



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 06:09 PM JST

PDB ID : 7VHK
EMDB ID : EMD-31997
Title : S1-S2 deletion S-2P trimer(3 down)
Authors : Wang, X.; Cui, Z.
Deposited on : 2021-09-22
Resolution : 3.60 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

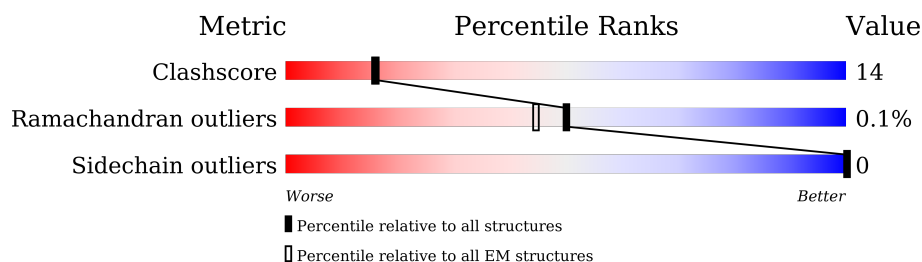
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	1114	<div> <div>37%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
1	B	1114	<div> <div>39%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	C	1114	<div> <div>37%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25191 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1077	Total	C	N	O	S	0	0
			8397	5352	1401	1606	38		
1	A	1077	Total	C	N	O	S	0	0
			8397	5352	1401	1606	38		
1	C	1077	Total	C	N	O	S	0	0
			8397	5352	1401	1606	38		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	SER	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	979	PRO	LYS	engineered mutation	UNP P0DTC2
B	980	PRO	VAL	engineered mutation	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	SER	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	979	PRO	LYS	engineered mutation	UNP P0DTC2
A	980	PRO	VAL	engineered mutation	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2

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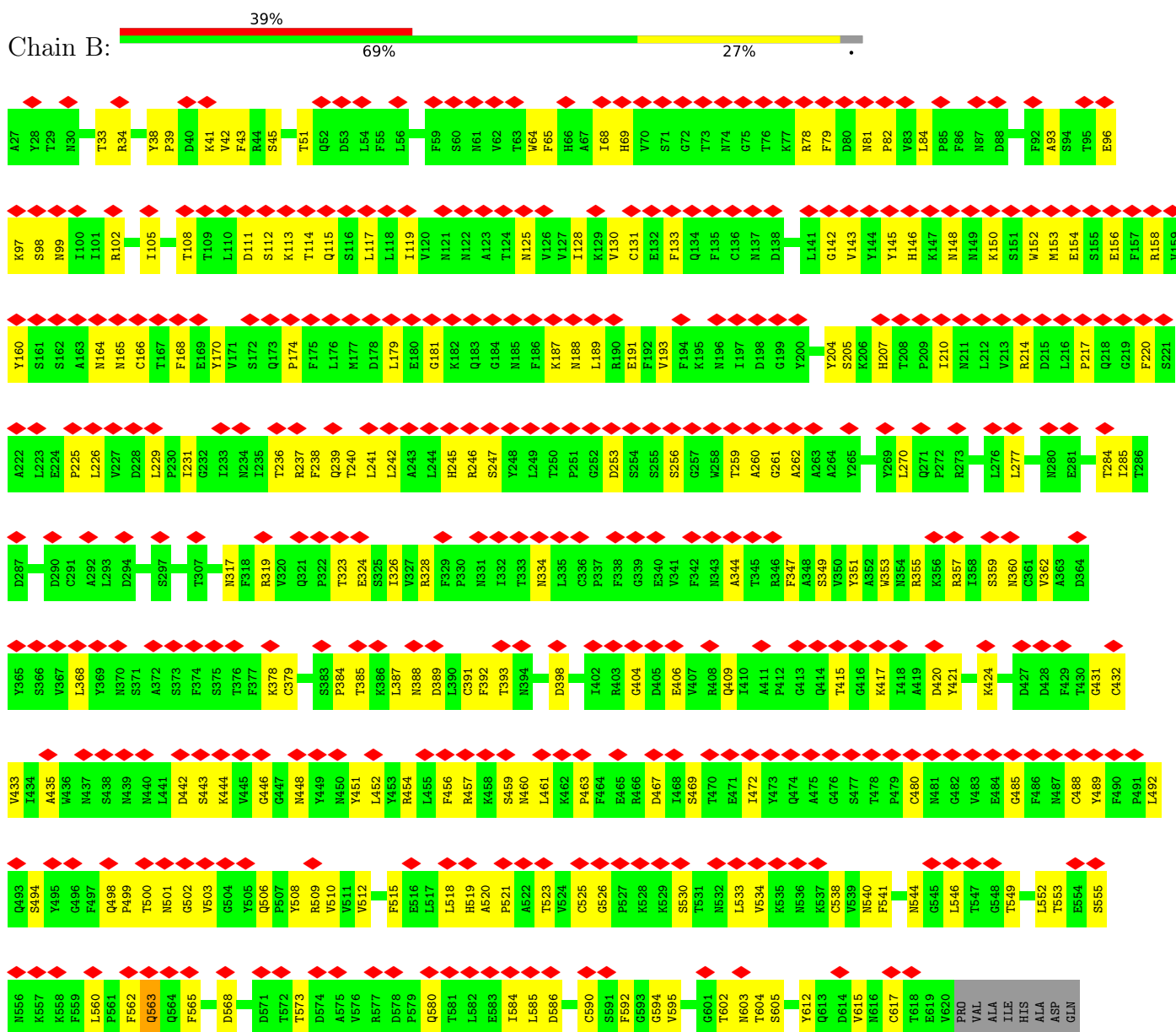
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P0DTC2
C	979	PRO	LYS	engineered mutation	UNP P0DTC2
C	980	PRO	VAL	engineered mutation	UNP P0DTC2

