



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:25 PM UTC

PDB ID : 8XCK / pdb_00008xck
EMDB ID : EMD-38246
Title : Closed state of central tail fiber of bacteriophage lambda
Authors : Ge, X.F.; Wang, J.W.
Deposited on : 2023-12-09
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

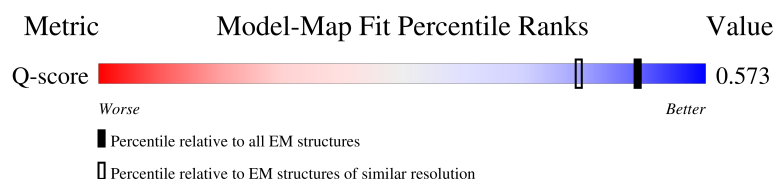
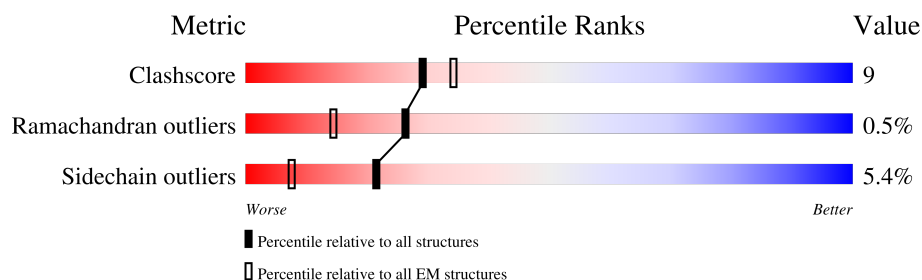
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 (2.25 - 3.25)

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	F	420	
1	J	420	
1	Z	420	
2	f	190	

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Mol	Chain	Length	Quality of chain
2	j	190	60%22%16%
2	z	190	63%19%16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10671 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 Tip attachment protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	305	Total	C	N	O	S	0	0
			2323	1459	401	453	10		
1	Z	305	Total	C	N	O	S	0	0
			2323	1459	401	453	10		
1	F	305	Total	C	N	O	S	0	0
			2323	1459	401	453	10		

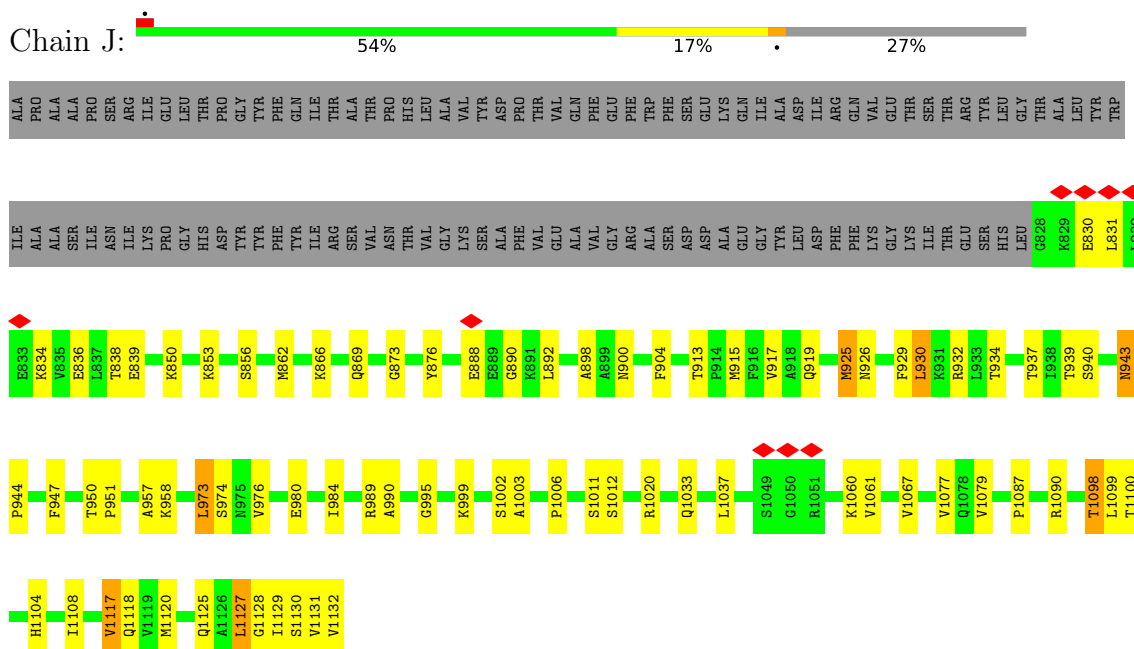
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	j	160	Total	C	N	O	S	0	0
			1234	780	216	234	4		
2	z	160	Total	C	N	O	S	0	0
			1234	780	216	234	4		
2	f	160	Total	C	N	O	S	0	0
			1234	780	216	234	4		

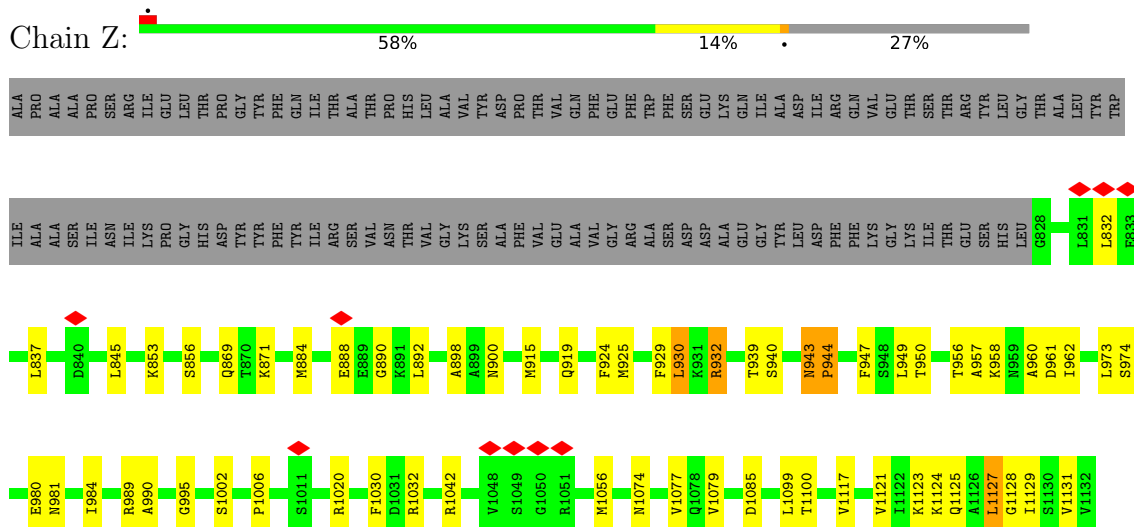
3 Residue-property plots

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: Tip attachment protein J



• Molecule 1: Tip attachment protein Z



Chain F:

Chain j:

A horizontal stacked bar chart for Chain j. The bar is divided into three segments: a green segment representing 60%, a yellow segment representing 22%, and a grey segment representing 16%. A small red dot is visible at the very beginning of the bar.

Category	Percentage
Green	60%
Yellow	22%
Grey	16%

Chain z:

Residue	Conservation (%)
K98	~10
D102	~10
N107	~10
T112	~10
A113	~10
R116	~10
D119	~10
K120	~10
D121	~10
S122	~10
A123	~10
T124	~10
S126	~10
F128	~10
N134	~10
D138	~10
Q141	~10
R142	~10
D143	~10
K154	~10
D157	~10
H158	~10
K187	~10
V188	~10
L189	~10
PRO	~10

Chain f:

Residue	Category
MET	Grey
PHE	Grey
LYS	Grey
SER	Grey
THR	Grey
LEU	Grey
ALA	Green
ALA	Green
MET	Green
ALA	Green
ALA	Green
VAL	Green
PHE	Green
LEU	Green
LEU	Green
SER	Green
ALA	Green
LEU	Green
SER	Green
PRO	Green
PRO	Green
ALA	Green
ALA	Green
LYS	Green
GLY	Green
ASP	Green
PRO	Green
H3O	Green
V31	Yellow
L32	Yellow
G38	Yellow
N39	Yellow
I40	Yellow
E41	Yellow
L42	Yellow
E43	Yellow
L44	Yellow
V53	Yellow
F56	Yellow
V57	Yellow
V60	Yellow
M67	Yellow
H71	Yellow
R72	Yellow
V73	Yellow
I74	Yellow
P75	Yellow
I79	Yellow
Q80	Yellow
G81	Yellow



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	369942	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.551	Depositor
Minimum map value	-3.650	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	497.28, 497.28, 497.28	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.036, 1.036, 1.036	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	F	1.13	7/2364 (0.3%)	1.19	4/3208 (0.1%)
1	J	1.13	6/2364 (0.3%)	1.18	2/3208 (0.1%)
1	Z	1.15	9/2364 (0.4%)	1.18	0/3208
2	f	1.06	1/1260 (0.1%)	1.13	3/1708 (0.2%)
2	j	1.07	1/1260 (0.1%)	1.12	1/1708 (0.1%)
2	z	1.07	2/1260 (0.2%)	1.16	2/1708 (0.1%)
All	All	1.11	26/10872 (0.2%)	1.17	12/14748 (0.1%)

