



wwPDB EM Validation Summary Report ⓘ

Dec 15, 2022 – 02:28 PM EST

PDB ID : 8F5P
EMDB ID : EMD-28867
Title : Structure of Leishmania tarentolae IFT-A (state 2)
Authors : Zhou, H.; Brown, A.
Deposited on : 2022-11-14
Resolution : 3.40 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

<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.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

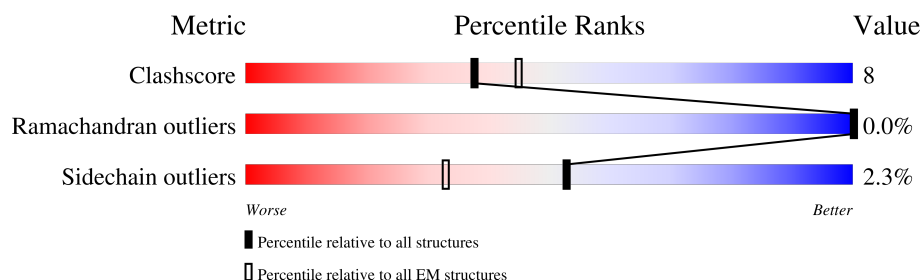
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	A	368	
2	B	1247	
3	C	1292	
4	D	1642	
5	E	1654	
6	F	1376	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39437 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 NET domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	75	Total	C	N	O	S	0	0
			585	361	97	120	7		

- Molecule 2 is a protein called Intraflagellar transport protein 122B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1128	Total	C	N	O	S	0	0
			8917	5645	1557	1652	63		

- Molecule 3 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1176	Total	C	N	O	S	0	0
			9337	5918	1619	1732	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	612	Total	C	N	O	S	0	0
			4826	3026	862	912	26		

- Molecule 5 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1057	Total	C	N	O	S	0	0
			8269	5228	1430	1561	50		

- Molecule 6 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	970	Total	C	N	O	S	0	0
			7499	4713	1315	1436	35		

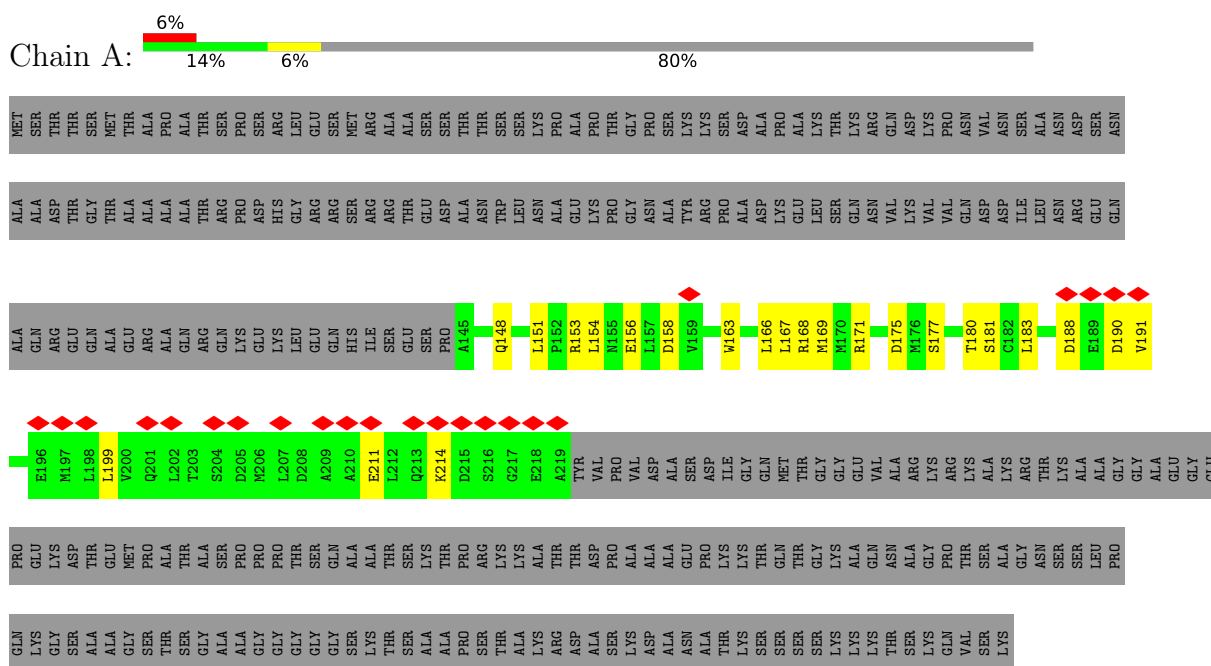
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

