



Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 06:50 AM EST

PDB ID : 8HQO
EMDB ID : EMD-34952
Title : Neck of DT57C bacteriophage in the full state
Authors : Ayala, R.; Moiseenko, A.V.; Chen, T.H.; Kulikov, E.E.; Golomidova, A.K.;
Orekhov, P.S.; Street, M.A.; Sokolova, O.S.; Letarov, A.V.; Wolf, M.
Deposited on : 2022-12-13
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

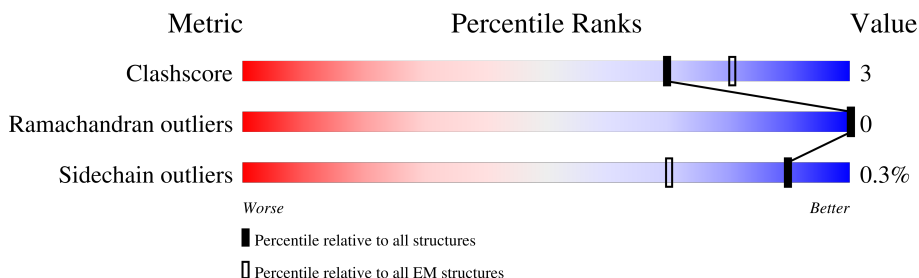
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



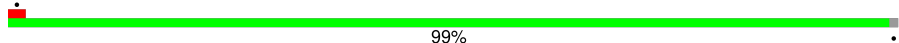
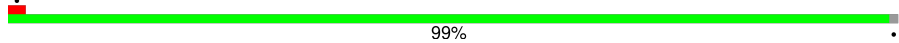
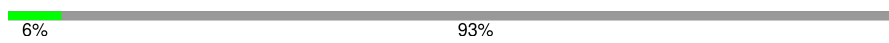
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	405	
1	C	405	
1	D	405	
1	E	405	
2	P	170	
2	Q	170	
2	R	170	
2	S	170	

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Mol	Chain	Length	Quality of chain
3	a	161	 99%
3	b	161	 99%
4	x	1227	 6%93%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20871 atoms, of which 634 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	368	Total	C	N	O	S	0	0
			2925	1858	494	559	14		
1	E	368	Total	C	N	O	S	0	0
			2925	1858	494	559	14		
1	B	368	Total	C	N	O	S	0	0
			2925	1858	494	559	14		
1	C	368	Total	C	N	O	S	0	0
			2925	1858	494	559	14		

- Molecule 2 is a protein called Head completion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	170	Total	C	N	O	S	0	0
			1345	853	222	262	8		
2	S	170	Total	C	N	O	S	0	0
			1345	853	222	262	8		
2	P	170	Total	C	N	O	S	0	0
			1345	853	222	262	8		
2	Q	170	Total	C	N	O	S	0	0
			1345	853	222	262	8		

- Molecule 3 is a protein called Tail terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	160	Total	C	N	O	S	0	0
			1279	805	215	255	4		
3	b	160	Total	C	N	O	S	0	0
			1279	805	215	255	4		

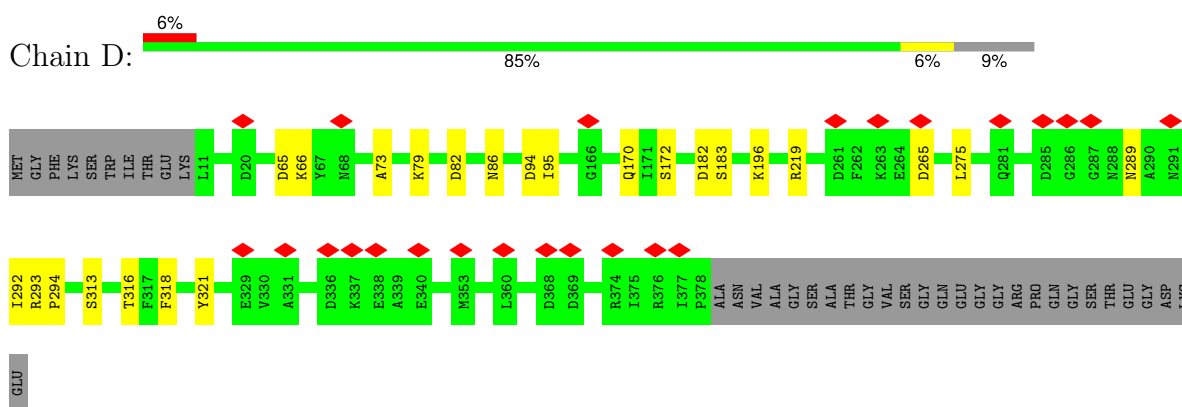
- Molecule 4 is a protein called Tape measure protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	x	80	Total	C	H	N	O	S	0	0
			1233	366	634	109	120	4		

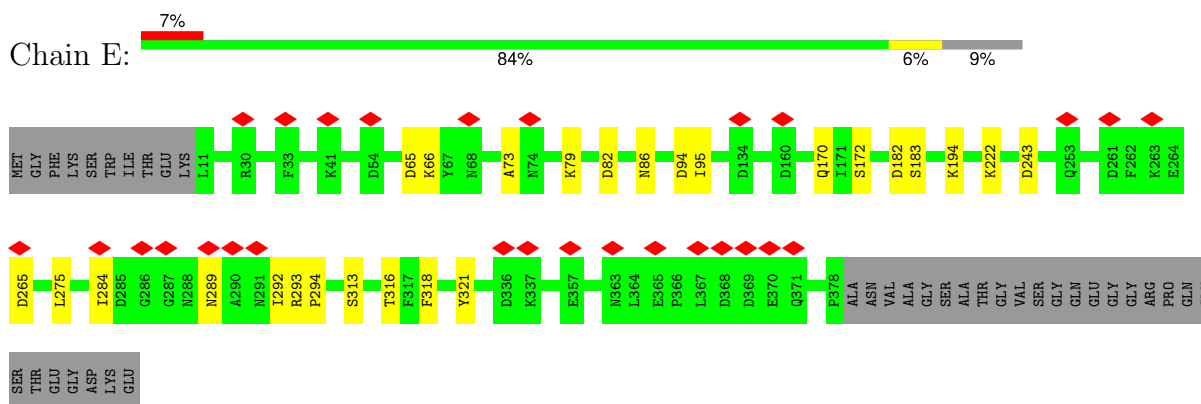
3 Residue-property plots

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.

