



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 04:30 PM EDT

PDB ID : 7JRJ
EMDB ID : EMD-22446
Title : Chlamydomonas reinhardtii radial spoke head and neck (recombinant)
Authors : Grossman-Haham, I.; Coudray, N.; Yu, Z.; Wang, F.; Zhang, N.; Bhabha, G.;
Vale, R.D.
Deposited on : 2020-08-12
Resolution : 3.03 Å(reported)
Based on initial model : 7JR9

This is a wwPDB EM Validation Summary 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) : 2.39

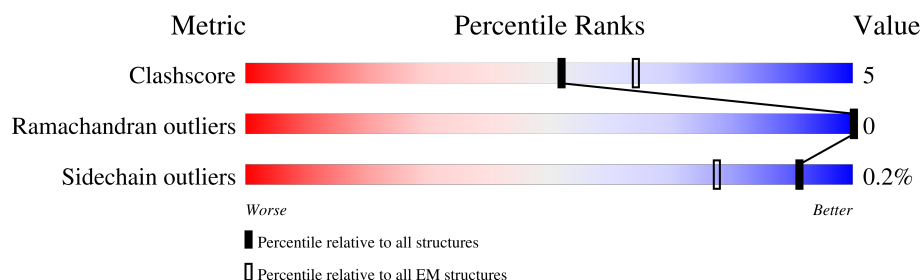
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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.



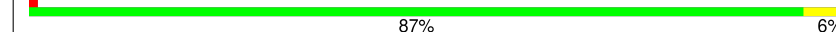
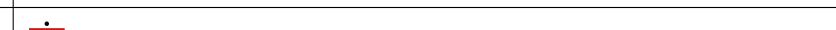

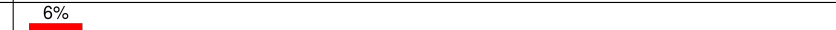


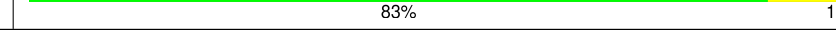
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	E	216	<div> <div>8%</div> <div>70%</div> <div>12%</div> <div>17%</div> </div>
2	F	814	<div> <div>5%</div> <div>39%</div> <div>5%</div> <div>56%</div> </div>
3	K	586	<div> <div>20%</div> <div>7%</div> <div>73%</div> </div>
4	I	738	<div> <div>9%</div> <div>38%</div> <div>6%</div> <div>56%</div> </div>
5	J	4	<div> <div>75%</div> <div>25%</div> </div>
6	G	362	<div> <div>7%</div> <div>34%</div> <div>7%</div> <div>59%</div> </div>
7	H	527	<div> <div>5%</div> <div>77%</div> <div>13%</div> <div>9%</div> </div>
8	A	269	<div> <div>86%</div> <div>8%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
8	B	269	
9	C	466	
10	D	459	
11	L	6	
12	M	5	
13	N	89	
14	O	69	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 22924 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 Radial spoke protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	180	Total	C	N	O	S	0	0
			1378	880	230	259	9		

- Molecule 2 is a protein called Flagellar radial spoke protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	356	Total	C	N	O	S	0	0
			2658	1689	449	514	6		

- Molecule 3 is a protein called Nucleoside diphosphate kinase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	158	Total	C	N	O	S	0	0
			1232	798	211	219	4		

- Molecule 4 is a protein called Flagellar radial spoke protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	327	Total	C	N	O	S	0	0
			2517	1601	435	477	4		

- Molecule 5 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	4	Total	C	N	O	0	0
			19	11	4	4		

- Molecule 6 is a protein called Flagellar radial spoke protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	148	Total	C	N	O	S	0	0
			1094	679	197	215	3		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	155	GLY	-	expression tag	UNP P12759
G	156	ALA	-	expression tag	UNP P12759
G	157	ALA	-	expression tag	UNP P12759
G	158	ALA	-	expression tag	UNP P12759
G	159	GLU	-	expression tag	UNP P12759

- Molecule 7 is a protein called Flagellar radial spoke protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	477	Total	C	N	O	S	0	0
			3611	2308	616	675	12		

- Molecule 8 is a protein called Radial spoke protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	252	Total	C	N	O	S	0	0
			1955	1249	331	370	5		
8	B	252	Total	C	N	O	S	0	0
			1955	1249	331	370	5		

- Molecule 9 is a protein called Flagellar radial spoke protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	359	Total	C	N	O	S	0	0
			2717	1740	458	512	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP Q01656

- Molecule 10 is a protein called Flagellar radial spoke protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	422	Total	C	N	O	S	0	0
			3168	2011	538	607	12		

- Molecule 11 is a protein called Flagellar radial spoke protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	6	Total	C	N	O	0	0
			30	18	6	6		

- Molecule 12 is a protein called Flagellar radial spoke protein 10.

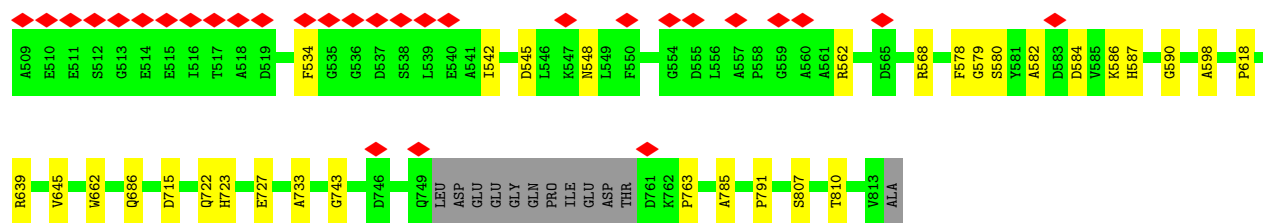
Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	5	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 13 is a protein called Flagellar radial spoke protein 1.