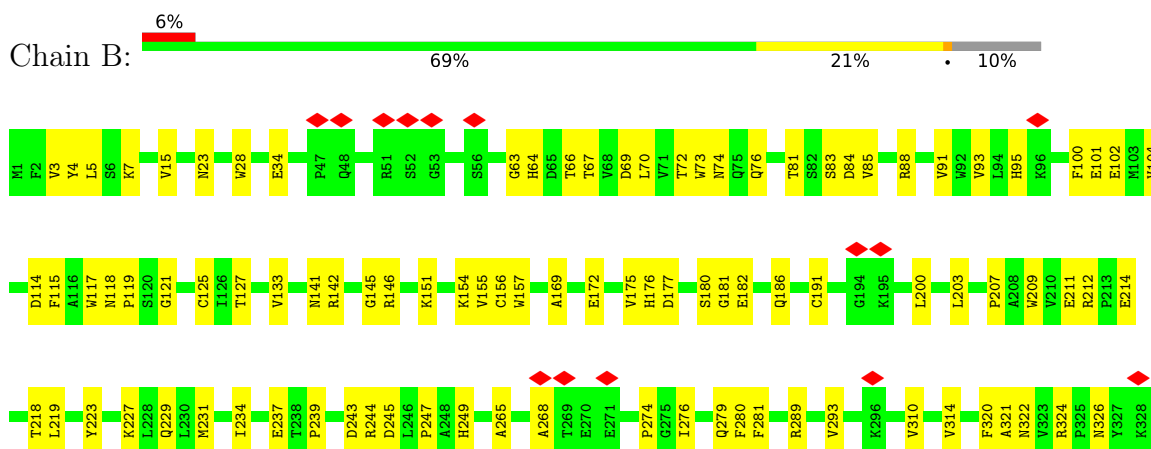
3 Residue-property plots

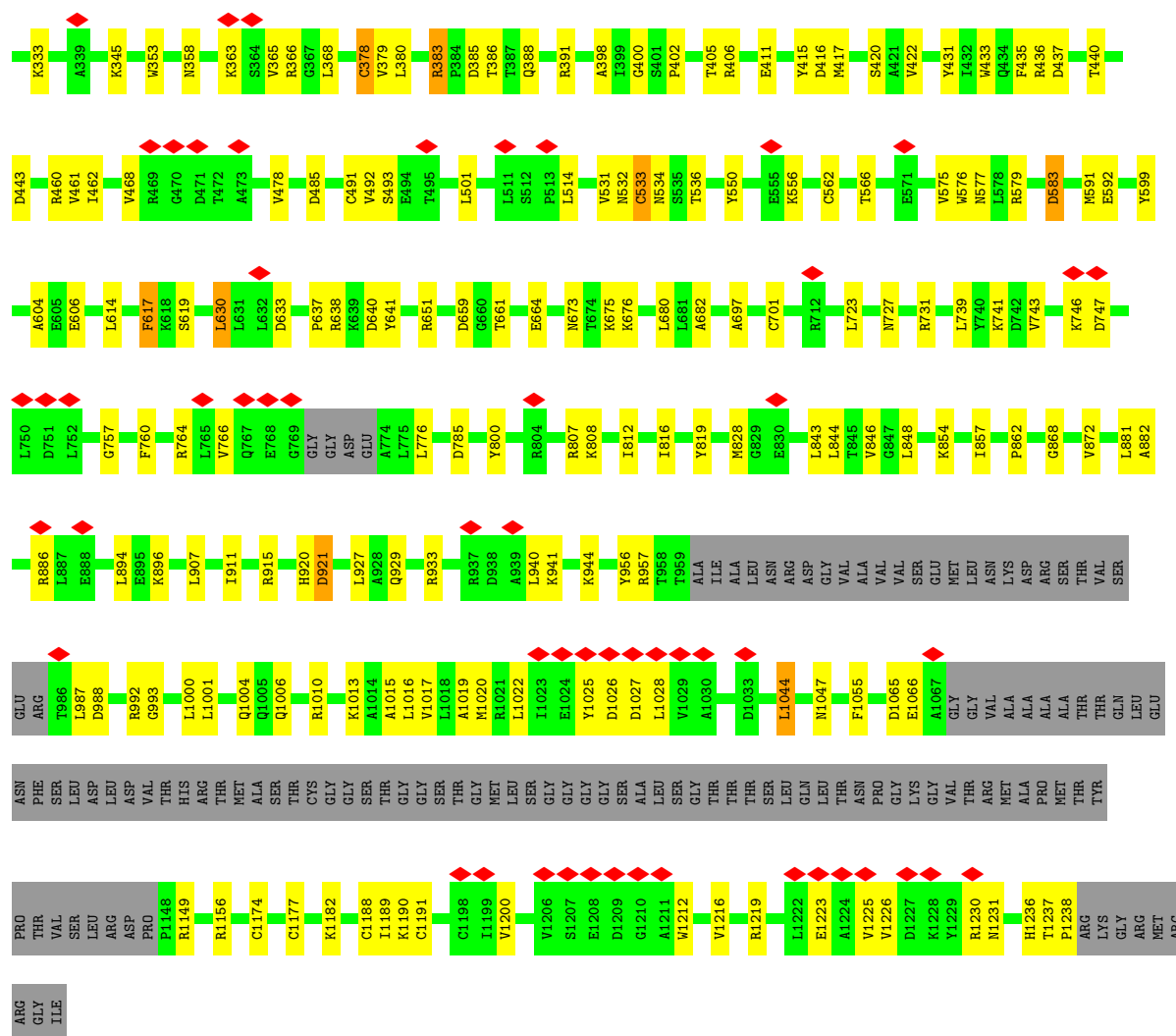
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

