



Full wwPDB EM Validation Report ⓘ

Dec 2, 2024 – 11:54 AM EST

PDB ID : 9CO9
EMDB ID : EMD-45774
Title : Local refinement of JN.1 spike/Nanosota-9 complex
Authors : Ye, G.; Bu, F.; Liu, B.; Li, F.
Deposited on : 2024-07-16
Resolution : 3.44 Å (reported)
Based on initial model : 8IOS

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:

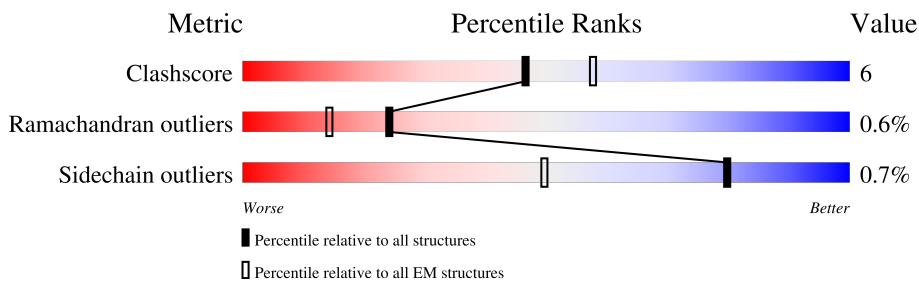
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.44 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	1243	
1	B	1243	
2	D	150	
2	E	150	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5198 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	200	1608	1042	270	288	8	0	0
1	A	203	1634	1059	276	291	8	0	0

There are 214 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	insertion	UNP P0DTC2
B	18	PRO	ASN	conflict	UNP P0DTC2
B	20	PHE	THR	conflict	UNP P0DTC2
B	21	ASN	THR	conflict	UNP P0DTC2
B	22	LEU	ARG	conflict	UNP P0DTC2
B	23	ILE	THR	conflict	UNP P0DTC2
B	24	THR	GLN	conflict	UNP P0DTC2
B	25	THR	LEU	conflict	UNP P0DTC2
B	26	THR	PRO	conflict	UNP P0DTC2
B	27	GLN	PRO	conflict	UNP P0DTC2
B	28	SER	ALA	conflict	UNP P0DTC2
B	51	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	126	PHE	VAL	conflict	UNP P0DTC2
B	141	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	155	SER	PHE	conflict	UNP P0DTC2
B	156	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	ILE	LEU	conflict	UNP P0DTC2
B	210	GLY	VAL	conflict	UNP P0DTC2
B	213	PHE	LEU	conflict	UNP P0DTC2
B	242	ASN	HIS	conflict	UNP P0DTC2
B	261	ASP	ALA	conflict	UNP P0DTC2
B	329	VAL	ILE	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	336	HIS	GLY	conflict	UNP P0DTC2
B	353	THR	LYS	conflict	UNP P0DTC2
B	368	PHE	SER	conflict	UNP P0DTC2
B	370	PRO	SER	conflict	UNP P0DTC2
B	372	PHE	SER	conflict	UNP P0DTC2
B	373	ALA	THR	conflict	UNP P0DTC2
B	400	LYS	ARG	conflict	UNP P0DTC2
B	402	ASN	ASP	conflict	UNP P0DTC2
B	405	SER	ARG	conflict	UNP P0DTC2
B	414	ASN	LYS	conflict	UNP P0DTC2
B	437	LYS	ASN	conflict	UNP P0DTC2
B	442	HIS	VAL	conflict	UNP P0DTC2
B	443	SER	GLY	conflict	UNP P0DTC2
B	447	ASP	ASN	conflict	UNP P0DTC2
B	449	TRP	LEU	conflict	UNP P0DTC2
B	452	SER	LEU	conflict	UNP P0DTC2
B	457	LYS	ASN	conflict	UNP P0DTC2
B	474	ASN	SER	conflict	UNP P0DTC2
B	475	LYS	THR	conflict	UNP P0DTC2
B	478	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	480	LYS	GLU	conflict	UNP P0DTC2
B	482	PRO	PHE	conflict	UNP P0DTC2
B	494	ARG	GLN	conflict	UNP P0DTC2
B	497	TYR	ASN	conflict	UNP P0DTC2
B	501	HIS	TYR	conflict	UNP P0DTC2
B	550	LYS	GLU	conflict	UNP P0DTC2
B	566	VAL	ALA	conflict	UNP P0DTC2
B	610	GLY	ASP	conflict	UNP P0DTC2
B	617	SER	PRO	conflict	UNP P0DTC2
B	651	TYR	HIS	conflict	UNP P0DTC2
B	675	LYS	ASN	conflict	UNP P0DTC2
B	677	ARG	PRO	conflict	UNP P0DTC2
B	678	ALA	ARG	conflict	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	760	LYS	ASN	conflict	UNP P0DTC2
B	792	TYR	ASP	conflict	UNP P0DTC2
B	813	PRO	PHE	conflict	UNP P0DTC2
B	888	PRO	ALA	conflict	UNP P0DTC2
B	895	PRO	ALA	conflict	UNP P0DTC2
B	935	PHE	SER	conflict	UNP P0DTC2
B	938	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	950	HIS	GLN	conflict	UNP P0DTC2
B	965	LYS	ASN	conflict	UNP P0DTC2
B	982	PRO	LYS	conflict	UNP P0DTC2
B	983	PRO	VAL	conflict	UNP P0DTC2
B	1139	LEU	PRO	conflict	UNP P0DTC2
B	1208	GLY	TRP	conflict	UNP P0DTC2
B	1209	SER	PRO	conflict	UNP P0DTC2
B	1210	GLY	TRP	conflict	UNP P0DTC2
B	1213	PRO	-	expression tag	UNP P0DTC2
B	1214	GLU	-	expression tag	UNP P0DTC2
B	1215	ALA	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	ARG	-	expression tag	UNP P0DTC2
B	1218	ASP	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	GLN	-	expression tag	UNP P0DTC2
B	1221	ALA	-	expression tag	UNP P0DTC2
B	1222	TYR	-	expression tag	UNP P0DTC2
B	1223	VAL	-	expression tag	UNP P0DTC2
B	1224	ARG	-	expression tag	UNP P0DTC2
B	1225	LYS	-	expression tag	UNP P0DTC2
B	1226	ASP	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	GLU	-	expression tag	UNP P0DTC2
B	1229	TRP	-	expression tag	UNP P0DTC2
B	1230	VAL	-	expression tag	UNP P0DTC2
