



Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 07:20 PM JST

PDB ID : 7V93
EMDB ID : EMD-31807
Title : Cryo-EM structure of the Cas12c2-sgRNA binary complex
Authors : Kurihara, N.; Hirano, H.; Tomita, A.; Kobayashi, K.; Kusakizako, T.;
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Deposited on : 2021-08-24
Resolution : 3.00 Å(reported)

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

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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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

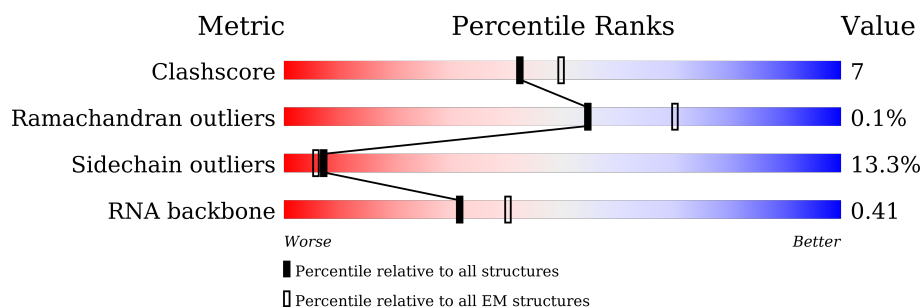
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1232	<div> <div>25%</div> <div>56%</div> <div>17%</div> <div>•</div> <div>25%</div> </div>
2	B	112	<div> <div>21%</div> <div>36%</div> <div>23%</div> <div>5%</div> <div>36%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8792 atoms, of which 0 are hydrogens and 0 are deuteriums.

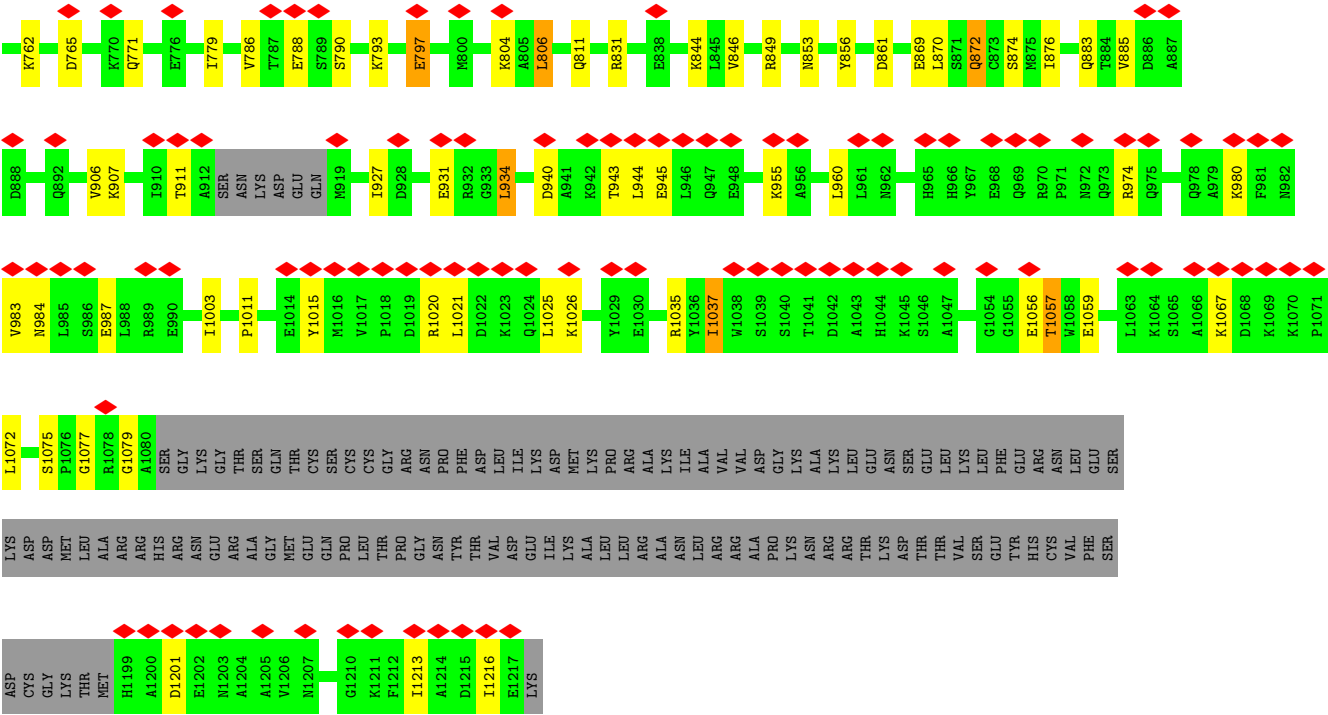
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cas12c2.

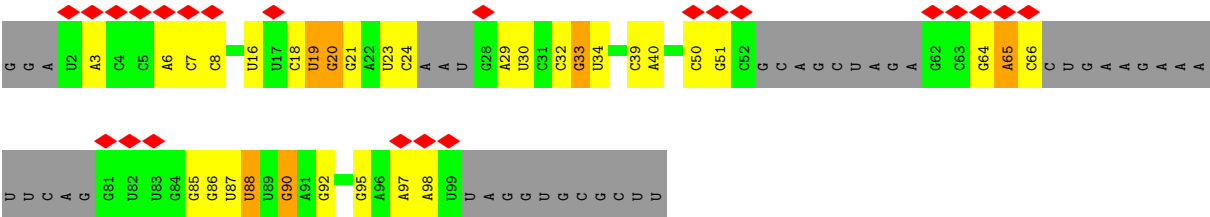
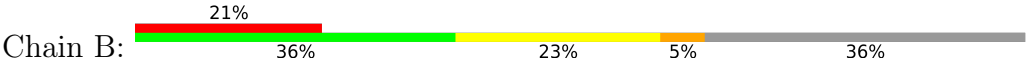
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	927	Total	C	N	O	S	0	0
			7260	4625	1254	1347	34		

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	72	Total	C	N	O	P	0	0
			1532	683	268	509	72		



● Molecule 2: sgRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	289394	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.348	Depositor
Minimum map value	-0.261	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.055	Depositor
Map size (\AA)	212.48065, 212.48065, 212.48065	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.10667, 1.10667, 1.10667	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.71	2/7405 (0.0%)	0.75	3/10013 (0.0%)
2	B	0.74	2/1707 (0.1%)	0.82	2/2651 (0.1%)
All	All	0.72	4/9112 (0.0%)	0.76	5/12664 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	32	C	O3'-P	-6.95	1.52	1.61
2	B	90	G	C8-N7	5.82	1.34	1.30
1	A	414	TYR	C-O	5.30	1.33	1.23
1	A	418	ASP	C-O	5.14	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	A	288	PRO	N-CA-CB	-6.00	96.00	102.60
2	B	92	G	O5'-P-OP2	-5.38	100.86	105.70
1	A	368	ARG	CG-CD-NE	5.22	122.77	111.80
2	B	21	G	OP1-P-OP2	-5.01	112.08	119.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1075	SER	Peptide
1	A	287	THR	Mainchain

