Full wwPDB EM Validation Report

May 18, 2025 – 09:39 AM EDT

PDB ID	:	8SQJ / pdb_00008sqj
EMDB ID	:	EMD-40707
Title	:	SARS-CoV-2 replication-transcription complex bound to RNA-nsp9, as a noncatalytic RNA-nsp9 binding mode
Authors	:	Small, G.I.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2023-05-04
Resolution	:	3.06 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:

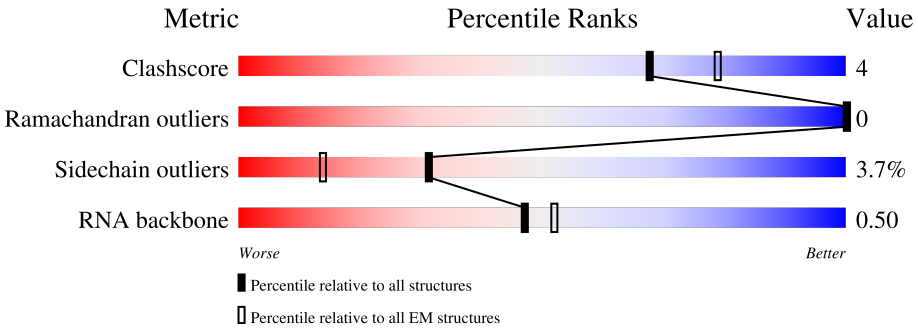
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.06 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	A	932	90% 9%
2	B	198	19% 84% 10% • 6%
2	D	198	17% 81% 11% • 7%
3	C	83	77% 10% 13%
4	G	113	12% 82% 16% •
5	P	37	16% 70% 16% 14%
6	T	55	20% 56% • 5% 36%

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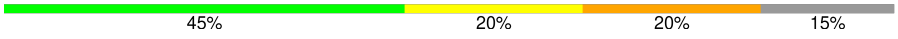
Mol	Chain	Length	Quality of chain
7	O	20	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26058 atoms, of which 12403 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	929	14700	4776	7219	1255	1396	54	0	0

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	187	2823	886	1408	244	274	11	0	0
2	D	185	Total	C	H	N	O	S	0	0
			2842	889	1428	242	272	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	72	1138	349	585	91	107	6	0	0

- Molecule 4 is a protein called Non-structural protein 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	G	113	1688	536	846	145	156	5	0	0

- Molecule 5 is a RNA chain called Primer RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
5	P	32	1023	303	346	119	223	32	0	0

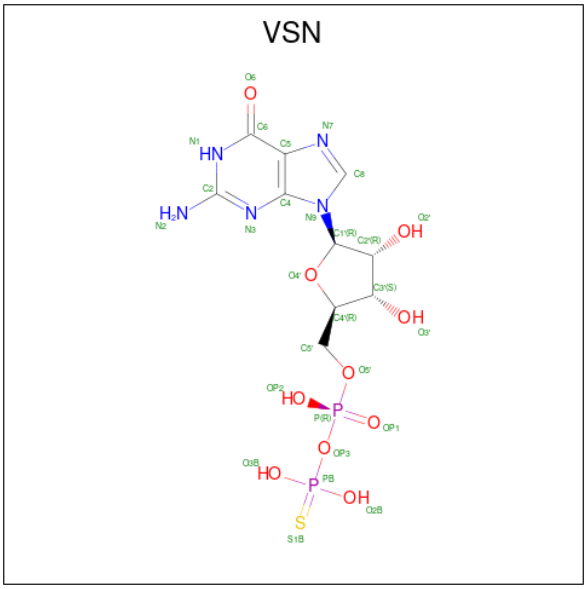
- Molecule 6 is a RNA chain called Template RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	T	35	Total	C	H	N	O	P	0	0
			1122	333	375	131	248	35		

- Molecule 7 is a RNA chain called SARS-CoV-2 5' UTR.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	17	Total	C	H	N	O	P	0	0
			538	160	182	59	120	17		

- Molecule 8 is 5'-O-[(R)-hydroxy(thiophosphonooxy)phosphoryl]guanosine (CCD ID: VSN) (formula: $C_{10}H_{15}N_5O_{10}P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
8	A	1	Total	C	H	N	O	P	S	0
			42	10	14	5	10	2	1	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Zn	0
			2	2	

- Molecule 11 is water.

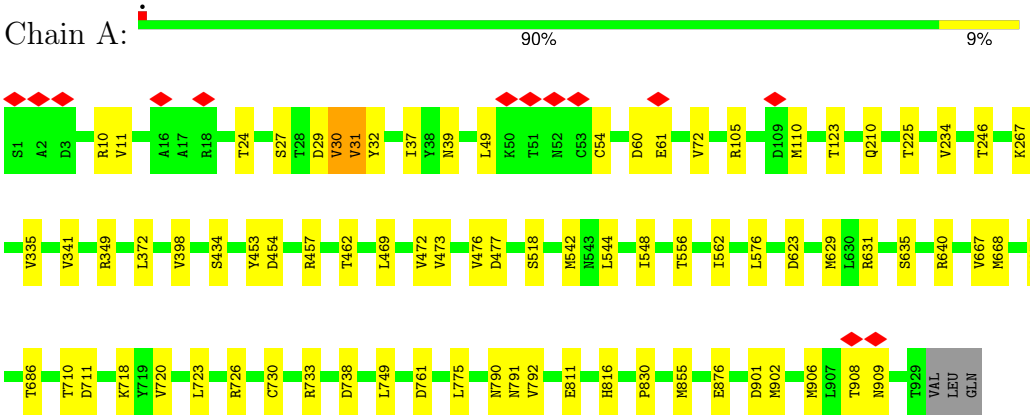
Mol	Chain	Residues	Atoms	AltConf
11	A	118	Total O 118 118	0
11	B	6	Total O 6 6	0
11	C	3	Total O 3 3	0
11	D	1	Total O 1 1	0
11	G	1	Total O 1 1	0
11	P	1	Total O 1 1	0
11	T	6	Total O 6 6	0
11	O	3	Total O 3 3	0

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.

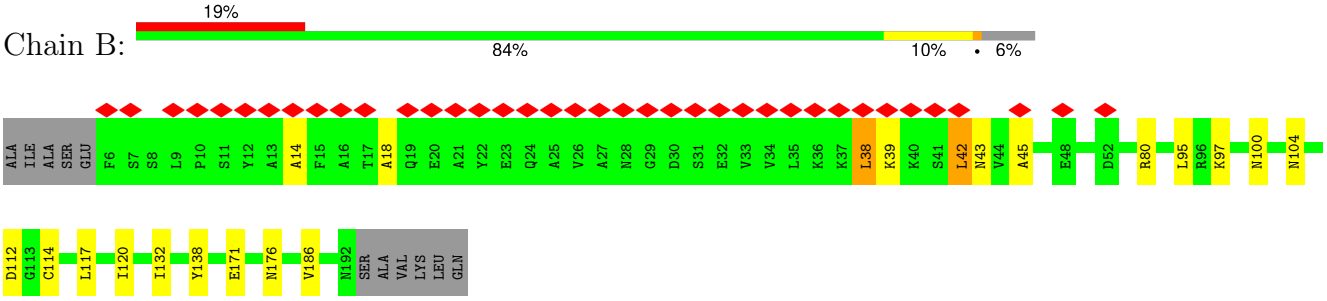
• Molecule 1: RNA-directed RNA polymerase

Chain A:



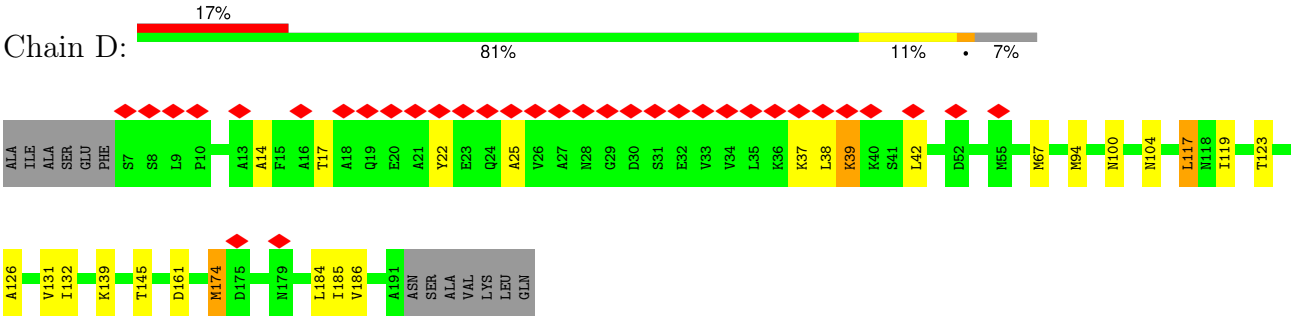
• Molecule 2: Non-structural protein 8

Chain B:



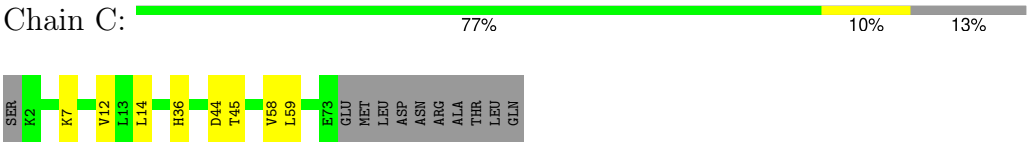
• Molecule 2: Non-structural protein 8

Chain D:



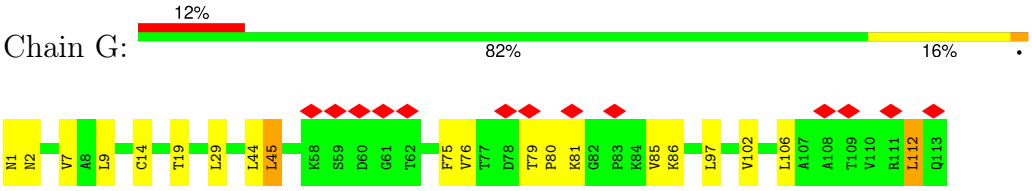
• Molecule 3: Non-structural protein 7

Chain C:



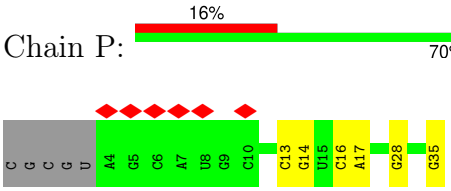
• Molecule 4: Non-structural protein 9

Chain G:



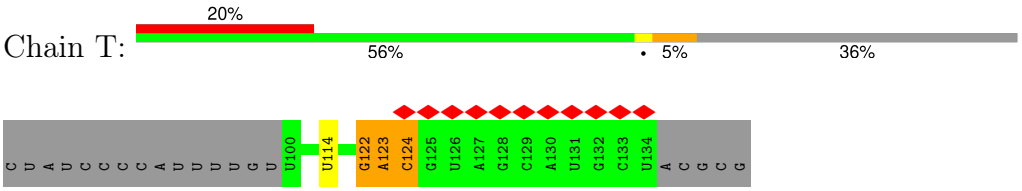
• Molecule 5: Primer RNA

Chain P:



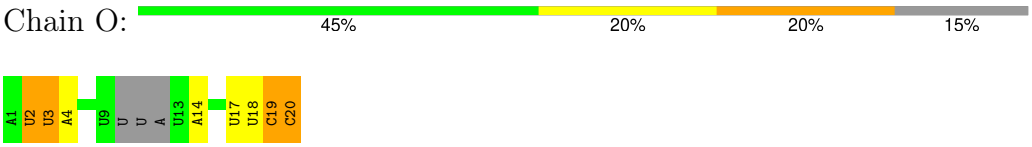
• Molecule 6: Template RNA

Chain T:



• Molecule 7: SARS-CoV-2 5' UTR

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113260	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.51	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	41.558	Depositor
Minimum map value	-27.921	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.023	Depositor
Recommended contour level	3.1	Depositor
Map size (Å)	277.12, 277.12, 277.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, VSN, 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	A	0.17	0/7670	0.28	0/10409
2	B	0.13	0/1434	0.25	0/1945
2	D	0.12	0/1433	0.28	0/1942
3	C	0.17	0/556	0.28	0/749
4	G	0.14	0/858	0.30	0/1169
5	P	0.10	0/755	0.20	0/1173
6	T	0.11	0/834	0.21	0/1298
7	O	0.15	0/395	0.38	0/609
All	All	0.15	0/13935	0.27	0/19294

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7481	7219	7219	39	0
2	B	1415	1408	1408	17	0
2	D	1414	1428	1428	17	0
3	C	553	585	585	7	0
4	G	842	846	831	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	677	346	346	1	0
6	T	747	375	376	3	0
7	O	356	182	183	8	0
8	A	28	14	0	3	0
9	A	1	0	0	0	0
10	A	2	0	0	0	0
11	A	118	0	0	2	0
11	B	6	0	0	0	0
11	C	3	0	0	1	0
11	D	1	0	0	0	0
11	G	1	0	0	0	0
11	O	3	0	0	0	0
11	P	1	0	0	0	0
11	T	6	0	0	0	0
All	All	13655	12403	12376	93	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 4.