B	1231	LEU	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	SER	-	expression tag	UNP P0DTC2
B	1234	THR	-	expression tag	UNP P0DTC2
B	1235	PHE	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	GLY	-	expression tag	UNP P0DTC2
B	1238	HIS	-	expression tag	UNP P0DTC2
B	1239	HIS	-	expression tag	UNP P0DTC2
B	1240	HIS	-	expression tag	UNP P0DTC2
B	1241	HIS	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
A	17	MET	-	insertion	UNP P0DTC2
A	18	PRO	ASN	conflict	UNP P0DTC2
A	20	PHE	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ASN	THR	conflict	UNP P0DTC2
A	22	LEU	ARG	conflict	UNP P0DTC2
A	23	ILE	THR	conflict	UNP P0DTC2
A	24	THR	GLN	conflict	UNP P0DTC2
A	25	THR	LEU	conflict	UNP P0DTC2
A	26	THR	PRO	conflict	UNP P0DTC2
A	27	GLN	PRO	conflict	UNP P0DTC2
A	28	SER	ALA	conflict	UNP P0DTC2
A	51	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	126	PHE	VAL	conflict	UNP P0DTC2
A	141	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	155	SER	PHE	conflict	UNP P0DTC2
A	156	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	209	ILE	LEU	conflict	UNP P0DTC2
A	210	GLY	VAL	conflict	UNP P0DTC2
A	213	PHE	LEU	conflict	UNP P0DTC2
A	242	ASN	HIS	conflict	UNP P0DTC2
A	261	ASP	ALA	conflict	UNP P0DTC2
A	329	VAL	ILE	conflict	UNP P0DTC2
A	336	HIS	GLY	conflict	UNP P0DTC2
A	353	THR	LYS	conflict	UNP P0DTC2
A	368	PHE	SER	conflict	UNP P0DTC2
A	370	PRO	SER	conflict	UNP P0DTC2
A	372	PHE	SER	conflict	UNP P0DTC2
A	373	ALA	THR	conflict	UNP P0DTC2
A	400	LYS	ARG	conflict	UNP P0DTC2
A	402	ASN	ASP	conflict	UNP P0DTC2
A	405	SER	ARG	conflict	UNP P0DTC2
A	414	ASN	LYS	conflict	UNP P0DTC2
A	437	LYS	ASN	conflict	UNP P0DTC2
A	442	HIS	VAL	conflict	UNP P0DTC2
A	443	SER	GLY	conflict	UNP P0DTC2
A	447	ASP	ASN	conflict	UNP P0DTC2
A	449	TRP	LEU	conflict	UNP P0DTC2
A	452	SER	LEU	conflict	UNP P0DTC2
A	457	LYS	ASN	conflict	UNP P0DTC2
A	474	ASN	SER	conflict	UNP P0DTC2
A	475	LYS	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	478	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	480	LYS	GLU	conflict	UNP P0DTC2
A	482	PRO	PHE	conflict	UNP P0DTC2
A	494	ARG	GLN	conflict	UNP P0DTC2
A	497	TYR	ASN	conflict	UNP P0DTC2
A	501	HIS	TYR	conflict	UNP P0DTC2
A	550	LYS	GLU	conflict	UNP P0DTC2
A	566	VAL	ALA	conflict	UNP P0DTC2
A	610	GLY	ASP	conflict	UNP P0DTC2
A	617	SER	PRO	conflict	UNP P0DTC2
A	651	TYR	HIS	conflict	UNP P0DTC2
A	675	LYS	ASN	conflict	UNP P0DTC2
A	677	ARG	PRO	conflict	UNP P0DTC2
A	678	ALA	ARG	conflict	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	760	LYS	ASN	conflict	UNP P0DTC2
A	792	TYR	ASP	conflict	UNP P0DTC2
A	813	PRO	PHE	conflict	UNP P0DTC2
A	888	PRO	ALA	conflict	UNP P0DTC2
A	895	PRO	ALA	conflict	UNP P0DTC2
A	935	PHE	SER	conflict	UNP P0DTC2
A	938	PRO	ALA	conflict	UNP P0DTC2
A	950	HIS	GLN	conflict	UNP P0DTC2
A	965	LYS	ASN	conflict	UNP P0DTC2
A	982	PRO	LYS	conflict	UNP P0DTC2
A	983	PRO	VAL	conflict	UNP P0DTC2
A	1139	LEU	PRO	conflict	UNP P0DTC2
A	1208	GLY	TRP	conflict	UNP P0DTC2
A	1209	SER	PRO	conflict	UNP P0DTC2
A	1210	GLY	TRP	conflict	UNP P0DTC2
A	1213	PRO	-	expression tag	UNP P0DTC2
A	1214	GLU	-	expression tag	UNP P0DTC2
A	1215	ALA	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	ASP	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	GLN	-	expression tag	UNP P0DTC2
A	1221	ALA	-	expression tag	UNP P0DTC2
A	1222	TYR	-	expression tag	UNP P0DTC2
A	1223	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	ARG	-	expression tag	UNP P0DTC2
A	1225	LYS	-	expression tag	UNP P0DTC2
A	1226	ASP	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	GLU	-	expression tag	UNP P0DTC2
A	1229	TRP	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	LEU	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	SER	-	expression tag	UNP P0DTC2
A	1234	THR	-	expression tag	UNP P0DTC2
A	1235	PHE	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	GLY	-	expression tag	UNP P0DTC2
A	1238	HIS	-	expression tag	UNP P0DTC2
A	1239	HIS	-	expression tag	UNP P0DTC2
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2

