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	I2T	2	1195	1	-	2/16/34/35	0/2/2/2
1	OMU	2	1384	1	-	1/9/27/28	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1195	I2T	C6-N1	7.65	1.55	1.36
1	2	1195	I2T	C4-N3	-7.46	1.26	1.40
1	2	1284	4AC	C4-N3	6.83	1.44	1.32
1	2	1384	OMU	C2-N1	6.79	1.49	1.38
1	2	1384	OMU	C2-N3	6.71	1.49	1.38
1	2	1284	4AC	C6-C5	6.53	1.50	1.35
1	2	1275	OMG	C4-N3	6.22	1.49	1.34
1	2	1434	OMG	C4-N3	6.20	1.49	1.34
1	2	1284	4AC	C2-N3	6.14	1.48	1.36
1	2	1219	OMC	C2-N3	6.13	1.48	1.36
1	2	1195	I2T	C2-N1	6.10	1.57	1.39
1	2	1384	OMU	C6-C5	5.91	1.48	1.35
1	2	1219	OMC	C6-C5	5.73	1.48	1.35
1	2	1195	I2T	C6-C5	5.61	1.42	1.34
1	2	1284	4AC	C7-N4	5.48	1.47	1.37
1	2	1284	4AC	C4-N4	5.26	1.47	1.39
1	2	1275	OMG	C2-N3	5.25	1.45	1.33
1	2	1219	OMC	C4-N3	5.23	1.45	1.34
1	2	1434	OMG	C2-N3	5.11	1.45	1.33
1	2	1219	OMC	C4-N4	4.75	1.45	1.33
1	2	1434	OMG	C2-N2	4.63	1.45	1.34
1	2	1275	OMG	C2-N2	4.61	1.45	1.34
1	2	1219	OMC	C2-N1	4.19	1.49	1.40
1	2	1284	4AC	C5-C4	3.95	1.49	1.40
1	2	1284	4AC	C2-N1	3.59	1.47	1.40
1	2	1384	OMU	C4-N3	3.42	1.44	1.38
1	2	1195	I2T	C1'-C5	3.41	1.58	1.50
1	2	1434	OMG	C5-N7	-3.30	1.32	1.39
1	2	1275	OMG	C5-N7	-3.23	1.32	1.39
1	2	1219	OMC	C6-N1	3.07	1.45	1.38
1	2	1284	4AC	C6-N1	3.04	1.45	1.38
1	2	1284	4AC	O2-C2	-2.87	1.18	1.23
1	2	1384	OMU	O2-C2	-2.81	1.17	1.23
1	2	1384	OMU	O4-C4	-2.78	1.19	1.24
1	2	1275	OMG	C2-N1	2.63	1.44	1.37
1	2	1219	OMC	C5-C4	2.63	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1275	OMG	O6-C6	-2.62	1.18	1.23
1	2	1434	OMG	O6-C6	-2.61	1.18	1.23
1	2	1219	OMC	O2-C2	-2.58	1.18	1.23
1	2	1434	OMG	C5-C6	2.53	1.53	1.44
1	2	1195	I2T	O2-C2	-2.53	1.17	1.22
1	2	1275	OMG	C5-C6	2.36	1.53	1.44
1	2	1434	OMG	C2-N1	2.36	1.43	1.37
1	2	1284	4AC	O7-C7	-2.20	1.18	1.23
1	2	1195	I2T	C32-C31	2.14	1.57	1.52
1	2	1275	OMG	C6-N1	2.02	1.42	1.38
1	2	1195	I2T	O4'-C1'	-2.01	1.41	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1434	OMG	C5-C4-N3	-5.90	118.90	128.46
1	2	1384	OMU	C4-N3-C2	-5.52	119.30	126.58
1	2	1275	OMG	C5-C4-N3	-5.34	119.80	128.46
1	2	1195	I2T	C5-C4-N3	5.25	125.89	116.17
1	2	1434	OMG	C2-N3-C4	4.80	120.86	112.30
1	2	1195	I2T	C4-N3-C2	-4.37	119.93	125.46
1	2	1275	OMG	C2-N3-C4	4.35	120.04	112.30
1	2	1384	OMU	N3-C2-N1	4.00	120.20	114.89
1	2	1275	OMG	C1'-N9-C4	-3.53	116.01	126.50
1	2	1434	OMG	N9-C4-N3	3.42	132.81	125.94
1	2	1384	OMU	C5-C4-N3	3.41	119.95	114.84
1	2	1275	OMG	C1'-N9-C8	3.31	136.11	126.70
1	2	1275	OMG	N9-C4-N3	3.28	132.52	125.94
1	2	1284	4AC	O3'-C3'-C4'	3.22	120.37	111.05
1	2	1284	4AC	O3'-C3'-C2'	3.12	121.93	111.82
1	2	1275	OMG	C2-N1-C6	-3.08	119.49	125.10
1	2	1434	OMG	C2-N1-C6	-3.06	119.52	125.10
1	2	1195	I2T	N3-C2-N1	3.05	121.07	116.76
1	2	1384	OMU	O4-C4-C5	-2.97	119.93	125.16
1	2	1195	I2T	C31-N3-C4	2.87	121.54	117.31
1	2	1434	OMG	C1'-N9-C8	2.84	134.78	126.70
1	2	1434	OMG	C1'-N9-C4	-2.78	118.24	126.50
1	2	1275	OMG	N9-C8-N7	-2.71	108.29	113.39
1	2	1275	OMG	C5-C6-N1	2.60	119.80	113.19
1	2	1434	OMG	C5-C6-N1	2.58	119.73	113.19
1	2	1275	OMG	O6-C6-C5	-2.50	119.97	126.60
1	2	1434	OMG	N9-C8-N7	-2.45	108.78	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1284	4AC	C6-C5-C4	2.43	119.93	116.96
1	2	1434	OMG	O6-C6-C5	-2.40	120.22	126.60
1	2	1384	OMU	O2-C2-N1	-2.34	119.67	122.79
1	2	1284	4AC	N4-C4-N3	2.16	117.48	113.85
1	2	1195	I2T	O4'-C1'-C2'	2.16	108.19	105.14
1	2	1195	I2T	O4-C4-N3	-2.14	116.35	119.98
1	2	1284	4AC	CM7-C7-N4	2.02	118.79	115.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1284	4AC	O4'-C4'-C5'-O5'
1	2	1284	4AC	C3'-C4'-C5'-O5'
1	2	1434	OMG	C4'-C5'-O5'-P
1	2	1434	OMG	O4'-C4'-C5'-O5'
1	2	1195	I2T	O4'-C1'-C5-C4
1	2	1275	OMG	C1'-C2'-O2'-CM2
1	2	1384	OMU	C1'-C2'-O2'-CM2
1	2	1195	I2T	O4'-C1'-C5-C6

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1219	OMC	3	0
1	2	1434	OMG	4	0
1	2	1284	4AC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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.