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	7260	0	7276	112	0
2	B	1532	0	778	14	0
All	All	8792	0	8054	121	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 (121) 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:324:GLU:O	1:A:328:PRO:HD2	1.84	0.76
1:A:599:ILE:HG12	1:A:607:PRO:HB3	1.70	0.73
1:A:259:PHE:CD2	1:A:281:ILE:HG21	2.23	0.73
1:A:272:LEU:HG	1:A:276:LYS:HG2	1.71	0.71
1:A:762:LYS:HD2	2:B:33:G:OP1	1.94	0.68
1:A:811:GLN:HG3	1:A:861:ASP:HB3	1.76	0.67
2:B:65:A:H2'	2:B:66:C:H6	1.61	0.64
1:A:595:SER:HB2	1:A:614:ILE:HD11	1.80	0.64
1:A:364:ASN:HB3	1:A:496:LEU:HD11	1.80	0.64
1:A:550:LYS:HD2	1:A:551:ARG:HH21	1.66	0.61
1:A:551:ARG:NH2	1:A:686:ASP:OD2	2.31	0.61
1:A:378:GLN:HB3	1:A:489:TRP:HB3	1.85	0.59
1:A:547:ALA:O	1:A:551:ARG:HD2	2.02	0.59
1:A:401:MET:HB2	1:A:405:GLU:HG2	1.84	0.58
1:A:41:PHE:CE1	1:A:856:TYR:HB3	2.37	0.58
1:A:698:ILE:HD13	1:A:727:TYR:HA	1.85	0.58
1:A:278:SER:HB2	1:A:363:ALA:HA	1.87	0.56
2:B:65:A:H2'	2:B:66:C:C6	2.40	0.56
1:A:372:LEU:HD11	1:A:493:VAL:HG21	1.89	0.55
1:A:621:ILE:HD12	1:A:636:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:HD12	1:A:646:TRP:HZ2	1.71	0.54
1:A:550:LYS:CD	1:A:551:ARG:HH21	2.21	0.53
1:A:399:ILE:HB	1:A:454:THR:HG23	1.90	0.53
1:A:368:ARG:HH21	1:A:368:ARG:HG3	1.73	0.53
2:B:39:C:H2'	2:B:40:A:O4'	2.08	0.53
1:A:276:LYS:NZ	1:A:276:LYS:HA	2.24	0.52
1:A:41:PHE:HE1	1:A:856:TYR:HB3	1.74	0.52
1:A:550:LYS:HD2	1:A:551:ARG:NH2	2.23	0.52
1:A:578:ARG:HD2	1:A:679:LEU:HD21	1.90	0.52
1:A:372:LEU:HD13	1:A:441:PHE:CE1	2.45	0.52
1:A:31:ARG:HB3	1:A:1057:THR:HB	1.91	0.51
1:A:527:ARG:NH2	1:A:695:LYS:O	2.44	0.51
1:A:940:ASP:HB3	1:A:943:THR:HG22	1.93	0.51
1:A:279:LYS:O	1:A:282:GLN:HG2	2.11	0.50
1:A:275:GLY:O	1:A:279:LYS:HG2	2.11	0.50
1:A:83:ALA:HA	1:A:325:SER:HB3	1.94	0.50
1:A:513:MET:HG3	1:A:738:LEU:HD21	1.93	0.50
1:A:551:ARG:NH2	1:A:554:GLU:OE2	2.45	0.49
1:A:580:GLY:HA3	1:A:613:PHE:HE2	1.78	0.49
1:A:269:ILE:HG21	1:A:428:LEU:HD13	1.95	0.49
1:A:8:LEU:HD21	1:A:1003:ILE:HG12	1.94	0.49
1:A:290:VAL:CG2	1:A:293:LEU:HD12	2.43	0.48
1:A:426:THR:HG23	1:A:431:GLY:O	2.13	0.48
1:A:305:ARG:NH1	1:A:336:ILE:O	2.46	0.48
1:A:339:MET:SD	1:A:341:VAL:HG22	2.53	0.48
1:A:517:PHE:HA	1:A:734:LEU:HD13	1.95	0.48
1:A:535:VAL:HG12	1:A:540:ALA:O	2.13	0.48
1:A:853:ASN:HB2	2:B:19:U:OP1	2.14	0.48
1:A:513:MET:SD	1:A:737:LYS:HB3	2.54	0.48
1:A:944:LEU:HD13	1:A:1213:ILE:HG23	1.95	0.48
1:A:348:ALA:O	1:A:351:ARG:HB3	2.14	0.47
1:A:278:SER:CB	1:A:363:ALA:HA	2.44	0.47
1:A:259:PHE:CZ	1:A:281:ILE:HG13	2.49	0.47
1:A:1037:ILE:HD11	1:A:1079:GLY:HA2	1.97	0.47
1:A:657:LEU:HB2	1:A:669:ALA:HB2	1.97	0.47
1:A:1021:LEU:HB2	1:A:1026:LYS:HG3	1.97	0.47
1:A:510:ILE:HA	1:A:513:MET:HG2	1.96	0.47
1:A:594:PHE:CD2	1:A:614:ILE:HG21	2.50	0.46
1:A:552:GLU:OE1	1:A:556:ILE:HD11	2.15	0.46
1:A:528:PHE:HB2	1:A:724:PHE:HZ	1.78	0.46
1:A:579:ILE:HD12	1:A:646:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:THR:HG23	1:A:657:LEU:HD11	1.97	0.46
1:A:1072:LEU:HD11	1:A:1216:ILE:HG21	1.97	0.46
1:A:357:LYS:HE2	1:A:499:ILE:HG23	1.96	0.46
1:A:80:LEU:HG	1:A:329:LEU:HD11	1.98	0.46
1:A:269:ILE:CG2	1:A:428:LEU:HD13	2.47	0.45
1:A:705:ALA:HA	1:A:708:MET:HE2	1.98	0.45
1:A:368:ARG:O	1:A:372:LEU:HD12	2.16	0.45
1:A:790:SER:HB3	1:A:793:LYS:HD3	1.97	0.45
1:A:379:ILE:HD13	1:A:489:TRP:HB2	1.99	0.45
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.80	0.45
1:A:605:LYS:HA	1:A:637:HIS:CE1	2.51	0.44
1:A:31:ARG:HE	1:A:1056:GLU:HB2	1.82	0.44
1:A:259:PHE:CE2	1:A:281:ILE:HG21	2.53	0.44
1:A:605:LYS:HB2	1:A:605:LYS:HE2	1.80	0.44
2:B:16:U:H3	2:B:40:A:H61	1.64	0.44
2:B:50:C:H2'	2:B:51:G:C8	2.53	0.44
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.81	0.44
1:A:745:LEU:HA	1:A:745:LEU:HD13	1.72	0.44
1:A:413:VAL:O	1:A:417:VAL:HG23	2.18	0.43
1:A:738:LEU:HA	1:A:883:GLN:HE22	1.83	0.43
1:A:788:GLU:HB3	1:A:793:LYS:HE2	1.99	0.43
1:A:10:ALA:HA	2:B:88:U:H5'	2.00	0.43
1:A:703:GLN:HG3	1:A:706:LEU:HB2	2.00	0.43
1:A:477:GLU:O	1:A:480:ILE:HG12	2.19	0.43
1:A:650:LEU:HD11	1:A:672:LEU:HD22	2.00	0.43
1:A:706:LEU:HD11	1:A:722:ARG:HB3	2.01	0.43
1:A:309:ILE:O	1:A:313:MET:HG2	2.19	0.43
1:A:746:LYS:HB3	1:A:746:LYS:HE3	1.78	0.42
1:A:786:VAL:HA	1:A:797:GLU:HG2	2.01	0.42
1:A:372:LEU:HD13	1:A:441:PHE:HE1	1.83	0.42
1:A:368:ARG:HH21	1:A:368:ARG:CG	2.32	0.42
1:A:376:LEU:HG	1:A:421:LYS:HG2	2.02	0.42
1:A:282:GLN:HE21	1:A:282:GLN:HB3	1.58	0.42
2:B:29:A:H2'	2:B:30:U:C6	2.53	0.42
1:A:345:LYS:H	1:A:345:LYS:HG3	1.65	0.42
1:A:305:ARG:NH1	1:A:333:ALA:O	2.52	0.42
2:B:65:A:C4	2:B:66:C:C5	3.08	0.42
1:A:1072:LEU:HD23	1:A:1072:LEU:HA	1.83	0.42
1:A:506:VAL:HG13	1:A:745:LEU:HD21	2.02	0.41
1:A:269:ILE:HD11	1:A:277:LEU:HD13	2.03	0.41
1:A:588:GLU:HA	1:A:591:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:GLN:H	1:A:872:GLN:HG2	1.61	0.41
1:A:15:GLY:HA3	2:B:20:G:OP2	2.19	0.41
1:A:276:LYS:O	1:A:280:LEU:HG	2.20	0.41
1:A:307:THR:HG22	1:A:312:ILE:HG13	2.02	0.41
2:B:23:U:H2'	2:B:24:C:C6	2.56	0.41
2:B:85:G:H2'	2:B:86:G:C8	2.54	0.41
1:A:78:ALA:HB1	1:A:254:LEU:HB3	2.02	0.41
1:A:263:ALA:HB2	1:A:281:ILE:HD11	2.02	0.41
1:A:849:ARG:HH22	2:B:34:U:H3'	1.86	0.41
1:A:597:LYS:HB3	1:A:649:LEU:HD21	2.02	0.41
1:A:927:ILE:HG23	1:A:934:LEU:HD13	2.01	0.41
1:A:677:LEU:HB3	1:A:724:PHE:HE2	1.86	0.41
1:A:476:LEU:HD12	1:A:476:LEU:HA	1.84	0.40
1:A:87:PHE:HB3	1:A:287:THR:CG2	2.51	0.40
1:A:528:PHE:HB2	1:A:724:PHE:CZ	2.55	0.40
1:A:1011:PRO:O	1:A:1077:GLY:HA2	2.21	0.40
1:A:617:GLN:HE21	1:A:617:GLN:HB2	1.64	0.40
1:A:1025:LEU:HD12	1:A:1025:LEU:HA	1.84	0.40
1:A:737:LYS:HD3	1:A:737:LYS:HA	1.95	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	915/1232 (74%)	894 (98%)	20 (2%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	PRO