All (93) 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:A:718:LYS:NZ	7:O:20:C:OP1	2.14	0.81
2:B:43:ASN:HD21	6:T:122:G:H5'	1.47	0.80
1:A:726:ARG:NH2	1:A:738:ASP:OD2	2.15	0.79
2:B:100:ASN:O	2:B:104:ASN:ND2	2.17	0.78
8:A:1001:VSN:O4'	5:P:35:G:O2'	2.02	0.77
6:T:123:A:O2'	6:T:124:C:OP1	2.06	0.73
1:A:331:ARG:NH2	2:B:114:CYS:SG	2.66	0.69
1:A:477:ASP:OD2	1:A:640:ARG:NH1	2.26	0.69
2:B:14:ALA:HB1	2:B:45:ALA:HB1	1.76	0.68
1:A:60:ASP:OD1	1:A:61:GLU:N	2.28	0.66
1:A:332:LYS:NZ	2:B:104:ASN:OD1	2.30	0.65
2:D:174:MET:SD	2:D:174:MET:N	2.68	0.64
1:A:278:GLU:N	1:A:278:GLU:OE1	2.30	0.64
1:A:631:ARG:NH1	1:A:635:SER:OG	2.31	0.64
1:A:518:SER:O	2:B:80:ARG:NH1	2.32	0.63
3:C:12:VAL:HG21	2:D:94:MET:CE	2.29	0.62
3:C:7:LYS:NZ	11:C:101:HOH:O	2.32	0.61
3:C:12:VAL:HG21	2:D:94:MET:HE3	1.82	0.61
4:G:75:PHE:CE2	4:G:112:LEU:HD12	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LEU:HD11	1:A:686:THR:HG22	1.84	0.58
4:G:45:LEU:HD22	4:G:86:LYS:HE3	1.86	0.58
1:A:901:ASP:OD1	1:A:902:MET:N	2.37	0.57
2:B:43:ASN:ND2	6:T:123:A:OP1	2.39	0.56
1:A:330:VAL:HG13	1:A:341:VAL:HG13	1.88	0.56
2:B:18:ALA:HB1	2:B:42:LEU:HD23	1.87	0.56
4:G:85:VAL:O	4:G:85:VAL:HG23	2.06	0.56
1:A:472:VAL:O	1:A:476:VAL:HG23	2.07	0.55
4:G:75:PHE:CD2	4:G:112:LEU:HD12	2.41	0.55
1:A:726:ARG:NH1	1:A:730:CYS:SG	2.80	0.54
2:D:14:ALA:O	2:D:17:THR:OG1	2.24	0.53
7:O:2:U:O2'	7:O:3:U:O5'	2.26	0.53
1:A:349:ARG:NH2	11:A:1107:HOH:O	2.40	0.53
1:A:32:TYR:CE1	1:A:49:LEU:HD11	2.43	0.53
1:A:453:TYR:CE1	1:A:667:VAL:HG21	2.44	0.53
2:B:95:LEU:C	2:B:95:LEU:HD23	2.34	0.53
1:A:105:ARG:NH2	1:A:110:MET:HE2	2.25	0.52
1:A:682:SER:O	8:A:1001:VSN:N2	2.43	0.51
1:A:720:VAL:O	1:A:720:VAL:HG12	2.10	0.51
2:D:132:ILE:HD12	2:D:186:VAL:HG21	1.91	0.51
2:D:117:LEU:HD13	2:D:131:VAL:CG2	2.40	0.51
2:D:22:TYR:OH	2:D:39:LYS:NZ	2.44	0.51
4:G:9:LEU:HD21	4:G:102:VAL:HG22	1.93	0.50
3:C:44:ASP:OD1	3:C:45:THR:N	2.42	0.50
2:D:117:LEU:HD13	2:D:131:VAL:HG23	1.93	0.49
2:B:112:ASP:OD1	2:B:112:ASP:N	2.46	0.49
1:A:469:LEU:O	1:A:473:VAL:HG23	2.13	0.49
1:A:27:SER:OG	1:A:54:CYS:HA	2.13	0.48
7:O:19:C:H2'	7:O:19:C:O2	2.12	0.48
8:A:1001:VSN:OP2	11:A:1101:HOH:O	2.20	0.48
4:G:79:THR:HB	4:G:80:PRO:CD	2.44	0.47
1:A:733:ARG:NH2	4:G:2:ASN:OD1	2.48	0.47
1:A:11:VAL:HG22	1:A:72:VAL:HG21	1.97	0.46
2:B:171:GLU:O	2:B:176:ASN:ND2	2.49	0.46
2:D:185:ILE:N	2:D:185:ILE:HD12	2.30	0.46
1:A:454:ASP:OD2	1:A:457:ARG:NH1	2.49	0.46
2:B:42:LEU:HD13	2:B:42:LEU:C	2.41	0.46
4:G:106:LEU:HD23	4:G:106:LEU:C	2.41	0.46
2:B:18:ALA:CB	2:B:42:LEU:HD23	2.46	0.45
7:O:17:U:C2	7:O:18:U:C6	3.04	0.45
2:D:145:THR:HG22	2:D:145:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ASN:O	2:D:104:ASN:ND2	2.38	0.45
7:O:18:U:N3	7:O:19:C:C5	2.84	0.45
4:G:14:CYS:SG	4:G:44:LEU:HD11	2.56	0.45
1:A:29:ASP:C	1:A:30:VAL:HG22	2.42	0.45
2:D:22:TYR:HA	2:D:38:LEU:HD21	1.99	0.44
1:A:544:LEU:HD12	1:A:556:THR:HG22	1.99	0.44
1:A:320:VAL:HG12	1:A:320:VAL:O	2.17	0.44
2:B:132:ILE:HG21	2:B:138:TYR:HB2	2.00	0.44
4:G:29:LEU:O	4:G:44:LEU:HD12	2.18	0.44
1:A:39:ASN:ND2	4:G:1:ASN:OD1	2.50	0.44
1:A:398:VAL:HG23	1:A:675:VAL:HG23	1.99	0.43
2:D:123:THR:OG1	2:D:126:ALA:HB2	2.19	0.43
1:A:434:SER:OG	1:A:876:GLU:OE1	2.35	0.42
1:A:710:THR:HG22	1:A:711:ASP:N	2.34	0.42
7:O:2:U:H1'	7:O:3:U:OP1	2.19	0.42
3:C:58:VAL:HG22	2:D:119:ILE:HG12	2.01	0.42
1:A:123:THR:OG1	1:A:210:GLN:O	2.34	0.42
7:O:18:U:C2	7:O:19:C:C5	3.08	0.42
7:O:19:C:H2'	7:O:20:C:C5'	2.49	0.42
1:A:462:THR:OG1	1:A:791:ASN:OD1	2.37	0.41
2:D:161:ASP:HA	2:D:184:LEU:HD12	2.02	0.41
1:A:720:VAL:HG11	1:A:775:LEU:HD13	2.03	0.41
2:B:38:LEU:C	2:B:38:LEU:HD12	2.45	0.41
3:C:59:LEU:HD23	3:C:59:LEU:C	2.45	0.41
1:A:31:VAL:O	1:A:32:TYR:CG	2.74	0.41
1:A:816:HIS:O	1:A:830:PRO:HA	2.21	0.41
2:B:42:LEU:O	2:B:42:LEU:HD22	2.21	0.41
3:C:14:LEU:HD22	3:C:36:HIS:CG	2.56	0.41
2:D:22:TYR:O	2:D:25:ALA:HB3	2.21	0.41
2:D:42:LEU:C	2:D:42:LEU:HD13	2.46	0.41
1:A:623:ASP:OD1	1:A:623:ASP:N	2.52	0.40
2:B:42:LEU:HD13	2:B:43:ASN:N	2.36	0.40
1:A:234:VAL:HG23	1:A:234:VAL:O	2.21	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	
1	A	927/932 (100%)	890 (96%)	37 (4%)	0	100	100
2	B	185/198 (93%)	183 (99%)	2 (1%)	0	100	100
2	D	183/198 (92%)	175 (96%)	8 (4%)	0	100	100
3	C	70/83 (84%)	69 (99%)	1 (1%)	0	100	100
4	G	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
All	All	1476/1524 (97%)	1418 (96%)	58 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	820/823 (100%)	793 (97%)	27 (3%)	33	59
2	B	149/167 (89%)	142 (95%)	7 (5%)	22	49
2	D	151/167 (90%)	145 (96%)	6 (4%)	27	55
3	C	67/77 (87%)	67 (100%)	0	100	100
4	G	86/94 (92%)	79 (92%)	7 (8%)	9	30
All	All	1273/1328 (96%)	1226 (96%)	47 (4%)	31	56

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	24	THR
1	A	30	VAL
1	A	31	VAL
1	A	37	ILE
1	A	225	THR
1	A	246	THR
1	A	267	LYS
1	A	330	VAL
1	A	335	VAL
1	A	372	LEU
1	A	542	MET
1	A	548	ILE
1	A	562	ILE
1	A	629	MET
1	A	668	MET
1	A	680	THR
1	A	723	LEU
1	A	749	LEU
1	A	761	ASP
1	A	790	ASN
1	A	792	VAL
1	A	811	GLU
1	A	855	MET
1	A	906	MET
1	A	908	THR
1	A	909	ASN
2	B	38	LEU
2	B	39	LYS
2	B	42	LEU
2	B	97	LYS
2	B	117	LEU
2	B	120	ILE
2	B	186	VAL
2	D	37	LYS
2	D	39	LYS
2	D	67	MET
2	D	117	LEU
2	D	139	LYS
2	D	174	MET
4	G	7	VAL
4	G	19	THR
4	G	45	LEU

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Mol	Chain	Res	Type
4	G	76	VAL
4	G	81	LYS
4	G	97	LEU
4	G	112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	ASN
1	A	39	ASN
1	A	52	ASN
1	A	75	HIS
1	A	133	HIS
1	A	191	GLN
1	A	209	ASN
1	A	297	ASN
1	A	381	HIS
1	A	468	GLN
1	A	570	GLN
1	A	599	HIS
1	A	600	ASN
1	A	611	ASN
1	A	650	HIS
2	B	43	ASN
4	G	33	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	P	31/37 (83%)	5 (16%)	0
6	T	34/55 (61%)	4 (11%)	1 (2%)
7	O	15/20 (75%)	6 (40%)	1 (6%)
All	All	80/112 (71%)	15 (18%)	2 (2%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	P	13	C
5	P	14	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	P	16	C
5	P	17	A
5	P	28	G
6	T	114	U
6	T	122	G
6	T	123	A
6	T	124	C
7	O	2	U
7	O	3	U
7	O	4	A
7	O	14	A
7	O	19	C
7	O	20	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	T	123	A
7	O	2	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	VSN	A	1001	-	25,30,30	3.66	14 (56%)	27,47,47	1.58	5 (18%)

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
8	VSN	A	1001	-	-	7/11/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1001	VSN	O4'-C1'	-8.49	1.29	1.40
8	A	1001	VSN	O4'-C4'	7.42	1.61	1.45
8	A	1001	VSN	C2'-C3'	-7.36	1.33	1.53
8	A	1001	VSN	P-OP3	6.07	1.66	1.59
8	A	1001	VSN	C2-N2	5.31	1.46	1.34
8	A	1001	VSN	C5'-C4'	-4.59	1.37	1.51
8	A	1001	VSN	PB-O2B	3.57	1.66	1.54
8	A	1001	VSN	PB-O3B	3.20	1.65	1.54
8	A	1001	VSN	C6-N1	-3.10	1.33	1.37
8	A	1001	VSN	O3'-C3'	2.48	1.49	1.43
8	A	1001	VSN	C5-C4	-2.41	1.37	1.43
8	A	1001	VSN	C5-C6	-2.39	1.42	1.47
8	A	1001	VSN	P-O5'	2.32	1.68	1.59
8	A	1001	VSN	C1'-N9	-2.10	1.44	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1001	VSN	C4'-O4'-C1'	-4.40	105.89	109.92
8	A	1001	VSN	C8-N7-C5	3.28	108.13	102.55
8	A	1001	VSN	C5-C6-N1	2.87	119.54	114.07
8	A	1001	VSN	C2-N1-C6	-2.48	120.56	125.11
8	A	1001	VSN	P-OP3-PB	-2.26	124.90	133.17