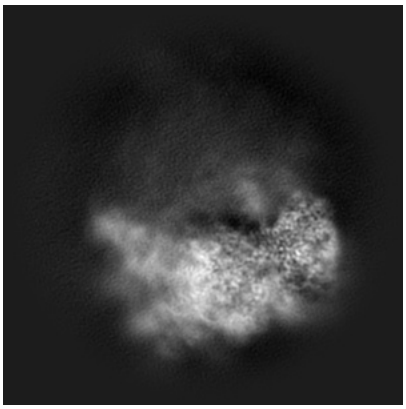
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-54790. These allow visual inspection of the internal detail of the map and identification of artifacts.

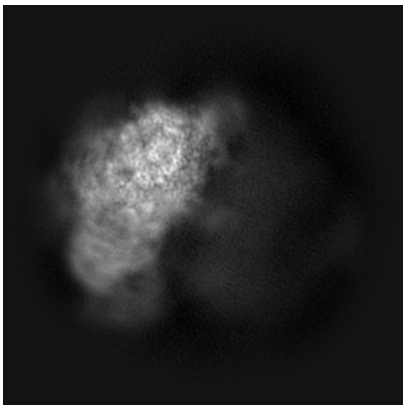
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

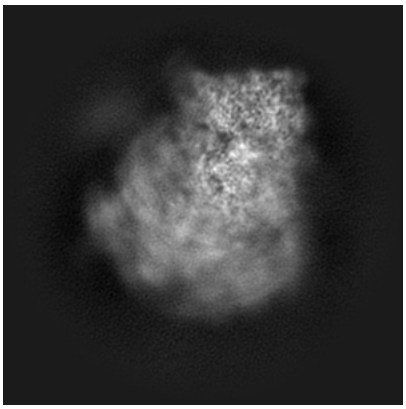
6.1.1 Primary map



X

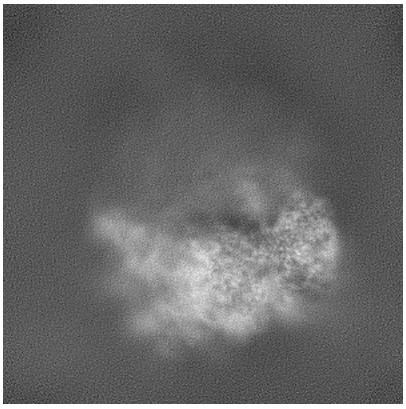


Y



Z

6.1.2 Raw map



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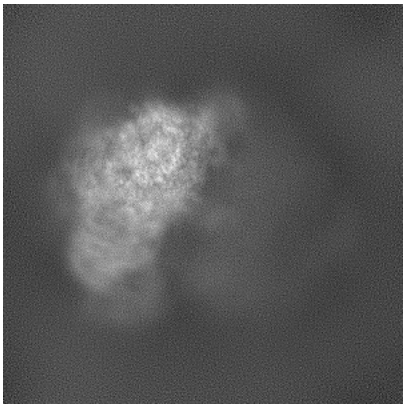
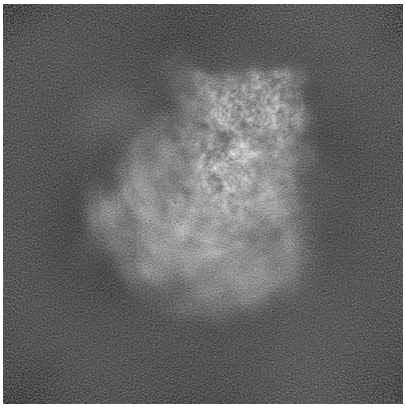


Y

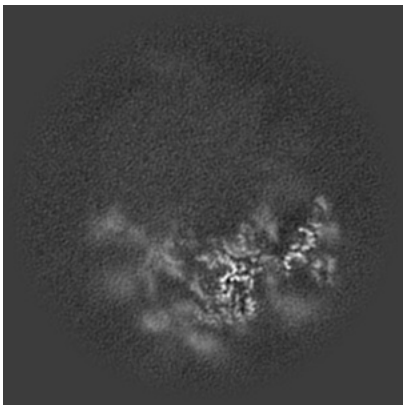


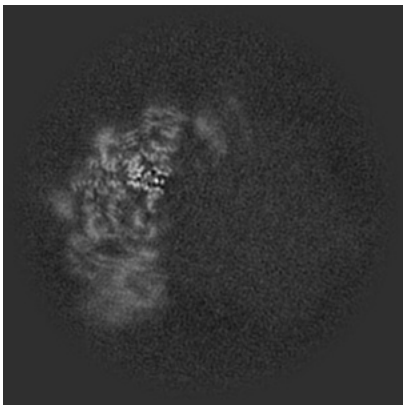
Z

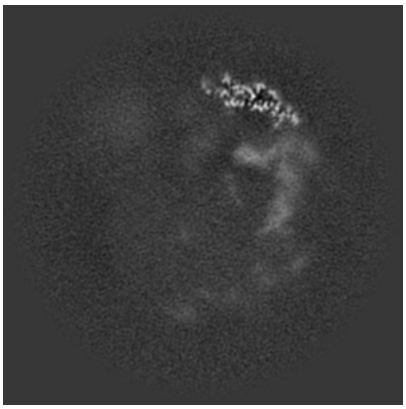
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