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	767/1039 (74%)	665 (87%)	102 (13%)	4 17

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	30	LYS
1	A	33	LYS
1	A	34	GLU
1	A	35	THR
1	A	45	MET
1	A	47	GLU
1	A	90	SER
1	A	245	ASP
1	A	271	ASP
1	A	276	LYS
1	A	282	GLN
1	A	341	VAL
1	A	342	LEU
1	A	345	LYS
1	A	346	ASN
1	A	351	ARG
1	A	368	ARG
1	A	372	LEU
1	A	376	LEU
1	A	378	GLN
1	A	384	GLU
1	A	392	ASN
1	A	396	MET
1	A	402	THR
1	A	411	GLU
1	A	443	GLN
1	A	459	SER
1	A	461	ARG
1	A	464	ARG

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Mol	Chain	Res	Type
1	A	475	ARG
1	A	478	LYS
1	A	483	LYS
1	A	493	VAL
1	A	503	LEU
1	A	506	VAL
1	A	507	GLU
1	A	510	ILE
1	A	551	ARG
1	A	555	GLN
1	A	573	ARG
1	A	592	GLN
1	A	603	VAL
1	A	610	LEU
1	A	617	GLN
1	A	618	LYS
1	A	621	ILE
1	A	623	ARG
1	A	635	GLN
1	A	649	LEU
1	A	678	GLN
1	A	698	ILE
1	A	703	GLN
1	A	706	LEU
1	A	710	LEU
1	A	715	VAL
1	A	718	ASP
1	A	720	LEU
1	A	721	GLN
1	A	724	PHE
1	A	725	ASN
1	A	731	LEU
1	A	736	PHE
1	A	739	LEU
1	A	745	LEU
1	A	748	ARG
1	A	765	ASP
1	A	771	GLN
1	A	779	ILE
1	A	797	GLU
1	A	804	LYS
1	A	806	LEU

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Mol	Chain	Res	Type
1	A	831	ARG
1	A	844	LYS
1	A	846	VAL
1	A	869	GLU
1	A	870	LEU
1	A	872	GLN
1	A	874	SER
1	A	876	ILE
1	A	885	VAL
1	A	906	VAL
1	A	907	LYS
1	A	911	THR
1	A	931	GLU
1	A	934	LEU
1	A	945	GLU
1	A	955	LYS
1	A	960	LEU
1	A	974	ARG
1	A	980	LYS
1	A	983	VAL
1	A	984	ASN
1	A	987	GLU
1	A	1015	TYR
1	A	1020	ARG
1	A	1035	ARG
1	A	1037	ILE
1	A	1057	THR
1	A	1059	GLU
1	A	1067	LYS
1	A	1201	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	317	ASN
1	A	346	ASN
1	A	392	ASN
1	A	439	GLN
1	A	452	ASN
1	A	611	ASN
1	A	665	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	703	GLN
1	A	883	GLN
1	A	947	GLN
1	A	959	ASN
1	A	975	GLN
1	A	978	GLN
1	A	1001	ASN
1	A	1008	ASN
1	A	1034	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	68/112 (60%)	15 (22%)	3 (4%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	3	A
2	B	6	A
2	B	7	C
2	B	8	C
2	B	18	C
2	B	19	U
2	B	20	G
2	B	33	G
2	B	65	A
2	B	87	U
2	B	88	U
2	B	90	G
2	B	95	G
2	B	97	A
2	B	98	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	19	U
2	B	64	G
2	B	87	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

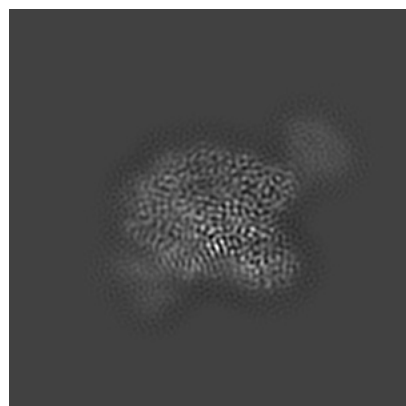
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31807. These allow visual inspection of the internal detail of the map and identification of artifacts.

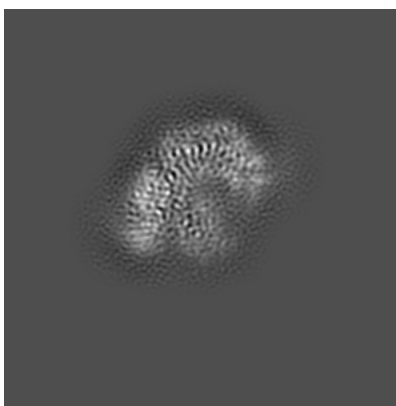
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