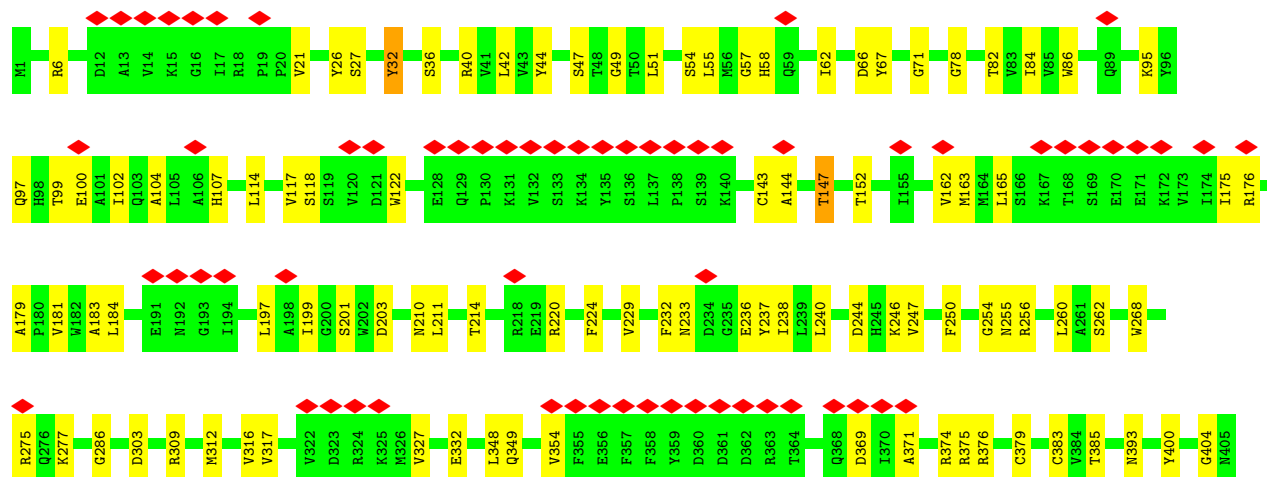


• Molecule 2: Intraflagellar transport protein 122B, putative



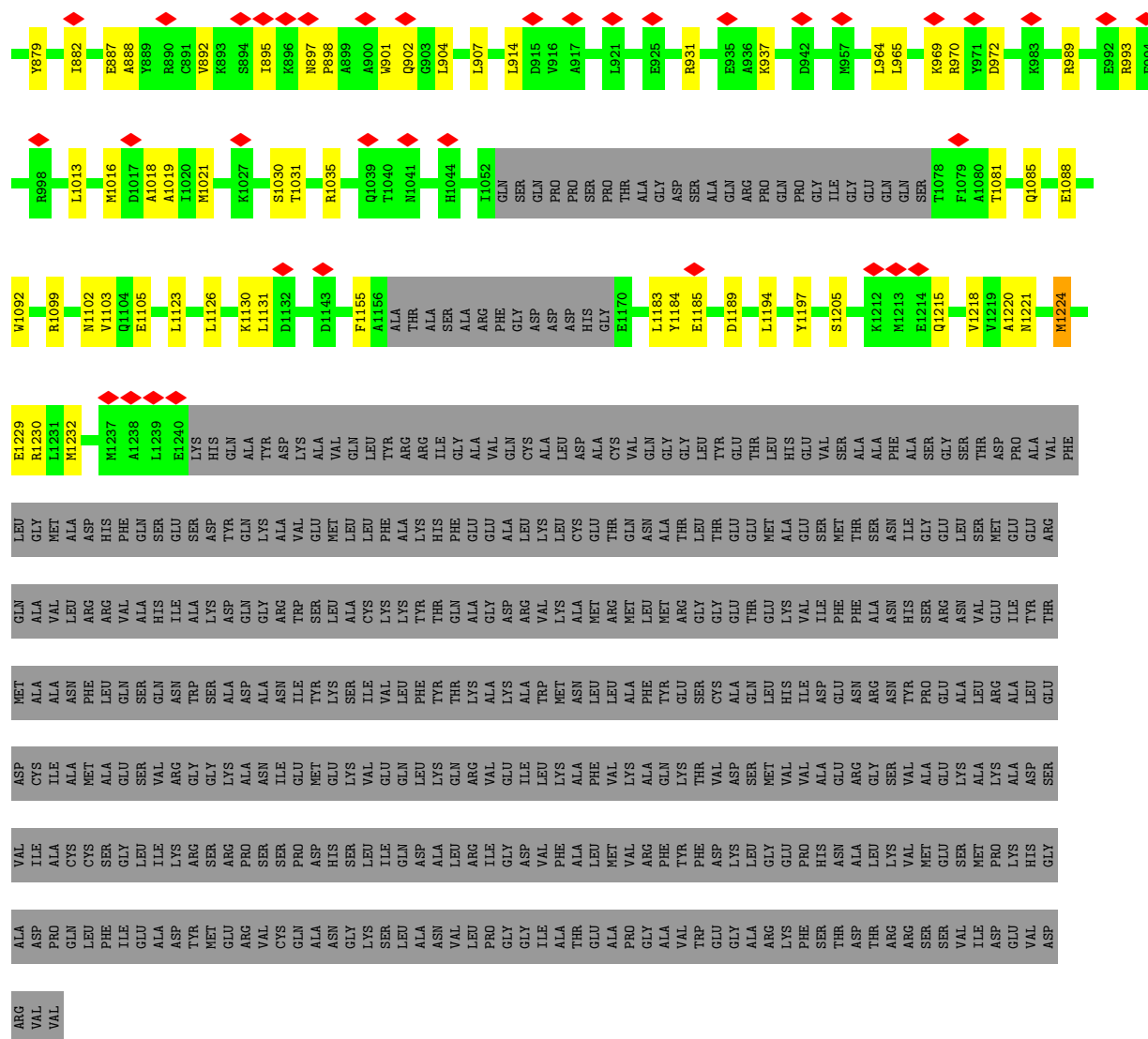


• Molecule 3: Intraflagellar transport protein 122 homolog

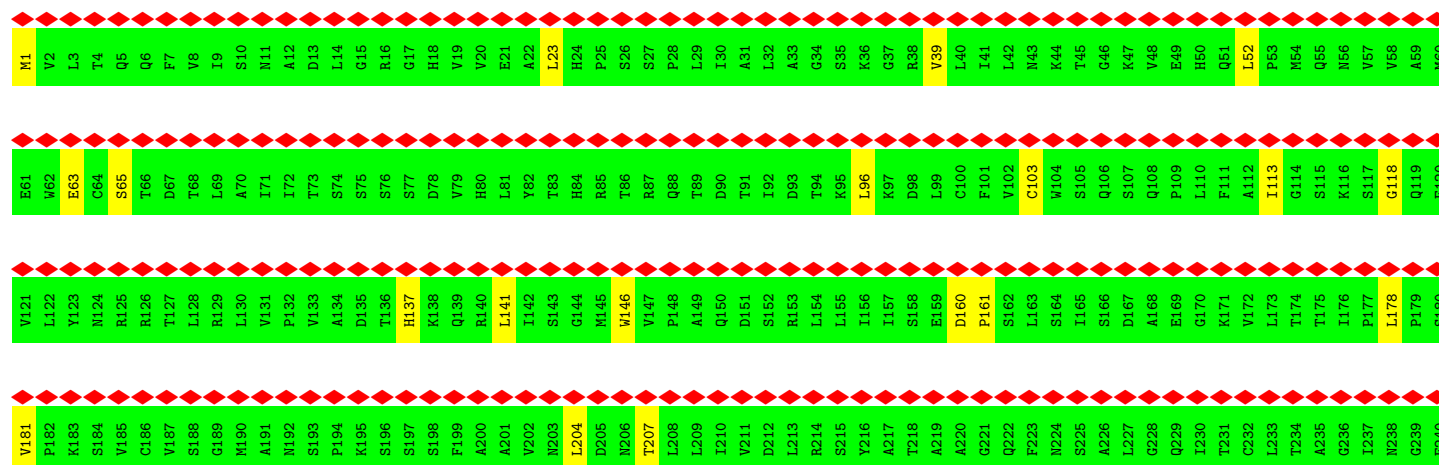








● Molecule 6: WD_REPEATS_REGION domain-containing protein



ALA	GLU	ASP	PRO	ALA	GLU	V939	H879	G812	V718	P625	H526	T441	I367	D301	F241
THR	PHE	LEU	LYS	GLY	PHE	E940	Q880	L813	L721	G626	L529	V442	G368	G302	L242
GLY	ASP	ARG	PRO	ALA	VAL	A941	K881	R814	E722	Y627	F533	E443	N371	I303	A243
LEU	LEU	ALA	SER	GLY	LEU	E942	H882	G819	K723	T631	A532	Y444	L372	A304	G244
ASP	LEU	LEU	TYR	MET	ALA	F943	E883	H820	I724	L632	A534	S446	Q373	P305	F245
CYS	LEU	LEU	ILE	TYR	LYS	A944	E884	H820	I727	L632	A534	S446	Q373	T306	A246
GLY	LEU	LEU	PHE	TYR	LYS	F945	A885	H820	I727	L632	A534	S446	Q373	G307	S247
ALA	LEU	LEU	LEU	LEU	LEU	F946	A886	H820	I727	L632	A534	S446	Q373	D308	G248
CYS	LEU	LEU	LEU	LEU	LEU	A947	Q887	H820	I727	L632	A534	S446	Q373	E309	T249
ASN	LEU	LEU	LEU	LEU	LEU	Q948	Q887	H820	I727	L632	A534	S446	Q373	A310	V250
THR	LEU	LEU	LEU	LEU	LEU	A948	Q887	H820	I727	L632	A534	S446	Q373	S311	A251
ILE	LEU	LEU	LEU	LEU	LEU	E949	Y889	H820	I727	L632	A534	S446	Q373	L312	L252
PRO	GLN	VAL	GLY	ALA	GLY	D950	E890	H820	I727	L632	A534	S446	Q373	E313	L253
PHE	ASN	VAL	GLY	LYS	LYS	W951	K891	H820	I727	L632	A534	S446	Q373	D254	L255
CYS	GLU	ASP	TYR	ALA	ALA	D952	K892	H820	I727	L632	A534	S446	Q373	S314	L256
ILE	LEU	LEU	GLY	LEU	LEU	W953	G893	H820	I727	L632	A534	S446	Q373	E315	L257
VAL	HIS	LEU	LYS	ASN	ASN	A954	G893	H820	I727	L632	A534	S446	Q373	R316	A256
THR	ARG	LYS	ALA	LYS	ASP	D955	G893	H820	I727	L632	A534	S446	Q373	G317	G257
GLY	ILE	LYS	ALA	LYS	ASP	W955	I895	H820	I727	L632	A534	S446	Q373	V318	S258
HIS	LYS	LEU	THR	LEU	PHE	R956	E896	H820	I727	L632	A534	S446	Q373	P319	E259
LYS	THR	ASP	VAL	GLY	PHE	L957	R897	H820	I727	L632	A534	S446	Q373	D320	V260
VAL	ILE	ASP	ILE	GLN	PHE	R958	A898	H820	I727	L632	A534	S446	Q373	L321	R261
LYS	LYS	ASP	ILE	GLN	PHE	I959	A899	H820	I727	L632	A534	S446	Q373	L322	L262
SER	SER	THR	ILE	PRO	SER	E960	T900	H820	I727	L632	A534	S446	Q373	A323	R263
ARG	ARG	THR	ILE	GLU	ALA	F961	K901	H820	I727	L632	A534	S446	Q373	W324	G264
LYS	LYS	CYS	ALA	ASP	ALA	L962	Y902	H820	I727	L632	A534	S446	Q373	S325	S265
THR	ILE	MET	GLY	GLU	GLU	N963	E904	H820	I727	L632	A534	S446	Q373	R326	L266
GLU	GLY	LEU	GLY	LYS	LYS	D964	E904	H820	I727	L632	A534	S446	Q373	D327	R267
GLY	ILE	ARG	ILE	VAL	VAL	L965	R905	H820	I727	L632	A534	S446	Q373	G328	L268
CYS	VAL	SER	ILE	GLU	GLU	W966	E905	H820	I727	L632	A534	S446	Q373	Q329	L269
VAL	VAL	ARG	ILE	VAL	VAL	R967	K907	H820	I727	L632	A534	S446	Q373	L331	N271
PHE	VAL	ARG	TYR	VAL	ASP	A968	E908	H820	I727	L632	A534	S446	Q373	F332	A272
PRO	GLY	ASN	LYS	GLY	GLY	G967	R908	H820	I727	L632	A534	S446	Q373	V333	V273
ALA	ILE	ASN	ALA	ILE	ILE	I969	L909	H820	I727	L632	A534	S446	Q373	G334	E274
LYS	LYS	GLN	ALA	LYS	LYS	W970	K910	H820	I727	L632	A534	S446	Q373	T335	M275