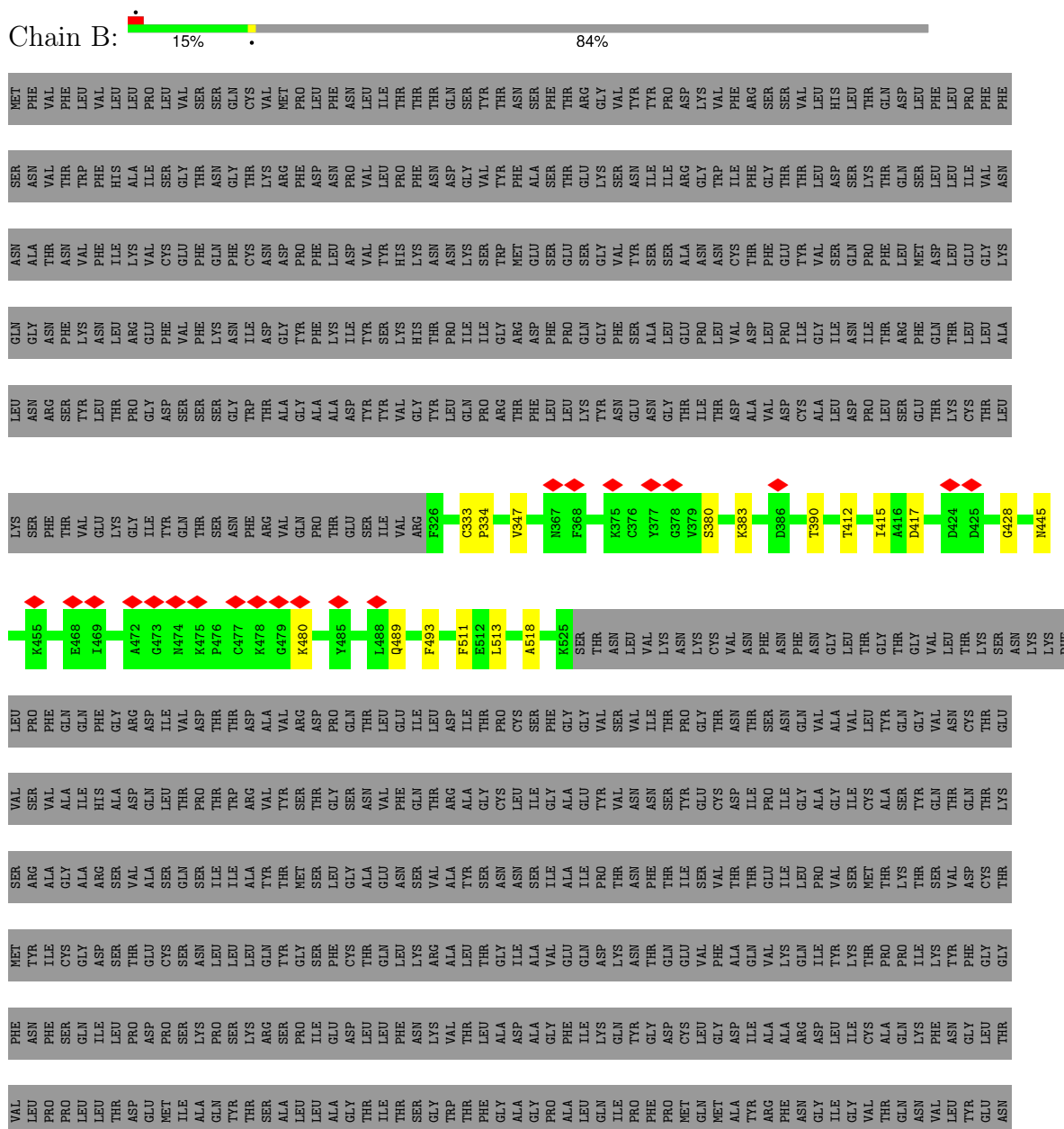
- Molecule 2 is a protein called Nanosota-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	129	Total	C	N	O	S	0	0
			978	602	168	203	5		
2	E	129	Total	C	N	O	S	0	0
			978	602	168	203	5		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248315	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 ($e^-/\text{\AA}^2$)	54.8	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.090	Depositor
Minimum map value	-0.374	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	339.96786, 339.96786, 339.96786	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.885333, 0.885333, 0.885333	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	0.42	0/1688	0.65	1/2296 (0.0%)
1	B	0.29	0/1662	0.59	0/2261
2	D	0.34	0/998	0.71	1/1353 (0.1%)
2	E	0.30	0/998	0.59	0/1353
All	All	0.35	0/5346	0.63	2/7263 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	110	TYR	CA-CB-CG	5.31	123.49	113.40
1	A	388	CYS	CA-CB-SG	5.04	123.07	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1634	0	1564	26	0
1	B	1608	0	1531	11	0
2	D	978	0	905	17	0
2	E	978	0	905	8	0
All	All	5198	0	4905	60	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 (60) 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:418:TYR:HD2	1:A:454:ARG:HB2	1.47	0.79
1:A:481:GLY:H	1:A:484:CYS:HB2	1.52	0.74
2:D:33:ALA:HB3	2:D:103:VAL:HG12	1.74	0.68
2:D:105:HIS:HB2	2:D:110:TYR:HD1	1.59	0.67
1:A:418:TYR:CD2	1:A:454:ARG:HB2	2.30	0.66
2:D:110:TYR:HD2	2:D:112:THR:HG23	1.60	0.66
2:D:114:ASP:O	2:D:116:PHE:N	2.33	0.61
1:A:494:ARG:HB2	1:A:497:TYR:CE1	2.36	0.61
1:B:489:GLN:HE21	2:D:100:PRO:HB3	1.65	0.60
2:D:29:LEU:O	2:D:72:ARG:NH1	2.35	0.60
1:A:390:THR:HG21	1:A:516:ALA:HB3	1.83	0.59
2:D:117:TYR:O	2:D:118:TYR:C	2.41	0.58
1:A:481:GLY:N	1:A:484:CYS:HB2	2.18	0.58
2:D:109:TYR:CE1	2:D:113:ASP:HB2	2.39	0.57
1:A:449:TRP:CE3	1:A:490:SER:HB3	2.38	0.57
1:A:476:PRO:HG2	1:A:478:LYS:HZ1	1.71	0.55
2:E:40:ALA:HB3	2:E:43:LYS:HD3	1.90	0.54
2:E:33:ALA:HB3	2:E:103:VAL:HG12	1.89	0.54
1:A:389:PHE:HE1	1:A:392:VAL:HB	1.72	0.53
2:D:9:GLY:HA2	2:D:125:VAL:HG22	1.91	0.53
1:B:380:SER:HB3	1:B:383:LYS:HB2	1.92	0.51
1:B:347:VAL:HG11	1:B:415:ILE:HD12	1.93	0.51
2:E:24:ALA:HB2	2:E:29:LEU:HD21	1.92	0.50
1:B:480:LYS:HE2	2:D:26:GLY:HA2	1.94	0.50
2:D:37:PHE:HB2	2:D:45:ARG:HH21	1.77	0.50
2:D:52:SER:OG	2:D:104:CYS:SG	2.69	0.50
1:A:362:TYR:HD2	1:A:384:LEU:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ALA:HA	1:A:463:ARG:HD3	1.93	0.49
1:A:340:ASN:HB2	1:A:368:PHE:CE1	2.48	0.49
1:B:390:THR:HG22	1:B:513:LEU:HA	1.94	0.48
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.95	0.48
2:E:28:ALA:HB1	2:E:30:HIS:CD2	2.48	0.48
1:A:430:VAL:HG22	1:A:508:VAL:HG22	1.96	0.47
2:D:104:CYS:HB2	2:D:111:TYR:HD2	1.80	0.47
1:A:398:VAL:HG22	1:A:505:ARG:HG2	1.97	0.47
1:B:445:ASN:HB3	1:B:493:PHE:HB2	1.96	0.46
1:A:347:VAL:HG12	1:A:419:ASN:HB3	1.96	0.46
2:D:33:ALA:CB	2:D:103:VAL:HG12	2.45	0.45
1:B:412:THR:OG1	1:B:417:ASP:OD2	2.35	0.45
1:A:388:CYS:HB2	1:A:521:CYS:HA	1.98	0.45
1:B:383:LYS:HB3	1:B:383:LYS:HE2	1.78	0.45
1:A:340:ASN:HB2	1:A:368:PHE:CZ	2.52	0.45
1:A:449:TRP:CZ3	1:A:490:SER:HB3	2.53	0.44
1:A:348:TYR:HE1	1:A:449:TRP:HB2	1.82	0.44
1:B:428:GLY:HA2	1:B:511:PHE:HD2	1.83	0.44
2:D:20:LEU:HD11	2:D:125:VAL:HG21	1.99	0.44
2:D:105:HIS:HB2	2:D:110:TYR:CD1	2.45	0.44
1:B:333:CYS:HA	1:B:334:PRO:HD3	1.88	0.43
1:A:362:TYR:CD2	1:A:384:LEU:HB3	2.53	0.43
1:A:469:ILE:HG12	1:A:484:CYS:HB3	2.00	0.43
2:E:33:ALA:CB	2:E:103:VAL:HG12	2.49	0.43
1:B:390:THR:HB	1:B:518:ALA:HA	2.00	0.43
2:D:18:LEU:HD12	2:D:18:LEU:HA	1.92	0.42
2:E:103:VAL:HG22	2:E:109:TYR:HE2	1.84	0.42
1:A:335:PHE:CE2	1:A:362:TYR:HE1	2.38	0.42
1:A:383:LYS:HB3	1:A:383:LYS:HE2	1.81	0.42
1:A:451:ARG:NH2	1:A:466:SER:O	2.50	0.41
2:E:54:GLY:O	2:E:56:GLY:N	2.53	0.41
1:A:469:ILE:CG1	1:A:484:CYS:HB3	2.50	0.41
1:A:358:CYS:H	1:A:520:VAL:HG12	1.86	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	201/1243 (16%)	190 (94%)	10 (5%)	1 (0%)	25	58
1	B	198/1243 (16%)	188 (95%)	10 (5%)	0	100	100
2	D	127/150 (85%)	115 (91%)	10 (8%)	2 (2%)	8	34
2	E	127/150 (85%)	115 (91%)	11 (9%)	1 (1%)	16	49
All	All	653/2786 (23%)	608 (93%)	41 (6%)	4 (1%)	24	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	115	ASP
2	D	118	TYR
2	E	55	ASP
1	A	333	CYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/1085 (16%)	174 (98%)	3 (2%)	56	75
1	B	174/1085 (16%)	174 (100%)	0	100	100
2	D	104/120 (87%)	103 (99%)	1 (1%)	73	84
2	E	104/120 (87%)	104 (100%)	0	100	100
All	All	559/2410 (23%)	555 (99%)	4 (1%)	80	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	ARG
1	A	457	LYS
1	A	465	ILE
2	D	117	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	489	GLN