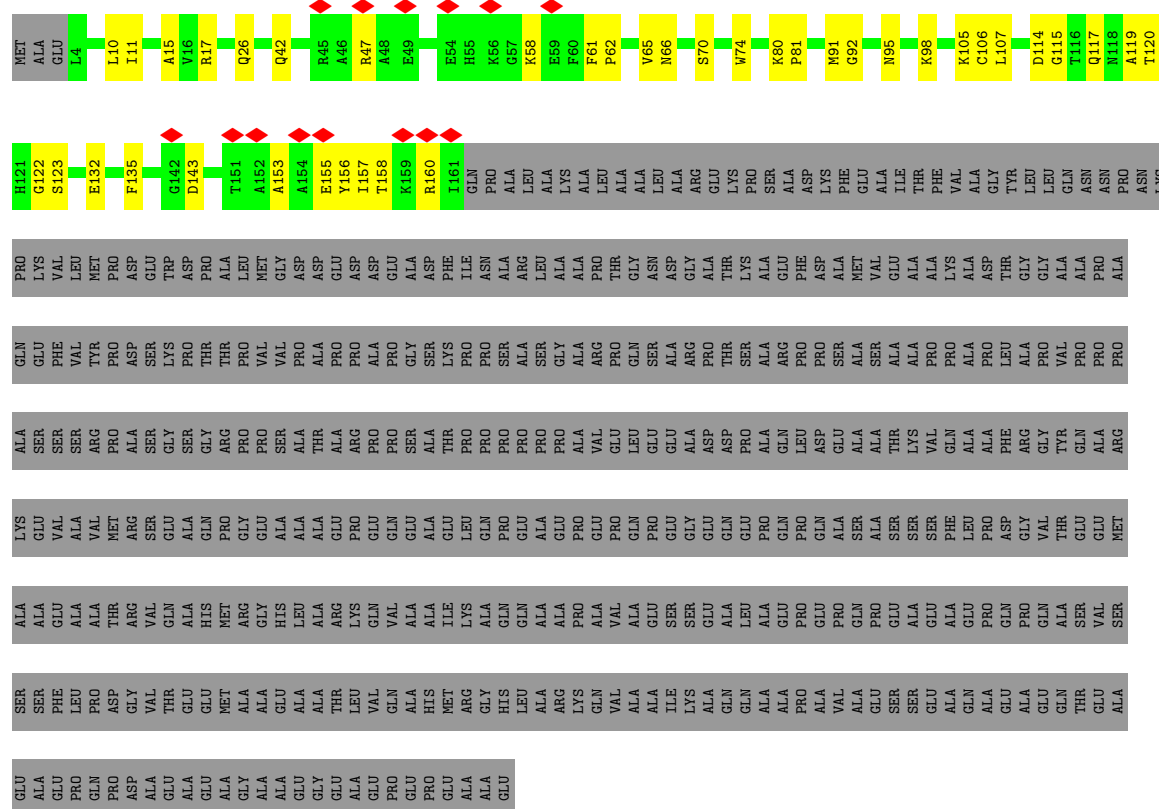
Mol	Chain	Residues	Atoms				AltConf	Trace
13	N	64	Total	C	N	O	0	0
			320	192	64	64		

- Molecule 14 is a protein called Flagellar radial spoke protein 2.

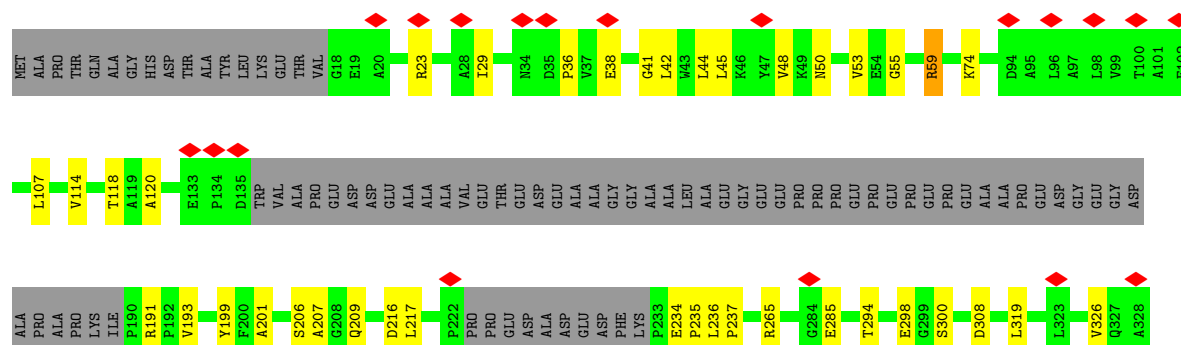
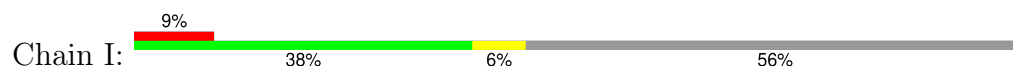
Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	49	Total	C	N	O	0	0
			245	147	49	49		

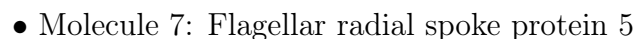


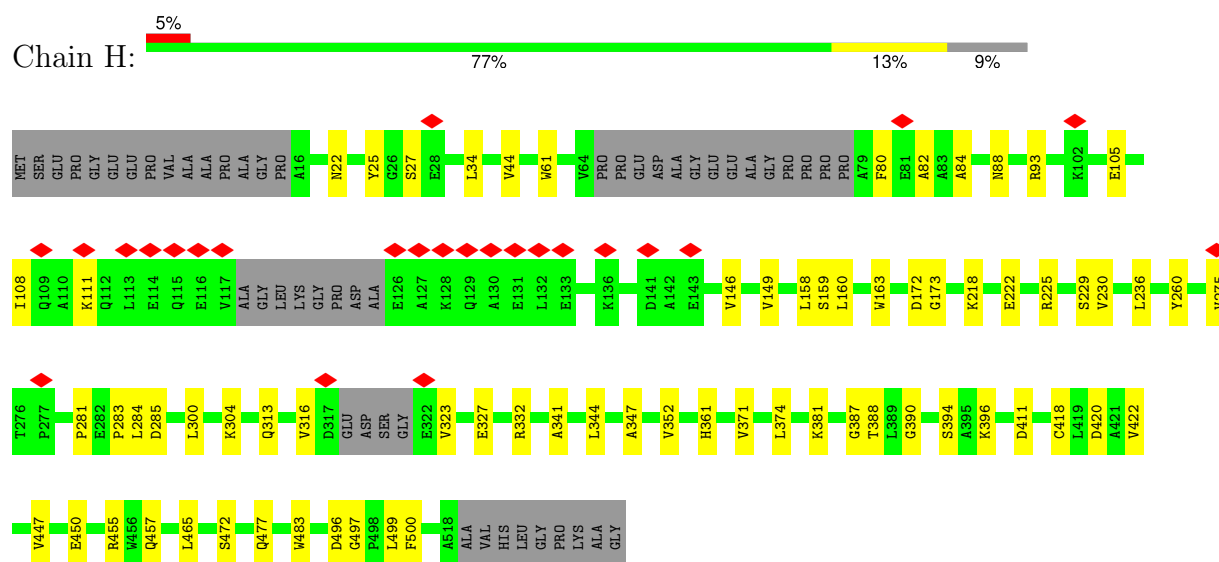
• Molecule 3: Nucleoside diphosphate kinase 6