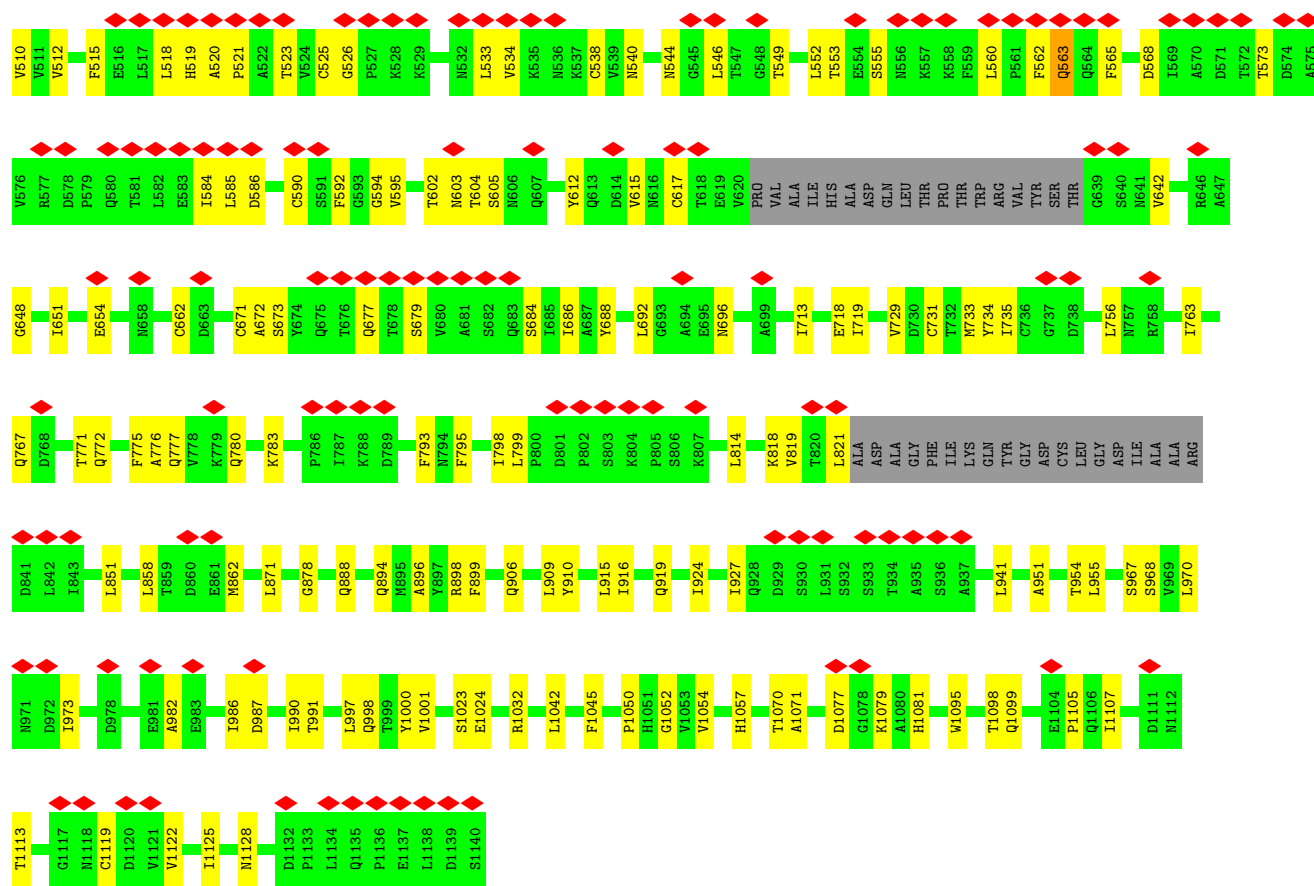
3 Residue-property plots

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.

