



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2024 – 02:35 am BST

PDB ID : 8BDA
EMDB ID : EMD-15980
Title : IFTA complex in anterograde intraflagellar transport trains (*Chlamydomonas reinhardtii*)
Authors : Lacey, S.E.; Foster, H.E.; Pigino, G.
Deposited on : 2022-10-18
Resolution : 20.70 Å(reported)

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

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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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

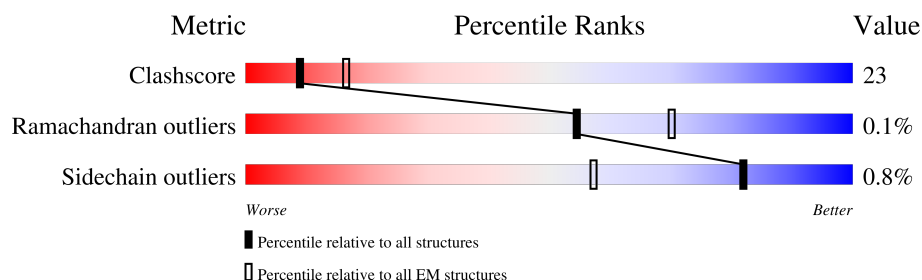
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	1224	<div> <div>8%</div> <div>51%</div> <div>37%</div> <div>12%</div> </div>
2	E	1355	<div> <div>14%</div> <div>60%</div> <div>37%</div> <div>.</div> </div>
3	G	1409	<div> <div>9%</div> <div>50%</div> <div>46%</div> <div>.</div> </div>
4	I	1367	<div> <div>22%</div> <div>53%</div> <div>46%</div> <div>.</div> </div>
5	L	1239	<div> <div>.</div> <div>38%</div> <div>42%</div> <div>20%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48086 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 Intraflagellar transport protein 121.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1074	Total	C	N	O	S	0	0
			8511	5406	1464	1579	62		

- Molecule 2 is a protein called Intraflagellar transport protein 139.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1325	Total	C	N	O	S	0	0
			10464	6587	1860	1956	61		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	188	GLN	GLU	variant	UNP A9XPA6

- Molecule 3 is a protein called Intraflagellar transport particle protein 140.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	1354	Total	C	N	O	S	0	0
			10600	6657	1867	1998	78		

- Molecule 4 is a protein called Intraflagellar transport protein 144.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	1367	Total	C	N	O	S	0	0
			10579	6654	1857	1998	70		

- Molecule 5 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	997	Total	C	N	O	S	0	0
			7932	5064	1373	1455	40		

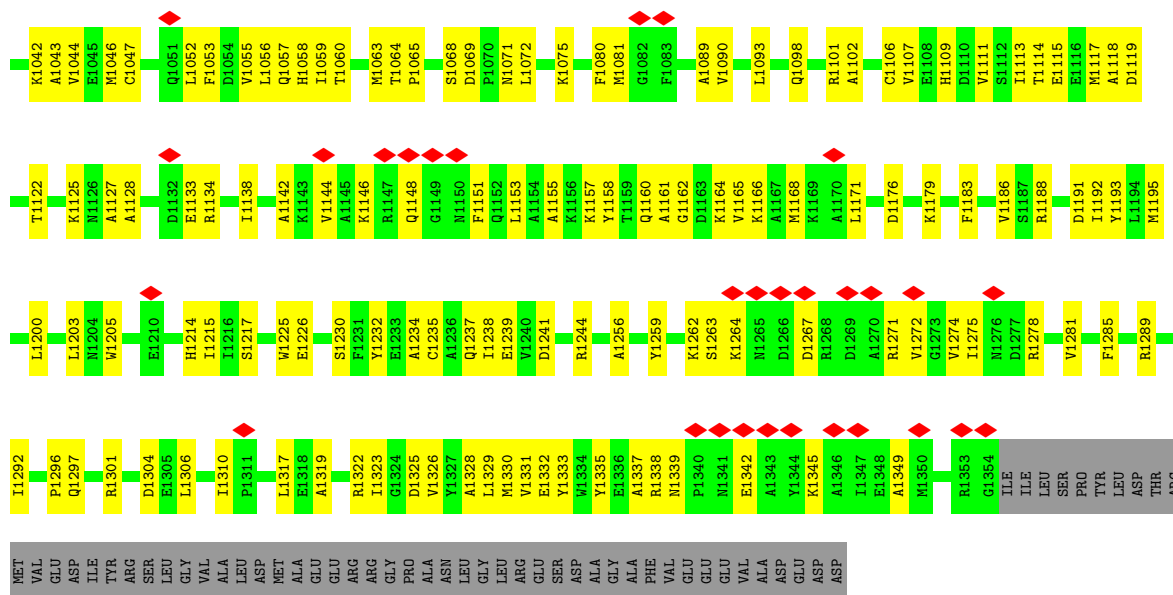
3 Residue-property plots

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.

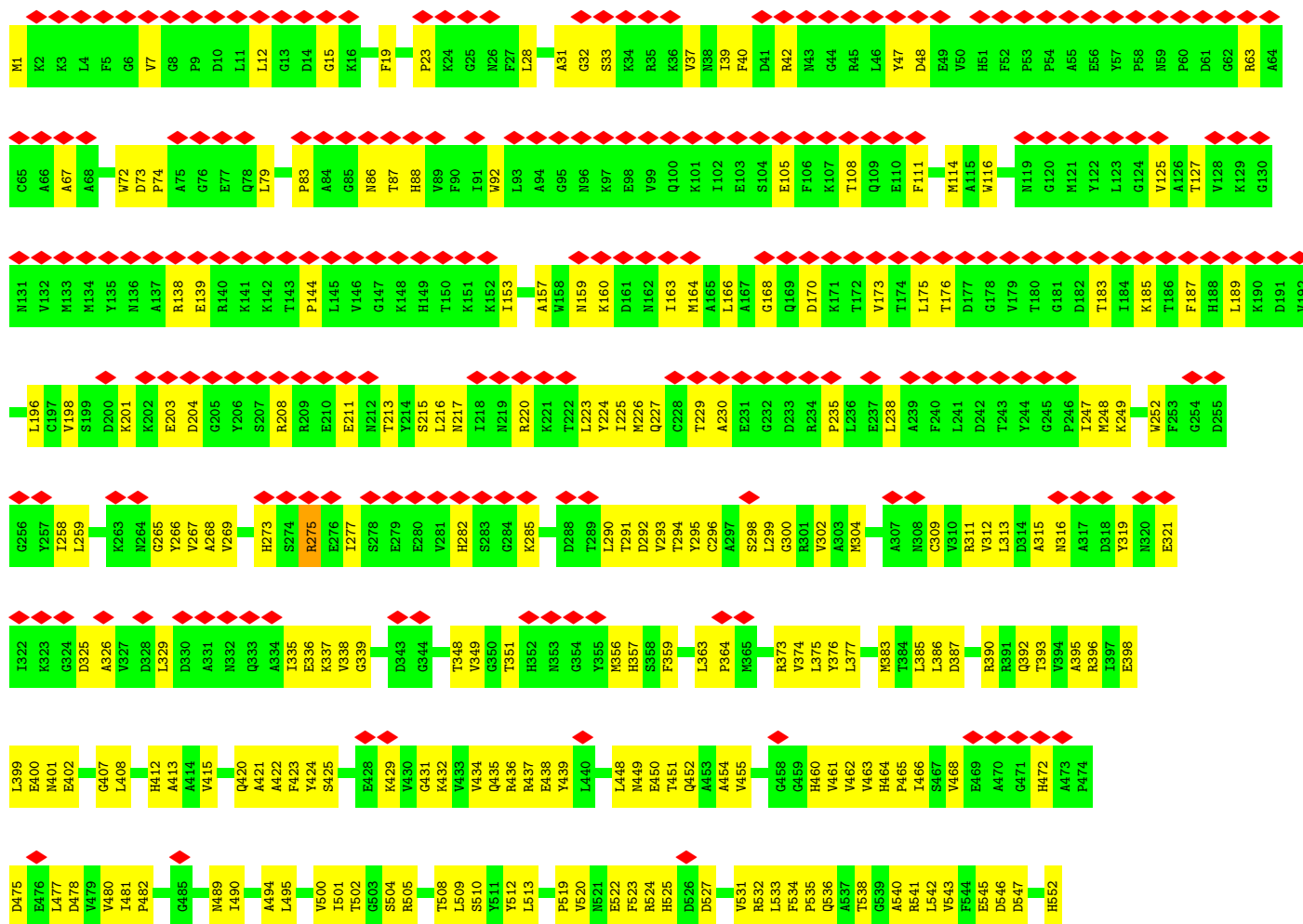
• Molecule 1: Intraflagellar transport protein 121

