



## wwPDB EM Validation Summary Report ⓘ

Dec 15, 2022 – 02:30 PM EST

PDB ID : 8F5O  
EMDB ID : EMD-28866  
Title : Structure of Leishmania tarentolae IFT-A (state 1)  
Authors : Zhou, H.; Brown, A.  
Deposited on : 2022-11-14  
Resolution : 3.50 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

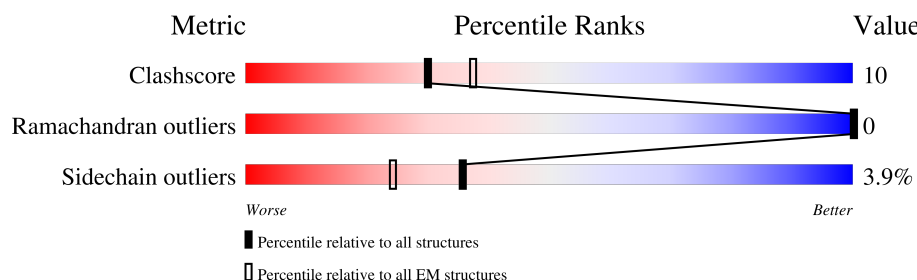
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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  $\geq 3$ , 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	1247	
2	C	1292	
3	E	1654	
4	A	368	
5	F	1376	
6	D	1642	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43398 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 122B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1134	Total	C	N	O	S	0	0
			8965	5674	1570	1658	63		

- Molecule 2 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1179	Total	C	N	O	S	0	0
			9354	5929	1622	1735	68		

- Molecule 3 is a protein called WD\_REPEATS\_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1076	Total	C	N	O	S	0	0
			8380	5291	1451	1588	50		

- Molecule 4 is a protein called NET domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	53	Total	C	N	O	S	0	0
			427	264	69	87	7		

- Molecule 5 is a protein called WD\_REPEATS\_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	911	Total	C	N	O	S	0	0
			7045	4431	1231	1349	34		

- Molecule 6 is a protein called TPR\_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	1180	Total	C	N	O	S	0	0
			9223	5796	1638	1738	51		

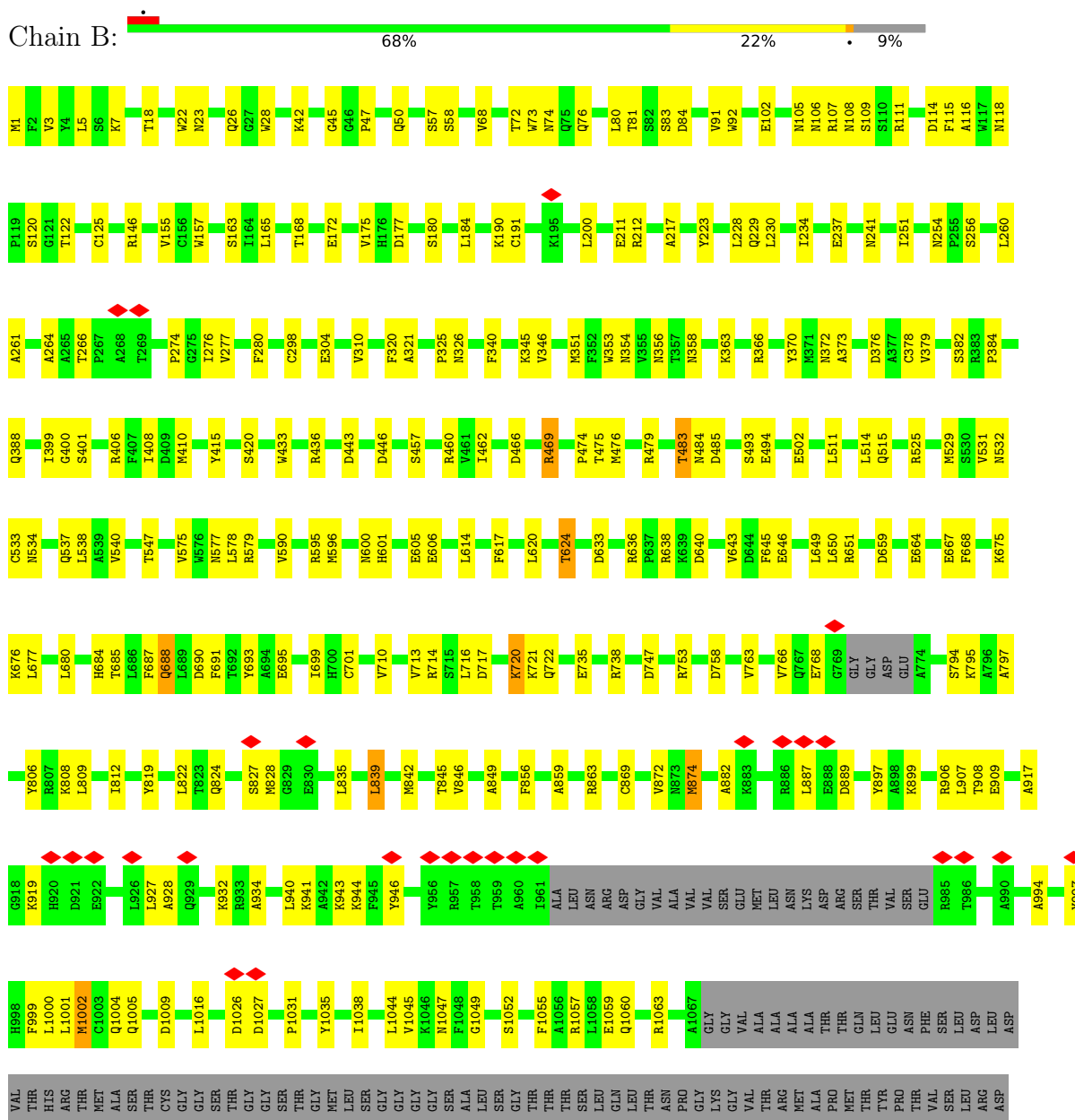
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