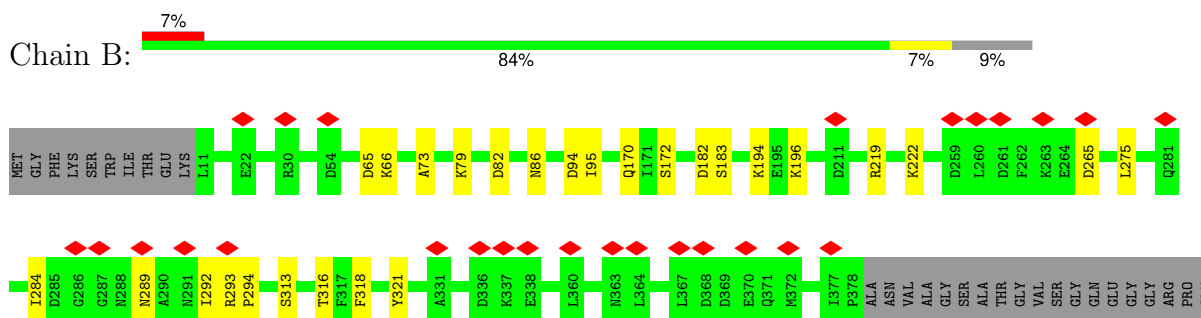
- Molecule 1: Portal protein



- Molecule 1: Portal protein

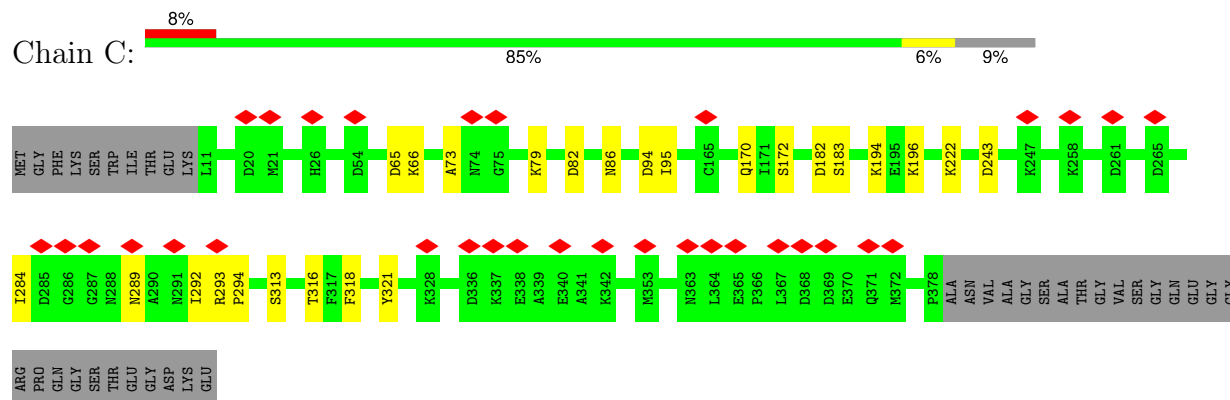


- Molecule 1: Portal protein

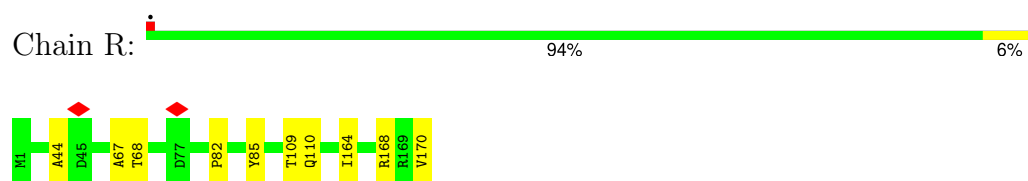


GLY
SER
THR
GLU
GLY
ASP
LYS
GLU

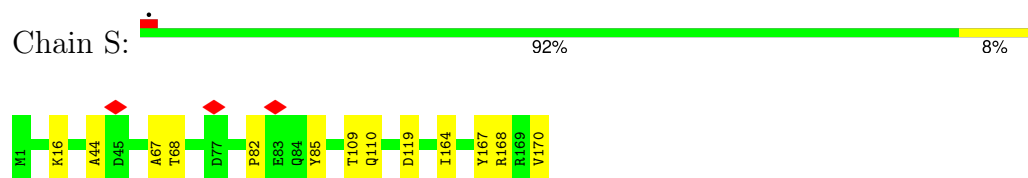
• Molecule 1: Portal protein



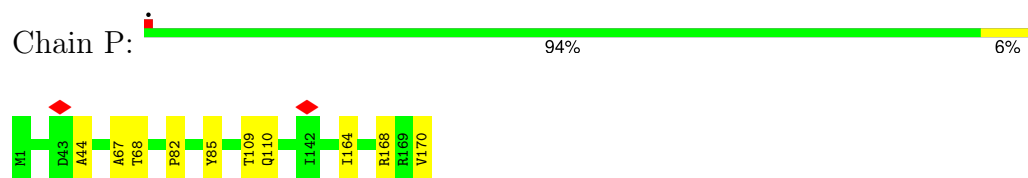
• Molecule 2: Head completion protein



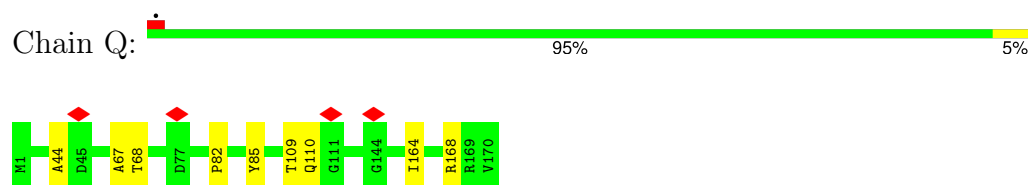
• Molecule 2: Head completion protein



• Molecule 2: Head completion protein



• Molecule 2: Head completion protein



• Molecule 3: Tail terminator protein



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34102	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 ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	31.963	Depositor
Minimum map value	-9.475	Depositor
Average map value	-0.017	Depositor
Map value standard deviation	0.972	Depositor
Recommended contour level	3.1	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	B	0.36	0/2976	0.54	0/4024
1	C	0.36	0/2976	0.54	0/4024
1	D	0.36	0/2976	0.54	0/4024
1	E	0.36	0/2976	0.54	0/4024
2	P	0.38	0/1371	0.55	0/1856
2	Q	0.38	0/1371	0.55	0/1856
2	R	0.38	0/1371	0.55	0/1856
2	S	0.38	0/1371	0.55	0/1856
3	a	0.33	0/1305	0.55	0/1773
3	b	0.33	0/1305	0.55	0/1773
4	x	0.24	0/600	0.52	0/802
All	All	0.36	0/20598	0.54	0/27868

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 [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	B	2925	0	2950	20	0
1	C	2925	0	2950	17	0
1	D	2925	0	2950	16	0
1	E	2925	0	2950	19	0
2	P	1345	0	1347	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	1345	0	1347	5	0
2	R	1345	0	1347	6	0
2	S	1345	0	1347	8	0
3	a	1279	0	1244	0	0
3	b	1279	0	1244	0	0
4	x	599	634	634	0	0
All	All	20237	634	20310	83	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 3.