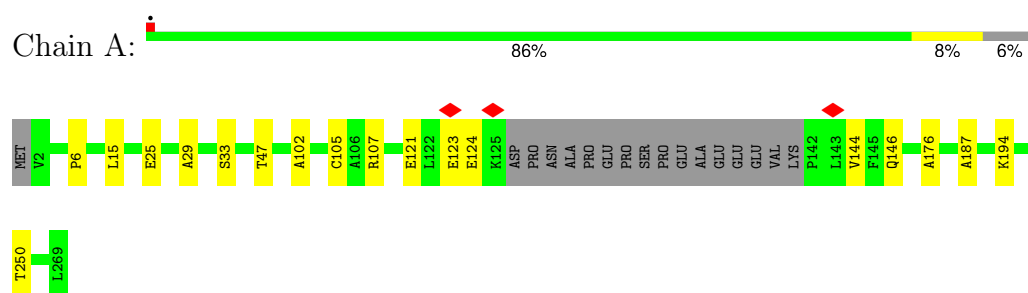
• Molecule 4: Flagellar radial spoke protein 2



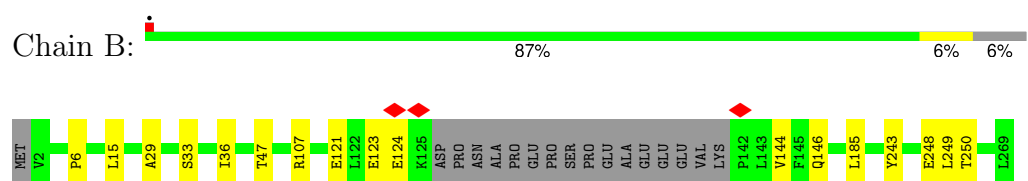




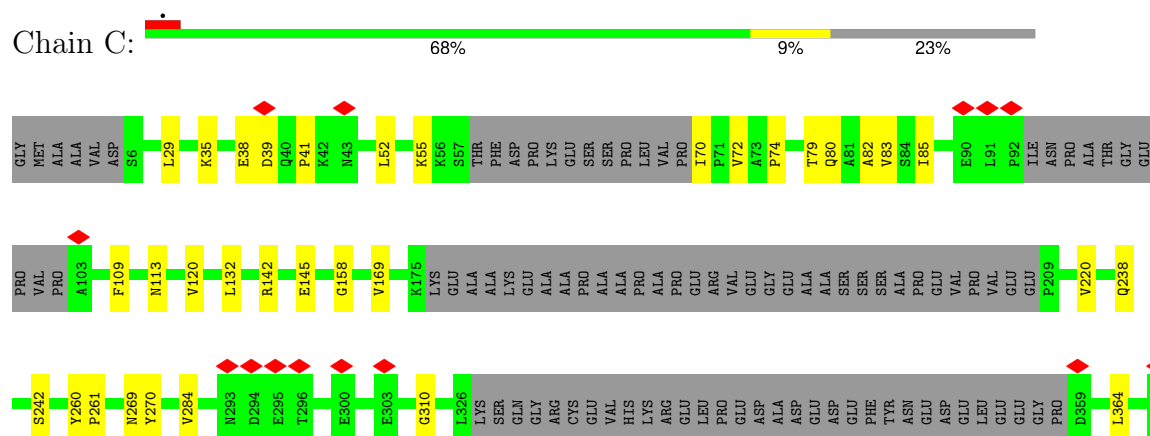
• Molecule 8: Radial spoke protein 9



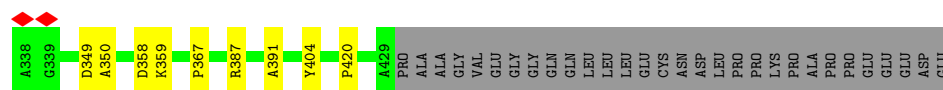
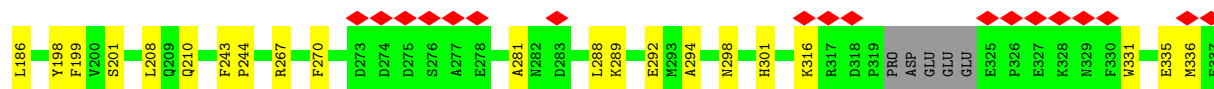
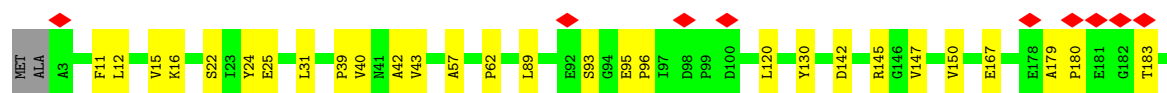
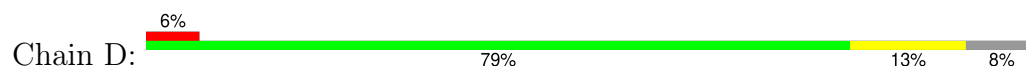
• Molecule 8: Radial spoke protein 9



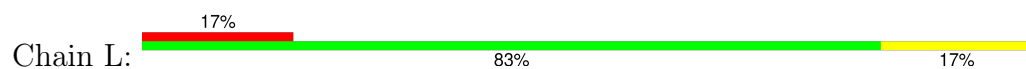
• Molecule 9: Flagellar radial spoke protein 4



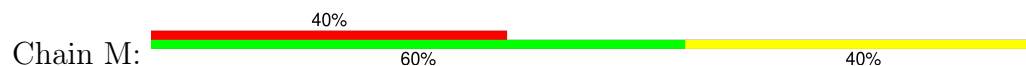
- Molecule 10: Flagellar radial spoke protein 6



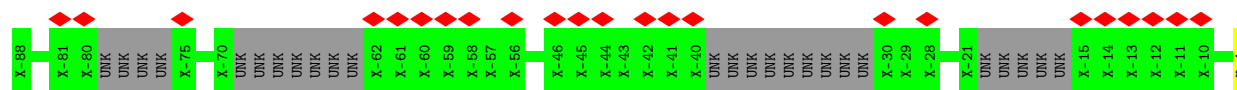
- Molecule 11: Flagellar radial spoke protein 6



- Molecule 12: Flagellar radial spoke protein 10



- Molecule 13: Flagellar radial spoke protein 1



- Molecule 14: Flagellar radial spoke protein 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	136659	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	450.9, 450.9, 450.9	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	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	E	0.38	0/1424	0.47	0/1918
2	F	0.36	0/2736	0.46	0/3722
3	K	0.32	0/1261	0.43	0/1705
4	I	0.31	0/2571	0.40	0/3487
6	G	0.28	0/1103	0.41	0/1493
7	H	0.36	0/3697	0.44	0/5042
8	A	0.42	0/1997	0.46	0/2715
8	B	0.43	0/1997	0.47	0/2715
9	C	0.38	0/2782	0.45	0/3794
10	D	0.38	0/3258	0.45	0/4461
All	All	0.37	0/22826	0.44	0/31052

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	E	1378	0	1264	17	0
2	F	2658	0	2493	31	0
3	K	1232	0	1262	26	0
4	I	2517	0	2493	30	0
5	J	19	0	7	1	0
6	G	1094	0	1111	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	3611	0	3588	44	0
8	A	1955	0	1937	13	0
8	B	1955	0	1939	10	0
9	C	2717	0	2698	31	0
10	D	3168	0	3071	38	0
11	L	30	0	9	1	0
12	M	25	0	7	2	0
13	N	320	0	90	2	0
14	O	245	0	55	0	0
All	All	22924	0	22024	232	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 5.