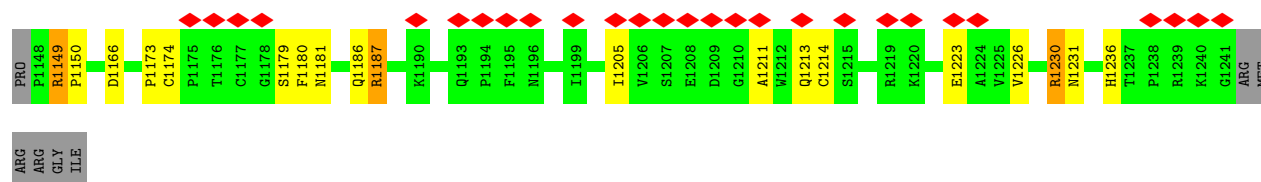
Mol	Chain	Residues	Atoms		AltConf
7	B	2	Total 2	Zn 2	0
7	C	2	Total 2	Zn 2	0

### 3 Residue-property plots

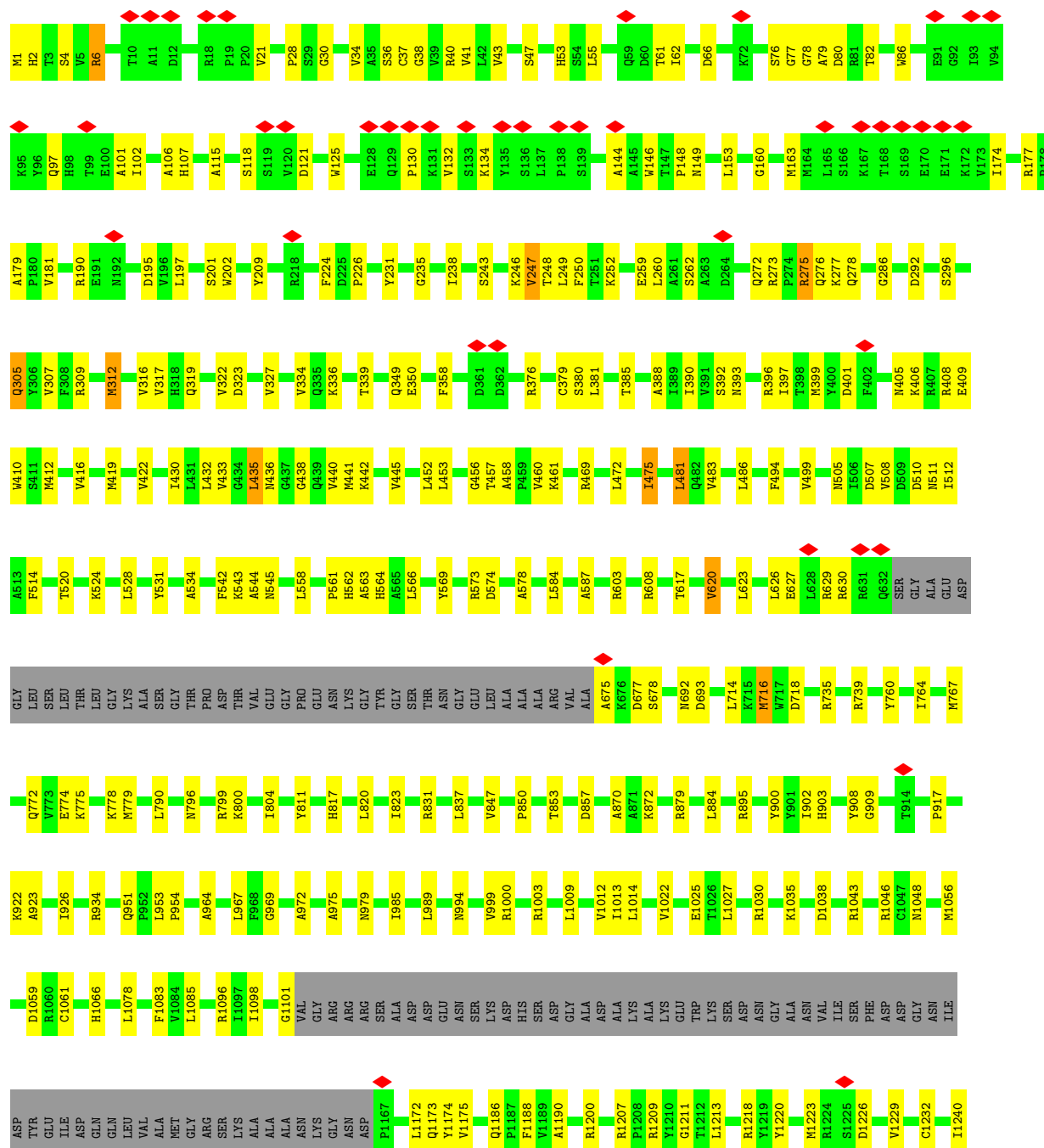
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

