



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:27 AM UTC

PDB ID : 9OS2 / pdb_00009os2
EMDB ID : EMD-70791
Title : Cryo-EM structure of the DDB1/CRBN-MRT-5702-G3BP2 ternary complex
Authors : Quan, C.; Petzold, G.; Gainza, P.; Tsai, J.; Bunker, R.D.; Wiedmer, L.; Donckele, E.J.
Deposited on : 2025-05-23
Resolution : 2.50 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

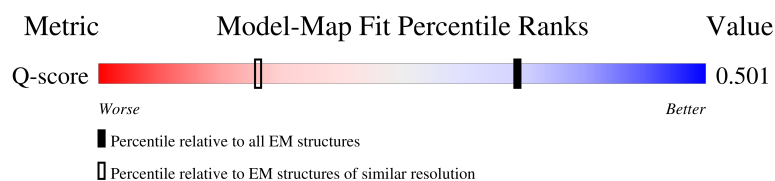
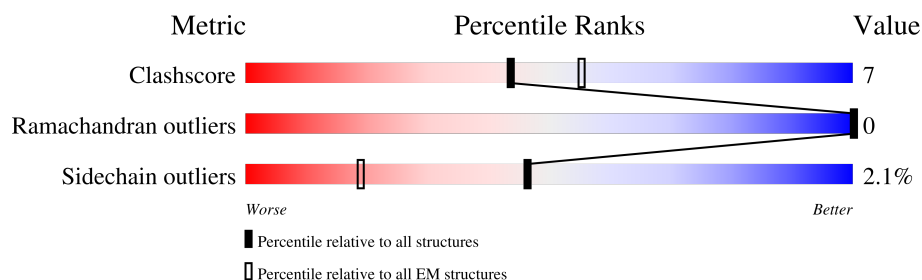
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	B	378	 5% 74% 22% ..
2	A	1140	 60% 9% 31%
3	C	482	 5% 21% 5% 74%
3	D	482	 15% 21% . 74%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	369	Total	C	N	O	S	0	0
			2912	1859	492	538	23		

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	790	Total	C	N	O	S	0	0
			6169	3918	1031	1186	34		

- Molecule 3 is a protein called Ras GTPase-activating protein-binding protein 2.

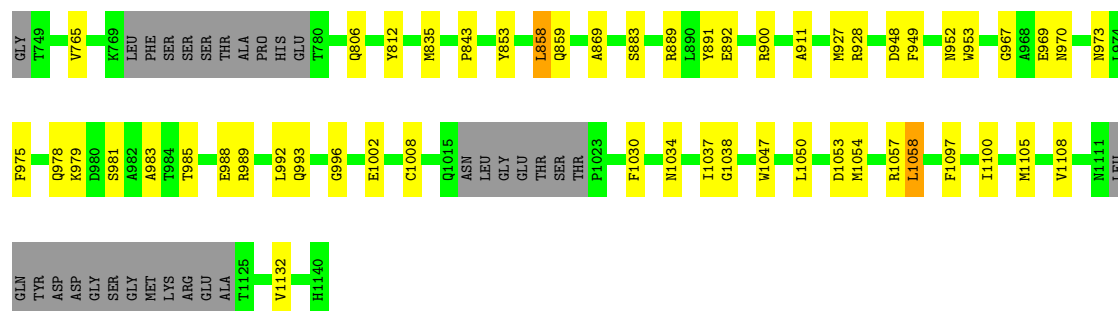
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	124	Total	C	N	O	S	0	0
			1012	647	178	183	4		
3	D	124	Total	C	N	O	S	0	0
			995	637	176	178	4		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

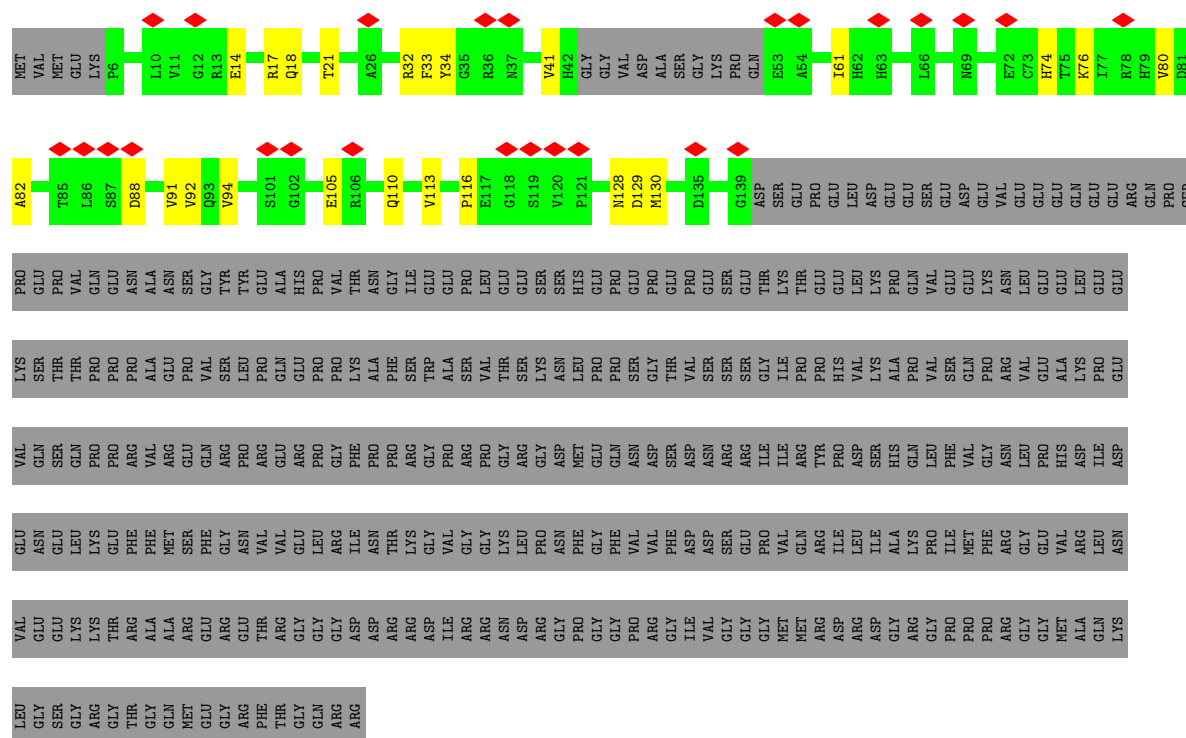
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	

- Molecule 5 is (1S,3S)-2-[(2-chlorophenyl)methanesulfonyl]-N-{[(4R)-3-(2,4-dioxo-1,3-diazinan-1-yl)imidazo[1,2-a]pyridin-7-yl]methyl}-1-methyl-1,2,3,4-tetrahydroisoquinoline-3-carboxamide (CCD ID: A1CED) (formula: C₃₀H₂₉ClN₆O₅S) (labeled as "Ligand of Interest" by depositor).