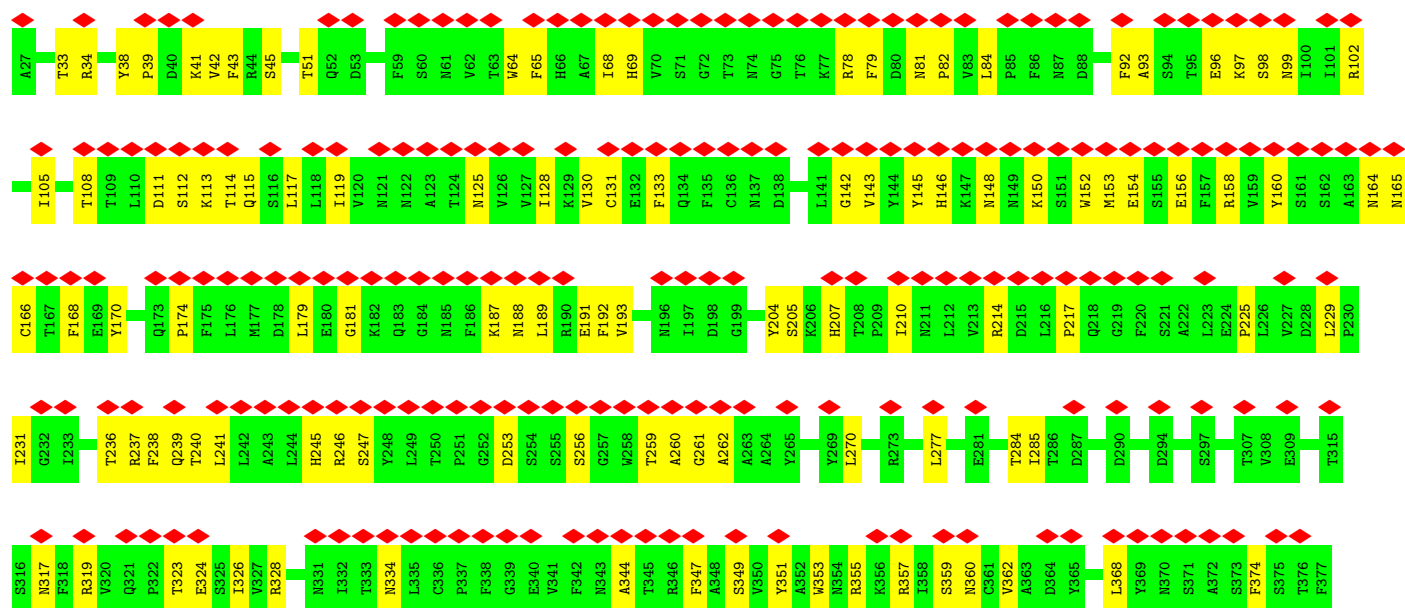
• Molecule 1: Spike glycoprotein







• Molecule 1: Spike glycoprotein



G1117	N1118	C1119	D1120	V1121	V1122	I1125	N1128	D1132	P1133	L1134	Q1135	P1136	E1137	L1138	D1139	S1140	N971	D972	I973	D978	E981	A982	E983	I986	D987	T990	T991	L997	Q998	T999	V1000	V1001	S1023	E1024	R1032	L1042	F1045	P1050	H1051	G1052	V1053	V1054	H1057	N1067	T1070	A1071	D1077	G1078	H1081	W1095	T1098	Q1099	E1104	P1105	D1111	N1112	T1113																																																														
L851	L858	T859	D860	E861	M862	L871	G878	Q888	Q894	R895	A896	R898	F899	Q906	L909	Y910	L915	I916	Q919	I924	G925	K926	I927	Q928	D929	S930	L931	S932	S933	T934	A935	S936	A937	L941	Q942	D943	A951	T954	L955	S967	S968	V969	L970	N971	D972	I973	D978	E981	A982	E983	I986	D987	T990	T991	L997	Q998	T999	V1000	V1001	S1023	E1024	R1032	L1042	F1045	P1050	H1051	G1052	V1053	V1054	H1057	N1067	T1070	A1071	D1077	G1078	H1081	W1095	T1098	Q1099	E1104	P1105	D1111	N1112	T1113																																			
T771	Q772	A776	Q777	V778	K779	Q780	K783	P786	I787	K788	D789	F793	N794	F795	I798	D801	P802	S803	K804	P805	S806	K807	L814	K818	V819	T820	L821	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	ARG	D841	L842	I843	C844	T771	Q772	A776	Q777	V778	K779	Q780	K783	P786	I787	K788	D789	F793	N794	F795	I798	D801	P802	S803	K804	P805	S806	K807	L814	K818	V819	T820	L821	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	ARG	D841	L842	I843	C844																		
R646	A647	G648	I651	E654	N658	C662	D663	C671	A672	S673	T676	Q677	T678	S679	V680	A681	S682	Q683	S684	I685	I686	A687	Y688	L692	N696	A699	I713	E718	I719	V729	D730	C731	I732	M733	V734	I736	C736	G737	L756	N757	R758	I763	D767	D768	R646	A647	G648	I651	E654	N658	C662	D663	C671	A672	S673	T676	Q677	T678	S679	V680	A681	S682	Q683	S684	I685	I686	A687	Y688	L692	N696	A699	I713	E718	I719	V729	D730	C731	I732	M733	V734	I736	C736	G737	L756	N757	R758	I763	D767	D768																														
T572	T573	D574	R577	D578	P579	Q580	T581	L582	E583	I584	L585	D586	C590	S591	F592	T597	G593	G594	V595	G601	T602	N603	T604	S605	Y612	Q613	D614	V615	N616	C617	T618	E619	V620	PRO	VAL	ALA	ALA	ILE	HIS	ASP	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TTR	SER	THR	G639	S640	N641	V642	T572	T573	D574	R577	D578	P579	Q580	T581	L582	E583	I584	L585	D586	C590	S591	F592	T597	G593	G594	V595	G601	T602	N603	T604	S605	Y612	Q613	D614	V615	N616	C617	T618	E619	V620	PRO	VAL	ALA	ALA	ILE	HIS	ASP	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TTR	SER	THR	G639	S640	N641	V642						
Y508	R509	V510	V511	V512	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	K529	S530	T531	N532	L533	V534	K535	N536	K537	C538	V539	N540	F541	N544	G545	L546	T547	G548	T549	L552	T553	E554	S555	N556	K557	K558	F559	L560	P561	F562	Q563	Q564	F565	D568	I569	A570	D571	Y508	R509	V510	V511	V512	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	K529	S530	T531	N532	L533	V534	K535	N536	K537	C538	V539	N540	F541	N544	G545	L546	T547	G548	T549	L552	T553	E554	S555	N556	K557	K558	F559	L560	P561	F562	Q563	Q564	F565	D568	I569	A570	D571								
M448	Y449	M450	L451	L452	Y453	R454	L455	F456	R457	K458	S459	M460	L461	K462	P463	F464	E465	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	S477	T478	P479	C480	M481	G482	V483	E484	G485	F486	M487	C488	Y489	F490	I491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	V503	G504	Y505	Q506	P507	M448	Y449	M450	L451	L452	Y453	R454	L455	F456	R457	K458	S459	M460	L461	K462	P463	F464	E465	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	S477	T478	P479	C480	M481	G482	V483	E484	G485	F486	M487	C488	Y489	F490	I491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	V503	G504	Y505	Q506	P507
K378	C379	Y380	S383	P384	T385	K386	L387	N388	D389	C390	F391	T392	T393	N394	D398	G404	D405	E406	V407	R408	A411	P412	G413	Q414	T415	G416	K417	I418	A419	D420	Y421	K424	L425	P426	D427	D428	G431	C432	V433	I434	A435	W436	N437	S438	N439	N440	L441	D442	S443	K444	V445	G446	G447	K378	C379	Y380	S383	P384	T385	K386	L387	N388	D389	C390	F391	T392	T393	N394	D398	G404	D405	E406	V407	R408	A411	P412	G413	Q414	T415	G416	K417	I418	A419	D420	Y421	K424	L425	P426	D427	D428	G431	C432	V433	I434	A435	W436	N437	S438	N439	N440	L441	D442	S443	K444	V445	G446	G447												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100907	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 ($e^-/\text{\AA}^2$)	1.875	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.139	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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	0.33	0/8592	0.47	0/11695
1	B	0.33	0/8592	0.47	0/11695
1	C	0.33	0/8592	0.47	0/11695
All	All	0.33	0/25776	0.47	0/35085