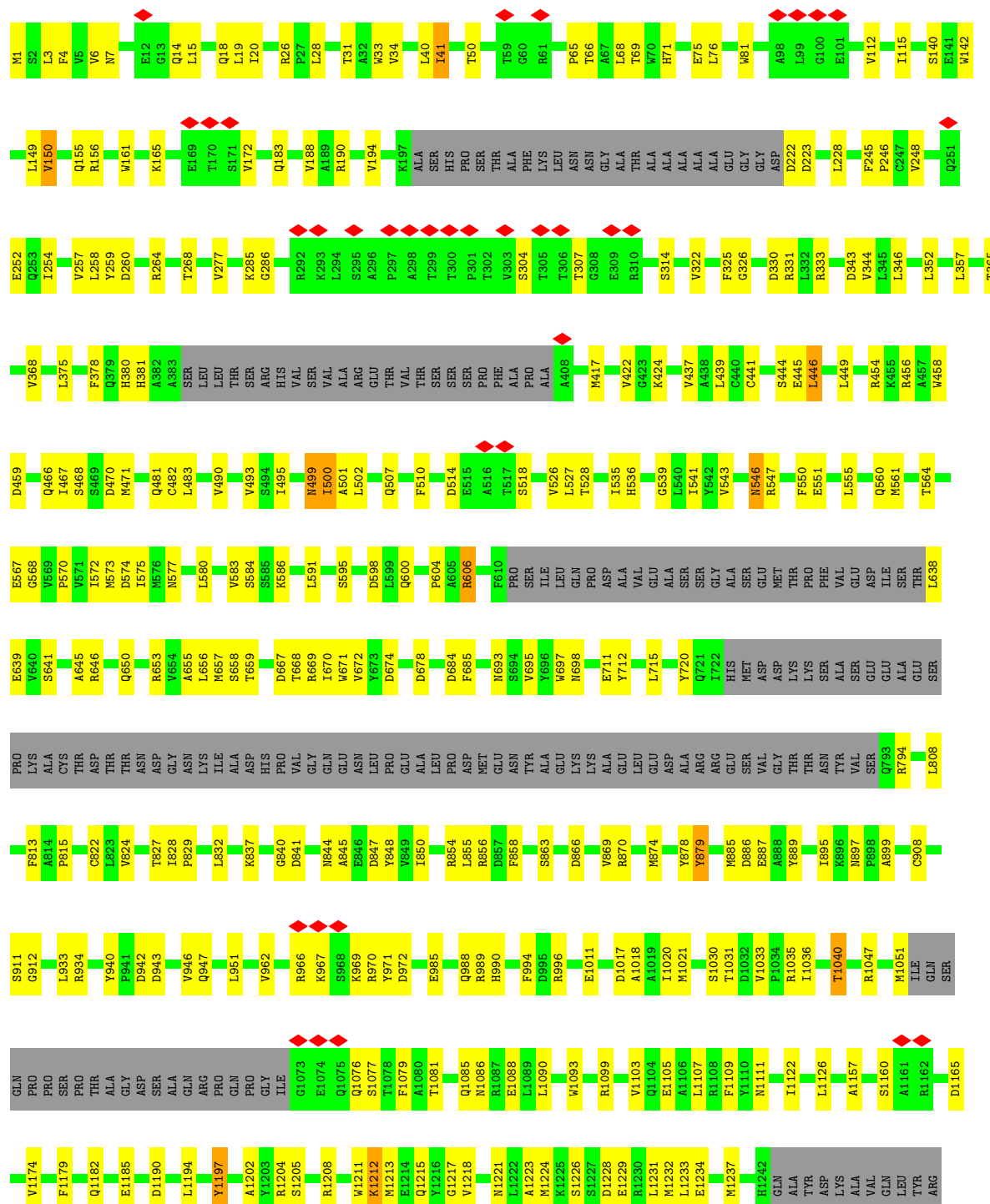
- Molecule 1: Intraflagellar transport protein 122B, putative

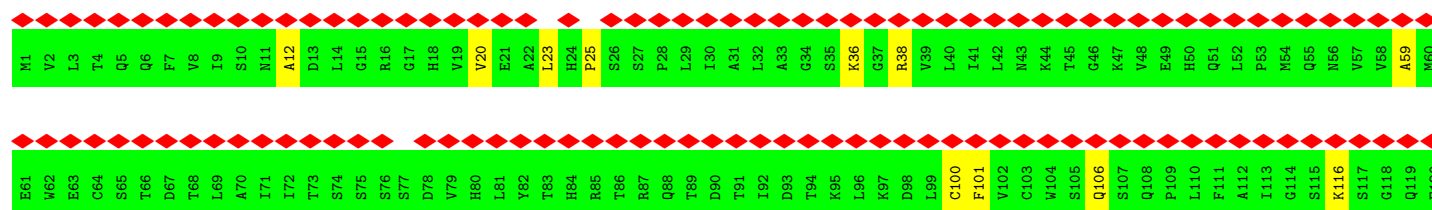




• Molecule 2: Intraflagellar transport protein 122 homolog











- Molecule 6: TPR REGION domain-containing protein

Chain D:



Q1607	P1608	P1609	K1610	A1611	I1612	D1613	K1616	R1617	T1624	Y1625	P1626	R1627	I1628	M1633	D1634	Y1637	S1638	M1639	L1640	R1641	P1642																									
L1433	A1511	A1512	C1435	K1436	V1437	P1440	F1443	L1446	T1452	Q1455	E1456	T1457	R1538	L1539	D1540	D1541	A1542	R1543	F1544	M1553	S1557	M1560	E1561	E1562	L1565	I1566	Y1567	K1572	M1573	K1574	A1575	A1576	S1577	Q1578	C1579	K1582	A1583	V1584	E1589	A1590	D1591	P1592	D1593	V1594	K1597	M1601
L1433	A1512	C1435	K1436	V1437	P1440	F1443	L1446	T1452	Q1455	E1456	T1457	R1538	L1539	D1540	D1541	A1542	R1543	F1544	M1553	S1557	M1560	E1561	E1562	L1565	I1566	Y1567	K1572	M1573	K1574	A1575	A1576	S1577	Q1578	C1579	K1582	A1583	V1584	E1589	A1590	D1591	P1592	D1593	V1594	K1597	M1601	
L1433	A1512	C1435	K1436	V1437	P1440	F1443	L1446	T1452	Q1455	E1456	T1457	R1538	L1539	D1540	D1541	A1542	R1543	F1544	M1553	S1557	M1560	E1561	E1562	L1565	I1566	Y1567	K1572	M1573	K1574	A1575	A1576	S1577	Q1578	C1579	K1582	A1583	V1584	E1589	A1590	D1591	P1592	D1593	V1594	K1597	M1601	
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	239280	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 ( $e^-/\text{\AA}^2$ )	57.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	86.420	Depositor
Minimum map value	-36.983	Depositor
Average map value	0.020	Depositor
Map value standard deviation	1.359	Depositor
Recommended contour level	9.0	Depositor
Map size (Å)	514.6, 514.6, 514.6	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.28	0/9156	0.51	0/12403
2	C	0.28	0/9548	0.52	0/12921
3	E	0.29	0/8546	0.52	0/11608
4	A	0.25	0/432	0.56	0/584
5	F	0.28	0/7173	0.51	0/9746
6	D	0.30	0/9377	0.54	1/12718 (0.0%)
All	All	0.29	0/44232	0.52	1/59980 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1003	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	B	8965	0	8873	170	0
2	C	9354	0	9301	185	0
3	E	8380	0	8309	173	0
4	A	427	0	413	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	7045	0	7054	101	0
6	D	9223	0	9265	253	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
All	All	43398	0	43215	868	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 10.

