



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 05:41 AM JST

PDB ID : 7V7B
EMDB ID : EMD-31765
Title : CryoEM structure of DDB1-VprBP complex in ARM-up conformation
Authors : Wang, D.; Xu, J.; Liu, Q.; Xiang, Y.
Deposited on : 2021-08-21
Resolution : 4.20 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

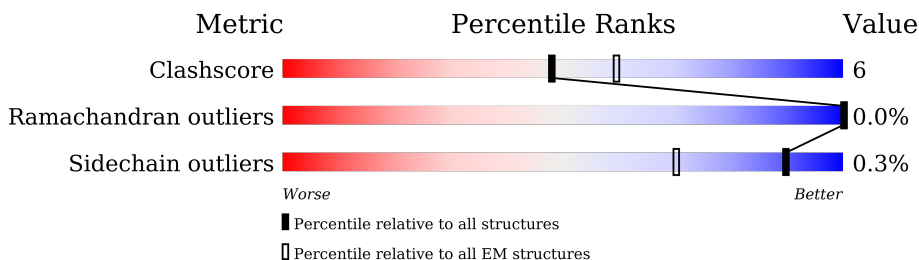
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1507	<div> <div>35%</div> <div>63%</div> <div>10%</div> <div>26%</div> </div>
1	C	1507	<div> <div>35%</div> <div>63%</div> <div>10%</div> <div>26%</div> </div>
2	B	1140	<div> <div>46%</div> <div>82%</div> <div>18%</div> <div>.</div> </div>
2	D	1140	<div> <div>46%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35366 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 DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1110	Total	C	N	O	S	0	0
			8809	5593	1515	1639	62		
1	C	1110	Total	C	N	O	S	0	0
			8809	5593	1515	1639	62		

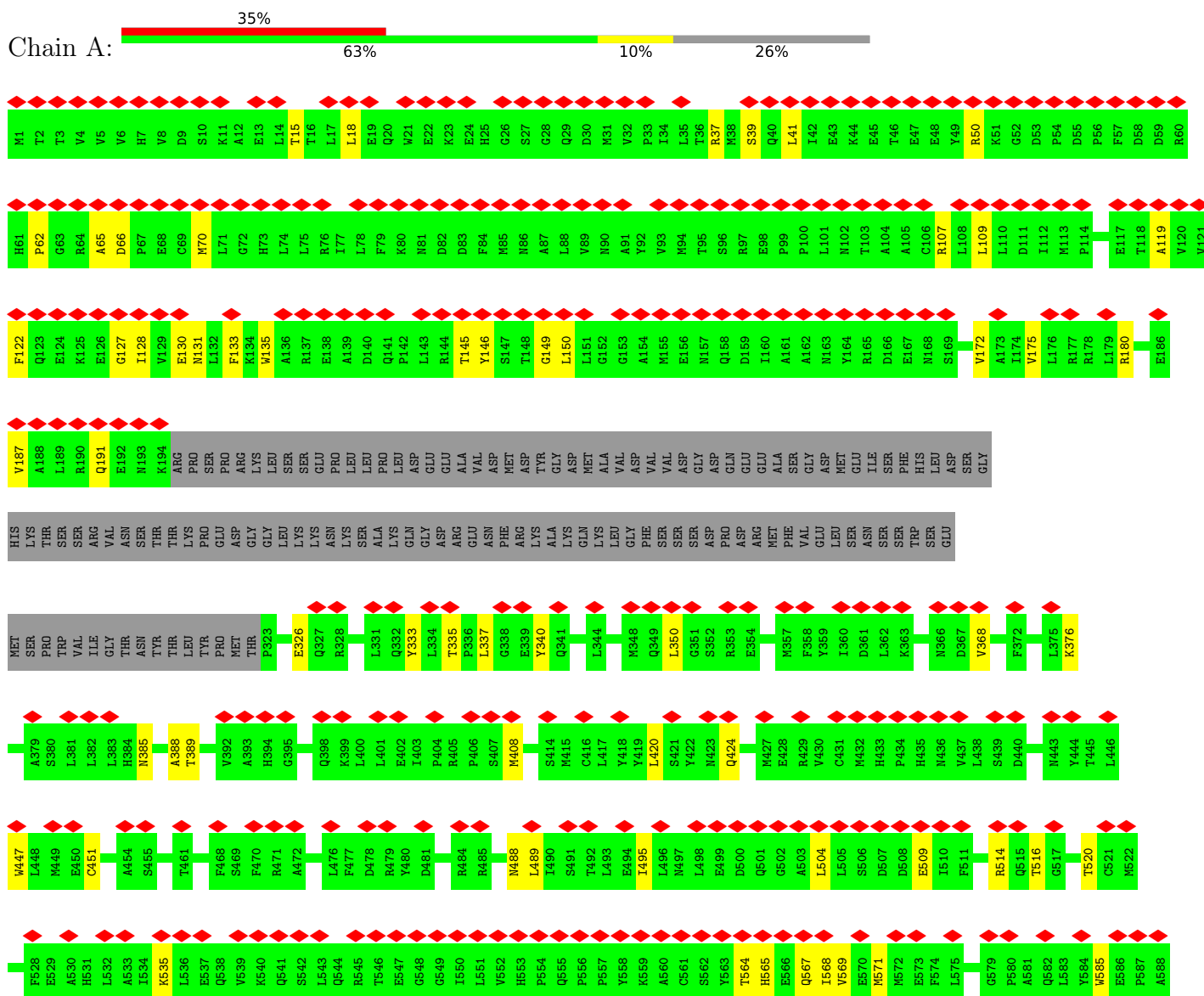
- Molecule 2 is a protein called DNA damage-binding protein 1.