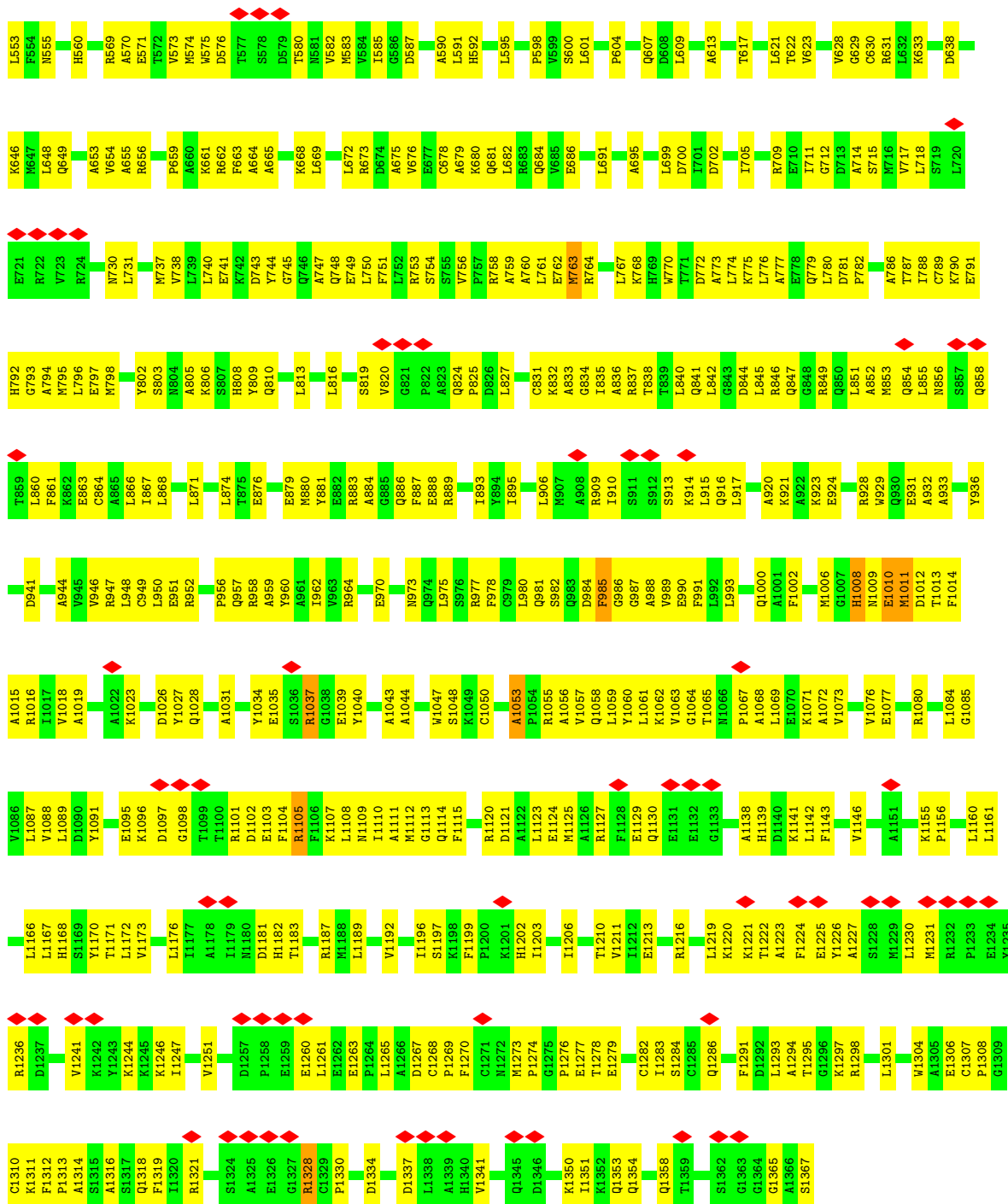




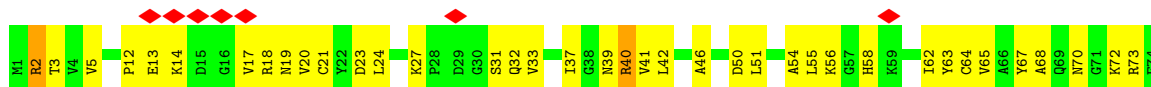
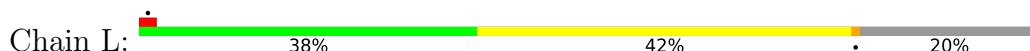