The worst 5 of 868 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)
3:E:441:CYS:O	3:E:445:GLU:HB3	1.71	0.89
2:C:76:SER:HG	2:C:86:TRP:HE1	1.25	0.80
5:F:446:SER:HB3	5:F:462:TYR:HB2	1.66	0.78
2:C:197:LEU:HB3	2:C:209:TYR:O	1.84	0.76
5:F:789:SER:HB3	5:F:808:MET:HB2	1.66	0.76

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	B	1126/1247 (90%)	1091 (97%)	35 (3%)	0	100	100
2	C	1173/1292 (91%)	1119 (95%)	54 (5%)	0	100	100
3	E	1064/1654 (64%)	1023 (96%)	41 (4%)	0	100	100
4	A	51/368 (14%)	45 (88%)	6 (12%)	0	100	100
5	F	907/1376 (66%)	865 (95%)	42 (5%)	0	100	100
6	D	1164/1642 (71%)	1118 (96%)	46 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5485/7579 (72%)	5261 (96%)	224 (4%)	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	960/1046 (92%)	926 (96%)	34 (4%)	36	67
2	C	1014/1094 (93%)	986 (97%)	28 (3%)	43	72
3	E	903/1373 (66%)	862 (96%)	41 (4%)	27	61
4	A	50/288 (17%)	47 (94%)	3 (6%)	19	52
5	F	779/1177 (66%)	763 (98%)	16 (2%)	53	79
6	D	971/1320 (74%)	910 (94%)	61 (6%)	18	51
All	All	4677/6298 (74%)	4494 (96%)	183 (4%)	36	64

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	707	ARG
6	D	733	TYR
5	F	833	GLU
6	D	518	ARG
6	D	974	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	540	GLN
6	D	1578	GLN
1	B	824	GLN
3	E	183	GLN
3	E	600	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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-28866. These allow visual inspection of the internal detail of the map and identification of artifacts.

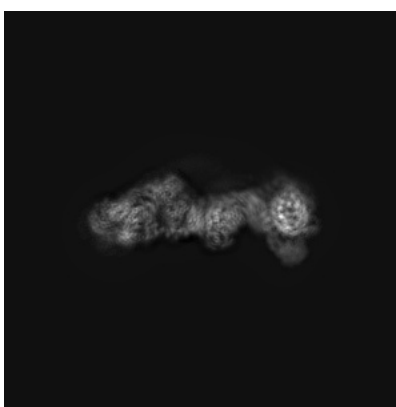
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

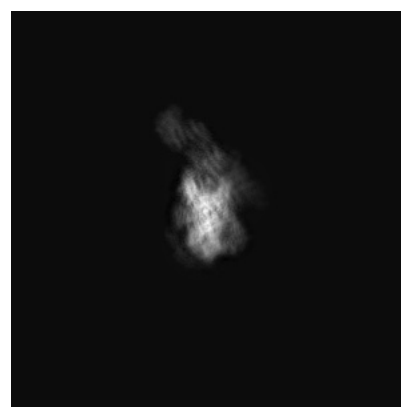
#### 6.1.1 Primary map



X



Y

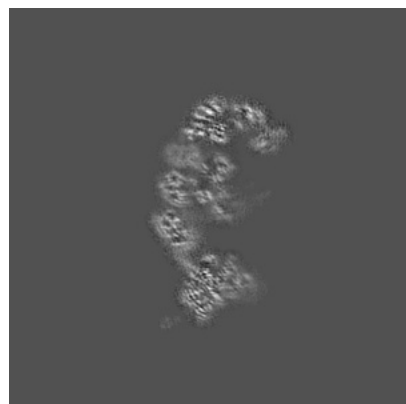


Z

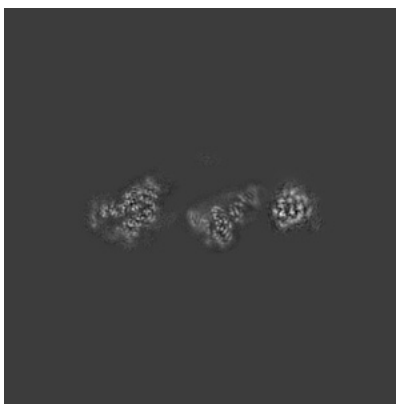
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