THR	ASP	PHE	LYS	HIS	PRO	V971	E911	H820	I727	L632	A534	S446	Q373	N336	V276
ALA	ASP	THR	LYS	SER	LEU	V972	A912	H820	I727	L632	A534	S446	Q373	Q337	N277
ALA	VAL	PRO	THR	ASP	SER	V973	E913	H820	I727	L632	A534	S446	Q373	ASP	F278
MET	ASP	HIS	VAL	SER	ASN	Q974	E914	H820	I727	L632	A534	S446	Q373	PRO	G279
THR	THR	THR	ALA	LEU	GLN	T975	R915	H820	I727	L632	A534	S446	Q373	V340	E280
GLY	GLY	VAL	THR	THR	ASP	R976	A856	H820	I727	L632	A534	S446	Q373	T341	G281
THR	THR	VAL	ARG	PHE	THR	S977	K857	H820	I727	L632	A534	S446	Q373	V342	S282
LEU	LEU	THR	ILE	ILE	THR	A978	E858	H820	I727	L632	A534	S446	Q373	F343	G283
PRO	PRO	THR	GLN	ASP	ILE	F917	T859	H820	I727	L632	A534	S446	Q373	T344	V284
CYS	THR	THR	GLN	GLY	GLY	R918	K861	H820	I727	L632	A534	S446	Q373	L345	V285
TYR	TYR	VAL	GLY	GLY	GLY	K920	E862	H820	I727	L632	A534	S446	Q373	K346	A286
MET	MET	VAL	GLY	GLY	GLY	S921	S863	H820	I727	L632	A534	S446	Q373	V347	A287
ASP	ASP	GLN	ASN	THR	THR	R922	S864	H820	I727	L632	A534	S446	Q373	L348	V288
GLY	GLY	CYS	ASN	THR	THR	E923	E865	H820	I727	L632	A534	S446	Q373	N349	A289
ALA	ALA	LEU	VAL	ASP	GLY	T924	R866	H820	I727	L632	A534	S446	Q373	V350	D290
VAL	VAL	SER	ASN	GLY	LYS	W984	E867	H820	I727	L632	A534	S446	Q373	A352	N291
						A985	K867	H820	I727	L632	A534	S446	Q373	S360	R292
						K986	E868	H820	I727	L632	A534	S446	Q373	F361	V293
						K987	Y869	H820	I727	L632	A534	S446	Q373	G294	L295
						C988	E870	H820	I727	L632	A534	S446	Q373	T362	L296
						T989	K871	H820	I727	L632	A534	S446	Q373	I298	R297
						A990	C872	H820	I727	L632	A534	S446	Q373	T299	E300
						Q991	K873	H820	I727	L632	A534	S446	Q373	S360	
						LYS	L875	H820	I727	L632	A534	S446	Q373	F361	
						GLU	E877	H820	I727	L632	A534	S446	Q373	G294	
						THR	E878	H820	I727	L632	A534	S446	Q373	T362	
						ALA	E878	H820	I727	L632	A534	S446	Q373	S363	
						VAL	E878	H820	I727	L632	A534	S446	Q373	N364	
								H820	I727	L632	A534	S446	Q373	R365	
								H820	I727	L632	A534	S446	Q373	T366	

ILE
ASP
ILE
SER
ASN
VAL
ASN
ARG
GLU
THR
ASN
PRO
GLU
LEU
LYS
ALA
LEU
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	563466	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	74.154	Depositor
Minimum map value	-32.225	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.778	Depositor
Recommended contour level	7.0	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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.25	0/592	0.47	0/800
2	B	0.28	0/9108	0.50	0/12341
3	C	0.26	0/9531	0.50	0/12900
4	D	0.26	0/4905	0.51	0/6650
5	E	0.25	0/8429	0.50	0/11438
6	F	0.24	0/7633	0.49	0/10368
All	All	0.26	0/40198	0.50	0/54497

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	A	585	0	565	22	0
2	B	8917	0	8815	162	0
3	C	9337	0	9275	168	0
4	D	4826	0	4799	105	0
5	E	8269	0	8212	125	0
6	F	7499	0	7503	91	0
7	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	2	0	0	0	0
All	All	39437	0	39169	636	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 8.