All (83) 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:82:ASP:OD1	1:B:86:ASN:ND2	2.13	0.81
1:C:82:ASP:OD1	1:C:86:ASN:ND2	2.13	0.81
1:D:82:ASP:OD1	1:D:86:ASN:ND2	2.13	0.80
1:E:82:ASP:OD1	1:E:86:ASN:ND2	2.13	0.80
2:S:44:ALA:O	2:S:110:GLN:NE2	2.30	0.62
2:Q:44:ALA:O	2:Q:110:GLN:NE2	2.30	0.62
1:D:294:PRO:HG2	1:E:289:ASN:HB2	1.83	0.60
1:B:294:PRO:HG2	1:C:289:ASN:HB2	1.83	0.60
2:P:44:ALA:O	2:P:110:GLN:NE2	2.30	0.60
1:E:289:ASN:HA	1:E:292:ILE:HG22	1.85	0.59
1:B:289:ASN:HA	1:B:292:ILE:HG22	1.85	0.58
2:R:44:ALA:O	2:R:110:GLN:NE2	2.30	0.58
1:C:289:ASN:HA	1:C:292:ILE:HG22	1.85	0.57
1:D:289:ASN:HA	1:D:292:ILE:HG22	1.85	0.57
1:E:294:PRO:HG2	1:B:289:ASN:HB2	1.86	0.57
1:D:313:SER:HA	1:D:316:THR:HG22	1.89	0.55
1:E:313:SER:HA	1:E:316:THR:HG22	1.89	0.54
1:C:222:LYS:HD3	2:P:170:VAL:HG13	1.89	0.54
1:E:222:LYS:HD3	2:R:170:VAL:HG13	1.89	0.54
1:C:313:SER:HA	1:C:316:THR:HG22	1.89	0.53
1:B:313:SER:HA	1:B:316:THR:HG22	1.89	0.53
2:S:170:VAL:HG13	1:B:222:LYS:HD3	1.93	0.51
1:D:182:ASP:OD1	1:D:183:SER:N	2.44	0.51
1:B:182:ASP:OD1	1:B:183:SER:N	2.44	0.51
2:S:82:PRO:HA	2:S:85:TYR:CE2	2.46	0.51
2:Q:82:PRO:HA	2:Q:85:TYR:CE2	2.46	0.51
1:C:182:ASP:OD1	1:C:183:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:ASP:OD1	1:E:183:SER:N	2.44	0.50
2:R:82:PRO:HA	2:R:85:TYR:CE2	2.46	0.50
2:P:82:PRO:HA	2:P:85:TYR:CE2	2.46	0.50
1:B:265:ASP:OD2	1:C:194:LYS:NZ	2.34	0.47
1:D:265:ASP:OD2	1:E:194:LYS:NZ	2.34	0.47
1:E:65:ASP:OD1	1:E:65:ASP:N	2.47	0.47
1:D:65:ASP:OD1	1:D:65:ASP:N	2.47	0.47
2:S:119:ASP:OD2	2:S:167:TYR:OH	2.24	0.46
1:B:65:ASP:OD1	1:B:65:ASP:N	2.47	0.46
1:B:293:ARG:HB3	1:B:294:PRO:HD3	1.99	0.45
1:D:293:ARG:HB3	1:D:294:PRO:HD3	1.99	0.45
1:E:293:ARG:HB3	1:E:294:PRO:HD3	1.99	0.45
1:C:293:ARG:HB3	1:C:294:PRO:HD3	1.99	0.44
1:D:275:LEU:HD13	1:E:284:ILE:HG23	2.00	0.44
1:D:170:GLN:O	1:D:172:SER:N	2.47	0.44
1:D:94:ASP:CG	1:D:95:ILE:N	2.71	0.43
1:C:94:ASP:CG	1:C:95:ILE:N	2.71	0.43
2:R:68:THR:HG22	2:R:109:THR:O	2.19	0.43
2:S:67:ALA:HA	2:S:110:GLN:HA	2.01	0.43
1:B:275:LEU:HD13	1:C:284:ILE:HG23	2.00	0.43
2:R:67:ALA:HA	2:R:110:GLN:HA	2.01	0.43
2:P:67:ALA:HA	2:P:110:GLN:HA	2.01	0.43
1:B:94:ASP:CG	1:B:95:ILE:N	2.72	0.43
1:E:94:ASP:CG	1:E:95:ILE:N	2.72	0.43
2:S:16:LYS:HB3	2:S:16:LYS:HE2	1.86	0.43
2:Q:67:ALA:HA	2:Q:110:GLN:HA	2.01	0.43
1:E:170:GLN:O	1:E:172:SER:N	2.47	0.43
2:S:68:THR:HG22	2:S:109:THR:O	2.19	0.43
1:B:66:LYS:HD3	1:B:321:TYR:CZ	2.54	0.43
2:P:68:THR:HG22	2:P:109:THR:O	2.19	0.43
1:E:265:ASP:OD2	1:B:194:LYS:NZ	2.35	0.42
2:Q:68:THR:HG22	2:Q:109:THR:O	2.19	0.42
1:C:66:LYS:HD3	1:C:321:TYR:CZ	2.54	0.42
1:E:66:LYS:HD3	1:E:321:TYR:CZ	2.54	0.42
1:D:66:LYS:HD3	1:D:321:TYR:CZ	2.54	0.42
1:B:170:GLN:O	1:B:172:SER:N	2.47	0.42
1:C:170:GLN:O	1:C:172:SER:N	2.47	0.42
1:C:196:LYS:HE3	1:C:196:LYS:HB2	1.93	0.42
1:D:196:LYS:HE3	1:D:196:LYS:HB2	1.93	0.41
2:Q:164:ILE:O	2:Q:168:ARG:N	2.53	0.41
1:E:66:LYS:HD3	1:E:321:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ALA:HB2	1:C:318:PHE:CE2	2.55	0.41
1:B:196:LYS:HE3	1:B:196:LYS:HB2	1.93	0.41
1:C:66:LYS:HD3	1:C:321:TYR:CE1	2.55	0.41
1:D:219:ARG:NH1	1:E:243:ASP:OD2	2.53	0.41
2:P:164:ILE:O	2:P:168:ARG:N	2.53	0.41
1:D:66:LYS:HD3	1:D:321:TYR:CE1	2.56	0.41
1:E:275:LEU:HD13	1:B:284:ILE:HG23	2.03	0.41
1:B:219:ARG:NH1	1:C:243:ASP:OD2	2.53	0.41
1:D:73:ALA:HB2	1:D:318:PHE:CE2	2.55	0.41
1:B:73:ALA:HB2	1:B:318:PHE:CE2	2.55	0.41
1:E:73:ALA:HB2	1:E:318:PHE:CE2	2.55	0.41
2:S:164:ILE:O	2:S:168:ARG:N	2.53	0.40
2:R:164:ILE:O	2:R:168:ARG:N	2.53	0.40
1:B:66:LYS:HD3	1:B:321:TYR:CE1	2.55	0.40
1:C:65:ASP:N	1:C:65:ASP:OD1	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	366/405 (90%)	353 (96%)	13 (4%)	0	100	100
1	C	366/405 (90%)	353 (96%)	13 (4%)	0	100	100
1	D	366/405 (90%)	353 (96%)	13 (4%)	0	100	100
1	E	366/405 (90%)	353 (96%)	13 (4%)	0	100	100
2	P	168/170 (99%)	168 (100%)	0	0	100	100
2	Q	168/170 (99%)	168 (100%)	0	0	100	100
2	R	168/170 (99%)	168 (100%)	0	0	100	100
2	S	168/170 (99%)	168 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	b	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
4	x	78/1227 (6%)	75 (96%)	3 (4%)	0	100	100
All	All	2530/3849 (66%)	2463 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	328/354 (93%)	327 (100%)	1 (0%)	91	96
1	C	328/354 (93%)	327 (100%)	1 (0%)	91	96
1	D	328/354 (93%)	327 (100%)	1 (0%)	91	96
1	E	328/354 (93%)	327 (100%)	1 (0%)	91	96
2	P	149/149 (100%)	149 (100%)	0	100	100
2	Q	149/149 (100%)	149 (100%)	0	100	100
2	R	149/149 (100%)	149 (100%)	0	100	100
2	S	149/149 (100%)	149 (100%)	0	100	100
3	a	142/143 (99%)	142 (100%)	0	100	100
3	b	142/143 (99%)	142 (100%)	0	100	100
4	x	63/967 (6%)	61 (97%)	2 (3%)	34	65
All	All	2255/3265 (69%)	2249 (100%)	6 (0%)	90	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	79	LYS
1	E	79	LYS
1	B	79	LYS
1	C	79	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	x	4	LYS
4	x	62	ARG

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

Mol	Chain	Res	Type
1	D	50	ASN
1	D	200	ASN
1	E	200	ASN
1	E	289	ASN
2	R	150	ASN
2	S	150	ASN
3	a	3	HIS
3	a	18	GLN
3	a	23	GLN
3	a	153	GLN
1	B	289	ASN
1	C	289	ASN
2	P	150	ASN
3	b	3	HIS
3	b	18	GLN
3	b	23	GLN
3	b	153	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.

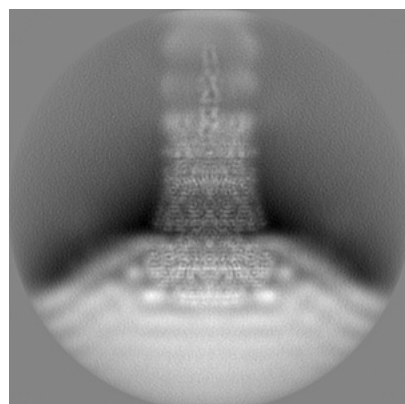
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34952. These allow visual inspection of the internal detail of the map and identification of artifacts.

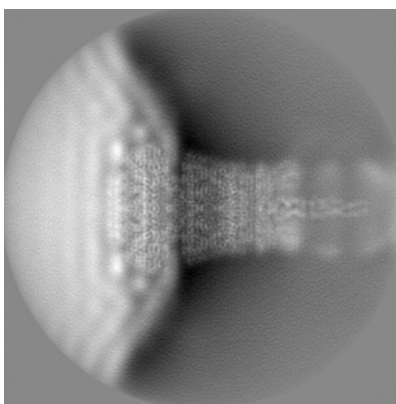
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