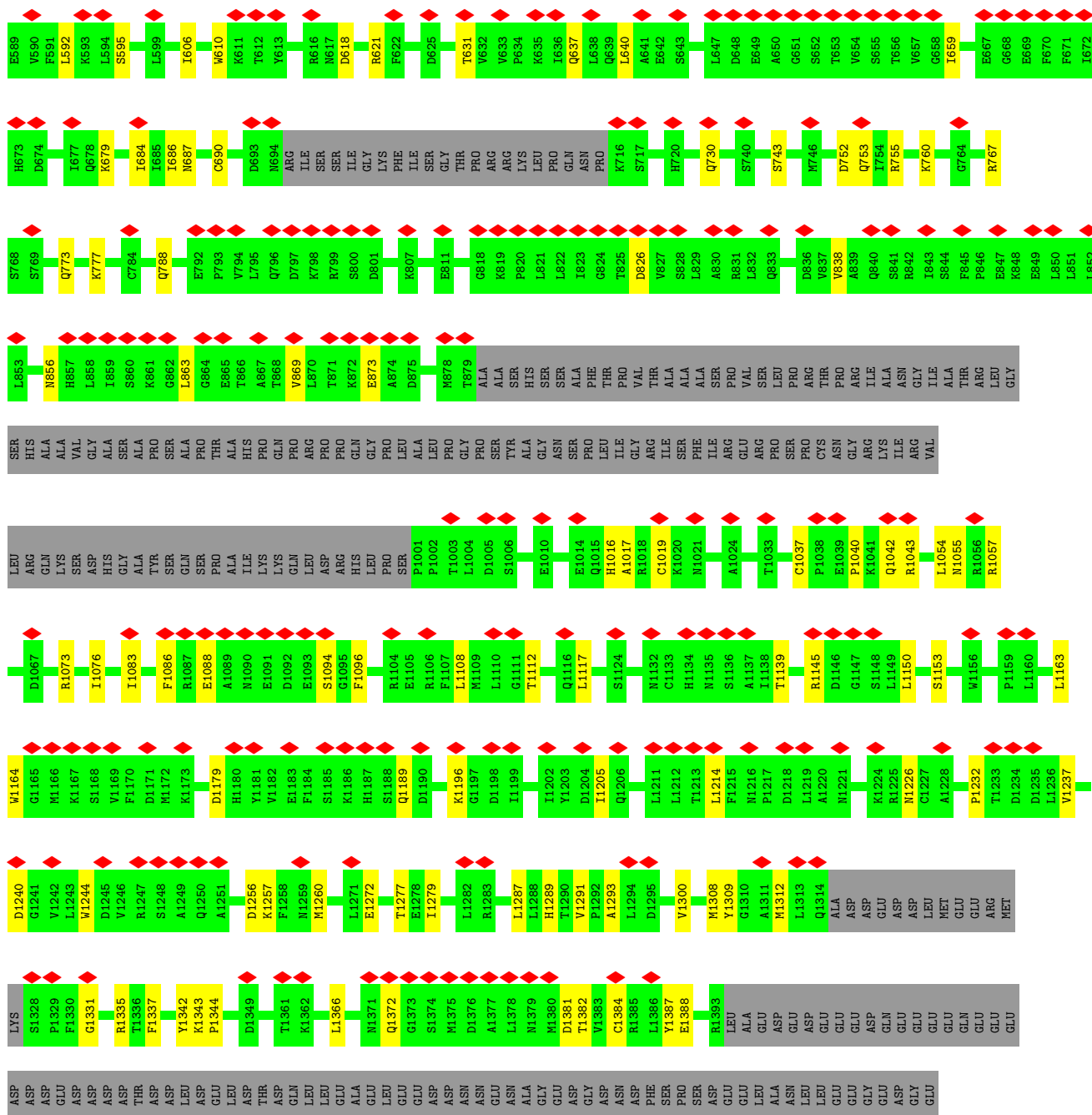
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1133	Total	C	N	O	S	0	0
			8874	5619	1496	1710	49		
2	D	1133	Total	C	N	O	S	0	0
			8874	5619	1496	1710	49		

3 Residue-property plots

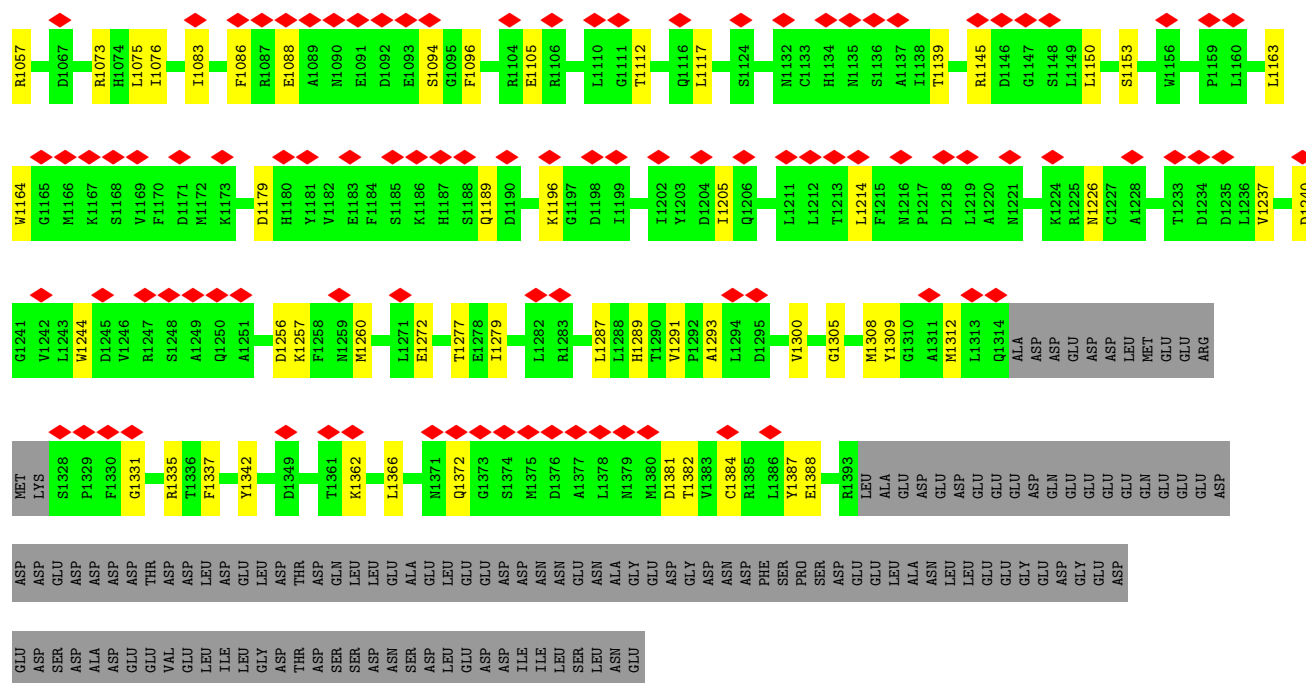
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DDB1- and CUL4-associated factor 1