The worst 5 of 636 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:E:539:GLY:HA3	5:E:551:GLU:O	1.71	0.91
3:C:1061:CYS:HB3	3:C:1064:CYS:SG	2.19	0.82
3:C:62:ILE:HA	3:C:78:GLY:HA2	1.66	0.76
5:E:656:LEU:HB2	5:E:671:TRP:HB2	1.68	0.76
2:B:1174:CYS:HB3	2:B:1177:CYS:SG	2.26	0.75

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	A	73/368 (20%)	69 (94%)	4 (6%)	0	100	100
2	B	1120/1247 (90%)	1070 (96%)	50 (4%)	0	100	100
3	C	1170/1292 (91%)	1133 (97%)	37 (3%)	0	100	100
4	D	596/1642 (36%)	567 (95%)	27 (4%)	2 (0%)	41	72
5	E	1039/1654 (63%)	1001 (96%)	38 (4%)	0	100	100
6	F	966/1376 (70%)	946 (98%)	20 (2%)	0	100	100
All	All	4964/7579 (66%)	4786 (96%)	176 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1058	VAL
4	D	1057	VAL

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	A	64/288 (22%)	64 (100%)	0	100	100
2	B	956/1046 (91%)	927 (97%)	29 (3%)	41	68
3	C	1012/1094 (92%)	987 (98%)	25 (2%)	47	72
4	D	505/1320 (38%)	487 (96%)	18 (4%)	35	63
5	E	892/1373 (65%)	879 (98%)	13 (2%)	65	82
6	F	822/1177 (70%)	809 (98%)	13 (2%)	62	81
All	All	4251/6298 (68%)	4153 (98%)	98 (2%)	53	74

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	1031	ARG
4	D	1624	THR
4	D	1118	GLU
4	D	1404	LEU
5	E	325	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	417	GLN
4	D	1221	ASN
4	D	1223	ASN
4	D	1622	HIS

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.

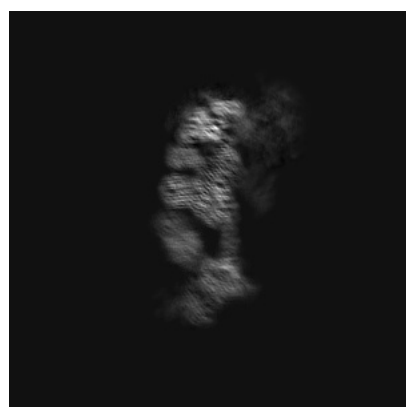
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28867. These allow visual inspection of the internal detail of the map and identification of artifacts.

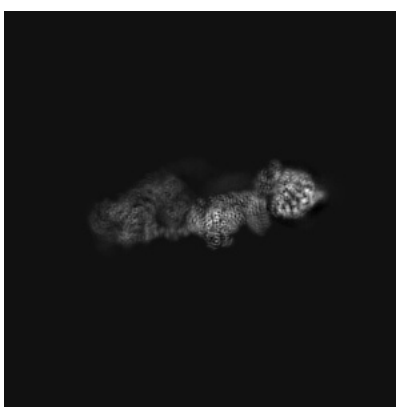
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

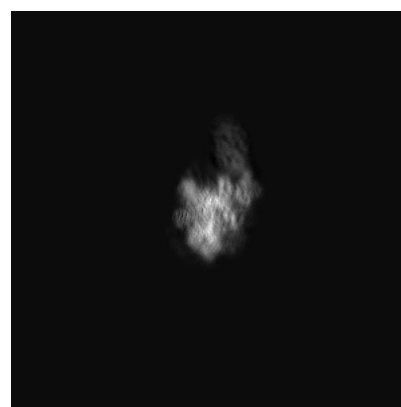
6.1.1 Primary map



X



Y

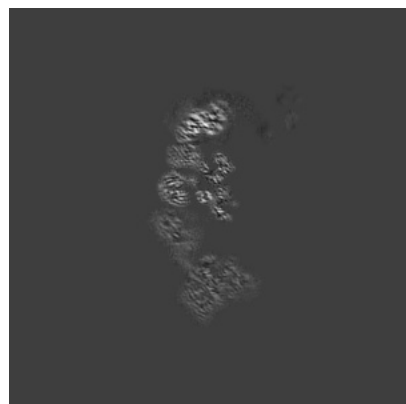


Z

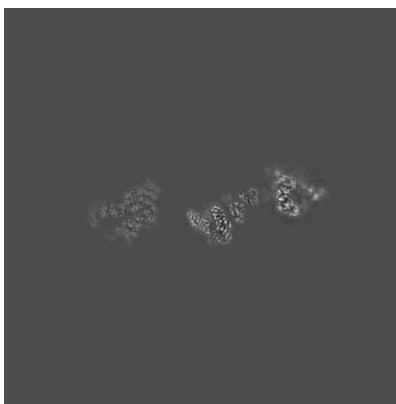
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

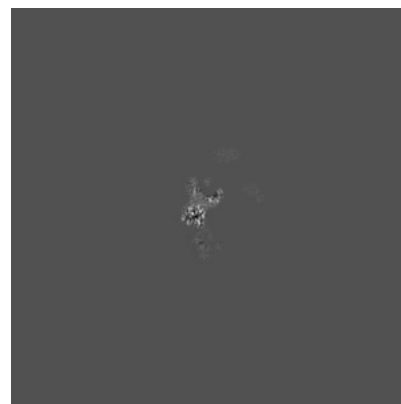
6.2.1 Primary map



X Index: 310



Y Index: 310

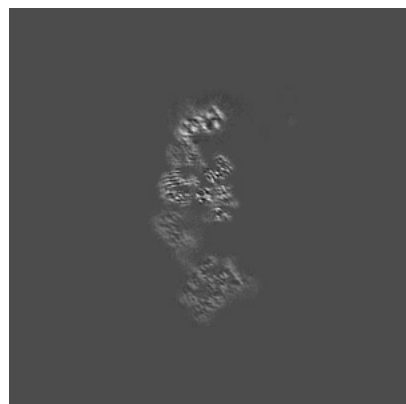


Z Index: 310

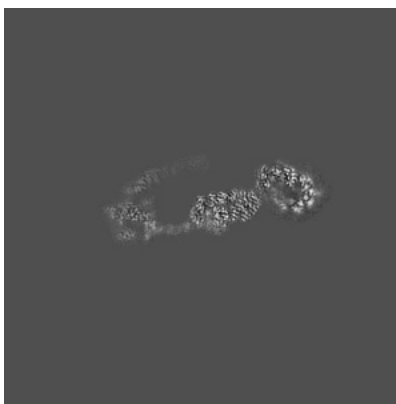
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 306



Y Index: 328



Z Index: 330

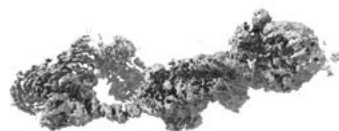
The images above show the largest variance slices of the map in three orthogonal directions.

