



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:43 PM UTC

PDB ID : 9RAF / pdb_00009raf
EMDB ID : EMD-53876
Title : Influenza A/H7N9 polymerase in complex with a 70-mer template in stalled elongation with backtracking and stem.
Authors : Arragain, B.; Cusack, S.
Deposited on : 2025-05-20
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

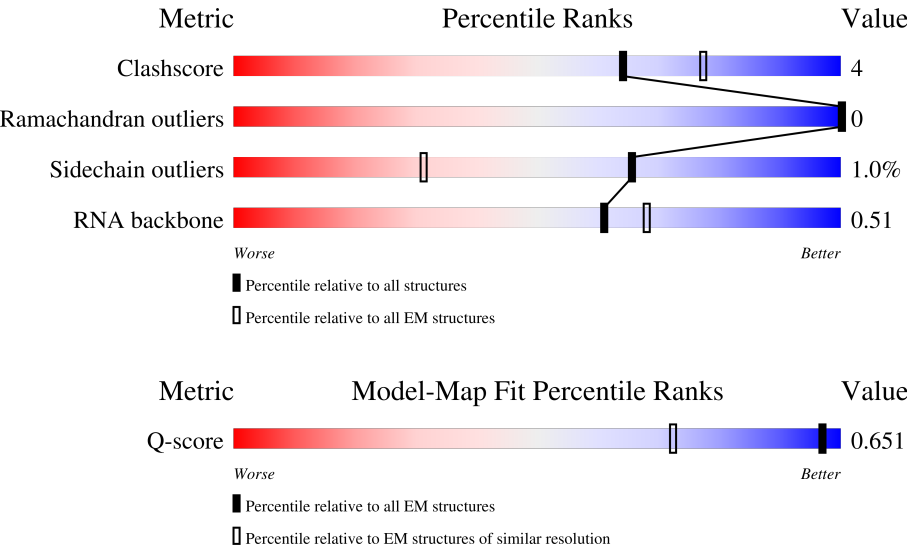
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.15 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	2551 (1.66 - 2.65)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	716	<div> <div>8%</div> <div>94%</div> <div>6%</div> </div>
2	C	788	<div> <div>30%</div> <div>68%</div> </div>
3	G	42	<div> <div>26%</div> <div>45%</div> <div>10%</div> <div>5%</div> <div>40%</div> </div>

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Mol	Chain	Length	Quality of chain
4	M	13	<div><div></div><div>8%</div><div>85%</div><div>8%</div><div>8%</div></div>
5	B	757	<div><div></div><div>5%</div><div>87%</div><div>9%</div><div></div></div>
6	T	70	<div><div></div><div>63%</div><div>46%</div><div>29%</div><div>26%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31095 atoms, of which 14762 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	716	Total	C	H	N	O	S	6	0
			11606	3692	5777	989	1107	41		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	LYS	GLU	engineered mutation	UNP M9TI86
A	490	ILE	ARG	engineered mutation	UNP M9TI86

- Molecule 2 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	250	Total	C	H	N	O	S	3	0
			4139	1288	2094	369	371	17		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	74	ARG	GLY	engineered mutation	UNP A0A024E1J5
C	760	GLY	-	expression tag	UNP A0A024E1J5
C	761	TRP	-	expression tag	UNP A0A024E1J5
C	762	SER	-	expression tag	UNP A0A024E1J5
C	763	HIS	-	expression tag	UNP A0A024E1J5
C	764	PRO	-	expression tag	UNP A0A024E1J5
C	765	GLN	-	expression tag	UNP A0A024E1J5
C	766	PHE	-	expression tag	UNP A0A024E1J5
C	767	GLU	-	expression tag	UNP A0A024E1J5
C	768	LYS	-	expression tag	UNP A0A024E1J5
C	769	GLY	-	expression tag	UNP A0A024E1J5
C	770	GLY	-	expression tag	UNP A0A024E1J5
C	771	GLY	-	expression tag	UNP A0A024E1J5
C	772	SER	-	expression tag	UNP A0A024E1J5
C	773	GLY	-	expression tag	UNP A0A024E1J5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	774	GLY	-	expression tag	UNP A0A024E1J5
C	775	GLY	-	expression tag	UNP A0A024E1J5
C	776	SER	-	expression tag	UNP A0A024E1J5
C	777	GLY	-	expression tag	UNP A0A024E1J5
C	778	GLY	-	expression tag	UNP A0A024E1J5
C	779	SER	-	expression tag	UNP A0A024E1J5
C	780	ALA	-	expression tag	UNP A0A024E1J5
C	781	TRP	-	expression tag	UNP A0A024E1J5
C	782	SER	-	expression tag	UNP A0A024E1J5
C	783	HIS	-	expression tag	UNP A0A024E1J5
C	784	PRO	-	expression tag	UNP A0A024E1J5
C	785	GLN	-	expression tag	UNP A0A024E1J5
C	786	PHE	-	expression tag	UNP A0A024E1J5
C	787	GLU	-	expression tag	UNP A0A024E1J5
C	788	LYS	-	expression tag	UNP A0A024E1J5

- Molecule 3 is a protein called RNA Pol II CTD 6 repeats (site 1A/2A).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	25	Total	C	H	N	O	P	0	0
			351	116	155	25	52	3		

- Molecule 4 is a RNA chain called RNA product.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	M	13	Total	C	H	N	O	P	0	0
			422	124	143	52	90	13		

- Molecule 5 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	725	Total	C	H	N	O	S	8	0
			11679	3672	5840	1028	1094	45		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	577	GLY	LYS	engineered mutation	UNP S5ME50

- Molecule 6 is a RNA chain called RNA template (70-mer).

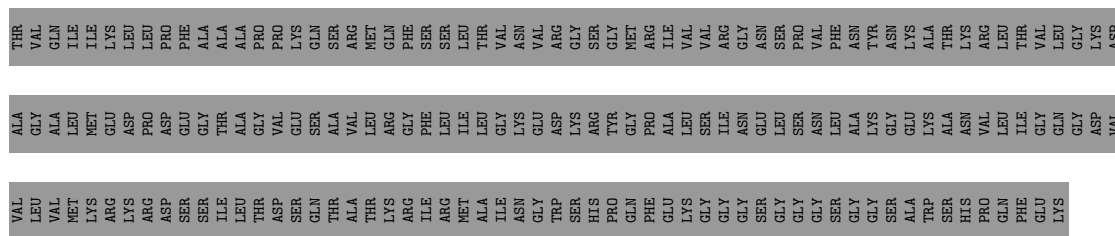
Mol	Chain	Residues	Atoms						AltConf	Trace
6	T	70	Total	C	H	N	O	P	0	0
			2243	665	753	262	493	70		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

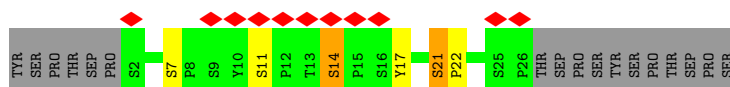
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	2	Total	Mg	0
			2	2	

- Molecule 8 is water.

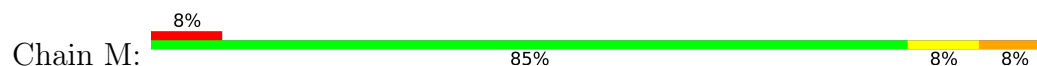
Mol	Chain	Residues	Atoms		AltConf
8	A	226	Total	O	0
			226	226	
8	C	54	Total	O	0
			54	54	
8	G	16	Total	O	0
			16	16	
8	M	19	Total	O	0
			19	19	
8	B	254	Total	O	0
			254	254	
8	T	83	Total	O	0
			83	83	