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	VSN	C5'-O5'-P-OP3
8	A	1001	VSN	C5'-O5'-P-OP1
8	A	1001	VSN	C3'-C4'-C5'-O5'
8	A	1001	VSN	PB-OP3-P-OP1
8	A	1001	VSN	C5'-O5'-P-OP2
8	A	1001	VSN	O4'-C4'-C5'-O5'
8	A	1001	VSN	PB-OP3-P-OP2

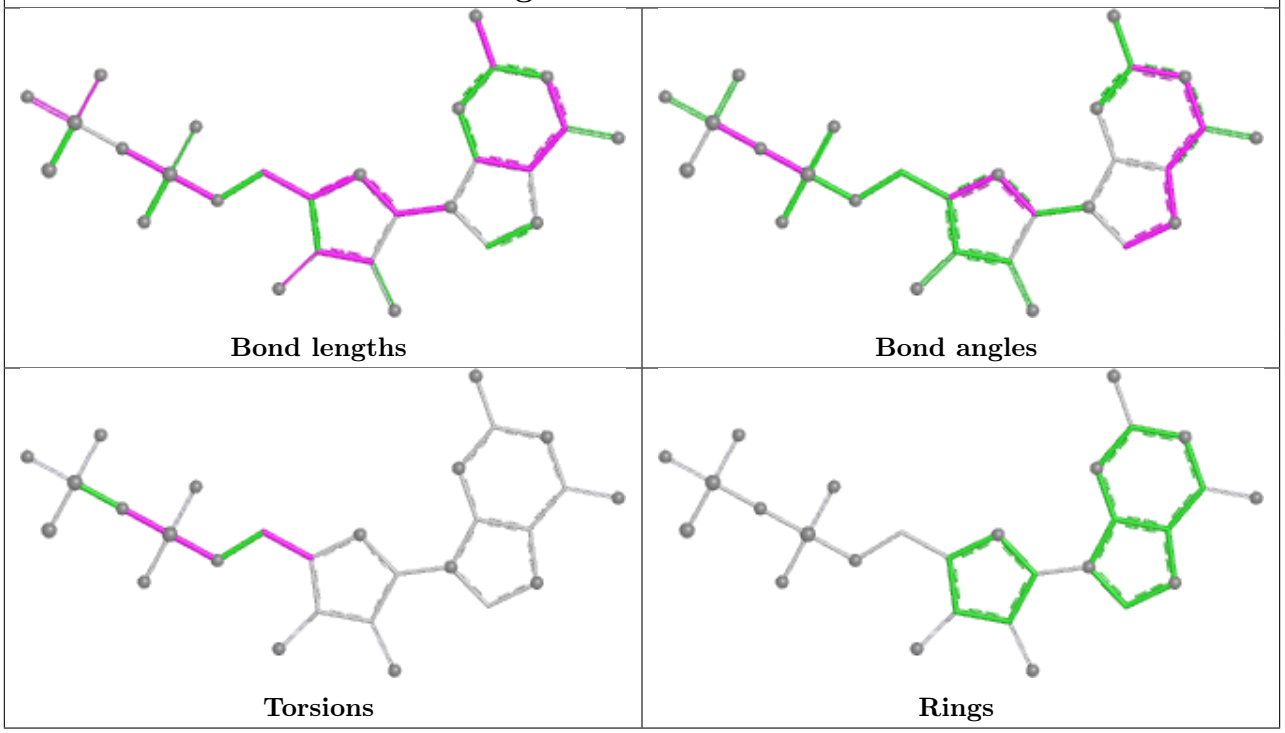
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1001	VSN	3	0

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

Ligand VSN A 1001



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.

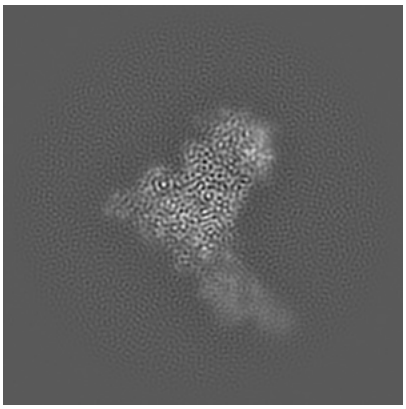
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40707. These allow visual inspection of the internal detail of the map and identification of artifacts.

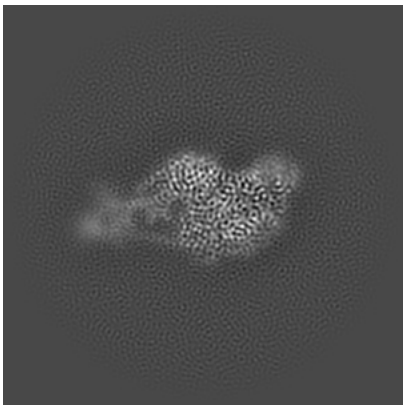
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

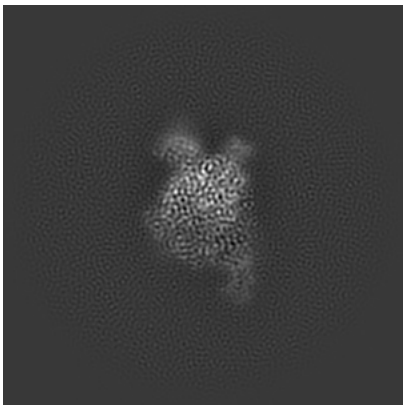
6.1.1 Primary map



X

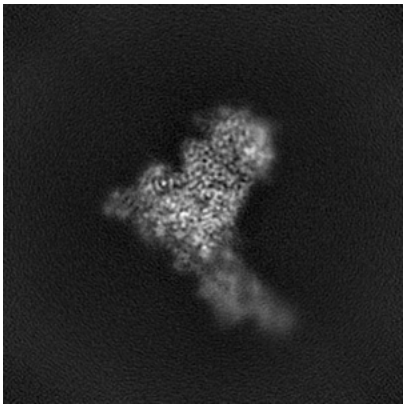


Y

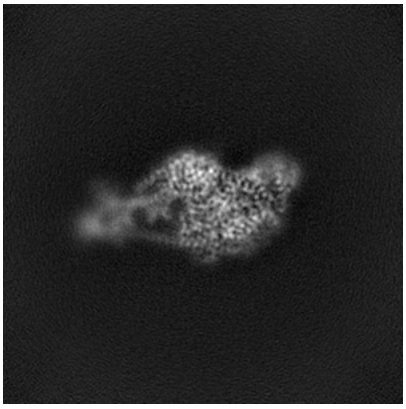


Z

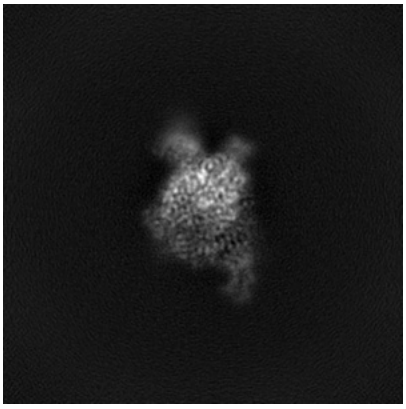
6.1.2 Raw map



X



Y

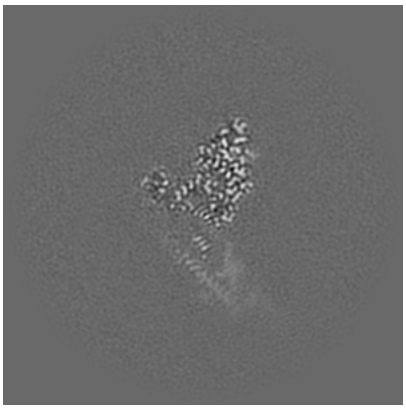


Z

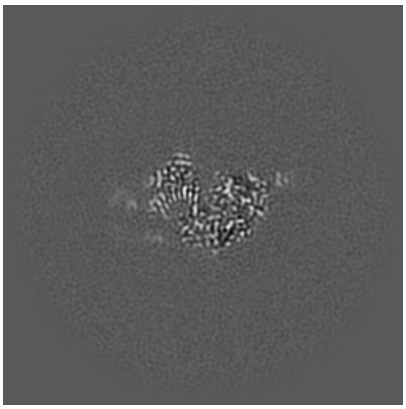
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