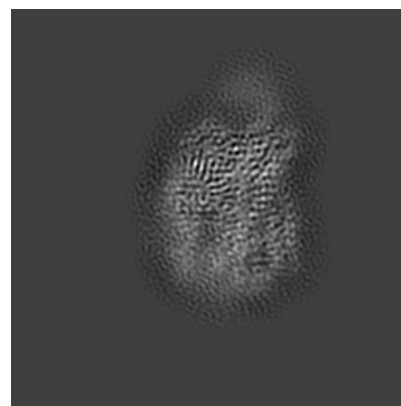
6.1.1 Primary map



X

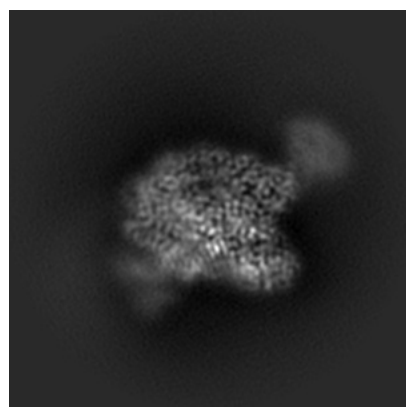


Y

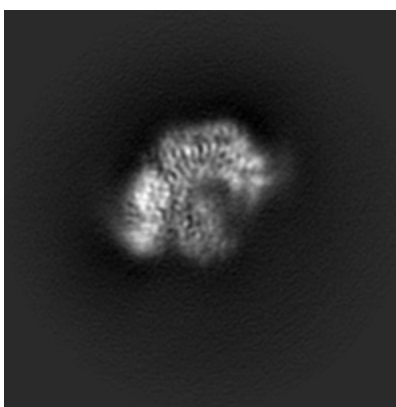


Z

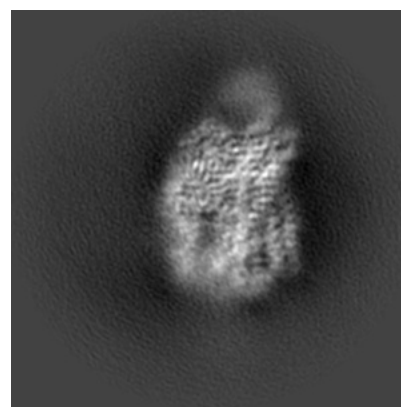
6.1.2 Raw map



X



Y

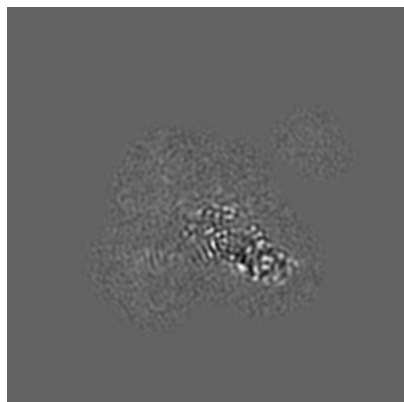


Z

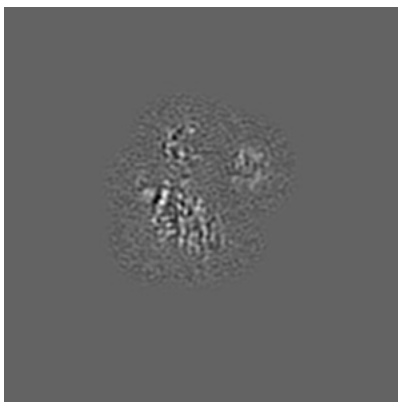
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

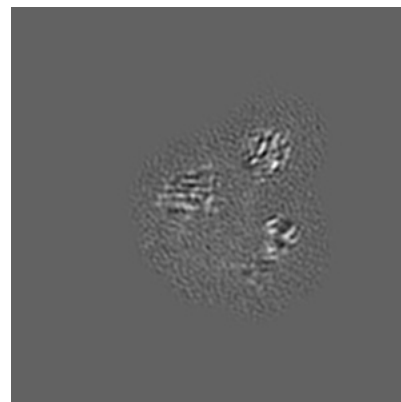
6.2.1 Primary map



X Index: 96

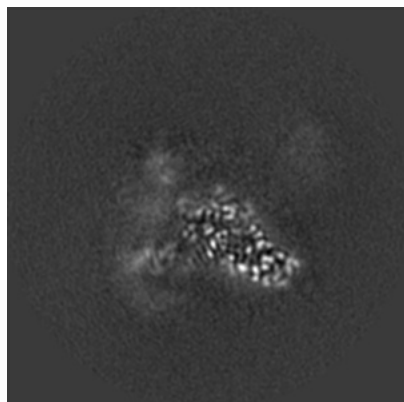


Y Index: 96

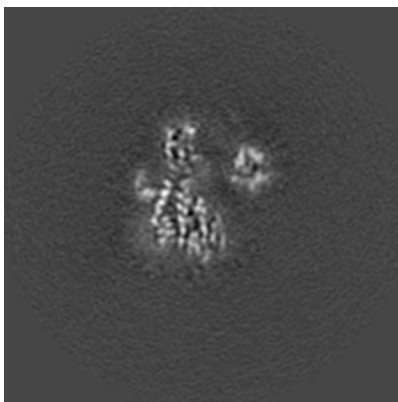


Z Index: 96

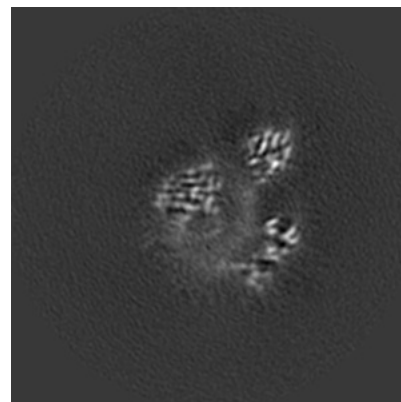
6.2.2 Raw map



X Index: 96



Y Index: 96

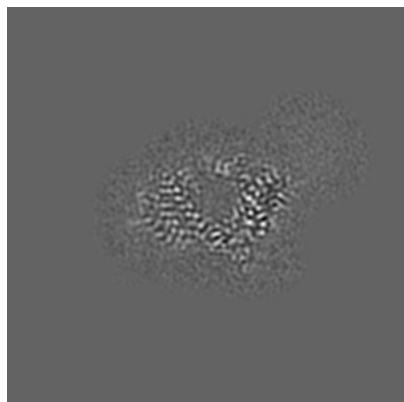


Z Index: 96

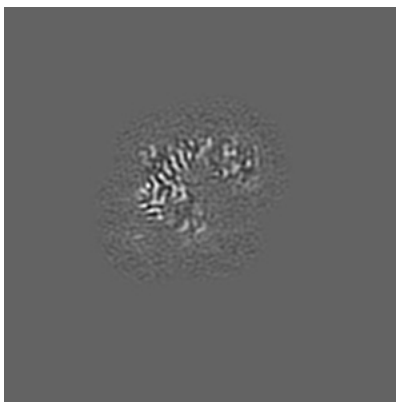
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

