



Full wwPDB EM Validation Report ⓘ

Sep 15, 2025 – 10:51 am BST

PDB ID : 9GQN / pdb_00009gqn
EMDB ID : EMD-51507
Title : Cryo-EM map of dimeric AvrSr35
Authors : Macha, A.; Gunkel, M.; Lawson, A.W.; Schulze-Lefert, P.; Behrmann, E.
Deposited on : 2024-09-09
Resolution : 3.10 Å(reported)
Based on initial model : 7XDS

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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

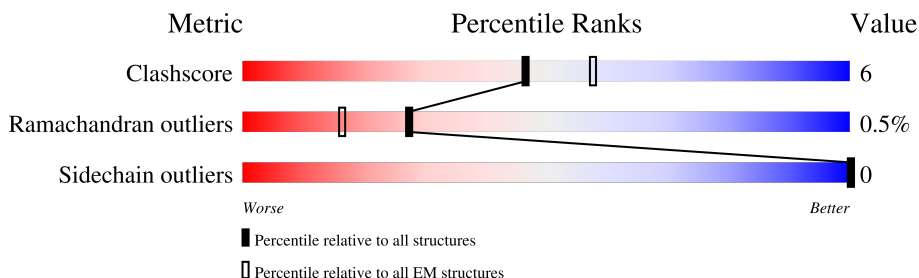
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	625	<div> <div>12%</div> <div>56%</div> <div>10%</div> <div>35%</div> </div>
1	B	625	<div> <div>12%</div> <div>56%</div> <div>10%</div> <div>35%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6718 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 Avirulence factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	408	Total	C	N	O	S	0	0
			3359	2165	550	634	10		
1	B	408	Total	C	N	O	S	0	0
			3359	2165	550	634	10		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP A0A5B0N367
A	576	ASN	-	expression tag	UNP A0A5B0N367
A	577	PRO	-	expression tag	UNP A0A5B0N367
A	578	ALA	-	expression tag	UNP A0A5B0N367
A	579	PHE	-	expression tag	UNP A0A5B0N367
A	580	LEU	-	expression tag	UNP A0A5B0N367
A	581	TYR	-	expression tag	UNP A0A5B0N367
A	582	LYS	-	expression tag	UNP A0A5B0N367
A	583	VAL	-	expression tag	UNP A0A5B0N367
A	584	VAL	-	expression tag	UNP A0A5B0N367
A	585	ASP	-	expression tag	UNP A0A5B0N367
A	586	ILE	-	expression tag	UNP A0A5B0N367
A	587	LYS	-	expression tag	UNP A0A5B0N367
A	588	ALA	-	expression tag	UNP A0A5B0N367
A	589	ALA	-	expression tag	UNP A0A5B0N367
A	590	ASP	-	expression tag	UNP A0A5B0N367
A	591	ILE	-	expression tag	UNP A0A5B0N367
A	592	THR	-	expression tag	UNP A0A5B0N367
A	593	SER	-	expression tag	UNP A0A5B0N367
A	594	LEU	-	expression tag	UNP A0A5B0N367
A	595	TYR	-	expression tag	UNP A0A5B0N367
A	596	LYS	-	expression tag	UNP A0A5B0N367
A	597	LYS	-	expression tag	UNP A0A5B0N367
A	598	VAL	-	expression tag	UNP A0A5B0N367
A	599	GLY	-	expression tag	UNP A0A5B0N367
A	600	TRP	-	expression tag	UNP A0A5B0N367

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Chain	Residue	Modelled	Actual	Comment	Reference
A	601	SER	-	expression tag	UNP A0A5B0N367
A	602	HIS	-	expression tag	UNP A0A5B0N367
A	603	PRO	-	expression tag	UNP A0A5B0N367
A	604	GLN	-	expression tag	UNP A0A5B0N367
A	605	PHE	-	expression tag	UNP A0A5B0N367
A	606	GLU	-	expression tag	UNP A0A5B0N367
A	607	LYS	-	expression tag	UNP A0A5B0N367
A	608	GLY	-	expression tag	UNP A0A5B0N367
A	609	GLY	-	expression tag	UNP A0A5B0N367
A	610	GLY	-	expression tag	UNP A0A5B0N367
A	611	SER	-	expression tag	UNP A0A5B0N367
A	612	GLY	-	expression tag	UNP A0A5B0N367
A	613	GLY	-	expression tag	UNP A0A5B0N367
A	614	GLY	-	expression tag	UNP A0A5B0N367
A	615	SER	-	expression tag	UNP A0A5B0N367
A	616	GLY	-	expression tag	UNP A0A5B0N367
A	617	GLY	-	expression tag	UNP A0A5B0N367
A	618	GLY	-	expression tag	UNP A0A5B0N367
A	619	SER	-	expression tag	UNP A0A5B0N367
A	620	TRP	-	expression tag	UNP A0A5B0N367
A	621	SER	-	expression tag	UNP A0A5B0N367
A	622	HIS	-	expression tag	UNP A0A5B0N367
A	623	PRO	-	expression tag	UNP A0A5B0N367
A	624	GLN	-	expression tag	UNP A0A5B0N367
A	625	PHE	-	expression tag	UNP A0A5B0N367
A	626	GLU	-	expression tag	UNP A0A5B0N367
A	627	LYS	-	expression tag	UNP A0A5B0N367
A	628	GLY	-	expression tag	UNP A0A5B0N367
A	629	THR	-	expression tag	UNP A0A5B0N367
A	630	GLU	-	expression tag	UNP A0A5B0N367
A	631	LEU	-	expression tag	UNP A0A5B0N367
A	632	GLY	-	expression tag	UNP A0A5B0N367
A	633	SER	-	expression tag	UNP A0A5B0N367
A	634	THR	-	expression tag	UNP A0A5B0N367
A	635	MET	-	expression tag	UNP A0A5B0N367
A	636	ALA	-	expression tag	UNP A0A5B0N367
A	637	SER	-	expression tag	UNP A0A5B0N367
A	638	TYR	-	expression tag	UNP A0A5B0N367
A	639	PRO	-	expression tag	UNP A0A5B0N367
A	640	TYR	-	expression tag	UNP A0A5B0N367
A	641	ASP	-	expression tag	UNP A0A5B0N367
A	642	VAL	-	expression tag	UNP A0A5B0N367