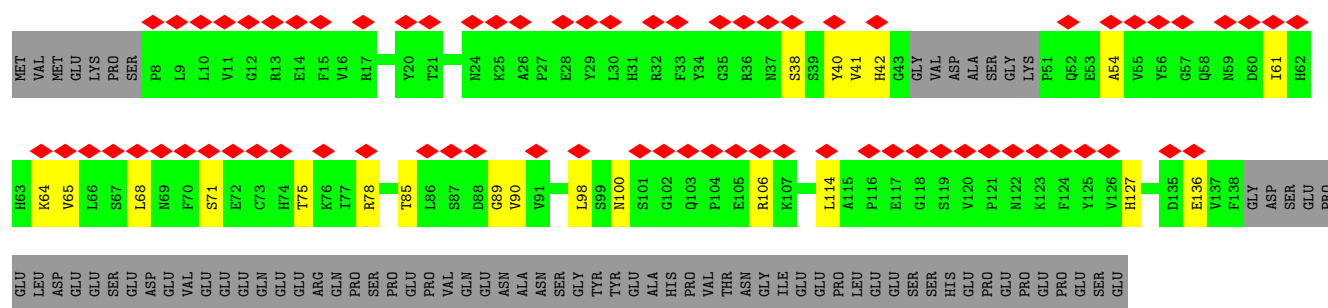




• Molecule 3: Ras GTPase-activating protein-binding protein 2



• Molecule 3: Ras GTPase-activating protein-binding protein 2



GLY	GLY	PRO	ILE	GLY	THR
MET	ILE	GLN	ARG	PRO	LYS
MET	TYR	ARG	PRO	ILE	LYS
ARG	ILE	ILE	ASP	VAL	GLU
ARG	SER	ILE	SER	LYS	LEU
ASP	ALA	ALA	HIS	ALA	LYS
GLY	LYS	GLN	LEU	PRO	PHO
ARG	LEU	PRO	GLY	VAL	GLN
PRO	ILE	ILE	PHE	VAL	GLU
PRO	MET	GLY	VAL	GLN	GLY
PRO	PHE	ARG	GLY	PRO	LYS
GLY	ARG	ARG	ASN	ARG	ASN
GLY	GLY	GLY	LEU	VAL	LEU
GLY	GLU	GLU	PRO	GLY	GLU
MET	VAL	VAL	HIS	ALA	GLU
ALA	ARG	ARG	ASP	LYS	LEU
GLN	LEU	LEU	ILE	PRO	GLU
LYS	ASN	LYS	ASP	GLY	GLY
LEU	VAL	LEU	GLU	VAL	GLU
GLY	GLU	GLU	ASN	GLN	LYS
SER	SER	GLY	GLU	SER	SER
GLY	LYS	LYS	LEU	GLN	THR
ARG	GLY	THR	THR	PRO	PRO
THR	THR	ARG	PHE	PRO	PHO
GLN	ALA	ALA	PHE	VAL	ALA
GLN	GLY	ALA	MET	ARG	GLY
MET	MET	ARG	SER	GLY	PRO
GLU	GLY	GLU	PHE	GLN	VAL
GLY	GLY	GLU	GLY	ARG	SER
ARG	ARG	THR	ASN	PRO	LEU
PHE	PHE	GLY	VAL	ARG	GLN
THR	THR	ARG	VAL	GLY	GLY
GLY	GLY	GLY	GLU	ARG	PHO
GLN	GLY	GLY	LEU	PRO	PHO
ARG	ARG	ASP	ILE	PHE	LYS
		ASP	ASN	PRO	ALA
		ARG	THR	PRO	PHE
		ARG	LYS	ARG	SER
		ASP	GLY	ARG	THR
		ILE	VAL	PRO	ALA
		ARG	GLY	ARG	SER
		ARG	GLY	PRO	VAL
		ASN	LYS	GLY	THR
		ASP	LEU	ARG	SER
		ARG	PRO	GLY	LYS
		GLY	ASN	ASP	ASN
		PRO	PHE	MET	PHO
		GLY	PHE	GLU	PRO
		GLY	PHE	GLN	PHO
		PRO	VAL	ASN	SER
		ARG	VAL	ASP	GLY
		ILE	PHE	SER	THR
		VAL	ASP	ASN	VAL
		VAL	ASP	ASN	SER
		GLY	THR	ARG	THR
		GLY	GLN	ARG	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	565661	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5056	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.486	Depositor
Minimum map value	-0.272	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.044	Depositor
Map size ($\text{\AA}$)	392.4, 392.4, 392.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.654, 0.654, 0.654	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, A1CED

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	B	0.38	0/2983	0.55	0/4060
2	A	0.38	0/6278	0.50	0/8498
3	C	0.26	0/1040	0.56	0/1406
3	D	0.16	0/1022	0.47	0/1382
All	All	0.36	0/11323	0.52	0/15346

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	B	2912	0	2819	60	0
2	A	6169	0	6096	58	0
3	C	1012	0	970	18	0
3	D	995	0	933	14	0
4	B	1	0	0	0	0
5	B	43	0	0	2	0
All	All	11132	0	10818	143	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 7.