The worst 5 of 232 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)
2:F:542:ILE:HG22	2:F:542:ILE:O	1.85	0.77
9:C:80:GLN:HA	9:C:83:VAL:HG12	1.68	0.74
1:E:57:ARG:HB2	1:E:79:GLY:HA2	1.70	0.71
9:C:72:VAL:O	9:C:72:VAL:HG13	1.91	0.70
3:K:106:CYS:SG	3:K:107:LEU:N	2.63	0.70

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	E	176/216 (82%)	167 (95%)	9 (5%)	0	100	100
2	F	352/814 (43%)	334 (95%)	18 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	156/586 (27%)	148 (95%)	8 (5%)	0	100	100
4	I	319/738 (43%)	306 (96%)	13 (4%)	0	100	100
6	G	144/362 (40%)	140 (97%)	4 (3%)	0	100	100
7	H	469/527 (89%)	448 (96%)	21 (4%)	0	100	100
8	A	248/269 (92%)	242 (98%)	6 (2%)	0	100	100
8	B	248/269 (92%)	242 (98%)	6 (2%)	0	100	100
9	C	349/466 (75%)	323 (93%)	26 (7%)	0	100	100
10	D	418/459 (91%)	397 (95%)	21 (5%)	0	100	100
All	All	2879/4706 (61%)	2747 (95%)	132 (5%)	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	E	133/164 (81%)	132 (99%)	1 (1%)	79	89
2	F	256/640 (40%)	256 (100%)	0	100	100
3	K	125/433 (29%)	125 (100%)	0	100	100
4	I	255/517 (49%)	254 (100%)	1 (0%)	89	94
6	G	104/269 (39%)	104 (100%)	0	100	100
7	H	374/406 (92%)	372 (100%)	2 (0%)	86	93
8	A	206/221 (93%)	206 (100%)	0	100	100
8	B	206/221 (93%)	206 (100%)	0	100	100
9	C	285/371 (77%)	285 (100%)	0	100	100
10	D	327/357 (92%)	327 (100%)	0	100	100
All	All	2271/3599 (63%)	2267 (100%)	4 (0%)	91	96

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

Mol	Chain	Res	Type
1	E	204	HIS
4	I	59	ARG
7	H	472	SER
7	H	483	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
8	B	247	ASN
9	C	293	ASN
10	D	426	GLN
10	D	305	HIS
4	I	209	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.

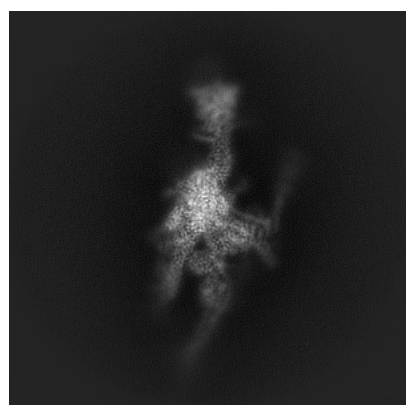
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22446. These allow visual inspection of the internal detail of the map and identification of artifacts.

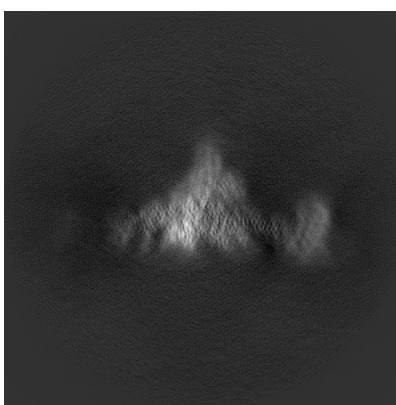
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

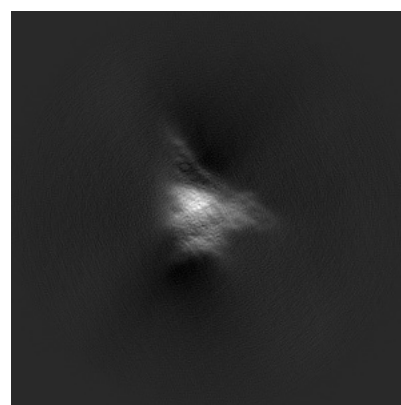
6.1.1 Primary map



X



Y

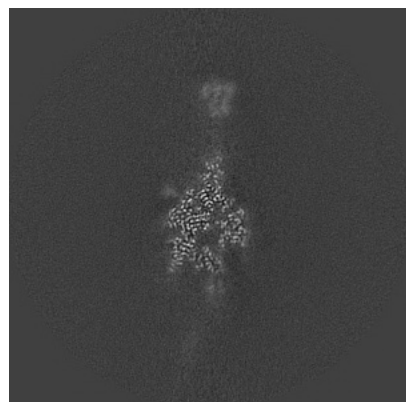


Z

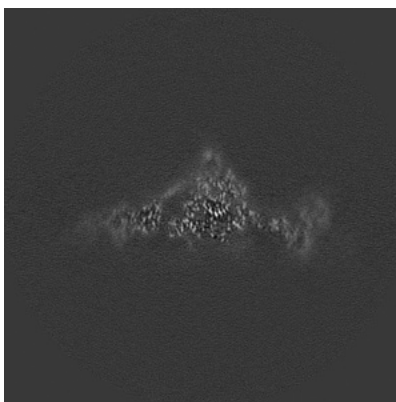
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