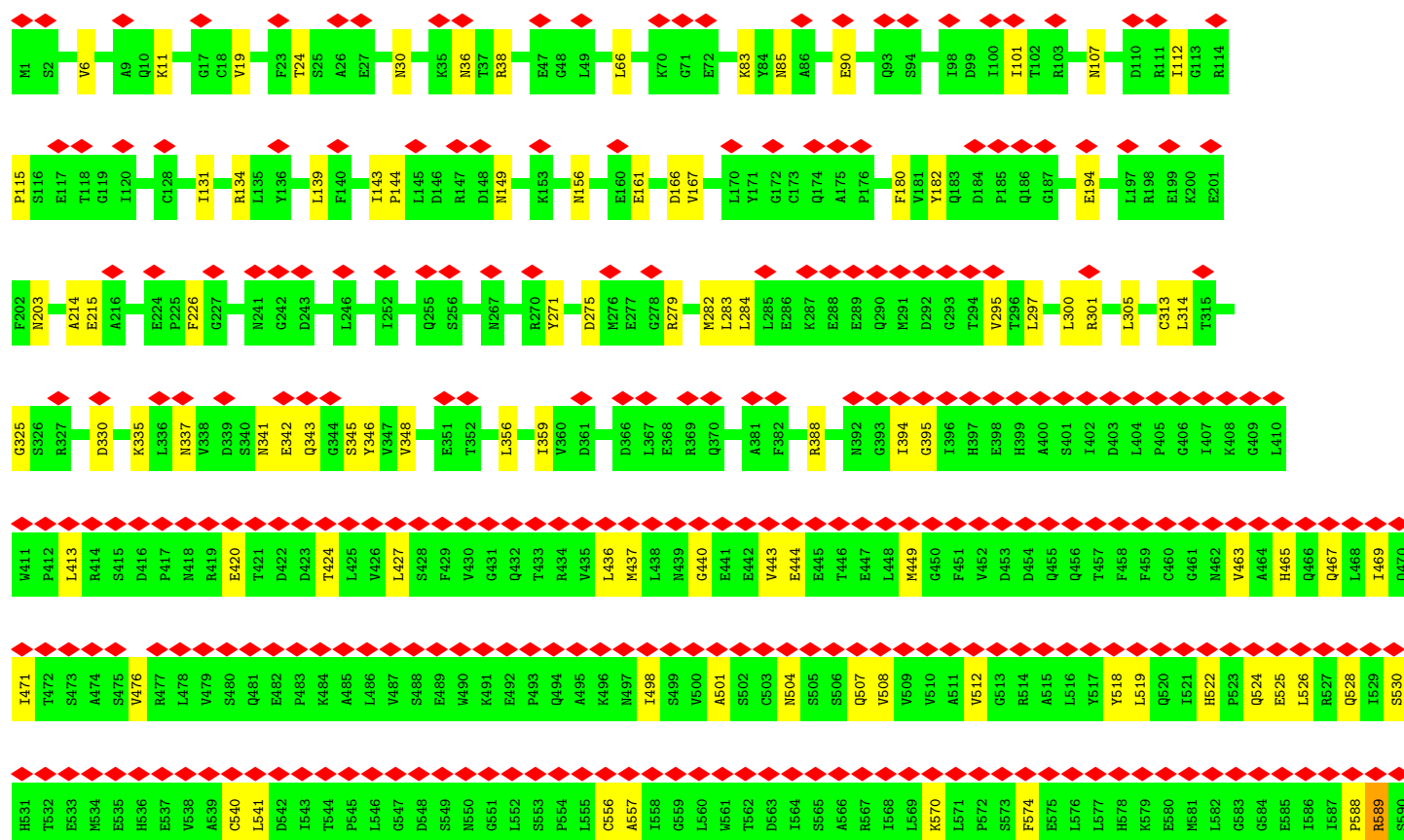
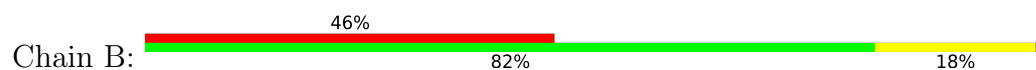








• Molecule 2: DNA damage-binding protein 1



I1094	F1097	L1098	D1099	I1100	S1101	R1102	P1103	K1104	M1105	V1109	Q1113	Y1114	D1115	D1116	GLY	SER	G1119	M1120	K1121	E1123	A1124	D1127	D1128	L1129	I1130	E1134	R1138	I1139	H1140																															
A971	F972	N973	K979	D980	S981	A982	A983	T984	T985	E987	E988	R989	Q990	Q993	G996	H999	E1002	N1005	G1010	S1011	M1014	Q1015	N1016	L1017	GLY	GLU	THR	SER	THR	P1023	G1026	G1031	E939	N1034	V1040	L1043	I1062	W1073	E1079	R1080	T1086																			
V866	E875	K879	L880	L881	A882	S883	I884	Y891	E892	W893	T894	T895	E896	K897	E898	L899	E902	C903	N904	M910	A911	L914	K915	T916	K917	G918	D919	F920	I921	L922	D925	L926	N927	R928	S929	V930	M938	E939	G940	I945	A946	R947	D948	F949	N950	P951	N952	D963												
P777	H778	E779	T780	S781	F782	G783	E784	N790	L791	I794	D795	Q796	H797	T798	Q806	S815	L816	K820	L821	G822	K823	D824	Y828	F829	I830	V831	A834	E839	E842	P843	K844	Q845	G846	V850	F851	Q852	Y853	S854	D855	G856	K857	L858	Q859	T860	V861	A862	E863	K864	E865											
I701	G702	T703	I704	D705	E706	I707	Q708	H711	I712	R713	T714	L717	Y718	E719	S720	F721	R722	K723	Y726	Q727	E728	Q731	L736	S737	S738	E741	V742	Q743	D744	T745	S746	G747	G748	T749	T750	A751	L752	S762	S763	S764	V765	S766	S767	S768	K769	L770	S771	S772	S773	S774	T775	A776								
F641	R642	S643	L644	S645	T646	T647	N648	V649	F650	A651	C652	S653	D654	R655	P656	T657	V658	I659	Y660	S661	S662	N663	H664	K665	L666	V667	F668	S669	N670	V671	N672	L673	K674	E675	V676	M677	Y678	M679	C680	P681	L682	N683	S684	D685	G686	H687	P688	D689	S690	L691	A692	L693	A694	N695	N696	S697	T698	L699	T700	
M581	L582	G583	G584	E585	I586	I587	P588	R589	S590	I591	C592	S593	T594	T595	F596	E597	S598	S599	H600	Y601	L602	L603	C604	A605	L606	G607	D608	G609	A610	L611	F612	Y613	F614	G615	L616	C556	N617	I618	E619	T620	G621	L622	L623	S624	D625	R626	K627	K628	V629	T630	L631	G632	T633	Q634	P635	T636	V637	L638	R639	T640
I521	H522	P523	Q524	E525	L526	R527	Q528	I529	S530	H531	T532	E533	M534	E535	H536	E537	V538	A539	C540	L541	D542	I543	T544	P545	L546	G547	D548	S549	A550	G551	L552	S553	P554	L555	C556	A557	I558	G559	L560	W561	T562	D563	I564	S565	A566	R567	I568	L569	K570	L571	P572	S573	F574	E575	L576	L577	H578	K579	E580	
G461	N462	V463	A464	H465	Q466	Q467	L468	I469	Q470	I471	T472	S473	A474	S475	V476	R477	L478	V479	S480	Q481	E482	P483	K484	A485	L486	V487	S488	E489	W490	K491	E492	P493	Q494	A495	K496	N497	I498	S499	V500	A501	S502	C503	N504	S505	S506	Q507	V508	V509	V510	A511	V512	G513	R514	A515	L516	Y517	Y518	L519	Q520	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84405	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	31.370	Depositor
Minimum map value	-15.818	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.5	Depositor
Map size (\AA)	314.20798, 314.20798, 314.20798	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