All (143) 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:B:61:GLY:HA3	1:B:145:ARG:NH1	1.80	0.95
1:B:61:GLY:CA	1:B:145:ARG:NH1	2.51	0.73
3:D:71:SER:H	3:D:100:ASN:HD21	1.36	0.73
1:B:346:MET:HB2	1:B:360:LEU:HD12	1.76	0.68
1:B:301:ILE:O	1:B:307:ARG:NH1	2.26	0.67
2:A:948:ASP:HB2	2:A:992:LEU:HB2	1.76	0.67
3:C:88:ASP:HB2	3:C:116:PRO:HG3	1.77	0.66
1:B:287:CYS:HB3	1:B:345:PRO:HD2	1.77	0.65
3:D:106:ARG:NH2	3:D:136:GLU:OE2	2.28	0.65
1:B:114:ILE:HA	1:B:118:ARG:HG2	1.78	0.65
1:B:61:GLY:C	1:B:145:ARG:HH12	2.04	0.65
3:D:38:SER:HA	3:D:127:HIS:O	1.95	0.65
2:A:327:ARG:NH2	2:A:1034:ASN:OD1	2.30	0.64
1:B:399:GLY:HA3	1:B:416:GLY:O	1.99	0.62
1:B:61:GLY:CA	1:B:145:ARG:HH12	2.13	0.61
2:A:883:SER:HB2	2:A:911:ALA:HB3	1.83	0.61
2:A:952:ASN:ND2	2:A:969:GLU:OE1	2.31	0.61
3:D:75:THR:HG22	3:D:98:LEU:HD12	1.82	0.61
1:B:110:VAL:O	1:B:114:ILE:HG13	2.01	0.60
2:A:230:ILE:HD11	2:A:285:LEU:HD21	1.83	0.60
1:B:351:ASN:ND2	5:B:502:A1CED:N1	2.50	0.60
2:A:983:ALA:HB3	2:A:989:ARG:HG2	1.83	0.60
1:B:351:ASN:HB3	1:B:355:TYR:H	1.67	0.59
2:A:739:ARG:NH1	2:A:741:GLU:OE2	2.36	0.57
3:C:113:VAL:HB	3:C:128:ASN:HB2	1.86	0.56
3:D:90:VAL:HB	3:D:114:LEU:HD12	1.87	0.56
2:A:143:ILE:HG12	2:A:154:ALA:HB2	1.86	0.56
2:A:333:LEU:HB2	2:A:351:GLU:HB2	1.87	0.56
1:B:59:TYR:HE1	1:B:350:VAL:HG12	1.69	0.55
1:B:374:PRO:HA	1:B:386:TRP:O	2.07	0.55
2:A:36:ASN:ND2	2:A:1002:GLU:OE2	2.40	0.54
1:B:241:PRO:HB3	2:A:812:TYR:CZ	2.43	0.54
1:B:48:ASN:HB2	1:B:410:SER:H	1.71	0.54
1:B:92:ILE:HD12	1:B:286:ALA:HA	1.89	0.54
1:B:86:GLN:NE2	1:B:106:GLU:OE1	2.37	0.54
1:B:370:LEU:HD21	1:B:401:LYS:HD2	1.90	0.53
1:B:320:SER:OG	1:B:330:GLU:OE2	2.27	0.53
1:B:48:ASN:H	1:B:410:SER:HB2	1.74	0.52
1:B:200:GLU:H	1:B:200:GLU:CD	2.17	0.52
2:A:969:GLU:HG3	2:A:975:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LYS:O	1:B:327:GLN:NE2	2.43	0.52
3:C:110:GLN:NE2	3:C:129:ASP:OD1	2.38	0.51
1:B:401:LYS:HE2	1:B:403:THR:HG22	1.93	0.51
2:A:979:LYS:HE2	2:A:981:SER:HB3	1.93	0.51
2:A:69:PRO:HD2	2:A:72:GLU:HG3	1.92	0.51
2:A:38:ARG:HD2	2:A:54:GLU:OE2	2.11	0.51
3:C:76:LYS:NZ	3:C:105:GLU:OE2	2.33	0.51
3:C:82:ALA:HB2	3:C:92:VAL:HG22	1.93	0.51
1:B:423:LEU:HD12	1:B:424:PRO:HD2	1.92	0.50
5:B:502:A1CED:C29	3:C:17:ARG:HD2	2.41	0.50
2:A:1053:ASP:O	2:A:1057:ARG:HG3	2.11	0.50
2:A:40:GLU:HG2	2:A:54:GLU:HG3	1.92	0.50
3:C:17:ARG:HG3	3:C:18:GLN:N	2.27	0.50
1:B:62:ALA:O	1:B:145:ARG:NH2	2.44	0.50
2:A:843:PRO:HG2	2:A:869:ALA:HB2	1.94	0.50
1:B:241:PRO:HB3	2:A:812:TYR:OH	2.12	0.50
3:C:91:VAL:HG12	3:C:113:VAL:HG22	1.94	0.50
1:B:60:LEU:O	1:B:145:ARG:NH1	2.44	0.49
3:C:113:VAL:HG11	3:D:85:THR:OG1	2.12	0.49
2:A:892:GLU:OE2	2:A:900:ARG:NH1	2.45	0.49
2:A:1050:LEU:O	2:A:1054:MET:HG2	2.12	0.49
2:A:983:ALA:HB1	2:A:988:GLU:HB3	1.93	0.49
3:C:14:GLU:HA	3:C:17:ARG:HG2	1.95	0.49
2:A:853:TYR:HB2	2:A:858:LEU:HD23	1.94	0.49
2:A:1058:LEU:HD21	2:A:1097:PHE:HB2	1.95	0.49
2:A:1057:ARG:HD3	2:A:1108:VAL:O	2.13	0.49
1:B:164:ARG:NH2	1:B:302:GLY:HA2	2.29	0.48
2:A:1047:TRP:CZ3	2:A:1132:VAL:HG13	2.49	0.48
2:A:207:TRP:HB3	2:A:242:GLY:HA2	1.95	0.48
3:D:42:HIS:H	3:D:64:LYS:NZ	2.11	0.48
1:B:370:LEU:HD11	1:B:415:TRP:HH2	1.79	0.47
2:A:1030:PHE:CZ	2:A:1038:GLY:HA3	2.49	0.47
1:B:187:GLU:HG2	1:B:278:ILE:HG12	1.96	0.47
2:A:38:ARG:NH1	2:A:54:GLU:OE1	2.48	0.47
2:A:92:LYS:HE2	2:A:92:LYS:HB2	1.72	0.46
3:D:65:VAL:HA	3:D:68:LEU:HD12	1.97	0.46
1:B:312:LEU:O	1:B:316:ASN:ND2	2.48	0.46
1:B:321:LEU:HB3	1:B:422:LEU:HD23	1.97	0.46
1:B:352:PRO:O	3:C:17:ARG:NH2	2.49	0.46
2:A:226:PHE:O	2:A:241:ASN:ND2	2.49	0.46
3:C:34:TYR:OH	3:C:129:ASP:OD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:HIS:CE1	1:B:105:GLN:HB2	2.50	0.46
1:B:323:CYS:SG	1:B:326:CYS:HB2	2.56	0.46
1:B:406:LYS:HD2	1:B:406:LYS:H	1.81	0.45
1:B:75:ASP:HB3	1:B:186:PRO:HB3	1.97	0.45
2:A:1100:ILE:HG13	2:A:1105:MET:HG3	1.97	0.45
1:B:61:GLY:C	1:B:145:ARG:NH1	2.74	0.45
2:A:250:PRO:HG2	2:A:253:ILE:HG12	1.98	0.45
2:A:970:ASN:O	2:A:973:ASN:ND2	2.50	0.45
2:A:290:GLN:NE2	2:A:296:THR:OG1	2.49	0.45
2:A:967:GLY:HA3	2:A:975:PHE:CE1	2.52	0.45
3:D:85:THR:HG22	3:D:89:GLY:C	2.41	0.45
3:D:61:ILE:O	3:D:65:VAL:HG23	2.16	0.45
3:D:40:TYR:HB3	3:D:61:ILE:HG12	1.99	0.44
3:C:80:VAL:HG22	3:C:94:VAL:HG22	1.99	0.44
2:A:927:MET:HE2	2:A:927:MET:HB3	1.90	0.44
2:A:765:VAL:HG12	2:A:806:GLN:HB3	2.00	0.44
1:B:152:ILE:HD11	3:C:32:ARG:HB2	2.00	0.43
1:B:229:LYS:HE3	1:B:229:LYS:HB2	1.73	0.43
2:A:49:LEU:HG	2:A:333:LEU:HD11	2.00	0.43
1:B:269:LYS:O	1:B:270:ASP:C	2.60	0.43
2:A:1058:LEU:HD12	2:A:1108:VAL:HG21	1.99	0.43
1:B:107:VAL:HG21	1:B:153:GLU:O	2.19	0.43
1:B:232:PHE:O	1:B:242:ARG:HG2	2.19	0.43
1:B:288:LEU:HD21	1:B:315:MET:HG2	2.00	0.43
1:B:150:PHE:HB3	3:C:33:PHE:CE1	2.54	0.43
1:B:385:ALA:O	1:B:402:PHE:HA	2.19	0.43
1:B:408:ASP:OD1	1:B:408:ASP:N	2.52	0.43
2:A:265:ASP:OD2	2:A:269:SER:HB2	2.18	0.43
1:B:118:ARG:NH1	1:B:141:ILE:O	2.52	0.42
2:A:118:THR:OG1	2:A:134:ARG:NH2	2.51	0.42
1:B:65:GLU:O	1:B:143:ALA:HA	2.19	0.42
1:B:89:MET:HE2	1:B:89:MET:HB3	1.79	0.42
3:D:41:VAL:HB	3:D:54:ALA:HB2	2.01	0.42
1:B:107:VAL:HG12	1:B:111:ARG:HH21	1.85	0.42
1:B:326:CYS:SG	1:B:393:ILE:HB	2.60	0.42
2:A:10:GLN:HB3	2:A:1037:ILE:HB	2.02	0.42
2:A:141:LYS:HE2	2:A:141:LYS:HB2	1.71	0.42
2:A:340:SER:HB3	2:A:344:GLY:HA2	2.02	0.42
1:B:401:LYS:HB2	1:B:415:TRP:CZ3	2.55	0.42
2:A:1047:TRP:HZ3	2:A:1132:VAL:HG13	1.84	0.41
2:A:130:MET:HE3	2:A:176:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:78:ARG:HA	3:D:78:ARG:HD3	1.84	0.41
1:B:381:PHE:HD2	1:B:402:PHE:CE2	2.39	0.41
2:A:978:GLN:OE1	2:A:993:GLN:NE2	2.53	0.41
1:B:155:VAL:HG12	1:B:157:VAL:HG23	2.02	0.41
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.78	0.41
2:A:985:THR:O	2:A:989:ARG:HG3	2.21	0.41
2:A:364:VAL:HG23	2:A:1008:CYS:SG	2.61	0.41
2:A:975:PHE:HA	2:A:996:GLY:O	2.21	0.41
2:A:190:VAL:O	2:A:209:GLN:HA	2.21	0.41
1:B:102:PHE:CZ	3:C:21:THR:HG21	2.56	0.41
2:A:261:HIS:HA	2:A:272:LEU:O	2.21	0.41
2:A:928:ARG:NE	2:A:969:GLU:OE2	2.45	0.41
2:A:948:ASP:C	2:A:949:PHE:HD1	2.28	0.41
2:A:953:TRP:HB2	2:A:970:ASN:HB2	2.03	0.41
3:C:41:VAL:HG13	3:C:130:MET:HA	2.03	0.41
1:B:54:PRO:HG3	1:B:381:PHE:HD1	1.86	0.40
2:A:889:ARG:HD2	2:A:891:TYR:CZ	2.57	0.40
3:D:71:SER:H	3:D:100:ASN:ND2	2.12	0.40
1:B:155:VAL:CG1	1:B:157:VAL:HG23	2.51	0.40
2:A:385:GLY:HA3	2:A:719:GLU:O	2.21	0.40
3:C:34:TYR:CD2	3:C:61:ILE:HD13	2.57	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	B	365/378 (97%)	350 (96%)	15 (4%)	0	100	100
2	A	778/1140 (68%)	753 (97%)	25 (3%)	0	100	100
3	C	120/482 (25%)	117 (98%)	3 (2%)	0	100	100
3	D	120/482 (25%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1383/2482 (56%)	1337 (97%)	46 (3%)	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	B	316/342 (92%)	303 (96%)	13 (4%)	27	53
2	A	680/999 (68%)	669 (98%)	11 (2%)	55	79
3	C	111/419 (26%)	110 (99%)	1 (1%)	70	87
3	D	104/419 (25%)	104 (100%)	0	100	100
All	All	1211/2179 (56%)	1186 (98%)	25 (2%)	46	74

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	ILE
1	B	123	LEU
1	B	132	GLU
1	B	144	TYR
1	B	153	GLU
1	B	157	VAL
1	B	197	VAL
1	B	198	GLN
1	B	268	LEU
1	B	323	CYS
1	B	356	VAL
1	B	387	THR
1	B	406	LYS
2	A	65	GLU
2	A	207	TRP
2	A	246	LEU
2	A	292	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	294	THR
2	A	307	GLU
2	A	391	ARG
2	A	835	MET
2	A	858	LEU
2	A	859	GLN
2	A	1058	LEU
3	C	74	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	GLN
1	B	173	GLN
1	B	179	GLN
1	B	198	GLN
1	B	203	ASN
1	B	225	GLN
1	B	228	GLN
1	B	233	HIS
1	B	316	ASN
1	B	357	HIS
1	B	412	GLN
2	A	109	GLN
2	A	174	GLN
2	A	203	ASN
2	A	234	GLN
2	A	290	GLN
2	A	374	GLN
2	A	789	HIS
2	A	810	ASN
2	A	907	ASN
2	A	978	GLN
2	A	993	GLN
2	A	1025	GLN
2	A	1056	ASN
2	A	1106	GLN
2	A	1140	HIS
3	D	31	HIS
3	D	42	HIS
3	D	63	HIS
3	D	74	HIS

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Mol	Chain	Res	Type
3	D	93	GLN
3	D	100	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
5	A1CED	B	502	-	46,48,48	0.21	0	55,71,71	0.53	1 (1%)

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
5	A1CED	B	502	-	-	9/20/53/53	0/6/6/6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	A1CED	C7-C8-C9	2.23	116.48	111.61

There are no chirality outliers.