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.

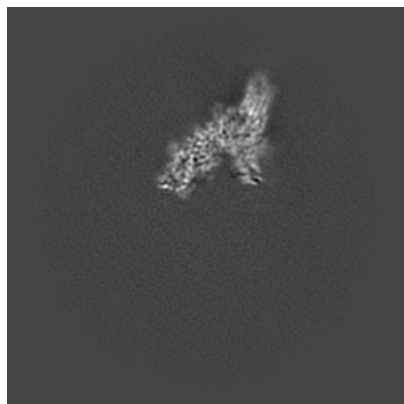
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45774. These allow visual inspection of the internal detail of the map and identification of artifacts.

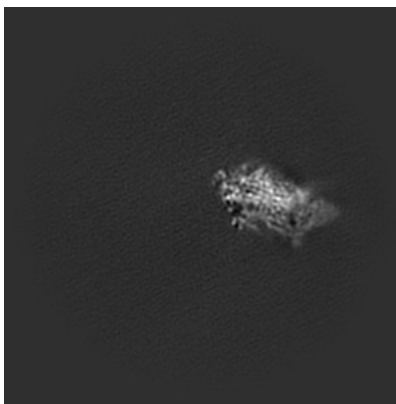
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

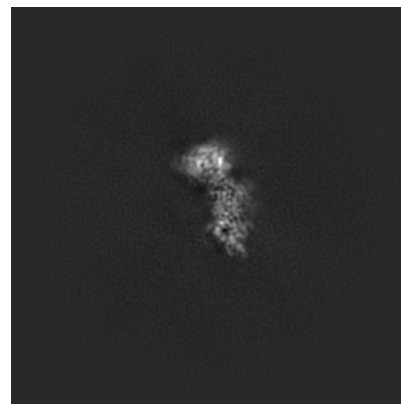
6.1.1 Primary map



X

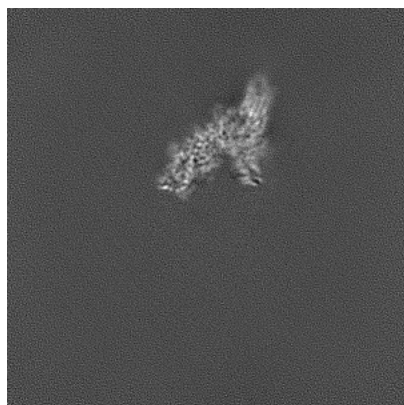


Y

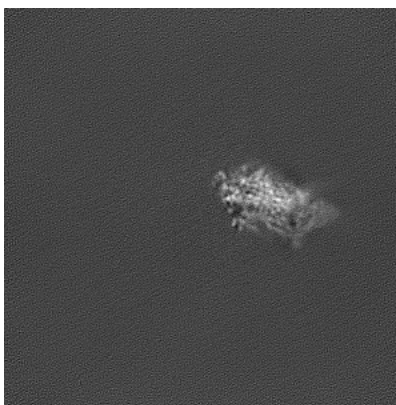


Z

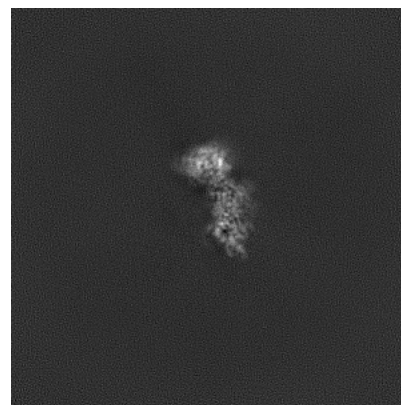
6.1.2 Raw map



X



Y

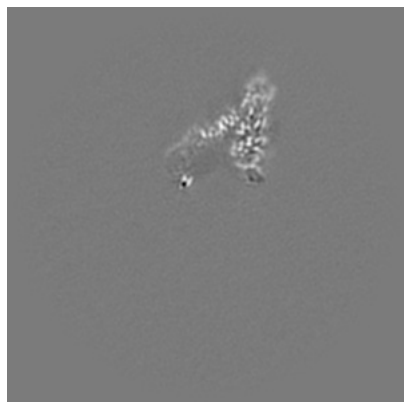


Z

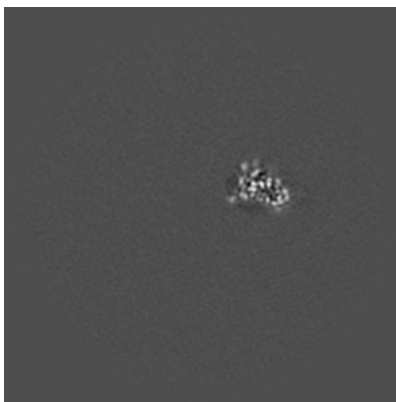
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