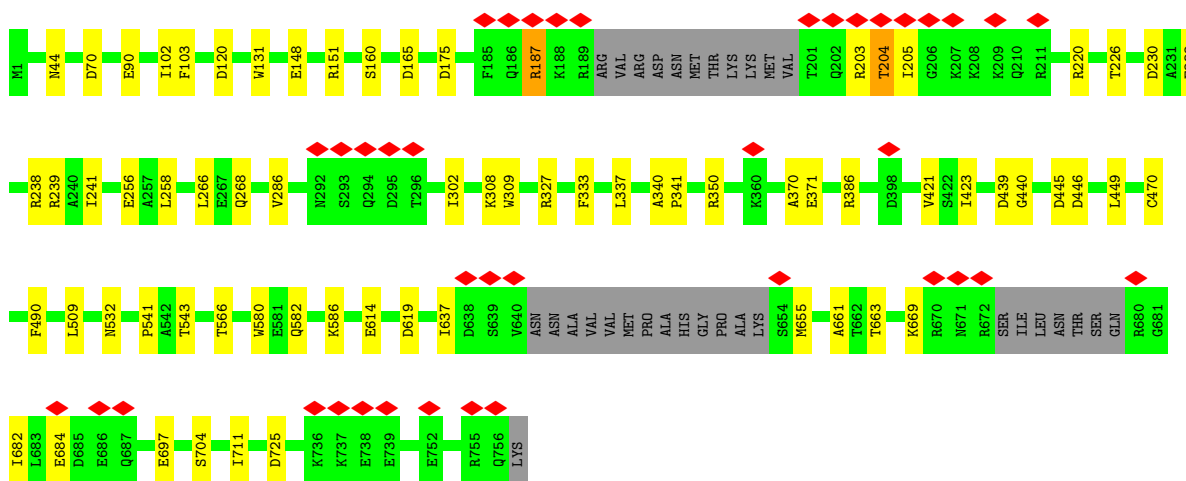
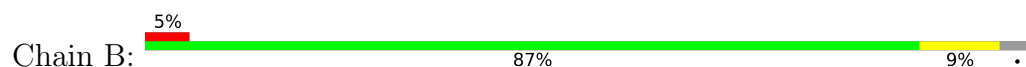
- Molecule 3: RNA Pol II CTD 6 repeats (site 1A/2A)



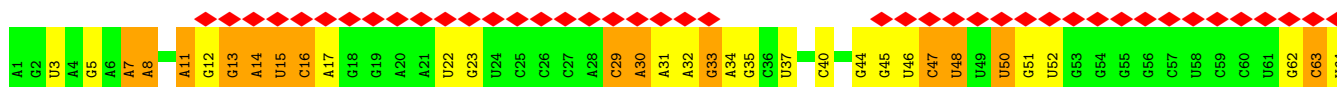
- Molecule 4: RNA product



- Molecule 5: RNA-directed RNA polymerase catalytic subunit



- Molecule 6: RNA template (70-mer)



165	166	167	168	169	170
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	195294	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 ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	4.697	Depositor
Minimum map value	-1.832	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	306.6, 306.6, 306.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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: SEP, 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	0.12	0/5974	0.23	0/8055
2	C	0.25	1/2093 (0.0%)	0.26	0/2821
3	G	0.12	0/173	0.23	0/235
4	M	0.14	0/311	0.18	0/483
5	B	0.12	0/5979	0.25	0/8055
6	T	0.13	0/1664	0.27	0/2589
All	All	0.15	1/16194 (0.0%)	0.25	0/22238