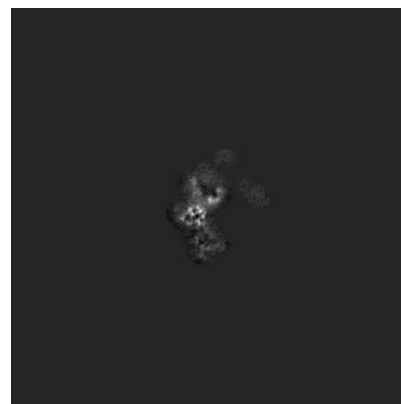
#### 6.2.1 Primary map



X Index: 310



Y Index: 310

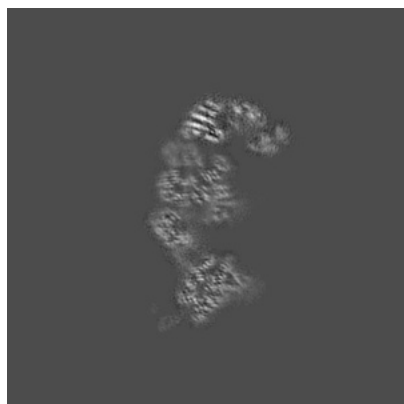


Z Index: 310

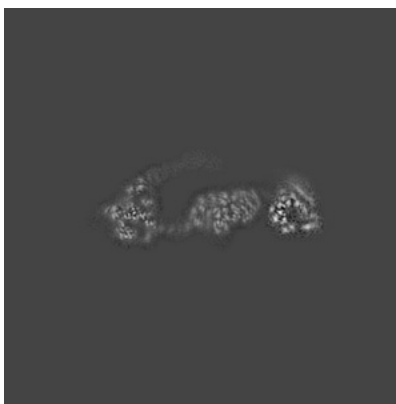
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

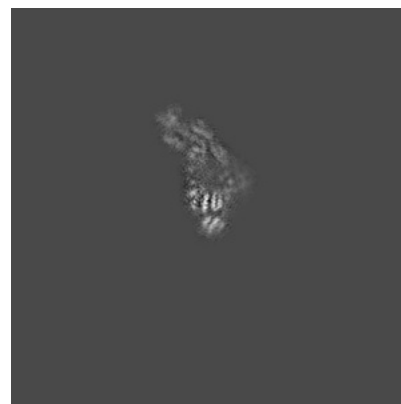
### 6.3.1 Primary map



X Index: 305



Y Index: 325



Z Index: 429

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

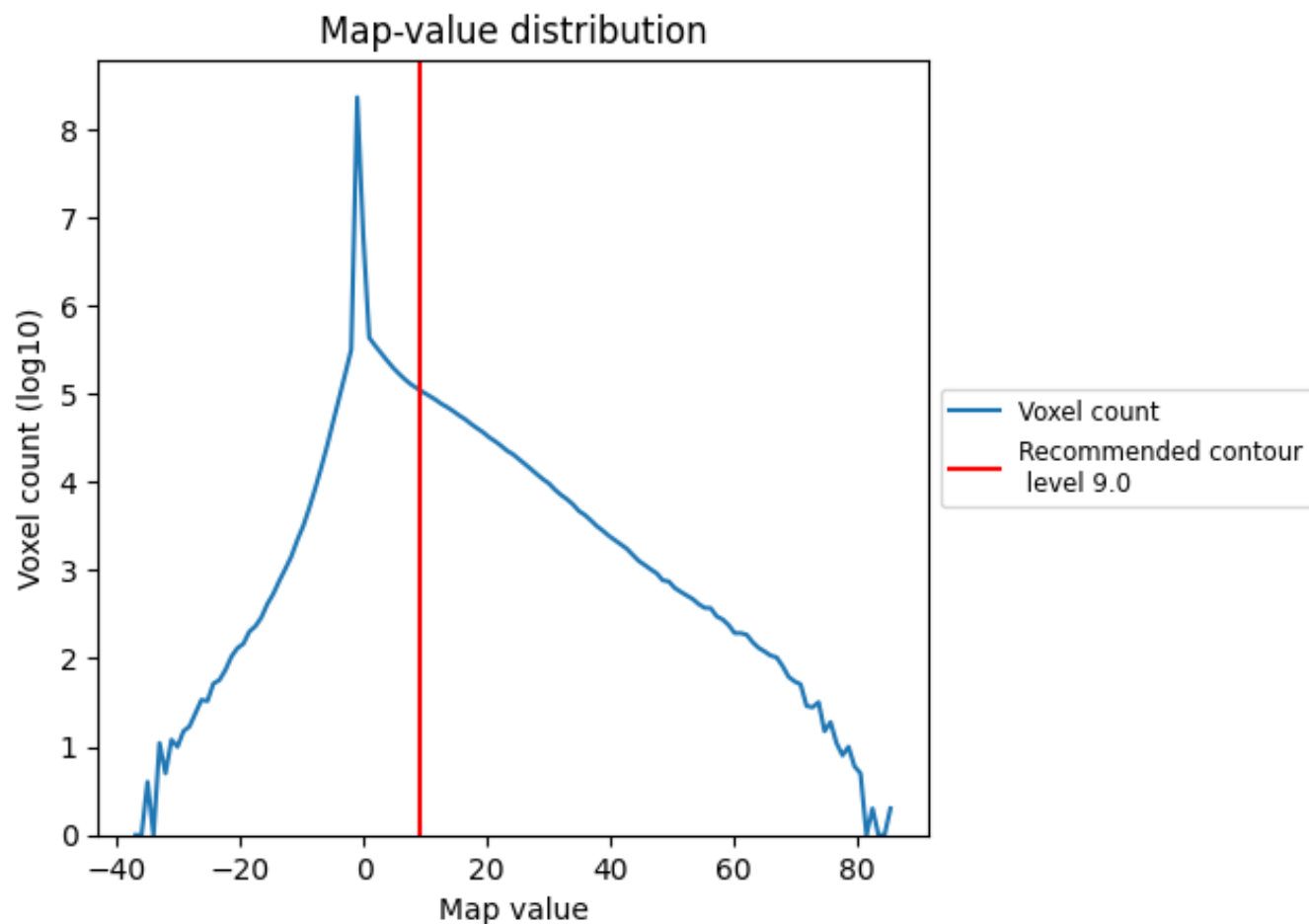
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