• Molecule 4: Intraflagellar transport protein 144





- Molecule 5: Intraflagellar transport protein 122 homolog



VAL	ASP	ARG	ALA	PHE	T919	T841	L775	L696	K627	L775	Q529	V458	H386	Q309	L155	A75
ASP	ARG	ALA	K776	SER	A928	R842	K777	R699	E632	Q530	A550	R459	V387	M310	L155	S76
ALA	LEU	LEU	D778	LVS	D778	R843	Q700	R699	Q633	L634	L531	C460	L388	T311	C157	G77
LEU	LEU	LEU	D779	GLU	D779	R844	LVS	R699	Q633	L634	F534	L461	L389	T237	F158	A79
ASP	LEU	LEU	T780	GLY	T780	Q846	E705	E705	L635	L636	V535		C390	I314		
LEU	LEU	LEU	L847	LEU	L847	R847	A713	A713	A637	L636	I543			I315	I162	V83
ASP	ASP	ASP	L848	ASP	L848	C848	A713	A713	A637	L636	I543			Q316	S163	V83
LEU	LEU	LEU	T784	PRO	T784	A849	T785	T785	E638	L636	L546			Q317	I164	R84
ALA	ALA	ALA	R786	VAL	R786	R850	Y717	Y717	E638	L636	L546			L318	R165	R85
GLY	GLY	GLY	L786	VAL	L786	R850	Y717	Y717	E638	L636	L546			E321	K243	L86
THR	THR	THR	L787	MET	L787	R850	A641	A641	M640	L636	M551				T244	T87
GLU	GLU	ALA	A720	GLU	A720	E854	A720	A720	A641	L636	M551			V324	V245	S88
TRP	TRP	TRP	K721	TRP	K721	E854	K721	K721	A641	L636	M551			R325	H246	K89
ARG	ARG	ARG	T788	ARG	T788	R855	T788	T788	F642	L636	M551			S170	L247	A90
CYS	CYS	CYS	E799	CYS	E799	R856	T792	T792	F642	L636	M551			E171	G172	
LEU	LEU	LEU	A790	LEU	A790	T857	Y723	Y723	R645	L636	M551			K172	H173	L94
THR	THR	THR	K792	THR	K792	Y646	Y724	Y724	Y646	L636	M551			R250	K172	K95
ASN	ASN	ASN	K792	ASN	K792	Q647	R725	R725	Q647	L636	M551			D251	H174	Y96
PRO	PRO	PRO	W793	PRO	W793	F648	A726	A726	F648	L636	M551			C328	I175	
LYS	LYS	LYS	A796	LYS	A796	R863	T727	T727	F648	L636	M551			K329	L265	A101
ALA	ALA	ALA	A796	ALA	A796	R863	A798	A798	F648	L636	M551			Q330	G178	I102
GLU	GLU	GLU	A796	GLU	A796	R863	A798	A798	F648	L636	M551			Y331	F179	Q103
ASN	ASN	ASN	A796	ASN	A796	R863	A798	A798	F648	L636	M551			Y332	F179	C104
PRO	PRO	PRO	A796	PRO	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ASN	ASN	ASN	A796	ASN	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLN	GLN	GLN	A796	GLN	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
VAL	VAL	VAL	A796	VAL	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ILE	ILE	ILE	A796	ILE	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
LYS	LYS	LYS	A796	LYS	A796	R863	A798	A798	F648	L636	M551			Y333	F179	Y107
PRO	PRO	PRO	A796	PRO	A796	R863	A798	A798	F648	L636	M551			Y333	F179	N108
GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	P109
ASP	ASP	ASP	A796	ASP	A796	R863	A798	A798	F648	L636	M551			Y333	F179	T110
MET	MET	MET	A796	MET	A796	R863	A798	A798	F648	L636	M551			Y333	F179	T111
GLN	GLN	GLN	A796	GLN	A796	R863	A798	A798	F648	L636	M551			Y333	F179	Q112
TYR	TYR	TYR	A796	TYR	A796	R863	A798	A798	F648	L636	M551			Y333	F179	Q113
GLU	GLU	GLU	A796	GLU	A796	R863	A798	A798	F648	L636	M551			Y333	F179	L114
PHE	PHE	PHE	A796	PHE	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ARG	ARG	ARG	A796	ARG	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
VAL	VAL	VAL	A796	VAL	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ILE	ILE	ILE	A796	ILE	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
CYS	CYS	CYS	A796	CYS	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ASP	ASP	ASP	A796	ASP	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
PRO	PRO	PRO	A796	PRO	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ASP	ASP	ASP	A796	ASP	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLN	GLN	GLN	A796	GLN	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
LEU	LEU	LEU	A796	LEU	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLU	GLU	GLU	A796	GLU	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
LEU	LEU	LEU	A796	LEU	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
VAL	VAL	VAL	A796	VAL	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ILE	ILE	ILE	A796	ILE	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
CYS	CYS	CYS	A796	CYS	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
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GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
PRO	PRO	PRO	A796	PRO	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
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GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
PRO	PRO	PRO	A796	PRO	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ASP	ASP	ASP	A796	ASP	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
PRO	PRO	PRO	A796	PRO	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
ASP	ASP	ASP	A796	ASP	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
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GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
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GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
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GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
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GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
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GLY	GLY	GLY	A796	GLY	A796	R863	A798	A798	F648	L636	M551			Y333	F179	
PRO	PRO	PRO	A796	PRO	A796	R863	A798	A798	F648	L636	M551			Y333	F179	

THR	ALA	PRO	PHE	SER	ARG	THR	THR	VAL	ARG	GLY	GLY	GLY	LEU	ALA	PRO	GLY	GLU	ASP	ALA	GLU	ASP	GLU	GLY	ALA	GLY	GLY	ASN	LYS	LEU	GLY	GLY	PRO	LEU	GLY	SER	ALA	ARG	GLY	PRO	TLE	GLY	GLY	ALA	SER	LYS	ALA	ARG	MET	SER	VAL	PRO	PHE	GLN	GLN	GLY	ARG	PRO	LEU	VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	3897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Warp/Relion/M - CTF Refinement in M	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	104	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.122	Depositor
Minimum map value	-1.291	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	727.2, 727.2, 727.2	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.06, 6.06, 6.06	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	C	0.30	0/8701	0.57	0/11769
2	E	0.31	0/10649	0.61	0/14397
3	G	0.33	0/10815	0.63	0/14651
4	I	0.32	0/10781	0.61	0/14601
5	L	0.33	0/8108	0.61	0/10978
All	All	0.32	0/49054	0.61	0/66396

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	C	8511	0	8356	348	0
2	E	10464	0	10515	374	0
3	G	10600	0	10441	569	0
4	I	10579	0	10549	516	0
5	L	7932	0	7900	470	0
All	All	48086	0	47761	2227	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 23.

The worst 5 of 2227 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)
5:L:796:ALA:HB1	5:L:800:LEU:HG	1.44	0.98
3:G:1028:GLU:HA	3:G:1052:LEU:HD11	1.45	0.98
2:E:1144:ALA:O	2:E:1148:LEU:HB2	1.65	0.96
5:L:907:GLU:O	5:L:911:LYS:HB2	1.70	0.91
1:C:445:GLN:HE22	1:C:524:PRO:HB3	1.38	0.89

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	C	1070/1224 (87%)	974 (91%)	96 (9%)	0	100	100
2	E	1321/1355 (98%)	1229 (93%)	91 (7%)	1 (0%)	51	86
3	G	1352/1409 (96%)	1191 (88%)	160 (12%)	1 (0%)	51	86
4	I	1365/1367 (100%)	1245 (91%)	116 (8%)	4 (0%)	41	77
5	L	995/1239 (80%)	872 (88%)	121 (12%)	2 (0%)	47	81
All	All	6103/6594 (93%)	5511 (90%)	584 (10%)	8 (0%)	54	86

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	730	PRO
3	G	1165	VAL
4	I	1053	ALA
5	L	778	ASP
4	I	1008	HIS

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	904/1005 (90%)	897 (99%)	7 (1%)	81	89
2	E	1092/1114 (98%)	1082 (99%)	10 (1%)	78	87
3	G	1117/1162 (96%)	1107 (99%)	10 (1%)	78	87
4	I	1119/1119 (100%)	1112 (99%)	7 (1%)	86	92
5	L	840/1035 (81%)	834 (99%)	6 (1%)	84	90
All	All	5072/5435 (93%)	5032 (99%)	40 (1%)	82	89

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	763	MET
5	L	40	ARG
4	I	1011	MET
4	I	1221	LYS
5	L	418	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	227	GLN
4	I	811	GLN
4	I	792	HIS
4	I	1052	GLN
2	E	289	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 [i](#)