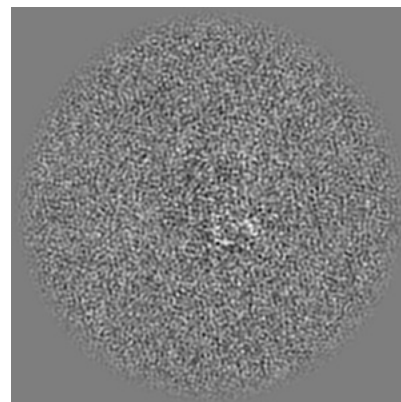
6.2.1 Primary map



X Index: 192

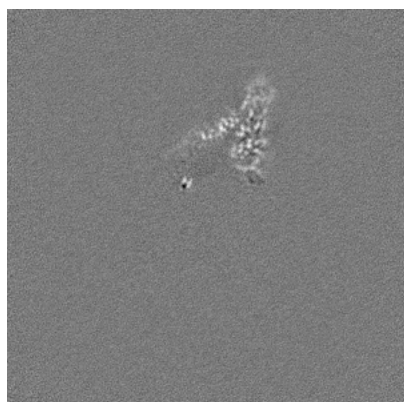


Y Index: 192

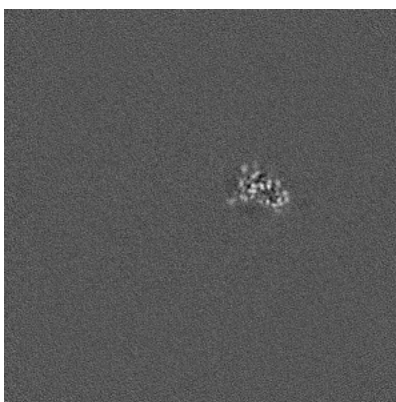


Z Index: 192

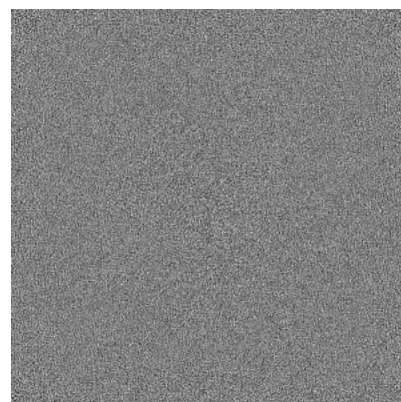
6.2.2 Raw map



X Index: 192



Y Index: 192

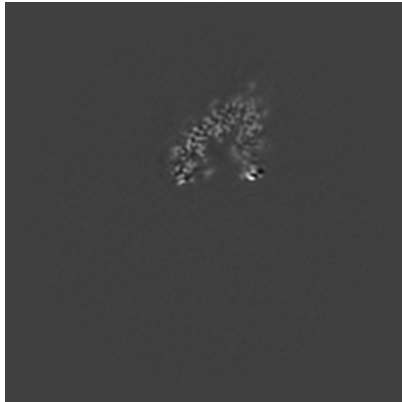


Z Index: 192

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

6.3 Largest variance slices [i](#)

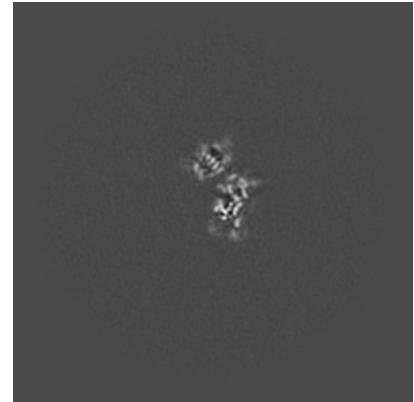
6.3.1 Primary map



X Index: 200

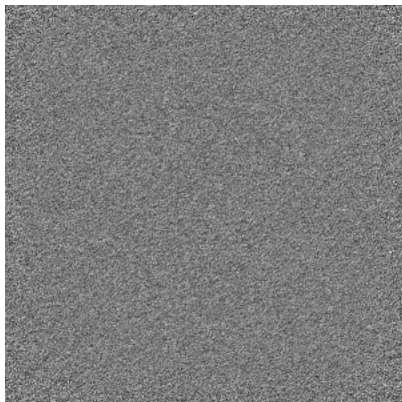


Y Index: 236

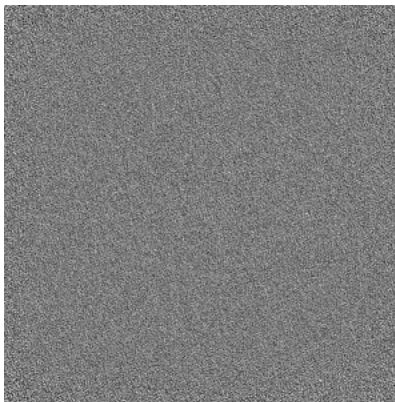


Z Index: 252

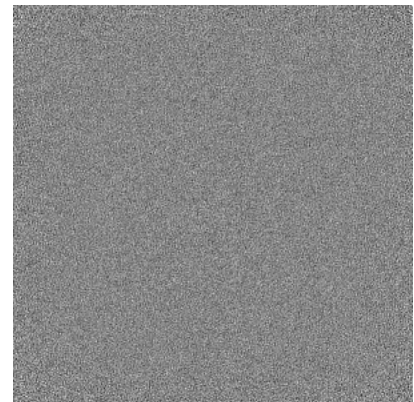
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

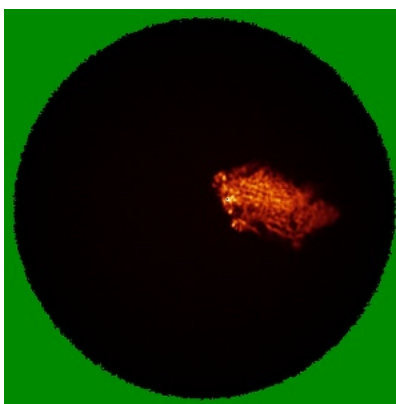
The images above show the largest variance slices of the map in three orthogonal directions.

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

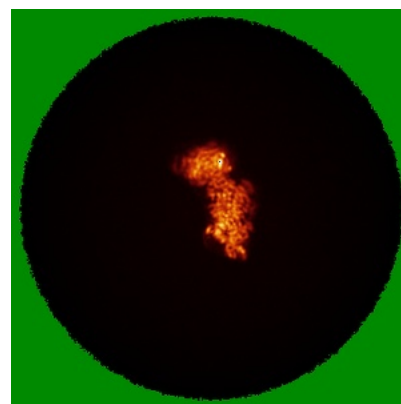
6.4.1 Primary map



X

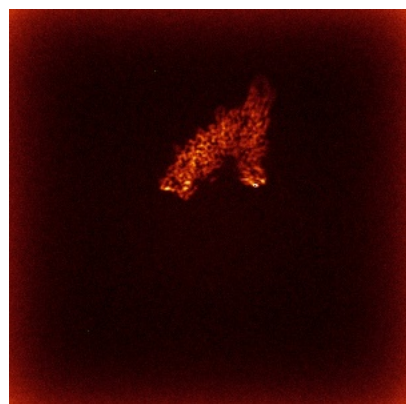


Y

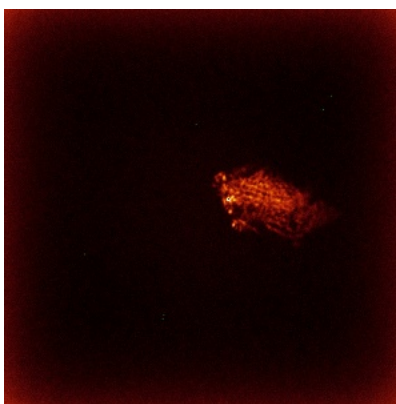


Z

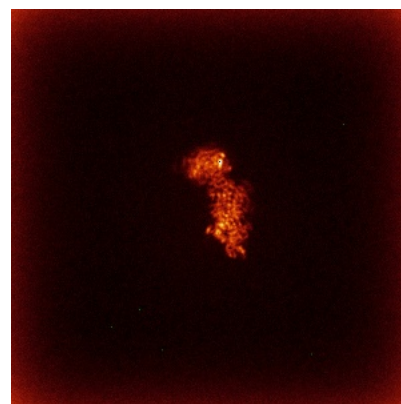
6.4.2 Raw map



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.

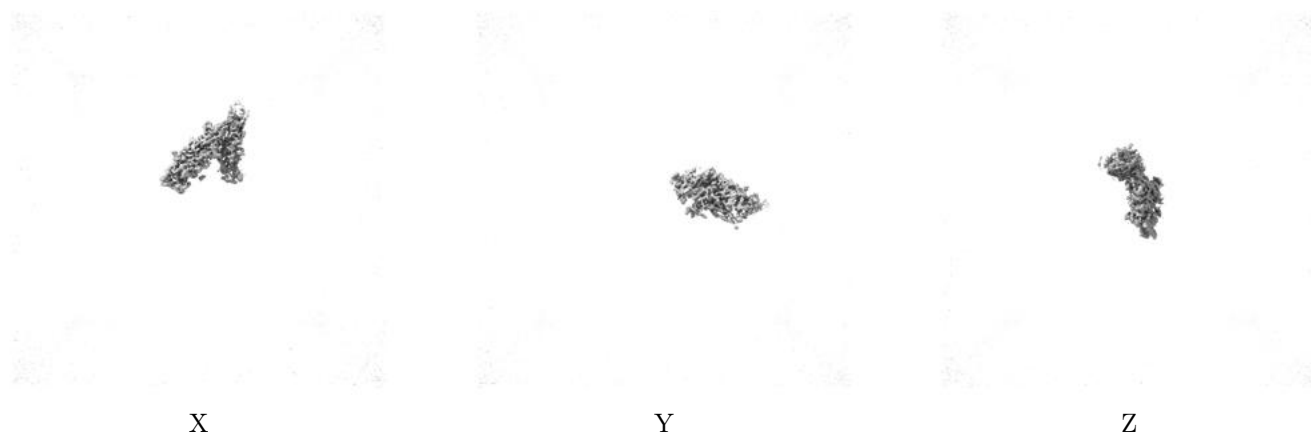
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

