



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 04:58 PM UTC

PDB ID : 6YRF / pdb_00006yrf
EMDB ID : EMD-10888
Title : Vip3Bc1 tetramer
Authors : Thompson, R.F.; Byrne, M.J.; Iadanza, M.I.; Arribas Perez, M.; Maskell, D.P.;
George, R.M.; Hesketh, E.L.; Beales, P.A.; Zack, M.D.; Berry, C.
Deposited on : 2020-04-20
Resolution : 3.90 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

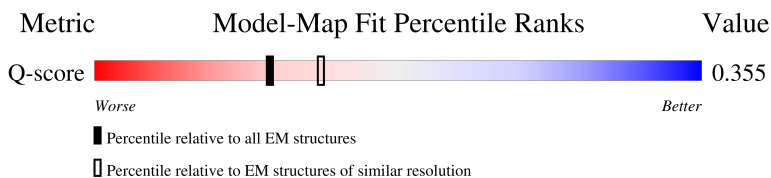
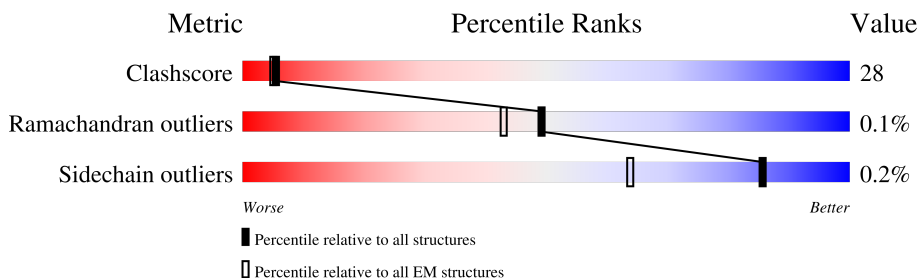
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	803	 44% 52%
1	B	803	 46% 50%
1	C	803	 44% 52%
1	D	803	 47% 49%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24828 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.

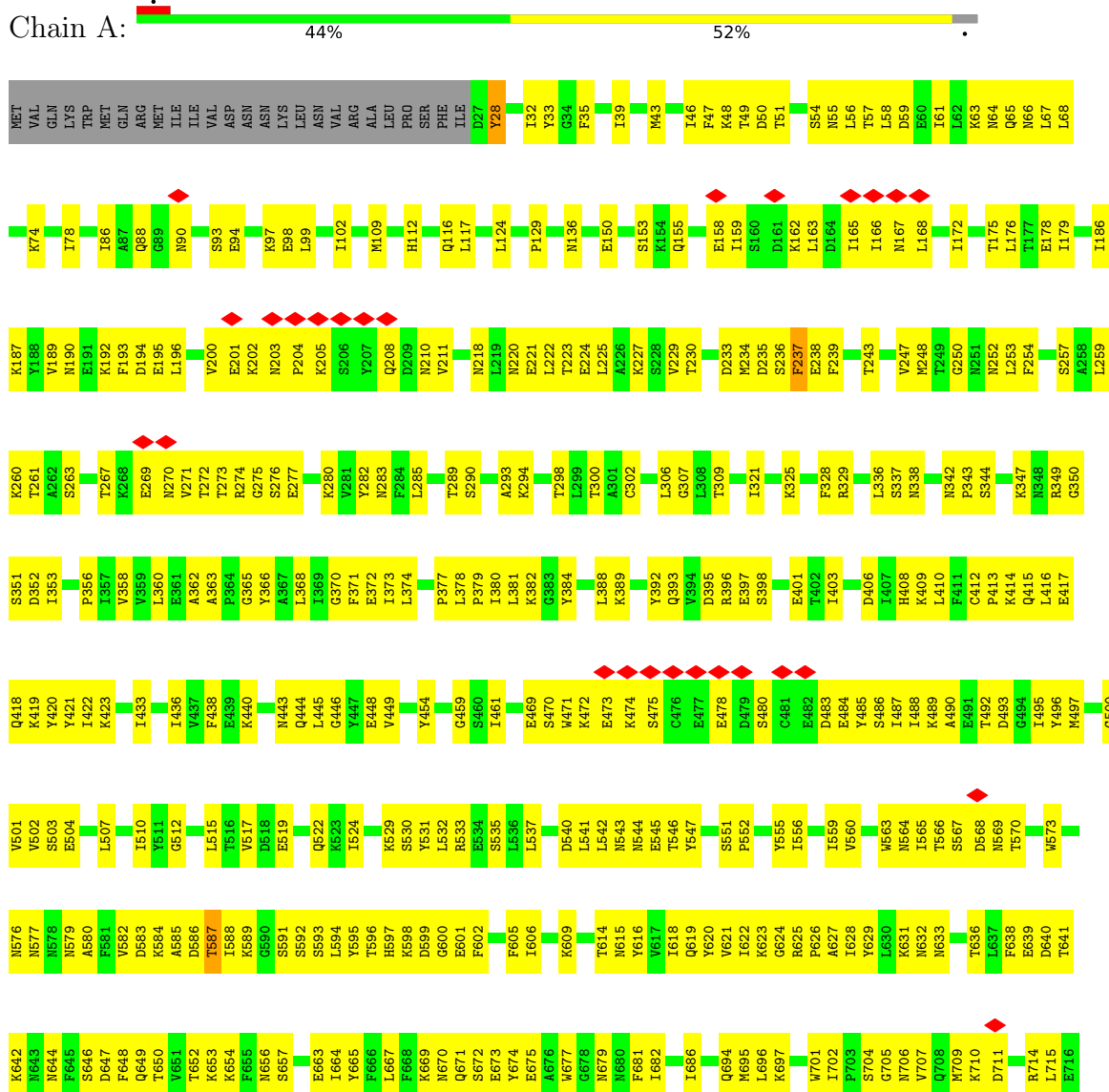
- Molecule 1 is a protein called Vegetative insecticidal protein.

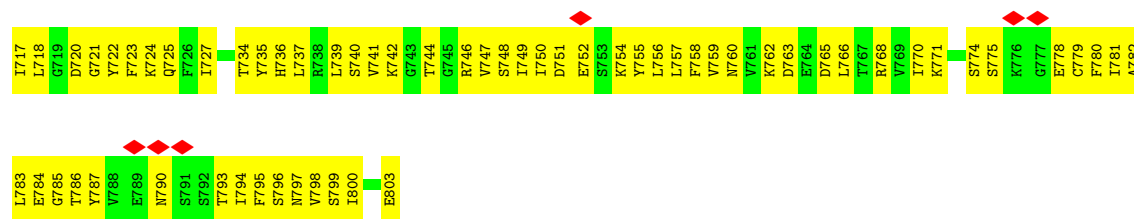
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	777	Total	C	N	O	S	0	0
			6207	3950	1009	1231	17		
1	B	777	Total	C	N	O	S	0	0
			6207	3950	1009	1231	17		
1	C	777	Total	C	N	O	S	0	0
			6207	3950	1009	1231	17		
1	D	777	Total	C	N	O	S	0	0
			6207	3950	1009	1231	17		

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.