All (9) torsion outliers are listed below:

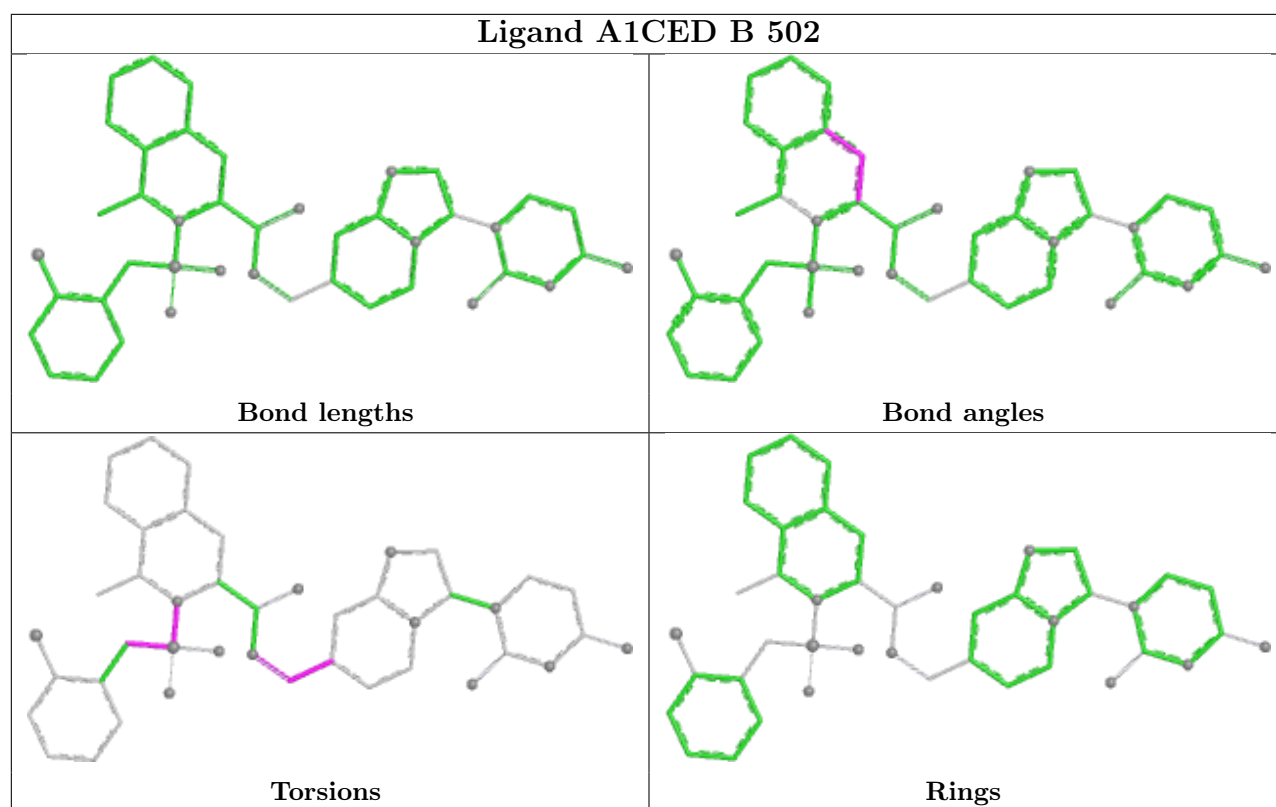
Mol	Chain	Res	Type	Atoms
5	B	502	A1CED	N-C11-C12-C13
5	B	502	A1CED	C24-C23-S-N5
5	B	502	A1CED	C24-C23-S-O3
5	B	502	A1CED	C24-C23-S-O4
5	B	502	A1CED	C1-N5-S-C23
5	B	502	A1CED	C1-N5-S-O3
5	B	502	A1CED	C9-N5-S-C23
5	B	502	A1CED	C9-N5-S-O3
5	B	502	A1CED	C12-C11-N-C10

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	A1CED	2	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 than 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.



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.

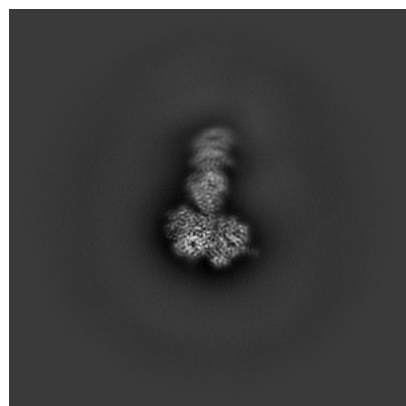
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70791. These allow visual inspection of the internal detail of the map and identification of artifacts.

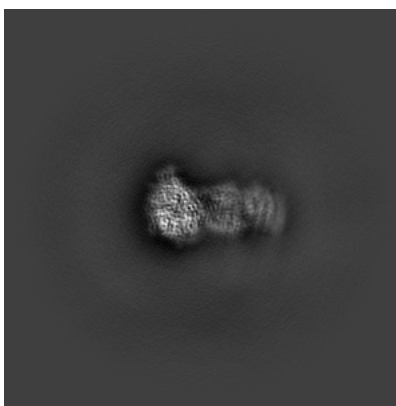
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

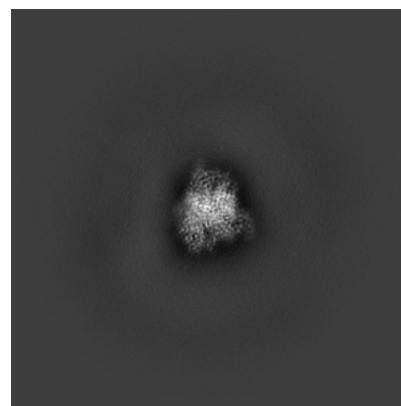
6.1.1 Primary map



X

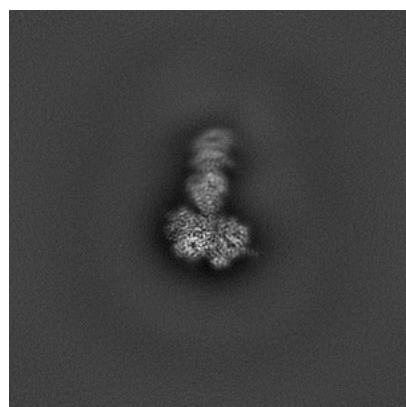


Y

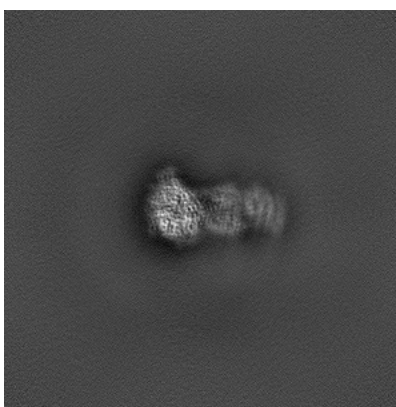


Z

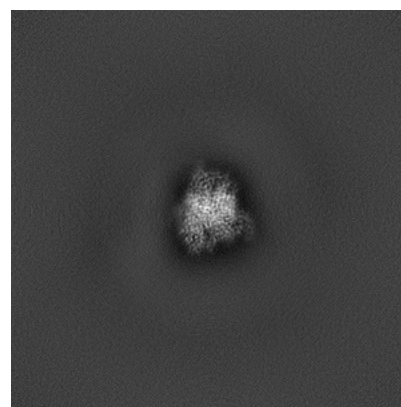
6.1.2 Raw map



X



Y

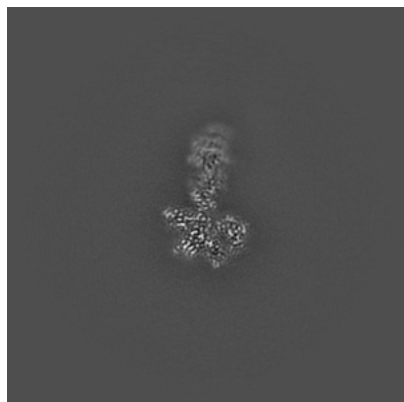


Z

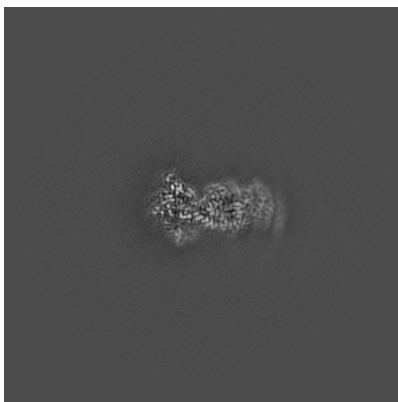
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