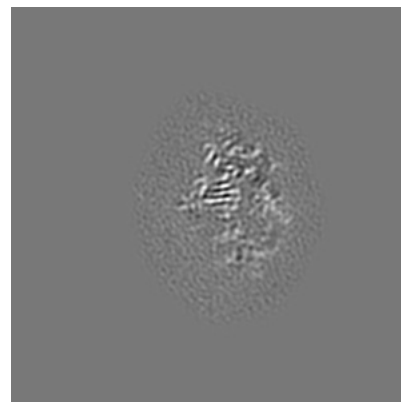
6.3.1 Primary map



X Index: 123

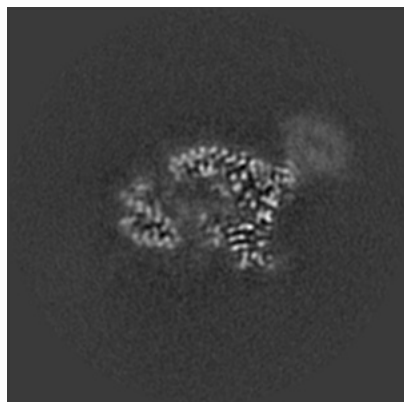


Y Index: 112

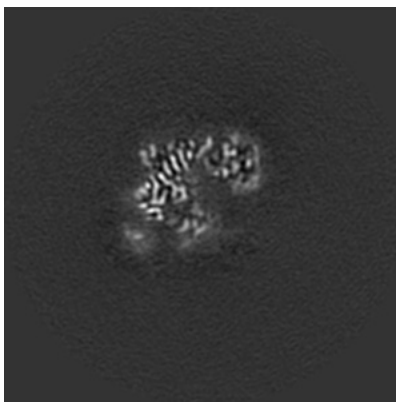


Z Index: 78

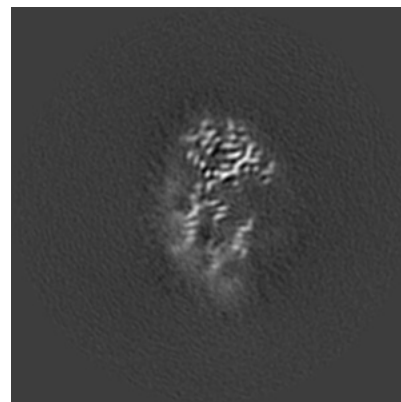
6.3.2 Raw map



X Index: 117



Y Index: 112

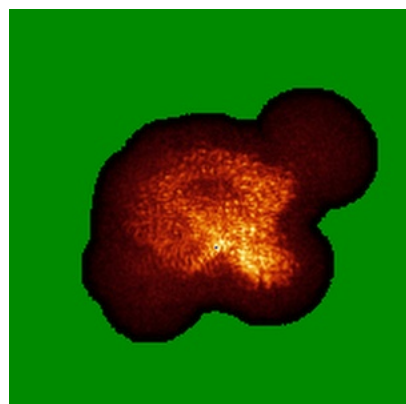


Z Index: 72

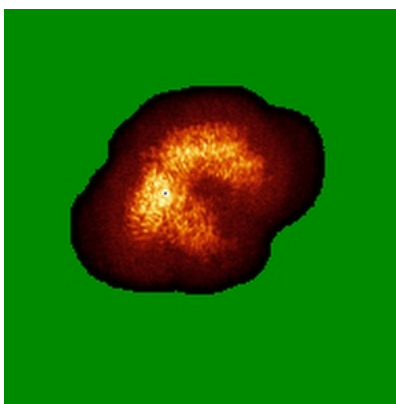
The images above show the largest variance slices of the map in three orthogonal directions.

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

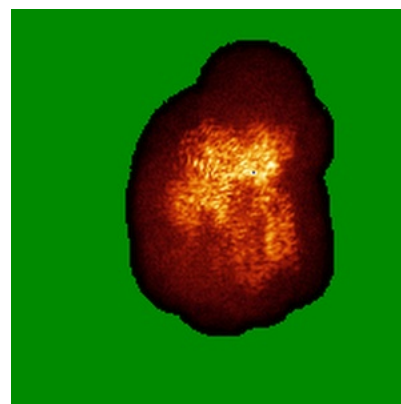
6.4.1 Primary map



X

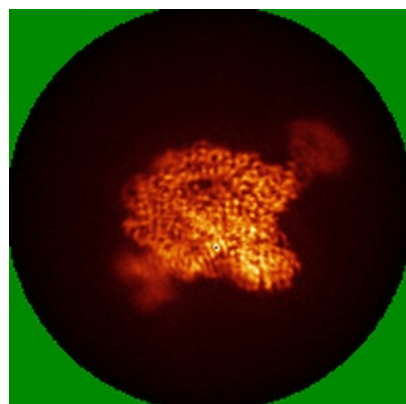


Y

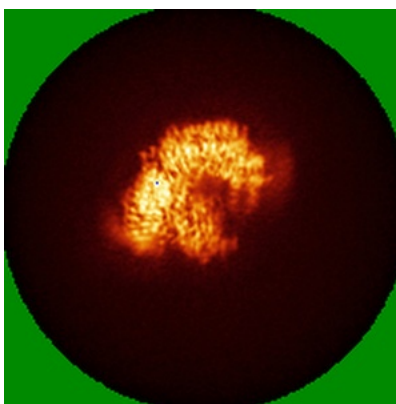


Z

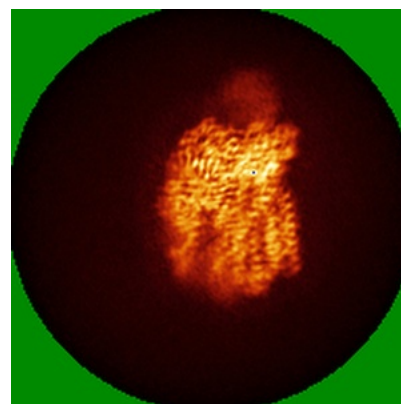
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



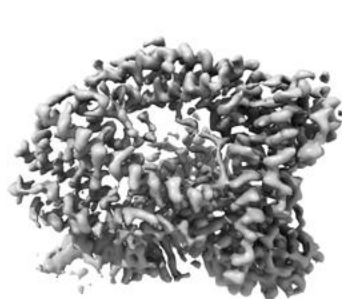
Y



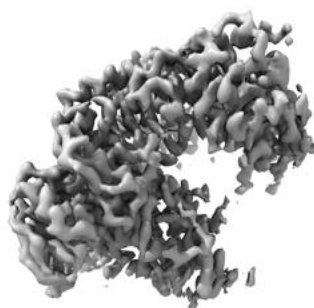
Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

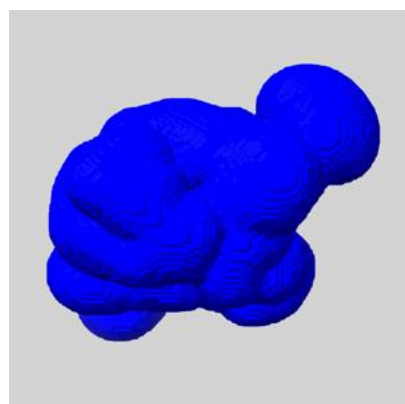
6.6 Mask visualisation [i](#)

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

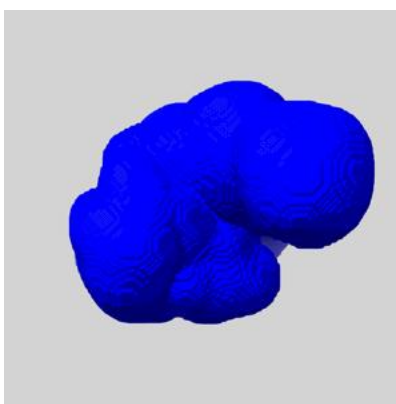
A mask typically either:

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

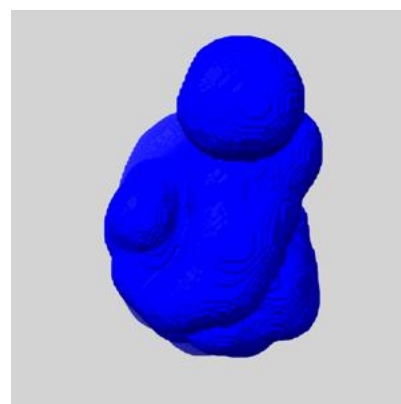
6.6.1 emd_31807_msk_1.map [i](#)