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	46	ARG	C-O	-9.39	1.13	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5829	5777	5754	33	0
2	C	2045	2094	2083	11	0
3	G	196	155	155	5	0
4	M	279	143	143	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5839	5840	5805	58	0
6	T	1490	753	753	34	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	A	226	0	0	9	0
8	B	254	0	0	17	0
8	C	54	0	0	2	0
8	G	16	0	0	3	0
8	M	19	0	0	0	0
8	T	83	0	0	9	0
All	All	16333	14762	14693	125	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 (125) 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:T:50:U:O2'	6:T:52:U:OP2	1.90	0.87
6:T:65:U:O2'	6:T:66:U:OP2	1.94	0.86
1:A:488:LYS:NZ	6:T:69:C:OP1	2.12	0.83
6:T:29:C:O2	6:T:51:G:N2	2.11	0.82
1:A:597:GLU:OE1	8:A:901:HOH:O	1.99	0.81
5:B:725:ASP:OD1	8:B:901:HOH:O	1.97	0.80
6:T:15:U:O2'	6:T:16:C:OP1	1.99	0.80
3:G:11:SER:OG	3:G:14:SEP:O1P	2.00	0.80
6:T:33:G:O2'	6:T:34:A:O4'	1.99	0.79
1:A:182:MET:HE1	1:A:191:PHE:CD2	2.17	0.79
6:T:3:U:O2'	8:T:102:HOH:O	2.03	0.76
6:T:44:G:OP2	8:T:101:HOH:O	2.03	0.76
1:A:267:PRO:O	8:A:902:HOH:O	2.05	0.74
5:B:582:GLN:OE1	8:B:902:HOH:O	2.05	0.74
3:G:17:TYR:OH	8:G:101:HOH:O	2.04	0.74
5:B:580:TRP:O	5:B:586:LYS:NZ	2.22	0.73
1:A:528:THR:OG1	8:A:903:HOH:O	2.06	0.72
6:T:37:U:O2	8:T:103:HOH:O	2.08	0.72
4:M:20:U:O2'	5:B:308:LYS:NZ	2.22	0.71
5:B:258:LEU:HD22	5:B:337[A]:LEU:HD13	1.73	0.71
5:B:44:ASN:O	8:B:903:HOH:O	2.09	0.70
6:T:29:C:N3	6:T:51:G:N1	2.34	0.70
5:B:160:SER:OG	5:B:165:ASP:OD2	2.02	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:697:GLU:OE2	6:T:45:G:N2	2.26	0.68
6:T:5:G:O6	8:T:104:HOH:O	2.10	0.68
2:C:50[B]:MET:SD	8:C:854:HOH:O	2.51	0.68
5:B:371:GLU:OE2	8:B:905:HOH:O	2.12	0.67
6:T:8:A:OP2	8:T:106:HOH:O	2.12	0.67
5:B:187:ARG:N	5:B:204:THR:O	2.28	0.67
5:B:661:ALA:O	8:B:904:HOH:O	2.11	0.66
4:M:21:C:N4	5:B:238:ARG:O	2.24	0.66
1:A:365:GLN:OE1	8:A:905:HOH:O	2.13	0.66
1:A:1:MET:HE1	1:A:182:MET:HE3	1.78	0.65
2:C:147:ILE:HD11	2:C:214:LYS:HD2	1.78	0.65
1:A:6:ARG:NH2	1:A:18:GLU:OE2	2.30	0.64
6:T:67:U:O2	8:T:105:HOH:O	2.11	0.64
5:B:327:ARG:NH1	8:B:916:HOH:O	2.30	0.64
2:C:19:ILE:HD11	5:B:684:GLU:HG2	1.80	0.64
6:T:3:U:OP2	8:T:107:HOH:O	2.16	0.63
5:B:386:ARG:NH1	8:B:920:HOH:O	2.32	0.63
5:B:258:LEU:HD22	5:B:337[B]:LEU:HD23	1.81	0.62
5:B:230:ASP:N	8:B:915:HOH:O	2.30	0.61
1:A:427:GLU:N	1:A:427:GLU:OE1	2.33	0.61
5:B:566:THR:OG1	8:B:906:HOH:O	2.16	0.61
6:T:29:C:O2'	6:T:30:A:N7	2.32	0.59
5:B:256:GLU:OE1	8:B:908:HOH:O	2.17	0.59
1:A:670:GLN:OE1	8:A:906:HOH:O	2.16	0.58
5:B:204:THR:HG22	5:B:205:ILE:H	1.68	0.58
1:A:362:LYS:NZ	1:A:478:ASP:O	2.29	0.58
3:G:21:SEP:O3P	8:G:103:HOH:O	2.17	0.58
3:G:21:SEP:O3P	8:G:102:HOH:O	2.17	0.58
5:B:226:THR:OG1	5:B:350[A]:ARG:O	2.18	0.57
5:B:232:GLU:OE2	5:B:239:ARG:NH2	2.36	0.57
5:B:440:GLY:O	8:B:907:HOH:O	2.17	0.57
5:B:226:THR:OG1	5:B:350[B]:ARG:O	2.18	0.57
5:B:232:GLU:OE1	8:B:910:HOH:O	2.18	0.57
5:B:175:ASP:OD1	8:B:909:HOH:O	2.17	0.56
5:B:423:ILE:HG21	5:B:470:CYS:SG	2.46	0.55
1:A:182:MET:HE1	1:A:191:PHE:CG	2.41	0.55
1:A:350:ASN:O	1:A:350:ASN:ND2	2.39	0.55
2:C:32:LYS:NZ	5:B:697:GLU:OE2	2.33	0.55
1:A:124:ARG:NH2	1:A:195:GLU:OE1	2.39	0.55
6:T:70:U:O3'	8:T:108:HOH:O	2.18	0.54
1:A:19:LYS:HE2	5:B:711:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:148:GLU:OE1	5:B:151:ARG:NH1	2.41	0.53
1:A:310:CYS:O	1:A:313:THR:OG1	2.24	0.53
1:A:300:GLU:OE1	6:T:70:U:O2'	2.26	0.53
5:B:258:LEU:HD22	5:B:337[B]:LEU:CD2	2.39	0.52
5:B:70:ASP:OD1	8:B:912:HOH:O	2.19	0.52
1:A:593:GLU:OE1	5:B:543:THR:OG1	2.20	0.52
5:B:286:VAL:HG21	5:B:490:PHE:CE1	2.46	0.51
5:B:637:ILE:HD12	5:B:655:MET:HB3	1.93	0.50
2:C:55:TYR:O	5:B:669:LYS:NZ	2.44	0.50
5:B:340:ALA:HB3	5:B:341:PRO:HD3	1.93	0.50
1:A:439:ALA:HB2	5:B:541:PRO:HB2	1.93	0.50
6:T:13:G:O2'	6:T:14:A:O5'	2.27	0.50
5:B:239:ARG:NH2	8:B:929:HOH:O	2.43	0.50
5:B:532:ASN:ND2	8:B:933:HOH:O	2.45	0.50
5:B:90:GLU:OE2	8:B:911:HOH:O	2.19	0.50
5:B:619:ASP:OD1	5:B:619:ASP:N	2.45	0.50
5:B:704:SER:OG	6:T:45:G:N1	2.45	0.50
6:T:47:C:H2'	6:T:48:U:O4'	2.11	0.49
6:T:62:G:H2'	6:T:63:C:O4'	2.12	0.49
5:B:697:GLU:CD	6:T:45:G:H22	2.20	0.49
1:A:326:HIS:N	1:A:331:ASN:OD1	2.42	0.48
1:A:538:GLU:O	8:A:907:HOH:O	2.20	0.48
2:C:99:TRP:CD1	5:B:663:THR:HG21	2.49	0.48
1:A:308:ILE:HD11	1:A:348:ILE:HD12	1.96	0.47
1:A:182:MET:HE1	1:A:191:PHE:CB	2.44	0.47
2:C:154:LEU:HD11	2:C:185:ILE:HD13	1.97	0.47
6:T:65:U:HO2'	6:T:66:U:P	2.30	0.47
6:T:17:A:C4	6:T:62:G:N2	2.83	0.47
6:T:7:A:O2'	6:T:8:A:OP2	2.29	0.46
5:B:704:SER:HG	6:T:45:G:H1	1.61	0.45
1:A:127:VAL:HG12	1:A:155:MET:HE3	1.98	0.45
6:T:29:C:H5'	6:T:30:A:OP1	2.16	0.45
2:C:67:ILE:HD11	2:C:99:TRP:HE3	1.83	0.44
1:A:393:TYR:O	8:A:908:HOH:O	2.20	0.44
5:B:203:ARG:HB2	6:T:51:G:OP1	2.17	0.44
5:B:268:GLN:NE2	5:B:439:ASP:OD1	2.44	0.43
5:B:241:ILE:HD12	6:T:35:G:C8	2.52	0.43
5:B:302:ILE:HD12	5:B:449:LEU:HD23	1.98	0.43
2:C:171:GLU:OE1	8:C:801:HOH:O	2.21	0.43
2:C:2:GLU:O	2:C:6:GLU:HG3	2.19	0.43
6:T:40:C:OP1	8:T:109:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:HA	1:A:155:MET:HE1	2.01	0.42
1:A:550:LEU:HD12	3:G:22:PRO:HB2	2.01	0.42
6:T:11:A:H2'	6:T:12:G:O4'	2.19	0.42
5:B:286:VAL:HG21	5:B:490:PHE:HE1	1.85	0.42
1:A:331:ASN:N	1:A:332:PRO:CD	2.83	0.42
6:T:31:A:H2'	6:T:32:A:C5	2.55	0.42
1:A:587:GLN:HB2	5:B:509:LEU:HD11	2.02	0.41
1:A:19:LYS:NZ	8:A:944:HOH:O	2.52	0.41
1:A:309:LYS:O	1:A:313:THR:HG23	2.20	0.41
1:A:288:LEU:HD21	1:A:548:MET:HE1	2.02	0.41
5:B:333:PHE:CZ	5:B:337[A]:LEU:HD11	2.56	0.41
5:B:131:TRP:O	5:B:220:ARG:NH1	2.48	0.41
5:B:266:LEU:HD13	5:B:421:VAL:HG11	2.03	0.41
1:A:442:ARG:NH2	1:A:606:ASP:OD2	2.50	0.41
5:B:102:ILE:HG23	5:B:103:PHE:N	2.36	0.41
6:T:65:U:C2'	6:T:66:U:OP2	2.68	0.41
5:B:309:TRP:CG	5:B:445:ASP:HB3	2.56	0.41
2:C:147:ILE:HD11	2:C:214:LYS:CD	2.47	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	720/716 (101%)	707 (98%)	13 (2%)	0	100	100
2	C	251/788 (32%)	249 (99%)	2 (1%)	0	100	100
3	G	20/42 (48%)	18 (90%)	2 (10%)	0	100	100
5	B	725/757 (96%)	713 (98%)	12 (2%)	0	100	100
All	All	1716/2303 (74%)	1687 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/645 (101%)	645 (99%)	6 (1%)	70	77
2	C	227/686 (33%)	224 (99%)	3 (1%)	61	68
3	G	22/36 (61%)	22 (100%)	0	100	100
5	B	647/667 (97%)	641 (99%)	6 (1%)	70	77
All	All	1547/2034 (76%)	1532 (99%)	15 (1%)	65	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	GLU
1	A	184	SER
1	A	237	GLU
1	A	353	LYS
1	A	550	LEU
1	A	700	VAL
2	C	16	THR
2	C	83	ASP
2	C	217	PHE
5	B	120	ASP
5	B	187	ARG
5	B	204	THR
5	B	446	ASP
5	B	614	GLU
5	B	682	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	346	GLN
1	A	519	ASN
5	B	367	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	375	ASN
5	B	428	GLN
5	B	690	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	12/13 (92%)	1 (8%)	0
6	T	69/70 (98%)	19 (27%)	4 (5%)
All	All	81/83 (97%)	20 (24%)	4 (4%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	20	U
6	T	7	A
6	T	8	A
6	T	11	A
6	T	14	A
6	T	16	C
6	T	22	U
6	T	23	G
6	T	29	C
6	T	30	A
6	T	33	G
6	T	47	C
6	T	48	U
6	T	50	U
6	T	63	C
6	T	64	U
6	T	65	U
6	T	66	U
6	T	69	C
6	T	70	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	T	13	G
6	T	15	U
6	T	46	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	65	U

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

3 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
3	SEP	G	21	3	8,9,10	1.56	1 (12%)	7,12,14	1.31	1 (14%)
3	SEP	G	14	3	8,9,10	1.62	1 (12%)	7,12,14	1.52	1 (14%)
3	SEP	G	7	3	8,9,10	1.57	1 (12%)	7,12,14	1.29	1 (14%)

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
3	SEP	G	21	3	-	0/6/8/10	-
3	SEP	G	14	3	-	4/6/8/10	-
3	SEP	G	7	3	-	3/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	14	SEP	P-O1P	3.56	1.61	1.50
3	G	21	SEP	P-O1P	3.44	1.61	1.50
3	G	7	SEP	P-O1P	3.43	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	14	SEP	OG-CB-CA	3.41	111.47	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	21	SEP	OG-CB-CA	2.74	110.81	108.14
3	G	7	SEP	OG-CB-CA	2.71	110.78	108.14

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	7	SEP	C-CA-CB-OG
3	G	14	SEP	N-CA-CB-OG
3	G	14	SEP	C-CA-CB-OG
3	G	14	SEP	CA-CB-OG-P
3	G	7	SEP	N-CA-CB-OG
3	G	14	SEP	CB-OG-P-O2P
3	G	7	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	21	SEP	2	0
3	G	14	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

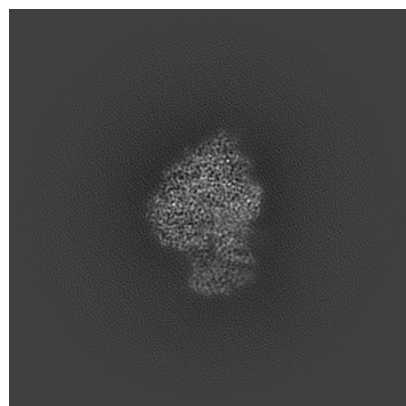
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53876. These allow visual inspection of the internal detail of the map and identification of artifacts.