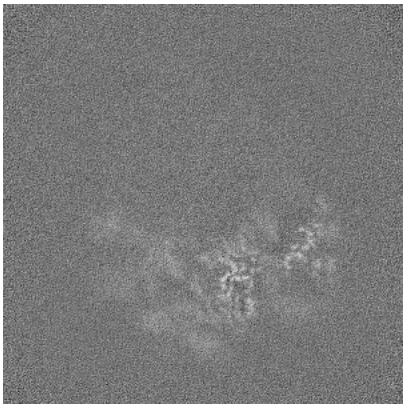
6.2.1 Primary map


X Index: 225


Y Index: 225


Z Index: 225

6.2.2 Raw map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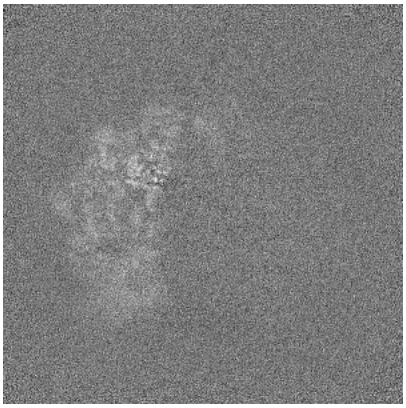
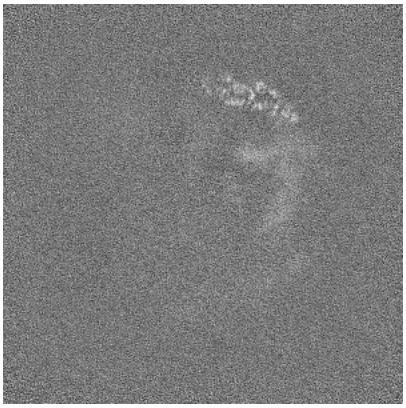
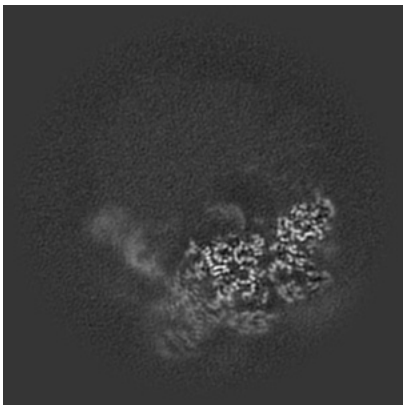

Y Index: 225


Z Index: 225

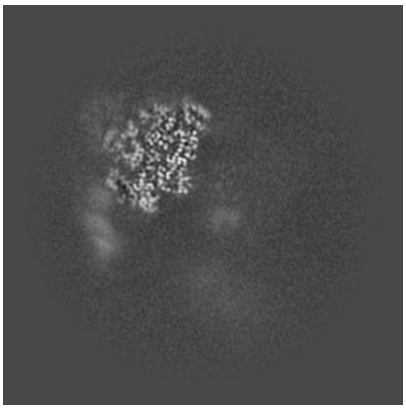
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