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

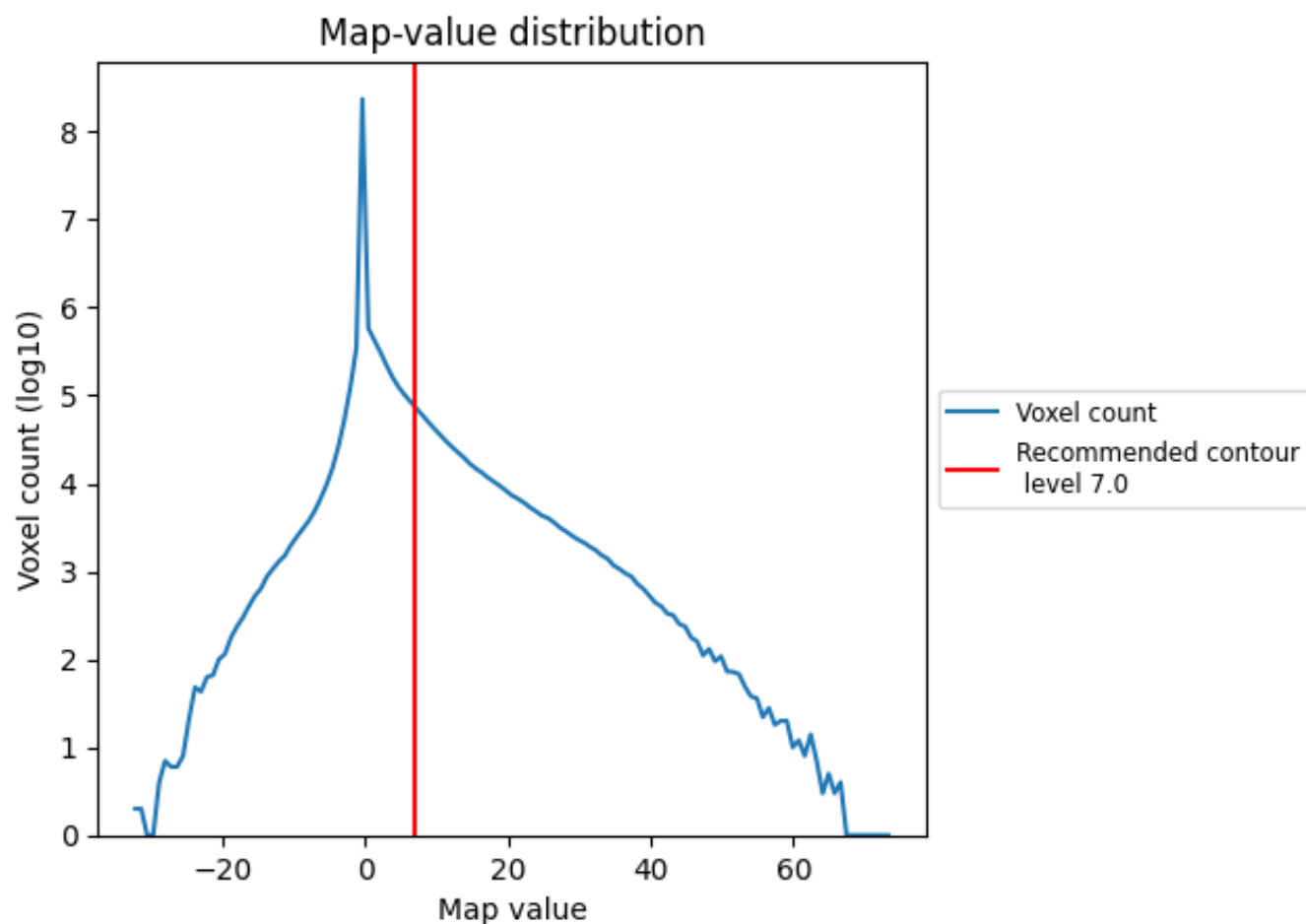
6.5 Mask visualisation

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

7 Map analysis [i](#)

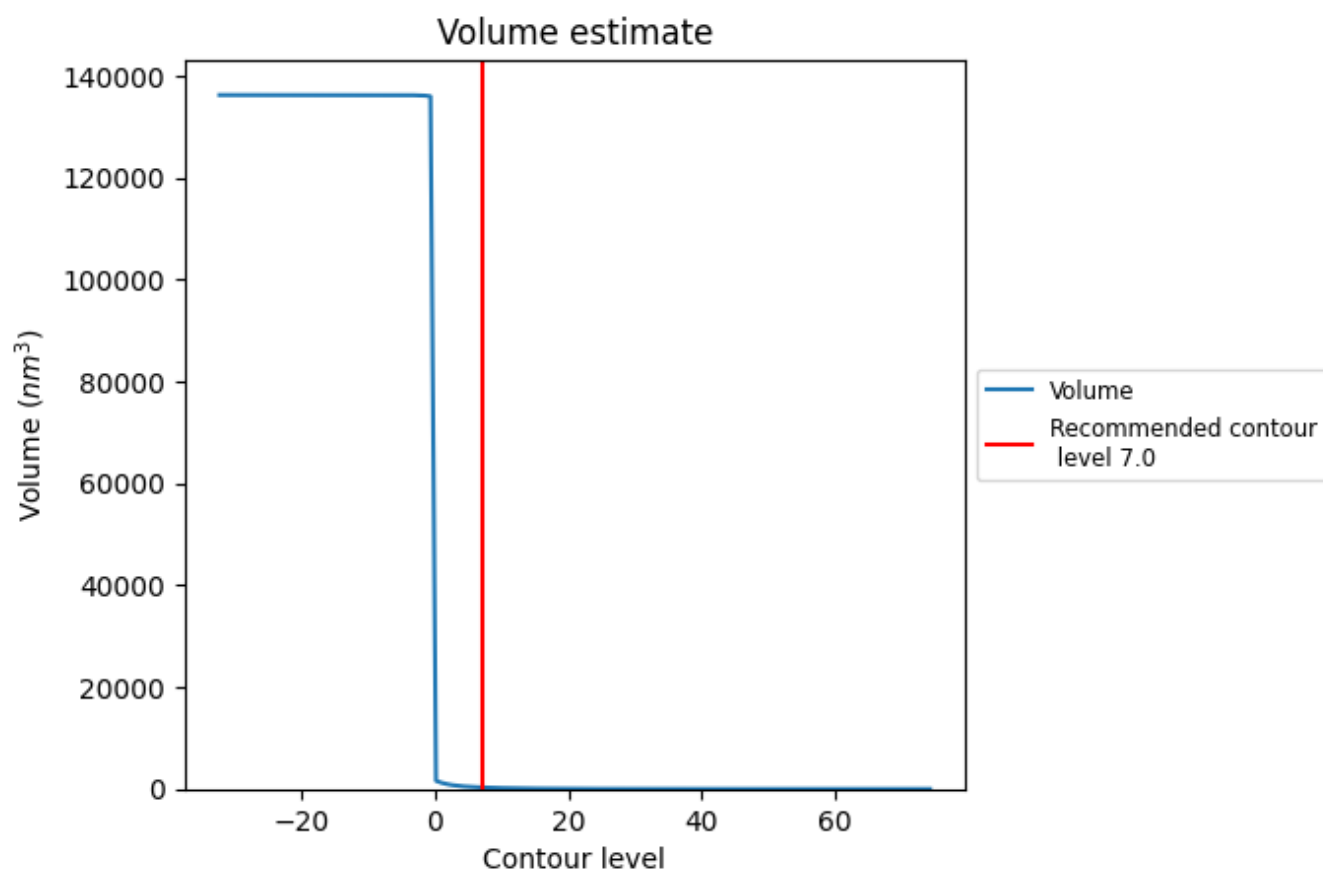
This section contains the results of statistical analysis of the map.