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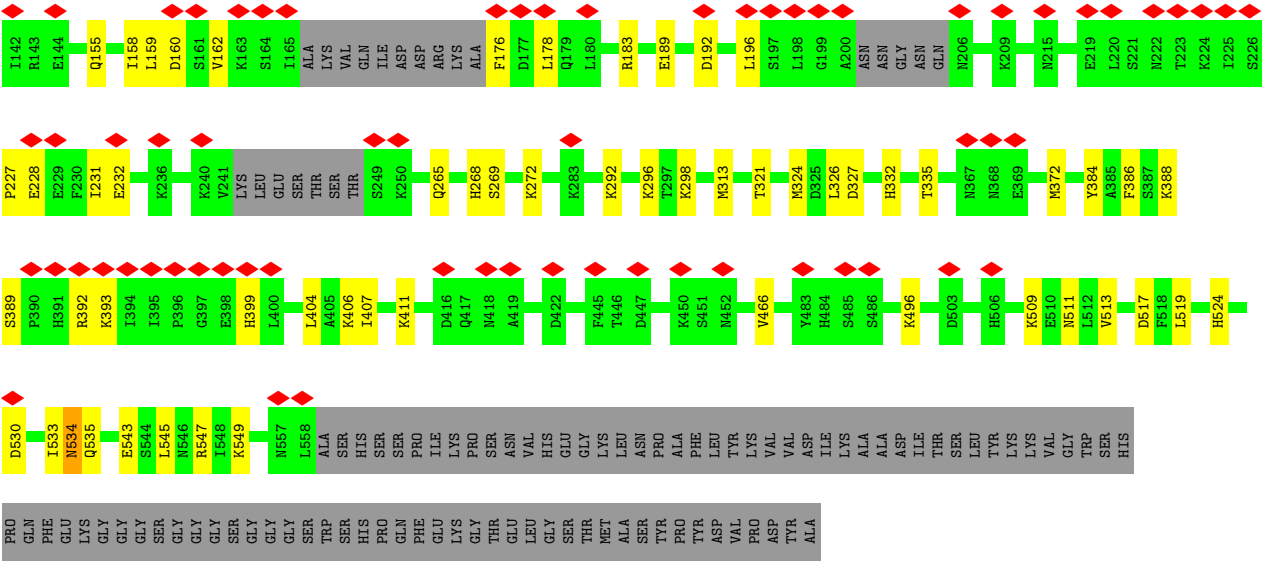
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Chain	Residue	Modelled	Actual	Comment	Reference
A	643	PRO	-	expression tag	UNP A0A5B0N367
A	644	ASP	-	expression tag	UNP A0A5B0N367
A	645	TYR	-	expression tag	UNP A0A5B0N367
A	646	ALA	-	expression tag	UNP A0A5B0N367
B	22	MET	-	initiating methionine	UNP A0A5B0N367
B	576	ASN	-	expression tag	UNP A0A5B0N367
B	577	PRO	-	expression tag	UNP A0A5B0N367
B	578	ALA	-	expression tag	UNP A0A5B0N367
B	579	PHE	-	expression tag	UNP A0A5B0N367
B	580	LEU	-	expression tag	UNP A0A5B0N367
B	581	TYR	-	expression tag	UNP A0A5B0N367
B	582	LYS	-	expression tag	UNP A0A5B0N367
B	583	VAL	-	expression tag	UNP A0A5B0N367
B	584	VAL	-	expression tag	UNP A0A5B0N367
B	585	ASP	-	expression tag	UNP A0A5B0N367
B	586	ILE	-	expression tag	UNP A0A5B0N367
B	587	LYS	-	expression tag	UNP A0A5B0N367
B	588	ALA	-	expression tag	UNP A0A5B0N367
B	589	ALA	-	expression tag	UNP A0A5B0N367
B	590	ASP	-	expression tag	UNP A0A5B0N367
B	591	ILE	-	expression tag	UNP A0A5B0N367
B	592	THR	-	expression tag	UNP A0A5B0N367
B	593	SER	-	expression tag	UNP A0A5B0N367
B	594	LEU	-	expression tag	UNP A0A5B0N367
B	595	TYR	-	expression tag	UNP A0A5B0N367
B	596	LYS	-	expression tag	UNP A0A5B0N367
B	597	LYS	-	expression tag	UNP A0A5B0N367
B	598	VAL	-	expression tag	UNP A0A5B0N367
B	599	GLY	-	expression tag	UNP A0A5B0N367
B	600	TRP	-	expression tag	UNP A0A5B0N367
B	601	SER	-	expression tag	UNP A0A5B0N367
B	602	HIS	-	expression tag	UNP A0A5B0N367
B	603	PRO	-	expression tag	UNP A0A5B0N367
B	604	GLN	-	expression tag	UNP A0A5B0N367
B	605	PHE	-	expression tag	UNP A0A5B0N367
B	606	GLU	-	expression tag	UNP A0A5B0N367
B	607	LYS	-	expression tag	UNP A0A5B0N367
B	608	GLY	-	expression tag	UNP A0A5B0N367
B	609	GLY	-	expression tag	UNP A0A5B0N367
B	610	GLY	-	expression tag	UNP A0A5B0N367
B	611	SER	-	expression tag	UNP A0A5B0N367
B	612	GLY	-	expression tag	UNP A0A5B0N367

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Chain	Residue	Modelled	Actual	Comment	Reference
B	613	GLY	-	expression tag	UNP A0A5B0N367
B	614	GLY	-	expression tag	UNP A0A5B0N367
B	615	SER	-	expression tag	UNP A0A5B0N367
B	616	GLY	-	expression tag	UNP A0A5B0N367
B	617	GLY	-	expression tag	UNP A0A5B0N367
B	618	GLY	-	expression tag	UNP A0A5B0N367
B	619	SER	-	expression tag	UNP A0A5B0N367
B	620	TRP	-	expression tag	UNP A0A5B0N367
B	621	SER	-	expression tag	UNP A0A5B0N367
B	622	HIS	-	expression tag	UNP A0A5B0N367
B	623	PRO	-	expression tag	UNP A0A5B0N367
B	624	GLN	-	expression tag	UNP A0A5B0N367
B	625	PHE	-	expression tag	UNP A0A5B0N367
B	626	GLU	-	expression tag	UNP A0A5B0N367
B	627	LYS	-	expression tag	UNP A0A5B0N367
B	628	GLY	-	expression tag	UNP A0A5B0N367
B	629	THR	-	expression tag	UNP A0A5B0N367
B	630	GLU	-	expression tag	UNP A0A5B0N367
B	631	LEU	-	expression tag	UNP A0A5B0N367
B	632	GLY	-	expression tag	UNP A0A5B0N367
B	633	SER	-	expression tag	UNP A0A5B0N367
B	634	THR	-	expression tag	UNP A0A5B0N367
B	635	MET	-	expression tag	UNP A0A5B0N367
B	636	ALA	-	expression tag	UNP A0A5B0N367
B	637	SER	-	expression tag	UNP A0A5B0N367
B	638	TYR	-	expression tag	UNP A0A5B0N367
B	639	PRO	-	expression tag	UNP A0A5B0N367
B	640	TYR	-	expression tag	UNP A0A5B0N367
B	641	ASP	-	expression tag	UNP A0A5B0N367
B	642	VAL	-	expression tag	UNP A0A5B0N367
B	643	PRO	-	expression tag	UNP A0A5B0N367
B	644	ASP	-	expression tag	UNP A0A5B0N367
B	645	TYR	-	expression tag	UNP A0A5B0N367
B	646	ALA	-	expression tag	UNP A0A5B0N367



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	250926	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	9.234	Depositor
Minimum map value	-6.434	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	1.35	Depositor
Map size (Å)	275.84, 275.84, 275.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.862, 0.862, 0.862	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/3429	0.63	0/4612
1	B	0.17	0/3429	0.63	0/4612
All	All	0.17	0/6858	0.63	0/9224