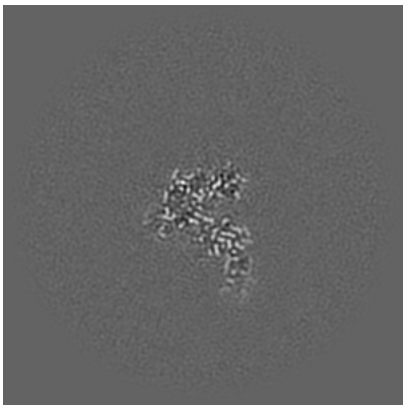
6.2.1 Primary map



X Index: 128

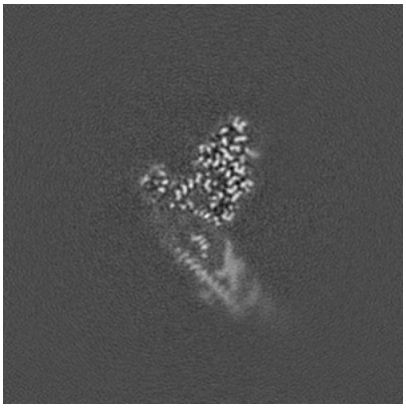


Y Index: 128

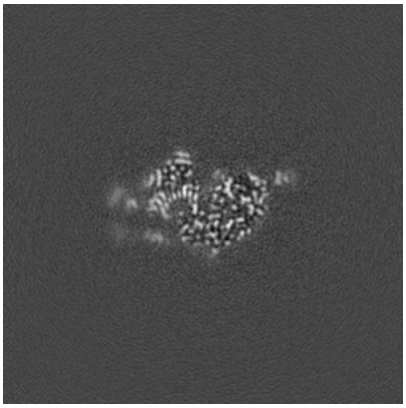


Z Index: 128

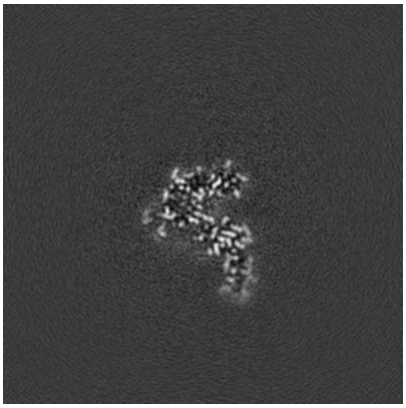
6.2.2 Raw map



X Index: 128



Y Index: 128

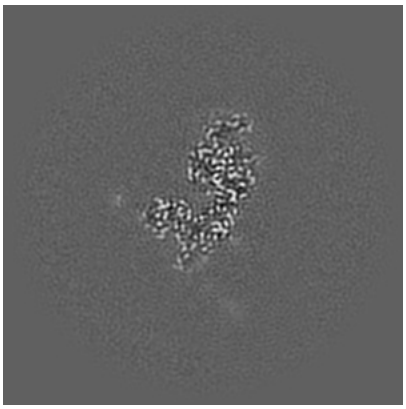


Z Index: 128

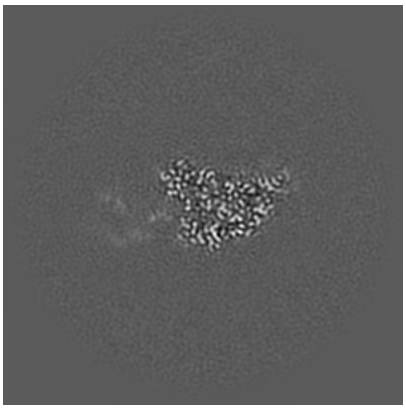
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

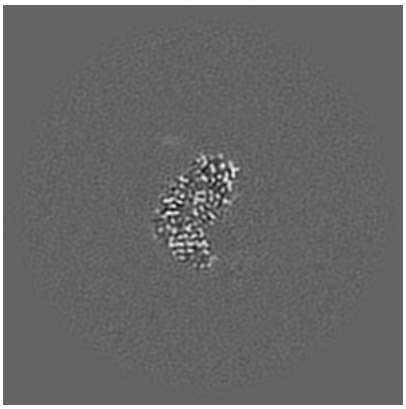
6.3.1 Primary map



X Index: 140

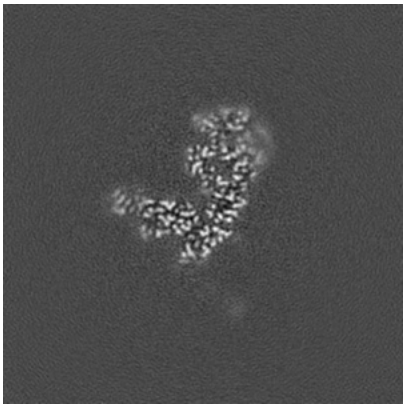


Y Index: 135

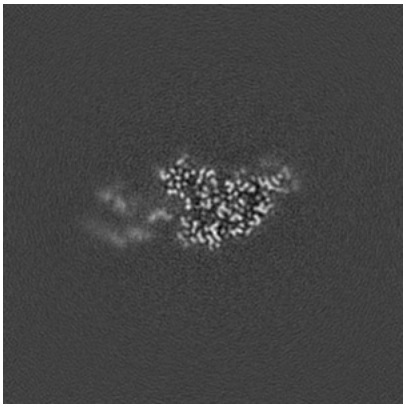


Z Index: 141

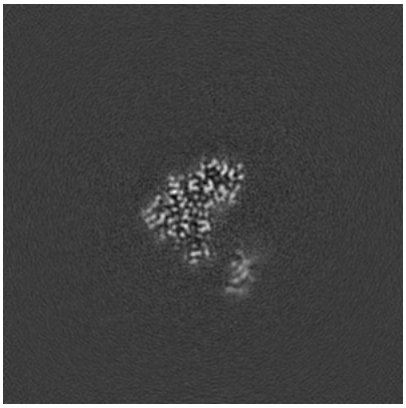
6.3.2 Raw map



X Index: 144



Y Index: 135

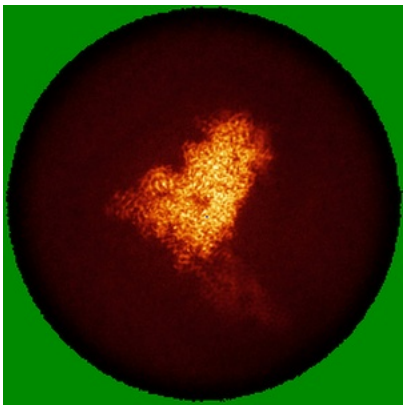


Z Index: 135

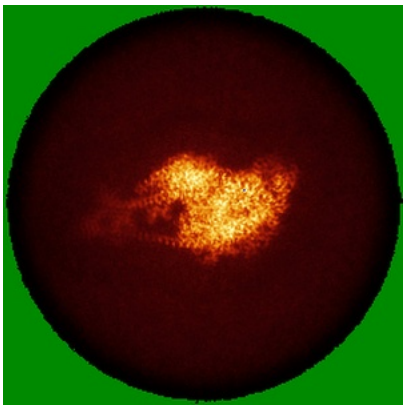
The images above show the largest variance slices of the map in three orthogonal directions.

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

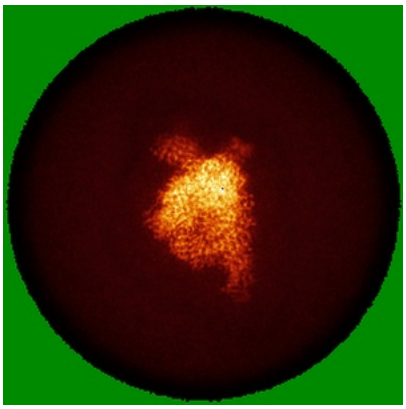
6.4.1 Primary map



X

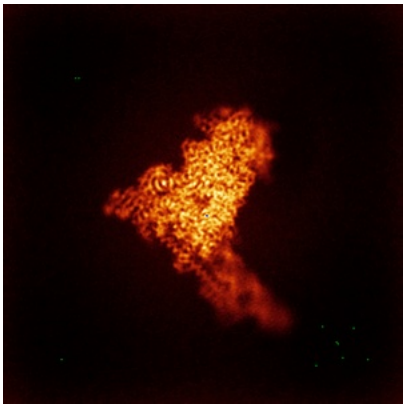


Y

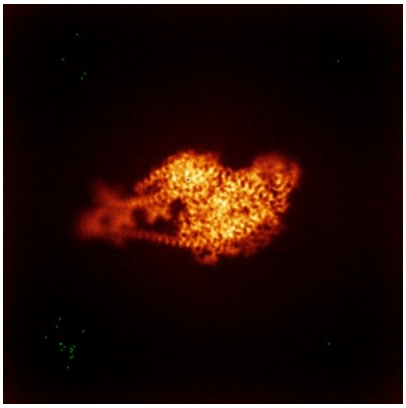


Z

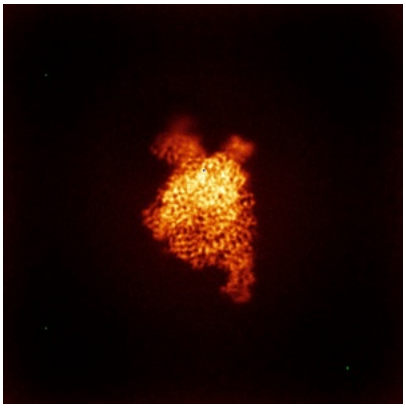
6.4.2 Raw map



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 3.1. 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.