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	0.29	0/8986	0.54	2/12169 (0.0%)
1	C	0.29	0/8986	0.54	2/12169 (0.0%)
2	B	0.29	0/9037	0.54	0/12241
2	D	0.29	0/9037	0.54	0/12241
All	All	0.29	0/36046	0.54	4/48820 (0.0%)

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
2	B	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	826	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	826	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	1117	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	1117	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	180	PHE	Peptide
2	B	589	ARG	Peptide
2	D	180	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	D	589	ARG	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	8809	0	8808	95	0
1	C	8809	0	8808	93	0
2	B	8874	0	8842	116	0
2	D	8874	0	8842	124	0
All	All	35366	0	35300	402	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 6.

The worst 5 of 402 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:720:SER:HB2	2:D:738:SER:HB3	1.74	0.69
2:B:720:SER:HB2	2:B:738:SER:HB3	1.74	0.67
1:C:1054:LEU:HD12	1:C:1057:ARG:HD3	1.80	0.63
2:B:284:LEU:HB2	2:B:301:ARG:HB2	1.80	0.63
2:B:437:MET:HB2	2:B:444:GLU:HB2	1.80	0.63

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	1100/1507 (73%)	1006 (92%)	94 (8%)	0	100	100
1	C	1100/1507 (73%)	1006 (92%)	94 (8%)	0	100	100
2	B	1127/1140 (99%)	1022 (91%)	104 (9%)	1 (0%)	48	82
2	D	1127/1140 (99%)	1020 (90%)	106 (9%)	1 (0%)	48	82
All	All	4454/5294 (84%)	4054 (91%)	398 (9%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	115	PRO
2	D	115	PRO

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	980/1323 (74%)	976 (100%)	4 (0%)	89	91
1	C	980/1323 (74%)	976 (100%)	4 (0%)	89	91
2	B	994/999 (100%)	993 (100%)	1 (0%)	92	94
2	D	994/999 (100%)	993 (100%)	1 (0%)	92	94
All	All	3948/4644 (85%)	3938 (100%)	10 (0%)	90	92

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	488	ASN
1	C	856	ASN
2	D	134	ARG
1	A	856	ASN
2	B	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1016	HIS
2	D	507	GLN
1	C	1035	HIS
1	C	1259	ASN
2	D	677	ASN

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.

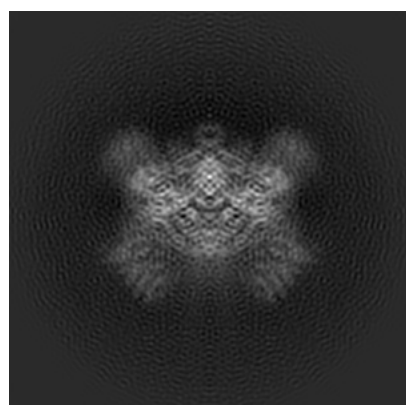
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31765. These allow visual inspection of the internal detail of the map and identification of artifacts.

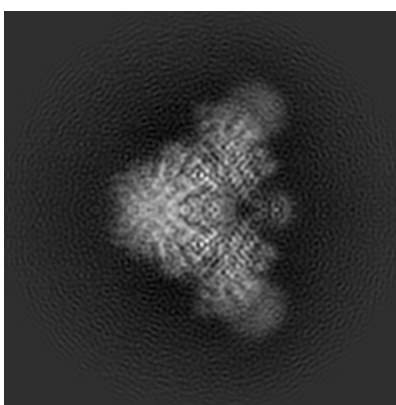
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

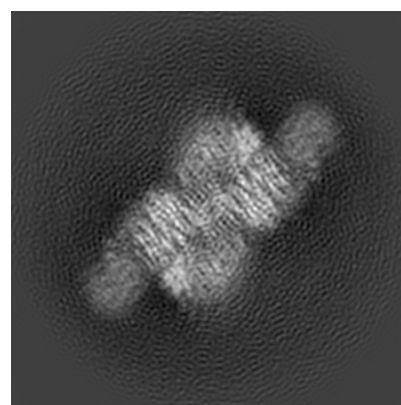
6.1.1 Primary map



X



Y

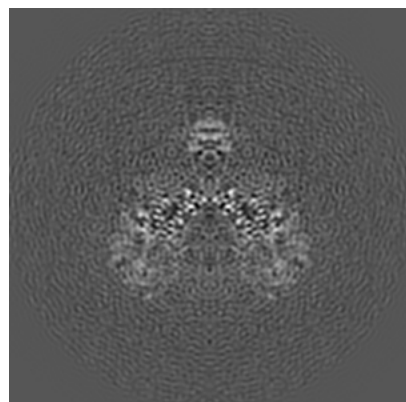


Z

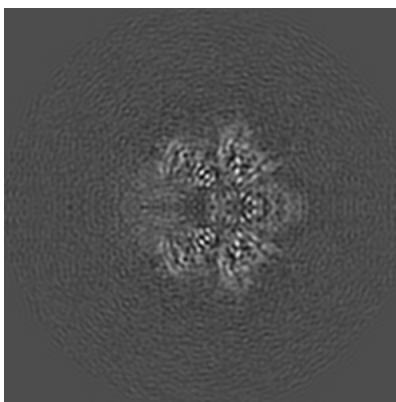
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