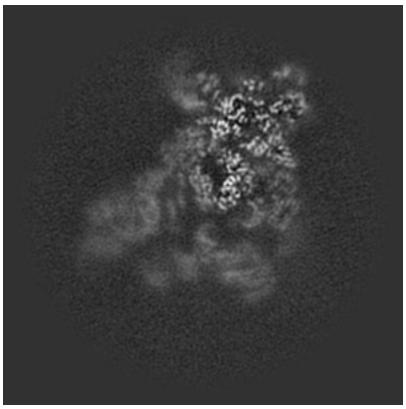
6.3.1 Primary map



X Index: 254

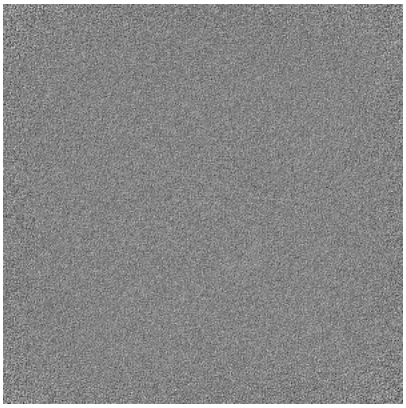


Y Index: 319

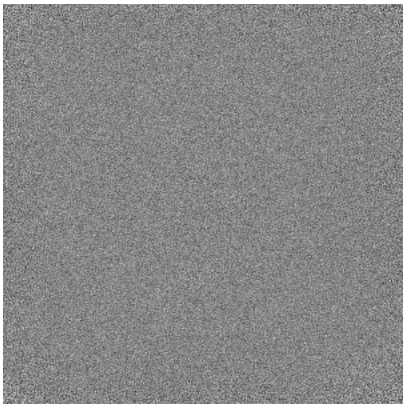


Z Index: 162

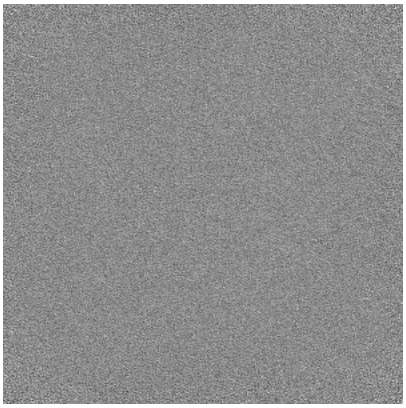
6.3.2 Raw map



X Index: 0



Y Index: 0

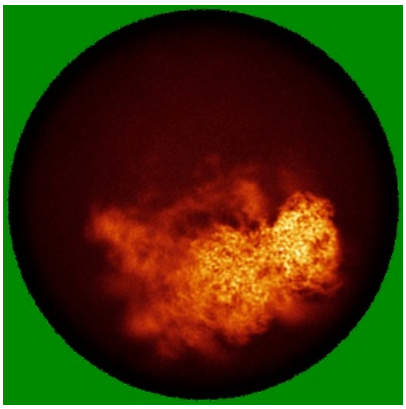


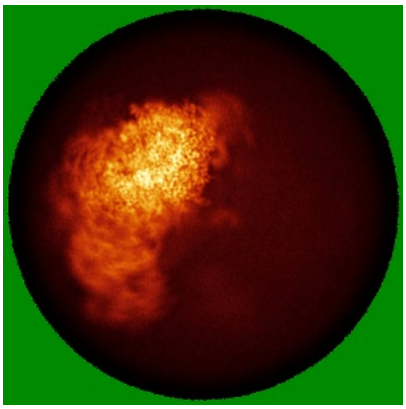
Z Index: 449

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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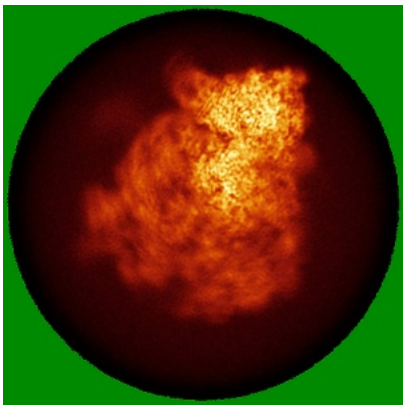
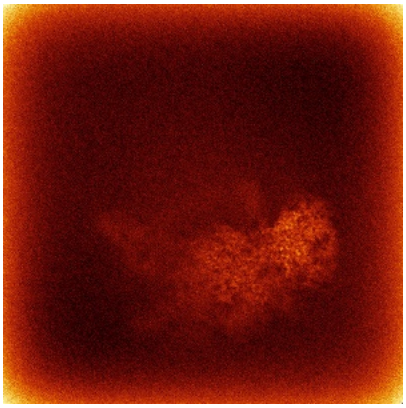

Z

6.4.2 Raw map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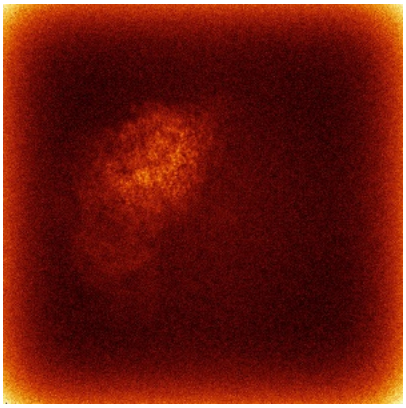
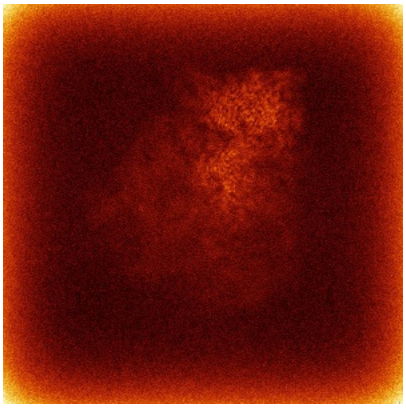

Y


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.

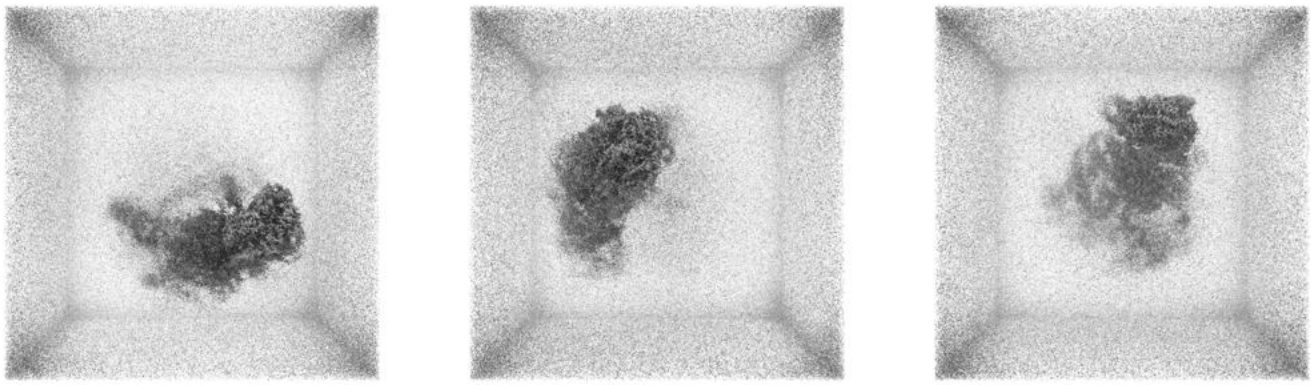
6.5 Orthogonal surface views (i)

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.