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	8397	0	8185	246	0
1	B	8397	0	8185	252	0
1	C	8397	0	8185	246	0
All	All	25191	0	24555	705	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 14.

The worst 5 of 705 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:A:393:THR:HG21	1:A:520:ALA:HB3	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:THR:HG21	1:C:520:ALA:HB3	1.39	1.03
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.39	1.02
1:B:909:LEU:HD12	1:B:916:ILE:HD12	1.44	0.99
1:C:909:LEU:HD12	1:C:916:ILE:HD12	1.44	0.99

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	1071/1114 (96%)	973 (91%)	97 (9%)	1 (0%)	48	79
1	B	1071/1114 (96%)	971 (91%)	99 (9%)	1 (0%)	48	79
1	C	1071/1114 (96%)	972 (91%)	98 (9%)	1 (0%)	48	79
All	All	3213/3342 (96%)	2916 (91%)	294 (9%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	563	GLN
1	A	563	GLN
1	C	563	GLN

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	937/966 (97%)	937 (100%)	0	100	100
1	B	937/966 (97%)	937 (100%)	0	100	100
1	C	937/966 (97%)	937 (100%)	0	100	100
All	All	2811/2898 (97%)	2811 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	460	ASN
1	C	580	GLN
1	C	962	ASN
1	A	146	HIS
1	A	49	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 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 ⓘ

There are no chain breaks in this entry.

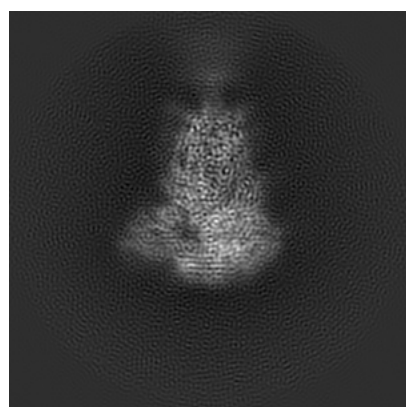
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31997. These allow visual inspection of the internal detail of the map and identification of artifacts.

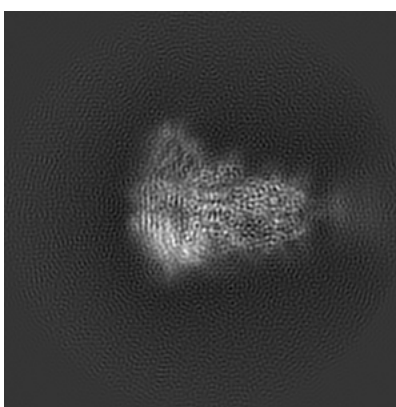
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

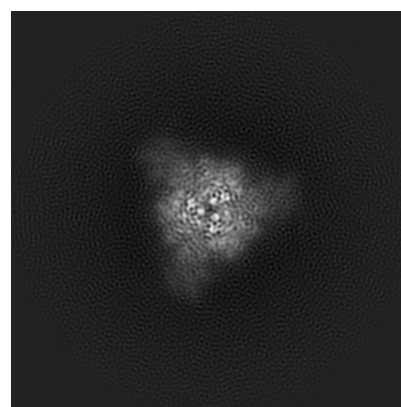
6.1.1 Primary map



X



Y

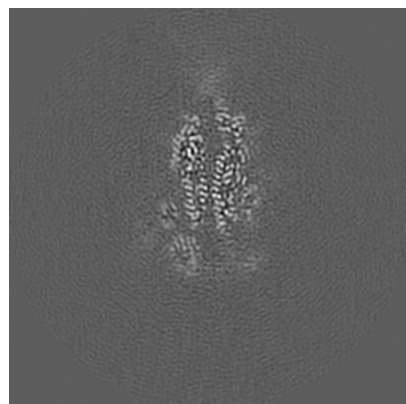


Z

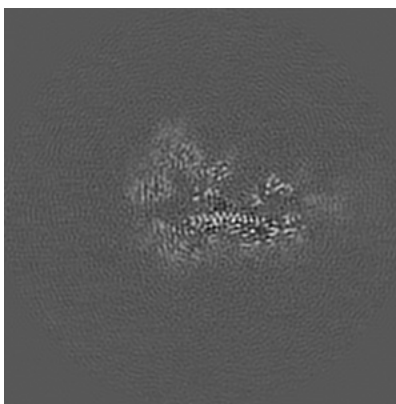
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