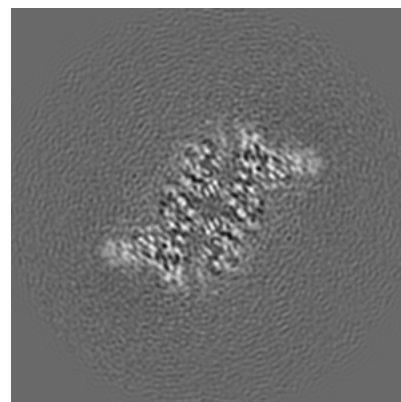
6.2.1 Primary map



X Index: 144



Y Index: 144

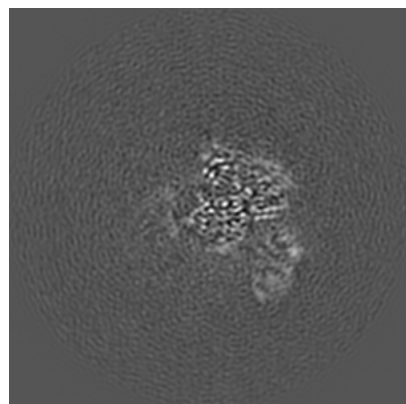


Z Index: 144

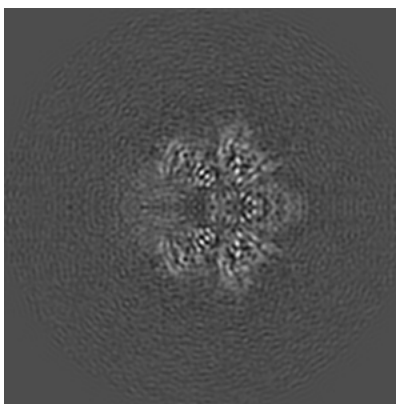
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

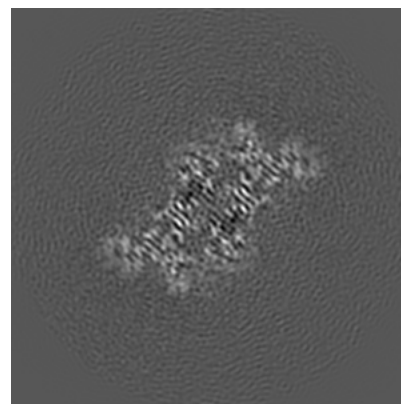
6.3.1 Primary map



X Index: 168



Y Index: 144

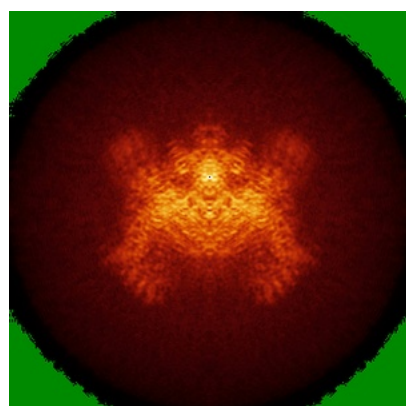


Z Index: 146

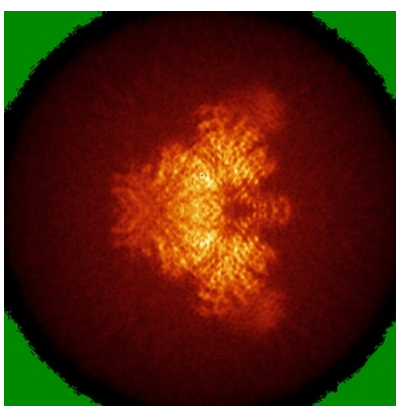
The images above show the largest variance slices of the map in three orthogonal directions.