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	F	0	1
1	J	0	1
1	Z	0	1
All	All	0	3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	961	ASP	CG-OD2	8.54	1.41	1.25
1	Z	957	ALA	C-O	8.48	1.34	1.23
1	J	1079	VAL	C-O	-7.60	1.15	1.24
1	Z	1079	VAL	C-O	-7.28	1.16	1.24
1	F	949	LEU	C-O	-7.14	1.15	1.24
1	F	1079	VAL	C-O	-7.08	1.16	1.24
2	z	81	GLY	C-O	-6.87	1.16	1.23
1	Z	949	LEU	C-O	-6.51	1.16	1.24
1	J	1117	VAL	C-O	-6.22	1.17	1.24
1	J	939	THR	C-O	-6.19	1.16	1.23
2	j	81	GLY	C-O	-6.05	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	957	ALA	C-O	6.03	1.31	1.23
1	F	1117	VAL	C-O	-5.99	1.17	1.24
1	J	957	ALA	C-O	5.84	1.31	1.23
2	f	81	GLY	C-O	-5.84	1.16	1.23
1	Z	924	PHE	C-O	-5.72	1.16	1.23
1	J	930	LEU	C-O	-5.71	1.16	1.23
1	Z	930	LEU	C-O	-5.68	1.16	1.23
1	F	930	LEU	C-O	-5.64	1.16	1.23
1	Z	961	ASP	CG-OD1	5.54	1.35	1.25
1	Z	932	ARG	C-O	-5.51	1.17	1.23
1	F	932	ARG	C-O	-5.40	1.17	1.23
1	Z	956	THR	C-O	5.14	1.29	1.24
1	F	924	PHE	C-O	-5.13	1.17	1.23
2	z	71	HIS	CE1-NE2	5.07	1.37	1.32
1	J	1061	VAL	C-O	-5.07	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	934	THR	CA-C-N	6.34	129.19	123.10
1	F	934	THR	C-N-CA	6.34	129.19	123.10
1	J	934	THR	CA-C-N	6.08	128.93	123.10
1	J	934	THR	C-N-CA	6.08	128.93	123.10
1	F	967	ASN	N-CA-CB	-5.88	102.23	111.23
2	j	75	PRO	N-CA-CB	5.74	108.41	103.36
2	f	75	PRO	N-CA-CB	5.69	108.36	103.36
2	f	187	LYS	CA-C-O	-5.55	114.77	120.54
1	F	967	ASN	OD1-CG-ND2	5.54	128.14	122.60
2	f	187	LYS	CB-CA-C	-5.35	102.22	110.78
2	z	187	LYS	CA-C-O	-5.30	114.92	120.80
2	z	75	PRO	N-CA-CB	5.25	107.98	103.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	943	ASN	Peptide
1	J	943	ASN	Peptide
1	Z	943	ASN	Peptide

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	F	2323	0	2322	48	0
1	J	2323	0	2322	51	0
1	Z	2323	0	2322	45	0
2	f	1234	0	1218	32	0
2	j	1234	0	1218	25	0
2	z	1234	0	1218	29	0
All	All	10671	0	10620	197	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 9.