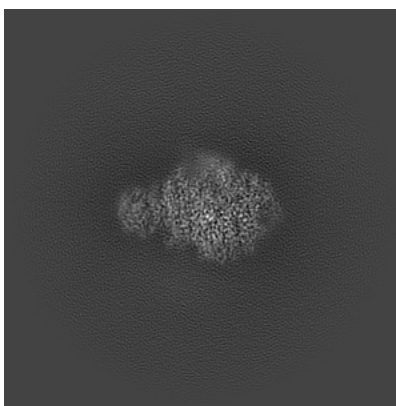
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

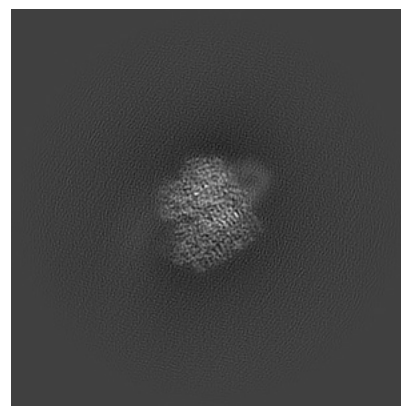
6.1.1 Primary map



X

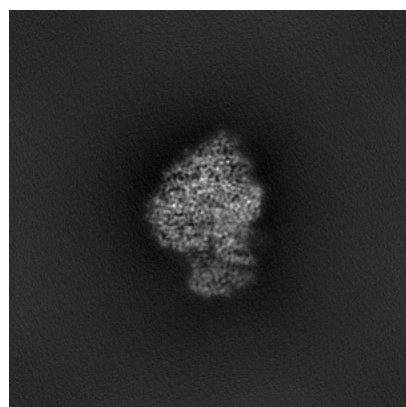


Y

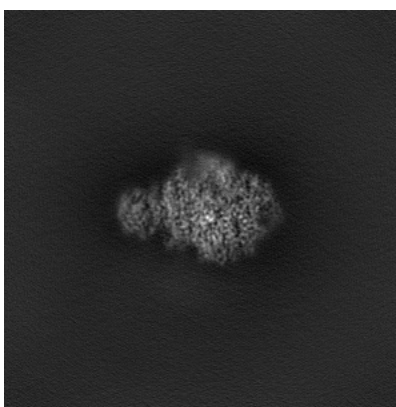


Z

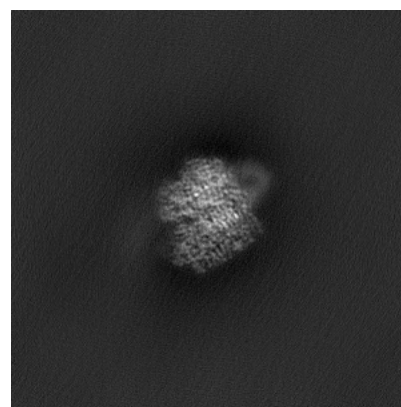
6.1.2 Raw map



X



Y

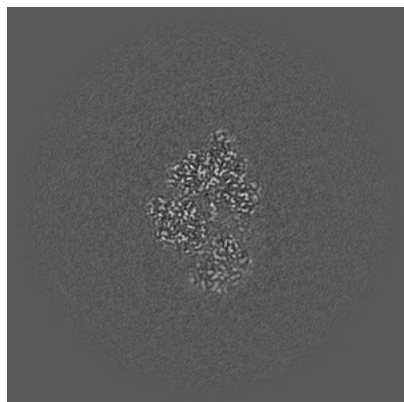


Z

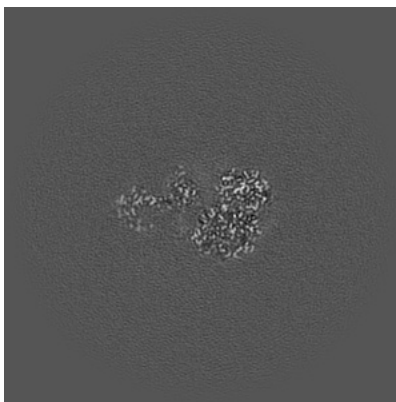
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

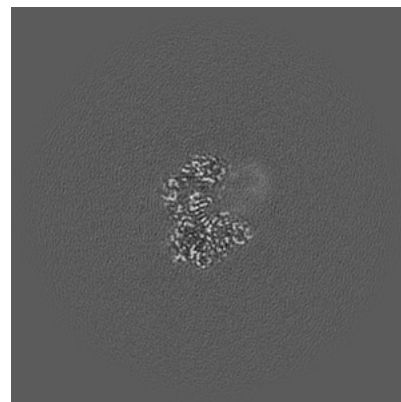
6.2.1 Primary map



X Index: 210

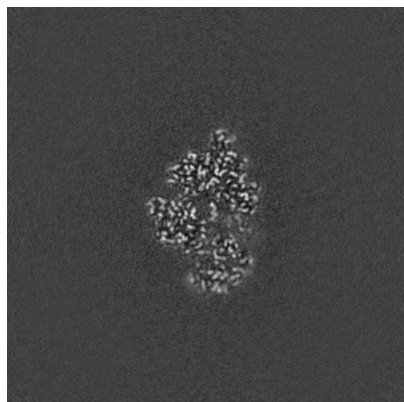


Y Index: 210

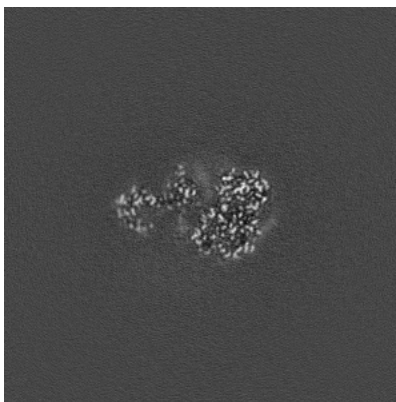


Z Index: 210

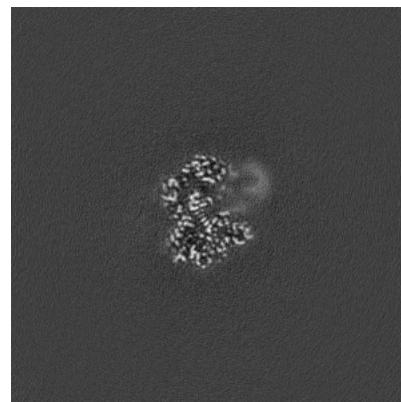
6.2.2 Raw map



X Index: 210



Y Index: 210

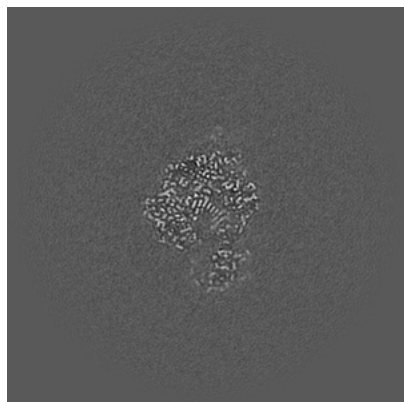


Z Index: 210

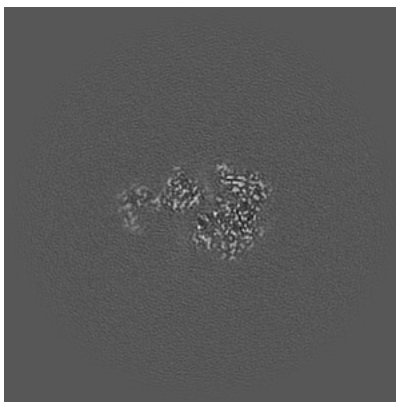
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