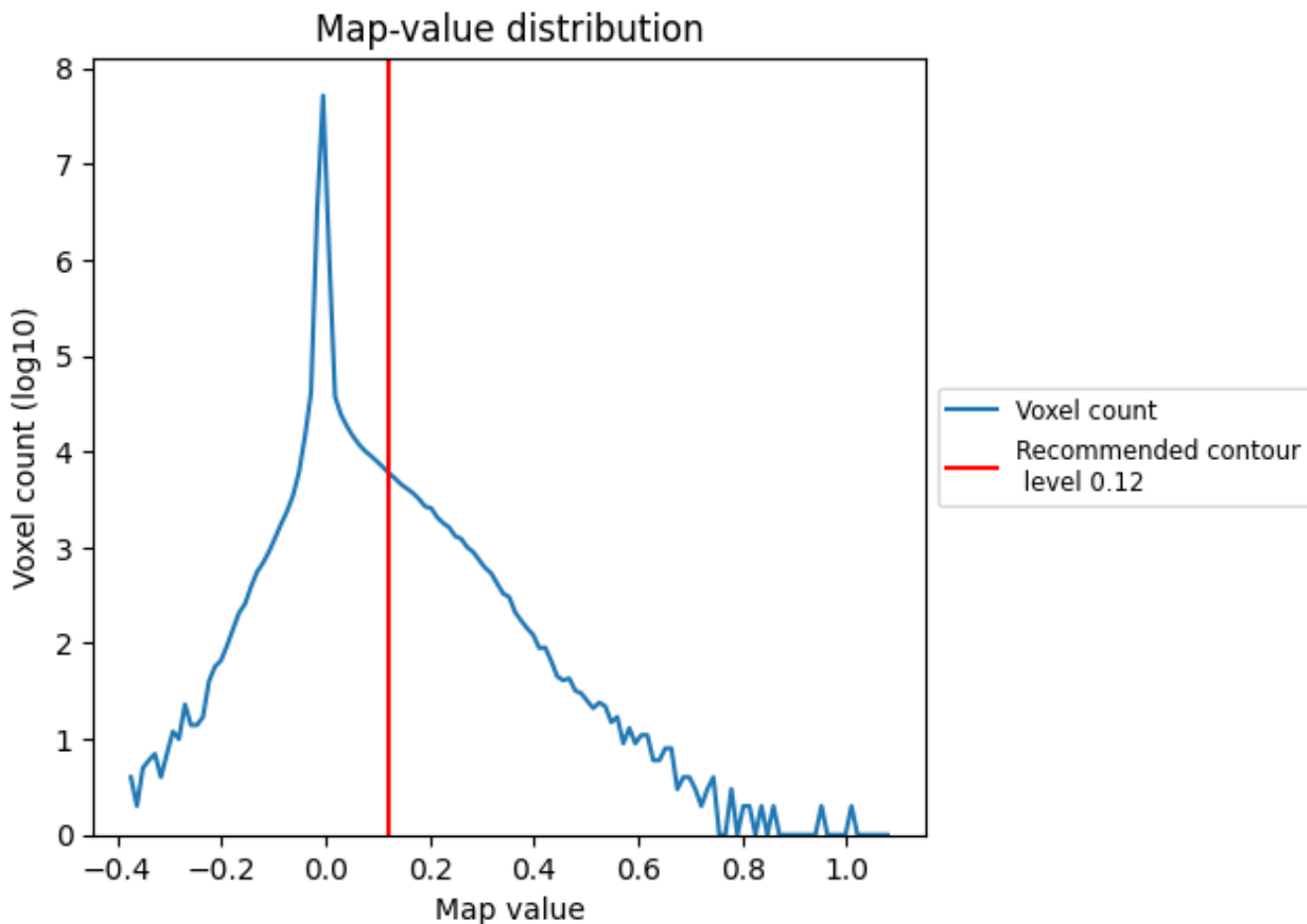
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

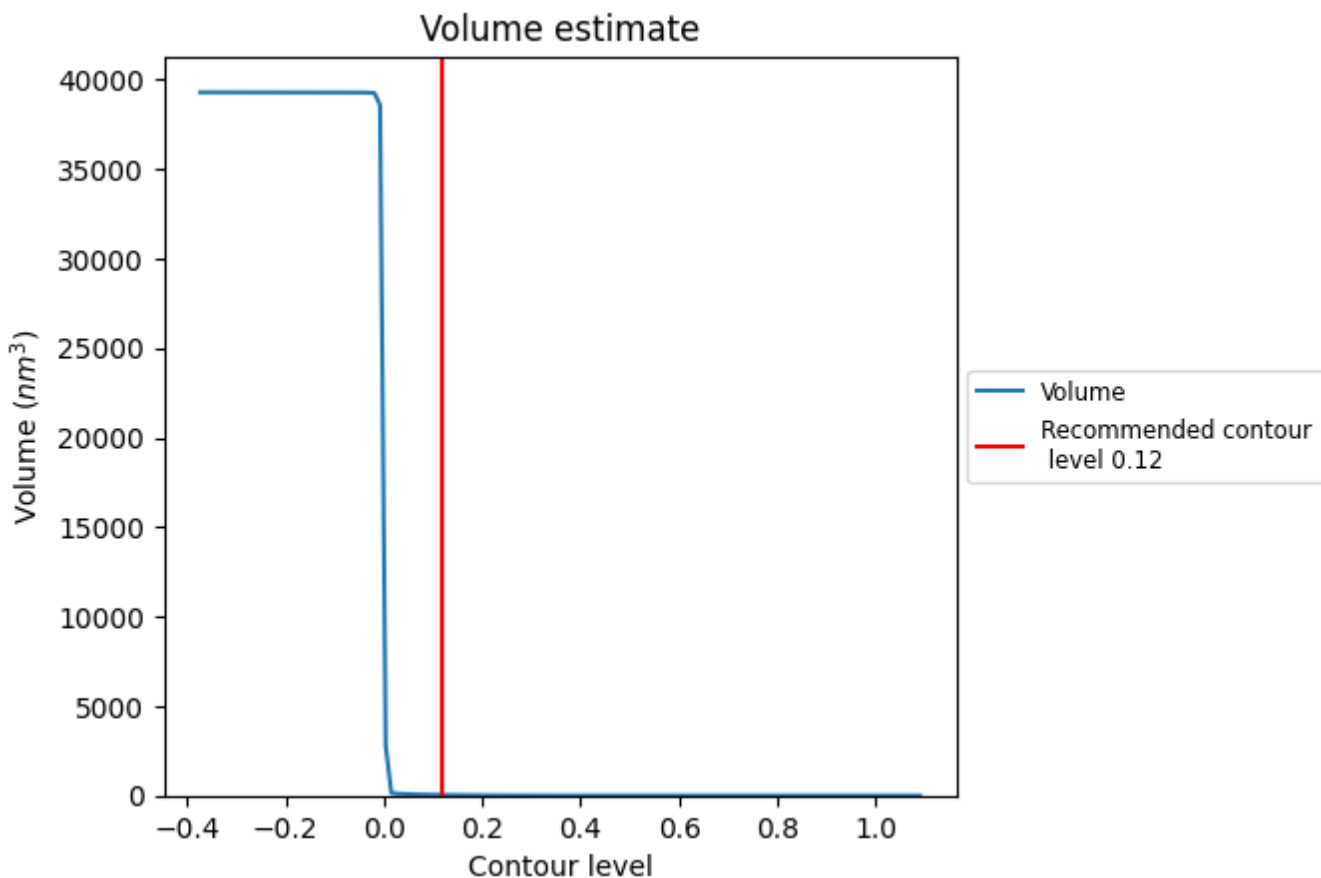
This section contains the results of statistical analysis of the map.

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.