All (197) 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:J:984:ILE:O	1:J:984:ILE:HG22	1.76	0.84
1:J:915:MET:HE3	1:Z:915:MET:HE1	1.59	0.82
1:J:915:MET:HE1	1:F:915:MET:HE3	1.65	0.78
2:f:141:GLN:HG3	2:f:143:ASP:H	1.47	0.78
1:J:915:MET:CE	1:Z:915:MET:HE1	2.15	0.77
1:Z:932:ARG:NH2	1:F:919:GLN:OE1	2.19	0.74
2:j:42:LEU:HD22	2:j:112:ILE:HD11	1.69	0.73
2:f:42:LEU:HD22	2:f:112:ILE:HD11	1.71	0.71
2:z:141:GLN:HG2	2:z:142:ARG:N	2.08	0.69
1:J:1087:PRO:HB2	1:J:1090:ARG:HD3	1.74	0.68
1:J:919:GLN:OE1	1:F:932:ARG:NH2	2.29	0.66
1:F:940:SER:HB3	1:F:947:PHE:HB3	1.76	0.66
1:J:1003:ALA:HB2	1:F:1131:VAL:HG11	1.78	0.65
1:J:995:GLY:HA3	1:Z:990:ALA:HB2	1.78	0.65
1:J:1037:LEU:HD12	1:J:1118:GLN:HB3	1.79	0.65
1:J:940:SER:HB3	1:J:947:PHE:HB3	1.77	0.64
2:f:32:LEU:HD11	2:f:39:ASN:HB3	1.79	0.64
2:f:67:ASN:ND2	2:f:86:GLU:OE2	2.31	0.64
1:Z:1085:ASP:OD2	1:Z:1124:LYS:NZ	2.27	0.64
2:j:139:HIS:ND1	2:j:141:GLN:OE1	2.30	0.63
1:F:929:PHE:O	1:F:930:LEU:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:42:LEU:HD22	2:z:112:ILE:HD11	1.80	0.63
1:Z:995:GLY:HA3	1:F:990:ALA:HB2	1.78	0.63
2:j:66:ASN:HD22	2:j:185:SER:HA	1.64	0.63
1:Z:940:SER:HB3	1:Z:947:PHE:HB3	1.80	0.63
2:f:119:ASP:HB3	2:f:122:SER:HB3	1.81	0.62
1:J:984:ILE:O	1:J:984:ILE:CG2	2.47	0.62
2:z:71:HIS:HB2	2:z:88:MET:HE1	1.82	0.62
1:J:929:PHE:O	1:J:930:LEU:HB2	2.01	0.60
1:F:1127:LEU:O	1:F:1129:ILE:N	2.33	0.60
2:f:141:GLN:HE21	2:f:142:ARG:HG3	1.67	0.60
1:F:984:ILE:O	1:F:984:ILE:HG22	2.02	0.59
1:J:1131:VAL:HG12	1:J:1132:VAL:HG23	1.85	0.59
1:F:1011:SER:OG	1:F:1012:SER:N	2.29	0.58
2:j:71:HIS:HB2	2:j:88:MET:HE1	1.85	0.58
1:F:1037:LEU:HD12	1:F:1118:GLN:HB3	1.84	0.58
2:z:116:ARG:O	1:Z:943:ASN:HB3	2.04	0.58
2:j:120:LYS:NZ	2:j:142:ARG:O	2.32	0.58
1:J:937:THR:HB	1:J:951:PRO:HD3	1.85	0.58
1:J:1011:SER:OG	1:J:1012:SER:N	2.30	0.58
1:Z:929:PHE:O	1:Z:930:LEU:HB2	2.04	0.58
1:J:1077:VAL:O	1:Z:1042:ARG:NH1	2.37	0.58
1:J:932:ARG:NH1	1:Z:919:GLN:OE1	2.37	0.57
1:Z:984:ILE:HG22	1:Z:984:ILE:O	2.02	0.57
1:Z:1123:LYS:HG3	1:Z:1123:LYS:O	2.03	0.57
1:J:904:PHE:HE2	1:J:915:MET:HG3	1.70	0.57
2:f:56:PHE:O	2:f:60:VAL:HG13	2.06	0.55
1:Z:915:MET:HE3	1:F:915:MET:HE1	1.89	0.55
1:J:862:MET:HE1	1:Z:884:MET:HE2	1.88	0.55
2:f:71:HIS:HB2	2:f:88:MET:HE1	1.89	0.55
2:f:116:ARG:O	1:F:943:ASN:HB3	2.06	0.55
1:J:1120:MET:HE1	1:F:1120:MET:HE3	1.89	0.54
2:z:46:LYS:HG2	2:z:53:VAL:HG11	1.90	0.53
1:J:943:ASN:HB3	2:j:116:ARG:O	2.07	0.53
1:J:990:ALA:HB2	1:F:995:GLY:HA3	1.89	0.53
2:z:46:LYS:HD2	2:z:46:LYS:C	2.34	0.53
1:F:1131:VAL:HG12	1:F:1132:VAL:HG23	1.90	0.53
2:f:72:ARG:HB3	2:f:80:GLN:HB3	1.91	0.52
2:j:44:LEU:HB3	2:j:53:VAL:HG21	1.91	0.52
2:j:67:ASN:ND2	2:j:86:GLU:OE2	2.43	0.52
2:f:138:ASP:O	2:f:139:HIS:HB2	2.09	0.52
2:z:119:ASP:HB3	2:z:122:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:1127:LEU:O	1:Z:1129:ILE:N	2.41	0.51
2:f:102:ASP:HB3	2:f:140:GLY:HA3	1.93	0.51
2:j:72:ARG:HB3	2:j:80:GLN:HB3	1.92	0.51
2:z:31:VAL:HG23	2:z:42:LEU:HB2	1.92	0.51
1:J:1127:LEU:O	1:J:1129:ILE:N	2.39	0.51
2:f:94:ASN:HB3	2:f:95:PRO:HD2	1.93	0.51
2:j:119:ASP:HB3	2:j:122:SER:HB3	1.92	0.50
1:Z:888:GLU:C	1:Z:890:GLY:H	2.20	0.50
2:f:31:VAL:HG23	2:f:42:LEU:HB2	1.92	0.50
1:Z:1074:ASN:OD1	1:Z:1074:ASN:N	2.44	0.50
2:f:113:ALA:HB3	2:f:128:PHE:CZ	2.47	0.50
1:F:904:PHE:HE2	1:F:915:MET:HG3	1.76	0.50
2:j:113:ALA:HB3	2:j:128:PHE:CZ	2.47	0.50
1:J:888:GLU:C	1:J:890:GLY:H	2.20	0.50
1:F:980:GLU:H	1:F:980:GLU:CD	2.20	0.49
1:F:888:GLU:C	1:F:890:GLY:H	2.19	0.49
1:J:944:PRO:HD2	2:j:72:ARG:NH1	2.28	0.49
2:f:72:ARG:NH1	1:F:944:PRO:HD2	2.28	0.49
2:z:41:GLU:HB2	2:z:154:LYS:HB3	1.94	0.49
2:f:73:VAL:HG13	2:f:79:ILE:HG22	1.94	0.48
1:Z:980:GLU:H	1:Z:980:GLU:CD	2.21	0.48
2:z:113:ALA:HB3	2:z:128:PHE:CZ	2.48	0.48
2:j:115:ALA:HB3	2:j:126:GLN:HB3	1.96	0.48
2:z:107:ASN:N	2:z:138:ASP:OD2	2.41	0.48
1:J:898:ALA:O	1:J:900:ASN:N	2.46	0.48
1:J:973:LEU:HG	1:J:976:VAL:HG21	1.95	0.48
1:J:866:LYS:HG3	1:J:892:LEU:HD21	1.96	0.48
2:j:116:ARG:HB3	2:j:123:ALA:HB2	1.95	0.48
2:f:38:GLY:C	2:f:39:ASN:HD22	2.22	0.47
2:f:107:ASN:ND2	2:f:138:ASP:OD1	2.39	0.47
1:F:830:GLU:HA	1:F:833:GLU:HG2	1.97	0.47
2:j:73:VAL:HG13	2:j:79:ILE:HG22	1.97	0.47
2:z:142:ARG:HD2	2:z:143:ASP:N	2.29	0.47
2:z:42:LEU:HD22	2:z:112:ILE:CD1	2.45	0.47
2:z:119:ASP:O	2:z:122:SER:OG	2.29	0.47
1:Z:898:ALA:O	1:Z:900:ASN:N	2.48	0.47
1:J:1060:LYS:HE3	1:J:1067:VAL:HG22	1.96	0.47
2:j:124:THR:OG1	2:j:125:SER:N	2.48	0.47
2:z:72:ARG:HB3	2:z:80:GLN:HB3	1.97	0.47
2:z:116:ARG:HB3	2:z:123:ALA:HB2	1.97	0.47
2:f:139:HIS:CD2	2:f:141:GLN:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:898:ALA:O	1:F:900:ASN:N	2.49	0.46
2:j:119:ASP:O	2:j:122:SER:OG	2.29	0.46
1:F:1045:LYS:HE2	1:F:1054:TYR:HE2	1.80	0.46
2:j:139:HIS:HD1	2:j:141:GLN:CD	2.20	0.46
1:F:1033:GLN:HG3	1:F:1124:LYS:HB2	1.97	0.46
2:z:124:THR:OG1	2:z:125:SER:N	2.48	0.46
2:j:57:VAL:HA	2:j:60:VAL:HG22	1.97	0.46
2:f:102:ASP:OD1	2:f:102:ASP:N	2.44	0.46
1:J:980:GLU:H	1:J:980:GLU:CD	2.23	0.46
1:Z:960:ALA:HB1	1:Z:962:ILE:HD13	1.97	0.46
1:J:869:GLN:OE1	1:J:873:GLY:HA2	2.16	0.45
1:Z:1002:SER:HA	1:Z:1117:VAL:O	2.17	0.45
1:Z:1125:GLN:CD	1:Z:1127:LEU:HB2	2.41	0.45
2:f:124:THR:OG1	2:f:125:SER:N	2.50	0.45
2:j:32:LEU:HB2	2:j:187:LYS:HB3	1.98	0.45
2:z:32:LEU:HD23	2:z:187:LYS:HB3	1.97	0.45
1:Z:930:LEU:HD23	1:F:925:MET:HG3	1.98	0.45
1:Z:1131:VAL:HG11	1:F:1003:ALA:HB2	1.97	0.45
2:f:32:LEU:HD13	2:f:41:GLU:OE1	2.16	0.45
1:Z:980:GLU:CD	1:Z:980:GLU:N	2.75	0.45
1:J:1120:MET:HE1	1:F:1120:MET:CE	2.47	0.45
1:Z:981:ASN:OD1	1:Z:981:ASN:N	2.50	0.45
1:F:837:LEU:HD23	1:F:837:LEU:HA	1.84	0.45
1:F:929:PHE:O	1:F:930:LEU:CB	2.59	0.45
1:F:1123:LYS:O	1:F:1123:LYS:HG3	2.17	0.45
1:Z:1131:VAL:HG11	1:F:1003:ALA:CB	2.47	0.44
2:z:72:ARG:NH1	1:Z:944:PRO:HD2	2.32	0.44
2:f:107:ASN:N	2:f:138:ASP:OD1	2.42	0.44
2:j:56:PHE:O	2:j:60:VAL:HG13	2.17	0.44
1:F:980:GLU:CD	1:F:980:GLU:N	2.75	0.44
1:F:1006:PRO:HD3	1:F:1020:ARG:CZ	2.47	0.44
1:J:980:GLU:CD	1:J:980:GLU:N	2.76	0.44
2:z:44:LEU:HB3	2:z:53:VAL:HG21	2.00	0.44
1:Z:837:LEU:HD23	1:Z:837:LEU:HA	1.83	0.44
1:J:917:VAL:HG23	1:J:926:ASN:HA	1.99	0.44
1:J:1002:SER:HA	1:J:1117:VAL:O	2.18	0.44
2:j:31:VAL:HG12	2:j:188:VAL:HG12	1.99	0.44
1:F:892:LEU:HD23	1:F:892:LEU:HA	1.86	0.44
1:J:973:LEU:HD21	1:Z:973:LEU:HD11	2.00	0.43
1:Z:1056:MET:HE1	1:Z:1074:ASN:HB3	2.00	0.43
1:F:913:THR:HG22	1:F:926:ASN:HD22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:845:LEU:HD23	1:Z:845:LEU:HA	1.88	0.43
1:Z:853:LYS:HA	1:Z:853:LYS:HD2	1.76	0.43
1:J:958:LYS:HA	1:F:963:SER:HB2	2.00	0.43
1:Z:1006:PRO:HD3	1:Z:1020:ARG:CZ	2.48	0.43
1:Z:890:GLY:C	1:Z:892:LEU:H	2.26	0.43
1:F:1124:LYS:HG3	1:F:1124:LYS:O	2.19	0.43
1:J:1006:PRO:HD3	1:J:1020:ARG:CZ	2.50	0.42
1:J:1129:ILE:HG23	1:J:1129:ILE:O	2.18	0.42
1:F:1062:LEU:HD23	1:F:1067:VAL:HG22	2.01	0.42
1:J:1104:HIS:HB2	1:J:1108:ILE:HB	2.01	0.42
2:j:119:ASP:OD1	2:j:120:LYS:N	2.52	0.42
2:f:119:ASP:O	2:f:122:SER:OG	2.31	0.42
1:J:919:GLN:CD	2:z:142:ARG:HH12	2.26	0.42
1:F:917:VAL:HG23	1:F:926:ASN:HA	2.01	0.42
2:z:141:GLN:HG2	2:z:142:ARG:H	1.82	0.42
1:F:850:LYS:HD3	1:F:850:LYS:HA	1.90	0.42
1:Z:898:ALA:HB2	1:F:876:TYR:CD2	2.55	0.42
1:Z:1030:PHE:CE2	1:F:990:ALA:HB3	2.54	0.42
2:f:41:GLU:OE1	2:f:41:GLU:HA	2.20	0.42
1:J:850:LYS:HD3	1:J:850:LYS:HA	1.86	0.42
1:Z:1129:ILE:HG23	1:Z:1129:ILE:O	2.19	0.42
2:z:77:PHE:CD1	1:Z:958:LYS:HG2	2.55	0.42
1:Z:929:PHE:O	1:Z:930:LEU:CB	2.64	0.42
1:J:890:GLY:C	1:J:892:LEU:H	2.28	0.41
1:J:913:THR:HG22	1:J:926:ASN:HD22	1.85	0.41
1:J:1060:LYS:HB3	1:J:1098:THR:HG23	2.00	0.41
2:z:119:ASP:OD1	2:z:120:LYS:N	2.53	0.41
1:J:1125:GLN:CD	1:J:1127:LEU:HB2	2.44	0.41
2:j:103:ASN:HD22	2:j:105:LEU:HD12	1.85	0.41
1:J:830:GLU:HB2	1:J:834:LYS:HE3	2.01	0.41
2:f:179:LYS:HD2	2:f:180:PRO:HD2	2.02	0.41
1:F:1127:LEU:HA	1:F:1127:LEU:HD12	1.79	0.41
2:z:44:LEU:HB3	2:z:53:VAL:CG2	2.50	0.41
1:J:836:GLU:OE1	1:J:836:GLU:N	2.53	0.41
2:f:112:ILE:HG12	2:f:129:ILE:HG12	2.03	0.41
1:J:876:TYR:CD2	1:F:898:ALA:HB2	2.56	0.41
1:J:925:MET:HE2	1:J:925:MET:HB3	1.86	0.41
1:F:1125:GLN:CD	1:F:1127:LEU:HB2	2.46	0.41
1:J:1127:LEU:HA	1:J:1127:LEU:HD23	1.75	0.41
2:z:79:ILE:O	2:z:79:ILE:HG13	2.19	0.41
2:z:85:THR:HG22	2:z:86:GLU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:1032:ARG:HD2	1:Z:1121:VAL:HG12	2.03	0.41
2:f:44:LEU:HB3	2:f:53:VAL:HG21	2.02	0.41
1:F:991:GLU:CD	1:F:991:GLU:H	2.25	0.41
2:j:109:ARG:HH12	2:j:156:MET:HG2	1.86	0.41
1:Z:871:LYS:H	1:Z:871:LYS:HD3	1.85	0.41
1:Z:1077:VAL:HG22	1:F:1077:VAL:HG11	2.03	0.40
2:f:115:ALA:HB3	2:f:126:GLN:HB2	2.02	0.40
2:f:141:GLN:HG3	2:f:143:ASP:N	2.26	0.40
2:z:157:ASP:OD1	2:z:157:ASP:N	2.54	0.40
2:f:79:ILE:O	2:f:79:ILE:HG13	2.20	0.40
2:z:134:ASN:OD1	1:Z:958:LYS:HE2	2.22	0.40
1:F:1102:THR:O	1:F:1110:PRO:HB3	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	F	303/420 (72%)	266 (88%)	35 (12%)	2 (1%)	18	34
1	J	303/420 (72%)	266 (88%)	35 (12%)	2 (1%)	18	34
1	Z	303/420 (72%)	266 (88%)	34 (11%)	3 (1%)	12	24
2	f	158/190 (83%)	142 (90%)	16 (10%)	0	100	100
2	j	158/190 (83%)	141 (89%)	17 (11%)	0	100	100
2	z	158/190 (83%)	138 (87%)	20 (13%)	0	100	100
All	All	1383/1830 (76%)	1219 (88%)	157 (11%)	7 (0%)	26	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	1127	LEU