There are no monosaccharides 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-15980. 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

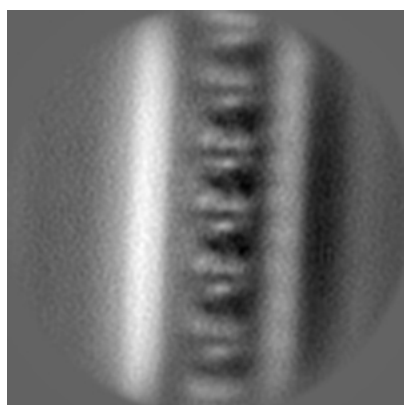


Y

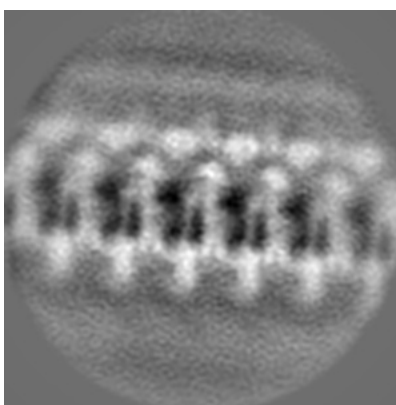


Z

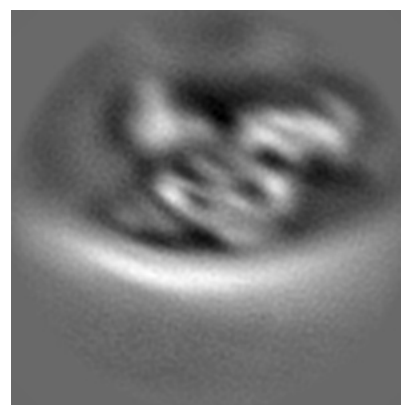
6.1.2 Raw map



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: 60

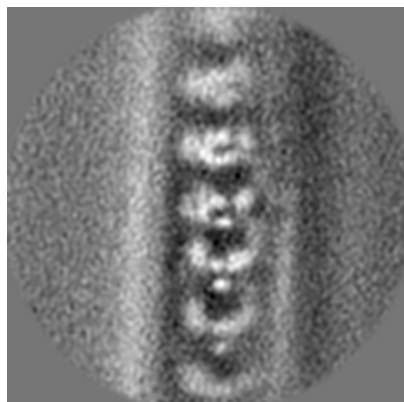


Y Index: 60

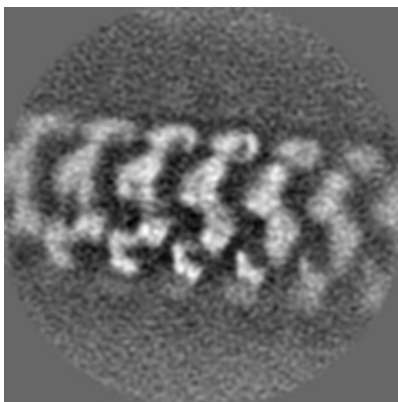


Z Index: 60

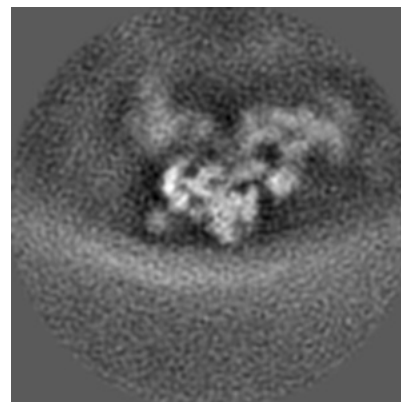
6.2.2 Raw map



X Index: 60



Y Index: 60



Z Index: 60

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: 48

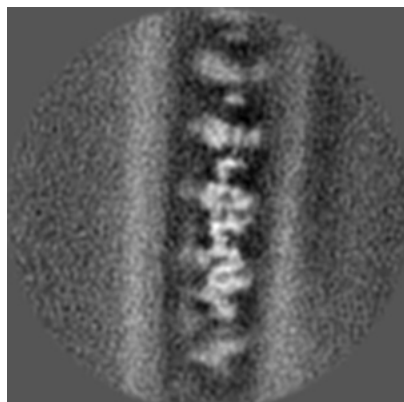


Y Index: 63

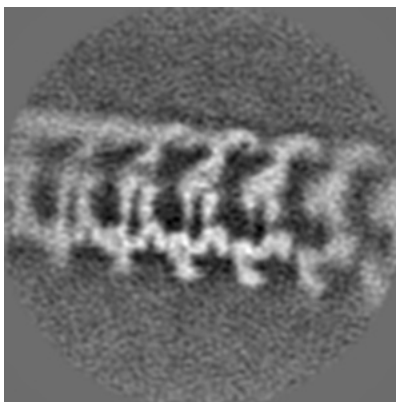


Z Index: 61

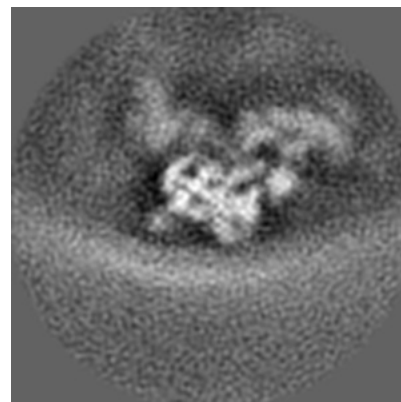
6.3.2 Raw map



X Index: 49



Y Index: 63



Z Index: 61

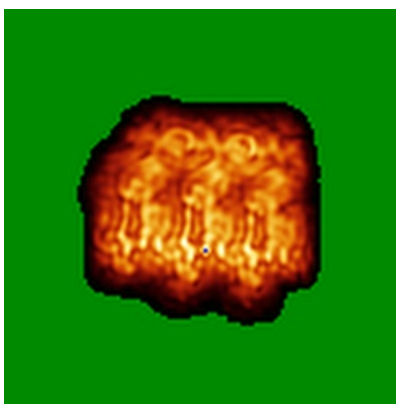
The images above show the largest variance slices of the map in three orthogonal directions.