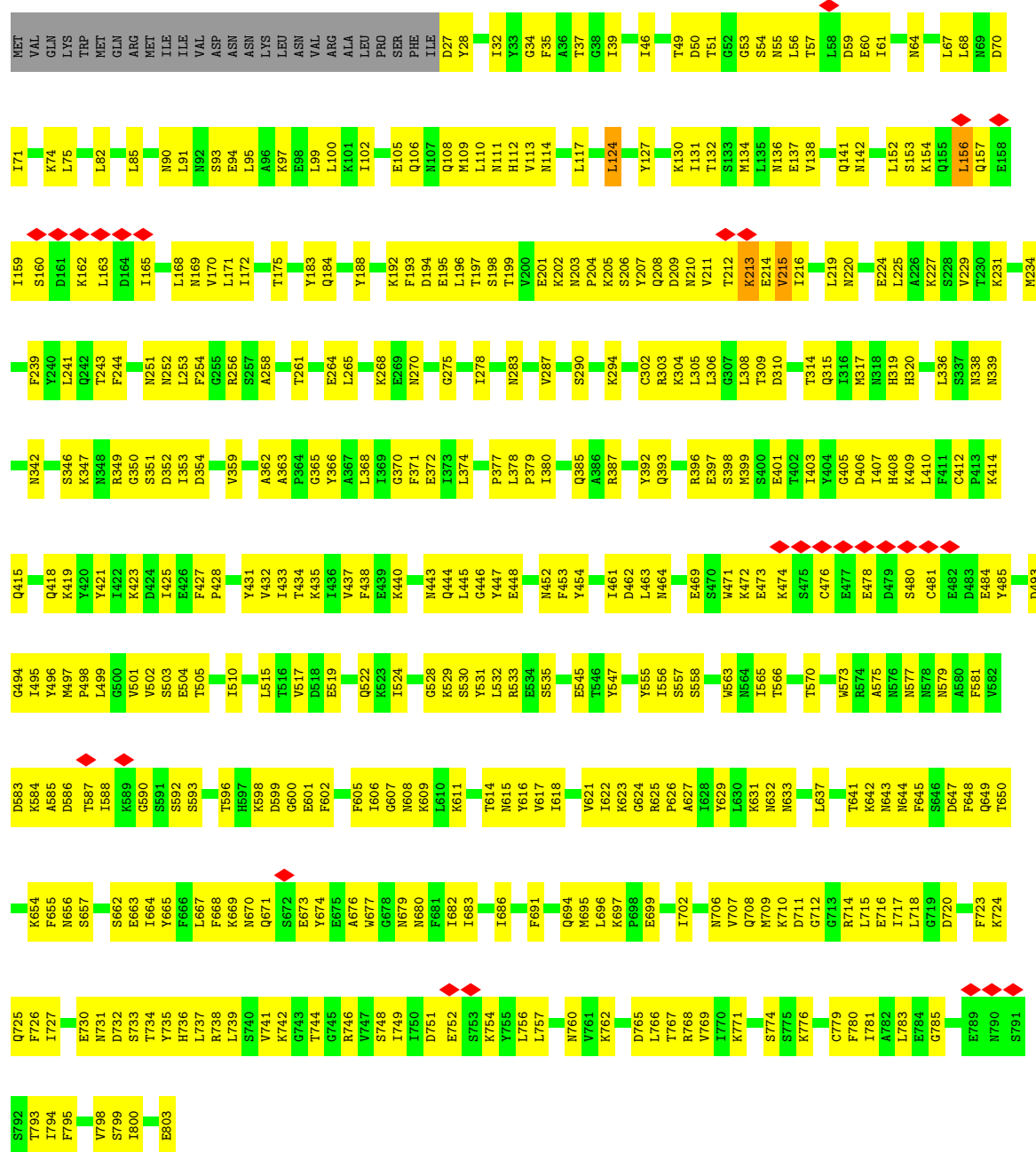
• Molecule 1: Vegetative insecticidal protein