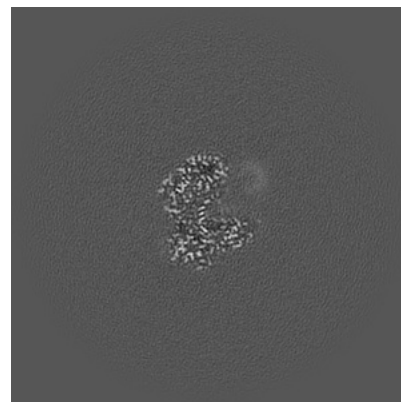
6.3.1 Primary map



X Index: 200

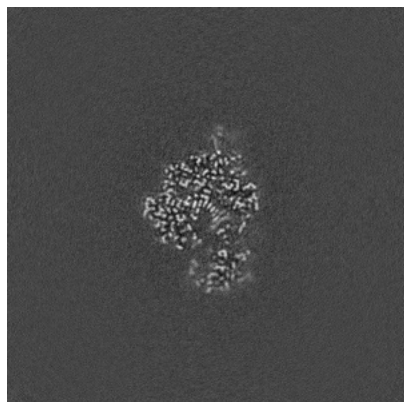


Y Index: 205

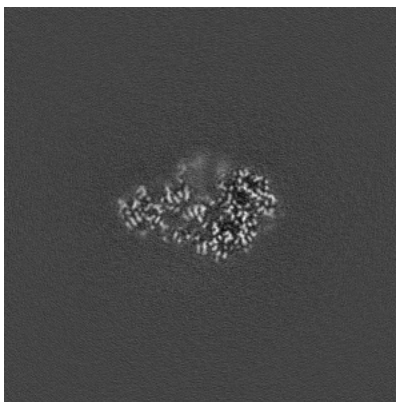


Z Index: 215

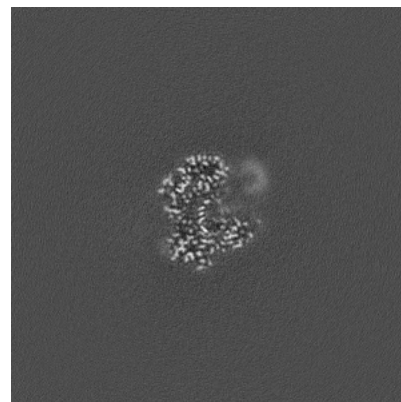
6.3.2 Raw map



X Index: 201



Y Index: 218

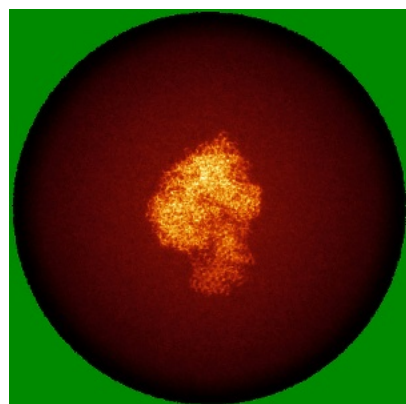


Z Index: 215

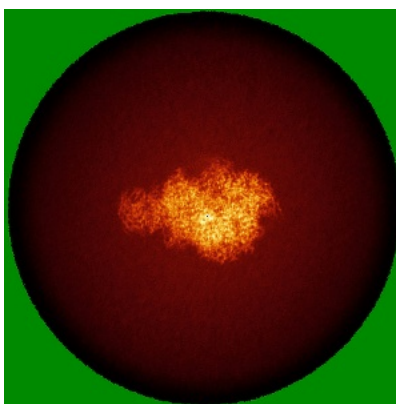
The images above show the largest variance slices of the map in three orthogonal directions.

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

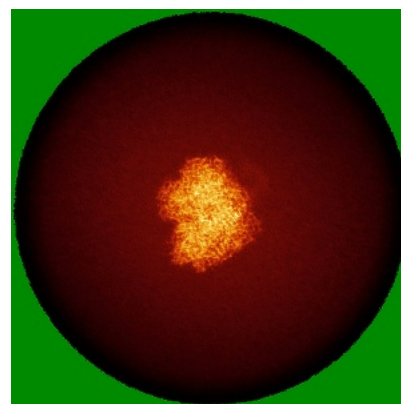
6.4.1 Primary map



X

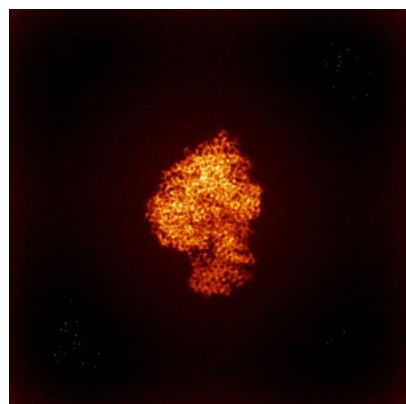


Y

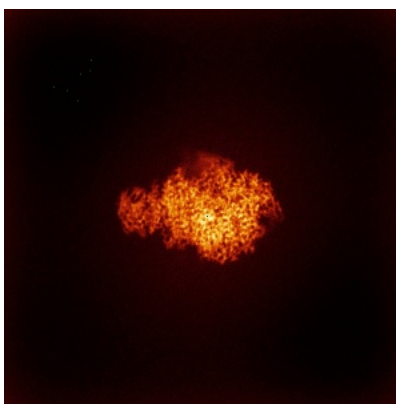


Z

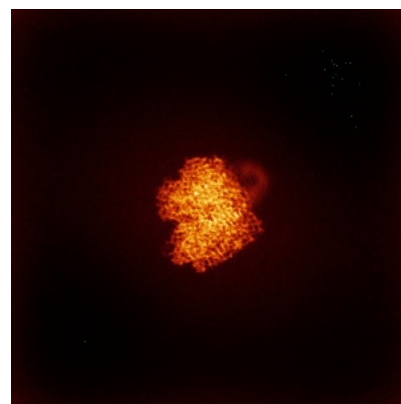
6.4.2 Raw map



X



Y

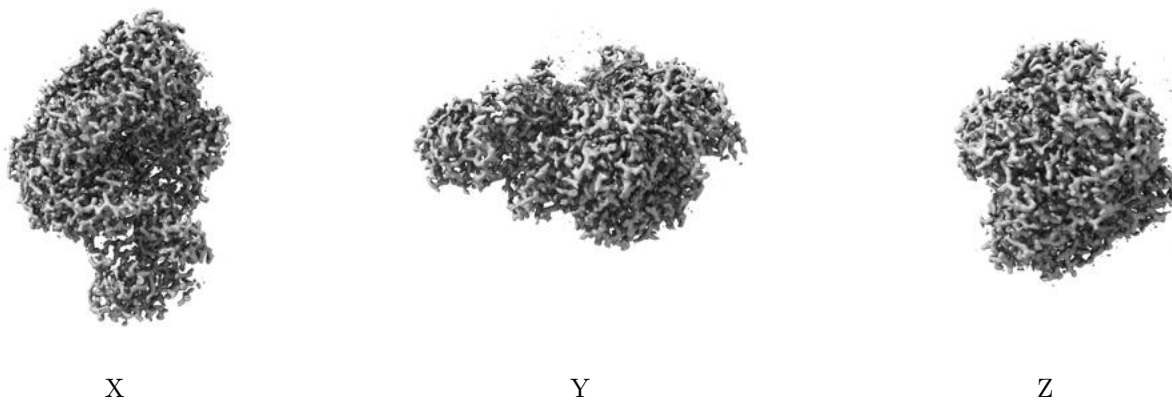


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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



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.