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Mol	Chain	Res	Type
1	J	1128	GLY
1	Z	1128	GLY
1	F	1127	LEU
1	Z	1127	LEU
1	F	1128	GLY
1	Z	944	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	254/349 (73%)	240 (94%)	14 (6%)	19	37
1	J	254/349 (73%)	238 (94%)	16 (6%)	16	30
1	Z	254/349 (73%)	244 (96%)	10 (4%)	28	51
2	f	135/154 (88%)	129 (96%)	6 (4%)	25	47
2	j	135/154 (88%)	125 (93%)	10 (7%)	13	24
2	z	135/154 (88%)	128 (95%)	7 (5%)	21	39
All	All	1167/1509 (77%)	1104 (95%)	63 (5%)	21	38

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	831	LEU
1	J	838	THR
1	J	839	GLU
1	J	853	LYS
1	J	856	SER
1	J	925	MET
1	J	950	THR
1	J	973	LEU
1	J	974	SER
1	J	989	ARG
1	J	999	LYS
1	J	1033	GLN

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Mol	Chain	Res	Type
1	J	1098	THR
1	J	1099	LEU
1	J	1100	THR
1	J	1130	SER
2	j	30	HIS
2	j	32	LEU
2	j	42	LEU
2	j	57	VAL
2	j	85	THR
2	j	102	ASP
2	j	114	MET
2	j	126	GLN
2	j	160	ASP
2	j	187	LYS
2	z	30	HIS
2	z	57	VAL
2	z	85	THR
2	z	98	LYS
2	z	102	ASP
2	z	143	ASP
2	z	187	LYS
1	Z	832	LEU
1	Z	856	SER
1	Z	869	GLN
1	Z	925	MET
1	Z	939	THR
1	Z	950	THR
1	Z	974	SER
1	Z	989	ARG
1	Z	1099	LEU
1	Z	1100	THR
2	f	40	ILE
2	f	42	LEU
2	f	57	VAL
2	f	85	THR
2	f	160	ASP
2	f	187	LYS
1	F	838	THR
1	F	856	SER
1	F	858	LYS
1	F	862	MET
1	F	950	THR

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Mol	Chain	Res	Type
1	F	969	ASN
1	F	974	SER
1	F	983	THR
1	F	989	ARG
1	F	991	GLU
1	F	1063	MET
1	F	1086	MET
1	F	1100	THR
1	F	1120	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	1028	HIS
2	j	66	ASN
2	z	55	ASN
2	z	71	HIS
1	Z	894	GLN
1	Z	926	ASN
1	Z	1008	GLN
1	Z	1028	HIS
1	Z	1118	GLN
2	f	39	ASN
2	f	71	HIS
2	f	141	GLN
1	F	841	ASN
1	F	875	HIS
1	F	894	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

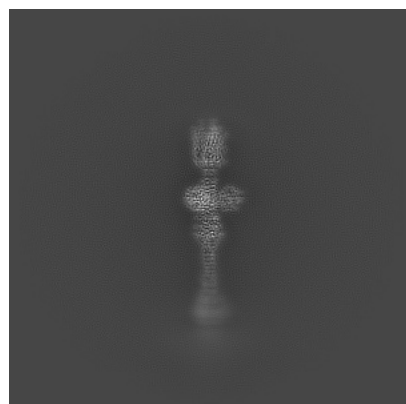
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38246. These allow visual inspection of the internal detail of the map and identification of artifacts.

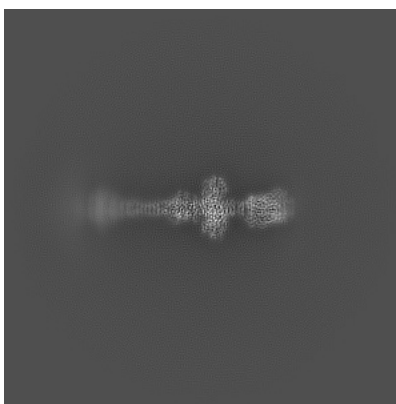
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