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

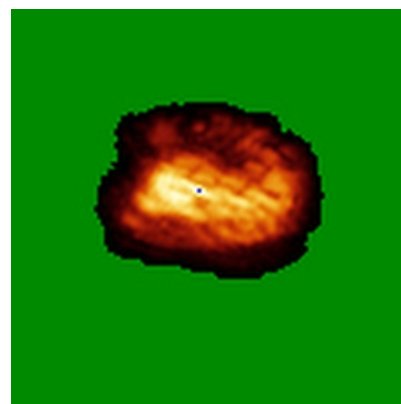
6.4.1 Primary map



X

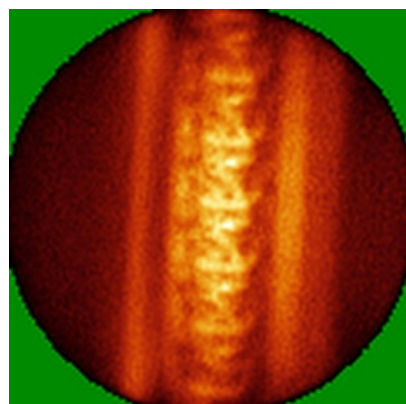


Y

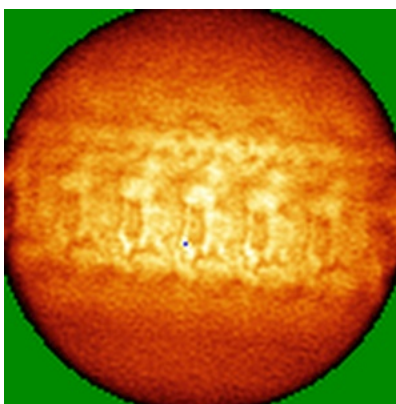


Z

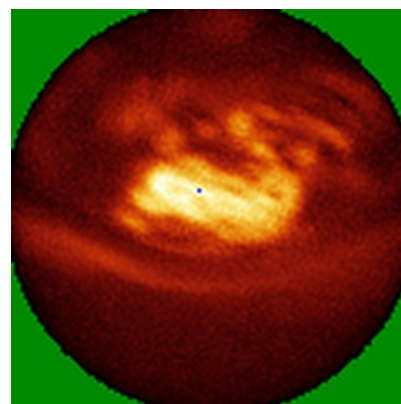
6.4.2 Raw map



X



Y



Z

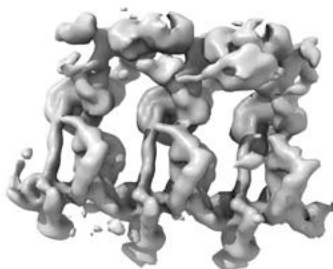
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

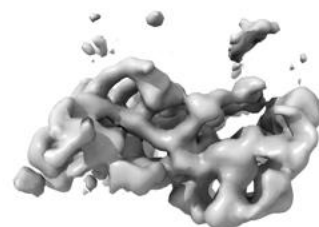
6.5.1 Primary map



X



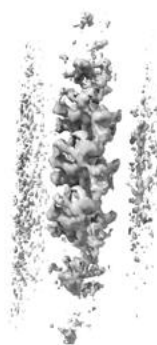
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



X



Y



Z

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.

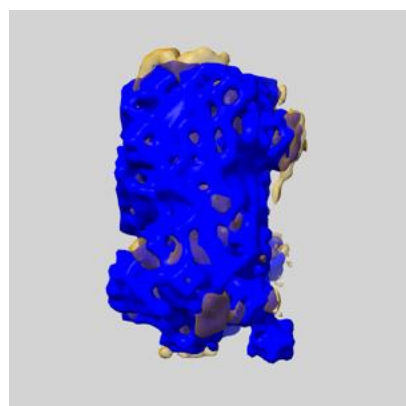
6.6 Mask visualisation [i](#)

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

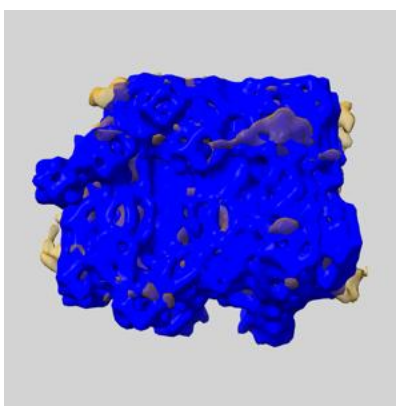
A mask typically either:

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

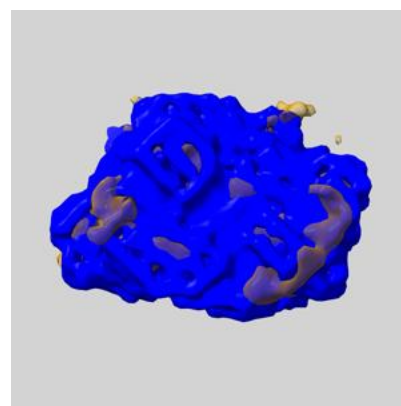
6.6.1 emd_15980_msk_1.map [i](#)