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

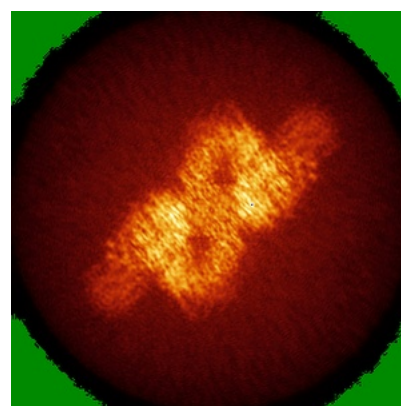
6.4.1 Primary map



X



Y

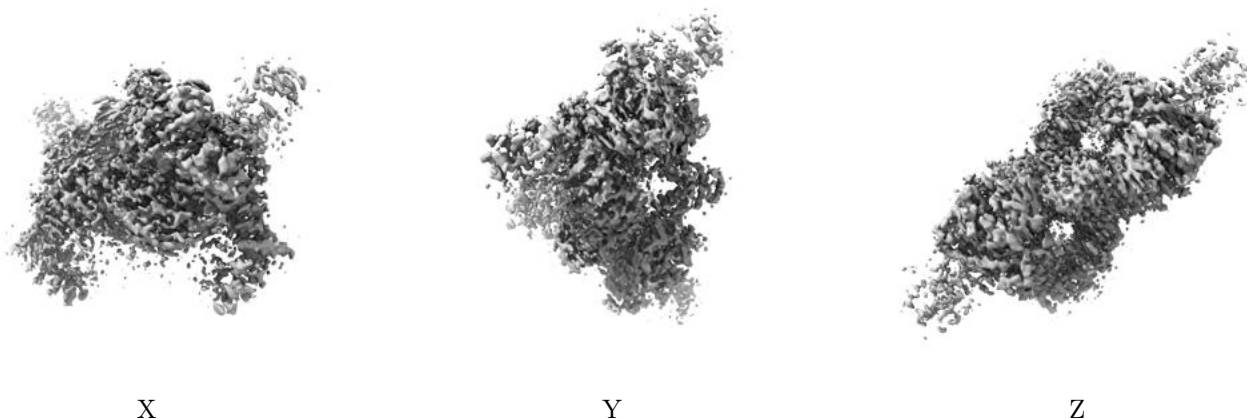


Z

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

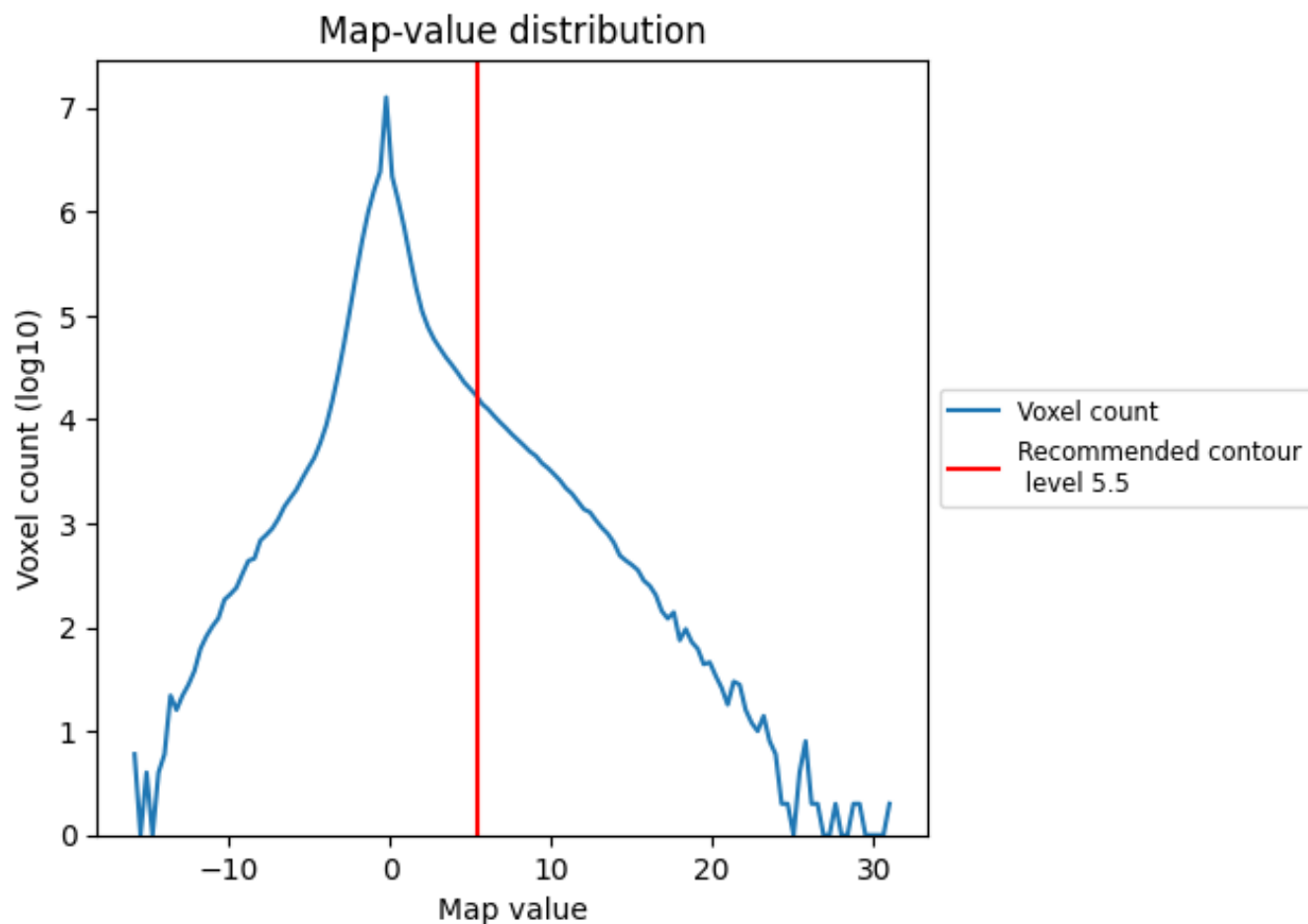
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

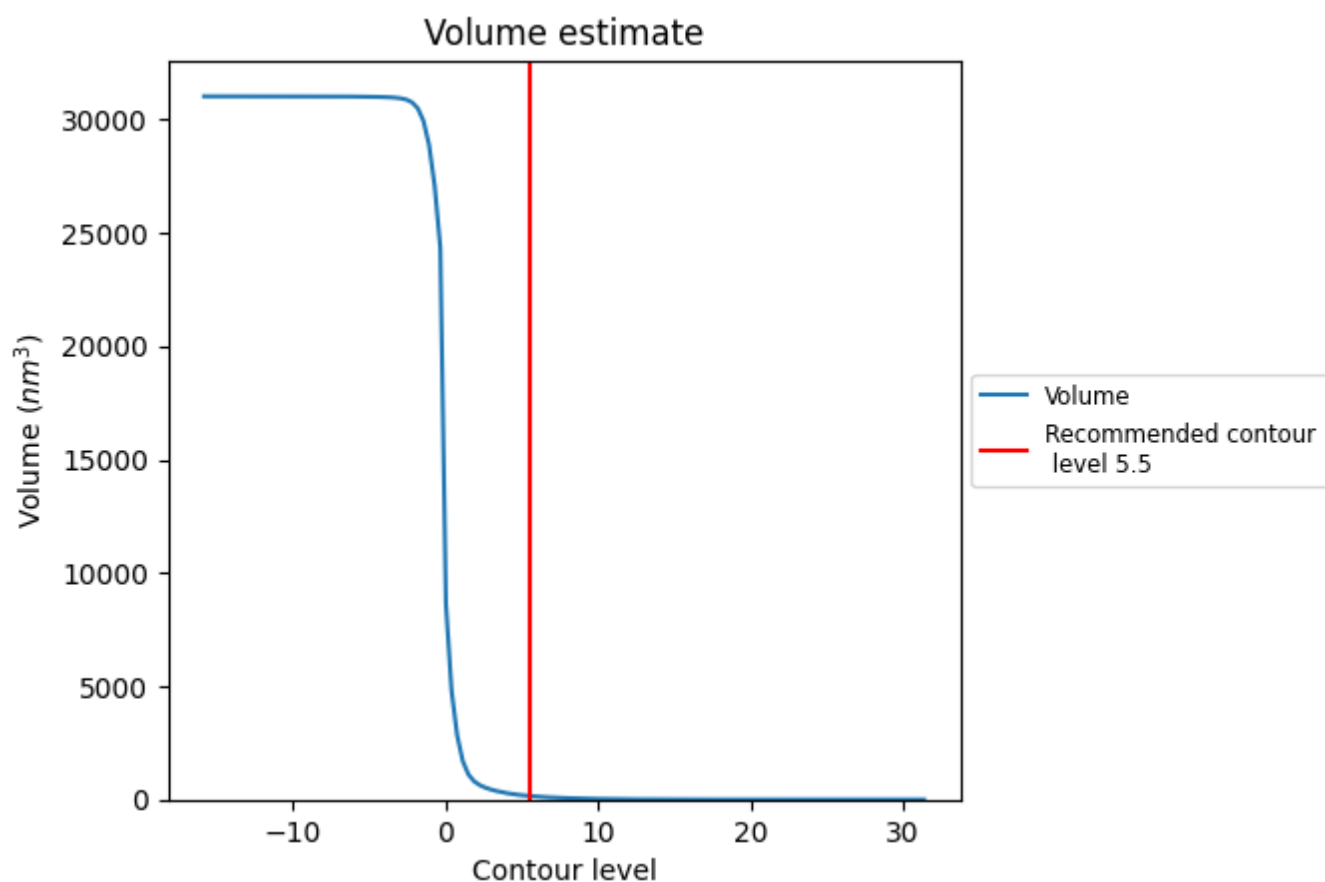
This section contains the results of statistical analysis of the map.

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.