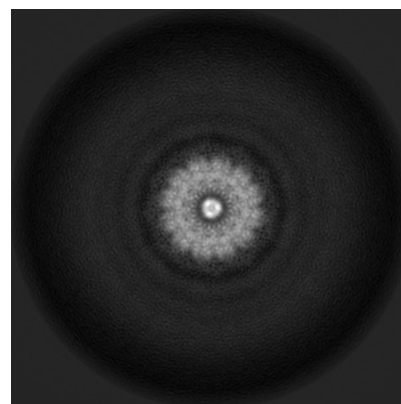
6.1.1 Primary map



X

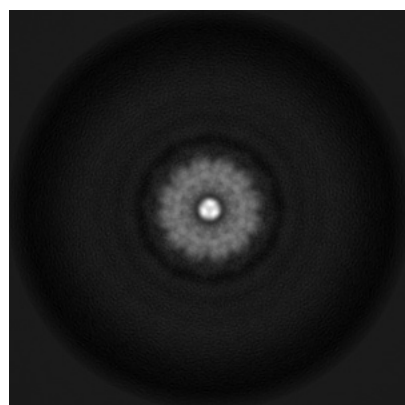


Y

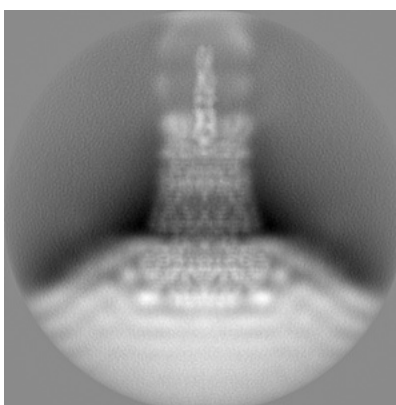


Z

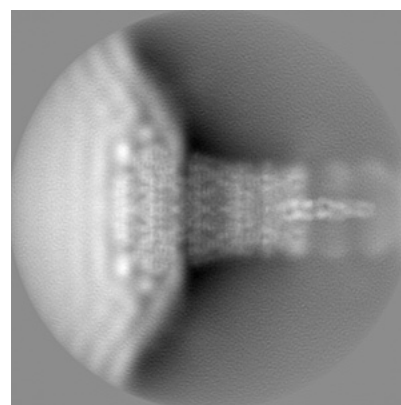
6.1.2 Raw map



X



Y

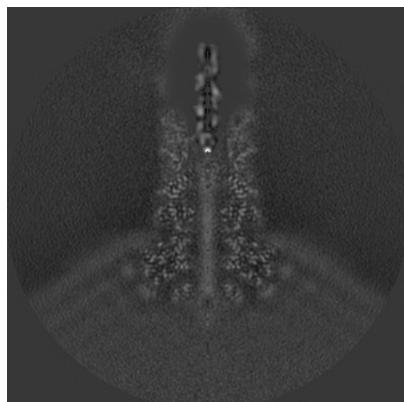


Z

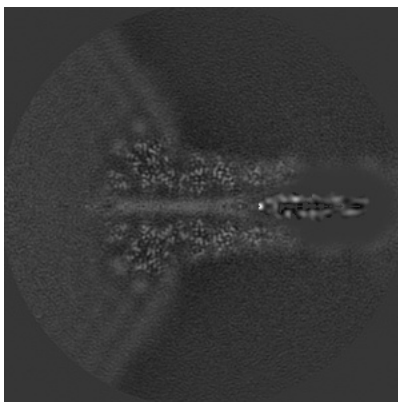
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

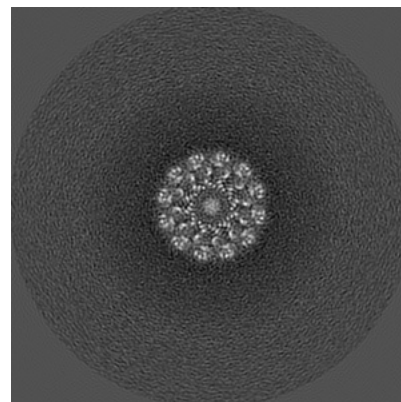
6.2.1 Primary map



X Index: 150

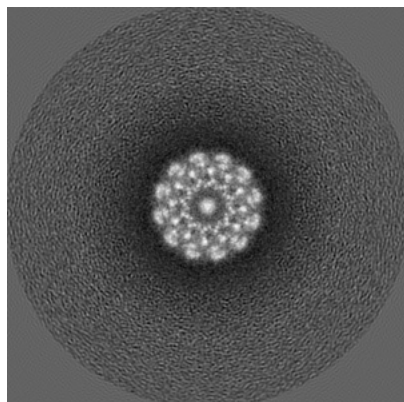


Y Index: 150

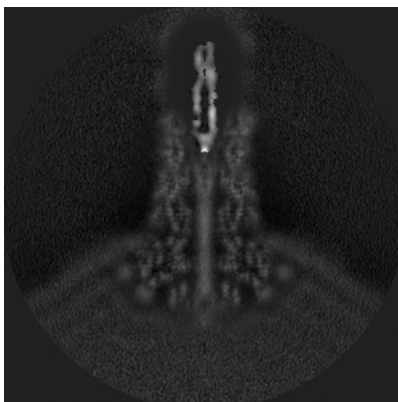


Z Index: 150

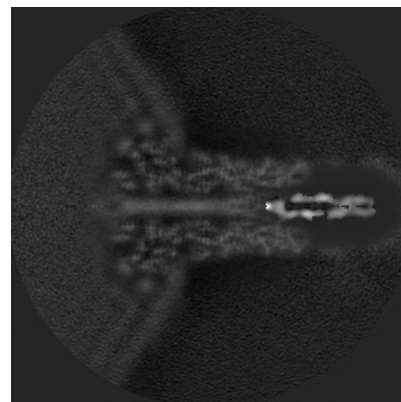
6.2.2 Raw map



X Index: 150



Y Index: 150

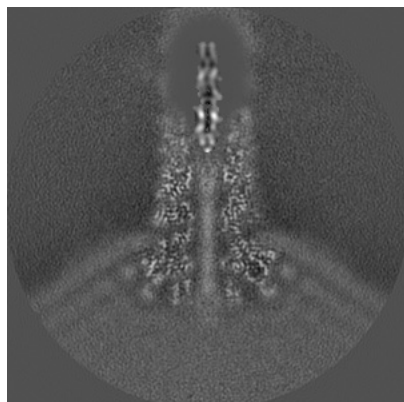


Z Index: 150

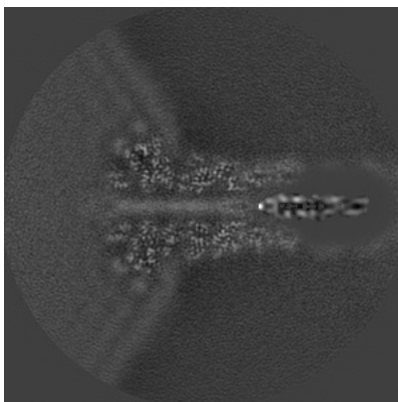
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

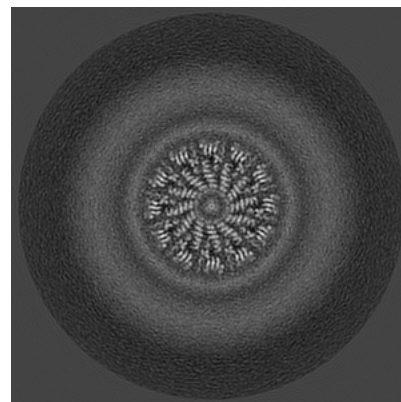
6.3.1 Primary map



X Index: 148

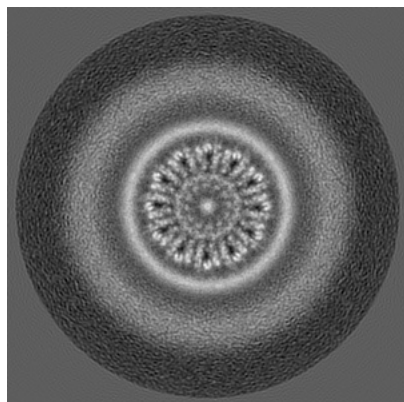


Y Index: 151

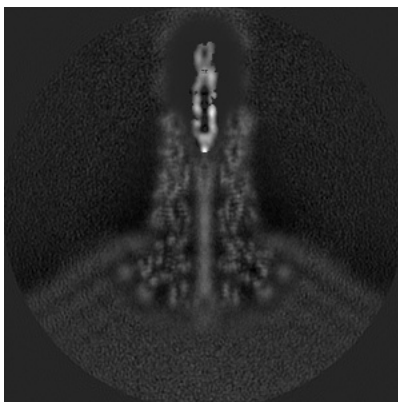


Z Index: 105

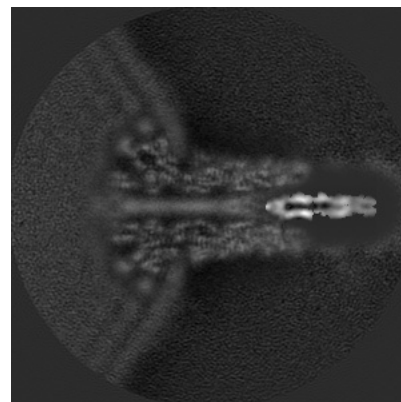
6.3.2 Raw map



X Index: 101



Y Index: 151

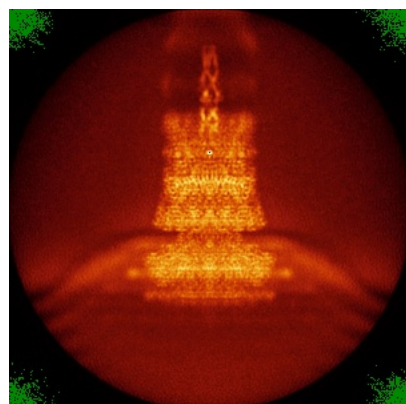


Z Index: 148

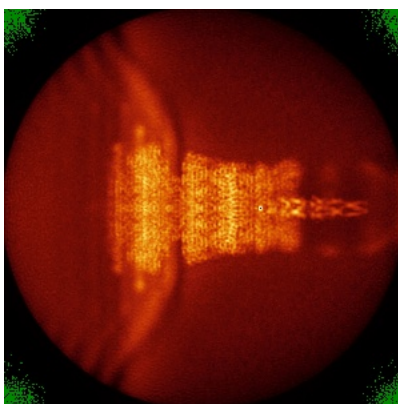
The images above show the largest variance slices of the map in three orthogonal directions.

