



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 10:57 AM UTC

PDB ID : 8QOX / pdb_00008qox
EMDB ID : EMD-18127
Title : Two-component assembly of SlaA and SlaB S-layer proteins of *Sulfolobus acidocaldarius*
Authors : Gambelli, L.; McLaren, M.; Isupov, M.; Conners, R.; Daum, B.
Deposited on : 2023-09-29
Resolution : 11.20 Å (reported)
Based on initial models : ., 7ZCX

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

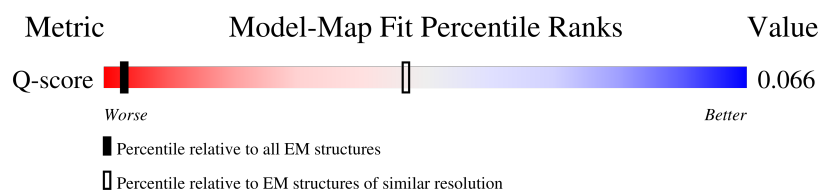
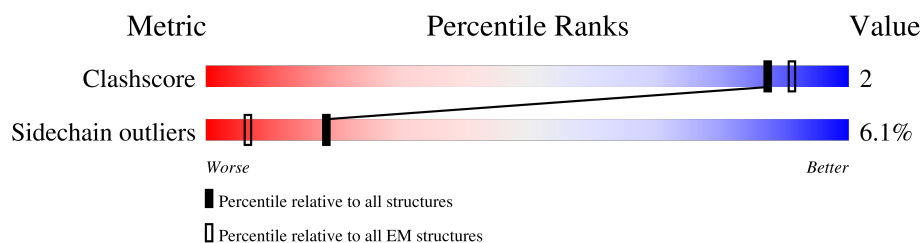
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

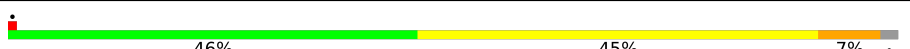
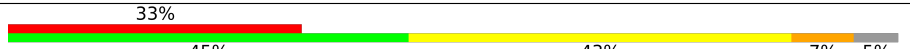
The reported resolution of this entry is 11.20 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	94 (10.70 - 11.70)

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	1424	
1	V	1424	
1	W	1424	
1	Z	1424	
2	B	475	

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Mol	Chain	Length	Quality of chain
2	C	475	36% 49% 40% 6% 5%
2	X	475	39% 47% 43% 5% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 51848 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 S-layer protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	V	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	W	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	Z	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		