X



Y

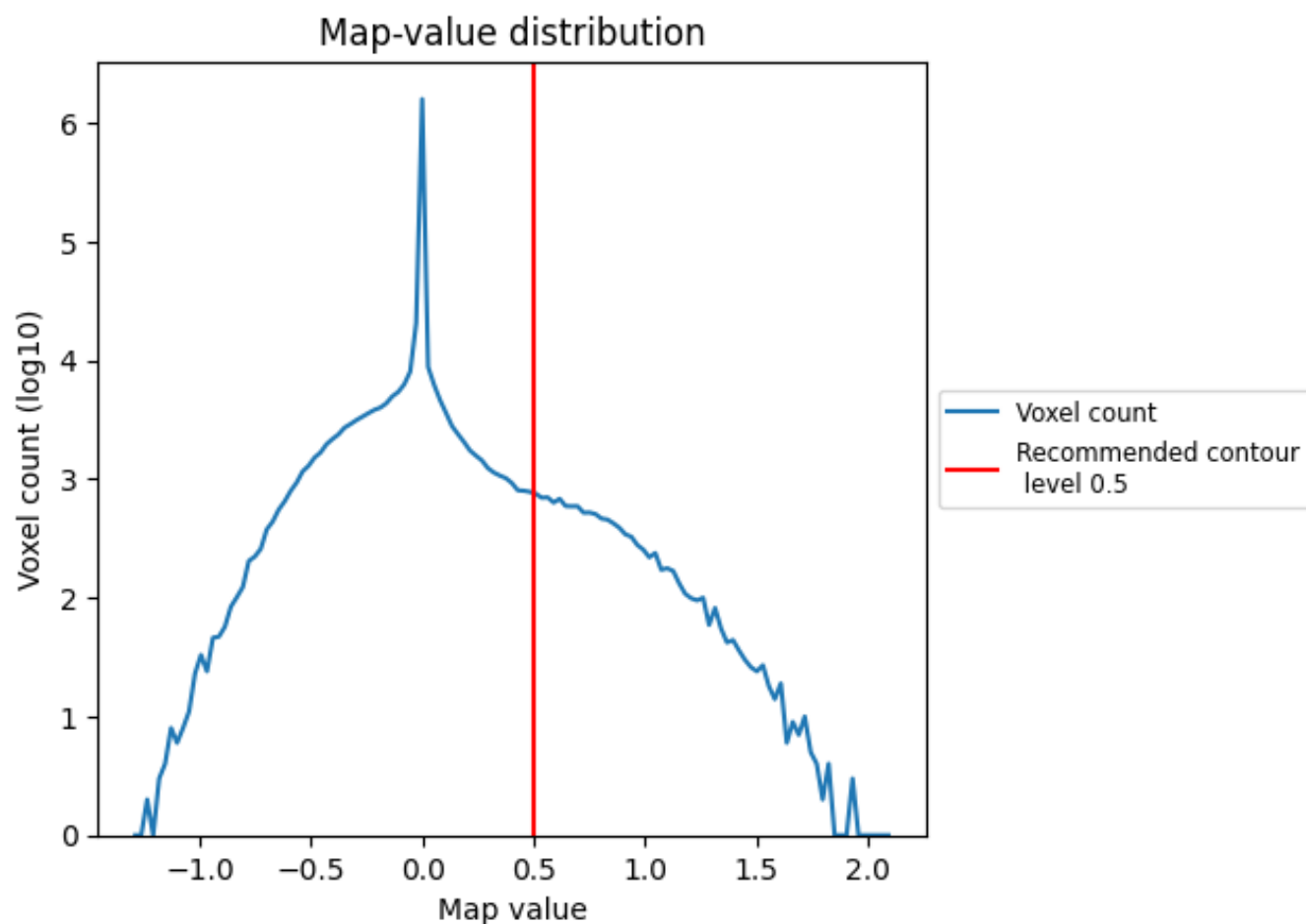


Z

7 Map analysis [i](#)

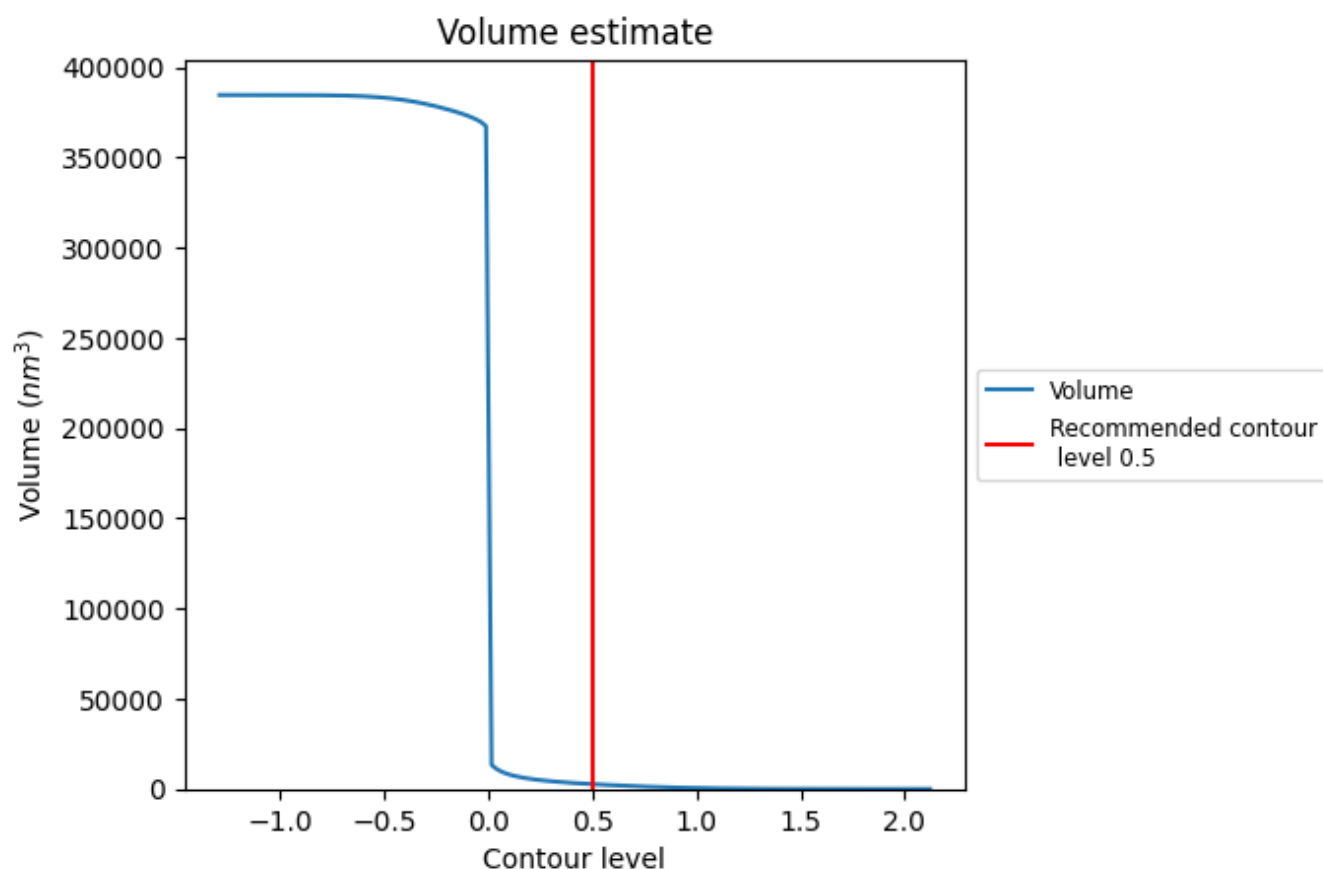
This section contains the results of statistical analysis of the map.

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.

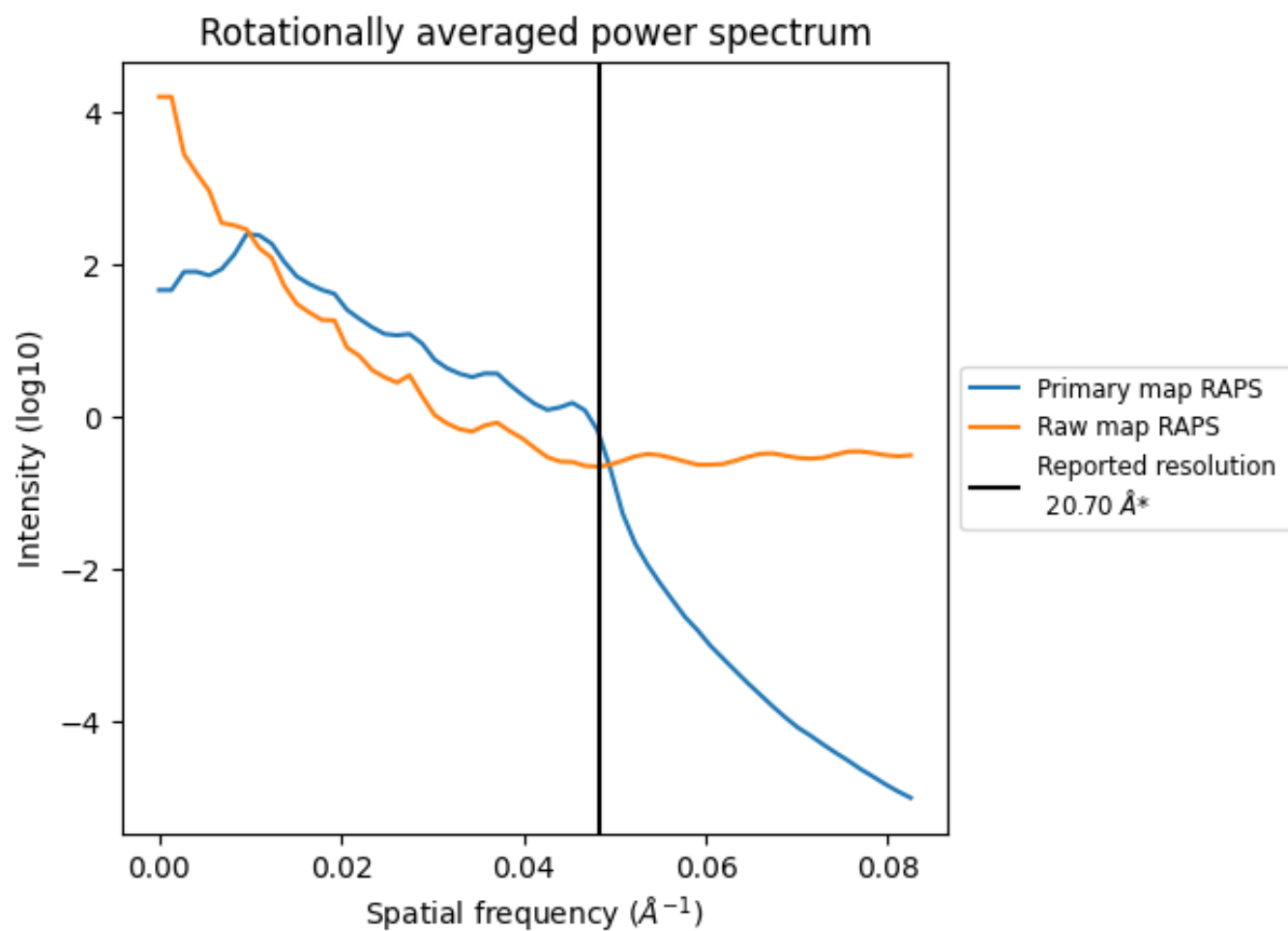
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2681 nm³; this corresponds to an approximate mass of 2422 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 ⓘ