X



Y

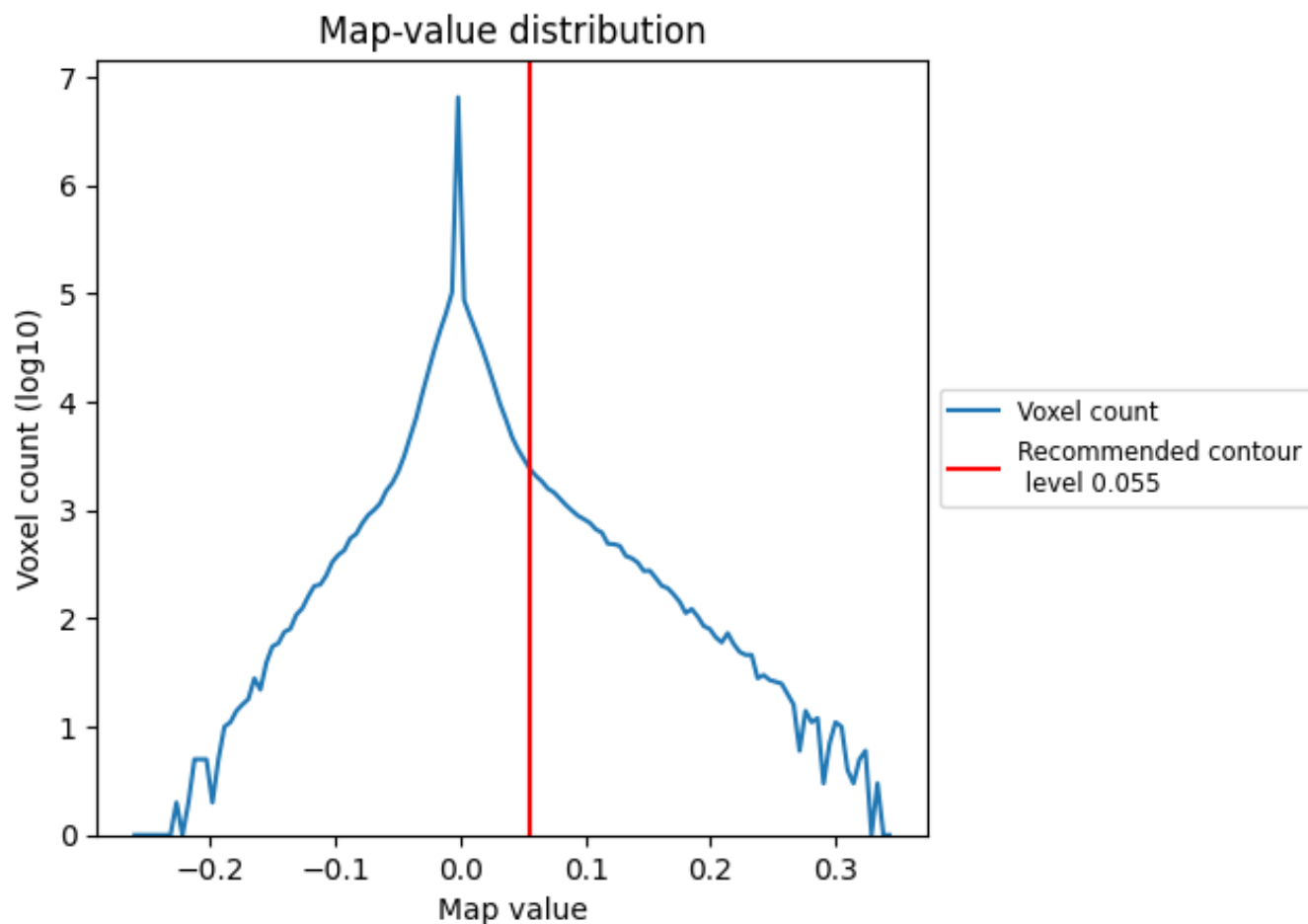


Z

7 Map analysis [i](#)

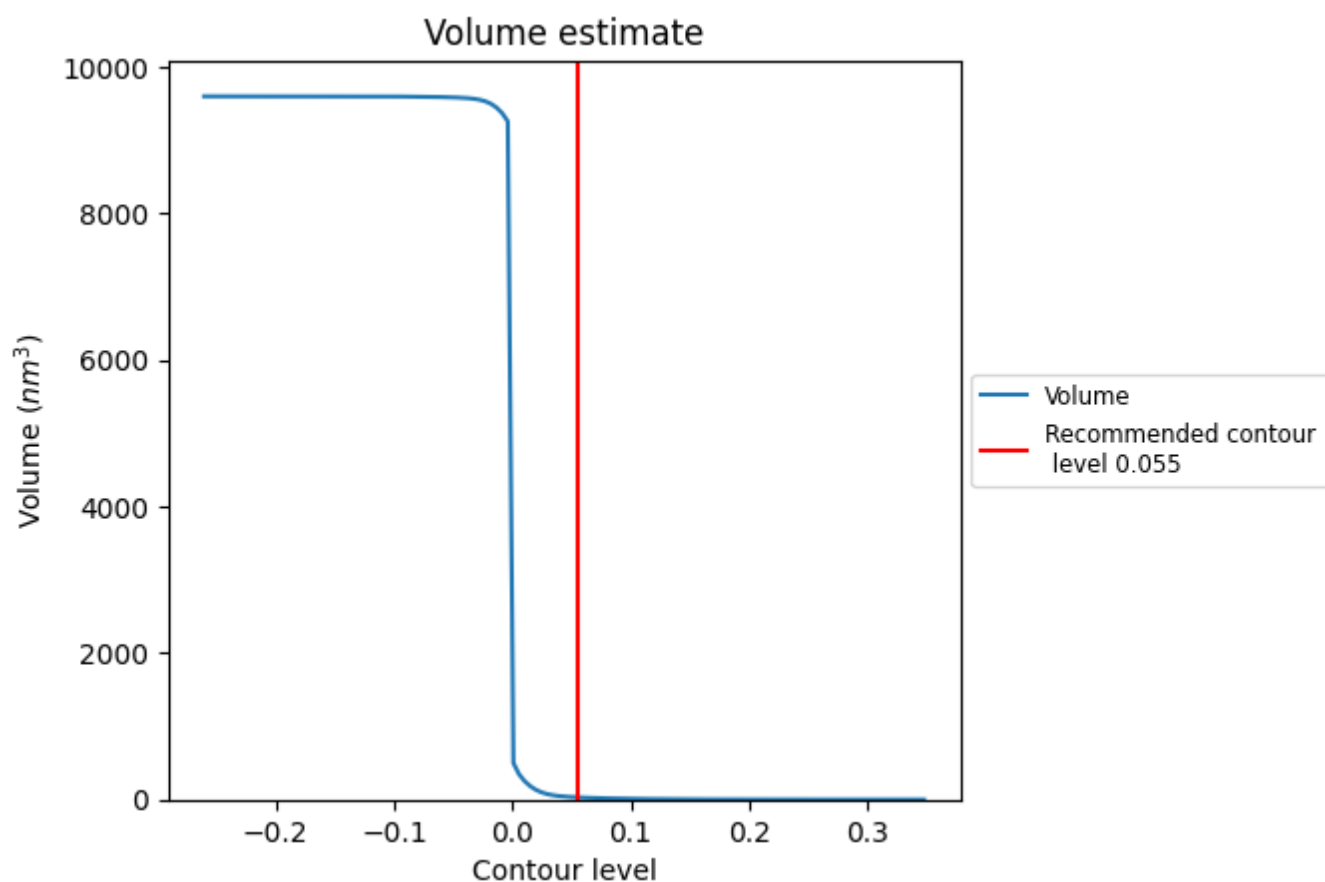
This section contains the results of statistical analysis of the map.

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.