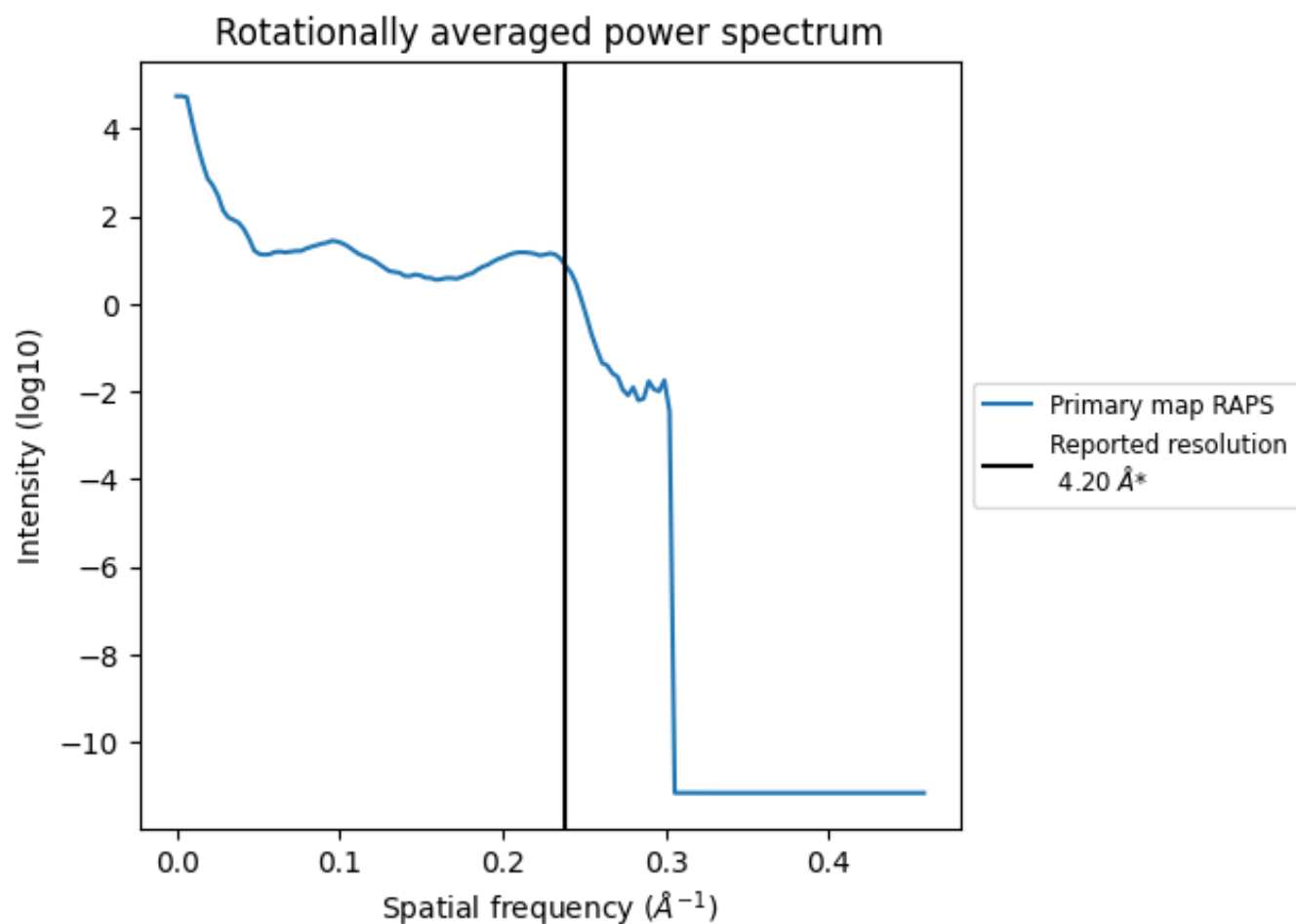
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm^3 ; this corresponds to an approximate mass of 143 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 0.238 Å⁻¹

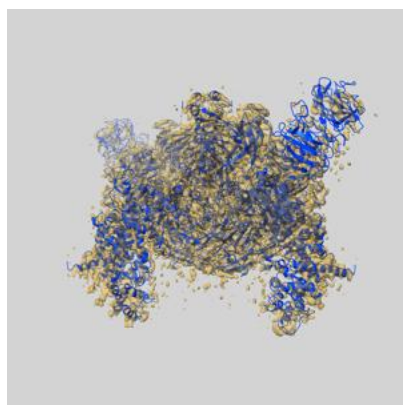
8 Fourier-Shell correlation ⓘ

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

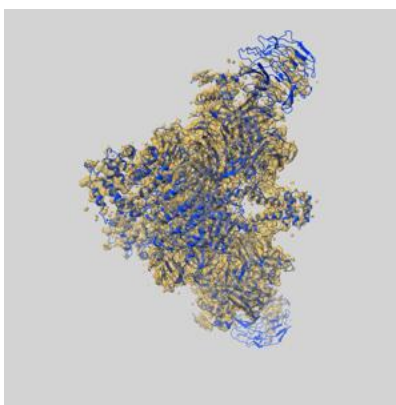
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31765 and PDB model 7V7B. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

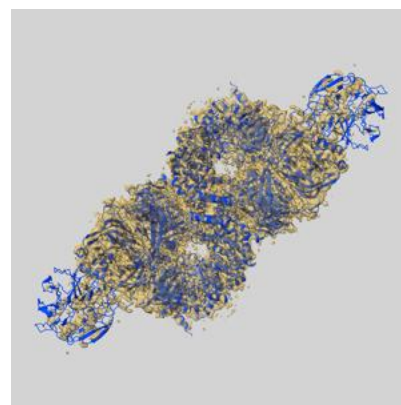
9.1 Map-model overlay [i](#)