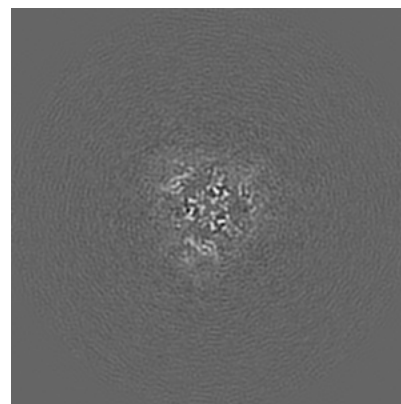
6.2.1 Primary map



X Index: 160



Y Index: 160

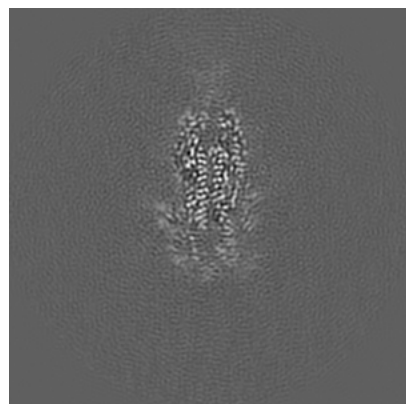


Z Index: 160

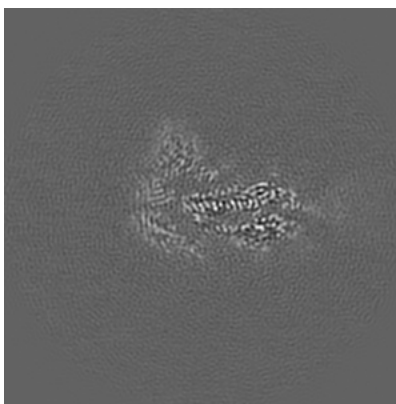
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

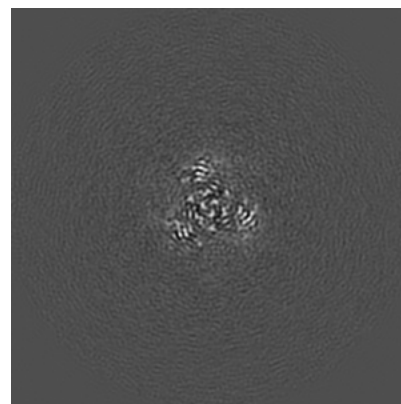
6.3.1 Primary map



X Index: 164



Y Index: 168

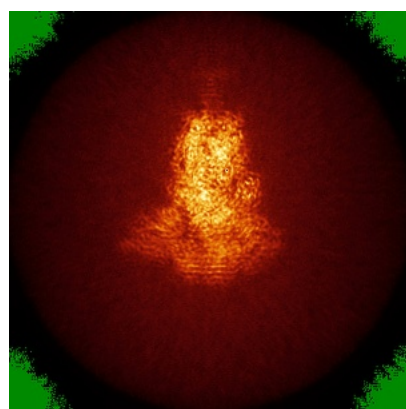


Z Index: 171

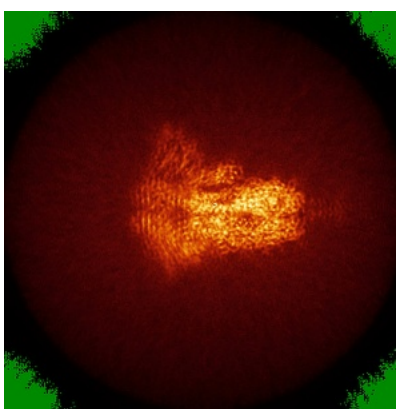
The images above show the largest variance slices of the map in three orthogonal directions.

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

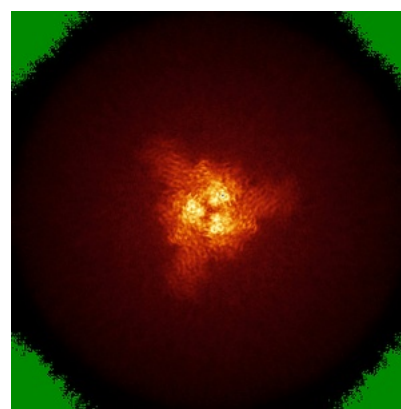
6.4.1 Primary map



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

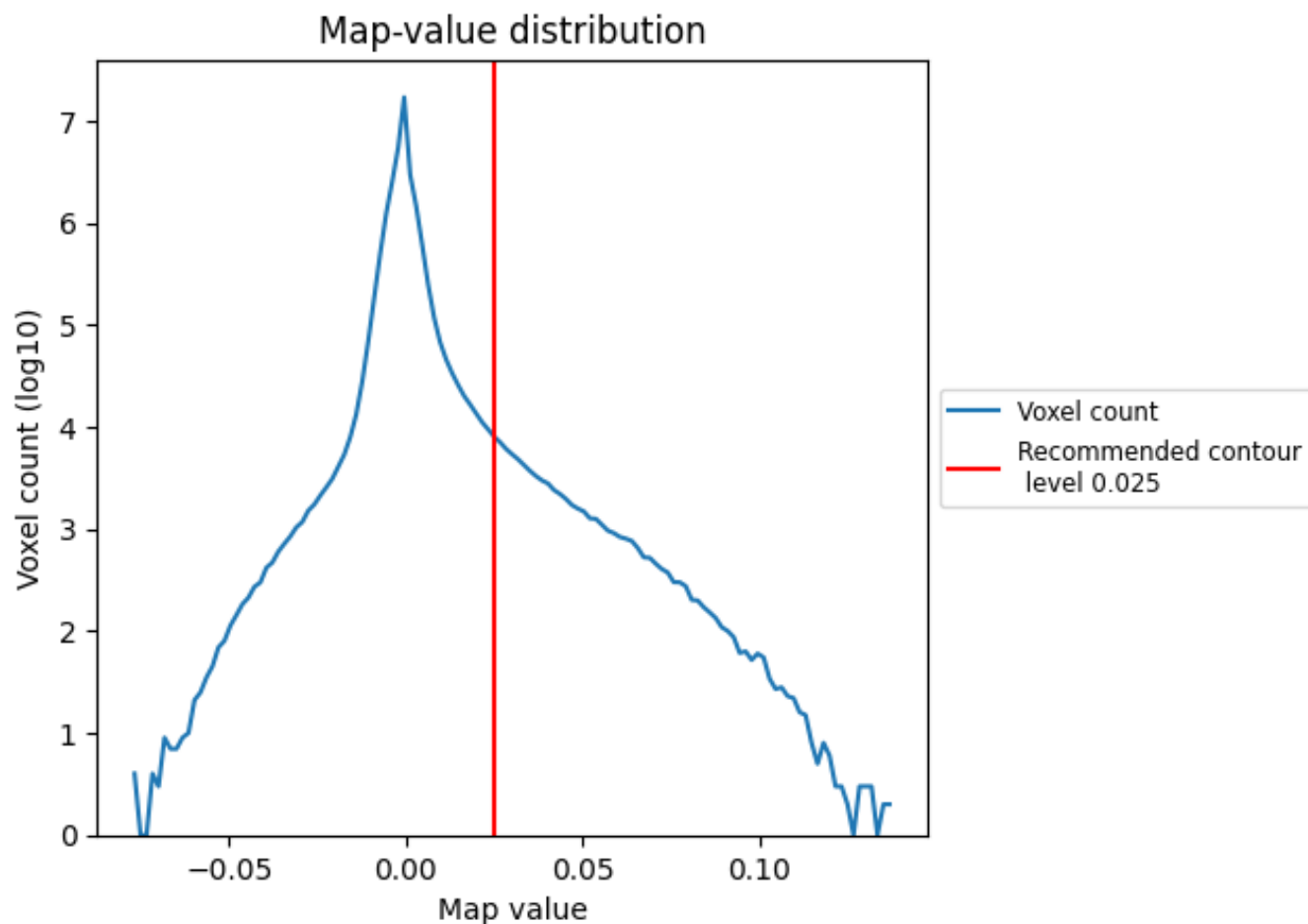
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