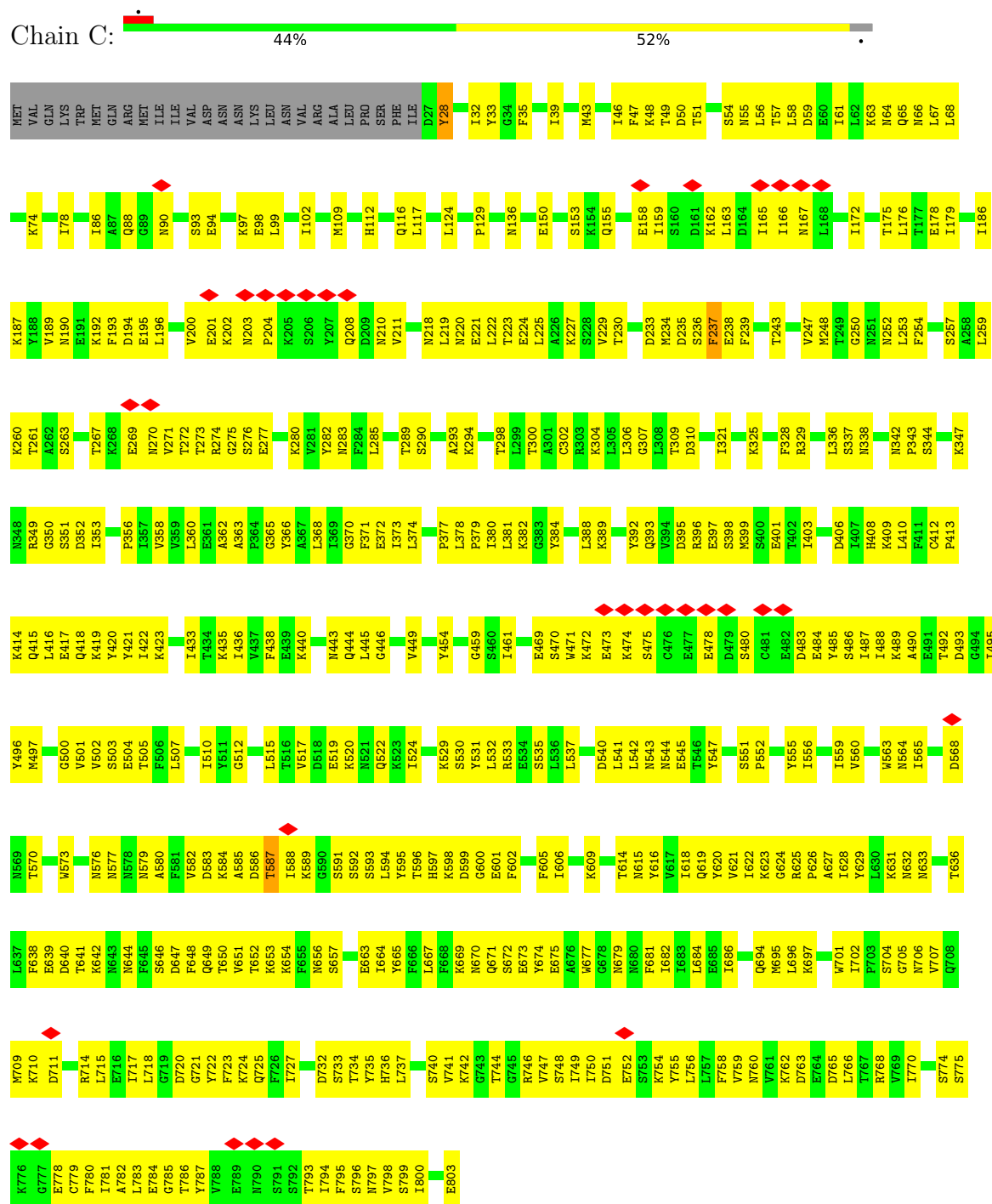


- Molecule 1: Vegetative insecticidal protein

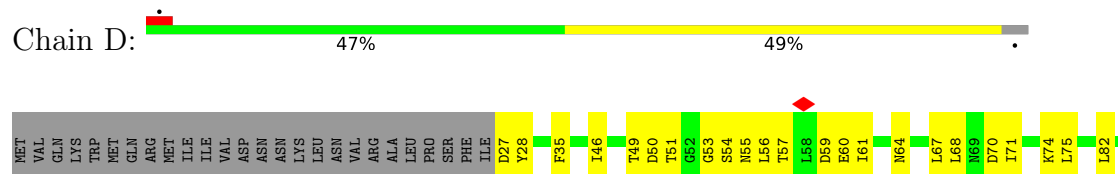
Chain B: 46% 50%



- Molecule 1: Vegetative insecticidal protein



- Molecule 1: Vegetative insecticidal protein



L85	V170	N252	D352	P428	H597	N670	L739
N90	L171	L253	I353	Y431	K598	Q671	S740
L91	I172	F254	D354	V432	D599	S672	V741
N92	T175	G255	V359	T516	G600	E673	K742
S93	L176	R256	V359	T517	F601	Y674	G743
E94	Y183	S257	A362	K435	F602	E675	T744
L95	Q184	A258	A363	T436	F605	A676	G745
A96	Y188	T261	A364	V437	I606	W677	R746
K97	Y188	E264	G365	F438	G607	G678	V747
I102	Y188	Y366	Y366	E439	N608	N680	S748
E105	K192	L265	A367	K440	K609	F681	I749
Q106	F193	L265	L368	M443	L610	I682	L750
M107	F193	K268	F371	Q444	K611	I683	D751
M108	D194	E269	E372	Q445	T614	I686	E752
Q109	E195	N270	E372	L445	N615	K687	S753
M110	L196	G275	I373	G446	Y616	F691	K754
M111	T197	L278	L374	Y447	L532	F691	Y755
H112	S198	I278	P379	E448	R533	F691	L756
V113	T199	I278	I380	M452	E534	I618	L757
M114	V200	E201	I380	F453	S535	Q694	N760
L117	K202	K202	Q385	Y454	E545	M695	M695
L124	N203	N203	A386	I461	T546	L696	K697
Y127	P204	P204	E387	D462	Y547	K697	P698
K130	K205	K205	Y392	L463	Y555	E699	D765
I131	S206	S206	Y392	D463	I556	I702	L766
T132	Y207	K294	Q393	M464	S557	I702	T767
S133	Q208	K294	R396	E469	S558	N706	R768
M134	D209	C302	E397	S470	W563	V707	V769
L135	N210	R303	S398	W471	N564	Q708	I770
N136	V211	K304	M399	K472	I565	M709	K771
E137	T212	L305	S400	E473	T570	K710	S774
V138	K213	L308	E401	K474	T570	D711	S775
Q141	E214	T309	I403	S475	W573	G712	K776
N142	V215	D310	Y404	C476	R574	G713	C779
L152	I216	T314	G405	E477	A575	R714	F780
S153	L219	Q315	I407	E478	N576	L715	I781
K154	N220	I316	H408	D479	N577	E716	A782
Q155	E224	M317	K409	S480	N578	L717	L783
L156	A226	N318	L410	C481	N579	L718	E784
Q157	L225	H319	F411	E482	A580	G719	G785
E158	H320	I321	C412	D483	F581	D720	E789
I159	S228	L336	Q414	E484	V582	F723	N790
S160	V229	S337	Q415	Y485	K584	K724	S791
D161	K231	N338	Q415	Y485	A585	Q725	S792
K162	K231	N339	Q415	Y485	D586	F726	I793
L163	M234	N342	Q418	D493	T587	I727	I794
D164	F239	S346	K419	G494	I588	E730	F795
I165	Y240	K347	Y421	Y496	K589	N731	V798
L168	L241	Q242	I422	M497	G590	S732	S799
N169	T243	N348	D424	L499	S591	S733	I800
	F244	R349	I425	G500	S592	Y734	Y735
	N251	G350	E426	V501	S593	H736	E803
		S351	F427	V502	T596	L737	
				E504	T505	R738	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1414999	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 ($e^-/\text{\AA}^2$)	76.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.103	Depositor
Minimum map value	-1.650	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.171	Depositor
Recommended contour level	0.83	Depositor
Map size (Å)	281.16, 281.16, 281.16	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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	A	0.28	0/6317	0.49	0/8542
1	B	0.29	0/6317	0.45	0/8542
1	C	0.28	0/6317	0.49	0/8542
1	D	0.29	0/6317	0.45	0/8542
All	All	0.28	0/25268	0.47	0/34168

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	LYS	Peptide
1	B	215	VAL	Peptide
1	D	213	LYS	Peptide
1	D	215	VAL	Peptide

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	6207	0	6174	358	0
1	B	6207	0	6174	352	0
1	C	6207	0	6174	358	0
1	D	6207	0	6174	352	0
All	All	24828	0	24696	1375	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 28.