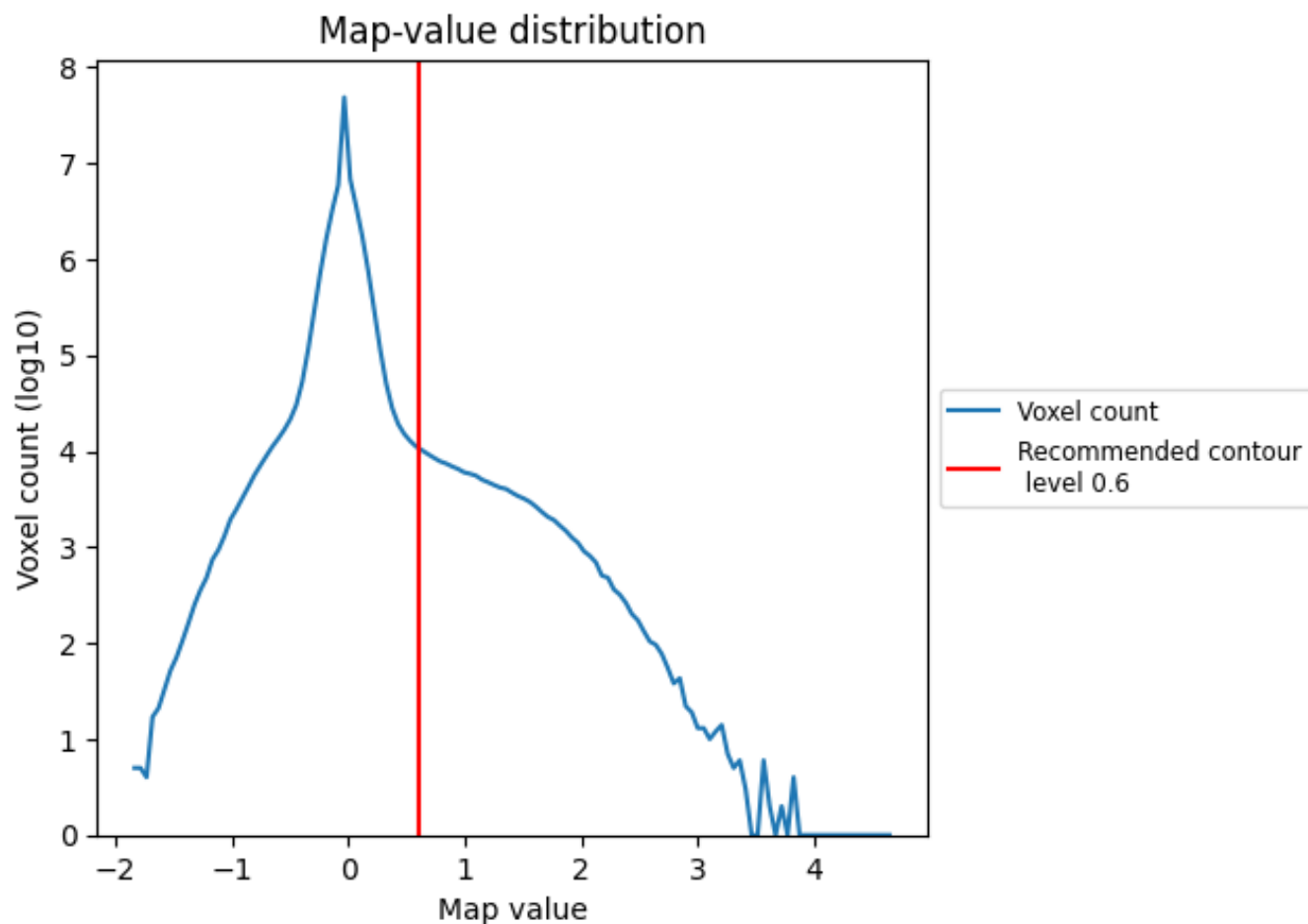
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

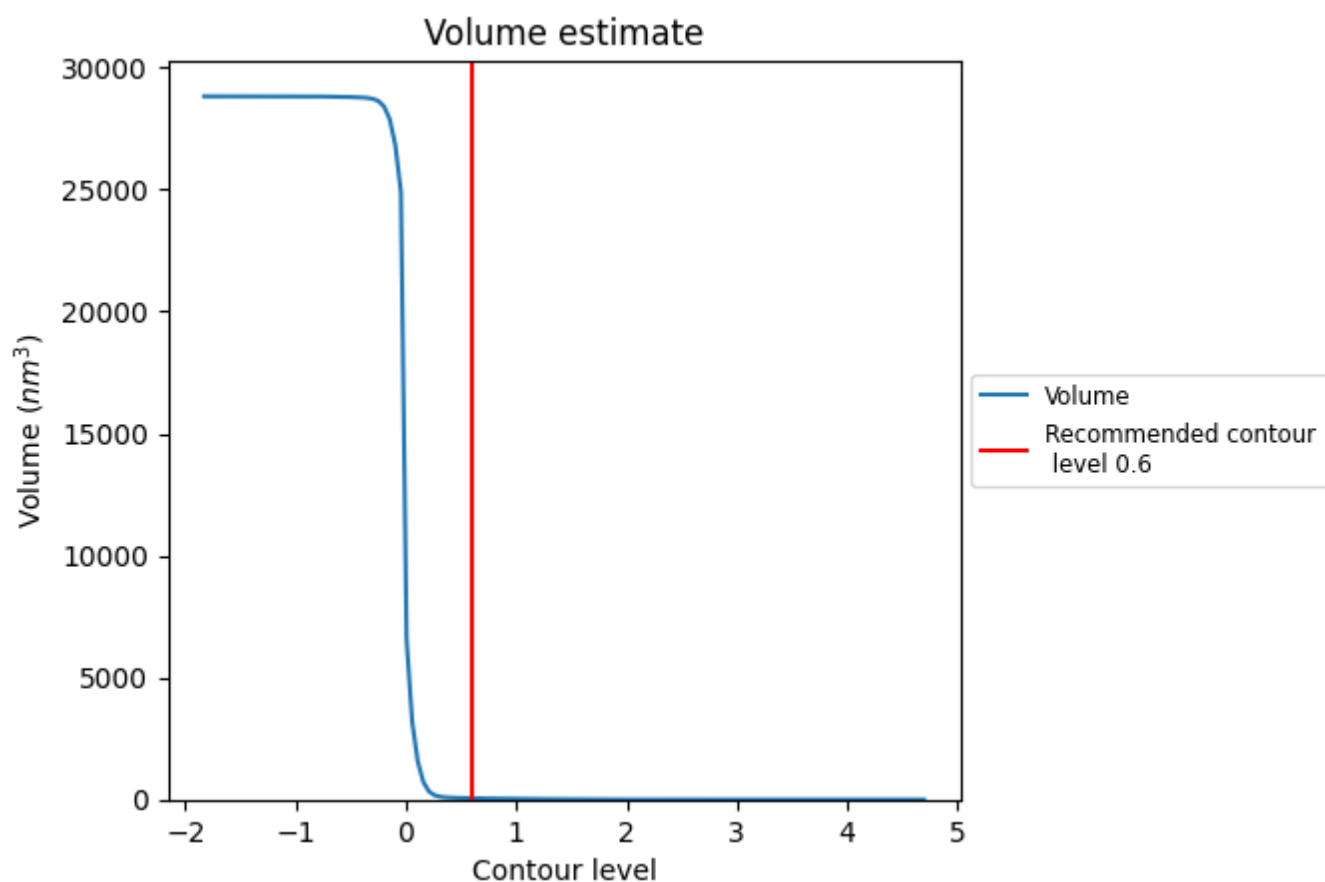
This section contains the results of statistical analysis of the map.

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.