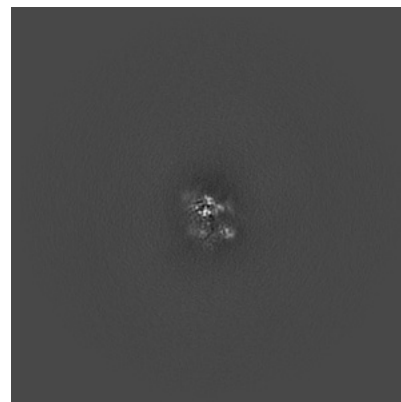
6.2.1 Primary map



X Index: 300

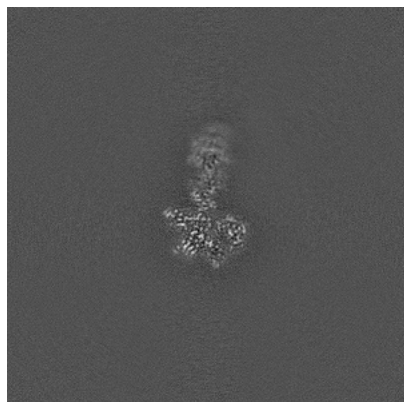


Y Index: 300

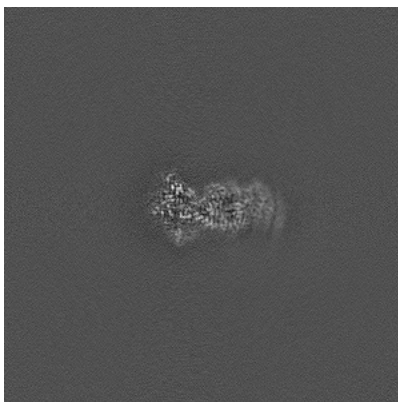


Z Index: 300

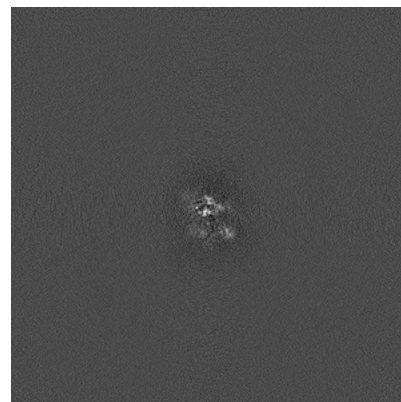
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

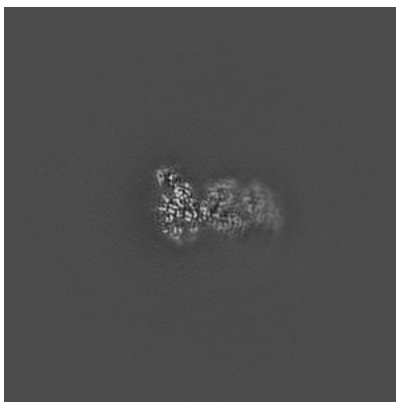
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

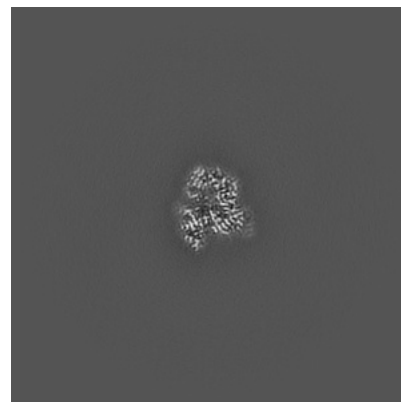
6.3.1 Primary map



X Index: 292

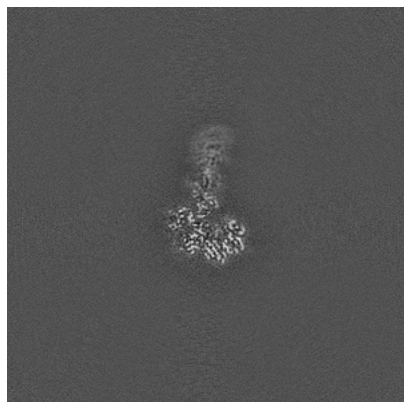


Y Index: 292

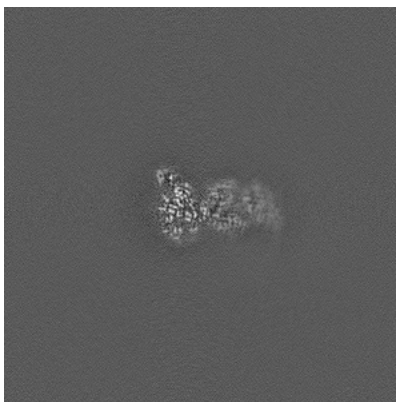


Z Index: 256

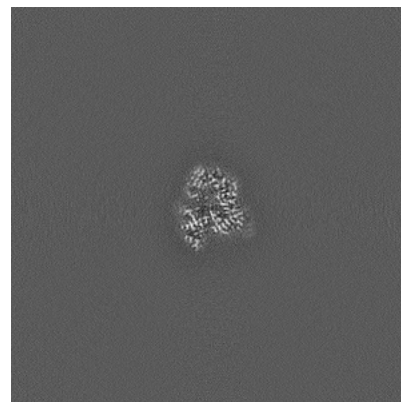
6.3.2 Raw map



X Index: 292



Y Index: 292

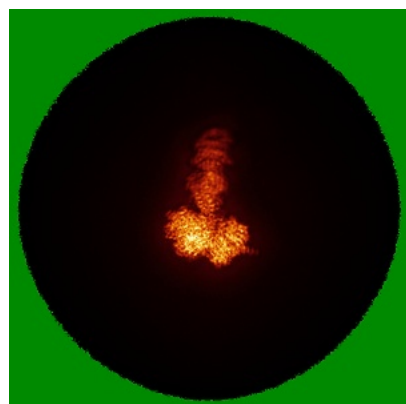


Z Index: 256

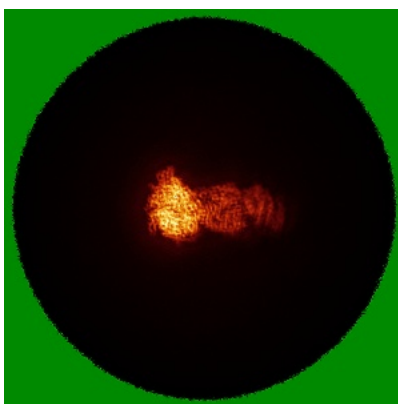
The images above show the largest variance slices of the map in three orthogonal directions.