The worst 5 of 1375 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:VAL:HG23	1:C:302:CYS:HB3	1.57	0.86
1:A:229:VAL:HG23	1:A:302:CYS:HB3	1.57	0.85
1:C:631:LYS:HG3	1:C:633:ASN:H	1.41	0.84
1:A:631:LYS:HG3	1:A:633:ASN:H	1.41	0.84
1:C:165:ILE:HD12	1:C:269:GLU:HB3	1.61	0.82

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	775/803 (96%)	675 (87%)	98 (13%)	2 (0%)	36	69
1	B	775/803 (96%)	675 (87%)	100 (13%)	0	100	100
1	C	775/803 (96%)	675 (87%)	98 (13%)	2 (0%)	36	69
1	D	775/803 (96%)	675 (87%)	100 (13%)	0	100	100
All	All	3100/3212 (96%)	2700 (87%)	396 (13%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	PHE
1	C	237	PHE
1	A	587	THR
1	C	587	THR

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	A	705/730 (97%)	704 (100%)	1 (0%)	88	89
1	B	705/730 (97%)	703 (100%)	2 (0%)	86	85
1	C	705/730 (97%)	704 (100%)	1 (0%)	88	89
1	D	705/730 (97%)	703 (100%)	2 (0%)	86	85
All	All	2820/2920 (97%)	2814 (100%)	6 (0%)	85	87

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	28	TYR
1	D	124	LEU
1	D	156	LEU
1	B	124	LEU
1	A	28	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	725	GLN
1	D	315	GLN
1	D	30	ASN
1	D	155	GLN
1	D	418	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.

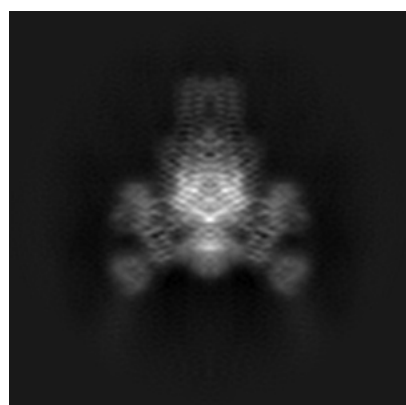
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10888. These allow visual inspection of the internal detail of the map and identification of artifacts.

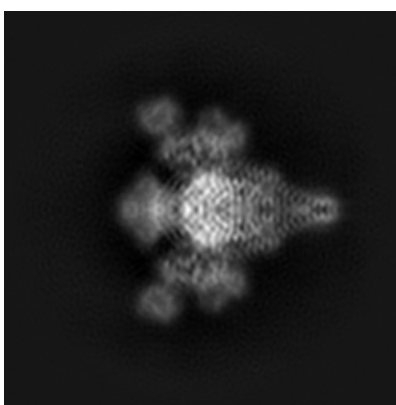
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

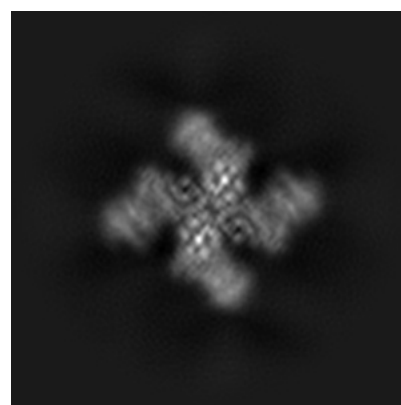
6.1.1 Primary map



X



Y

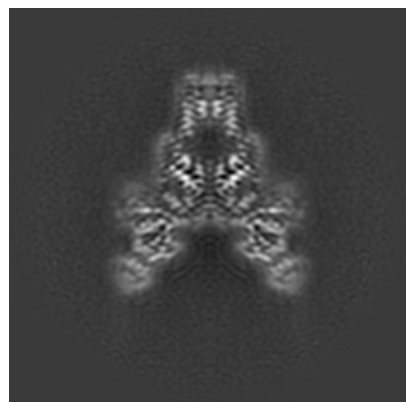


Z

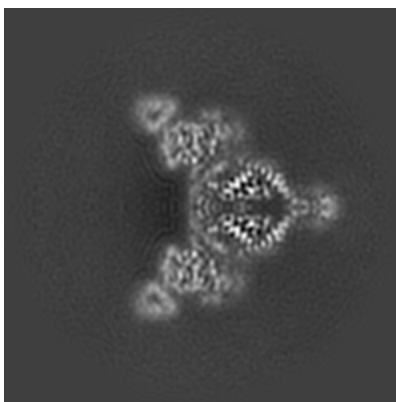
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

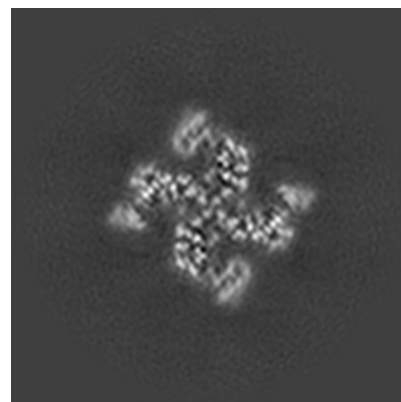
6.2.1 Primary map



X Index: 132



Y Index: 132

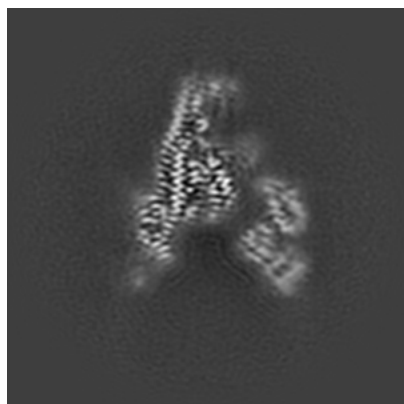


Z Index: 132

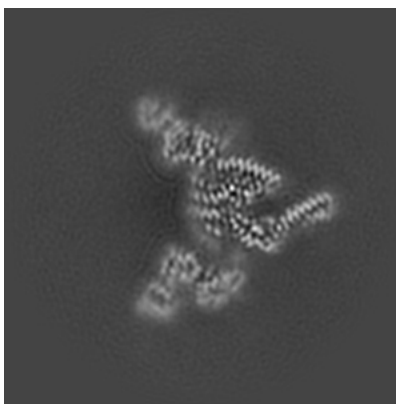
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