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

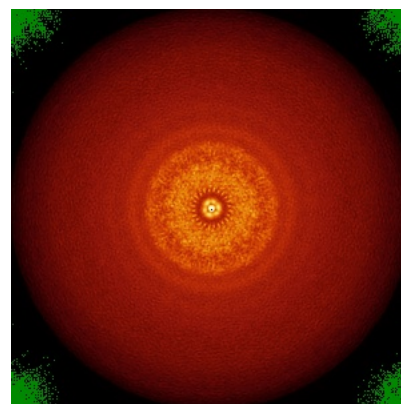
6.4.1 Primary map



X

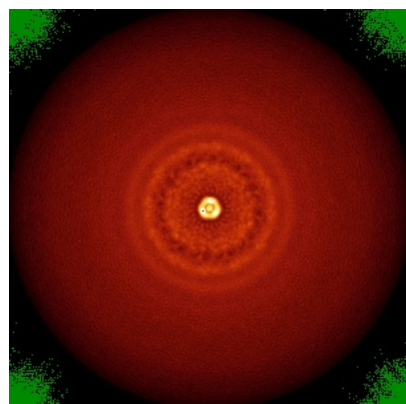


Y

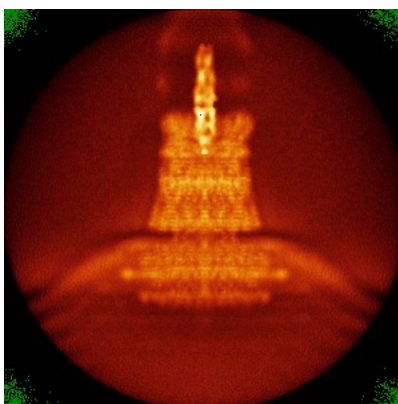


Z

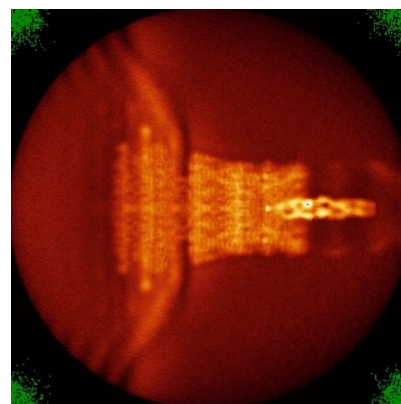
6.4.2 Raw map



X



Y

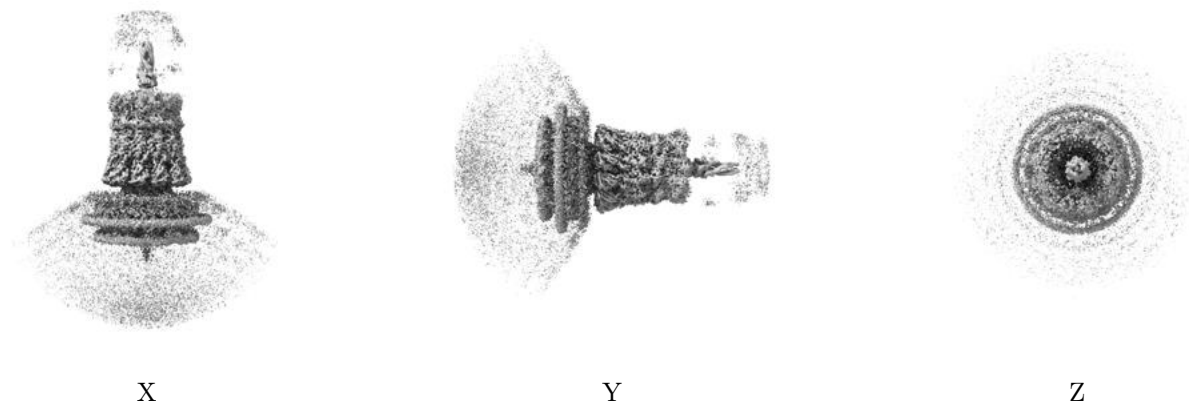


Z

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.

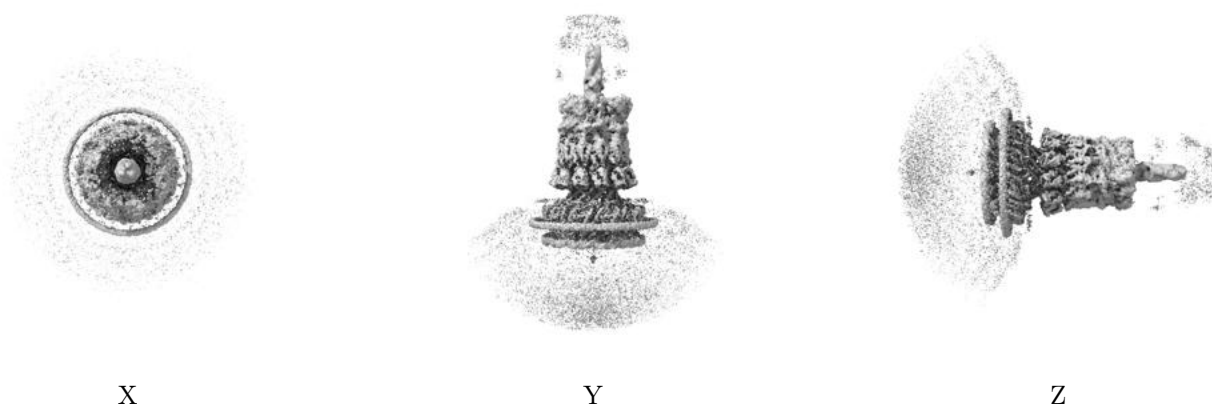
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.1. 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.

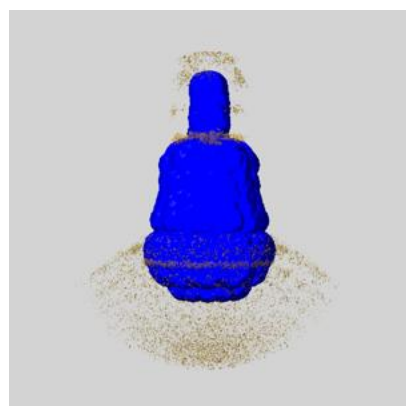
6.6 Mask visualisation [i](#)

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

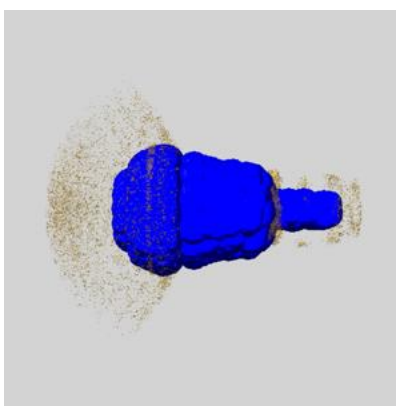
A mask typically either:

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

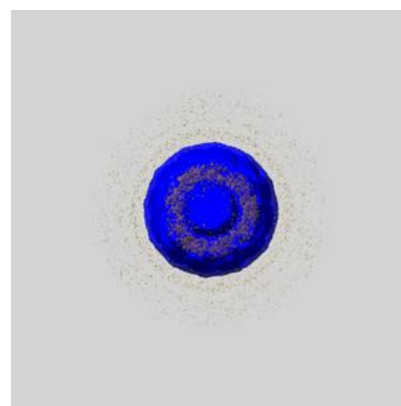
6.6.1 emd_34952_msk_1.map [i](#)