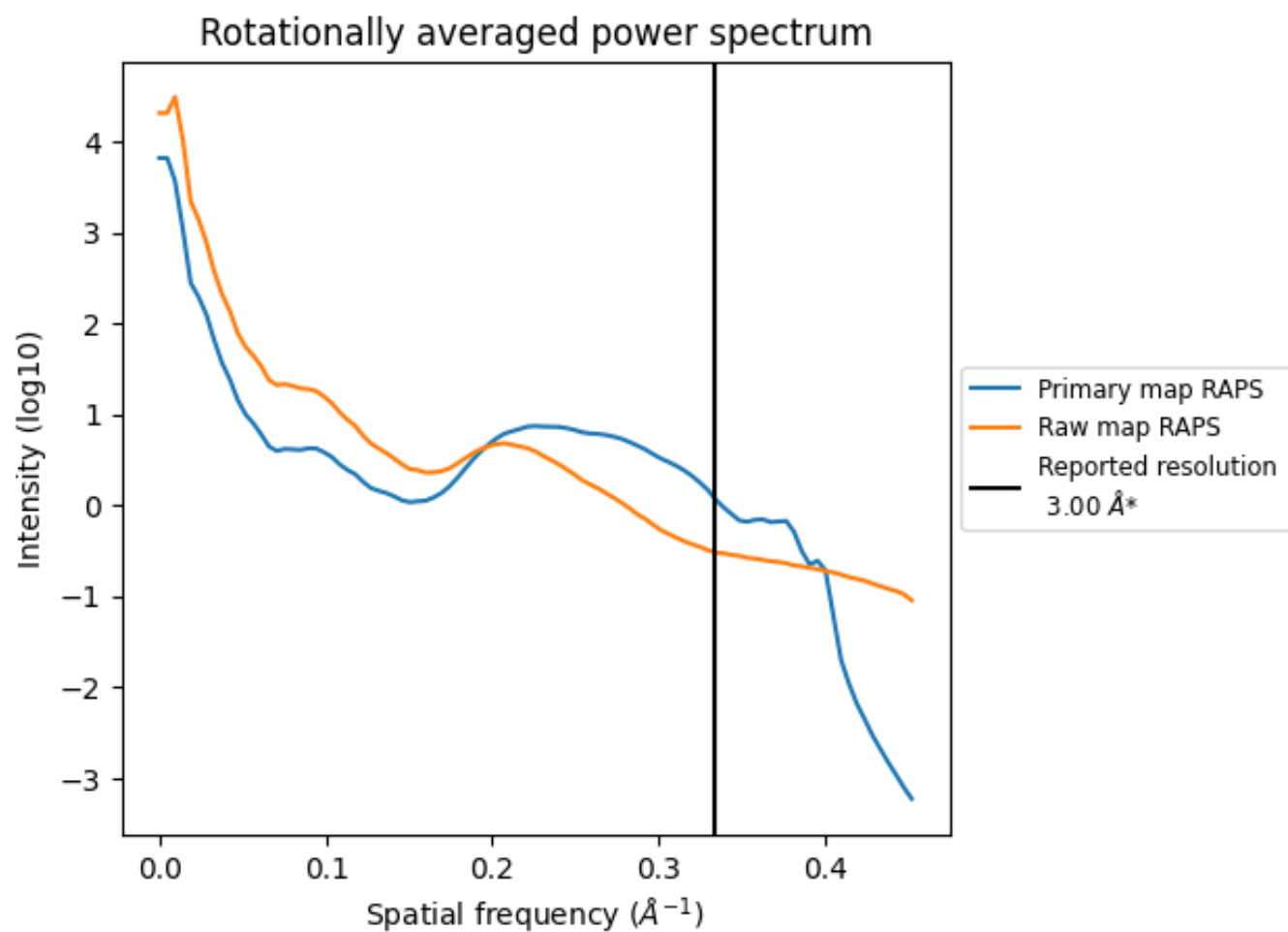
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 30 nm³; this corresponds to an approximate mass of 27 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 ⓘ

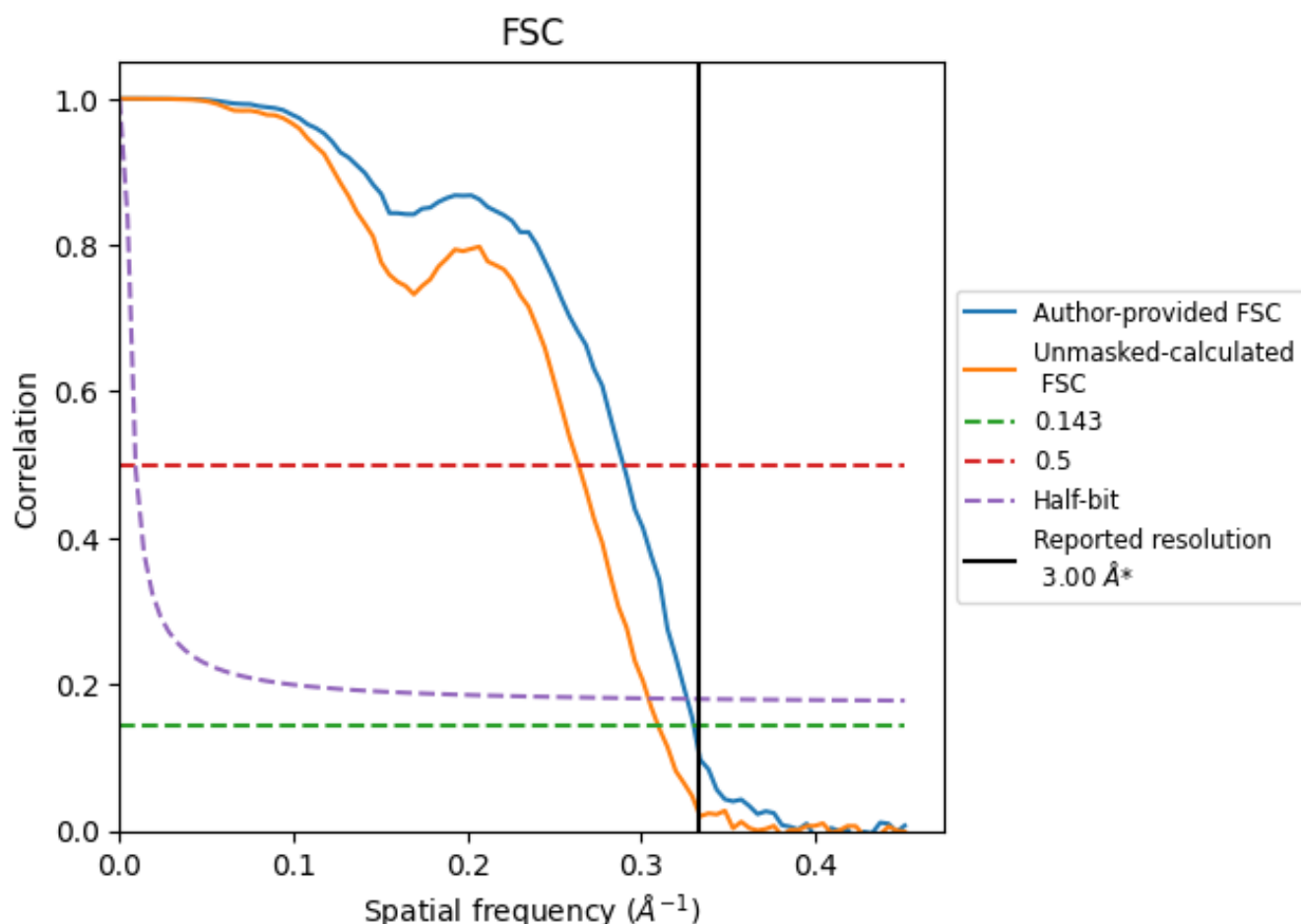


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

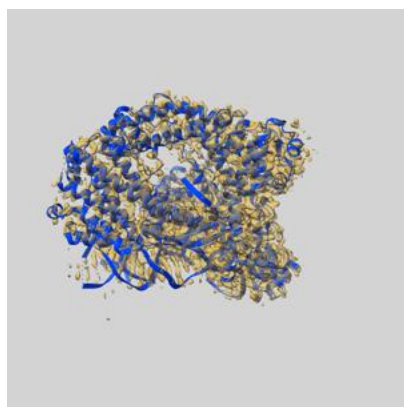
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.45	3.06
Unmasked-calculated*	3.23	3.79	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

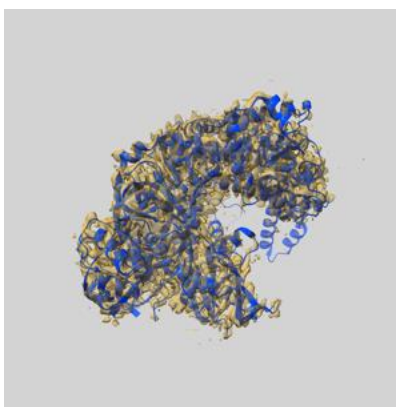
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31807 and PDB model 7V93. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

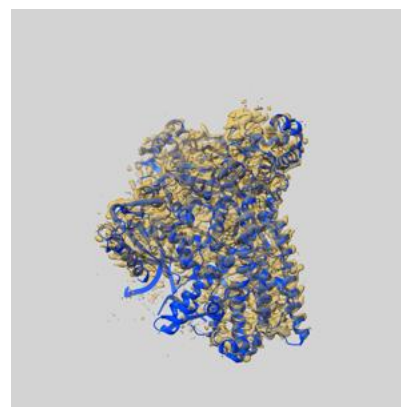
9.1 Map-model overlay [i](#)