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3359	0	3369	43	0
1	B	3359	0	3369	40	0
All	All	6718	0	6738	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (79) 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:372:MET:O	1:B:406:LYS:NZ	2.21	0.74
1:A:530:ASP:O	1:A:534:ASN:ND2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:ASP:O	1:B:534:ASN:ND2	2.20	0.74
1:A:372:MET:O	1:A:406:LYS:NZ	2.21	0.73
1:B:533:ILE:O	1:B:535:GLN:N	2.23	0.71
1:A:466:VAL:HG13	1:A:519:LEU:HD21	1.74	0.69
1:A:313:MET:O	1:A:547:ARG:NH1	2.25	0.69
1:B:313:MET:O	1:B:547:ARG:NH1	2.25	0.69
1:B:466:VAL:HG13	1:B:519:LEU:HD21	1.74	0.68
1:A:189:GLU:OE1	1:A:496:LYS:NZ	2.28	0.67
1:B:189:GLU:OE1	1:B:496:LYS:NZ	2.28	0.67
1:A:533:ILE:O	1:A:535:GLN:N	2.23	0.65
1:A:141:ASP:OD2	1:A:511:ASN:ND2	2.26	0.62
1:B:227:PRO:O	1:B:231:ILE:HG12	2.01	0.60
1:A:227:PRO:O	1:A:231:ILE:HG12	2.01	0.60
1:B:141:ASP:OD2	1:B:511:ASN:ND2	2.26	0.58
1:A:388:LYS:HE3	1:B:399:HIS:CD2	2.37	0.58
1:A:388:LYS:HE3	1:B:399:HIS:HD2	1.69	0.57
1:A:183:ARG:NH1	1:A:265:GLN:O	2.38	0.56
1:A:389:SER:O	1:A:392:ARG:NH2	2.34	0.56
1:B:192:ASP:O	1:B:196:LEU:HD13	2.04	0.56
1:A:192:ASP:O	1:A:196:LEU:HD13	2.04	0.56
1:B:183:ARG:NH1	1:B:265:GLN:O	2.38	0.56
1:B:136:GLU:HG2	1:B:162:VAL:HG11	1.89	0.54
1:A:399:HIS:HD2	1:B:388:LYS:HE3	1.73	0.54
1:A:399:HIS:CD2	1:B:388:LYS:HE3	2.43	0.54
1:B:389:SER:O	1:B:392:ARG:NH2	2.34	0.54
1:A:136:GLU:HG2	1:A:162:VAL:HG11	1.89	0.53
1:B:545:LEU:HD11	1:B:549:LYS:HE3	1.91	0.53
1:A:545:LEU:HD11	1:A:549:LYS:HE3	1.91	0.52
1:B:298:LYS:HE3	1:B:324:MET:HE3	1.93	0.51
1:B:543:GLU:OE2	1:B:547:ARG:NH2	2.44	0.51
1:A:543:GLU:OE2	1:A:547:ARG:NH2	2.44	0.50
1:A:298:LYS:HE3	1:A:324:MET:HE3	1.93	0.50
1:A:268:HIS:HD2	1:A:335:THR:HG21	1.77	0.50
1:A:131:LYS:HD2	1:A:524:HIS:CD2	2.47	0.49
1:B:292:LYS:HB3	1:B:296:LYS:HZ1	1.77	0.49
1:B:131:LYS:HD2	1:B:524:HIS:CD2	2.47	0.49
1:B:268:HIS:HD2	1:B:335:THR:HG21	1.77	0.48
1:A:292:LYS:HB3	1:A:296:LYS:NZ	2.28	0.48
1:B:292:LYS:HB3	1:B:296:LYS:NZ	2.28	0.48
1:A:292:LYS:HB3	1:A:296:LYS:HZ1	1.78	0.48
1:B:268:HIS:NE2	1:B:272:LYS:HE3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LYS:O	1:A:513:VAL:HG23	2.14	0.48
1:B:332:HIS:O	1:B:335:THR:HG22	2.14	0.47
1:A:332:HIS:O	1:A:335:THR:HG22	2.14	0.47
1:A:407:ILE:HG22	1:A:411:LYS:HE2	1.96	0.47
1:A:268:HIS:NE2	1:A:272:LYS:HE3	2.29	0.47
1:B:509:LYS:O	1:B:513:VAL:HG23	2.14	0.47
1:A:176:PHE:C	1:A:178:LEU:H	2.23	0.46
1:B:393:LYS:NZ	1:B:404:LEU:HD11	2.30	0.46
1:A:158:ILE:O	1:A:160:ASP:N	2.45	0.46
1:A:393:LYS:NZ	1:A:404:LEU:HD11	2.30	0.46
1:B:407:ILE:HG22	1:B:411:LYS:HE2	1.96	0.46
1:B:183:ARG:NH1	1:B:269:SER:HB2	2.31	0.46
1:A:183:ARG:NH1	1:A:269:SER:HB2	2.31	0.45
1:B:158:ILE:O	1:B:160:ASP:N	2.45	0.44
1:B:176:PHE:C	1:B:178:LEU:H	2.23	0.44
1:B:466:VAL:HG13	1:B:519:LEU:CD2	2.46	0.44
1:A:155:GLN:NE2	1:A:327:ASP:HA	2.33	0.44
1:B:155:GLN:NE2	1:B:327:ASP:HA	2.33	0.44
1:A:155:GLN:NE2	1:A:326:LEU:O	2.49	0.44
1:A:404:LEU:HD12	1:A:404:LEU:H	1.83	0.43
1:B:384:TYR:CZ	1:B:388:LYS:HD3	2.53	0.43
1:B:404:LEU:H	1:B:404:LEU:HD12	1.83	0.43
1:A:384:TYR:CZ	1:A:388:LYS:HD3	2.53	0.43
1:B:386:PHE:HE1	1:B:393:LYS:HE3	1.83	0.43
1:A:386:PHE:HE1	1:A:393:LYS:HE3	1.83	0.43
1:B:321:THR:HA	1:B:324:MET:HE2	2.00	0.43
1:A:321:THR:HA	1:A:324:MET:HE2	2.00	0.42
1:B:155:GLN:NE2	1:B:326:LEU:O	2.49	0.42
1:B:132:LYS:NZ	1:B:517:ASP:OD1	2.44	0.41
1:A:411:LYS:HB2	1:A:411:LYS:HE3	1.86	0.41
1:A:466:VAL:HG13	1:A:519:LEU:CD2	2.46	0.41
1:A:268:HIS:CD2	1:A:335:THR:HG21	2.56	0.41
1:B:228:GLU:O	1:B:232:GLU:HG3	2.21	0.41
1:A:228:GLU:O	1:A:232:GLU:HG3	2.21	0.41
1:A:505:LYS:HE3	1:A:505:LYS:HB2	1.88	0.41
1:A:519:LEU:O	1:A:522:THR:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	400/625 (64%)	376 (94%)	22 (6%)	2 (0%)	25	58
1	B	400/625 (64%)	376 (94%)	22 (6%)	2 (0%)	25	58
All	All	800/1250 (64%)	752 (94%)	44 (6%)	4 (0%)	27	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	534	ASN
1	B	534	ASN
1	A	159	LEU
1	B	159	LEU

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	382/566 (68%)	382 (100%)	0	100	100
1	B	382/566 (68%)	382 (100%)	0	100	100
All	All	764/1132 (68%)	764 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	A	268	HIS
1	A	399	HIS
1	A	474	HIS
1	A	529	GLN
1	A	534	ASN
1	B	265	GLN
1	B	268	HIS
1	B	399	HIS
1	B	474	HIS
1	B	529	GLN
1	B	534	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

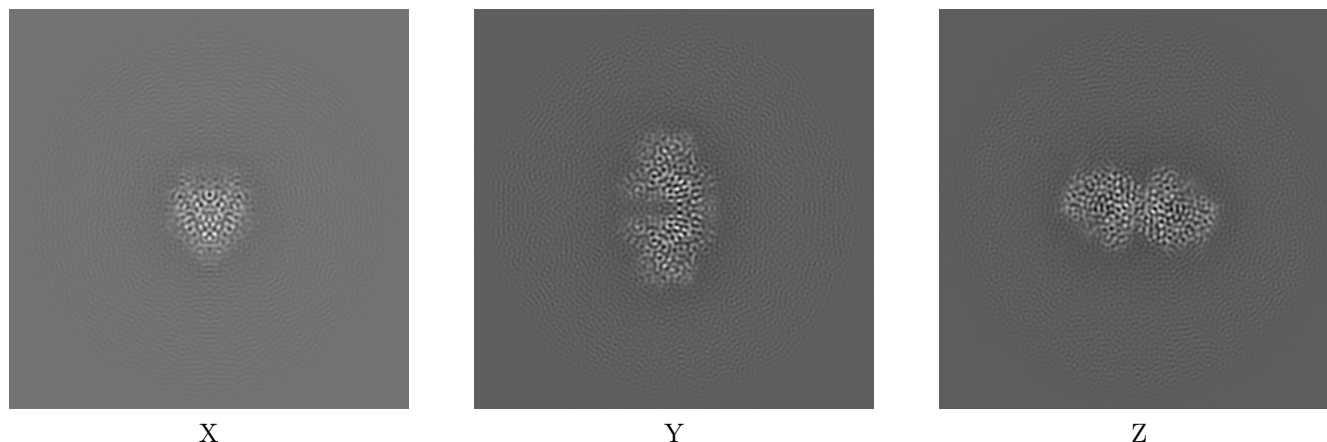
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51507. These allow visual inspection of the internal detail of the map and identification of artifacts.