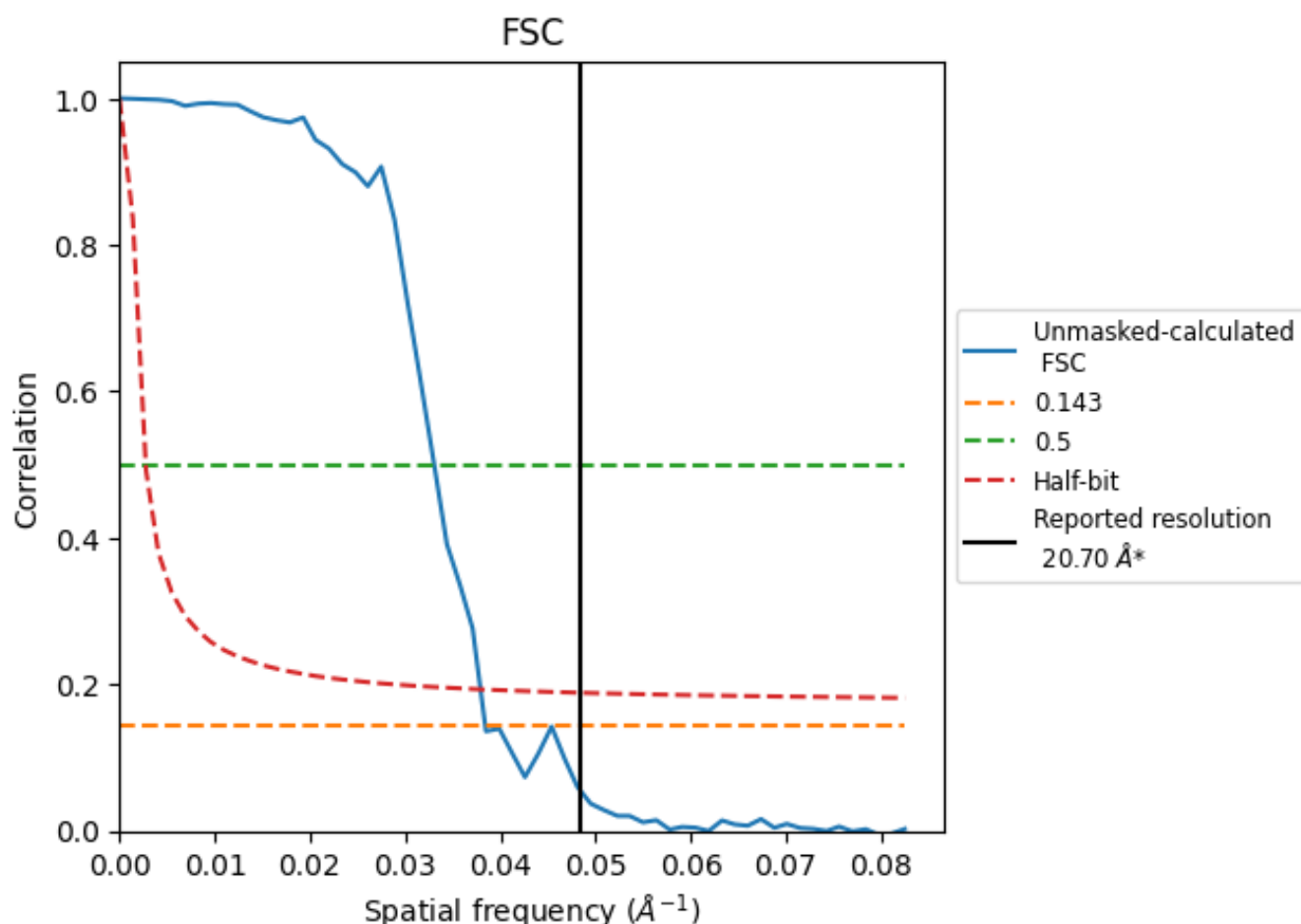


*Reported resolution corresponds to spatial frequency of 0.048 \AA^{-1}

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 0.048 Å⁻¹

8.2 Resolution estimates [i](#)

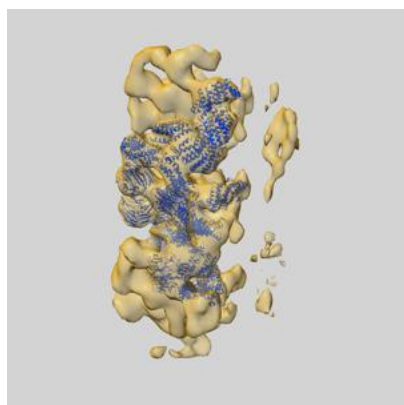
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	20.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	26.04	30.21	26.39

*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 26.04 differs from the reported value 20.7 by more than 10 %

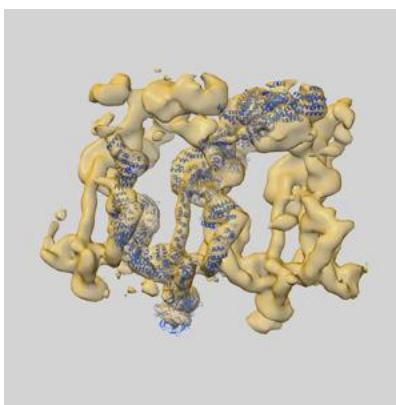
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15980 and PDB model 8BDA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

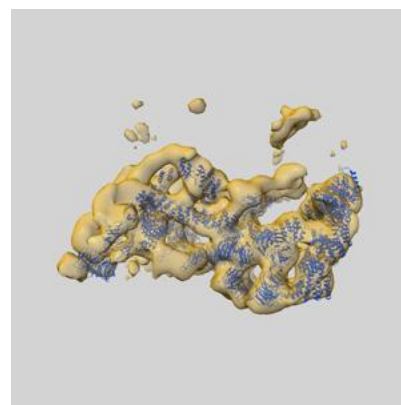
9.1 Map-model overlay [i](#)