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.

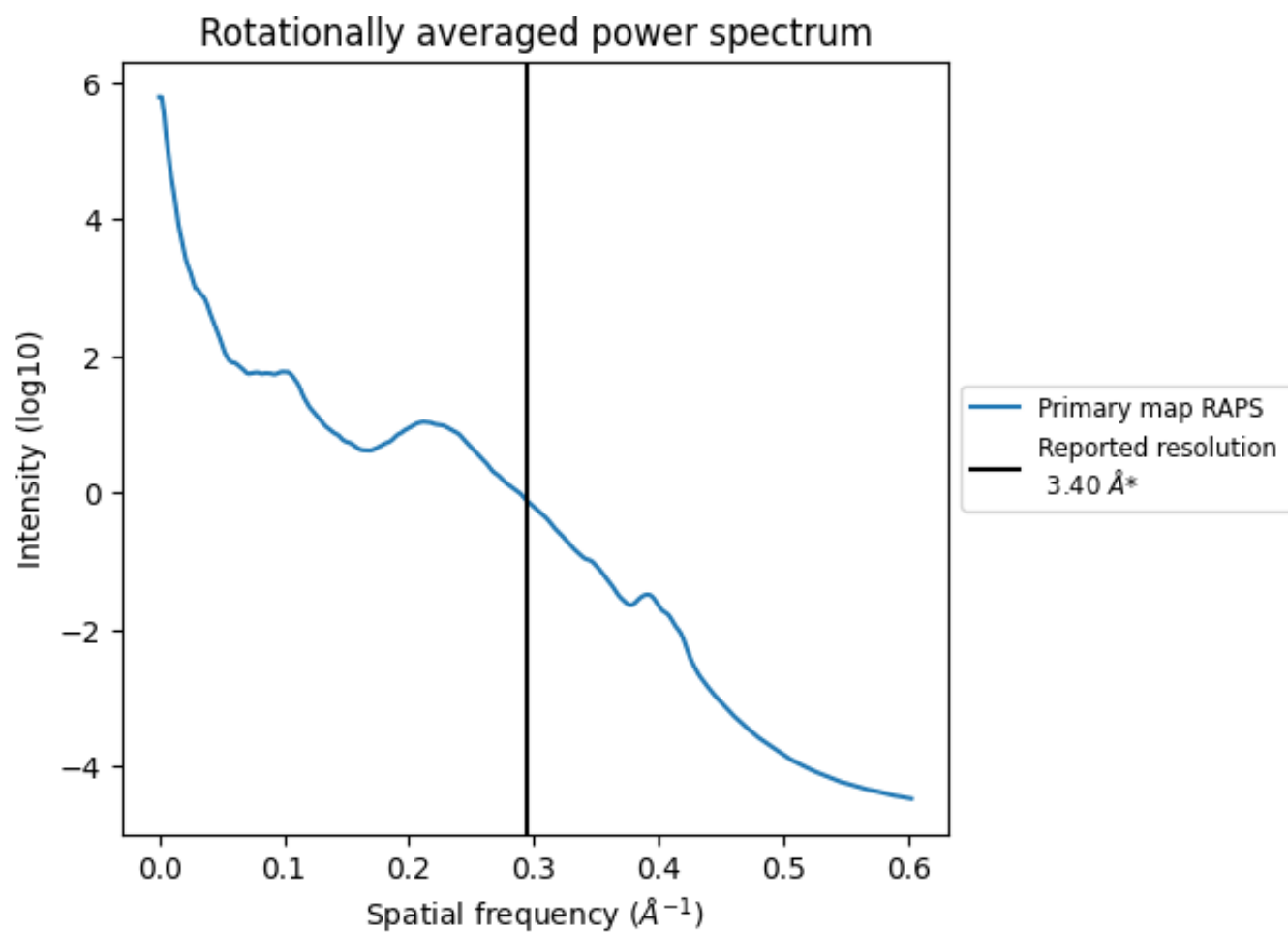
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 303 nm^3 ; this corresponds to an approximate mass of 273 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 0.294 Å⁻¹

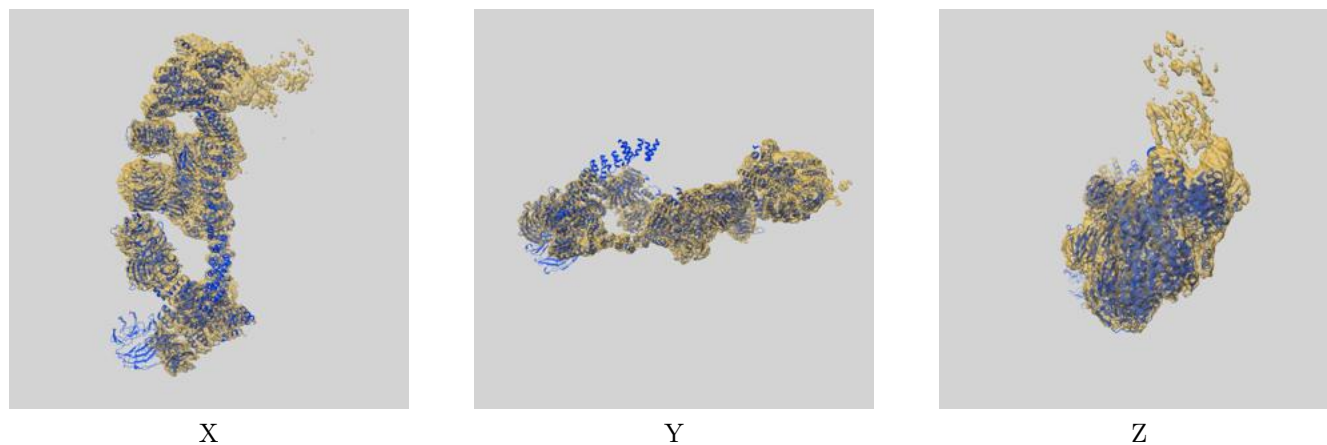
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