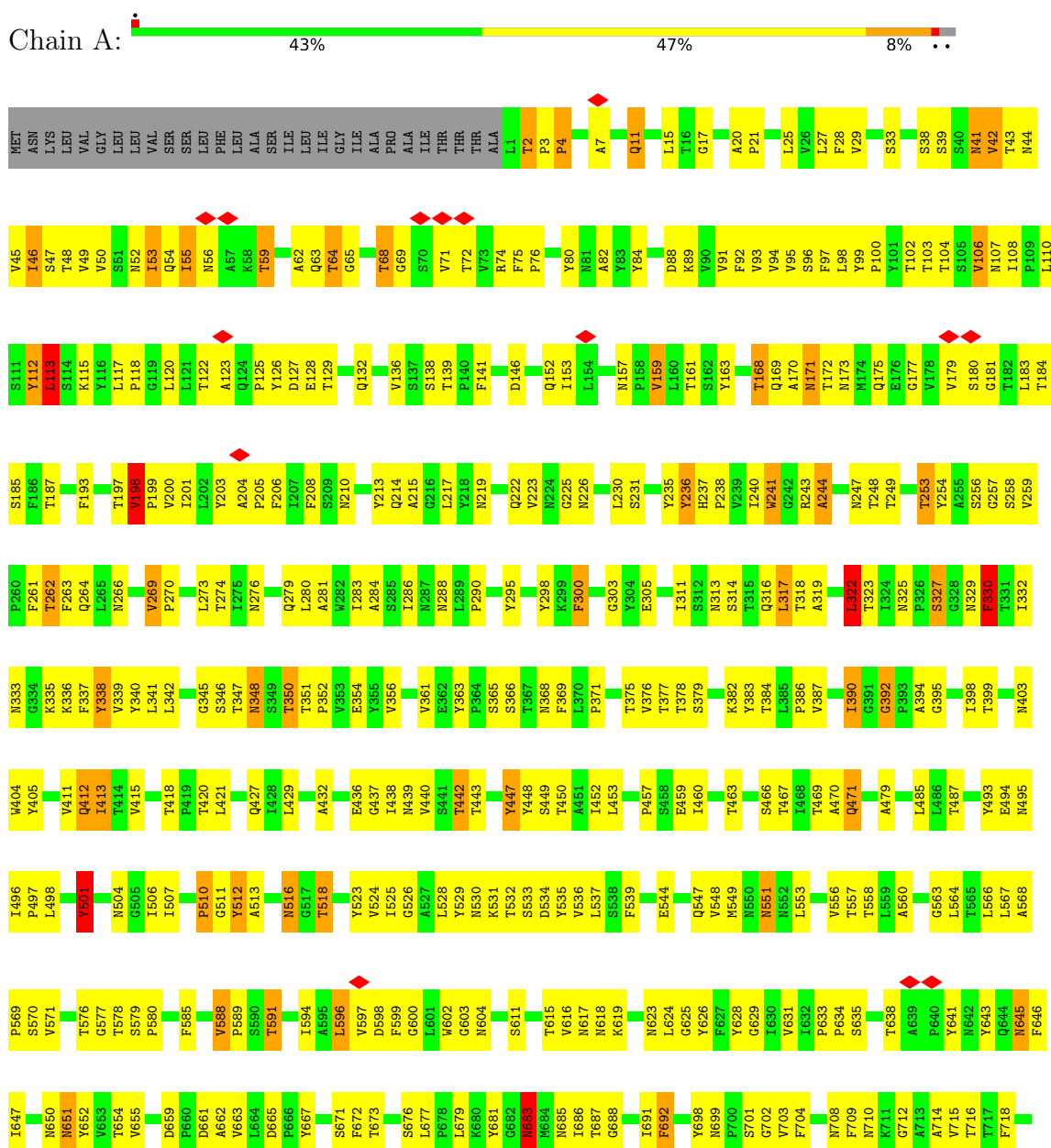
- Molecule 2 is a protein called Conserved membrane protein.