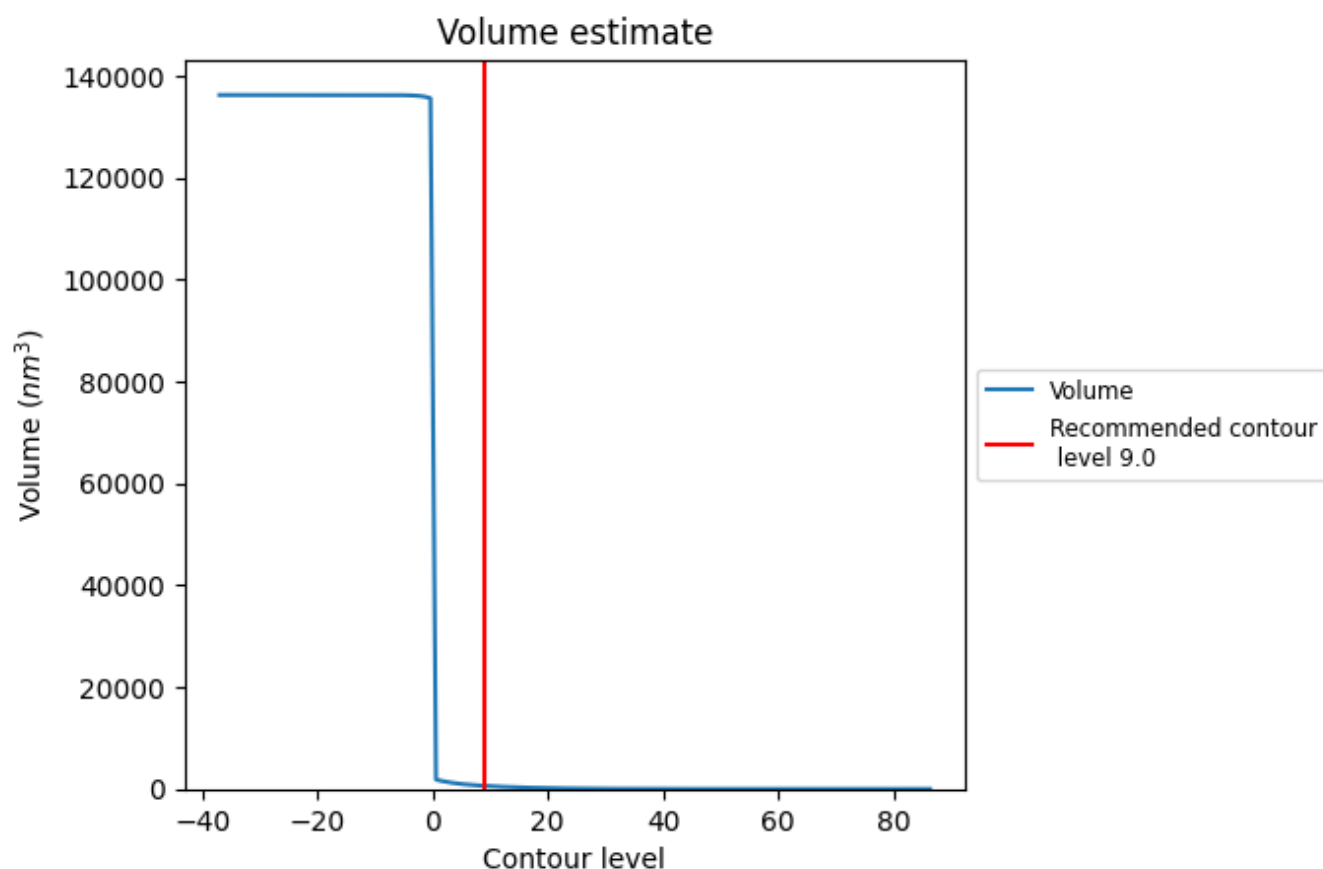
This section contains the results of statistical analysis of the map.

### 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.

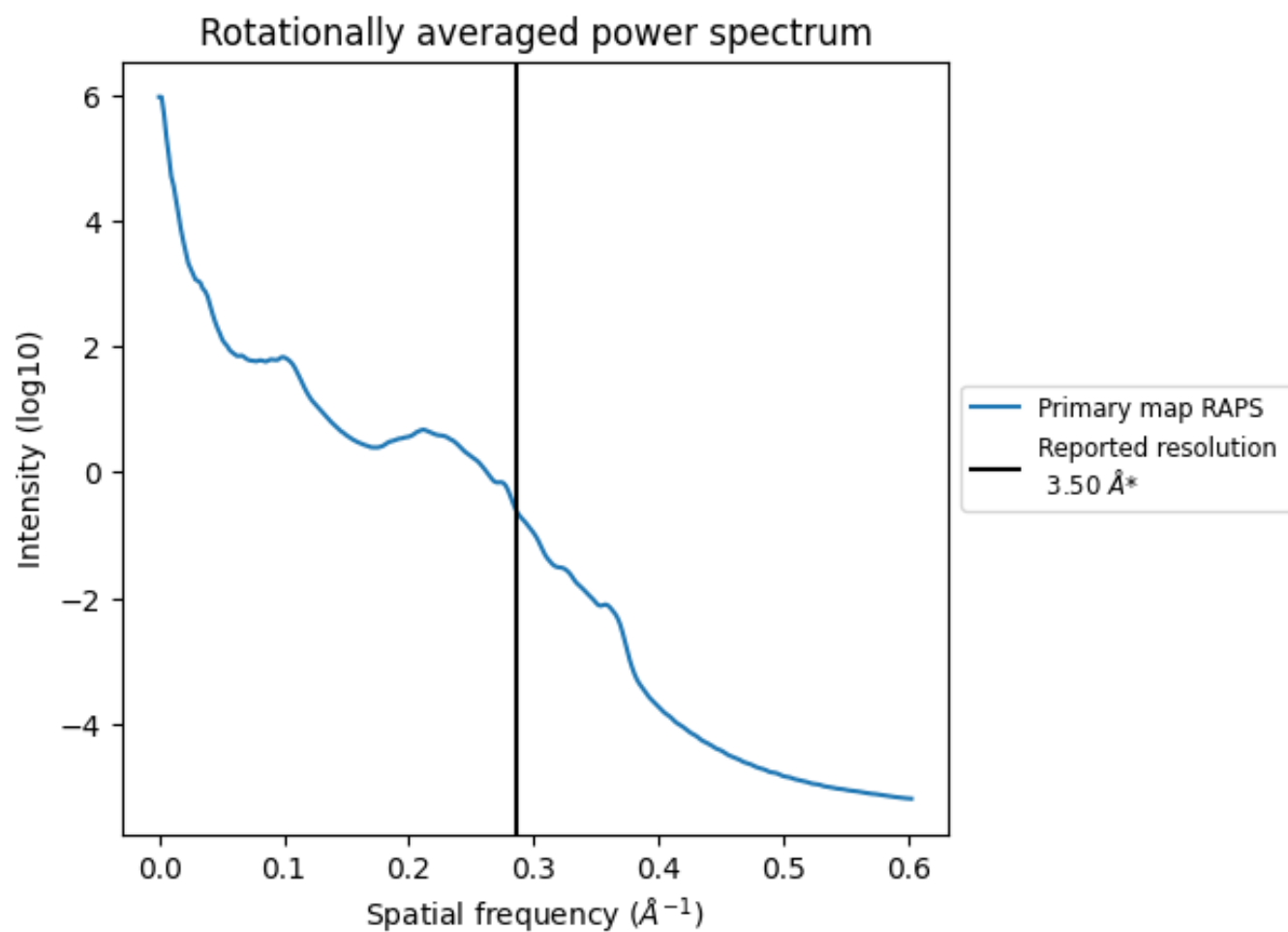
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 619  $\text{nm}^3$ ; this corresponds to an approximate mass of 559 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 0.286 Å<sup>-1</sup>