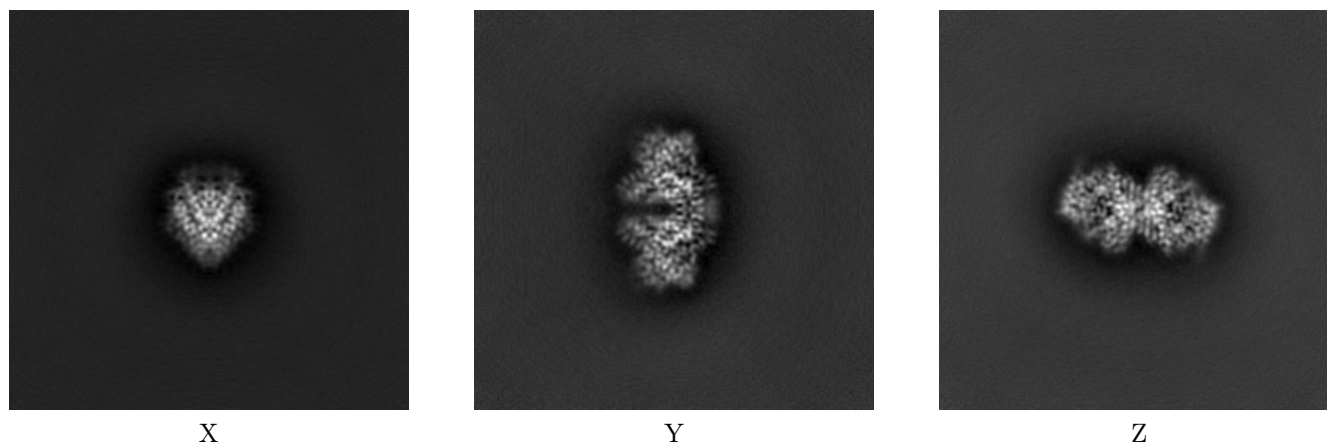
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



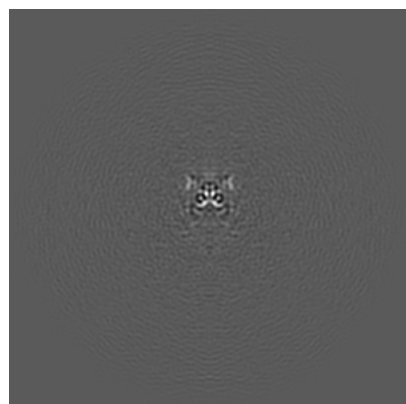
6.1.2 Raw map



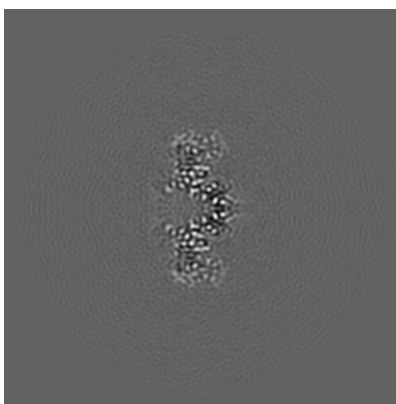
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

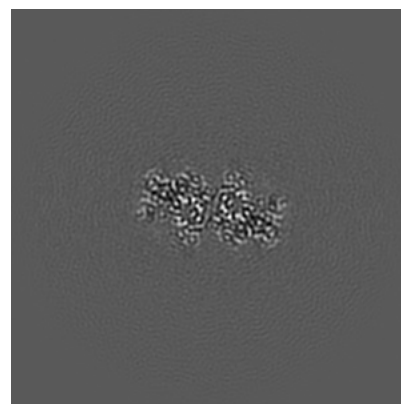
6.2.1 Primary map



X Index: 160

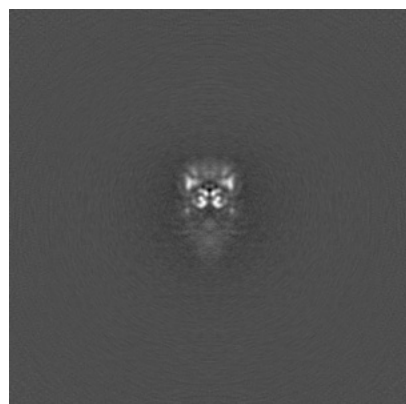


Y Index: 160

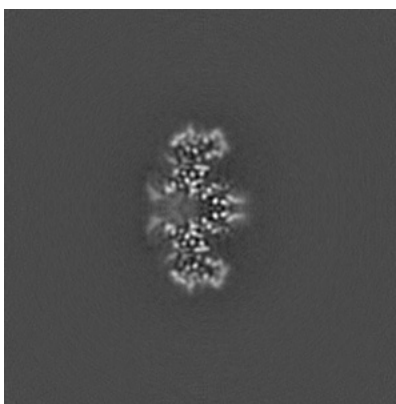


Z Index: 160

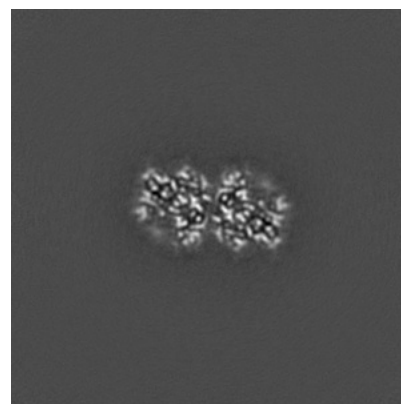
6.2.2 Raw map



X Index: 160



Y Index: 160

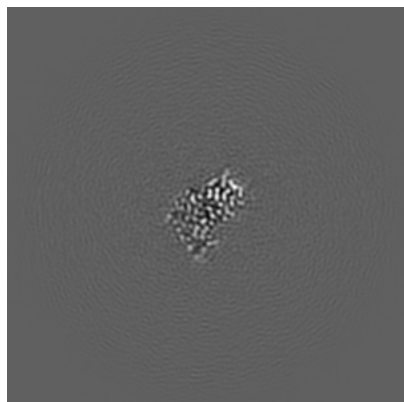


Z Index: 160

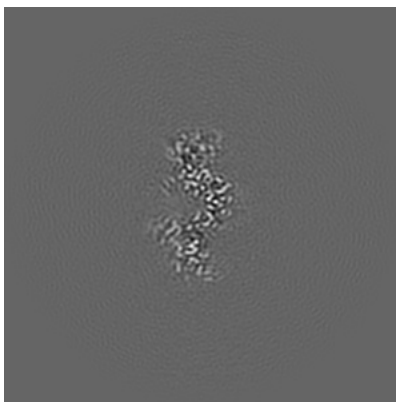
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