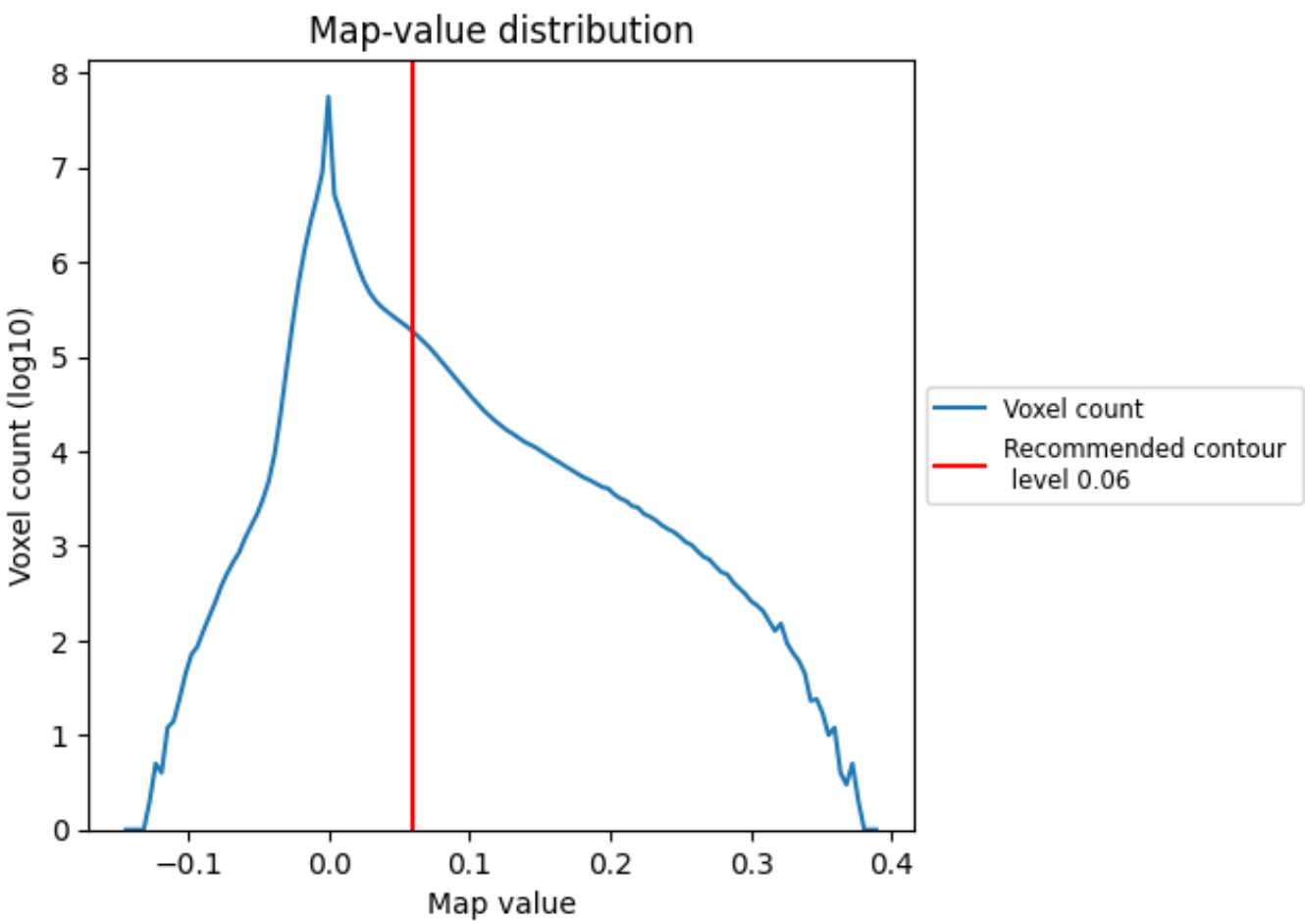
6.6 Mask visualisation (i)

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

7 Map analysis (i)

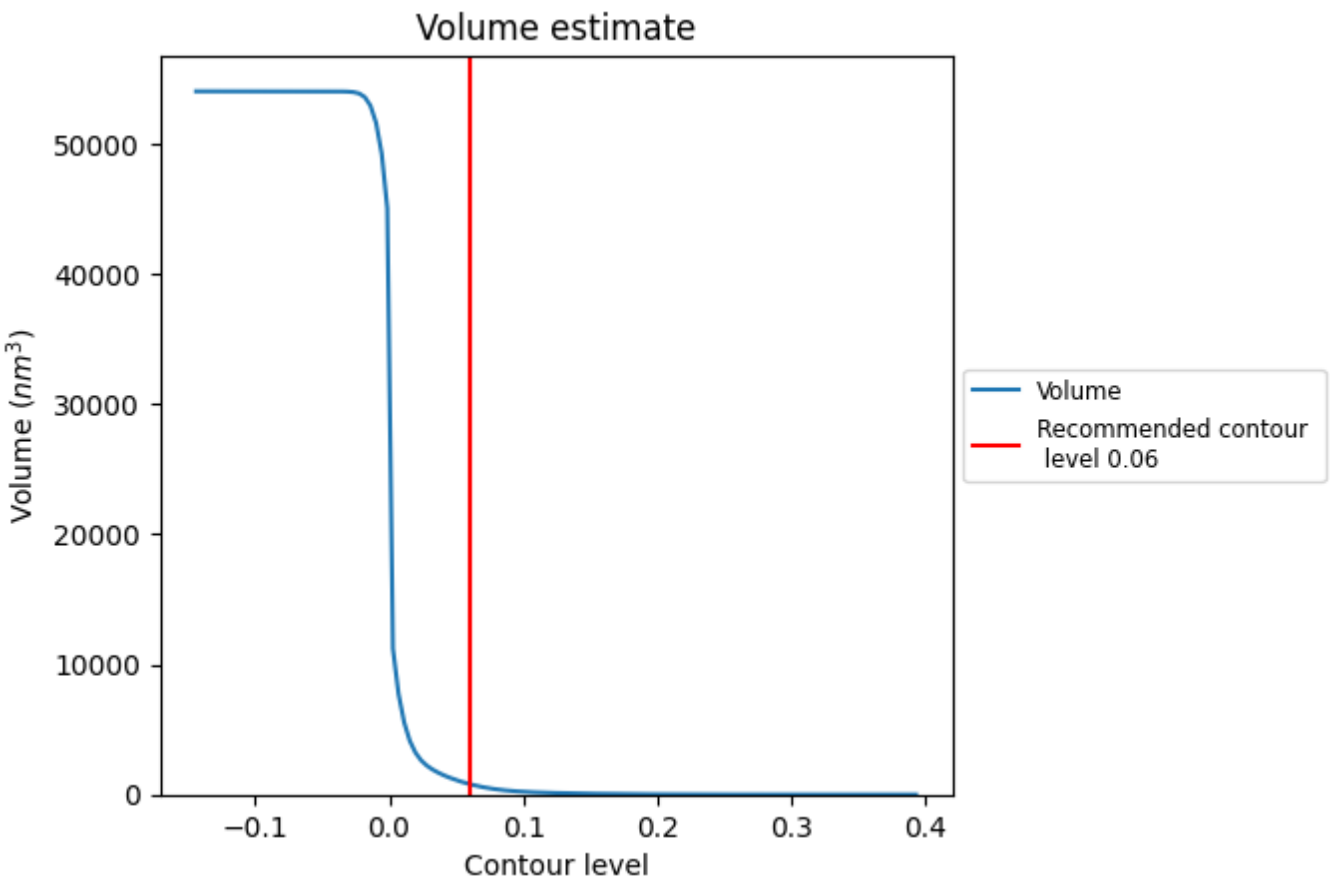
This section contains the results of statistical analysis of the map.