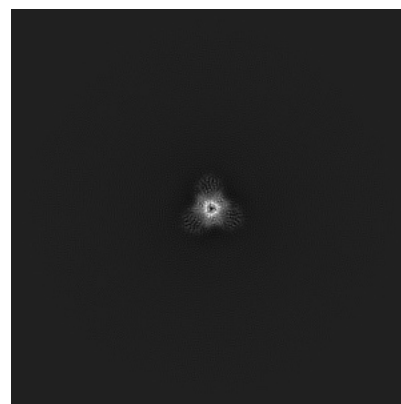
6.1.1 Primary map



X

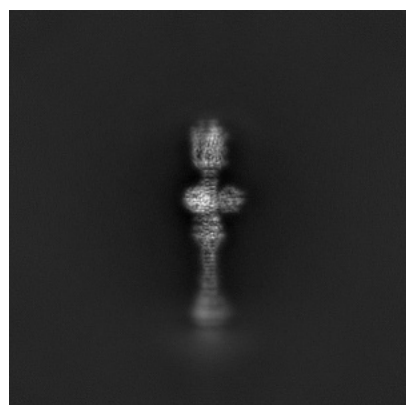


Y

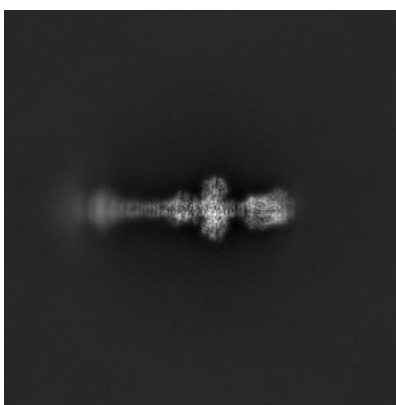


Z

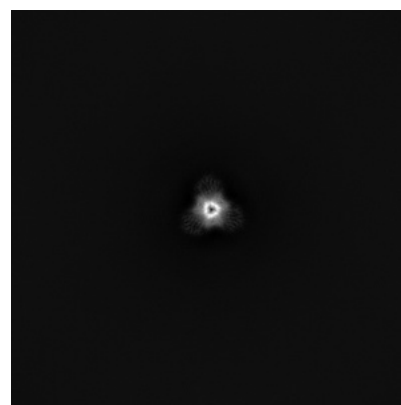
6.1.2 Raw map



X



Y

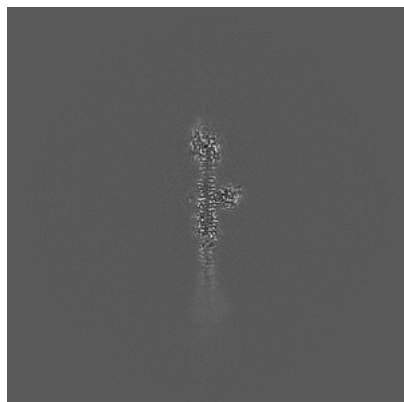


Z

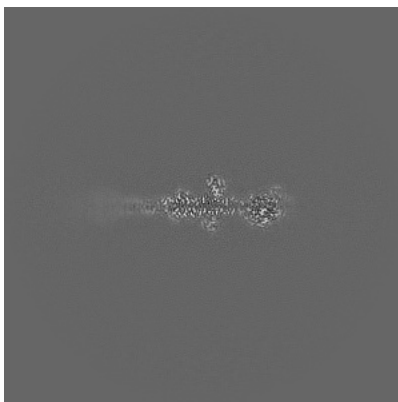
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

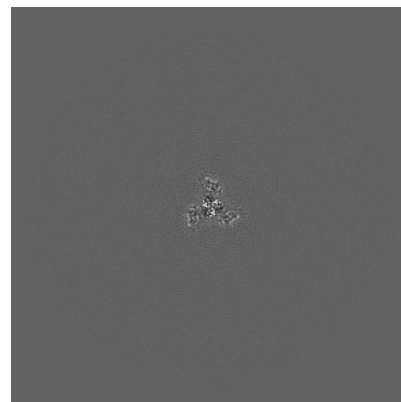
6.2.1 Primary map



X Index: 240

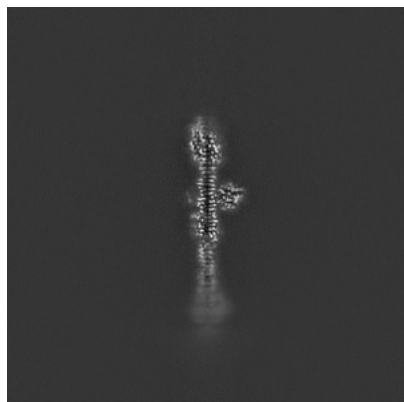


Y Index: 240



Z Index: 240

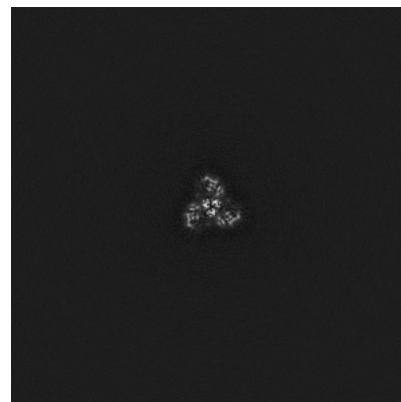
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

6.3 Largest variance slices [i](#)

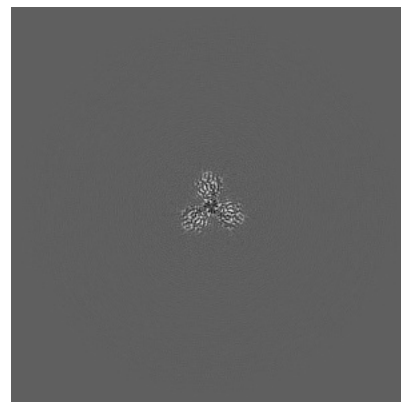
6.3.1 Primary map



X Index: 234

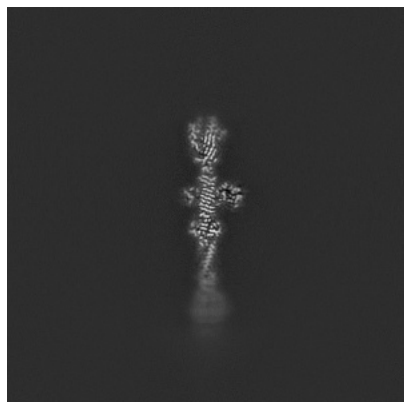


Y Index: 235

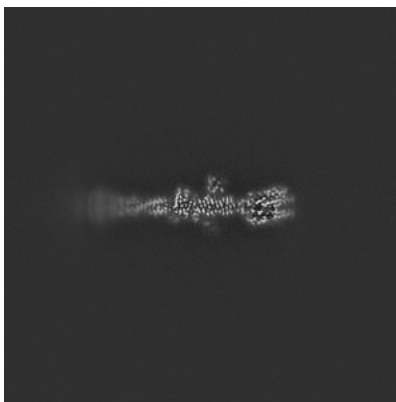


Z Index: 252

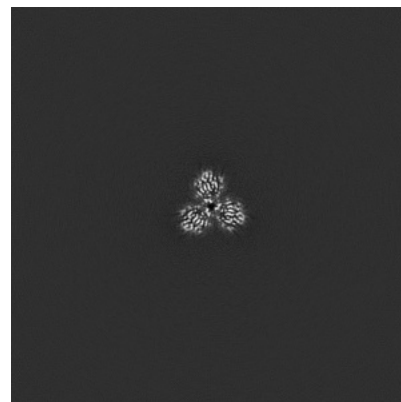
6.3.2 Raw map



X Index: 234



Y Index: 244

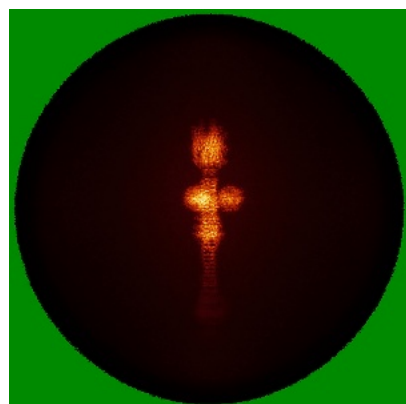


Z Index: 252

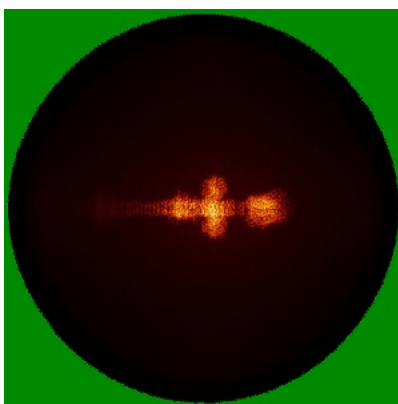
The images above show the largest variance slices of the map in three orthogonal directions.