X



Y

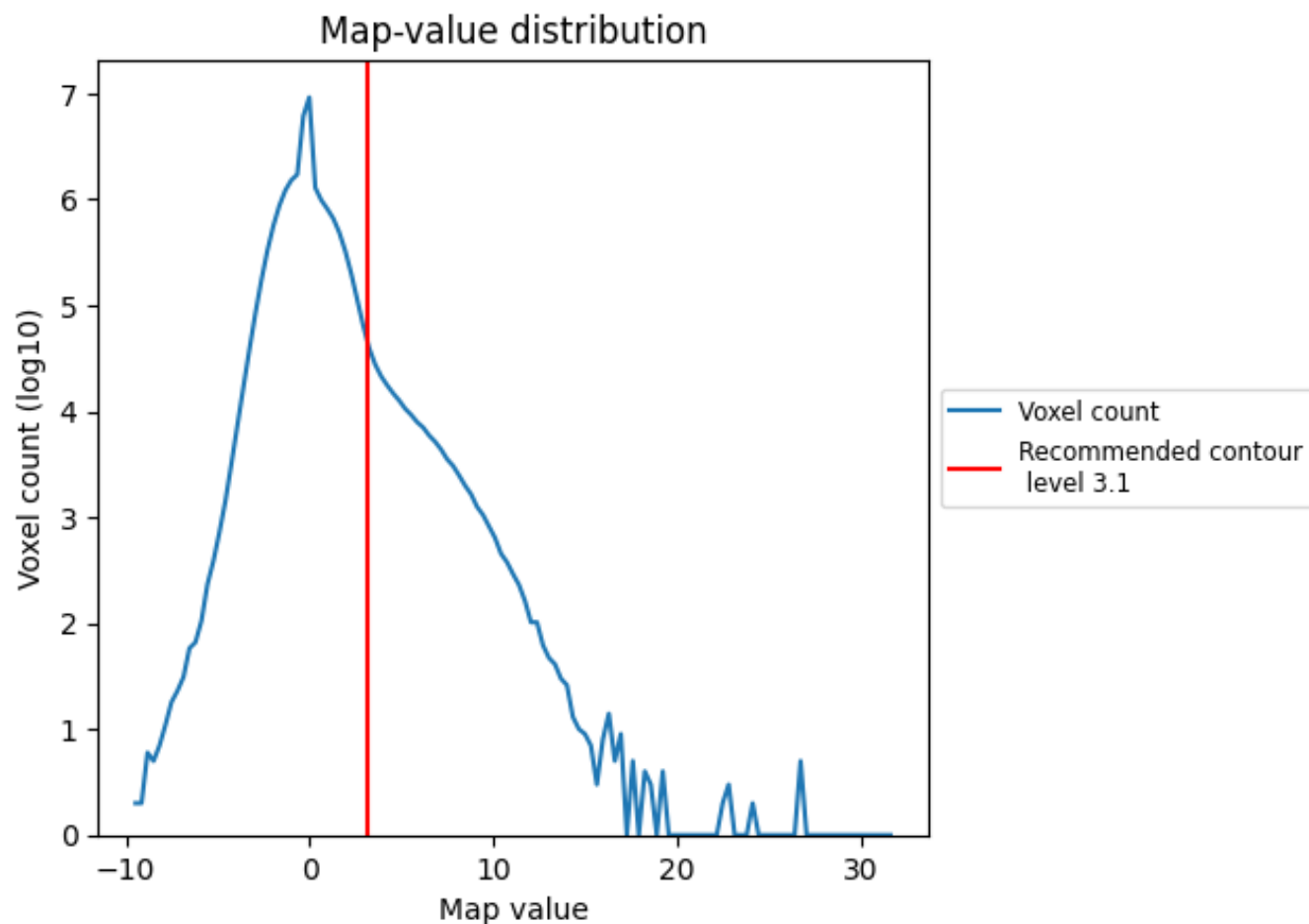


Z

7 Map analysis [i](#)

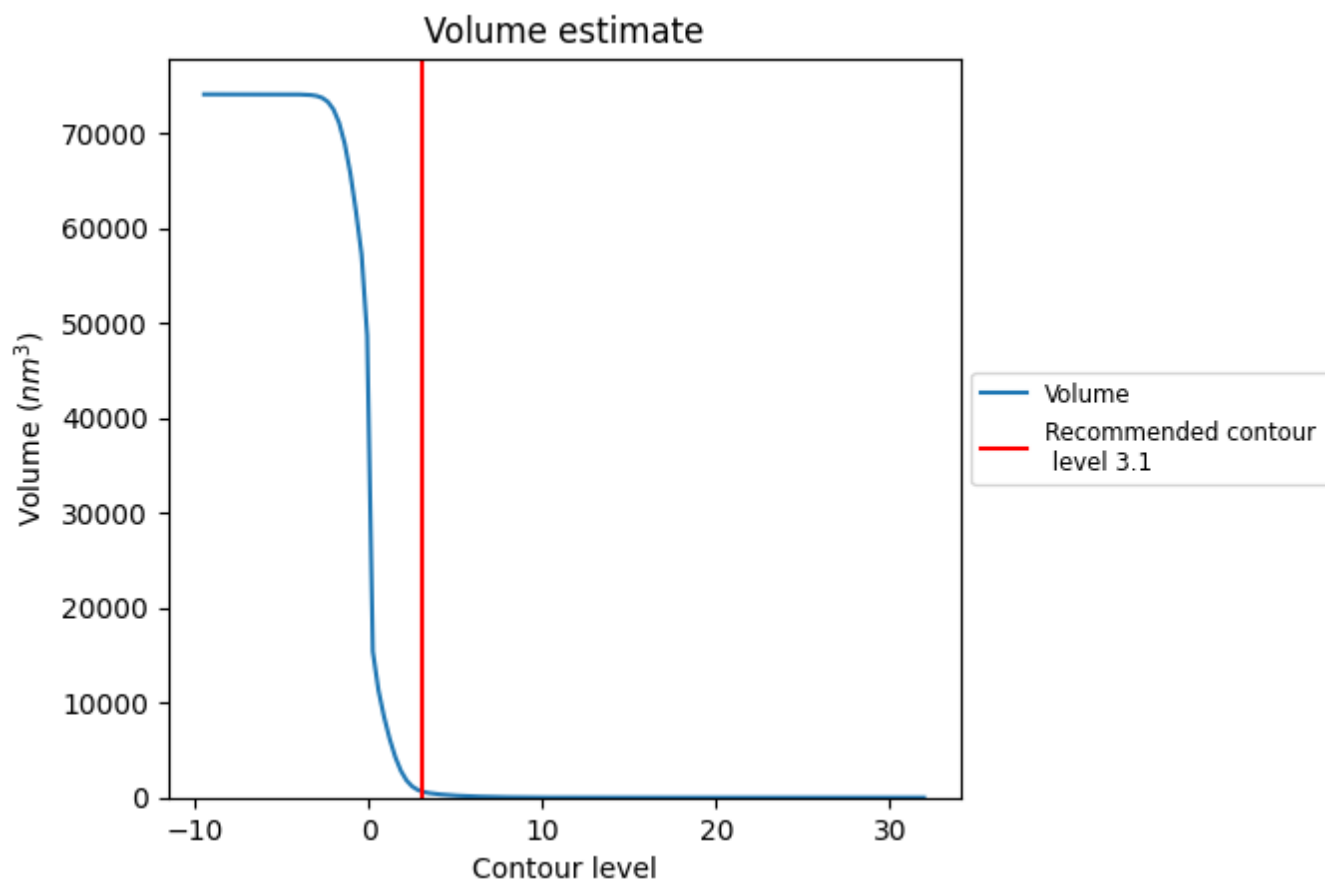
This section contains the results of statistical analysis of the map.

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.

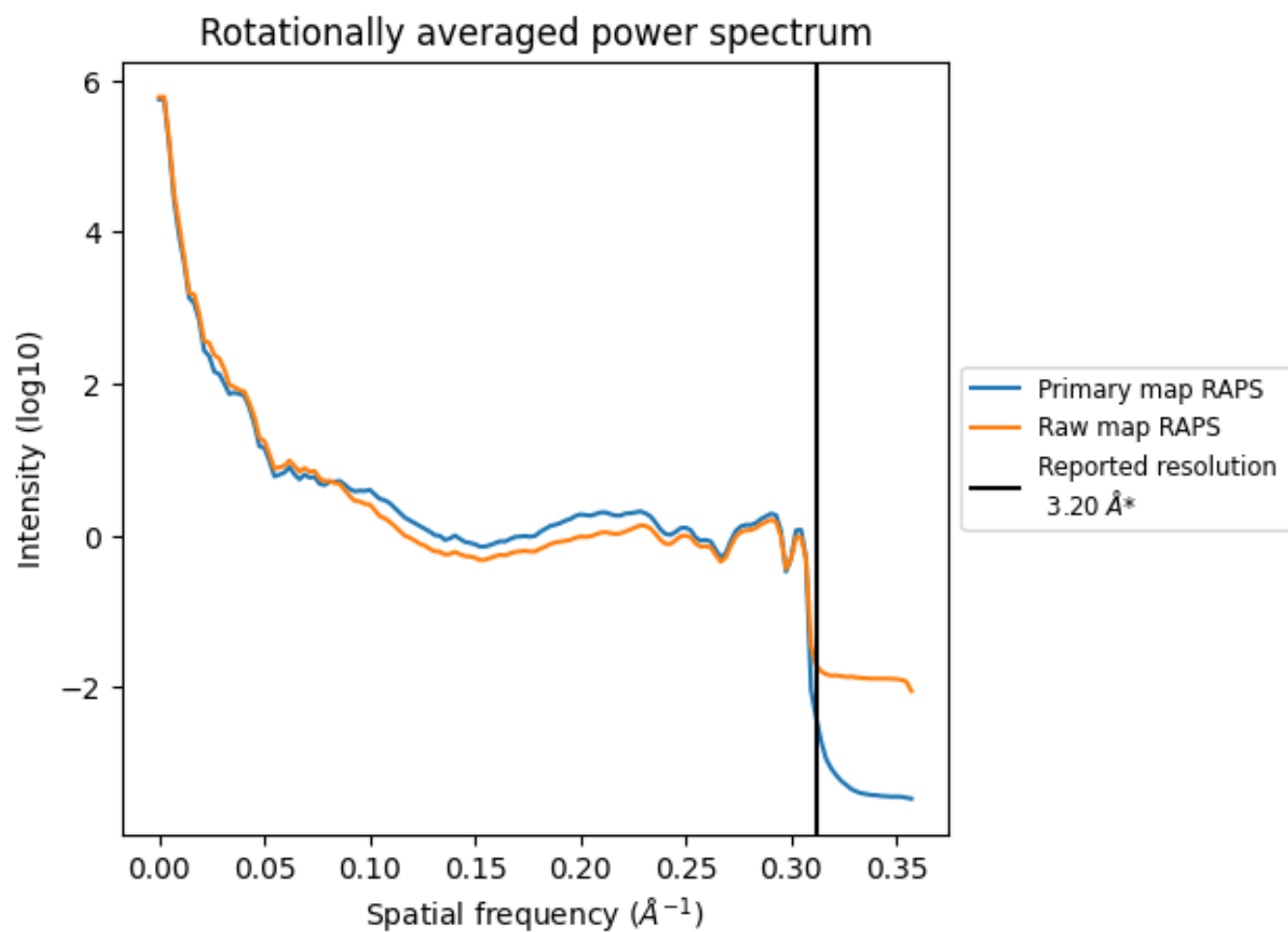
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 631 nm³; this corresponds to an approximate mass of 570 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 ⓘ