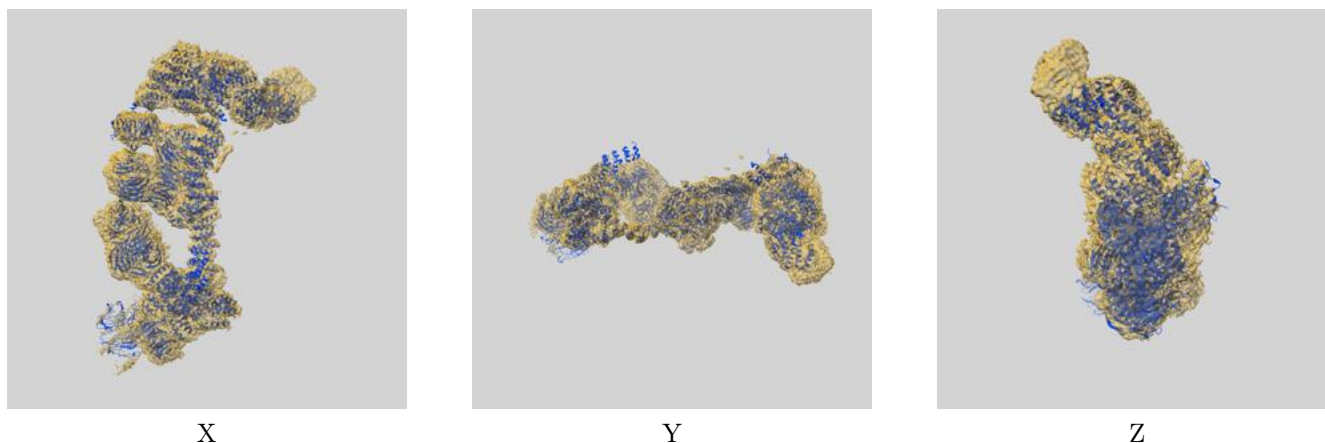
## 8 Fourier-Shell correlation ⓘ

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-28866 and PDB model 8F5O. Per-residue inclusion information can be found in section [3](#) on page [5](#).

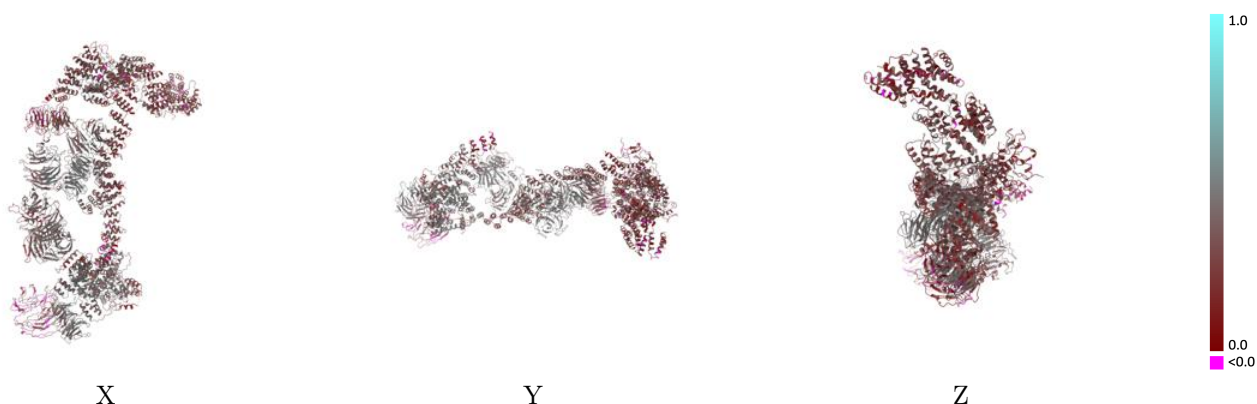
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 9.0 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.