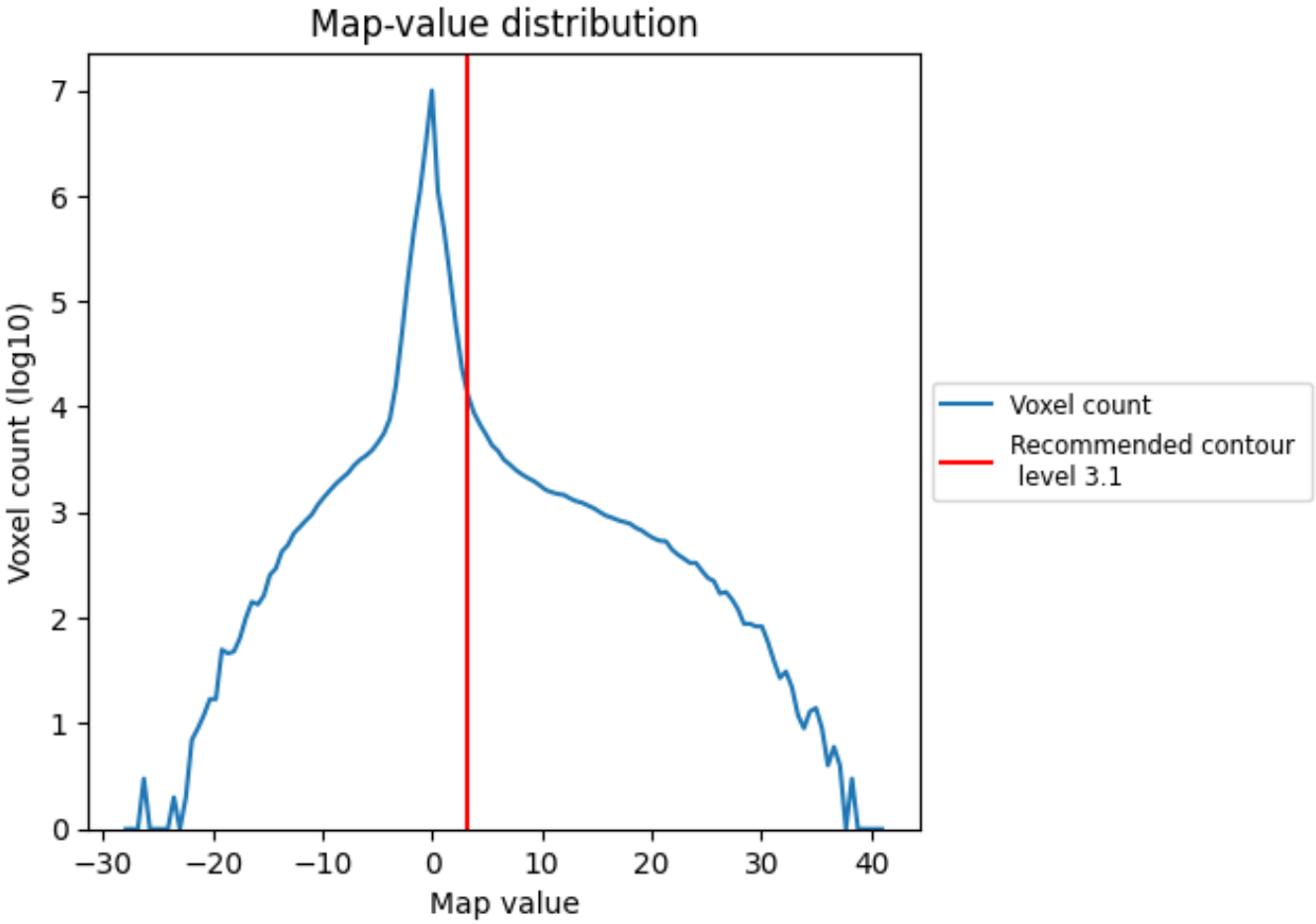
6.6 Mask visualisation (i)

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

7 Map analysis

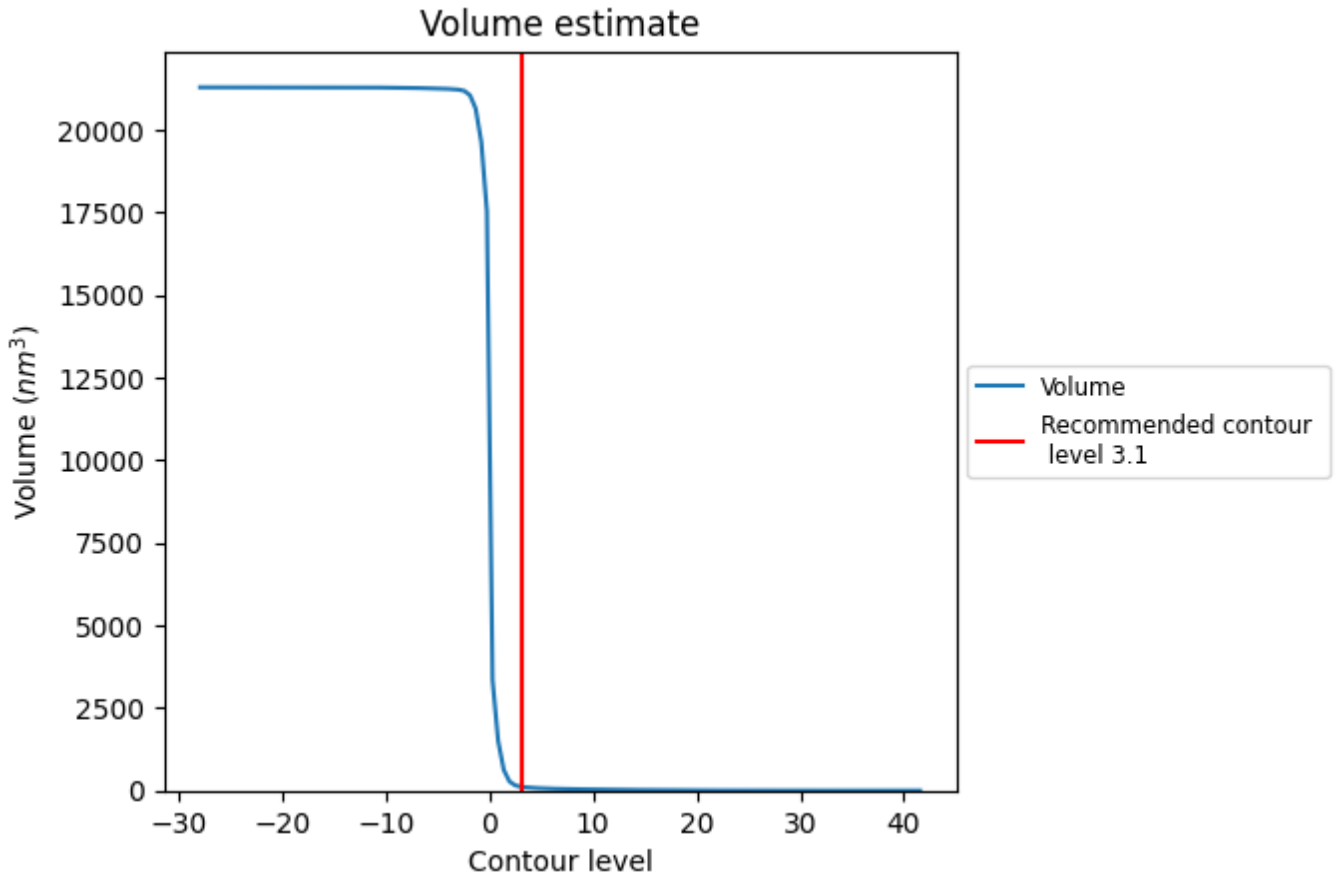
This section contains the results of statistical analysis of the map.