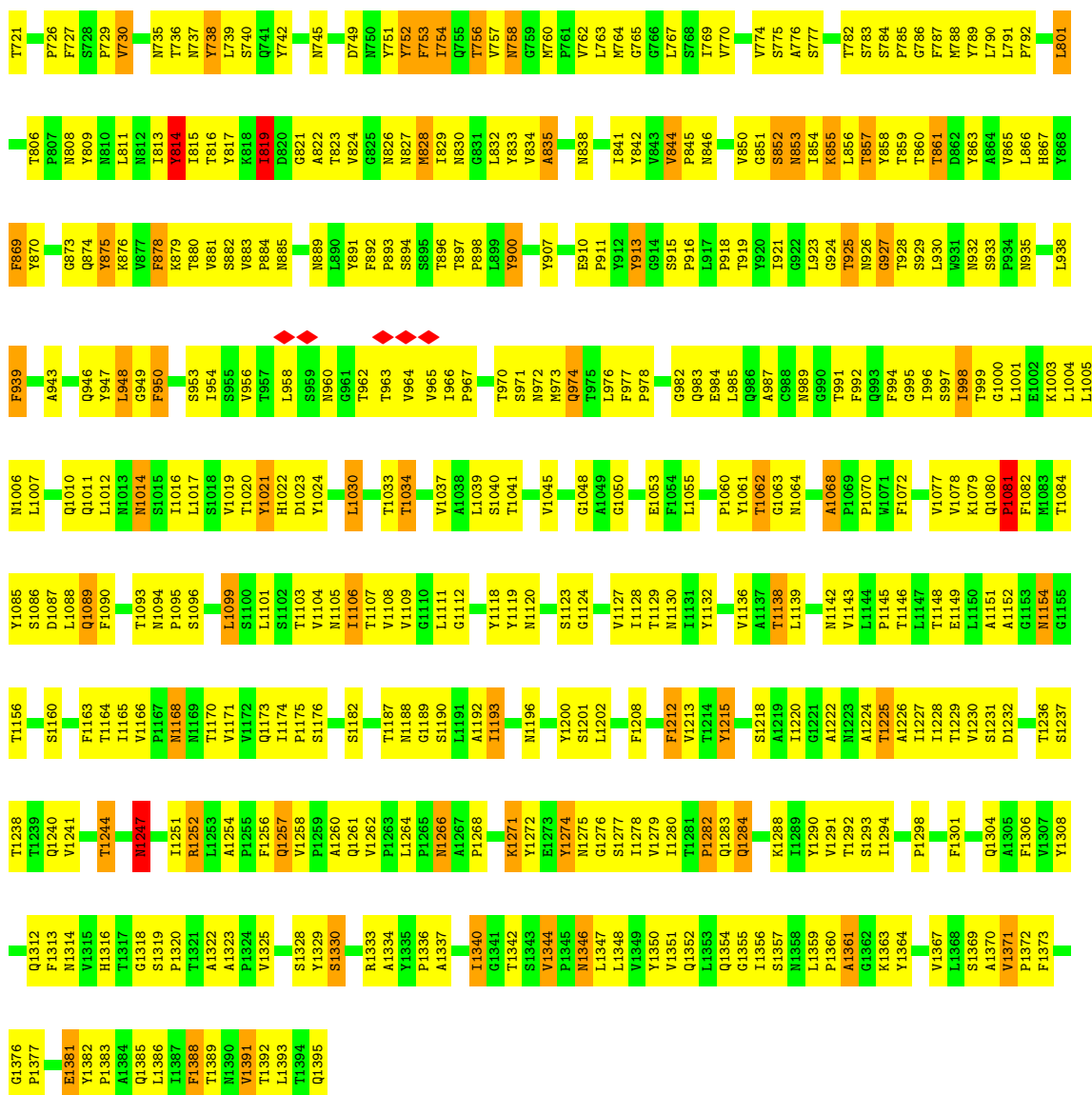
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		
2	C	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		
2	X	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		

3 Residue-property plots

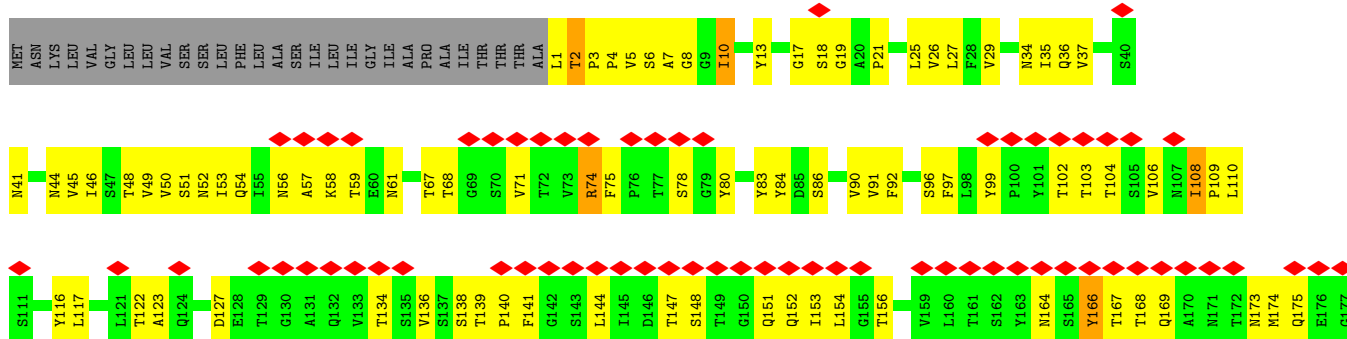
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