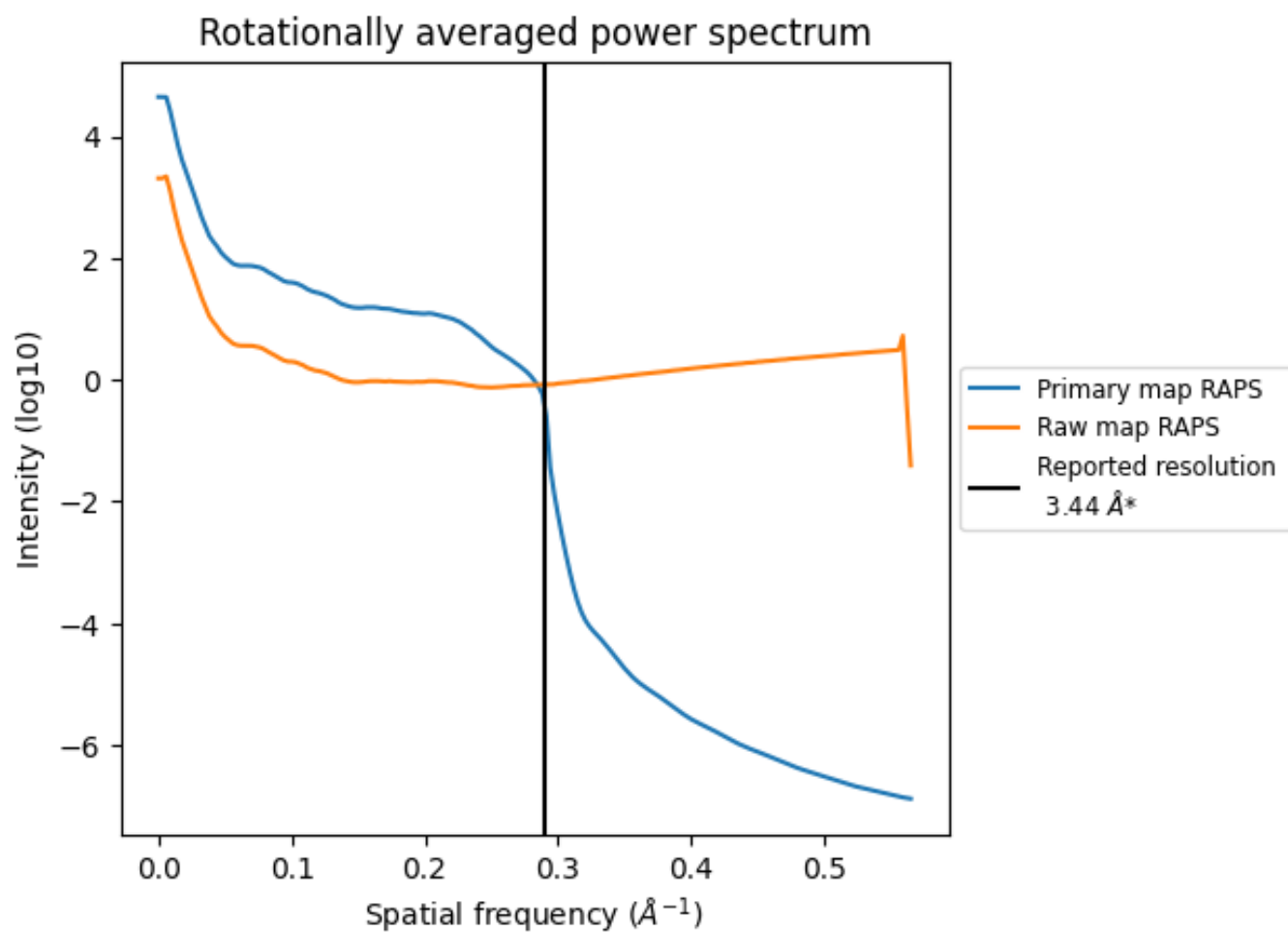
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm³; this corresponds to an approximate mass of 30 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](#)