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.

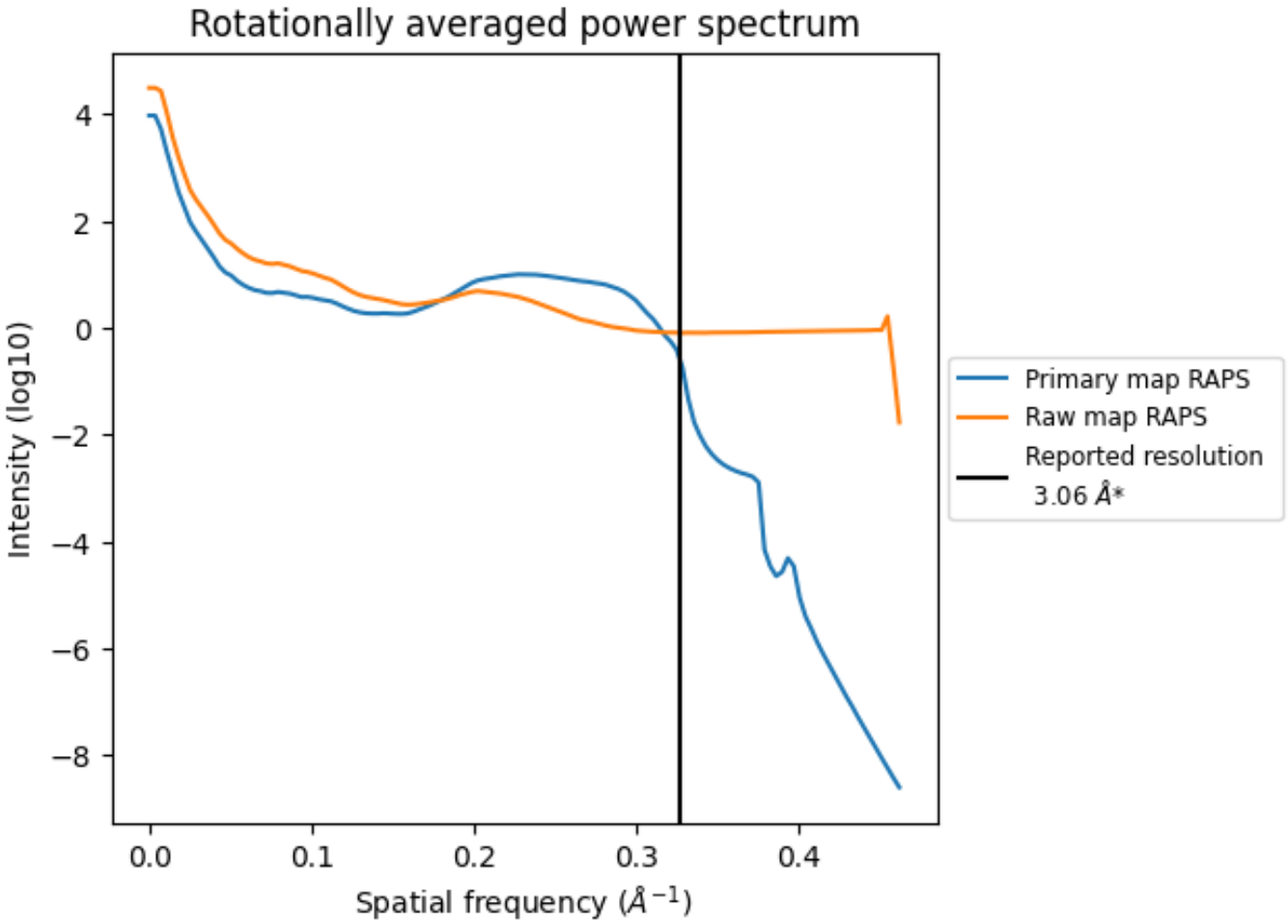
7.2 Volume estimate



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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)

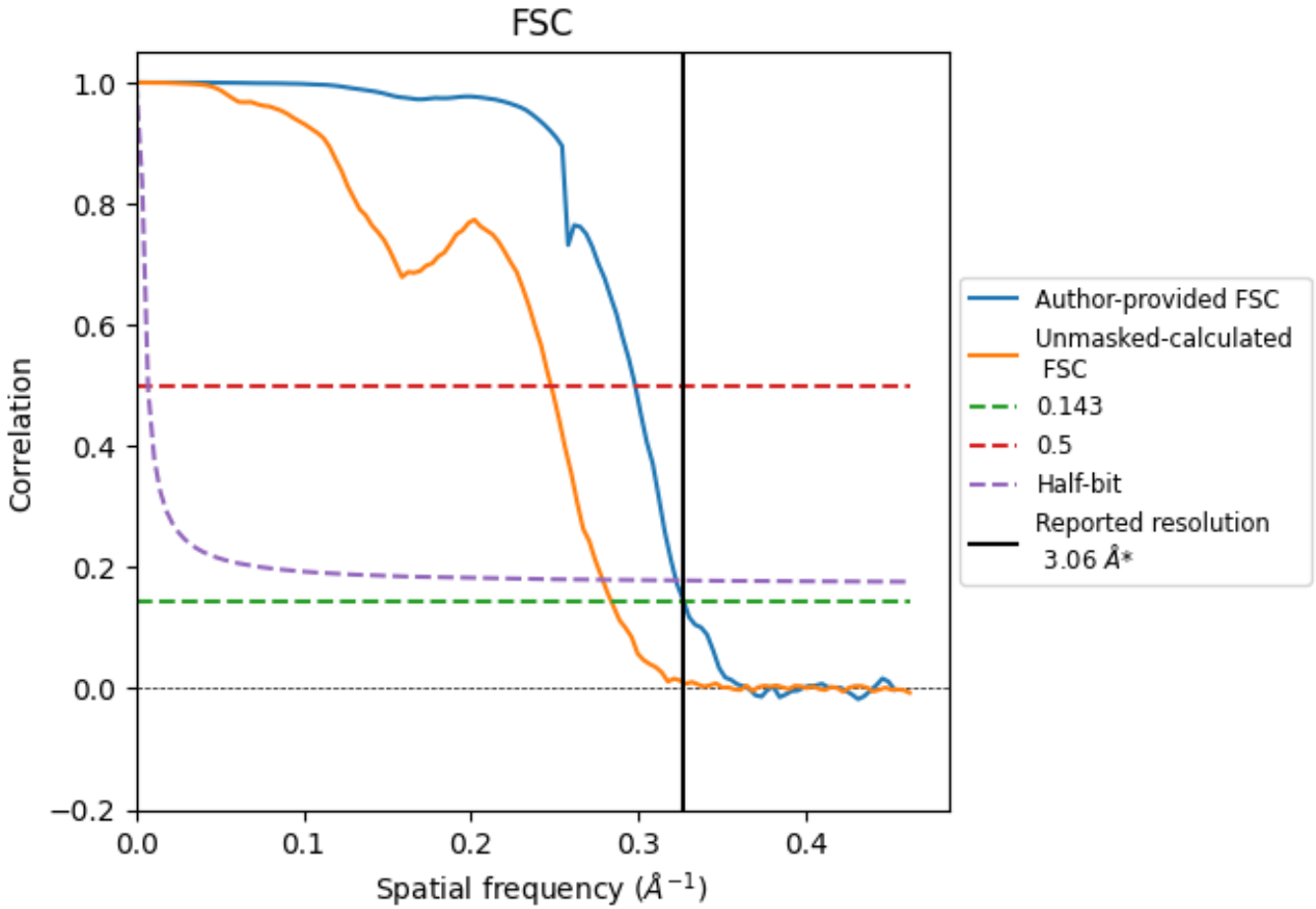


*Reported resolution corresponds to spatial frequency of 0.327 Å^{-1}

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 0.327 Å^{-1}

8.2 Resolution estimates (i)

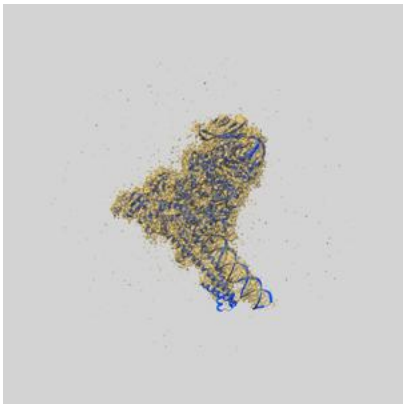
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.36	3.10
Unmasked-calculated*	3.52	4.04	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.52 differs from the reported value 3.06 by more than 10 %

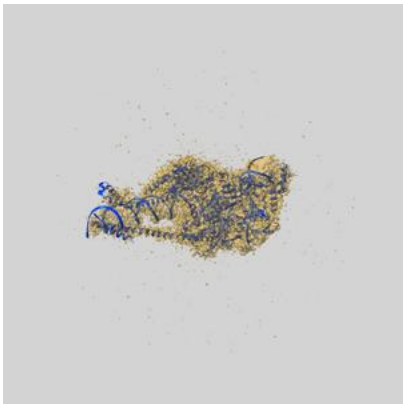
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40707 and PDB model 8SQJ. Per-residue inclusion information can be found in section 3 on page 7.