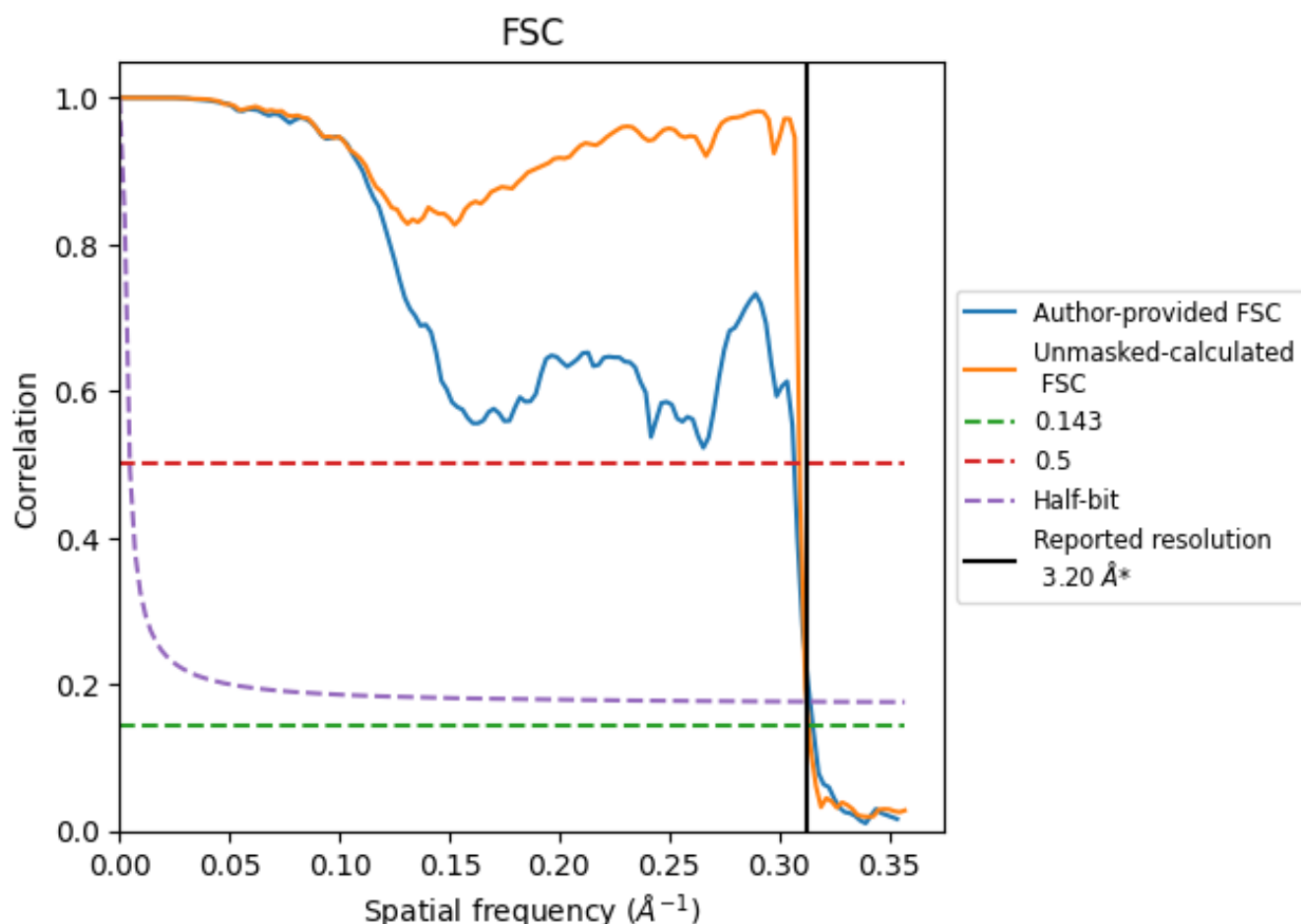


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.26	3.18
Unmasked-calculated*	3.19	3.23	3.20

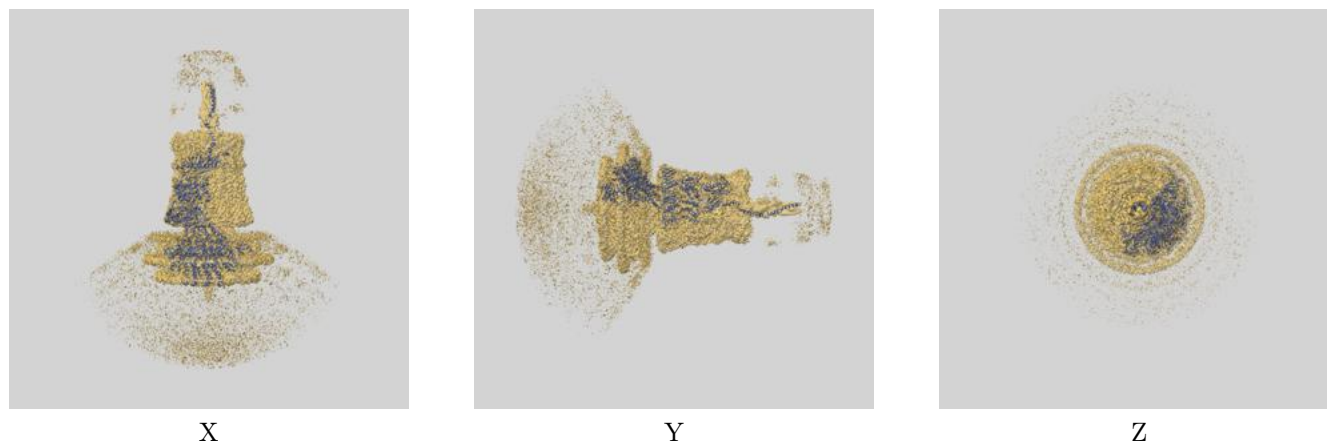
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

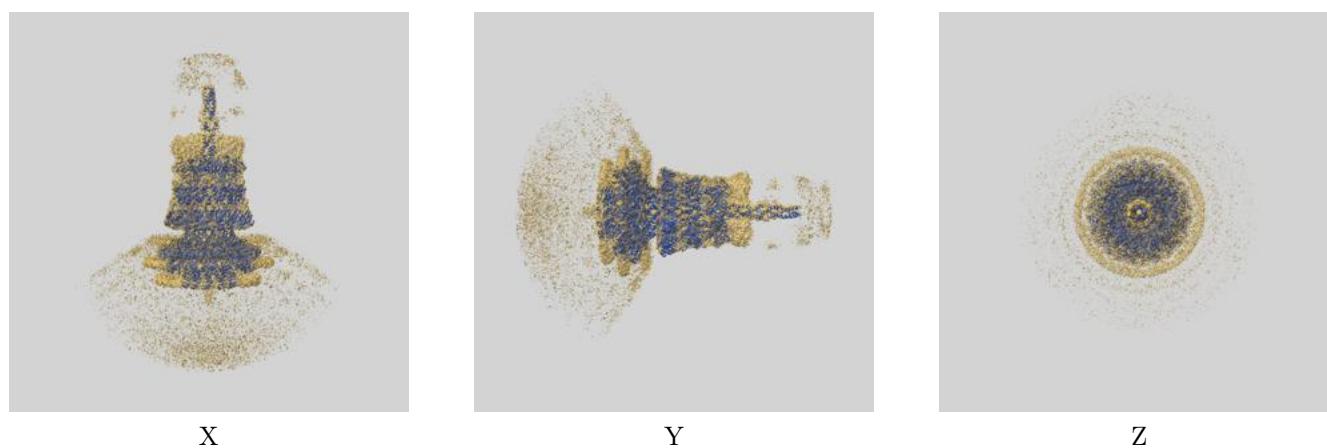
This section contains information regarding the fit between EMDB map EMD-34952 and PDB model 8HQO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