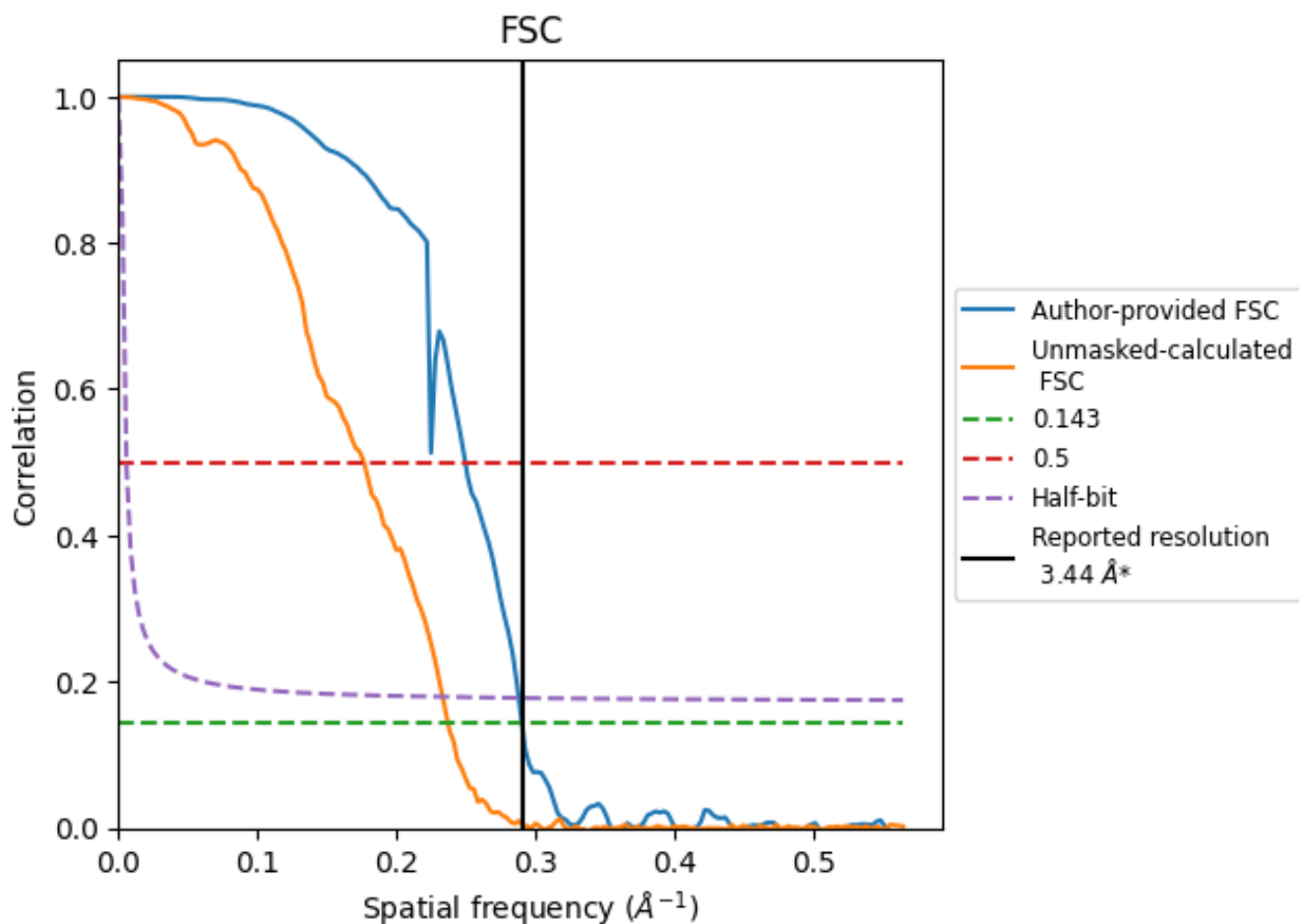


*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

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 0.291 Å⁻¹

8.2 Resolution estimates [i](#)

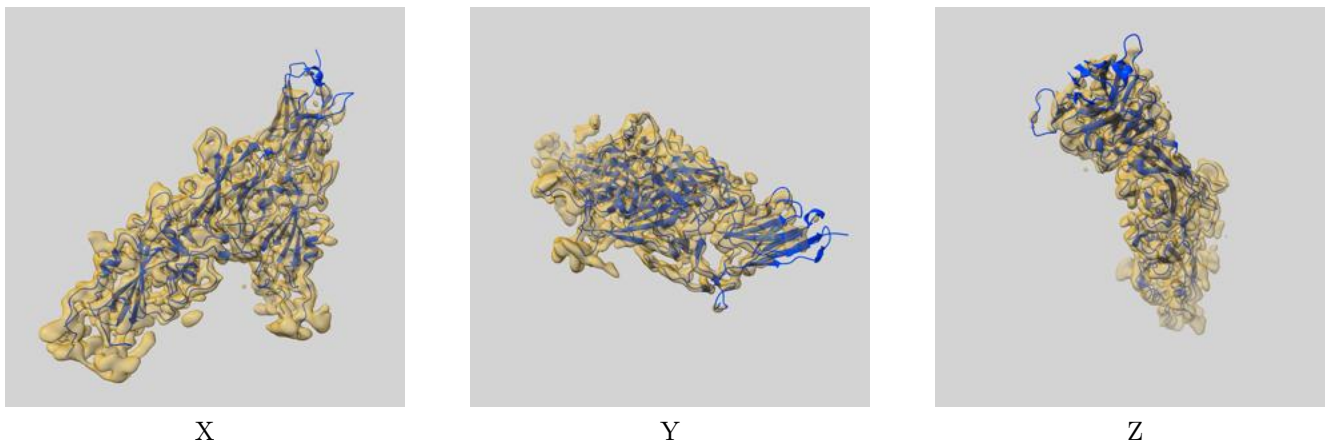
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	4.00	3.47
Unmasked-calculated*	4.22	5.66	4.28

*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 4.22 differs from the reported value 3.44 by more than 10 %

9 Map-model fit [i](#)

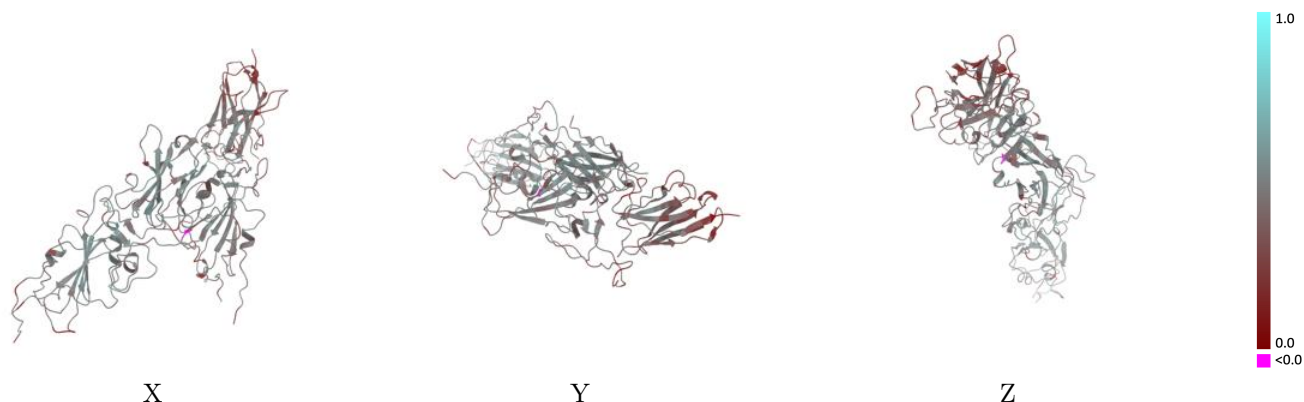
This section contains information regarding the fit between EMDB map EMD-45774 and PDB model 9CO9. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.12 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 [\(i\)](#)



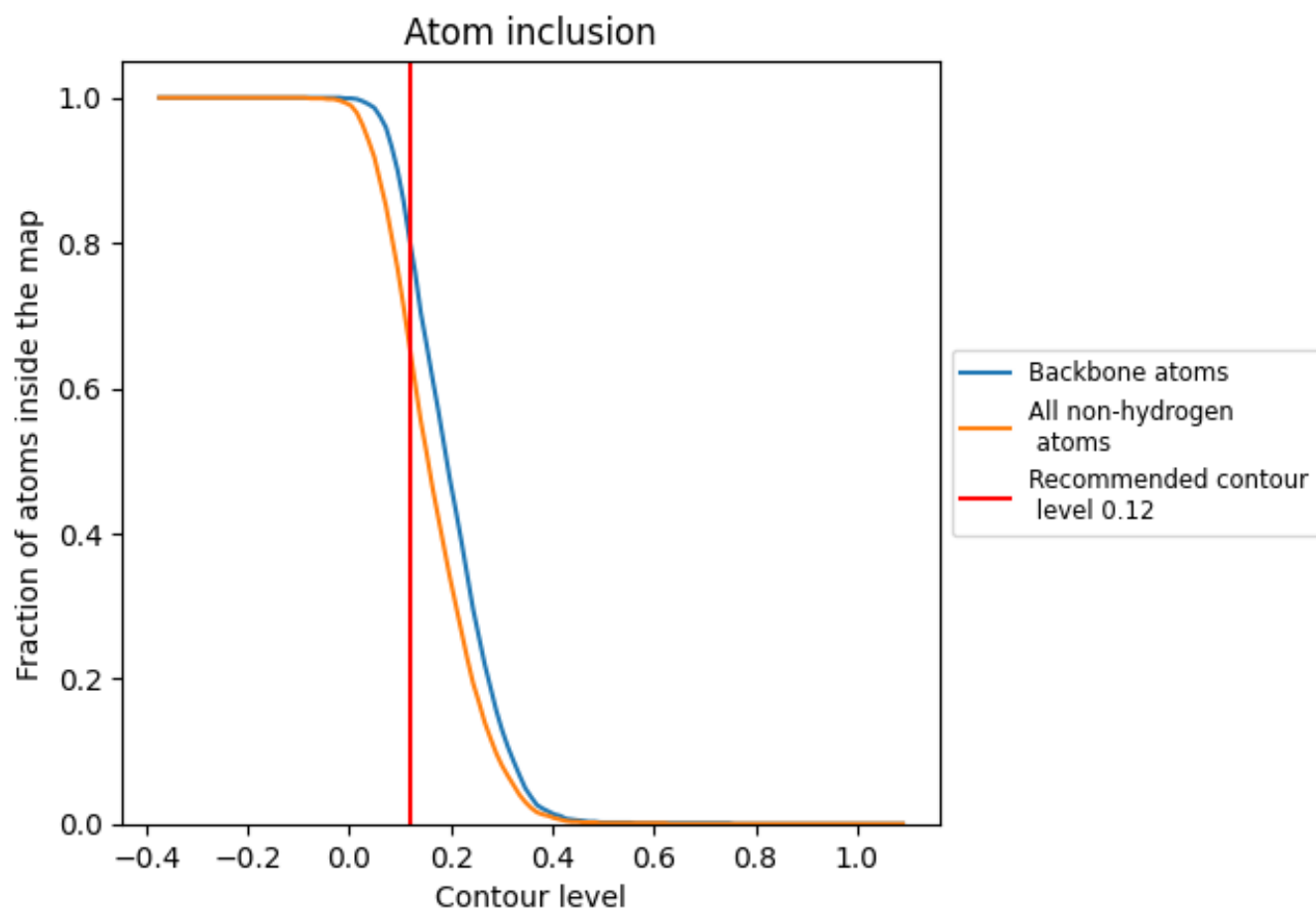
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).











9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 65% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6520	 0.4380
A	 0.7710	 0.4680
B	 0.6280	 0.4320
D	 0.3870	 0.3560
E	 0.7570	 0.4770