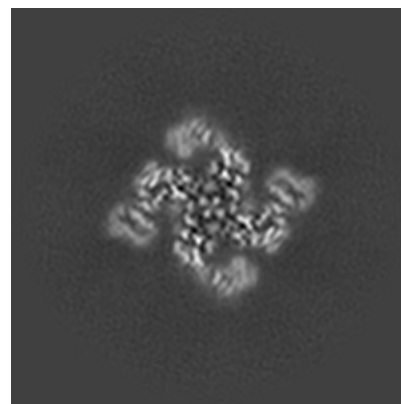
6.3.1 Primary map



X Index: 124



Y Index: 128

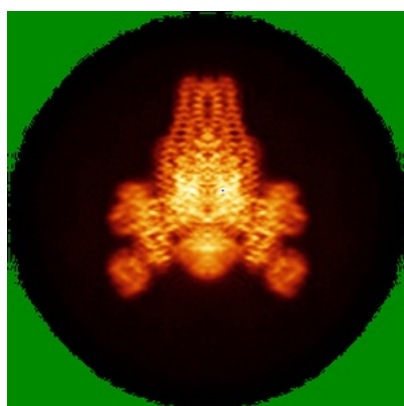


Z Index: 138

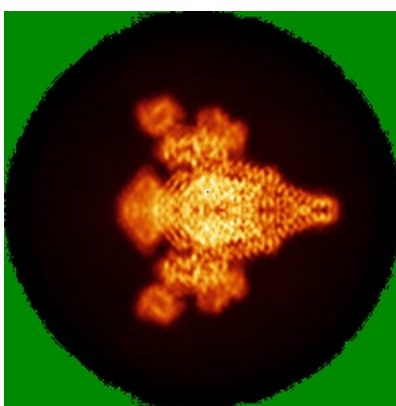
The images above show the largest variance slices of the map in three orthogonal directions.

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

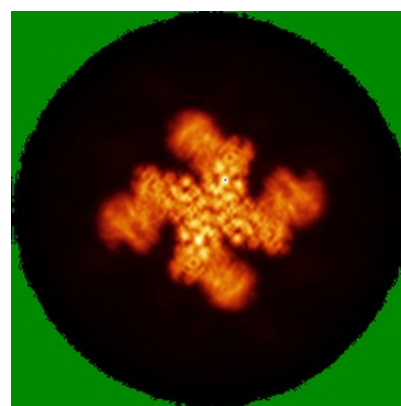
6.4.1 Primary map



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

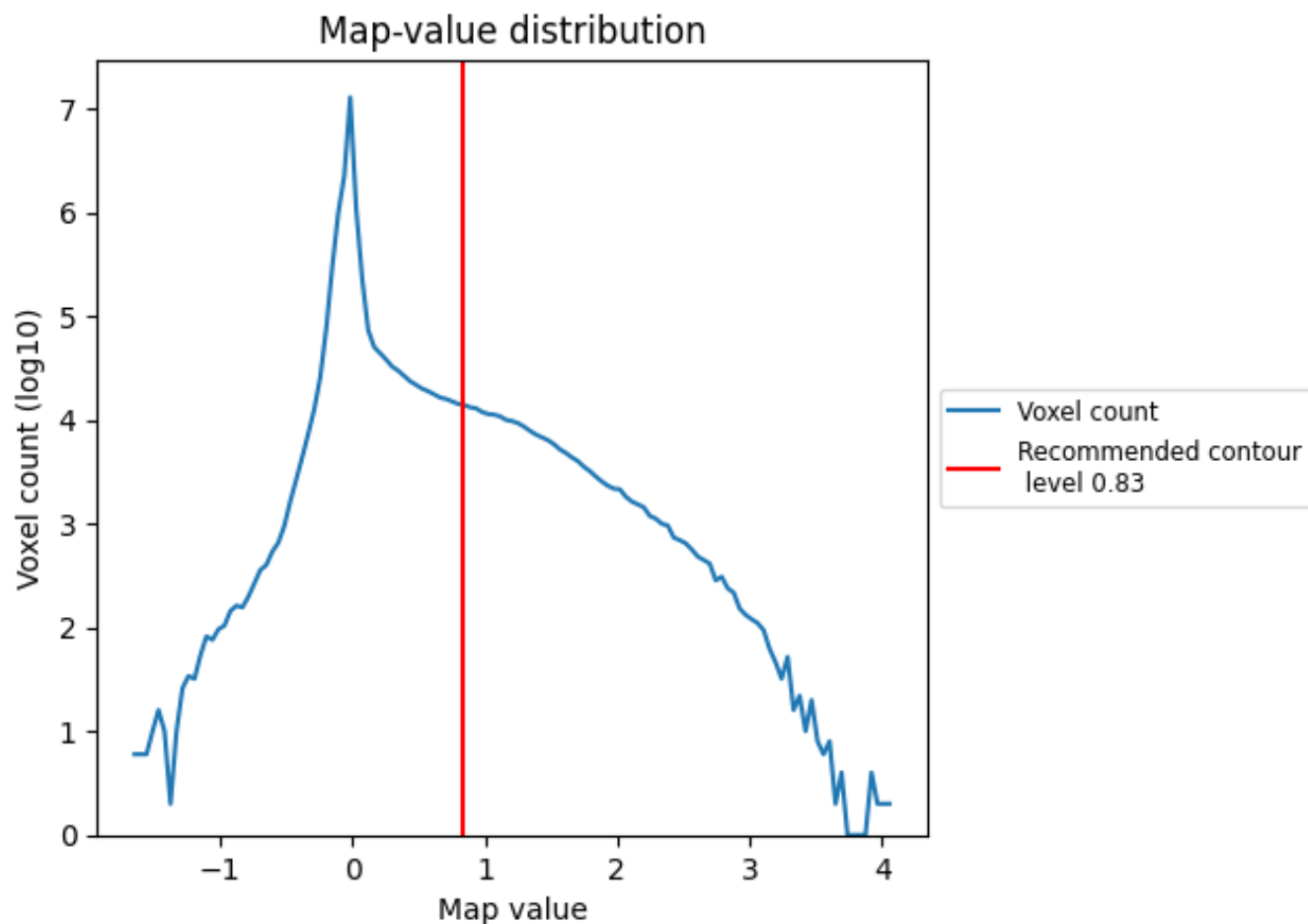
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