X



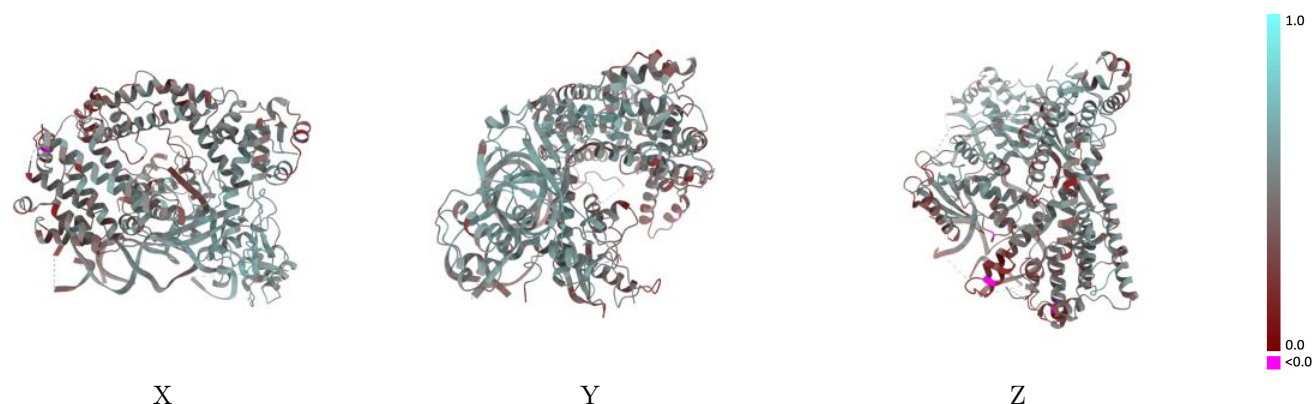
Y



Z

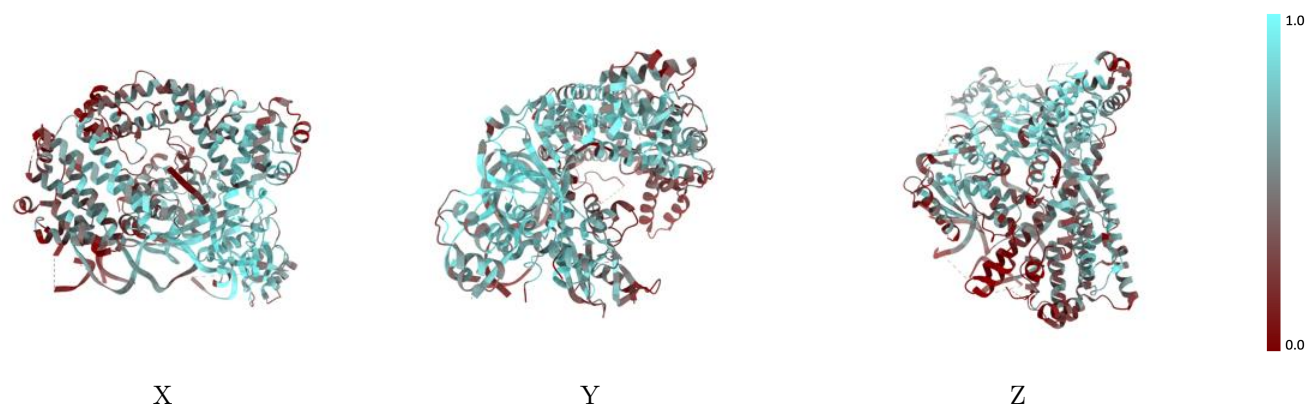
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



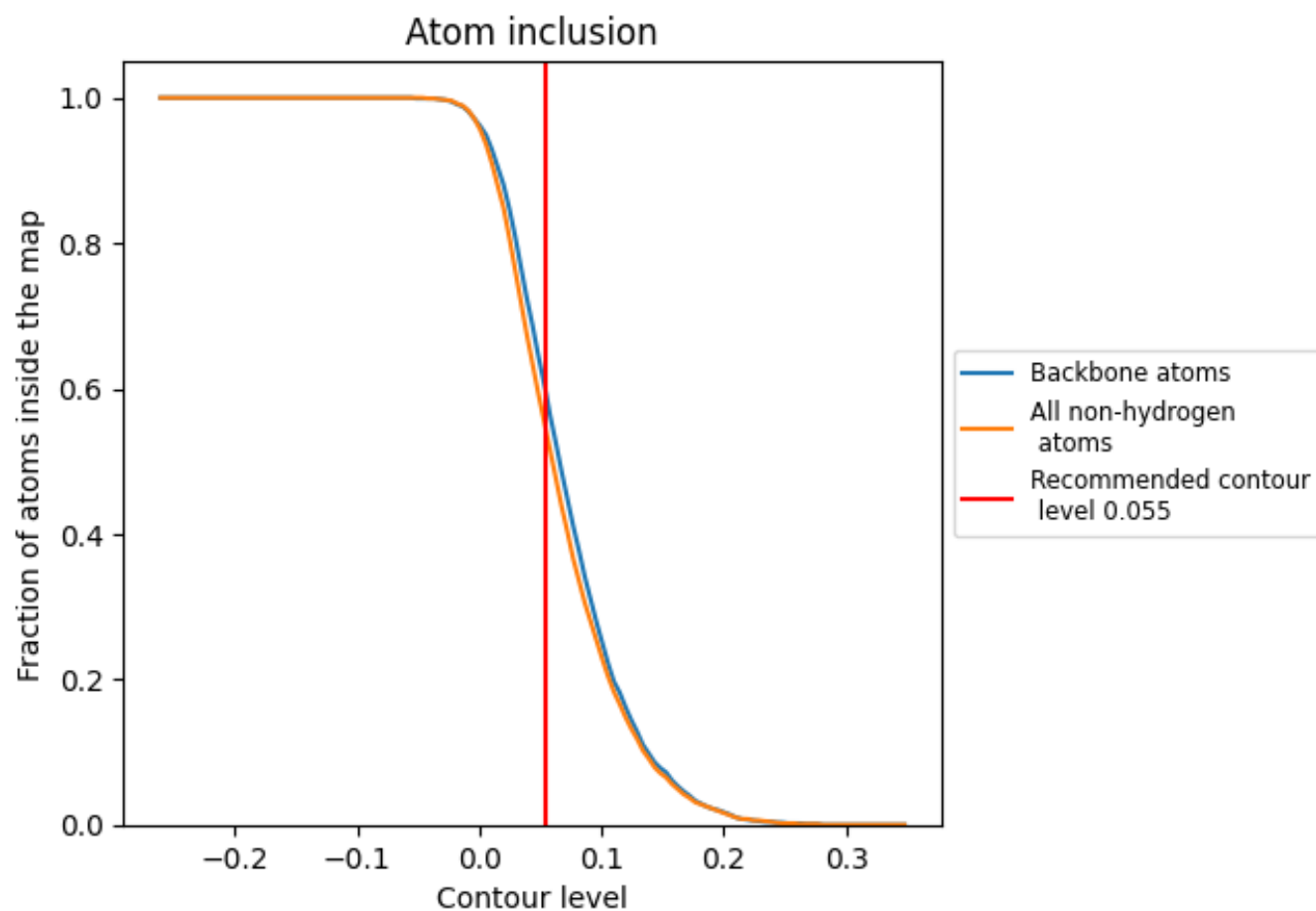
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 54% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5380	<div><div></div></div> 0.4720
A	<div><div></div></div> 0.5380	<div><div></div></div> 0.4700
B	<div><div></div></div> 0.5400	<div><div></div></div> 0.4830