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

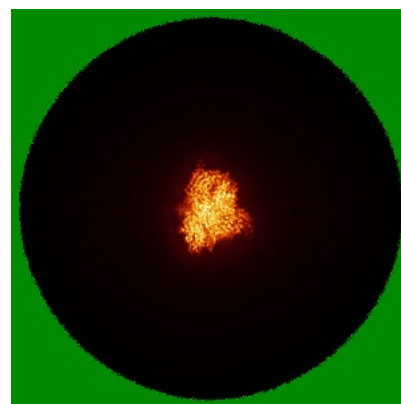
6.4.1 Primary map



X

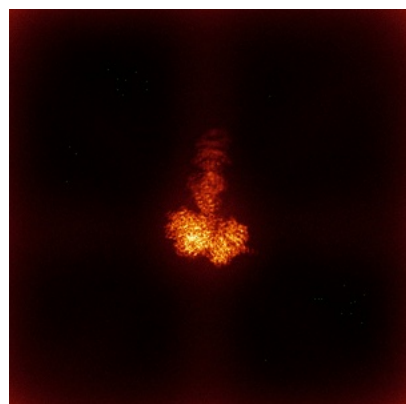


Y

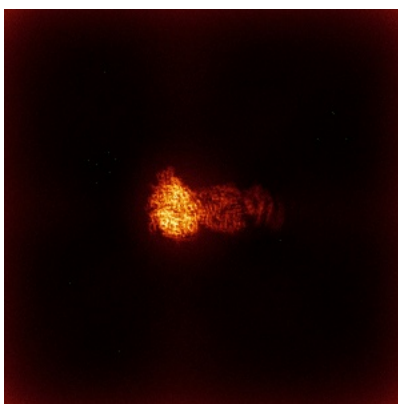


Z

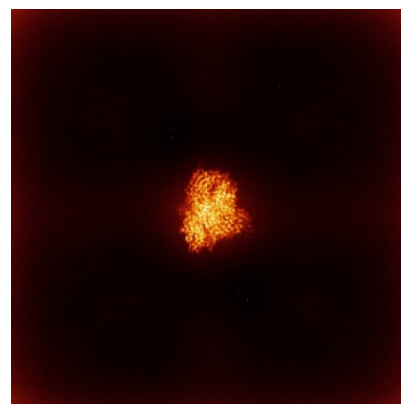
6.4.2 Raw map



X



Y

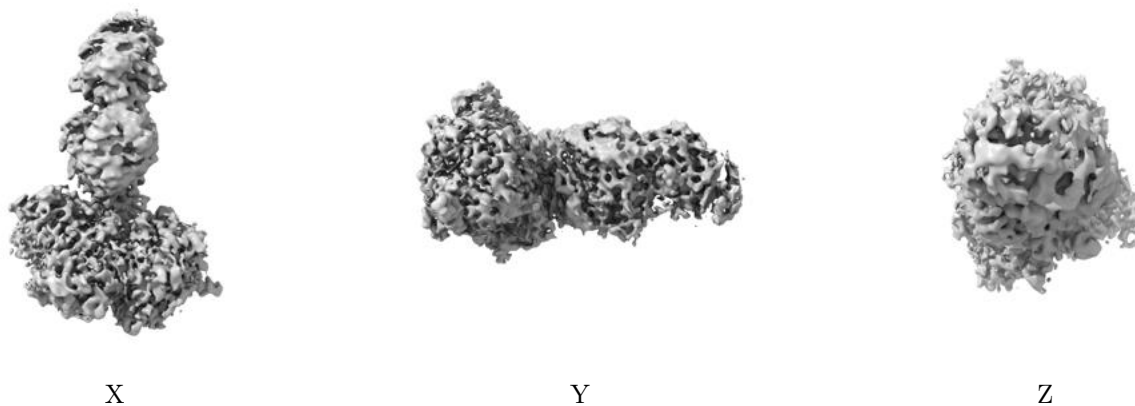


Z

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.

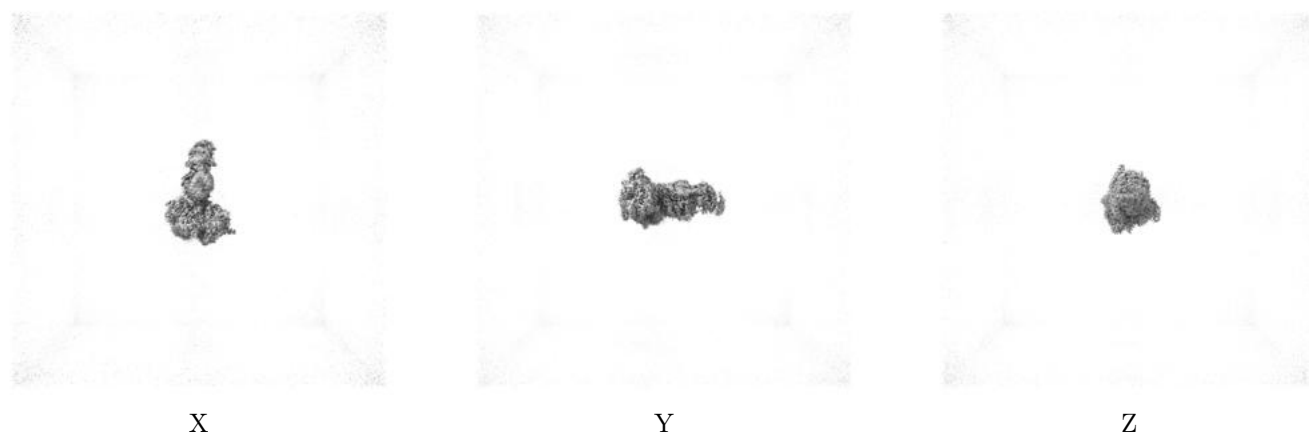
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.044. 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.

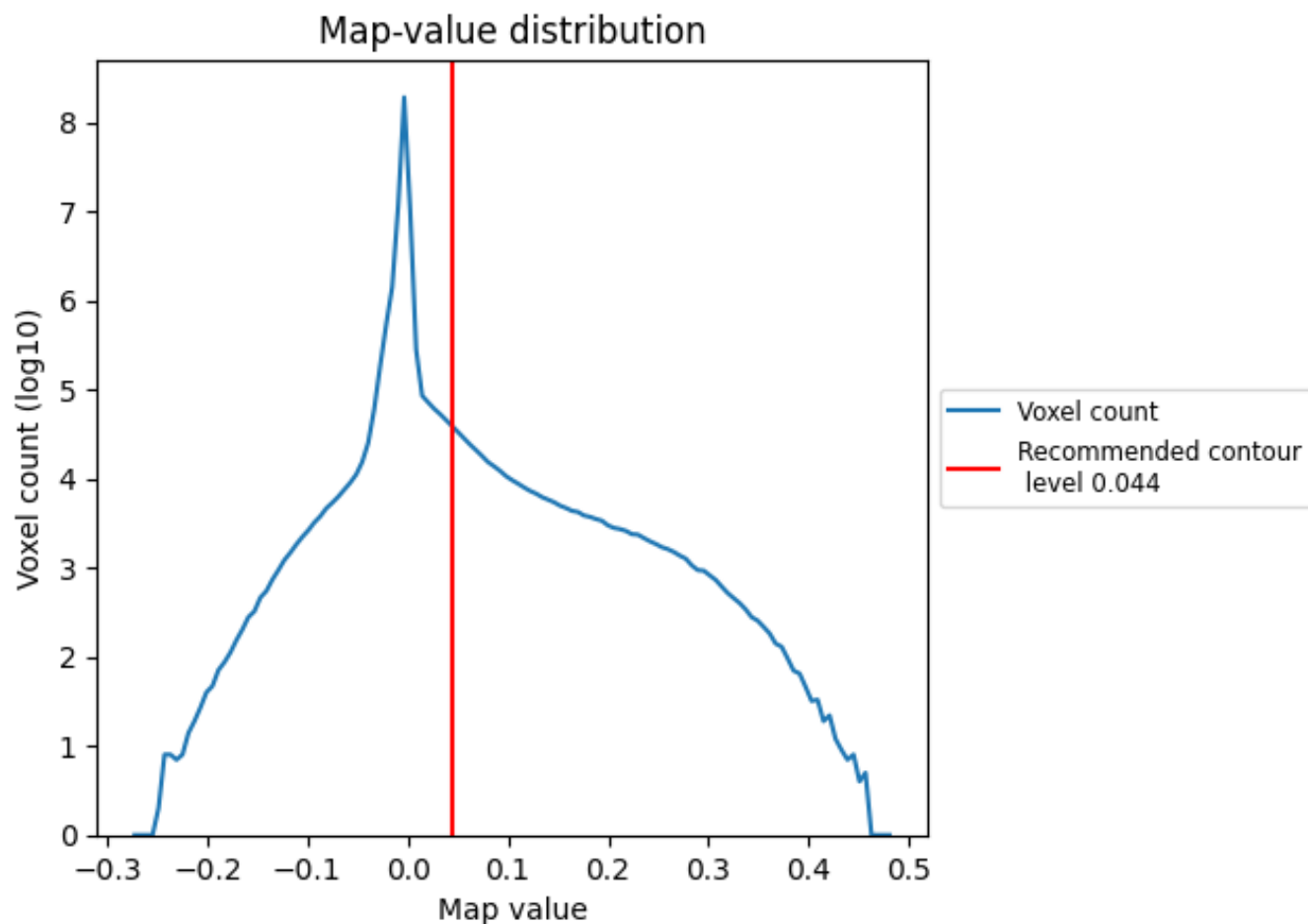
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