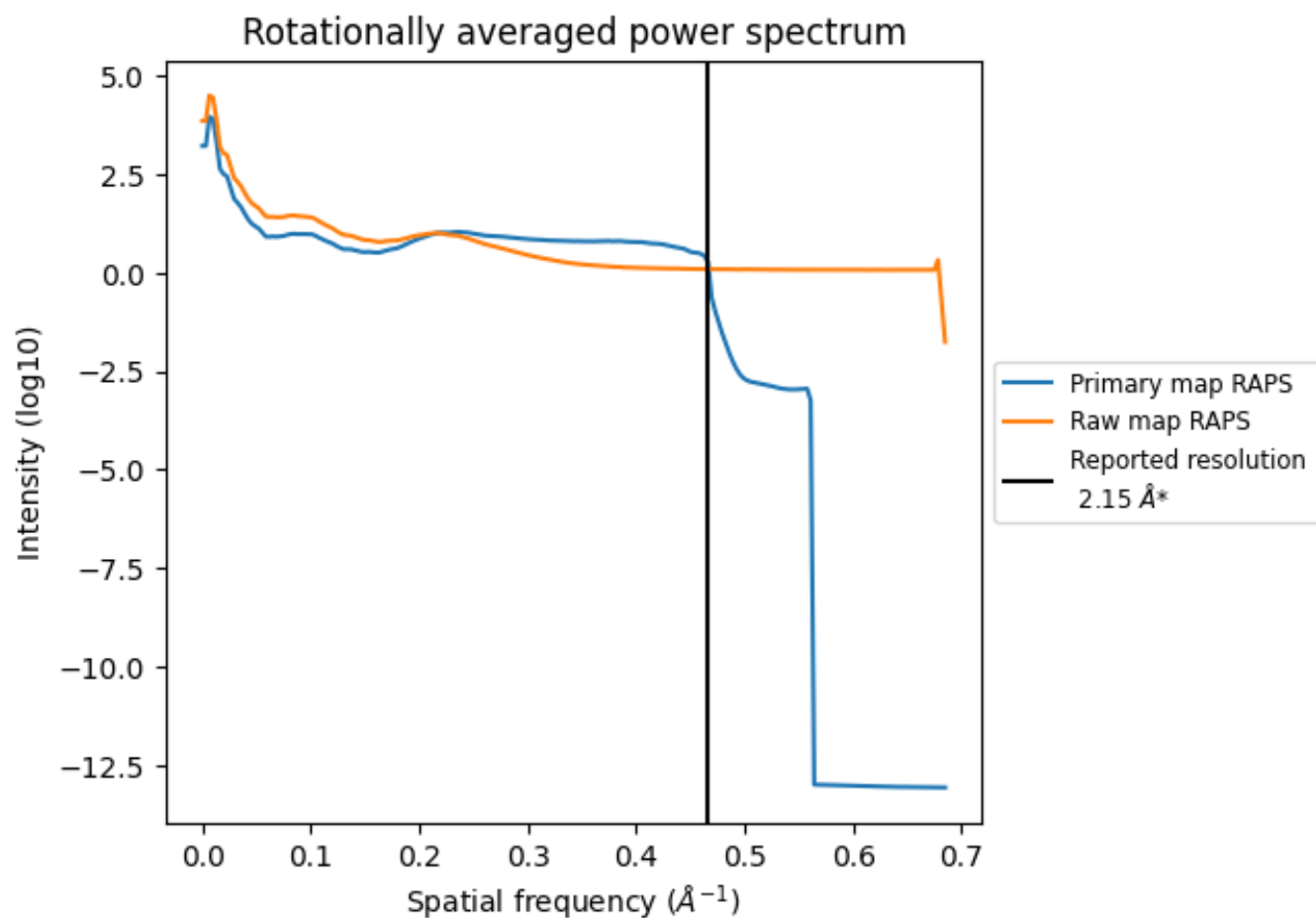
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53 nm³; this corresponds to an approximate mass of 48 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

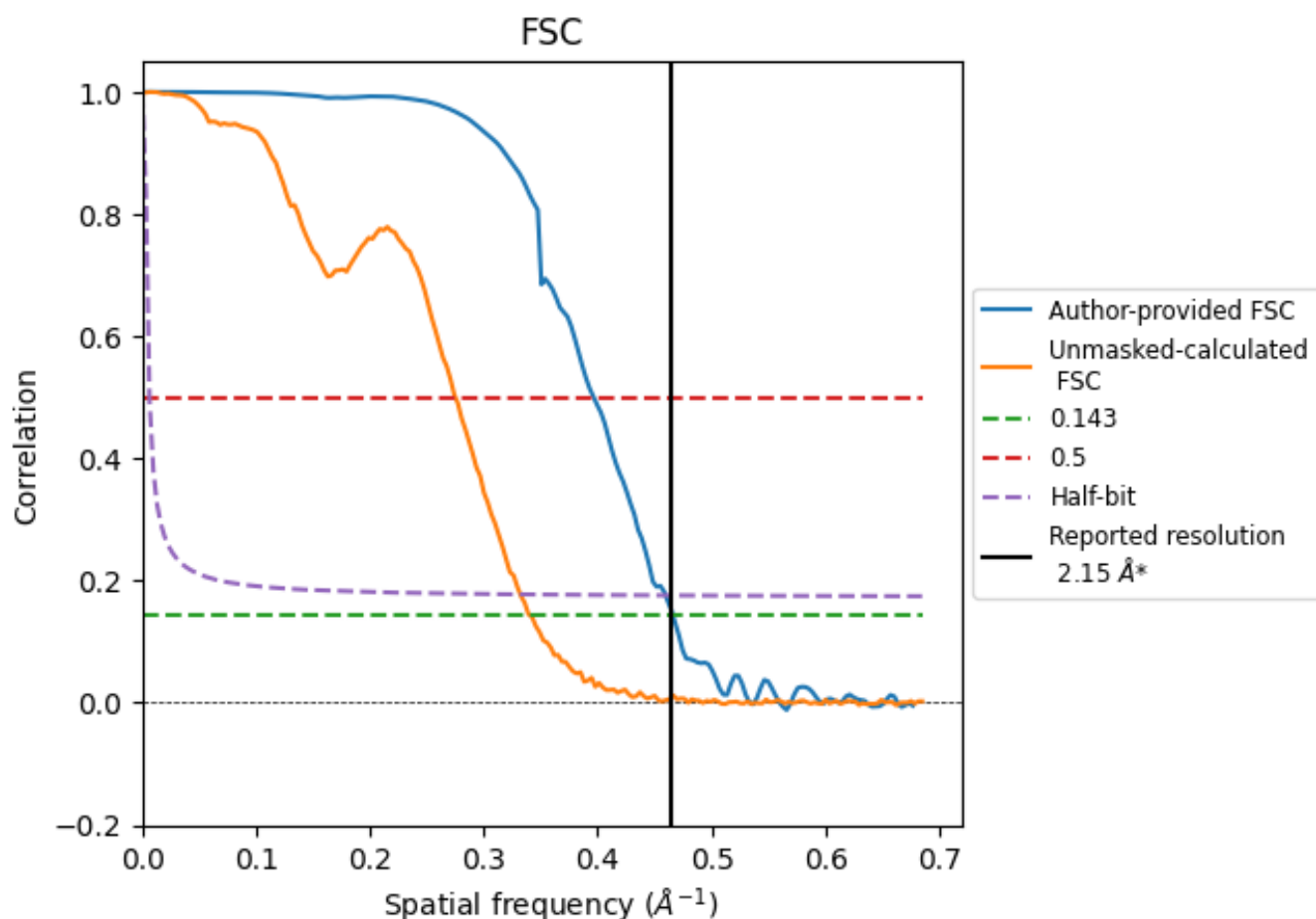


*Reported resolution corresponds to spatial frequency of 0.465 Å⁻¹

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 0.465 \AA^{-1}

8.2 Resolution estimates [i](#)

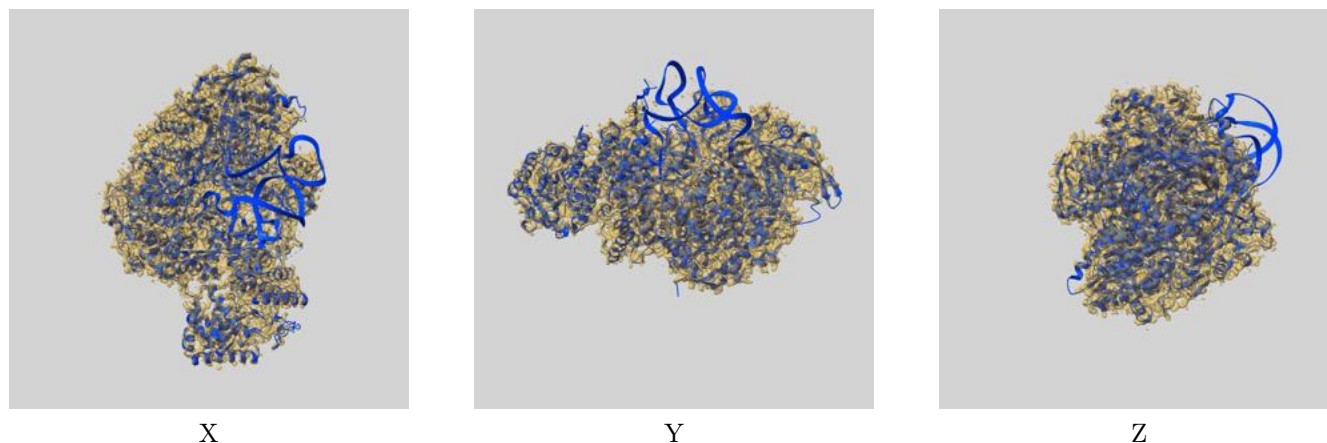
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.15	2.52	2.18
Unmasked-calculated*	2.94	3.64	3.01