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.

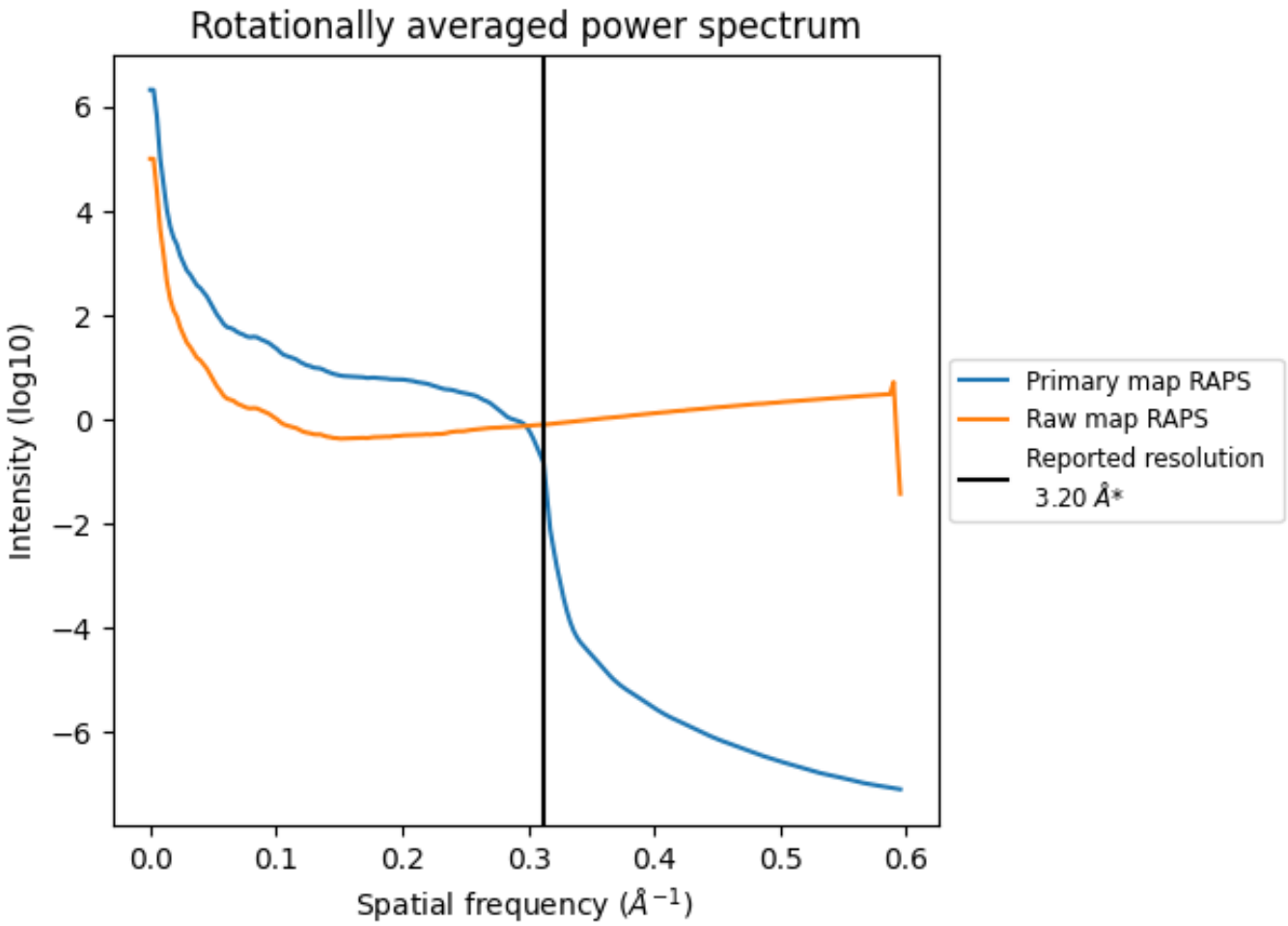
7.2 Volume estimate (i)



The volume at the recommended contour level is 805 nm^3; this corresponds to an approximate mass of 727 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)