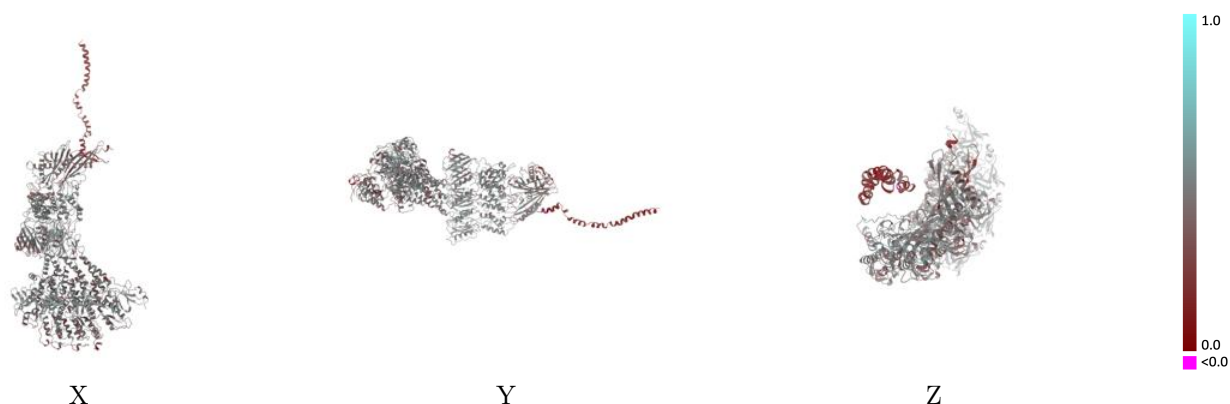


9.1.2 Map-model assembly overlay [i](#)



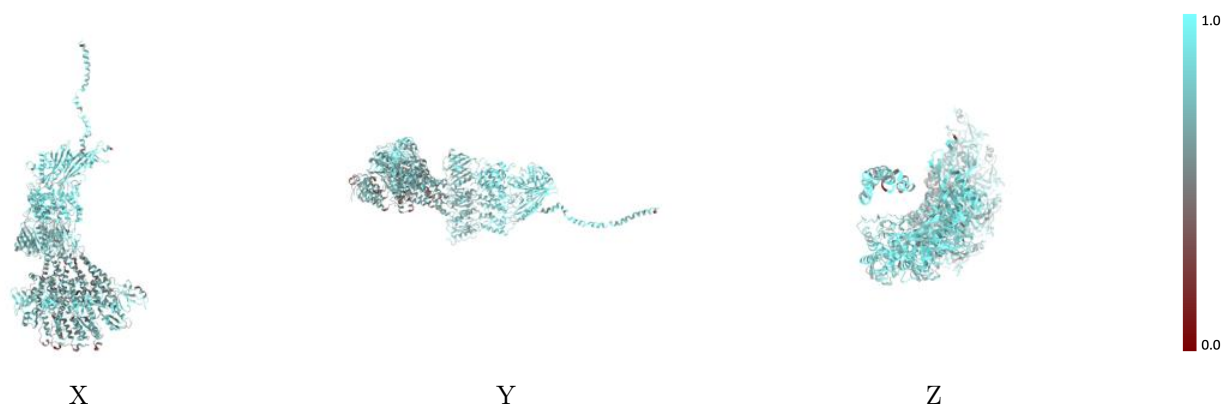
The images above show the 3D surface view of the map at the recommended contour level 3.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



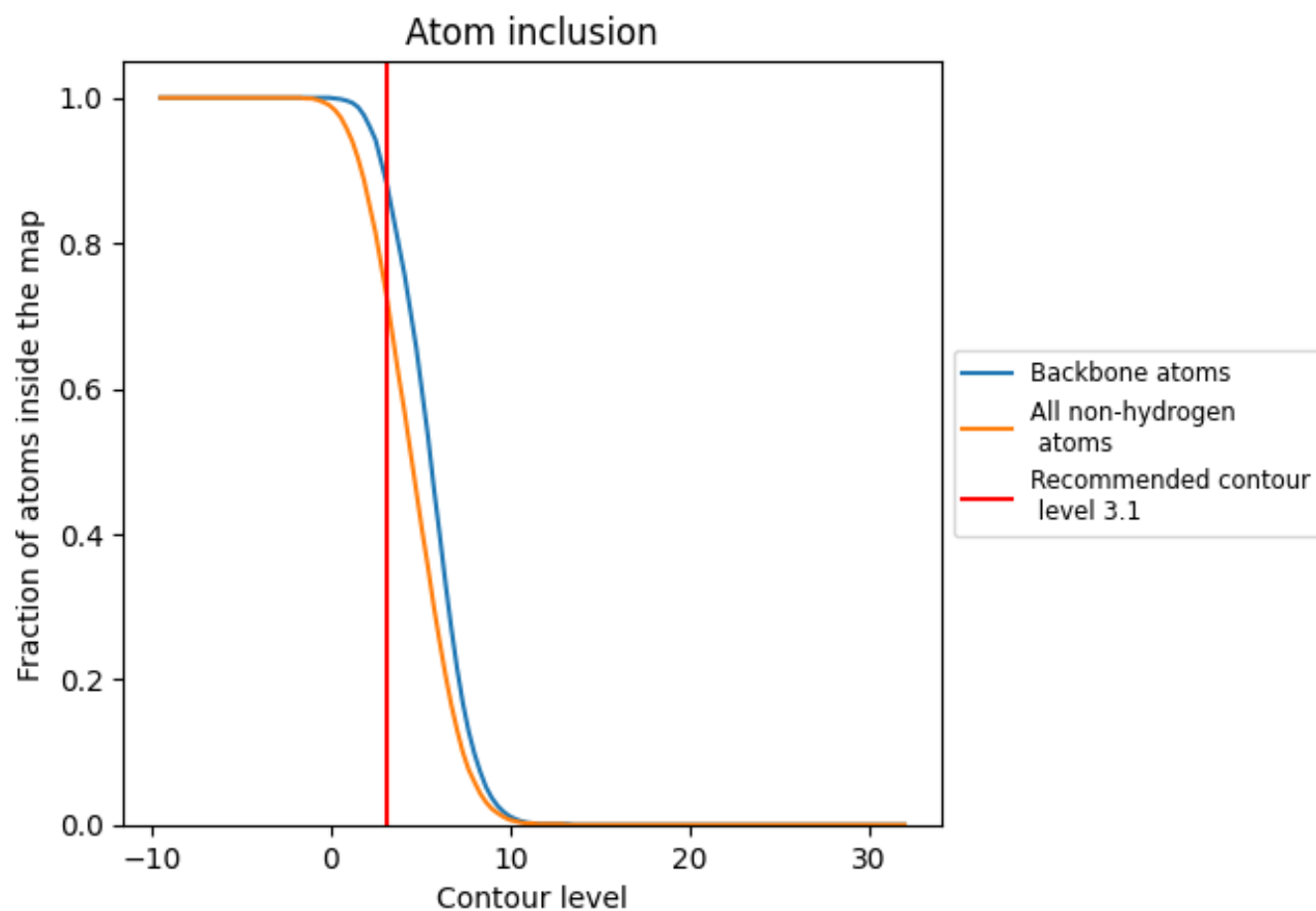
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.1).

























9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 73% 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 (3.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 0.4410
B	 0.6800	 0.4440
C	 0.6680	 0.4390
D	 0.6800	 0.4480
E	 0.6840	 0.4710
P	 0.7900	 0.4470
Q	 0.7970	 0.4730
R	 0.7930	 0.4540
S	 0.7830	 0.4530
a	 0.8630	 0.4420
b	 0.8280	 0.3940
x	 0.7430	 0.2120