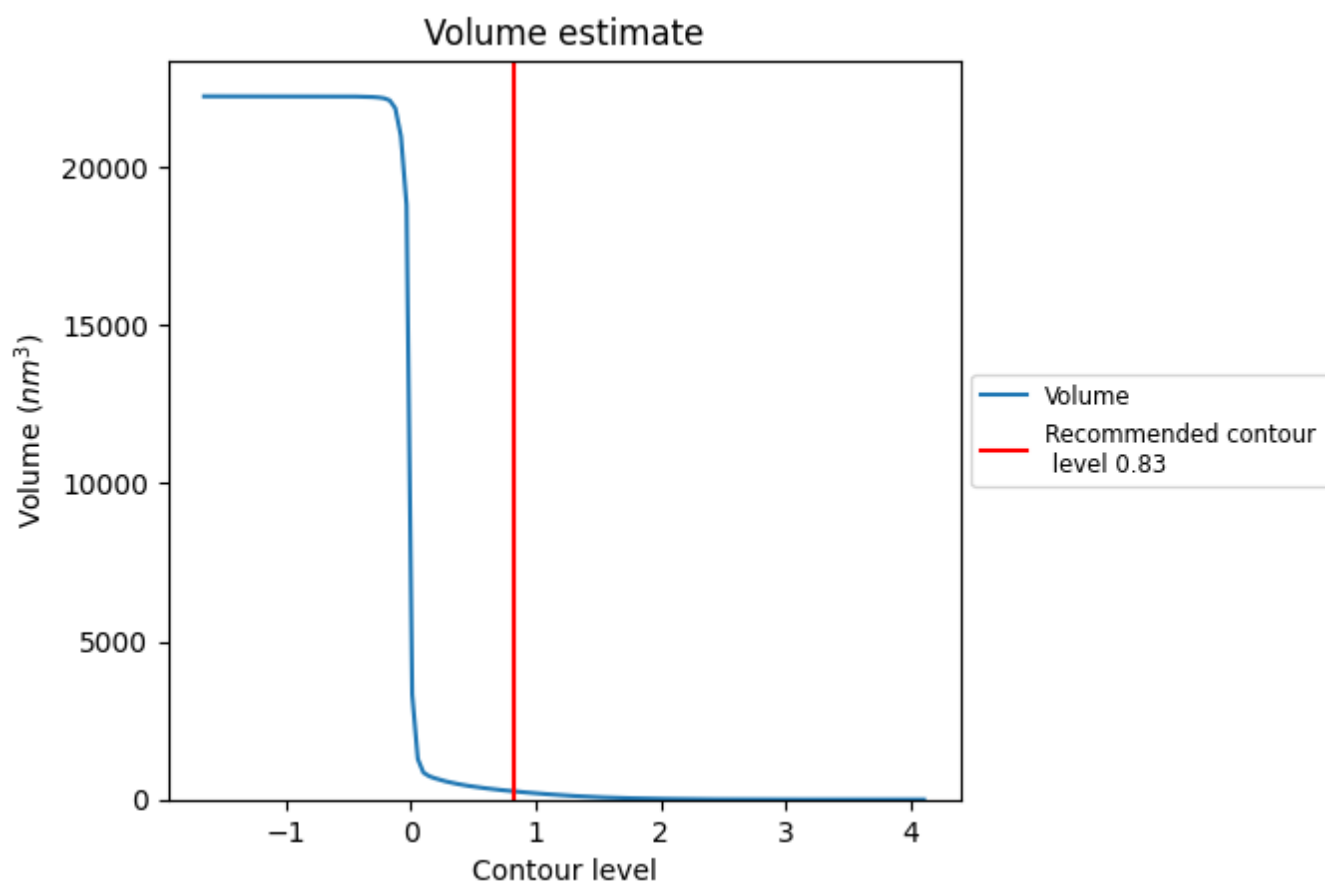
This section contains the results of statistical analysis of the map.

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.

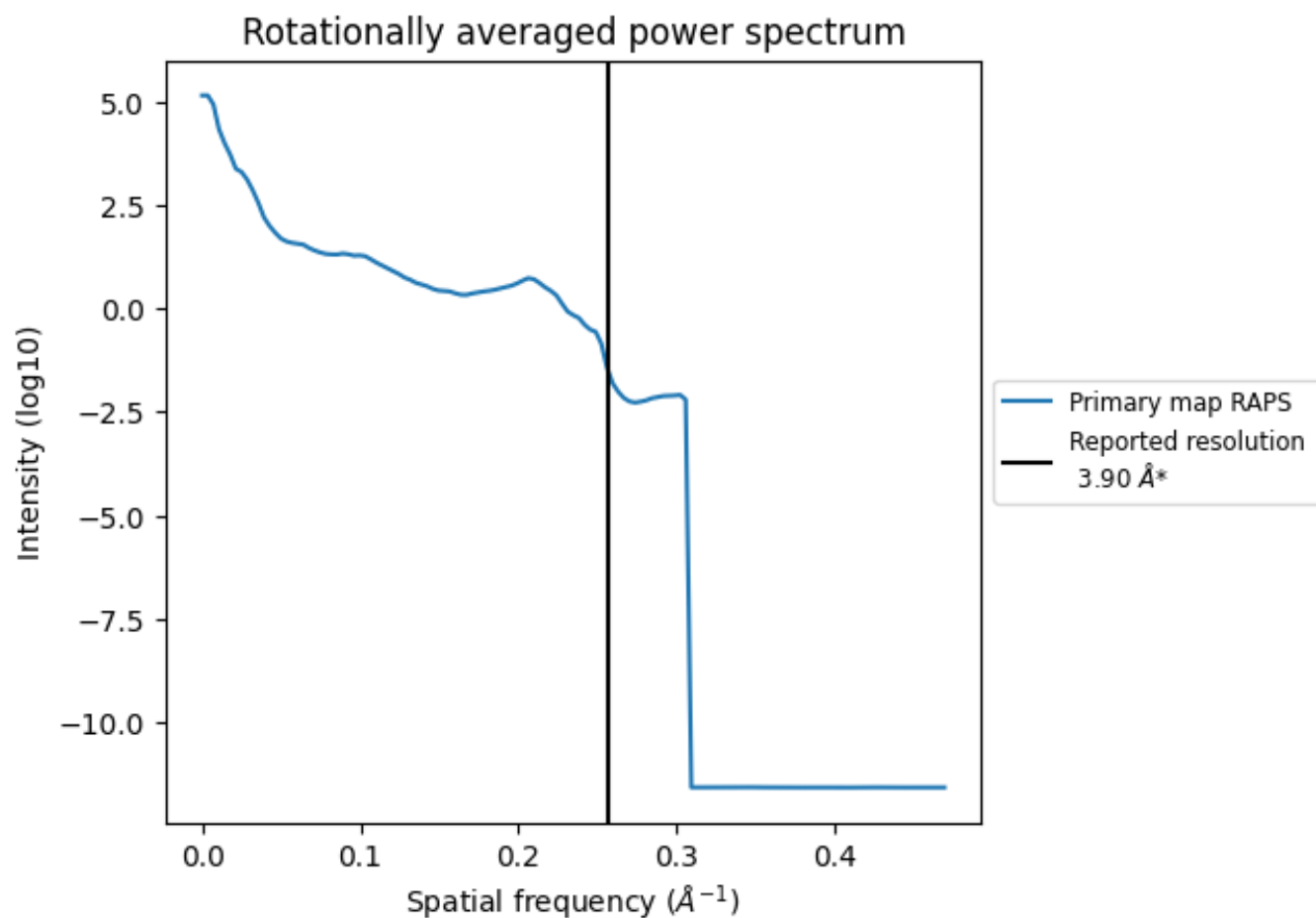
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm^3 ; this corresponds to an approximate mass of 234 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 ⓘ