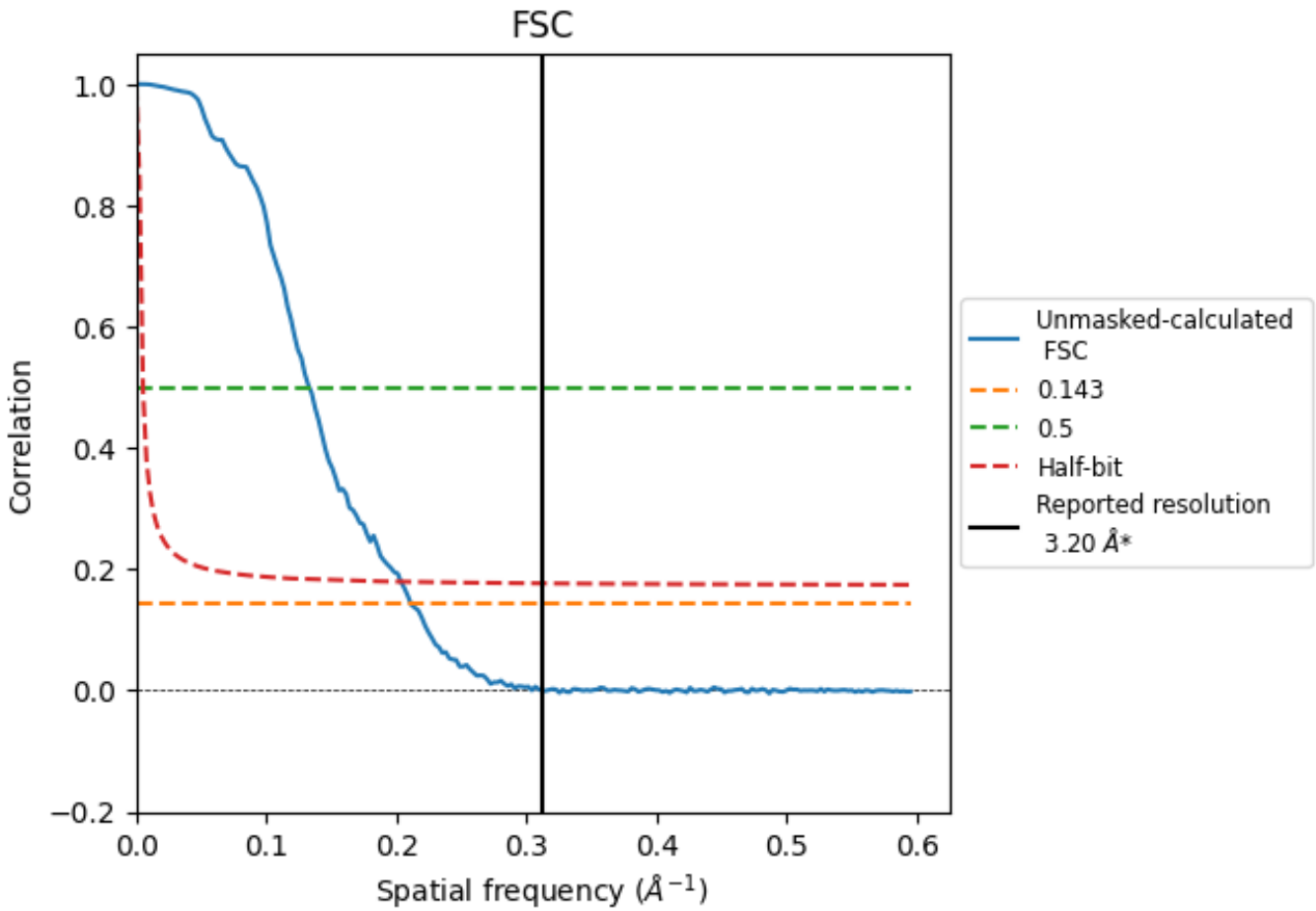


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (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 0.312 Å^{-1}

8.2 Resolution estimates (i)

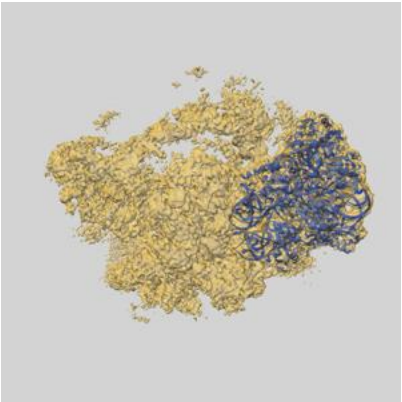
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.73	7.52	4.91

*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 4.73 differs from the reported value 3.2 by more than 10 %

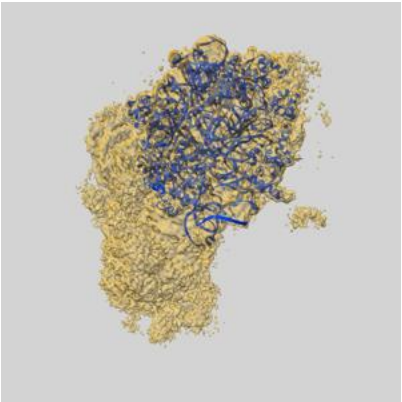
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-54790 and PDB model 9SDQ. Per-residue inclusion information can be found in section 3 on page 7.

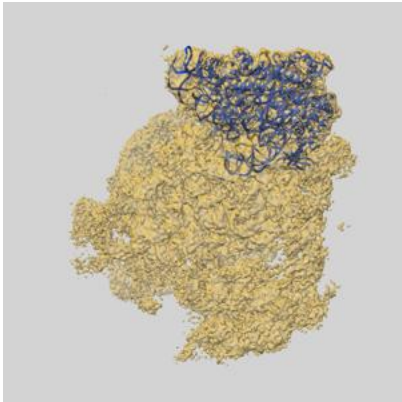
9.1 Map-model overlay (i)



X



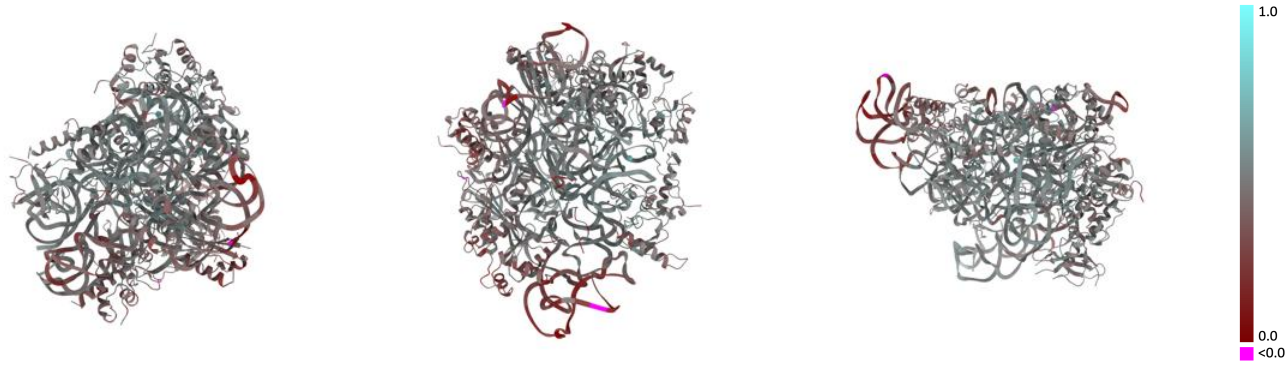
Y



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.