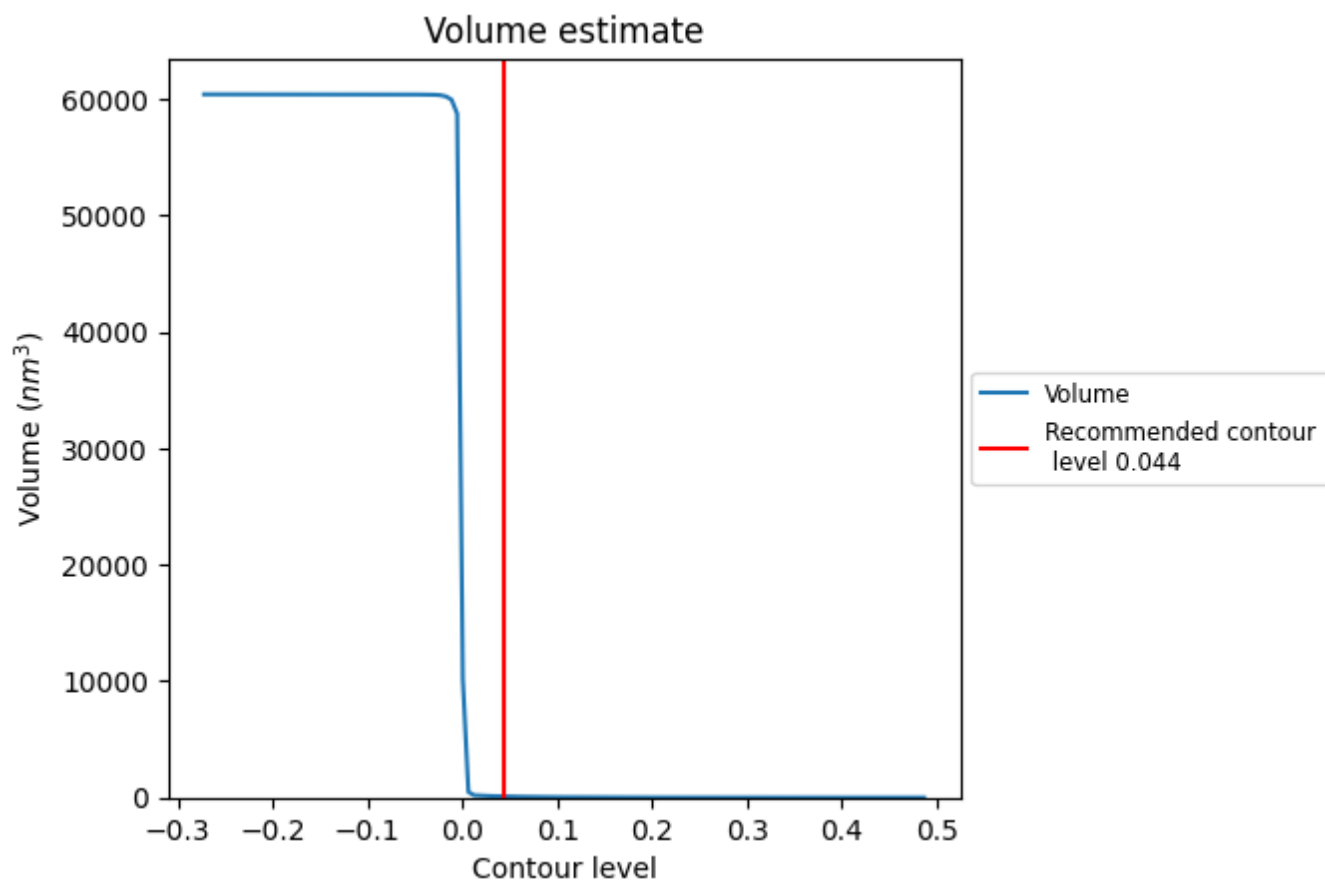
This section contains the results of statistical analysis of the map.

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.

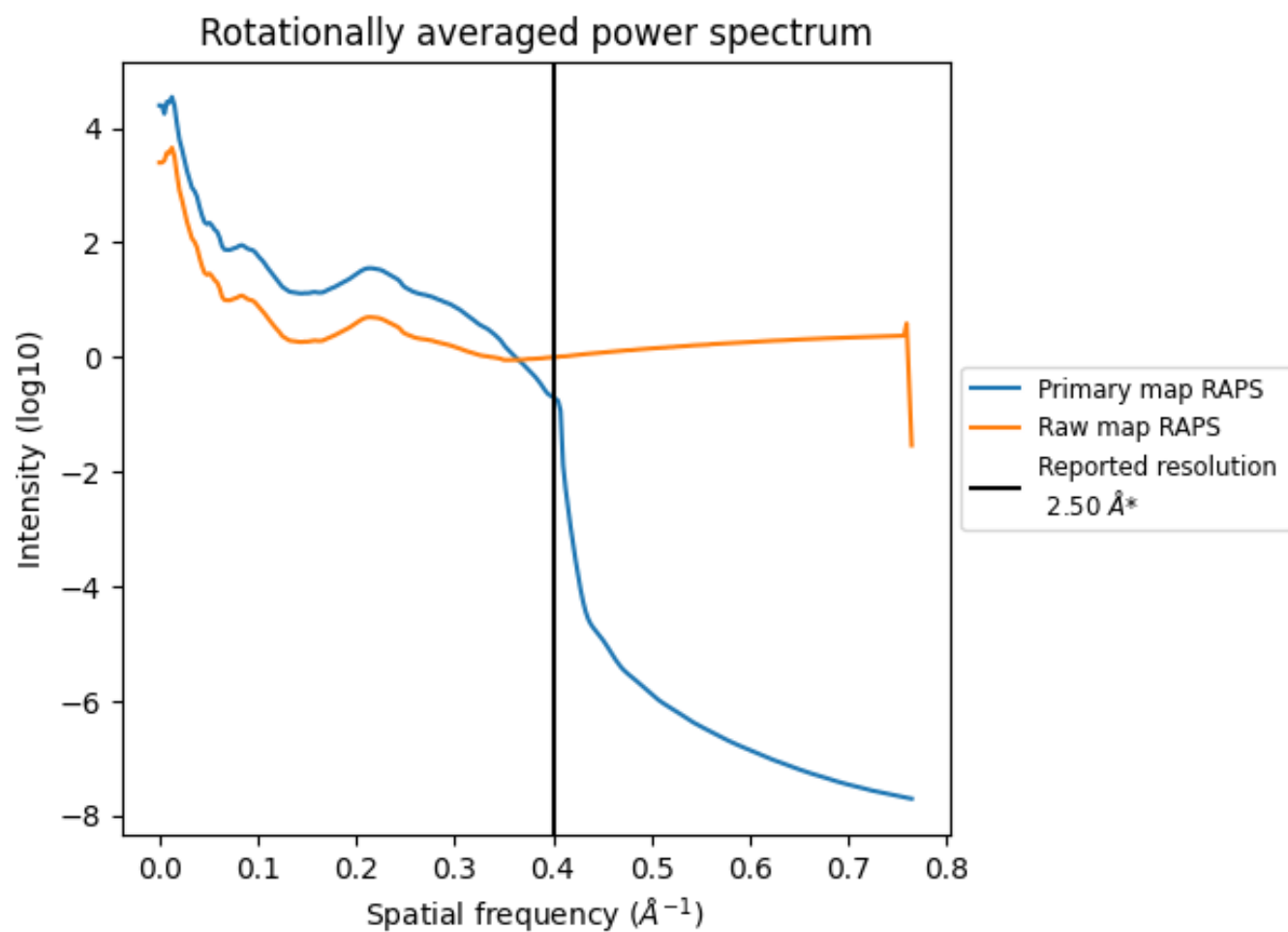
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm^3 ; this corresponds to an approximate mass of 88 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](#)

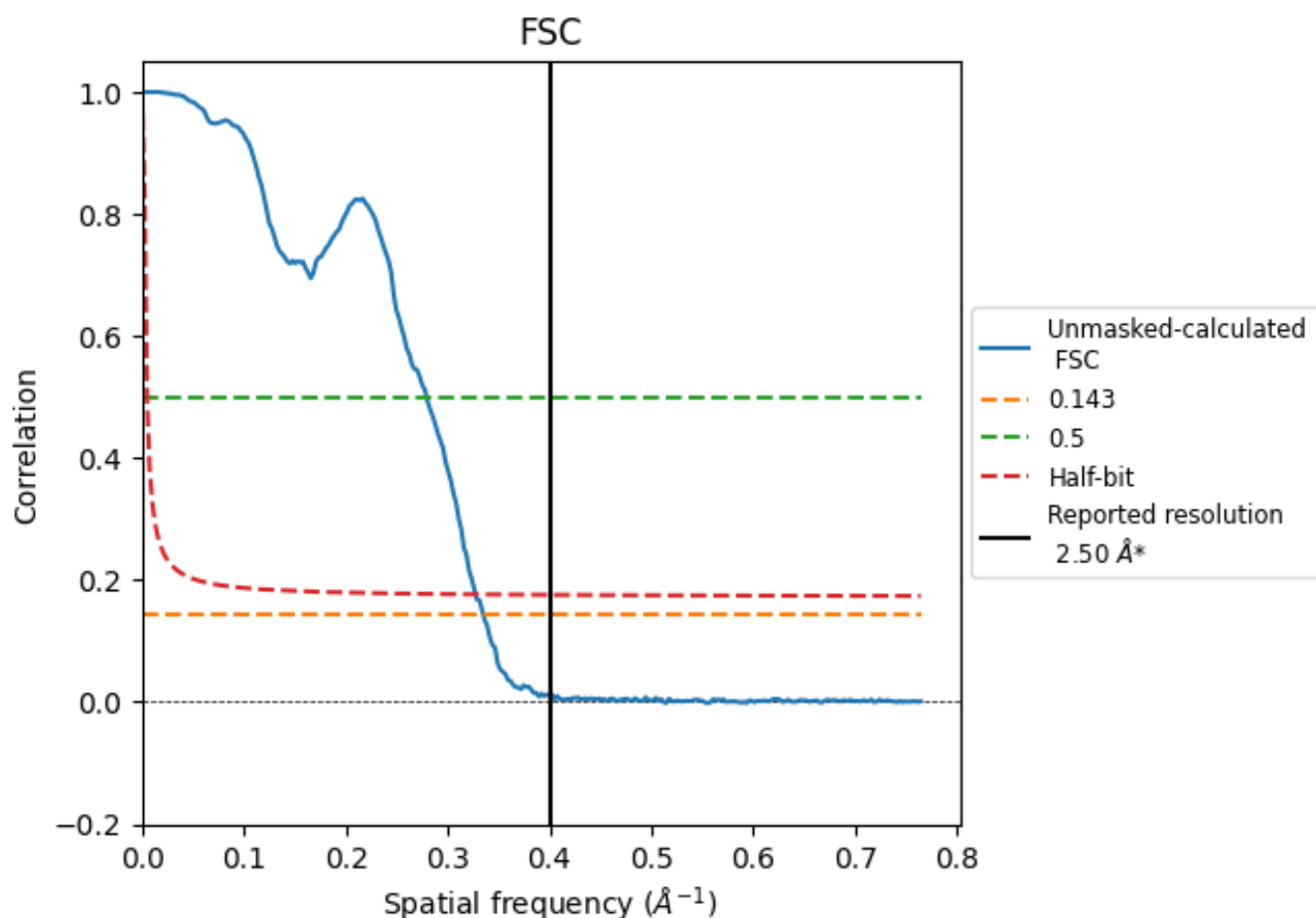


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 $0.400 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