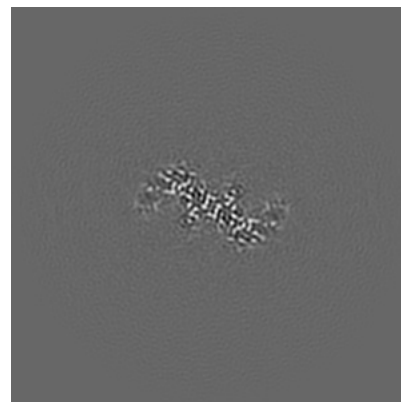
6.3.1 Primary map



X Index: 143

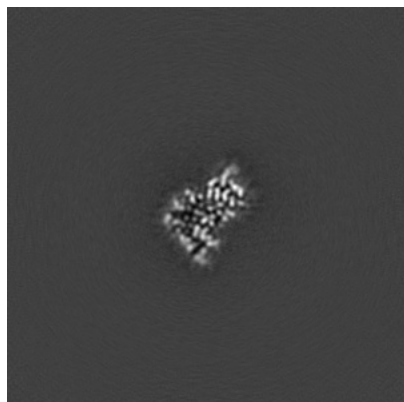


Y Index: 156

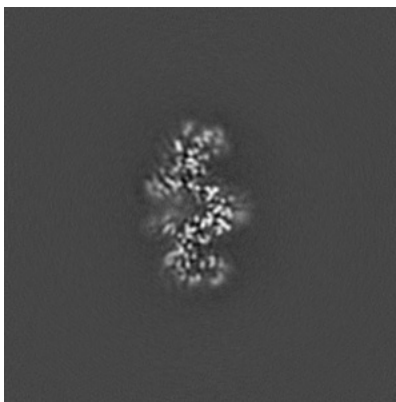


Z Index: 168

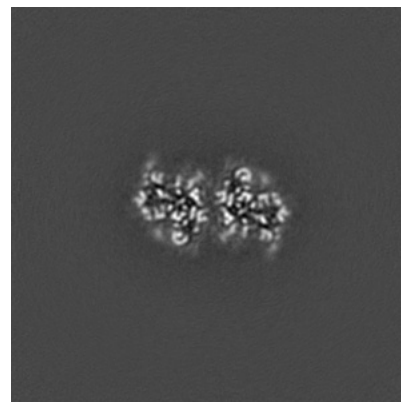
6.3.2 Raw map



X Index: 143



Y Index: 163

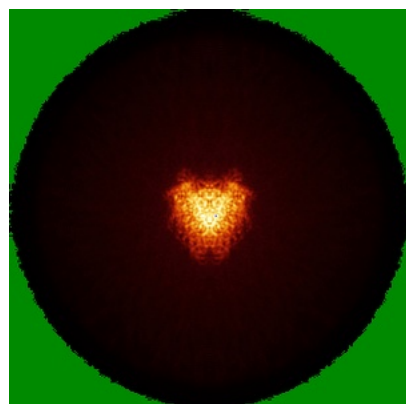


Z Index: 155

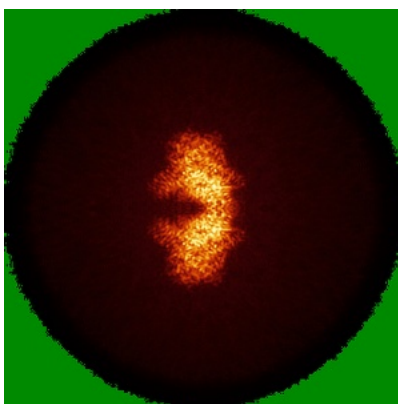
The images above show the largest variance slices of the map in three orthogonal directions.

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

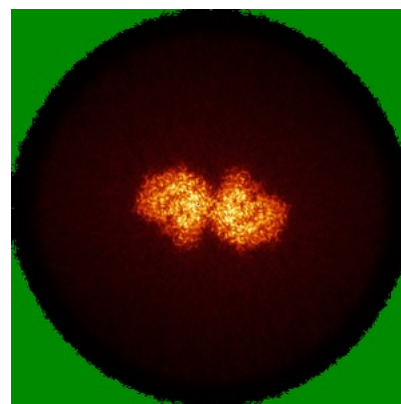
6.4.1 Primary map



X

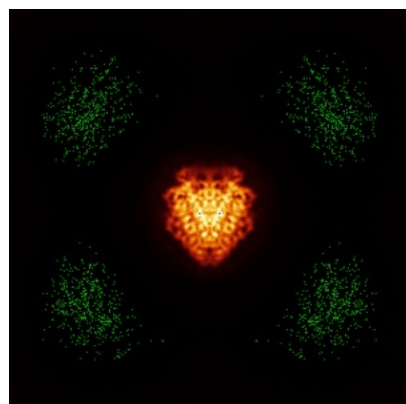


Y

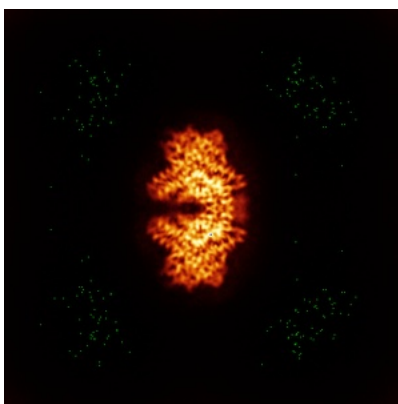


Z

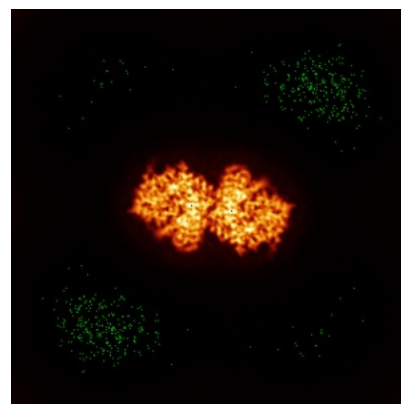
6.4.2 Raw map



X



Y

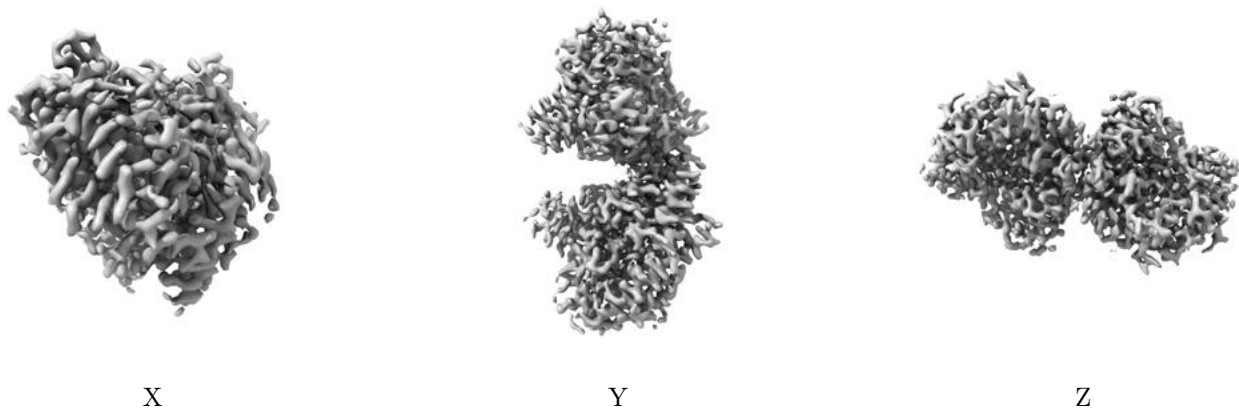


Z

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.

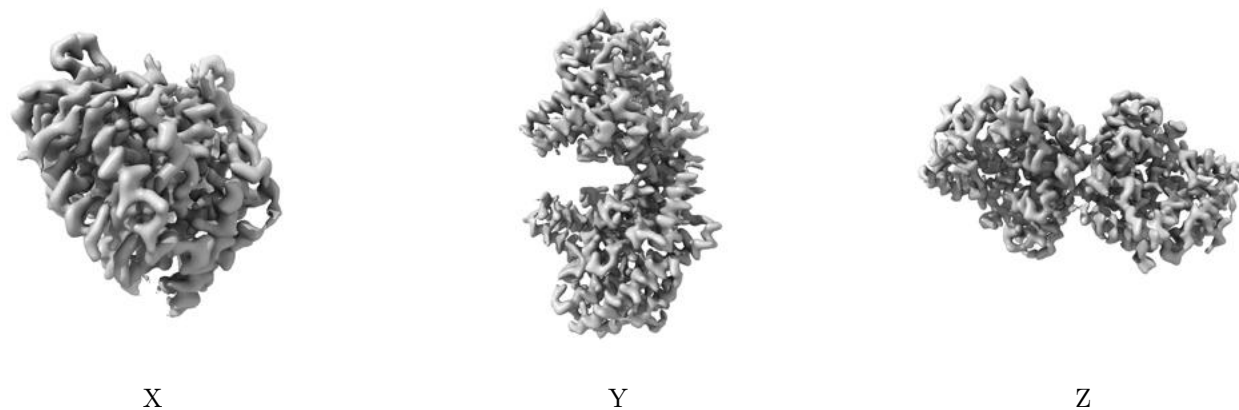
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.35. 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.