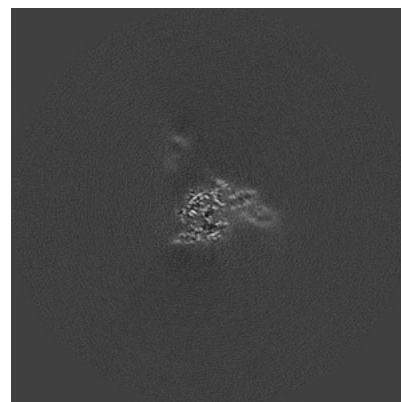
6.2.1 Primary map



X Index: 270



Y Index: 270

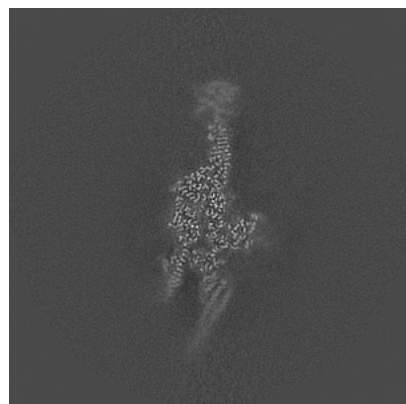


Z Index: 270

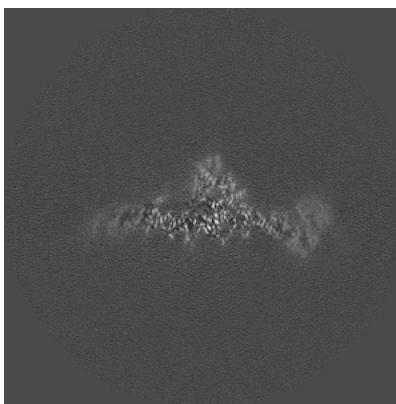
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

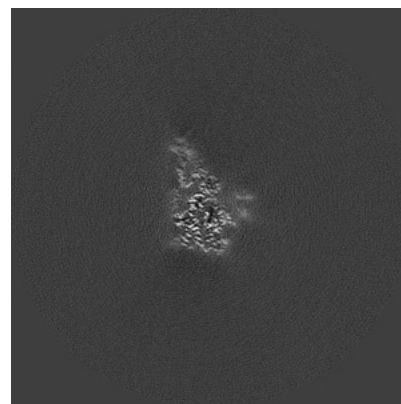
6.3.1 Primary map



X Index: 251



Y Index: 276

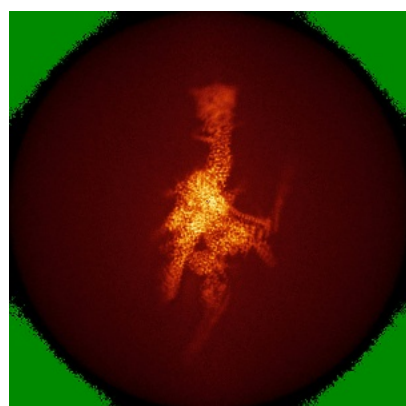


Z Index: 251

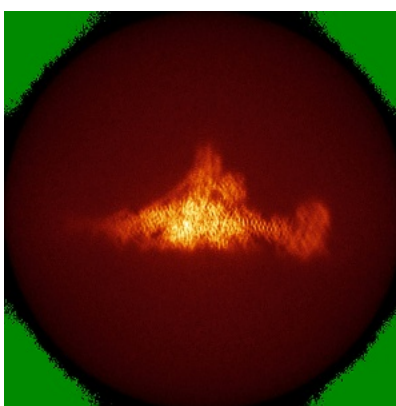
The images above show the largest variance slices of the map in three orthogonal directions.

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

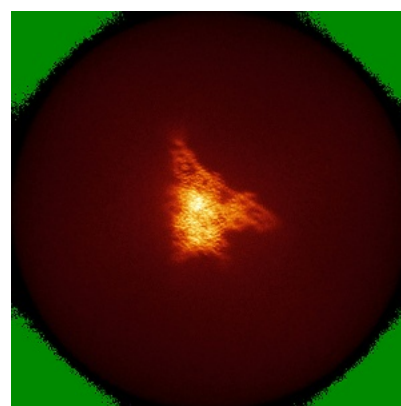
6.4.1 Primary map



X



Y

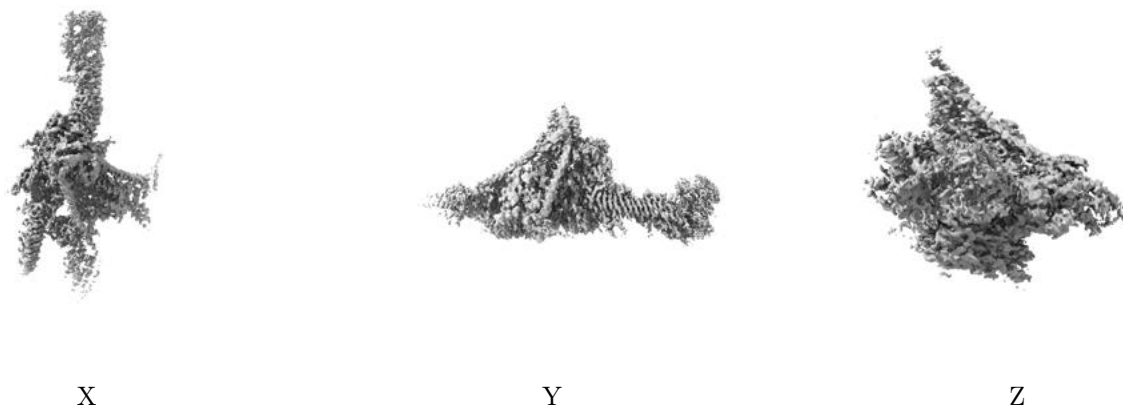


Z

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 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