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

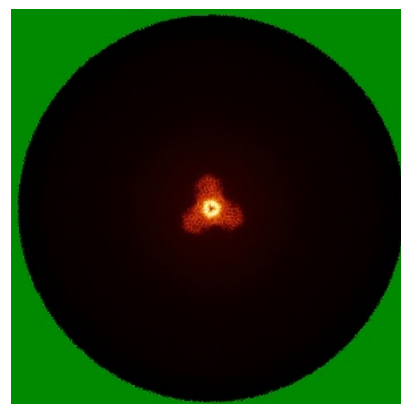
6.4.1 Primary map



X

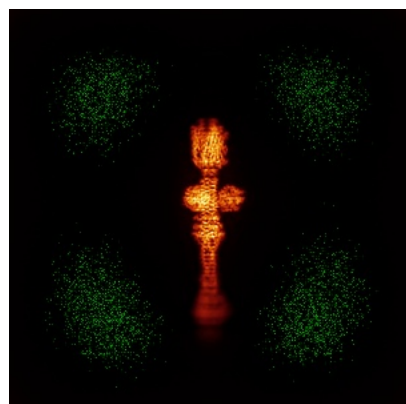


Y

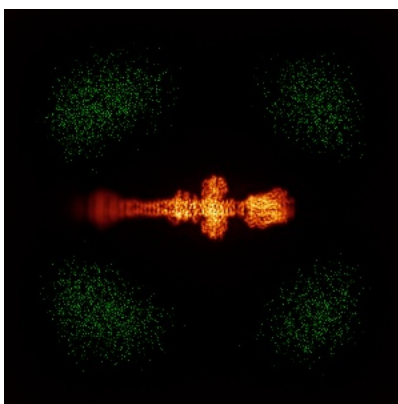


Z

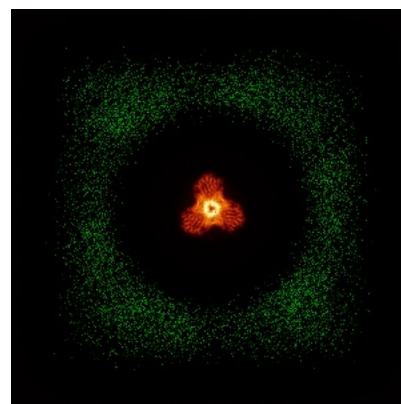
6.4.2 Raw map



X



Y

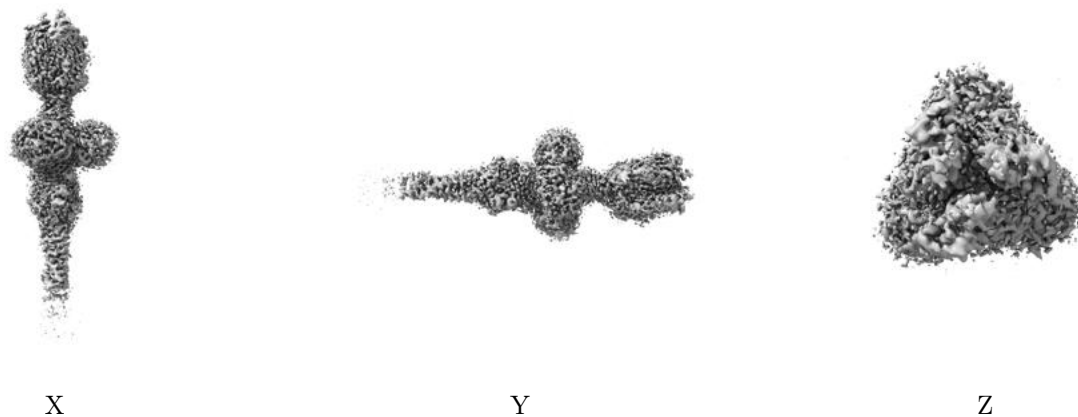


Z

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 0.4. 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.

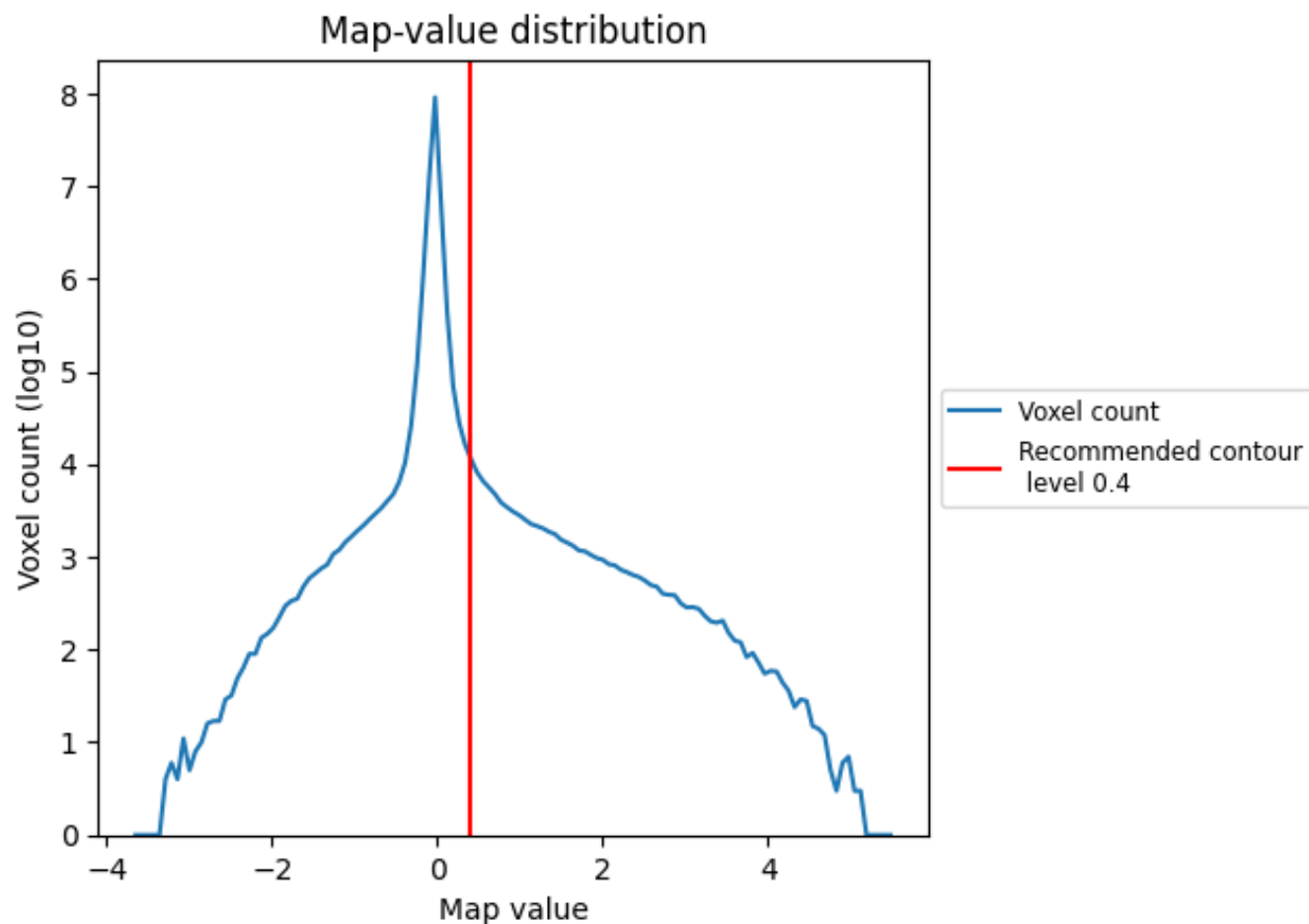
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

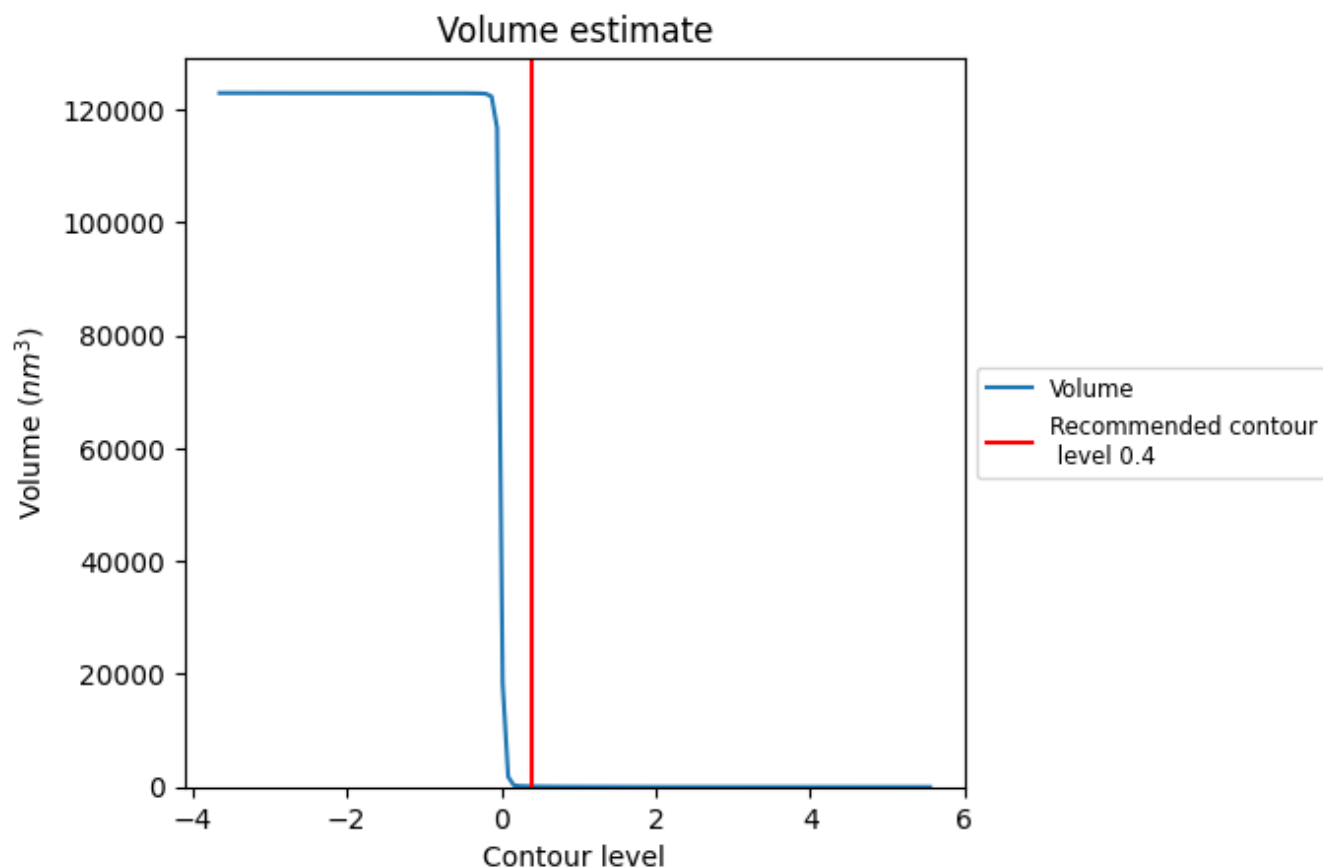
This section contains the results of statistical analysis of the map.