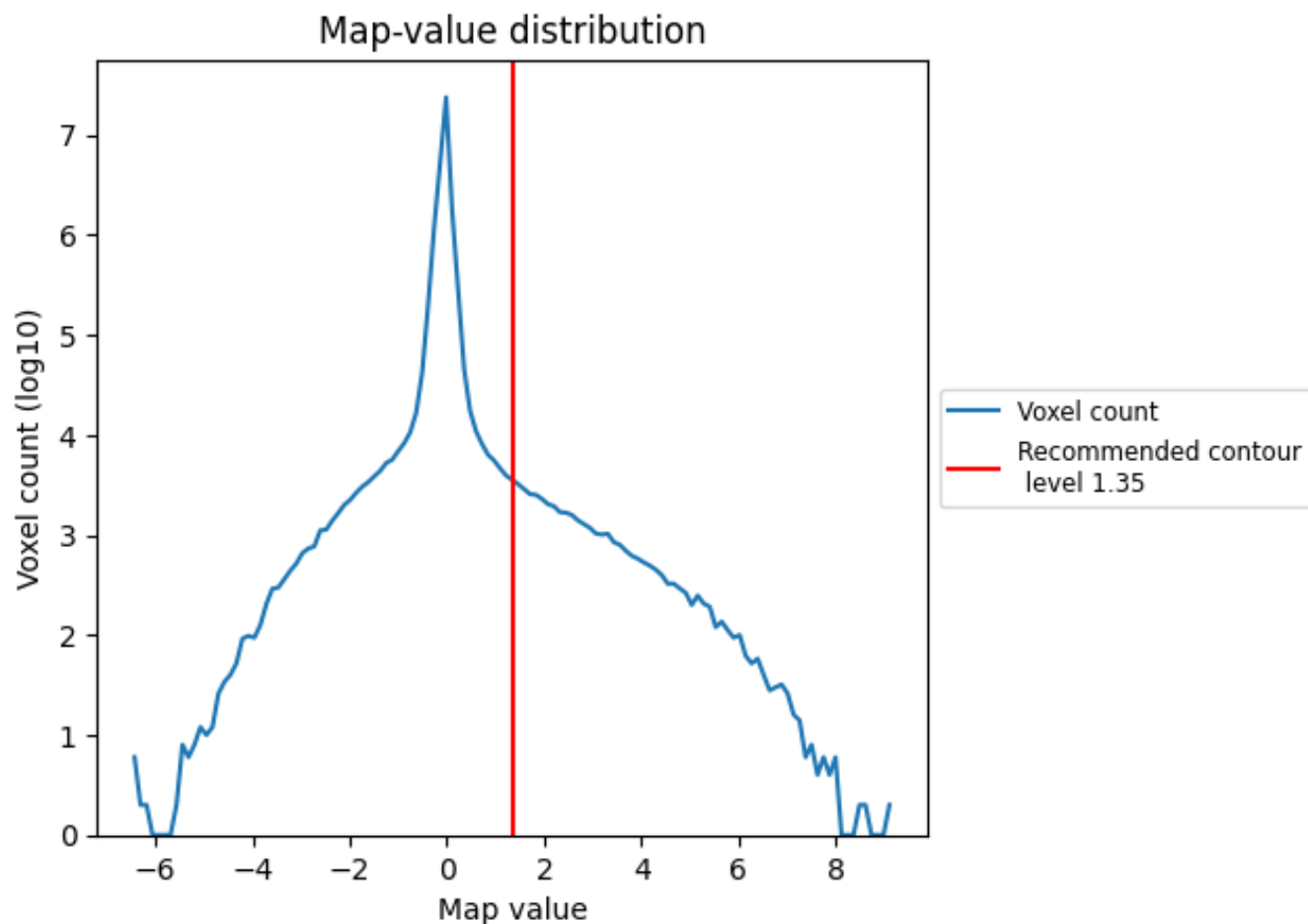
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

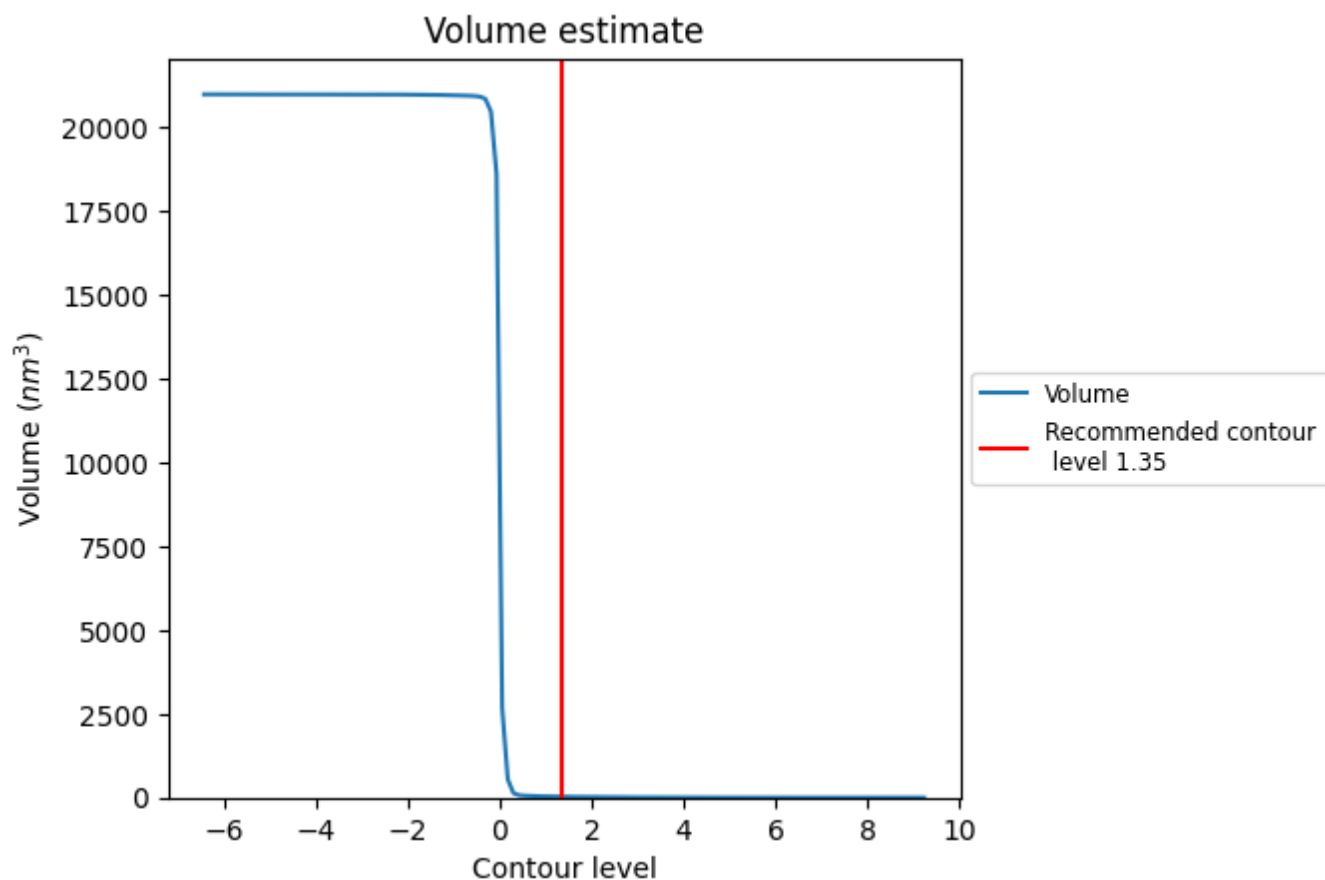
This section contains the results of statistical analysis of the map.

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.