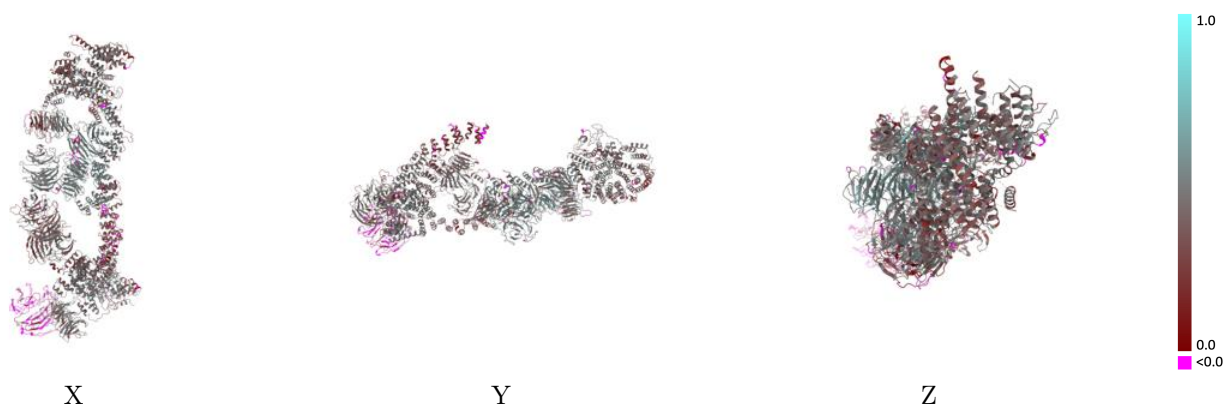
This section contains information regarding the fit between EMDB map EMD-28867 and PDB model 8F5P. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



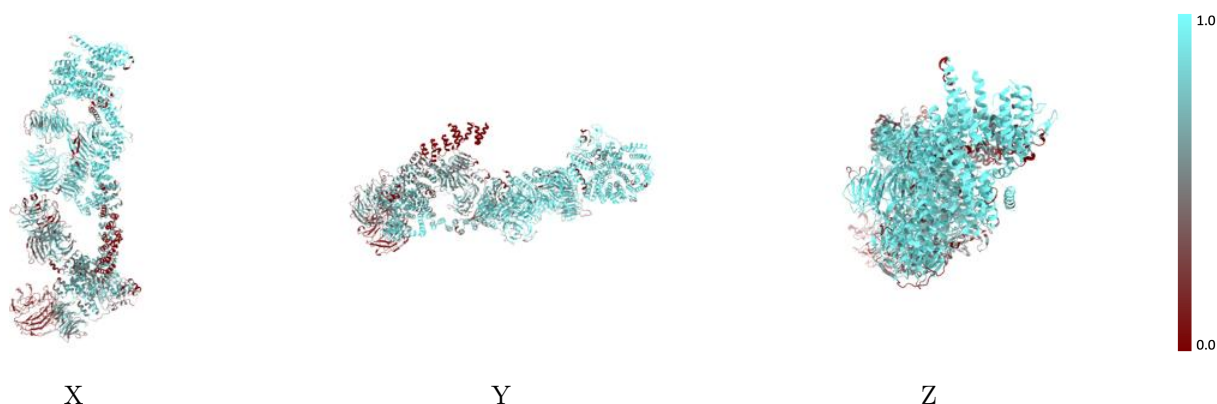
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



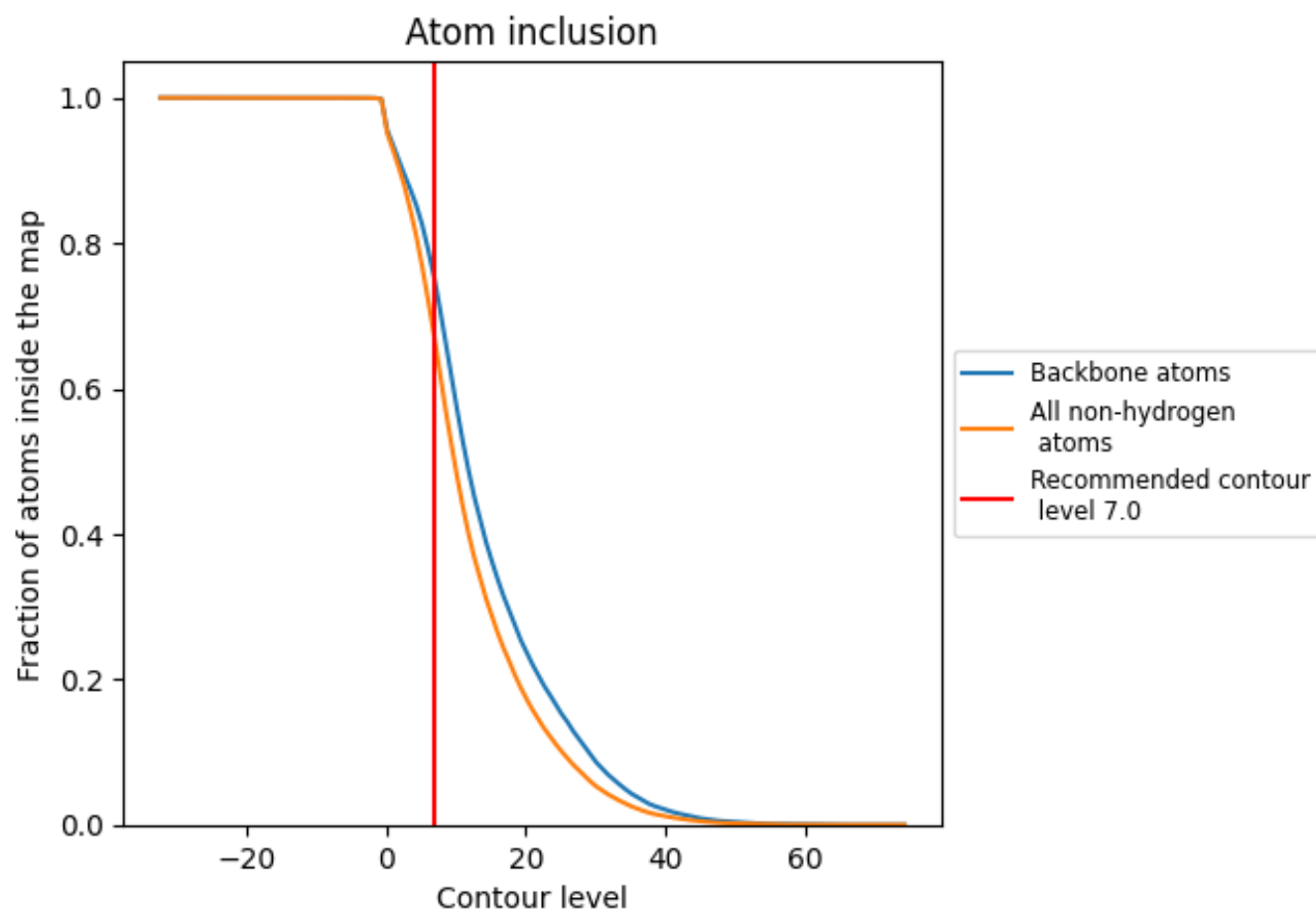
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6664	<div></div> 0.3860
A	<div></div> 0.6463	<div></div> 0.3640
B	<div></div> 0.8720	<div></div> 0.4660
C	<div></div> 0.7463	<div></div> 0.4180
D	<div></div> 0.9017	<div></div> 0.3900
E	<div></div> 0.5746	<div></div> 0.3960
F	<div></div> 0.2758	<div></div> 0.2390

1.0

0.0

<0.0