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.

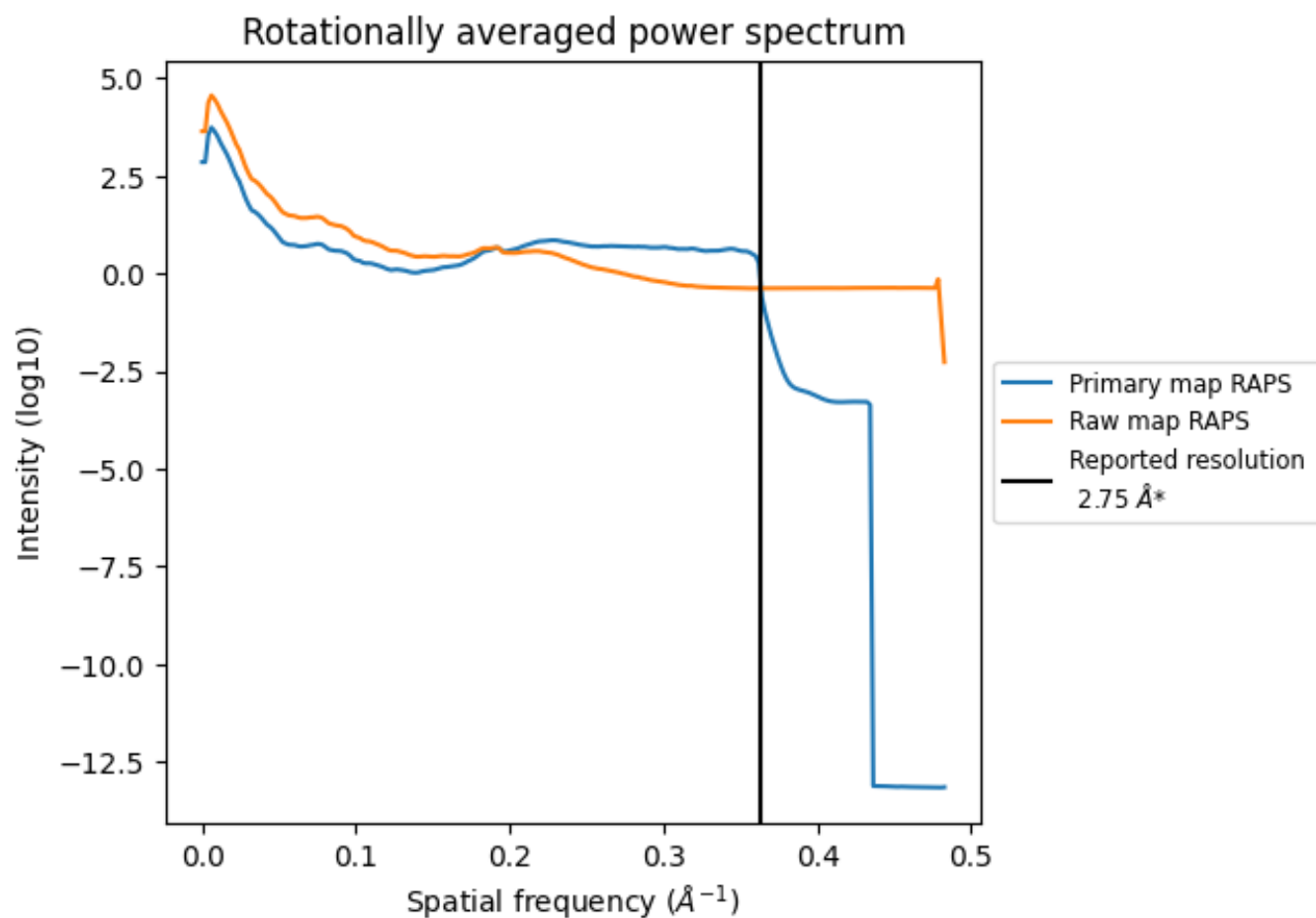
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 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 ⓘ

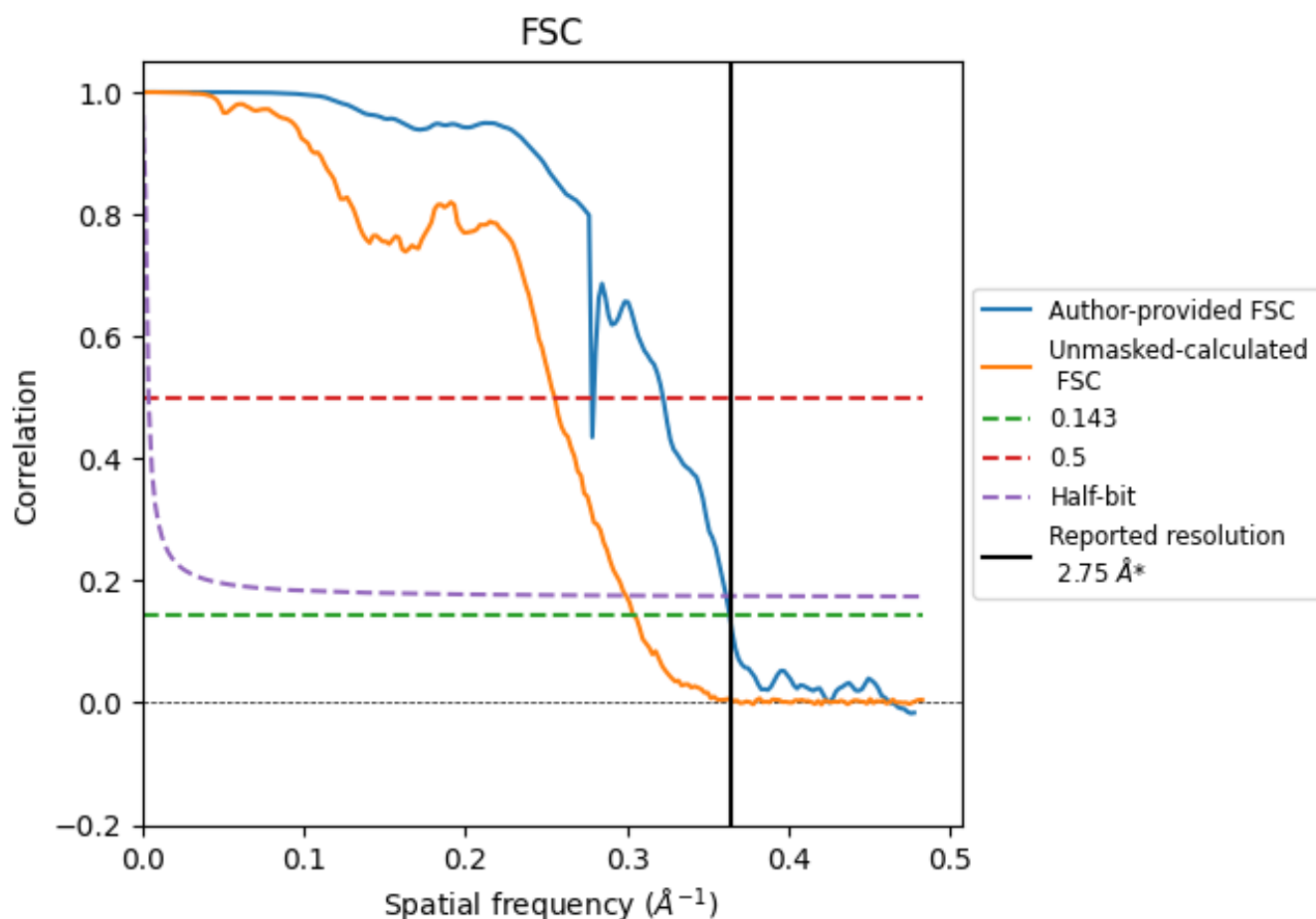


*Reported resolution corresponds to spatial frequency of 0.364 $\text{\AA}^{-1}$

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 0.364 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