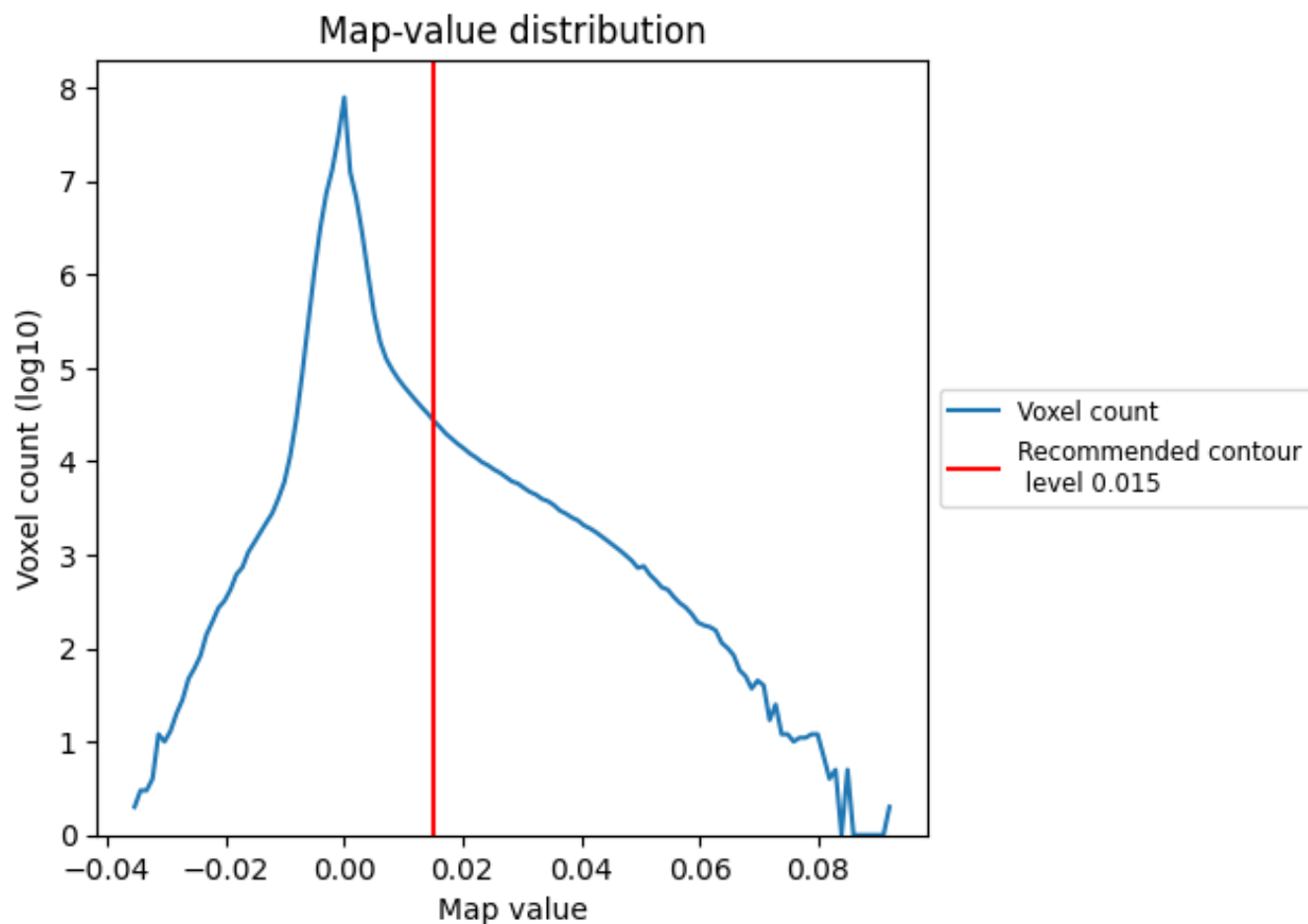
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

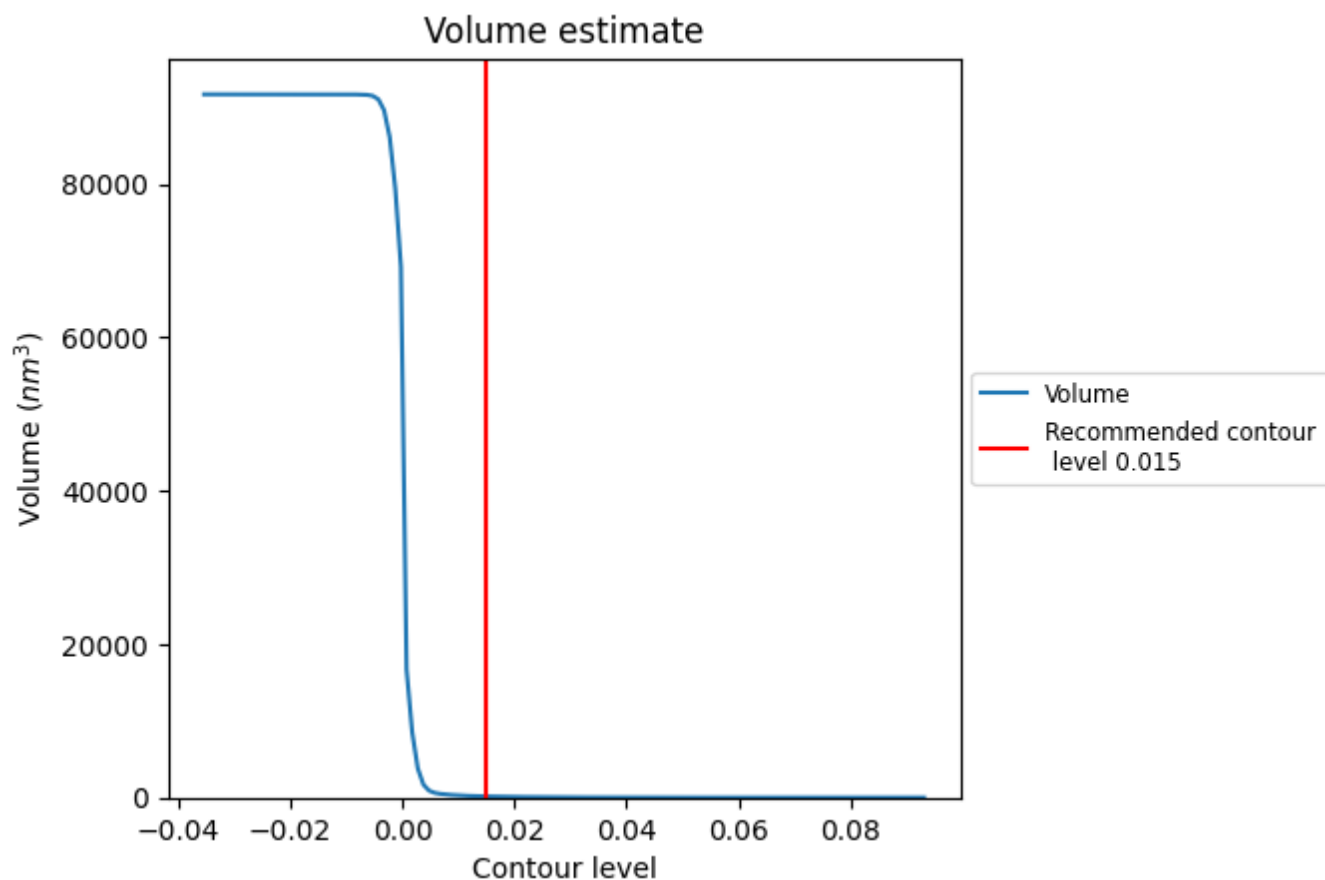
This section contains the results of statistical analysis of the map.

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.