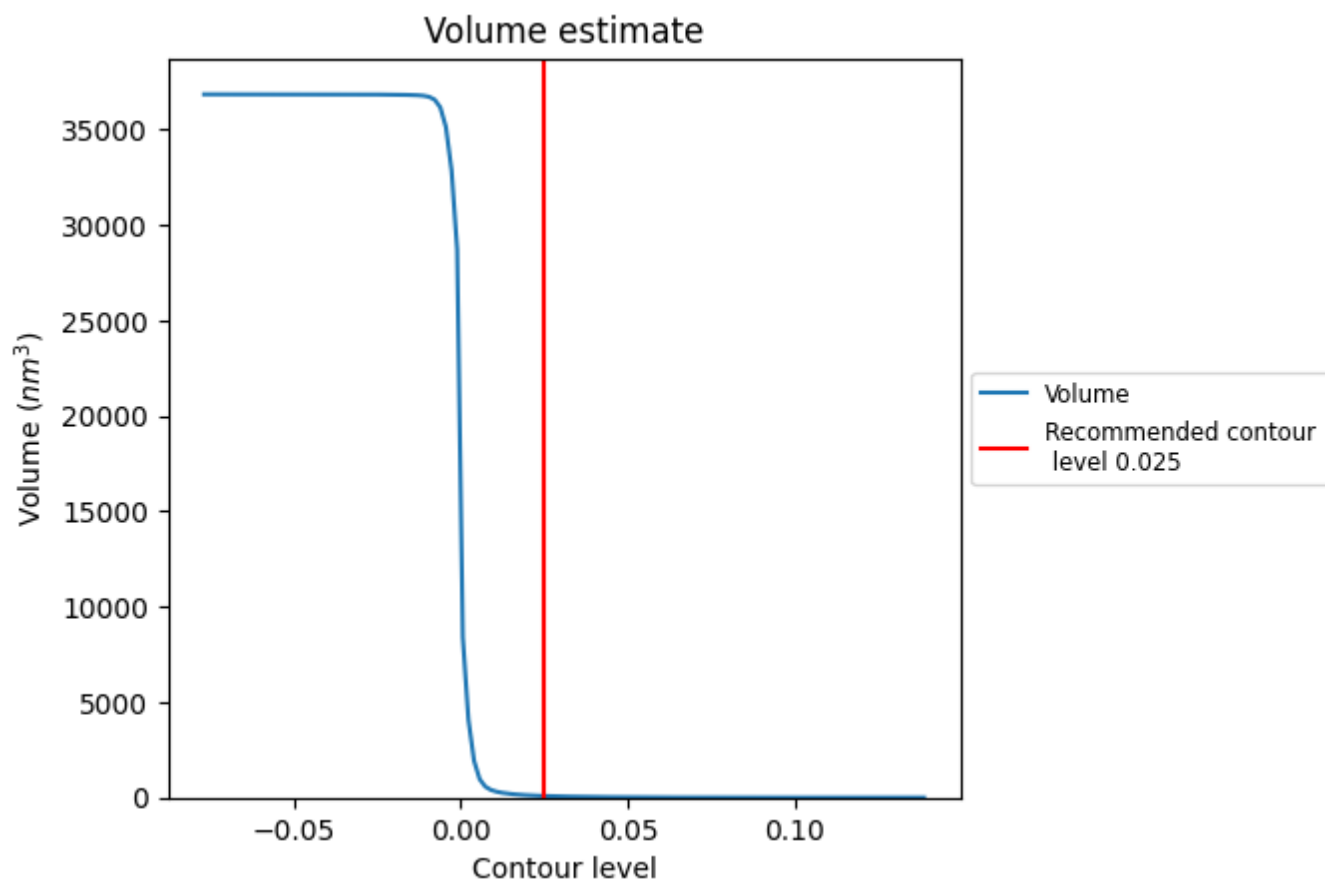
This section contains the results of statistical analysis of the map.

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.