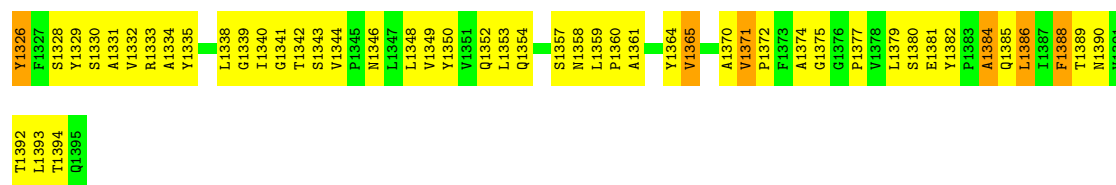




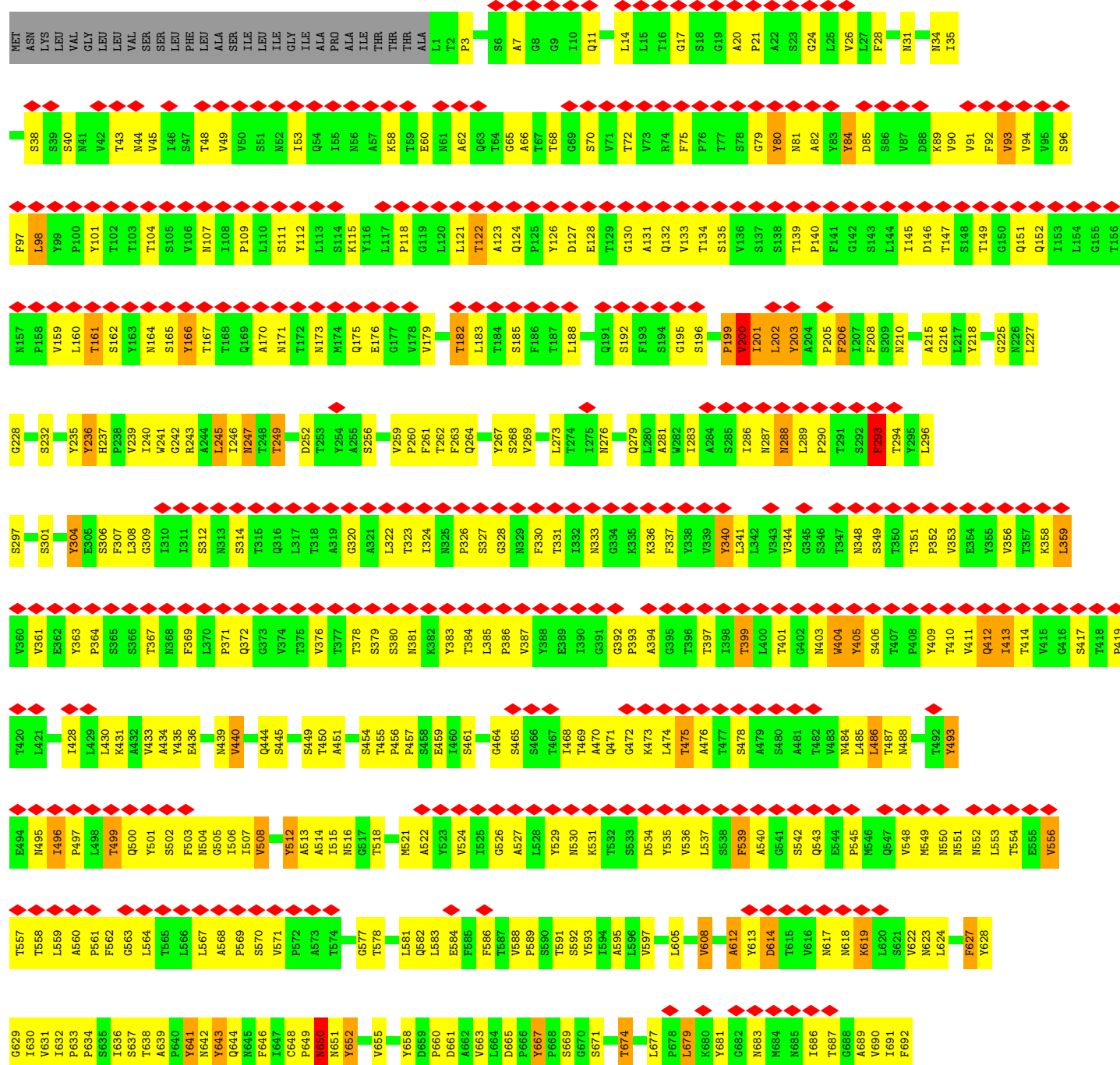
• Molecule 1: S-layer protein A

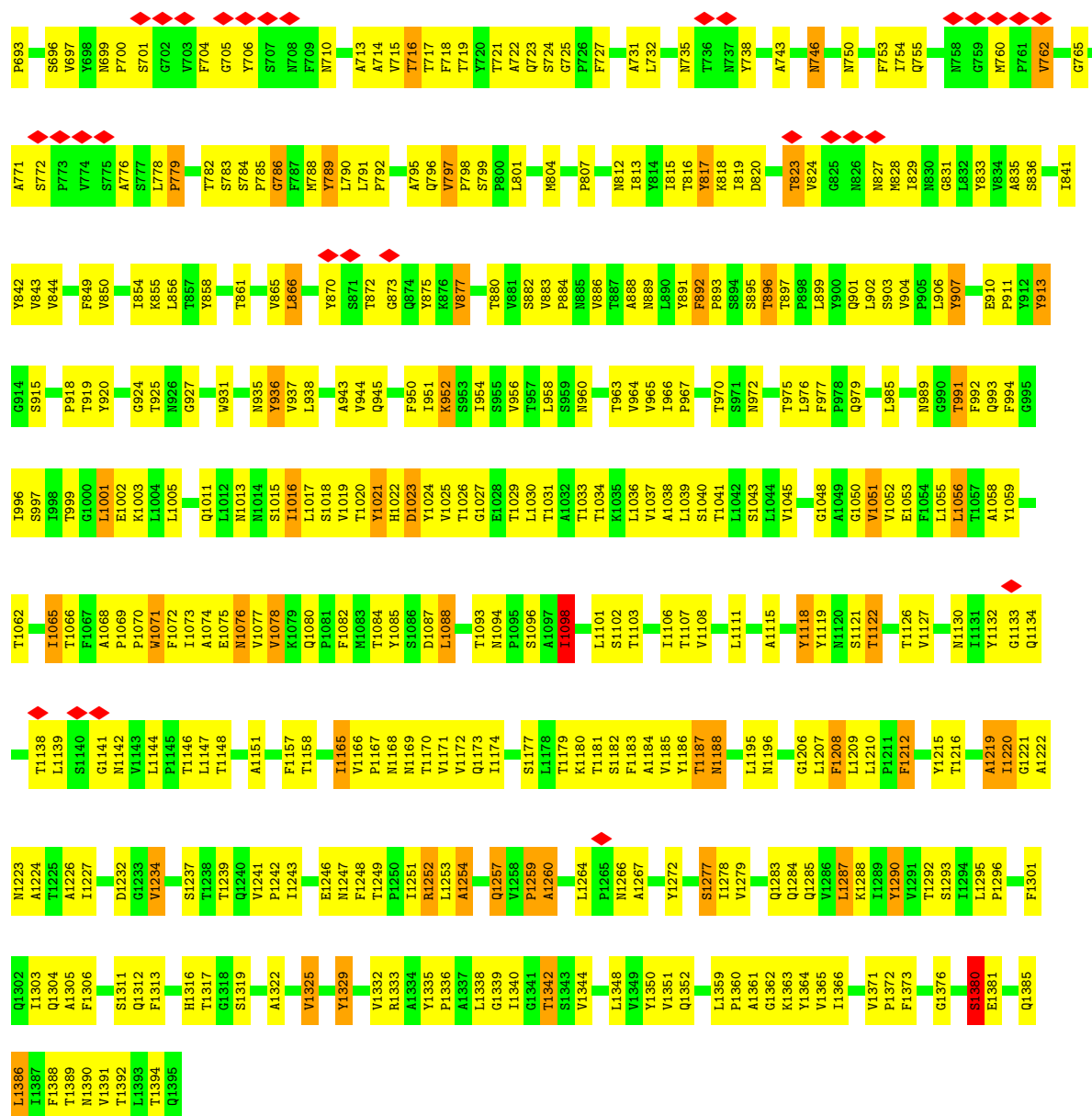


F1248	V1171	S1096	G1027	V877	V797	P729	T654	A568	N484	W404	N333	I251	V178
T1249	V1172	A1097	E1028	F878	P798	T733	V655	P569	T487	T407	G334	D252	V179
P1250	I1173	I1098	T1029	K879	L801	G734	T656	S570	T488	P408	K335	D253	S180
R1251	I1174	L1101	A1032	V881	A805	N735	D659	V571	A489	P409	K336	A255	G181
L1252	S1175	S955	S955	V882	T806	T736	D661	P580	A490	T410	Y337	G257	T182
A1254	S1177	T957	T1034	V883	P807	N737	D662	V588	L491	V411	Y338		L183
P1255	L1178	L958	K1035	F884	N808	Y738	A662	P589	T492		L342	Q264	T184
F1256	M1105	S959	L1036	N885	N810	L739	V663	P590	Y493	T418	V343	L265	S185