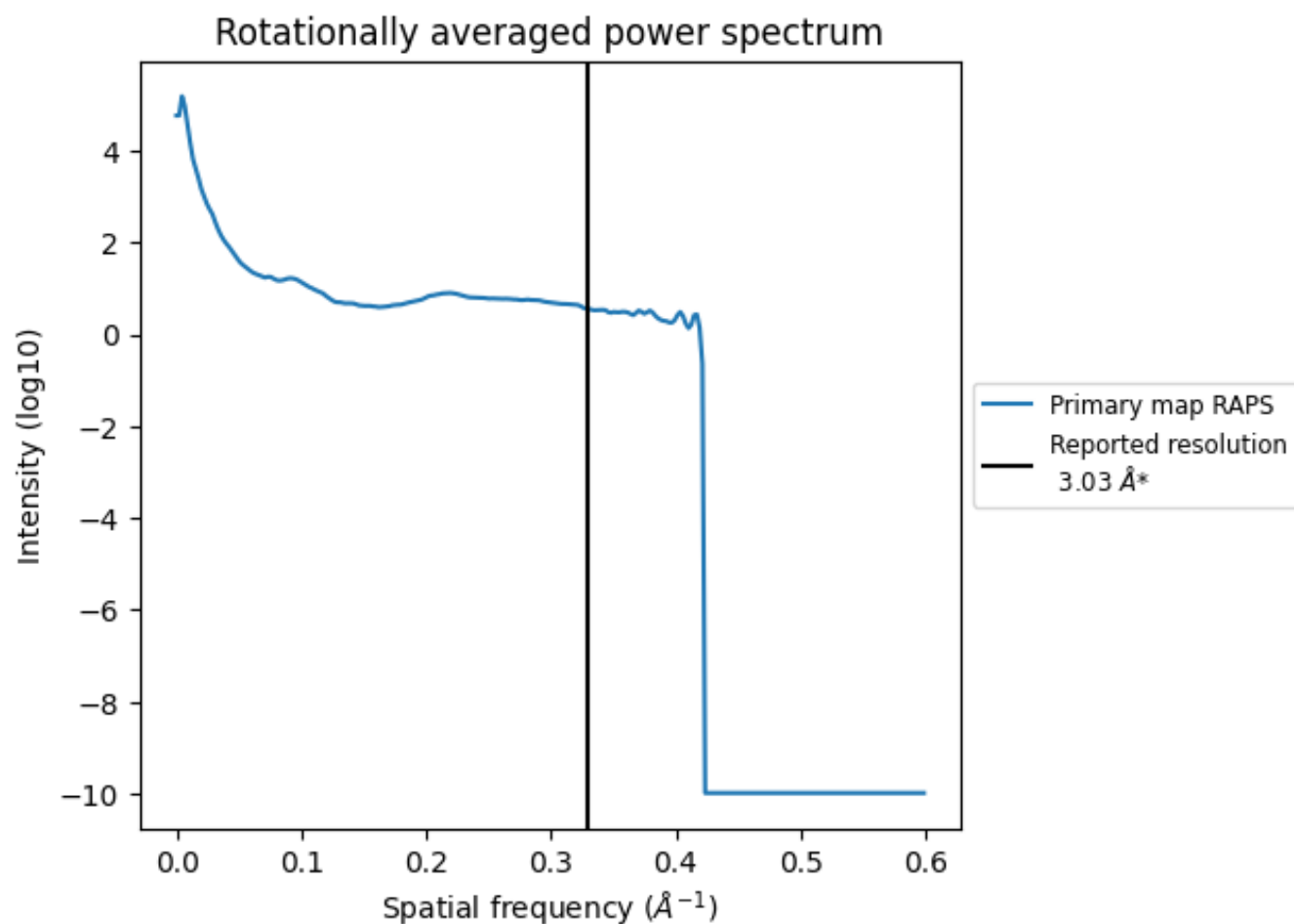
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm³; this corresponds to an approximate mass of 133 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 0.330 Å⁻¹

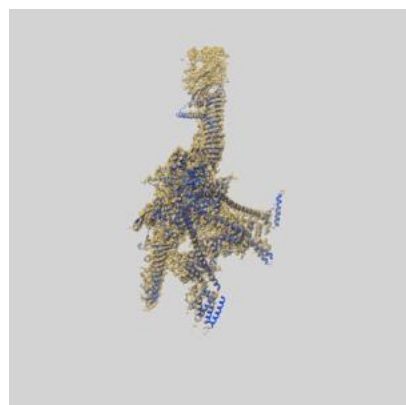
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

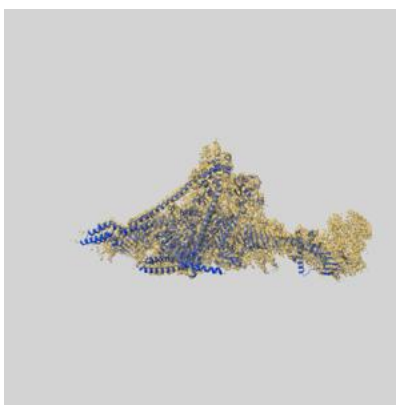
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22446 and PDB model 7JRJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

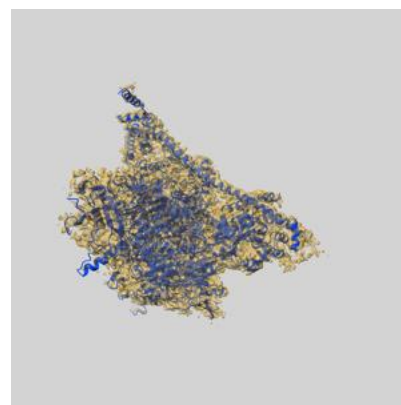
9.1 Map-model overlay [i](#)