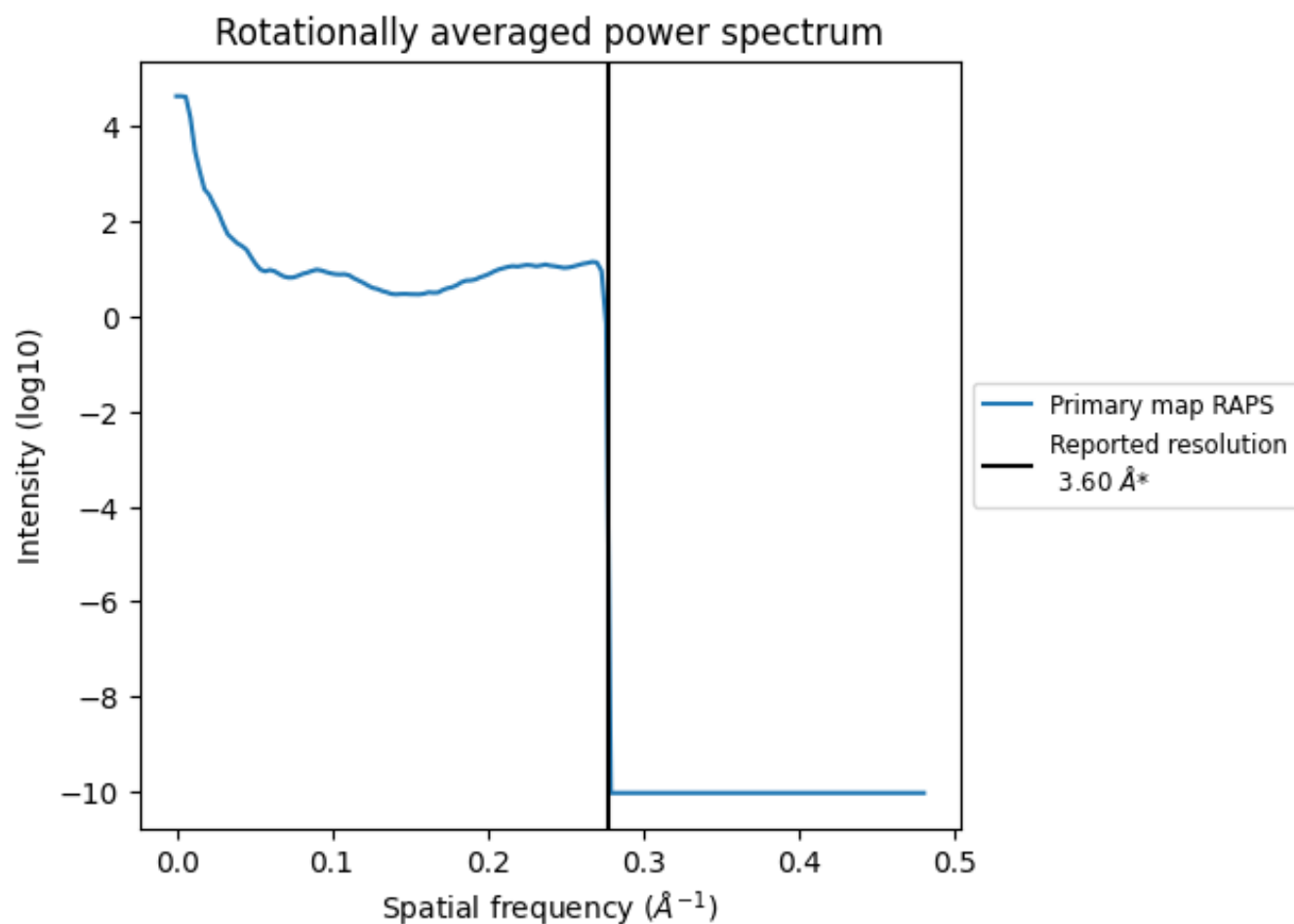
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 83 nm^3 ; this corresponds to an approximate mass of 75 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 0.278 Å⁻¹

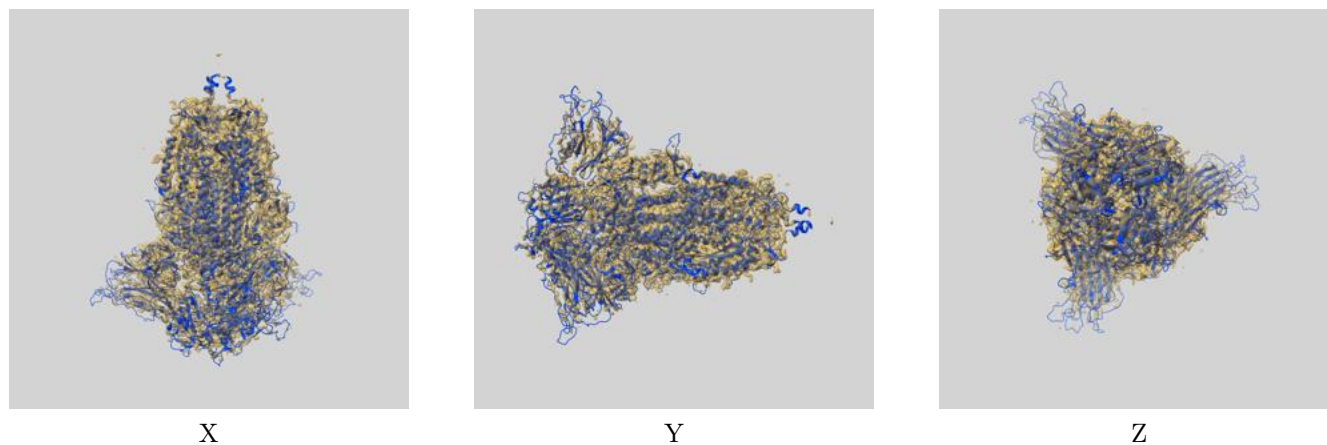
8 Fourier-Shell correlation

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-31997 and PDB model 7VHK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