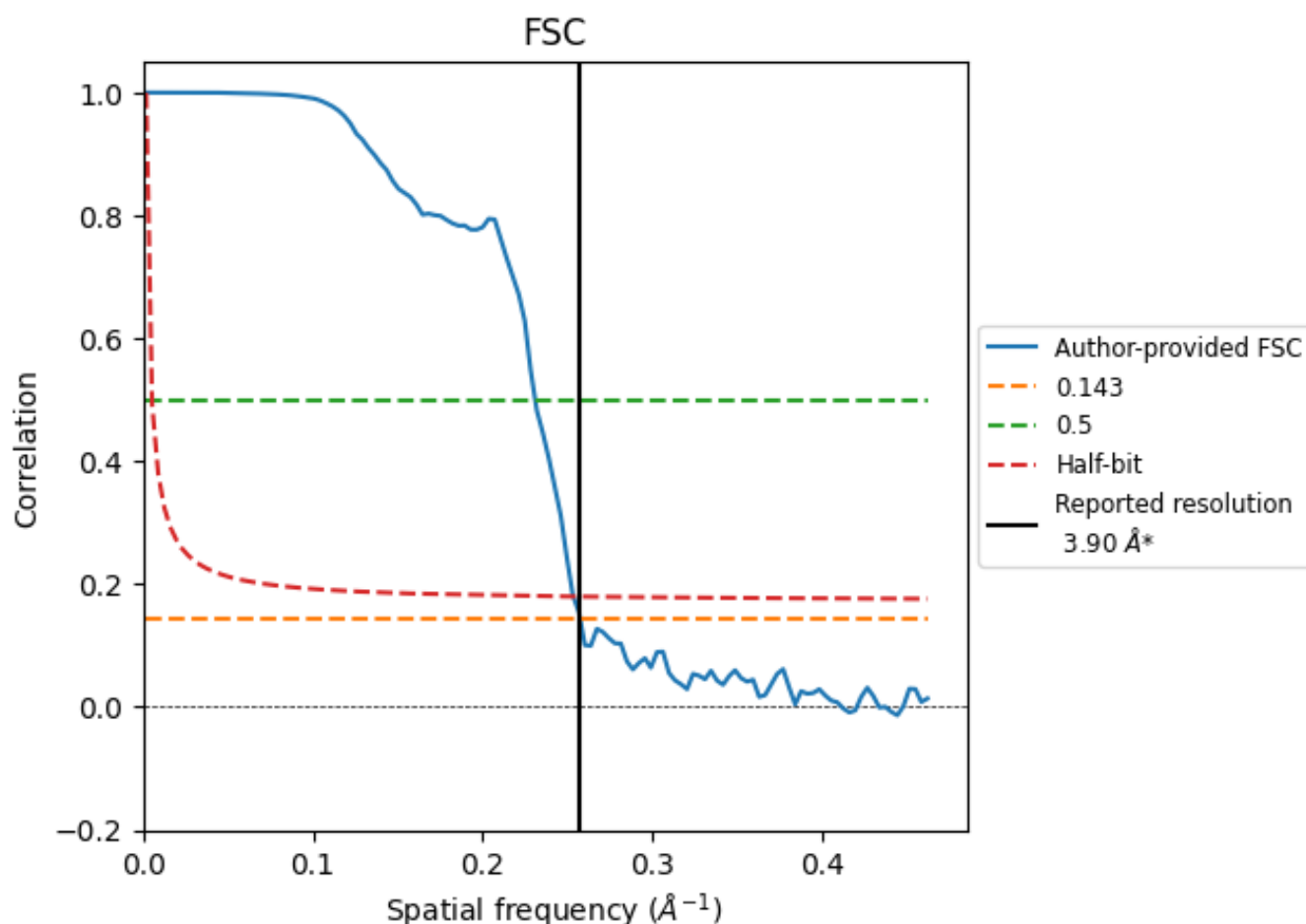


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

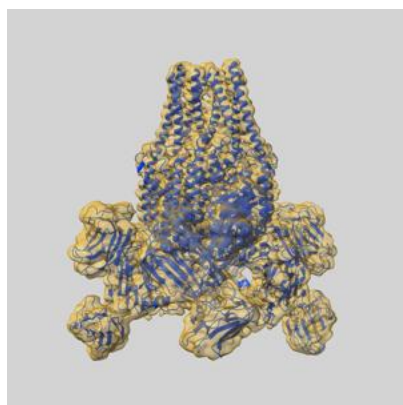
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	4.33	3.95
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

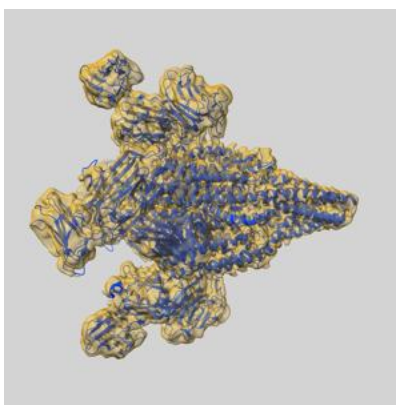
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10888 and PDB model 6YRF. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

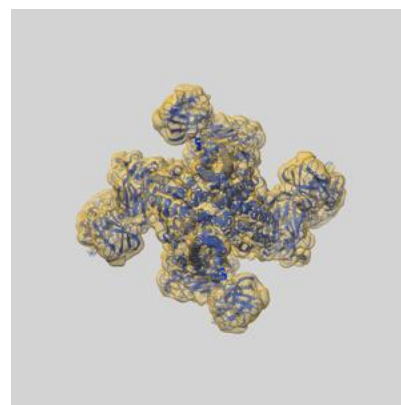
9.1 Map-model overlay [i](#)