*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 2.94 differs from the reported value 2.15 by more than 10 %

9 Map-model fit [i](#)

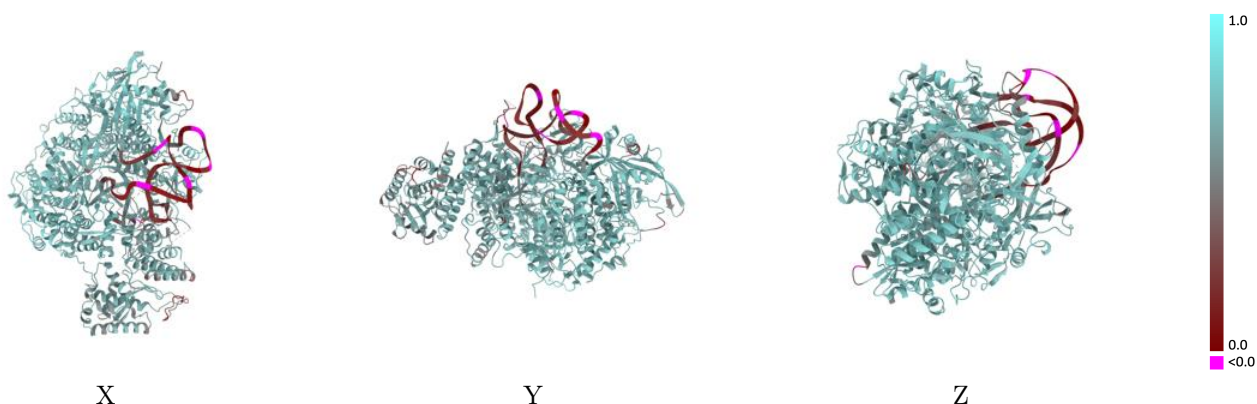
This section contains information regarding the fit between EMDB map EMD-53876 and PDB model 9RAF. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



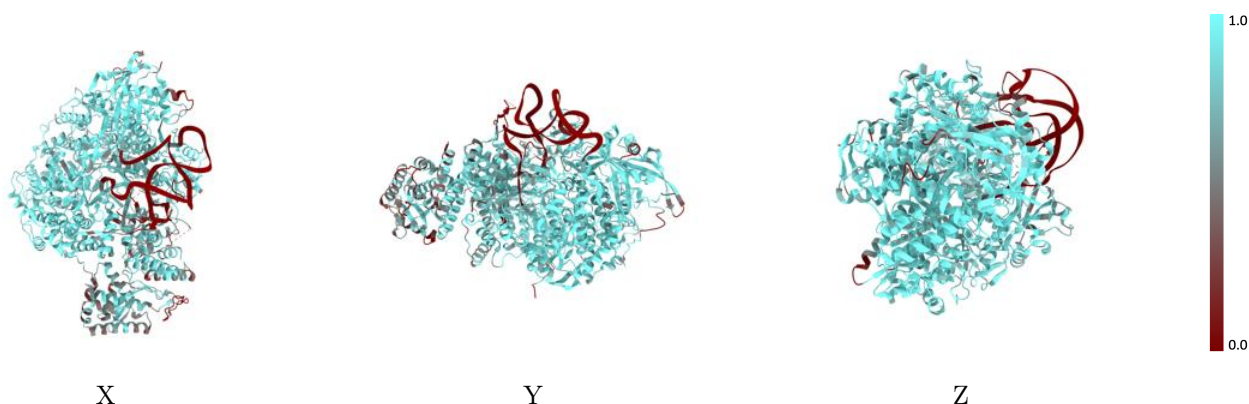
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



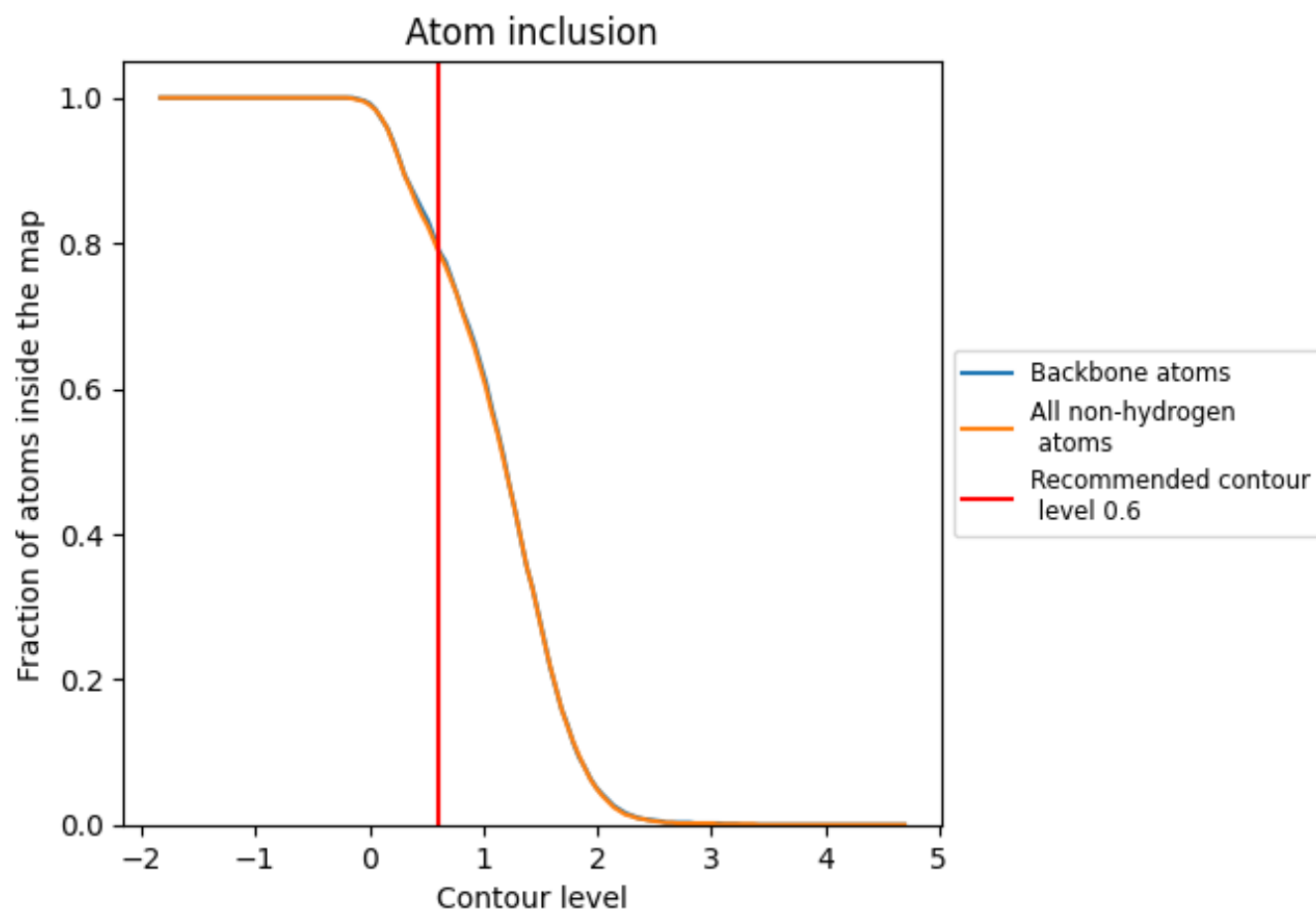
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7910	<div><div></div></div> 0.6510
A	<div><div></div></div> 0.8200	<div><div></div></div> 0.6770
B	<div><div></div></div> 0.8800	<div><div></div></div> 0.6980
C	<div><div></div></div> 0.8170	<div><div></div></div> 0.6700
G	<div><div></div></div> 0.5780	<div><div></div></div> 0.5810
M	<div><div></div></div> 0.7810	<div><div></div></div> 0.6310
T	<div><div></div></div> 0.3570	<div><div></div></div> 0.3560

1.0

0.0

<0.0