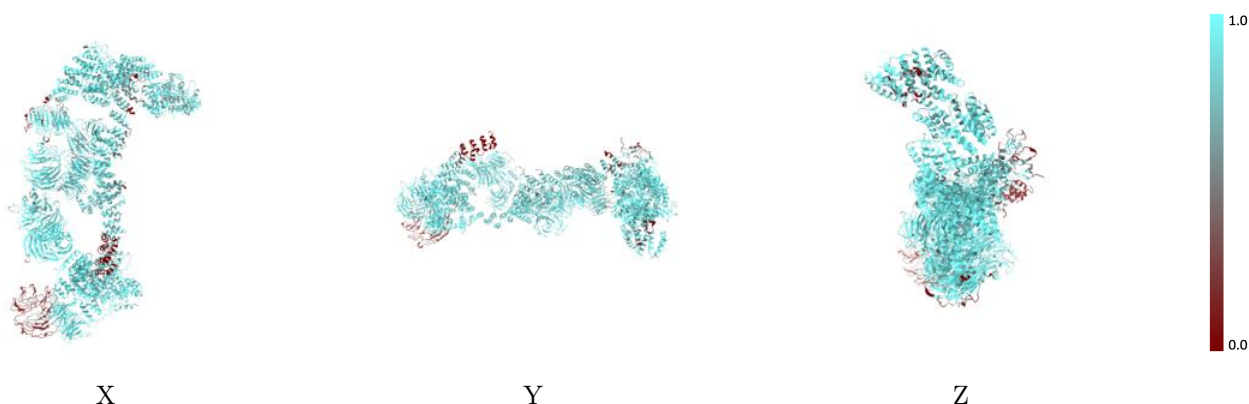


## 9.2 Q-score mapped to coordinate model [i](#)



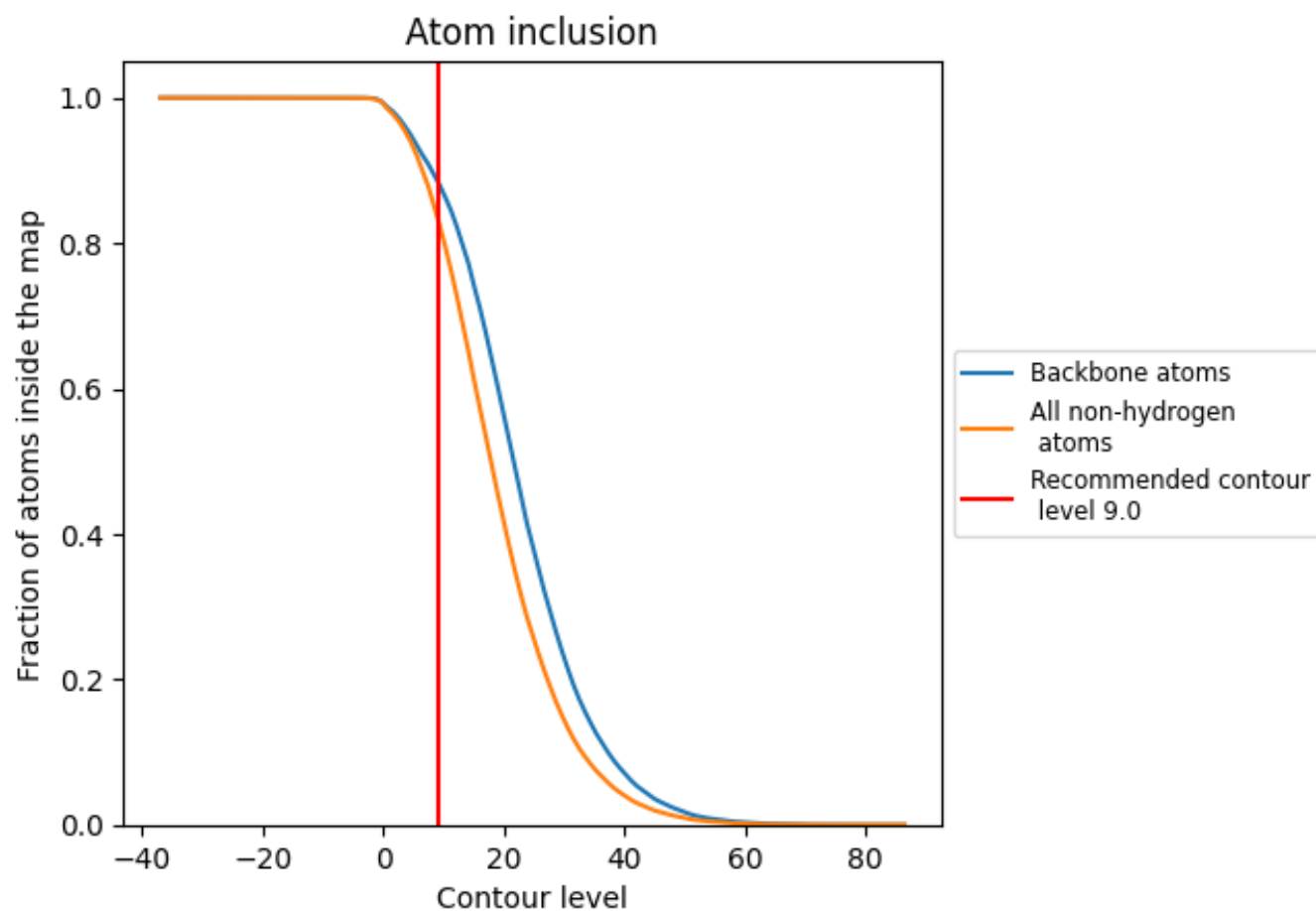
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9.0).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 83% 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 (9.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8342</div>	<div><div></div>0.3350</div>
A	<div><div></div>0.8158</div>	<div><div></div>0.2460</div>
B	<div><div></div>0.8775</div>	<div><div></div>0.3710</div>
C	<div><div></div>0.8765</div>	<div><div></div>0.3370</div>
D	<div><div></div>0.8970</div>	<div><div></div>0.2880</div>
E	<div><div></div>0.9351</div>	<div><div></div>0.3800</div>
F	<div><div></div>0.5228</div>	<div><div></div>0.2970</div>

1.0

0.0

<0.0