X



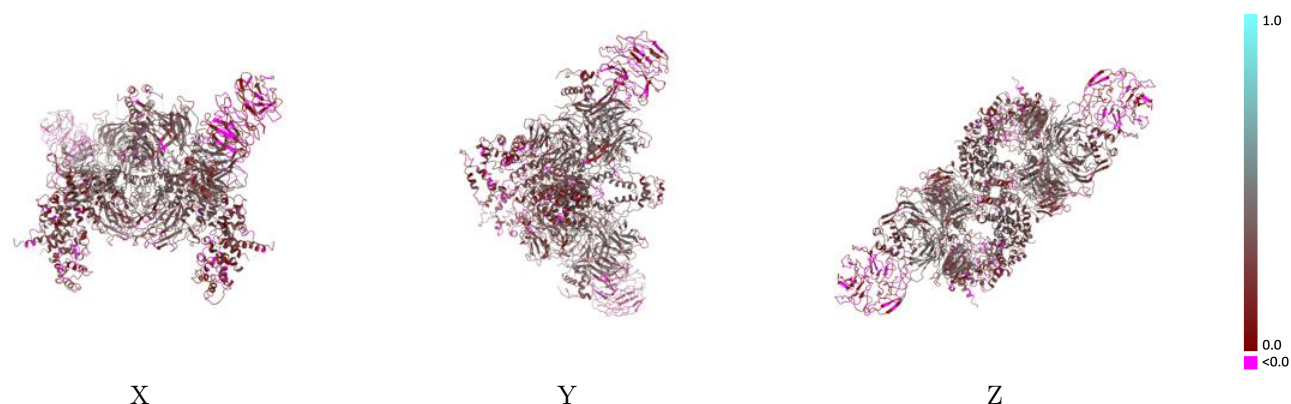
Y



Z

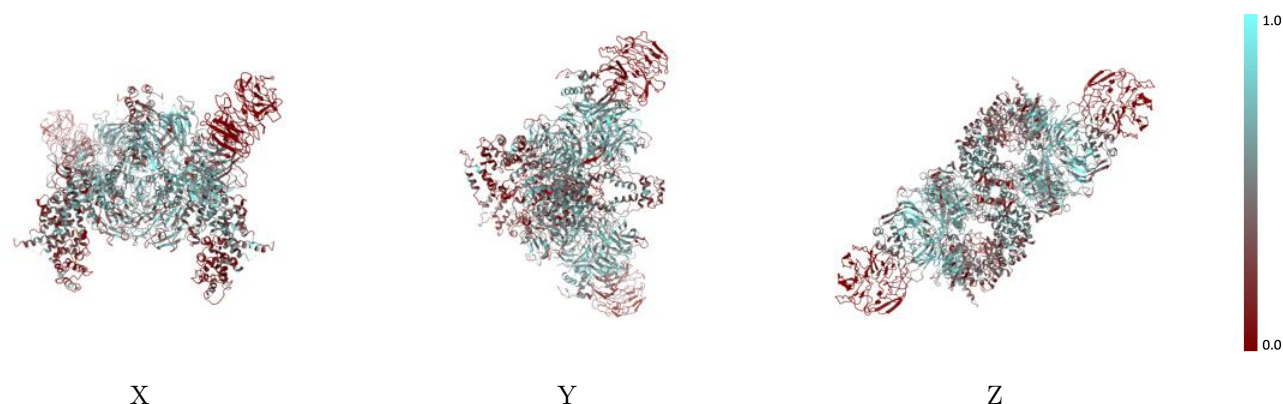
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



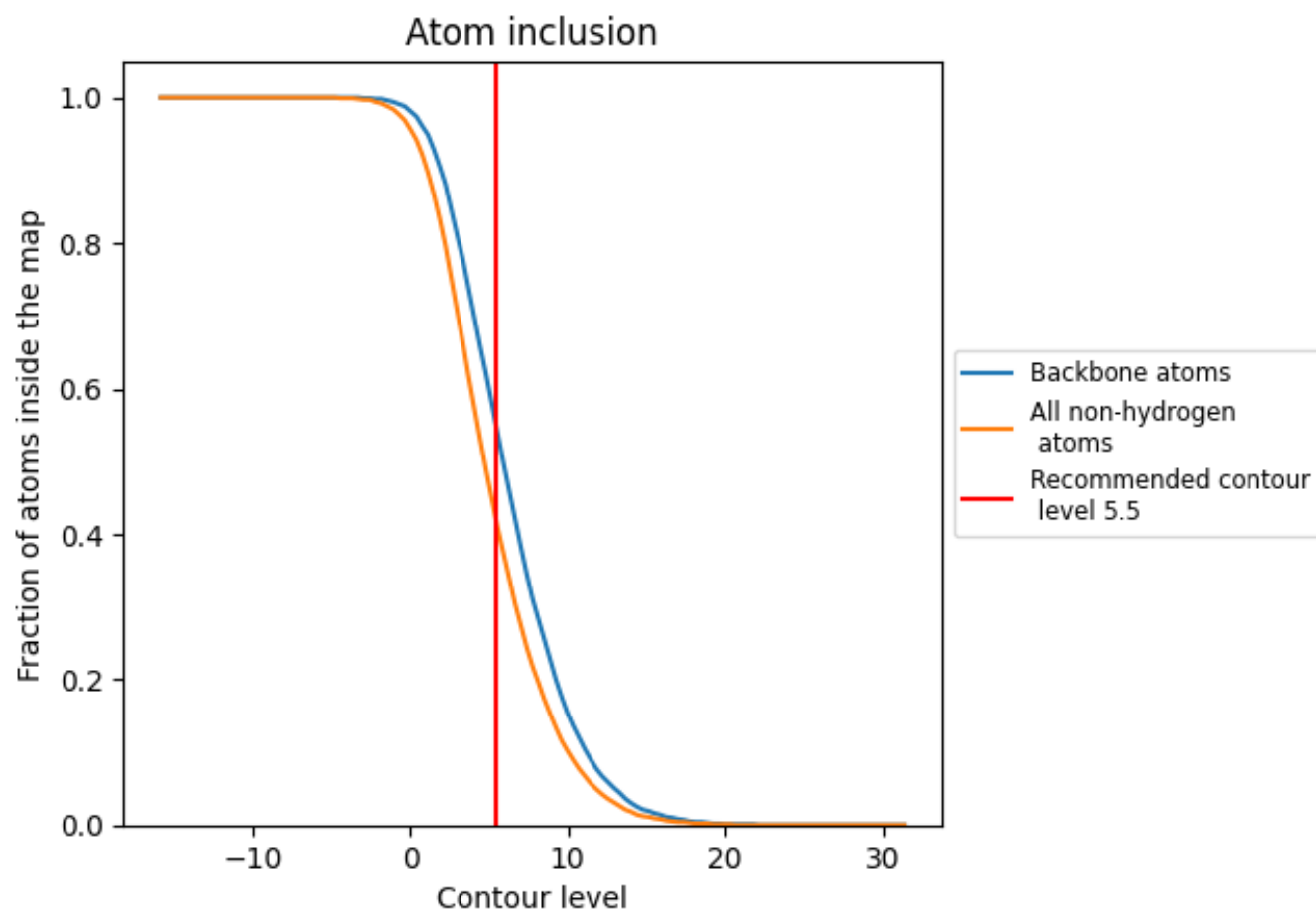
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 42% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4160	<div></div> 0.2620
A	<div></div> 0.4180	<div></div> 0.2650
B	<div></div> 0.4140	<div></div> 0.2610
C	<div></div> 0.4180	<div></div> 0.2640
D	<div></div> 0.4120	<div></div> 0.2600