X



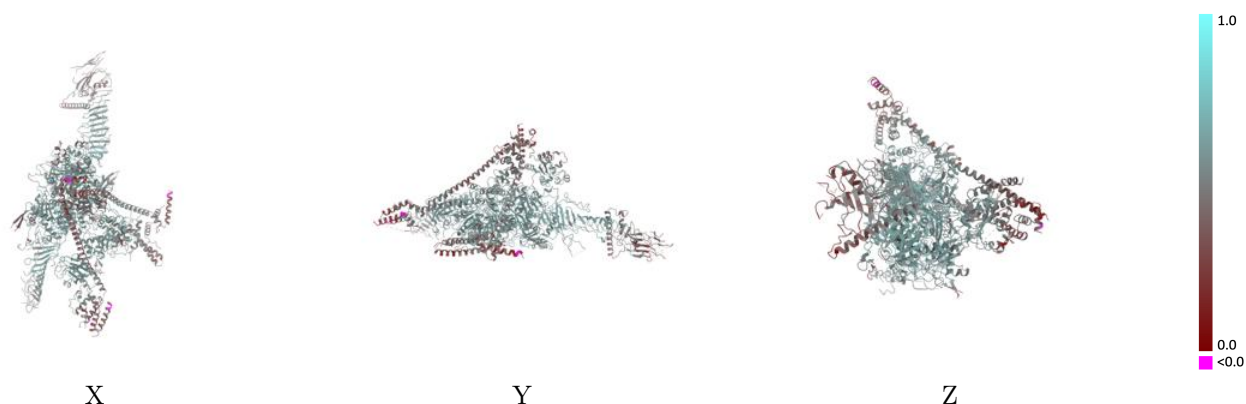
Y



Z

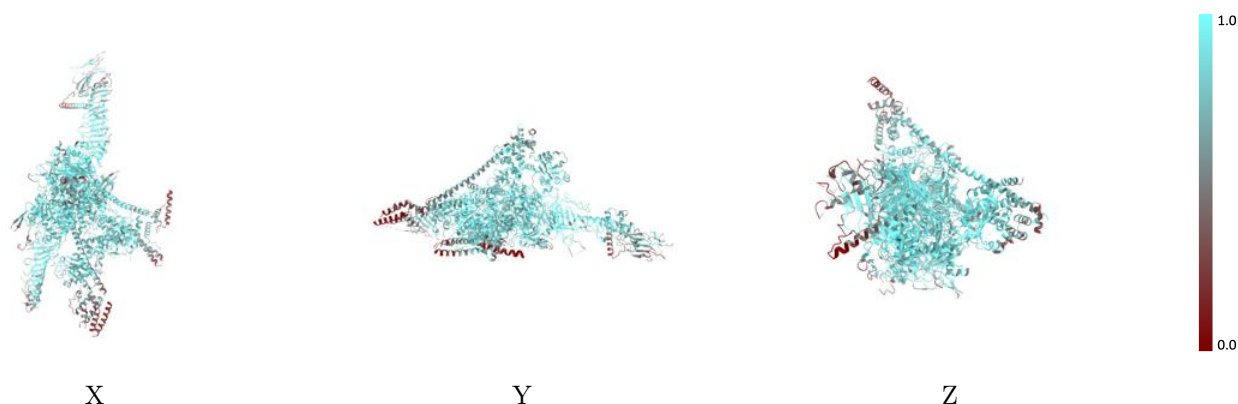
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



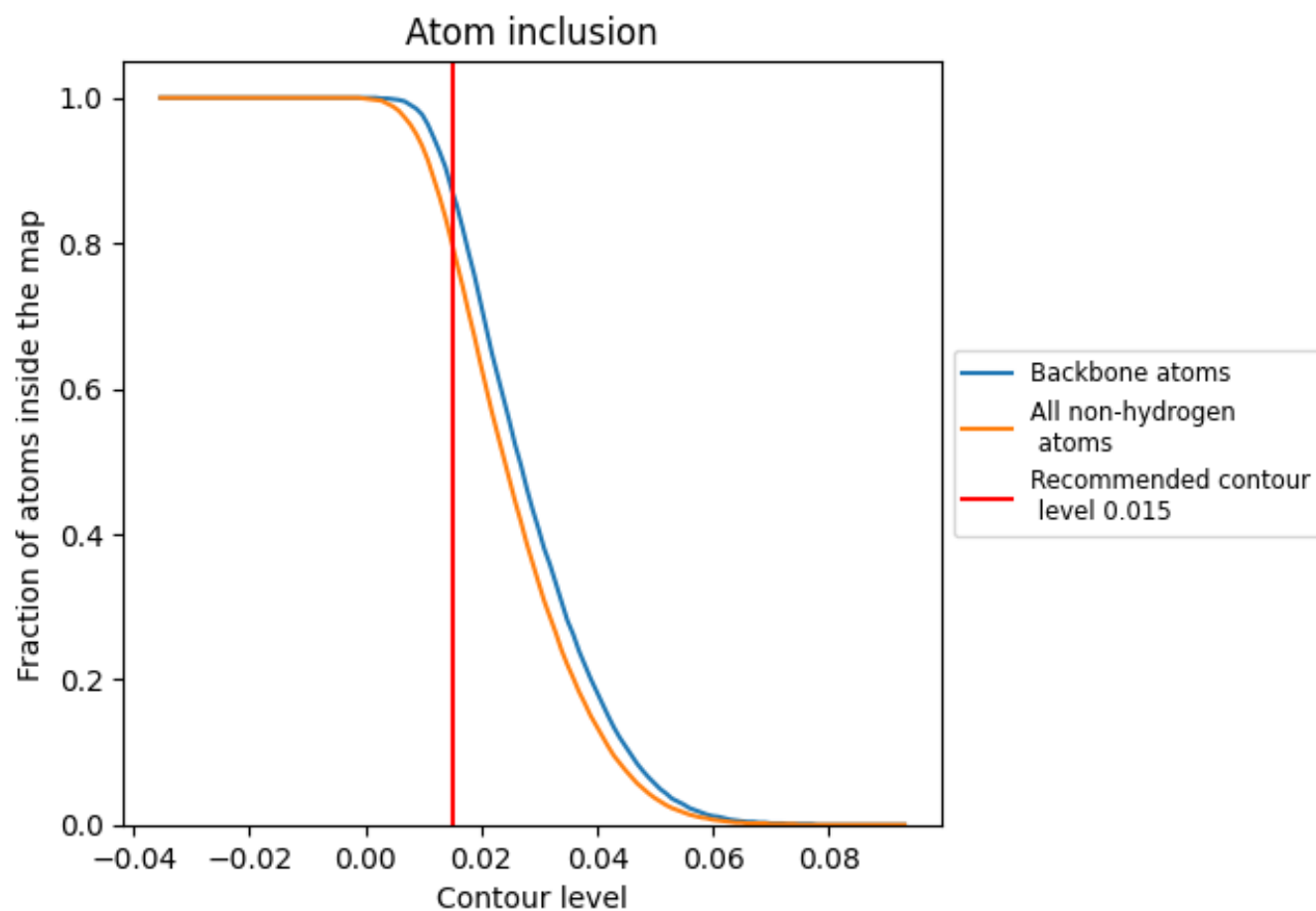
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7980	 0.5270
A	 0.9210	 0.5940
B	 0.9010	 0.5610
C	 0.8650	 0.5620
D	 0.8310	 0.5570
E	 0.7860	 0.5350
F	 0.7500	 0.5040
G	 0.6300	 0.3950
H	 0.8350	 0.5480
I	 0.6570	 0.4810
J	 0.7890	 0.6180
K	 0.8250	 0.4750
L	 0.6670	 0.4900
M	 0.6000	 0.5120
N	 0.5810	 0.3690
O	 0.2820	 0.3310