X



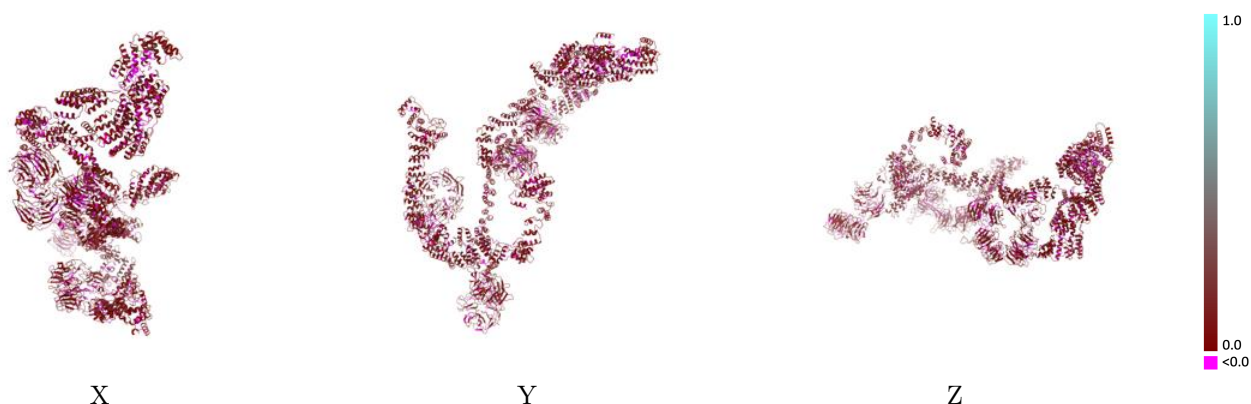
Y



Z

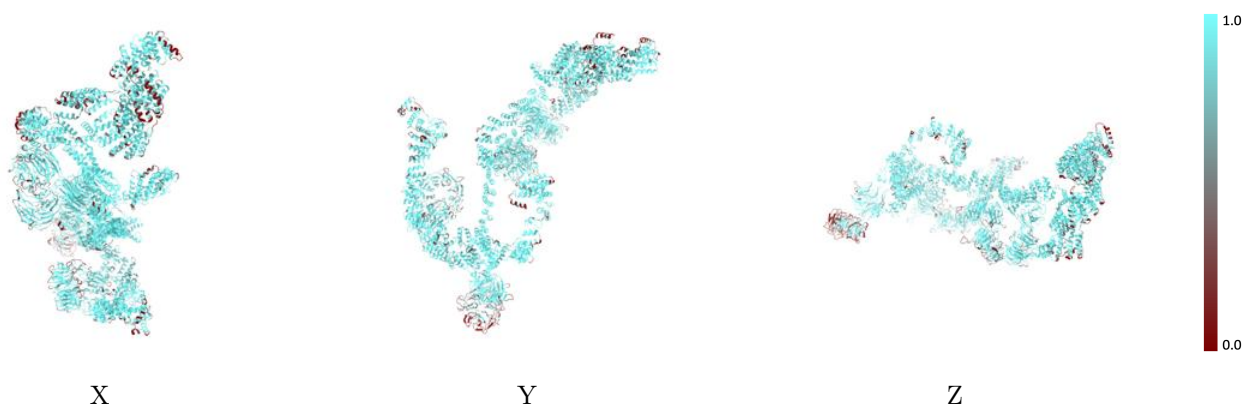
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



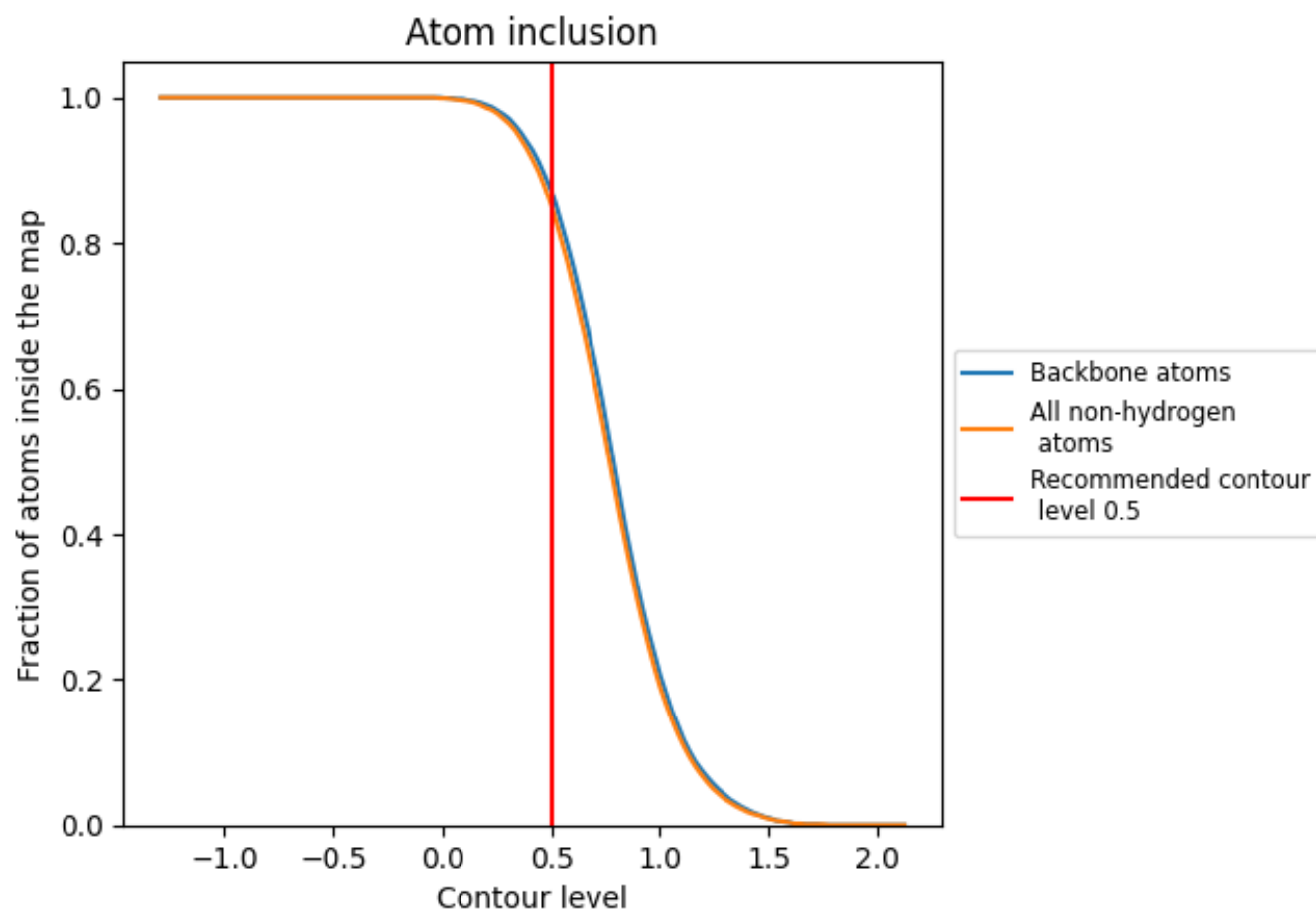
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8530	<div></div> 0.0800
C	<div></div> 0.8840	<div></div> 0.0780
E	<div></div> 0.8250	<div></div> 0.0740
G	<div></div> 0.8790	<div></div> 0.0840
I	<div></div> 0.7550	<div></div> 0.0810
L	<div></div> 0.9510	<div></div> 0.0840