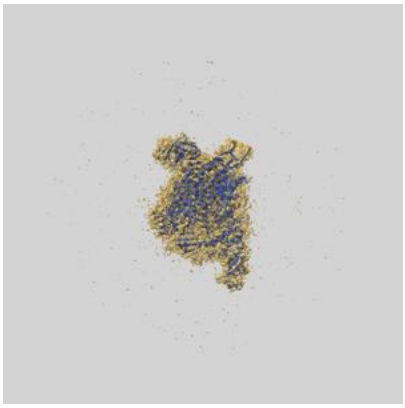
9.1 Map-model overlay



X



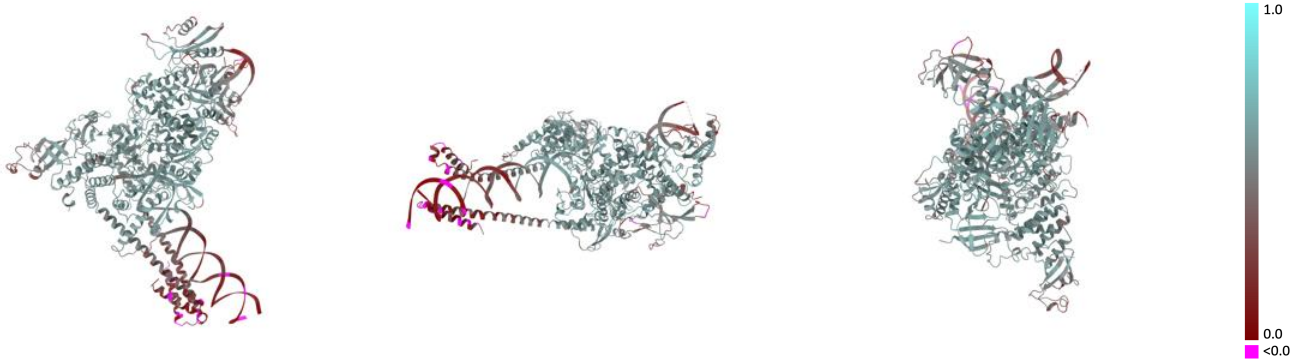
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.1 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.

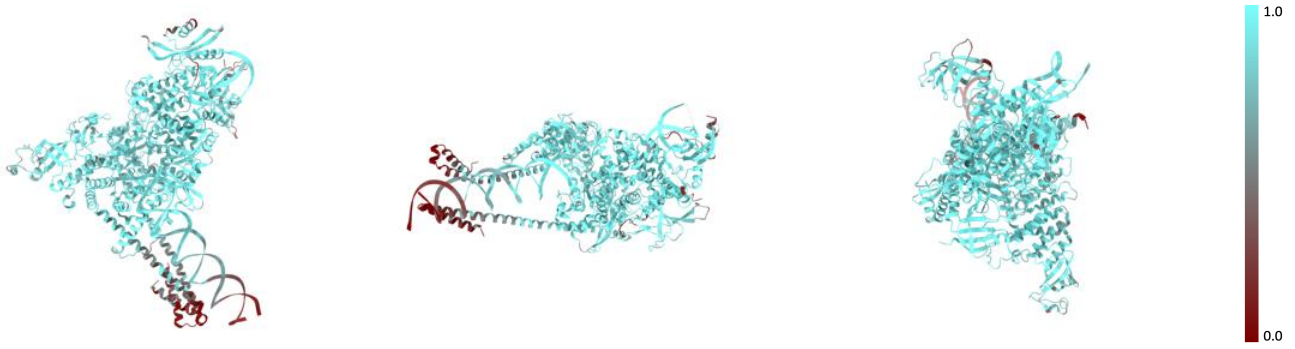
9.2 Q-score mapped to coordinate model (i)



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.

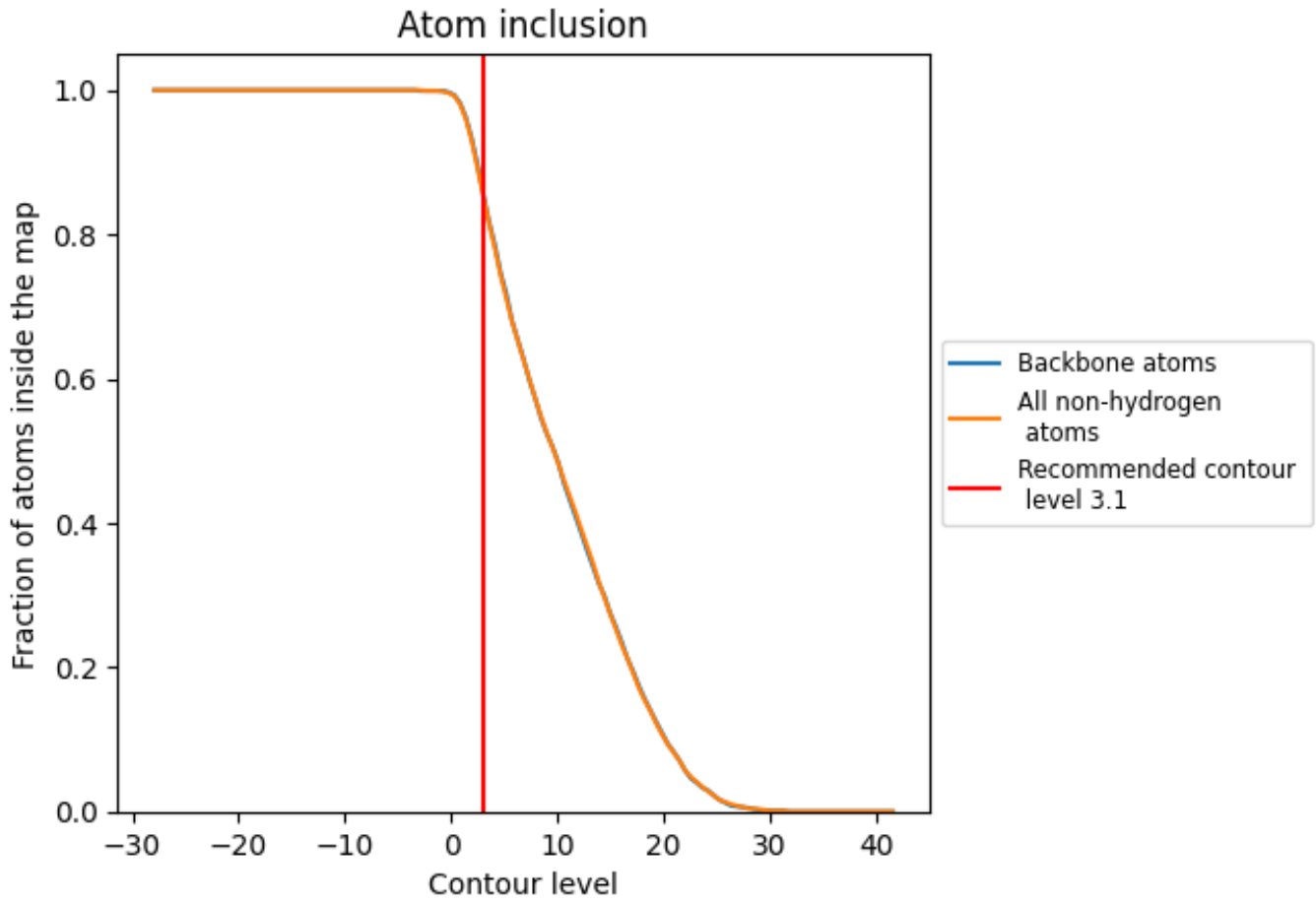
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.1).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.5110
A	0.9350	0.5860
B	0.7240	0.4390
C	0.8940	0.5580
D	0.7100	0.4310
G	0.7990	0.4550
O	0.8990	0.3840
P	0.6910	0.3250
T	0.6550	0.3010