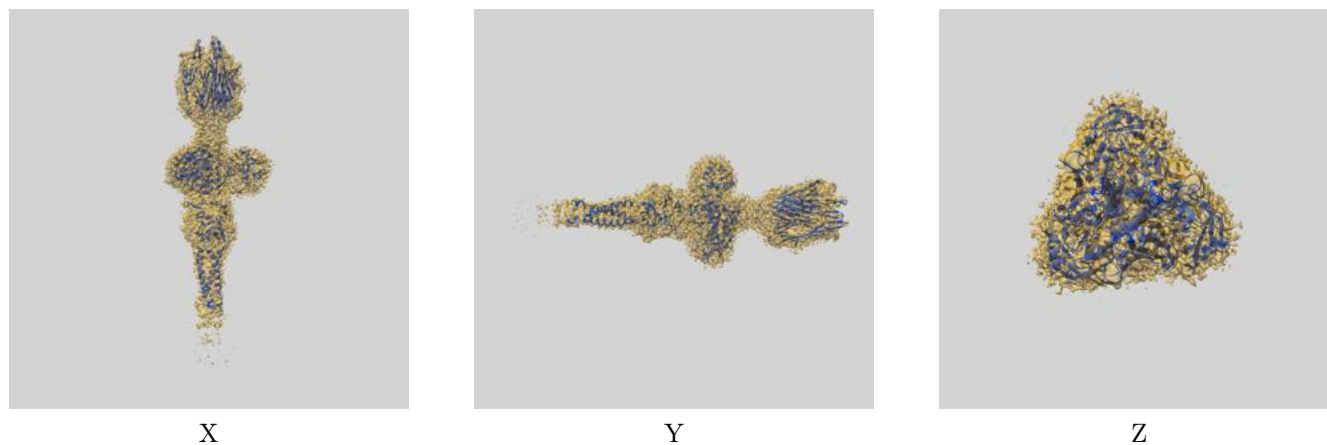
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.75	3.59	2.77
Unmasked-calculated*	3.29	3.92	3.34

*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 3.29 differs from the reported value 2.75 by more than 10 %

9 Map-model fit [i](#)

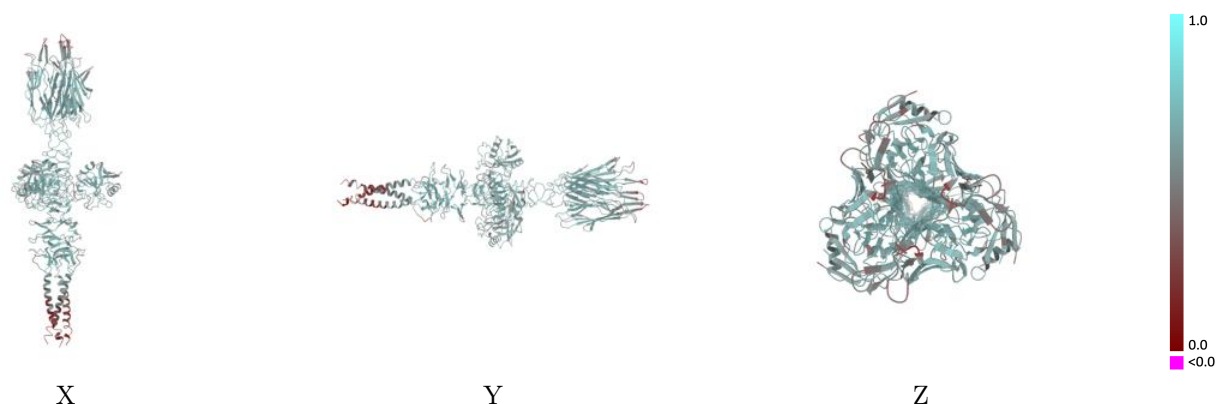
This section contains information regarding the fit between EMDB map EMD-38246 and PDB model 8XCK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



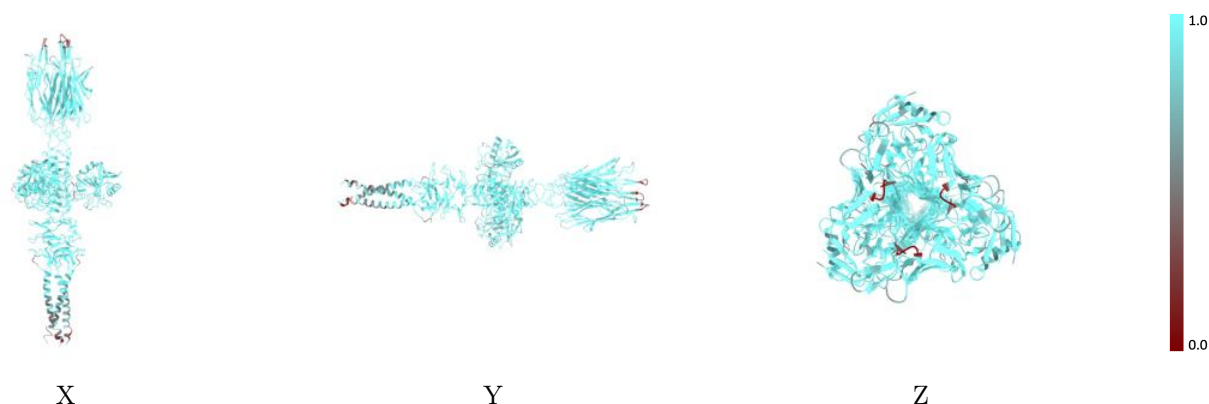
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



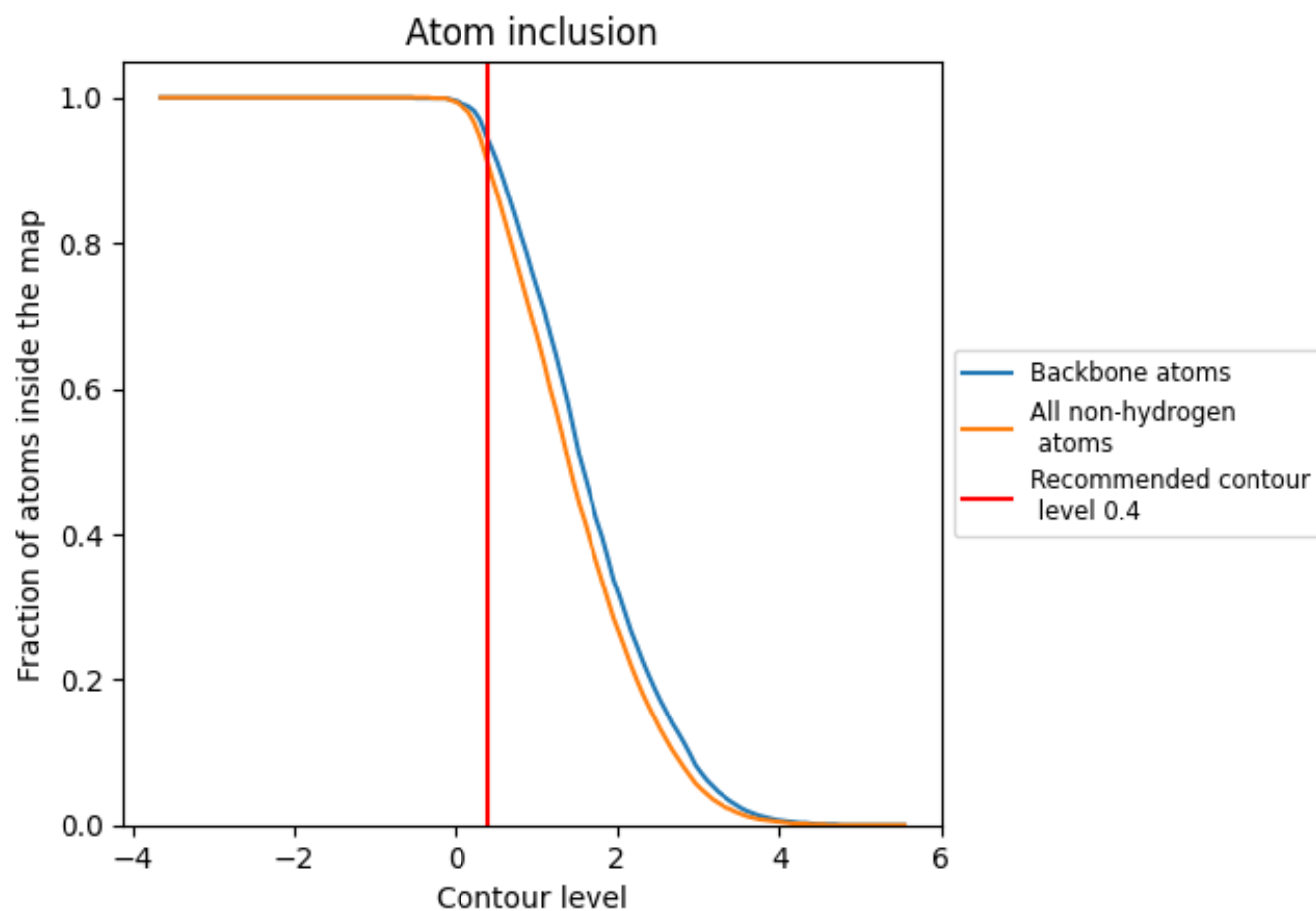
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.5730
F	0.9160	0.5750
J	0.9120	0.5680
Z	0.9130	0.5730
f	0.9060	0.5770
j	0.9080	0.5790
z	0.9020	0.5680

1.0

0.0

<0.0