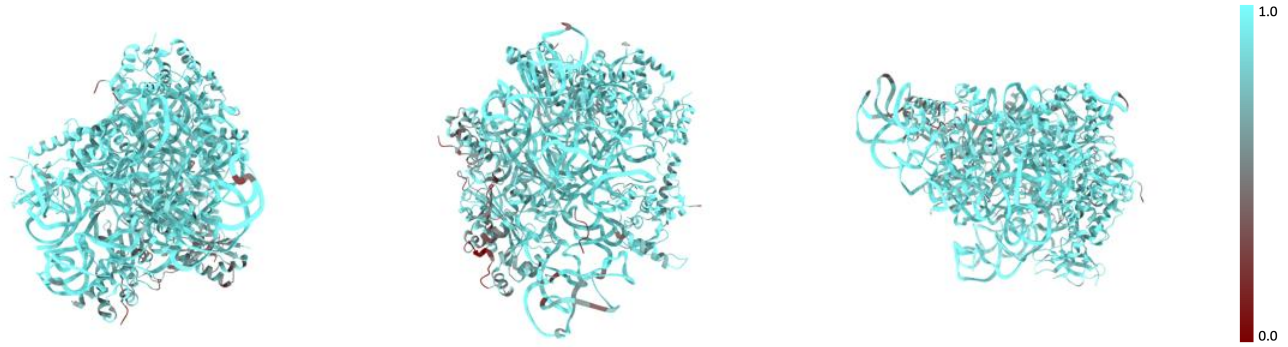
9.2 Q-score mapped to coordinate model (i)



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.

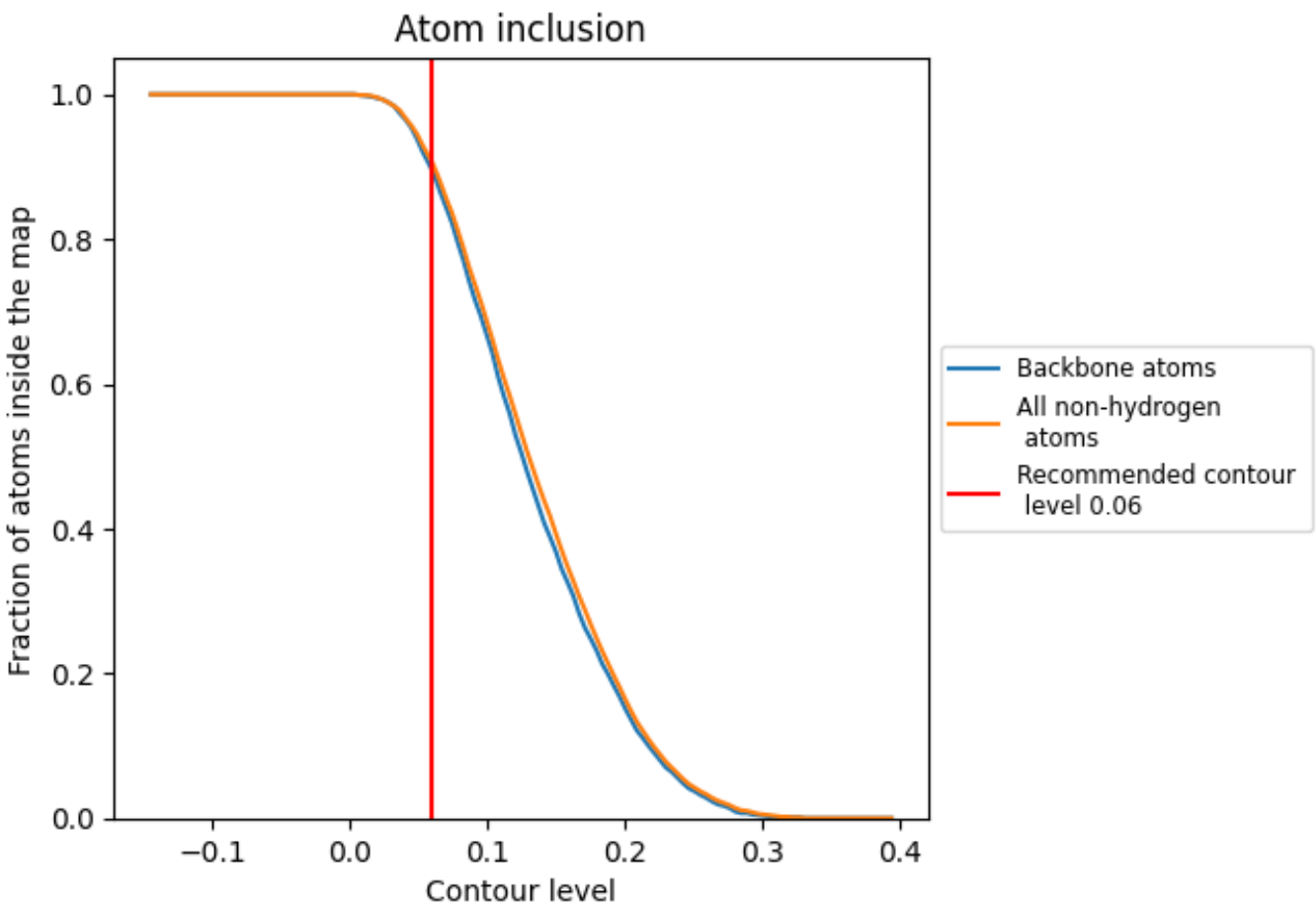
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.9060	0.4490
2	0.9690	0.4450
BD	0.7080	0.4290
BF	0.9110	0.4840
BK	0.7050	0.3610
BP	0.8900	0.4740
BQ	0.9030	0.4700
BR	0.8030	0.3850
BS	0.9090	0.4870
BT	0.9260	0.5020
BU	0.7770	0.4170
Bc	0.9330	0.4590
d	0.8110	0.4600
e	0.8880	0.4540