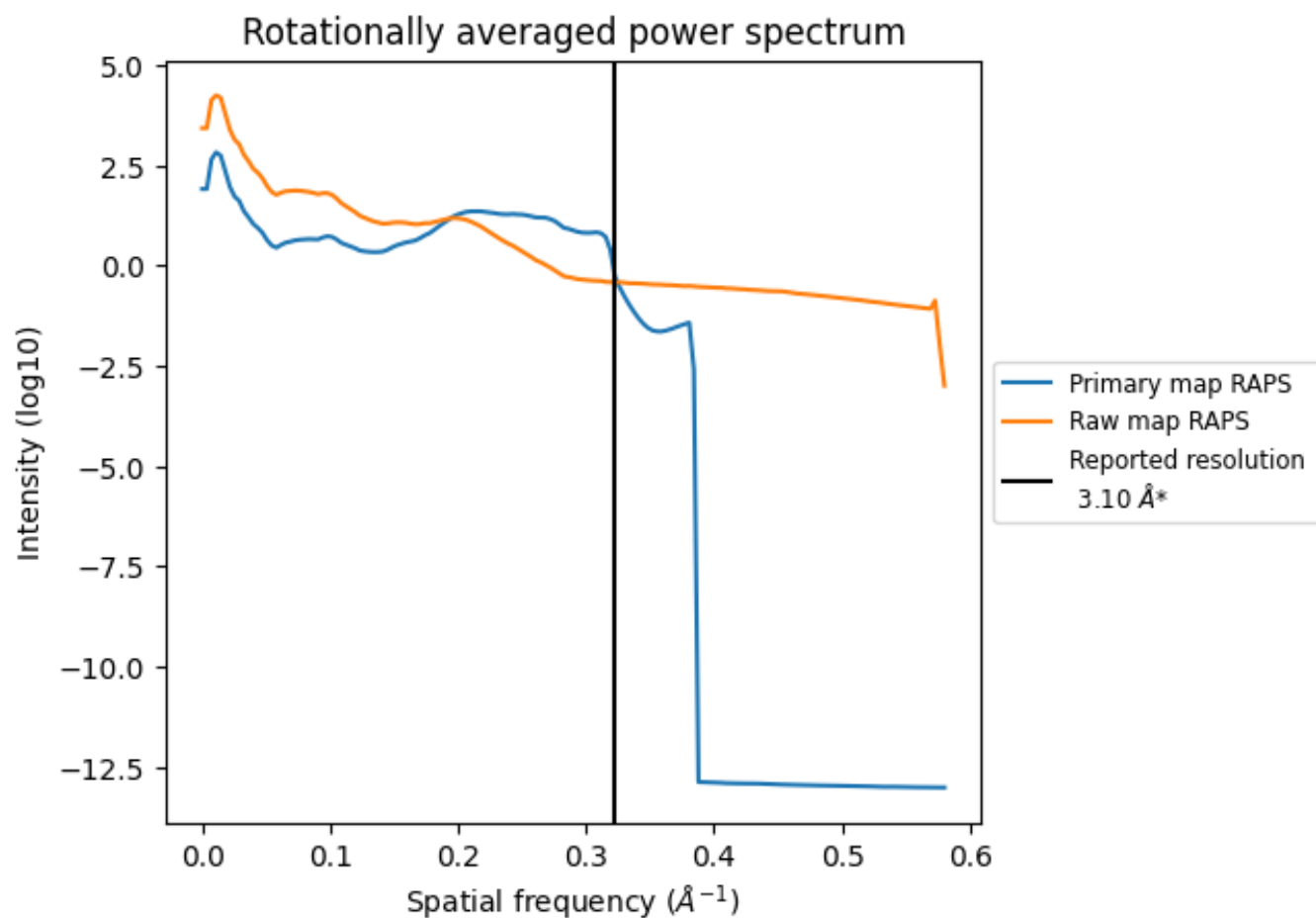
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 26 nm³; this corresponds to an approximate mass of 24 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 ⓘ

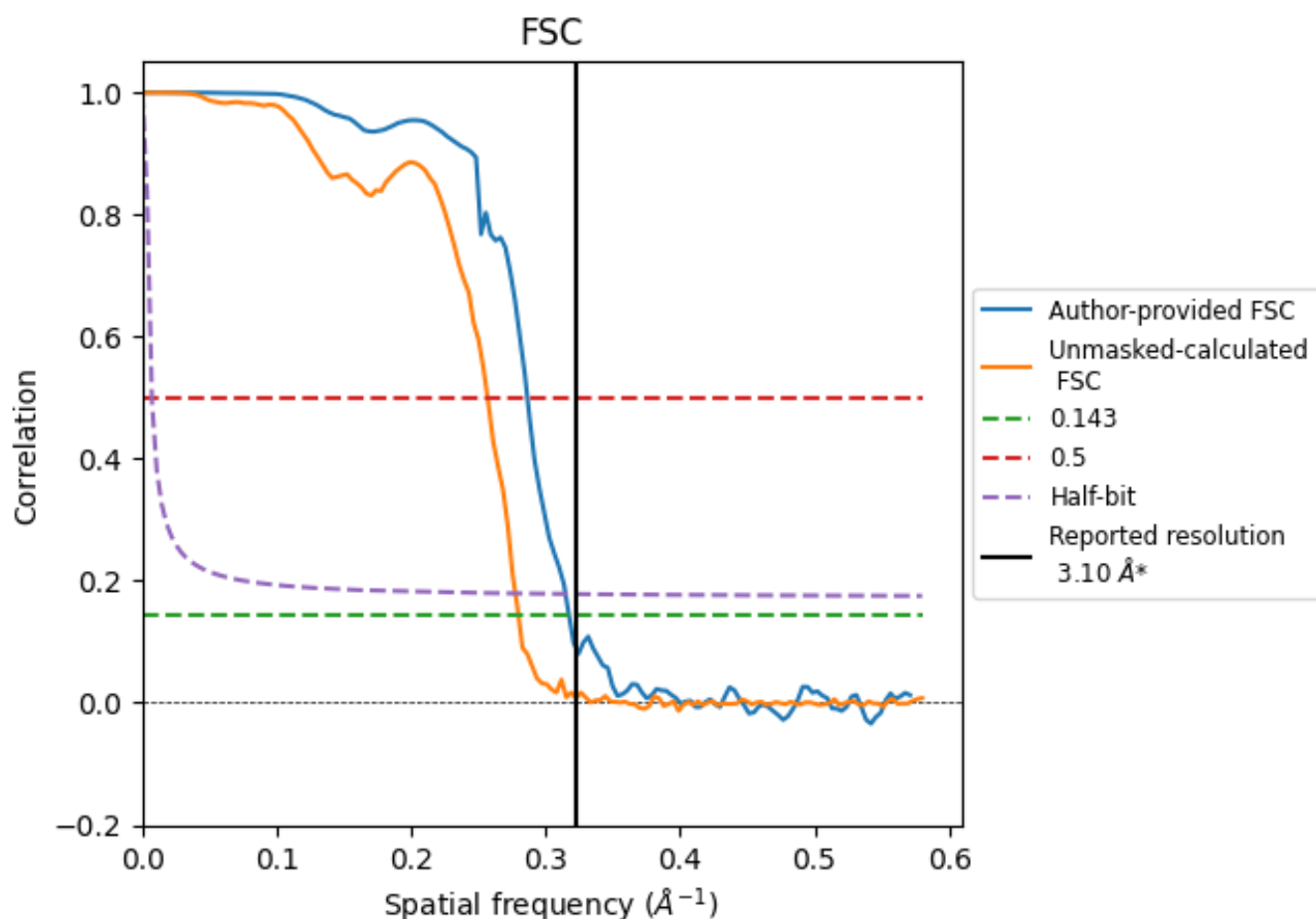


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

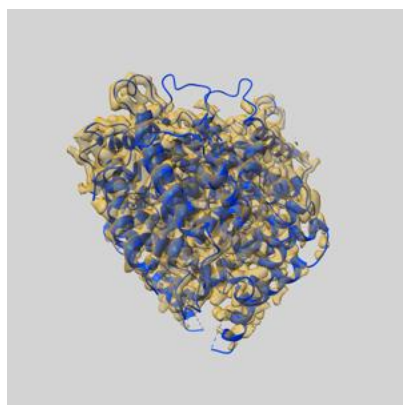
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.15	3.49	3.18
Unmasked-calculated*	3.57	3.89	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 3.1 by more than 10 %

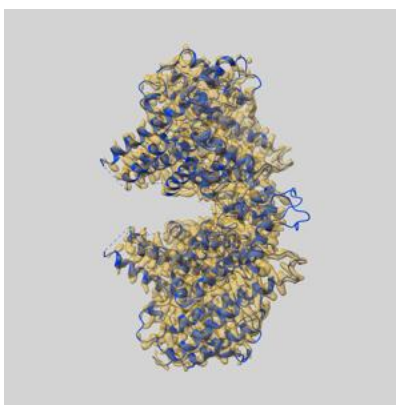
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51507 and PDB model 9GQN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