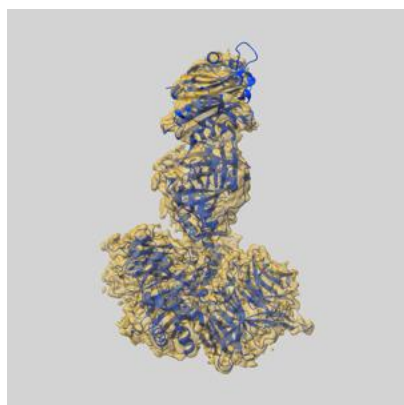
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.58	3.05

*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 2.99 differs from the reported value 2.5 by more than 10 %

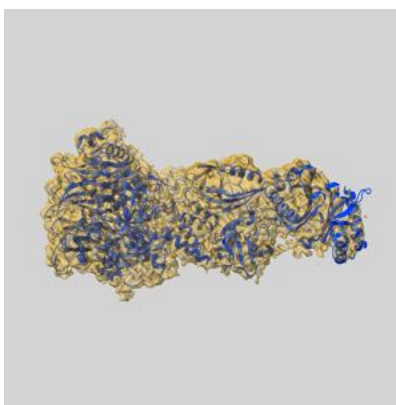
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70791 and PDB model 9OS2. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

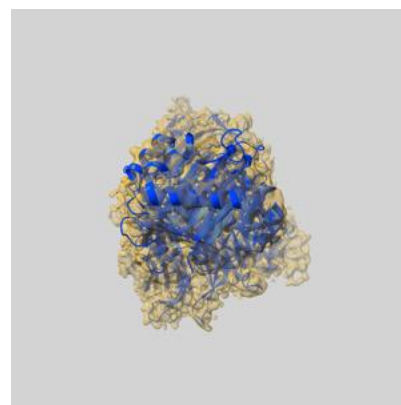
9.1 Map-model overlay [i](#)



X



Y



Z

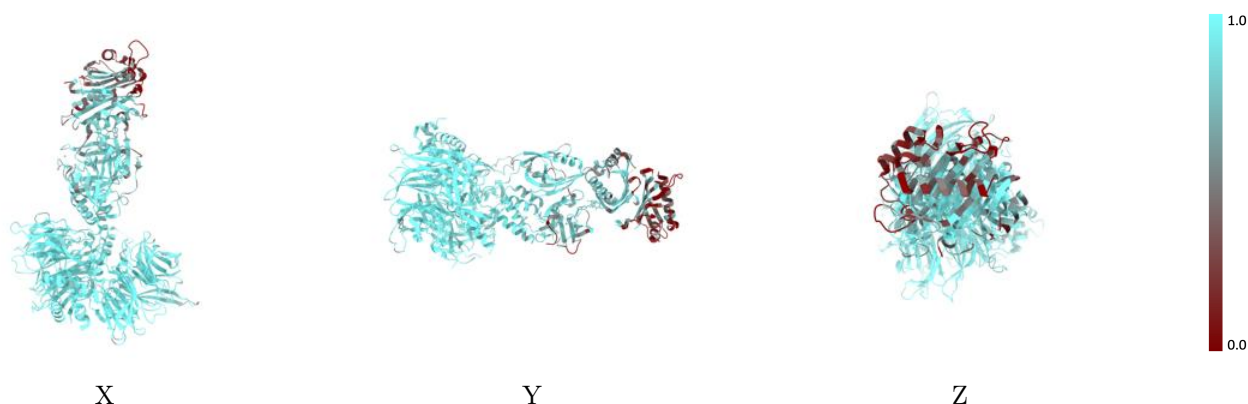
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



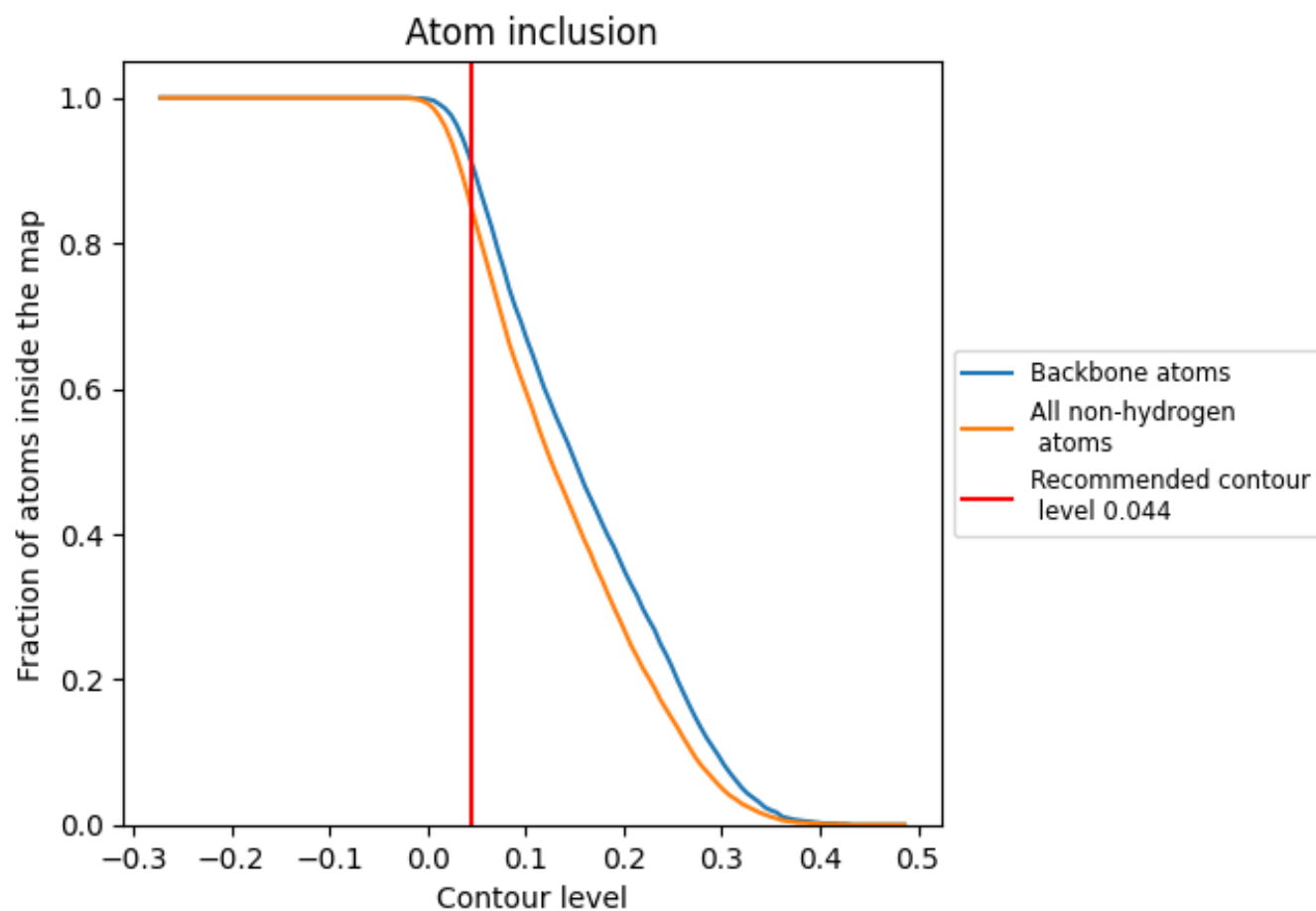
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8520	0.5010
A	0.9620	0.6120
B	0.8330	0.4430
C	0.7160	0.3130
D	0.3650	0.1830