X



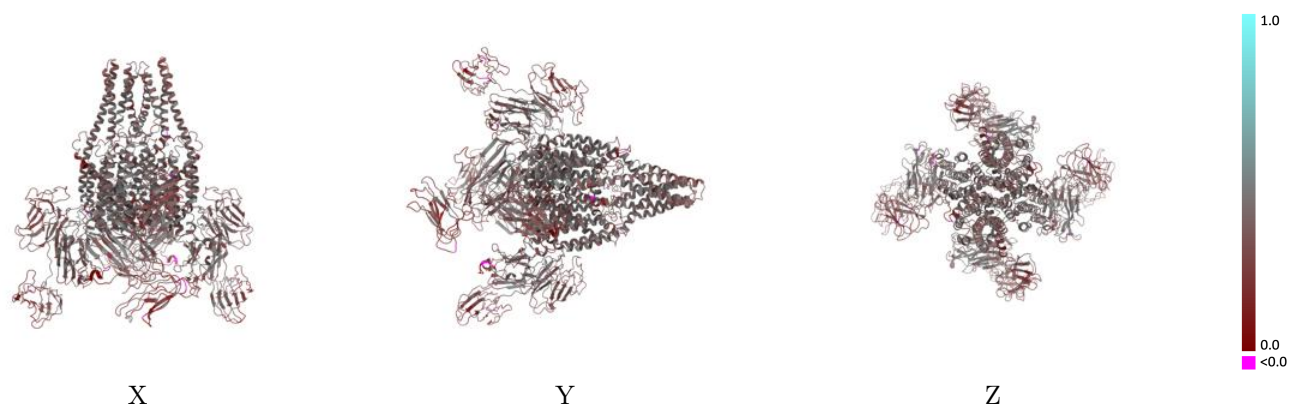
Y



Z

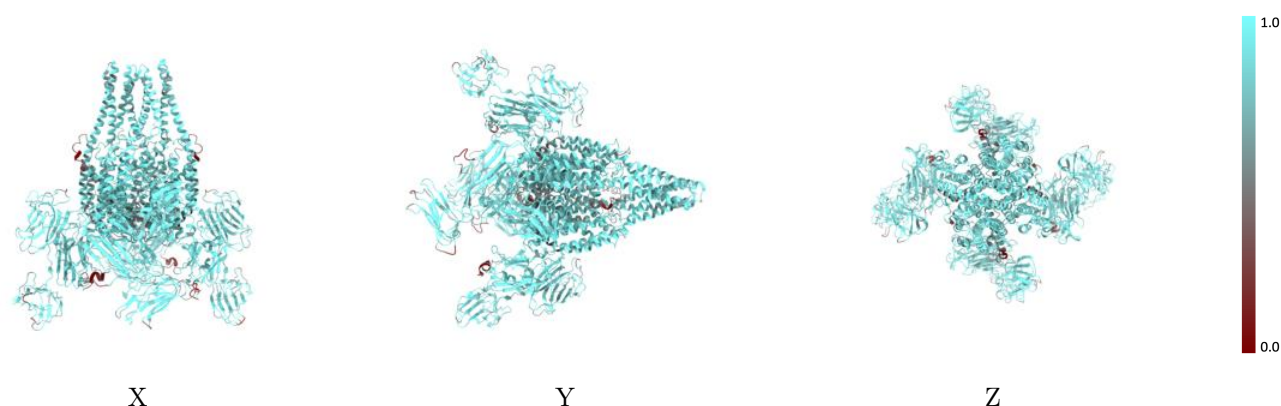
The images above show the 3D surface view of the map at the recommended contour level 0.83 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



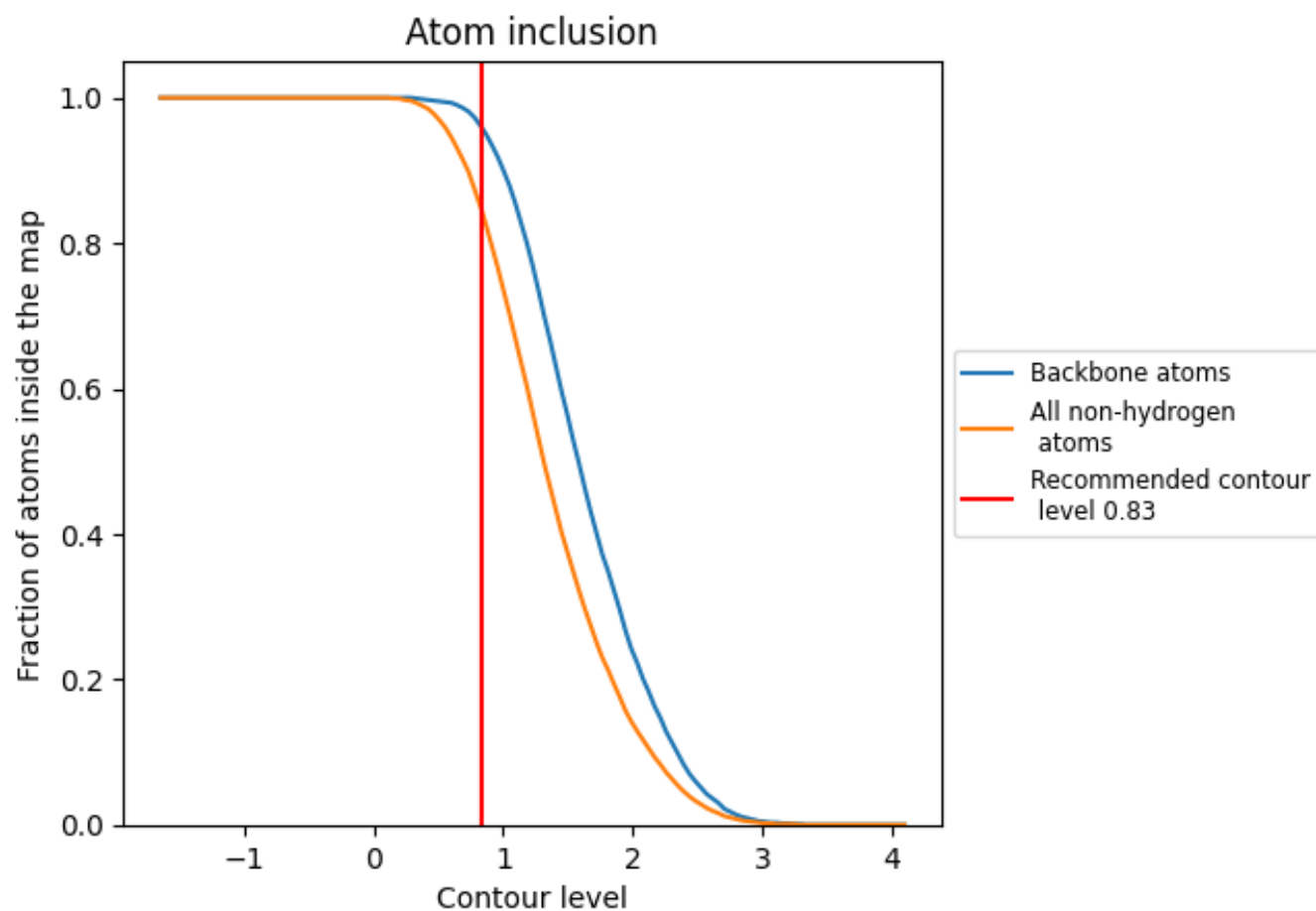
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.83).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.83) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.3550
A	0.8380	0.3540
B	0.8560	0.3560
C	0.8380	0.3530
D	0.8560	0.3560