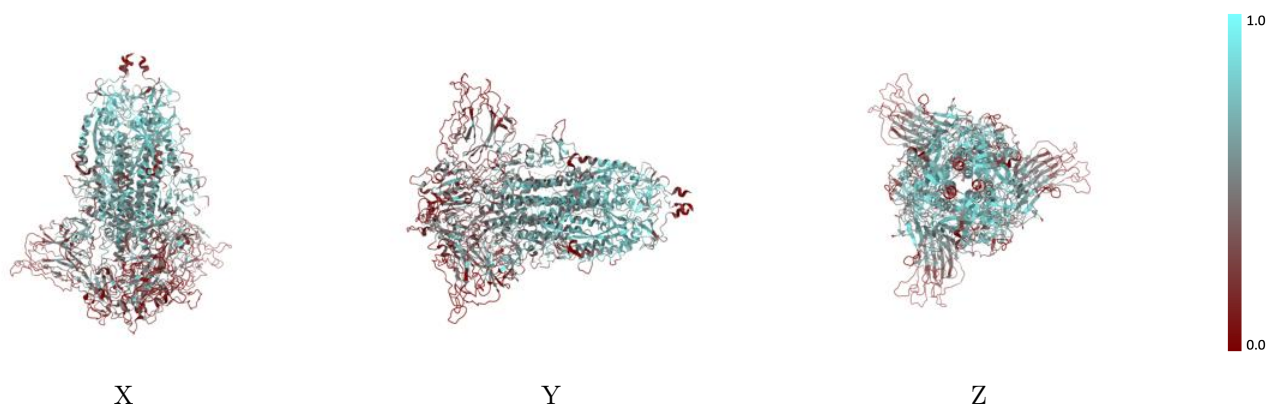
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



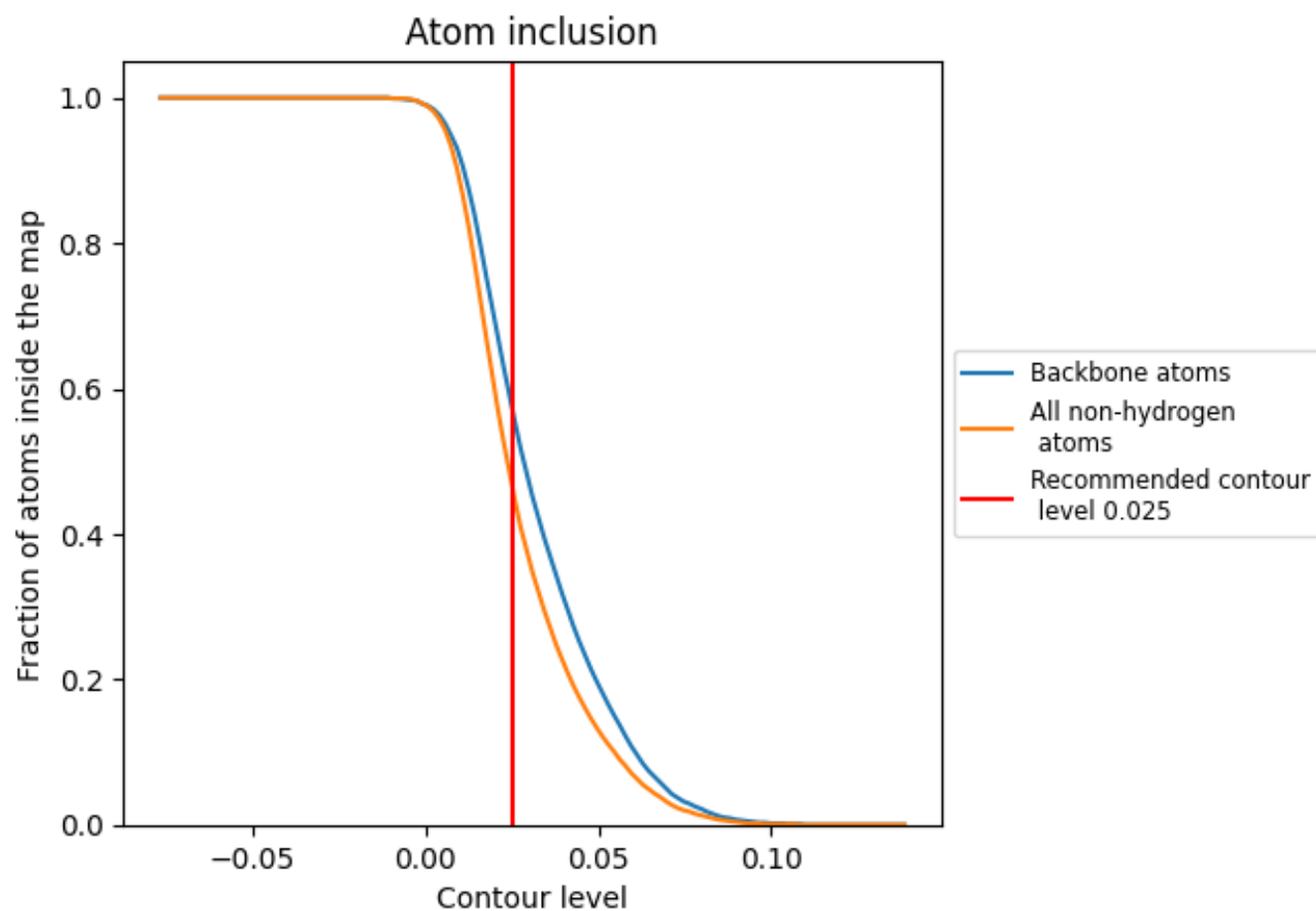
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 47% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4660	<div></div> 0.4380
A	<div></div> 0.4690	<div></div> 0.4380
B	<div></div> 0.4620	<div></div> 0.4410
C	<div></div> 0.4670	<div></div> 0.4350