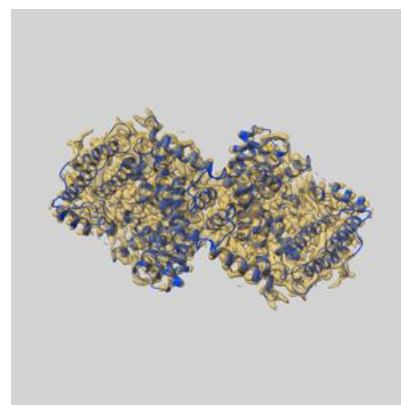
9.1 Map-model overlay [i](#)



X



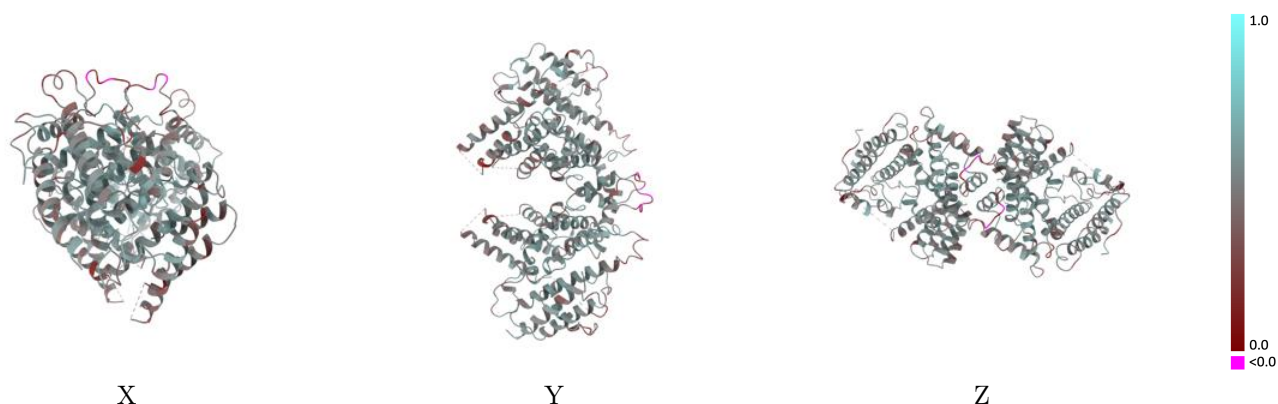
Y



Z

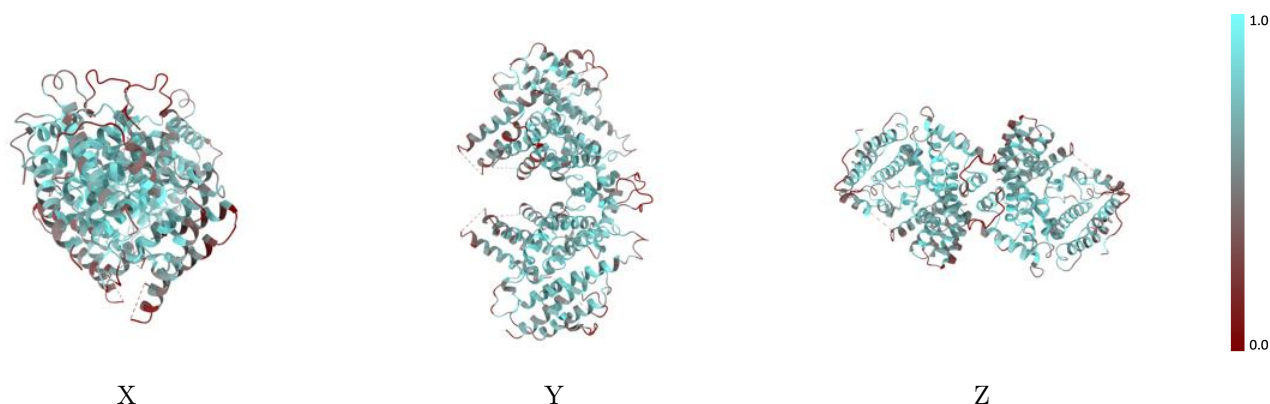
The images above show the 3D surface view of the map at the recommended contour level 1.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



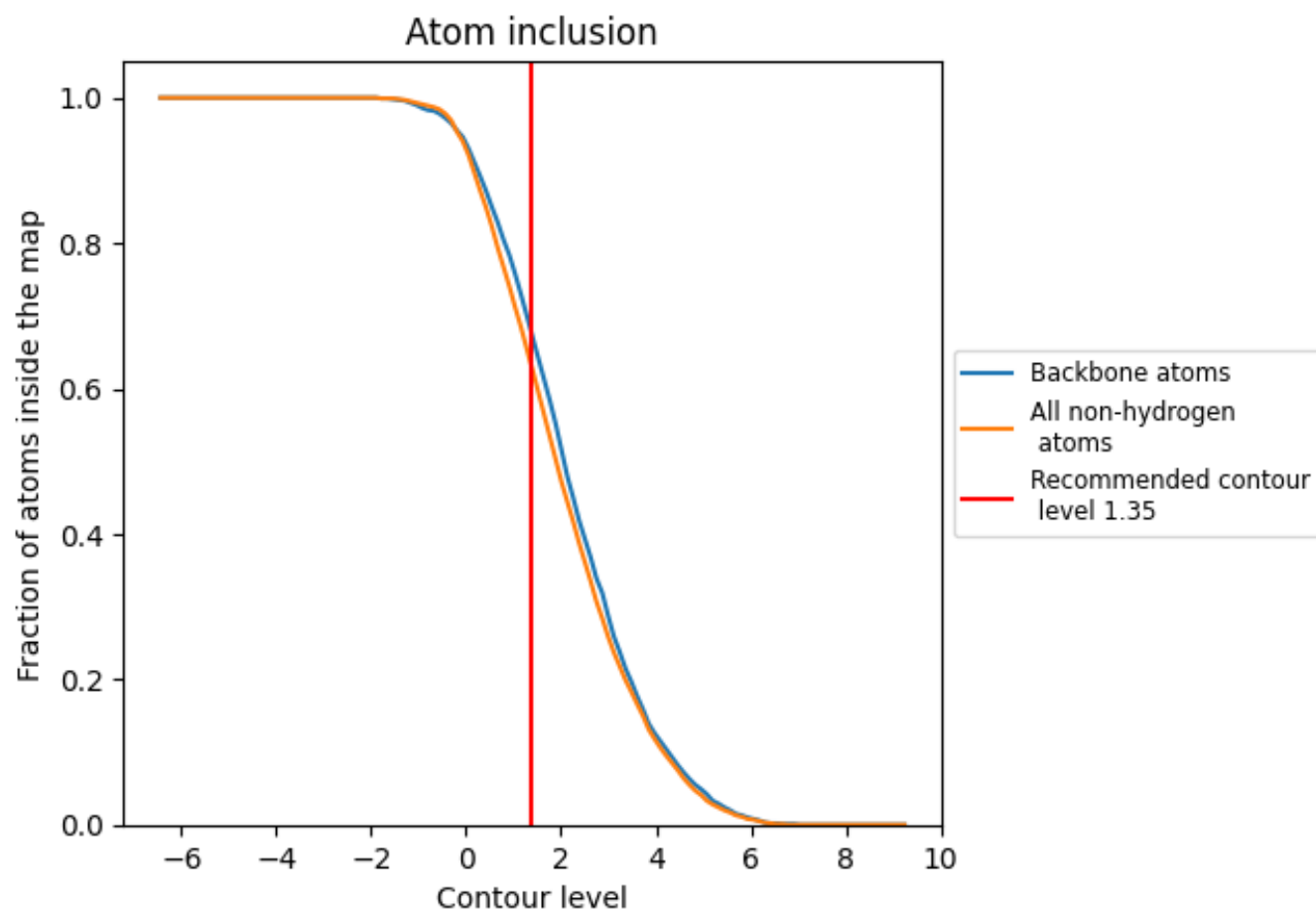
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 64% 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 (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6370	<div></div> 0.4910
A	<div></div> 0.6350	<div></div> 0.4900
B	<div></div> 0.6380	<div></div> 0.4910