	V1108	T962	V1037	V886	N810	Q741	L664	Y593	E494	T419	G344	L266	F186
			L1038	T887	N810	Y742		Y594		T420	V345	Y267	T187
			L1039	A888		A743	S669	I594	L498	T421	S346	S268	L188
	G1113	T966	S1040	Y817	Y817	Y744	G670	V597	T499	T422	T347	V269	F193
	K1114	P967	T1041	K818	K818	D744	S671	D598	I507	N423	K348	P270	
	V1117	L968		F892	L819	F745	F672	F598	V508	Y424	S349	G271	T197
	Y1118	T969	V1045	P893	D820	T754	T673	T509	T509	Y425	V350	G272	V198
	Y1119	T970		S894		T755		G600	Y512	Q427	T351	L273	P199
	N1120	S971	G1048	T897	T823	D749	S676	L601		K431	E354	T274	V200
		N972	A1049	P898	N826	Y750	L677	V602	Y516	A432	Y355	I275	I201
		N973		P898	N827	Y751	Y681	G603		A433	Y356	M277	L202
		L976	E1053	P899	M828	F752	Y682	Y613	Y523	A434	V360	Q279	Y203
		P978	L1055	Q901	M829	T754	N683	T615	V524	Y435	V361	W282	F206
		P978	L1056	L902	N830	T755	I686	V616	I525	E436	E362	I283	I207
			T1057	G831	G831	T757	T687	M617	G526	G437	Y363	W284	F208
			A1058			Y757	G888	N618	Y529	I438	T367	I284	S209
			P1059	P905	A835	N758	G889	K619	N530	G437	N368	I285	S211
			P1060	L906		G759	A689	V690	N531	S441	N369	P212	P212
			Y1061	Y907	N838	M760	V690	G621	K531	T442	L370	Y213	Y213
			G1063	P911	T839	P761	I687	G622	T532		P371	Q214	Q214
			N1064	P915	L840	M764	S695	N623	S533	S445	V374	A215	A215
			L1065	P916	Y842		S696	L624	S534	Y447	V374	F293	
			T1066	S915	Y842		V697	L624	I537	Y447	T295	Y295	P220
			F1067	Y920	N843	L767	Y698	G625	L537	Y448	L296	Y296	M221
			A1068	I921	V844	T769	N699	Y626	S538	Y449	T378	S297	W224
			P1069	G922	P845	W770	P700	F627	F539	S449	T379	Y298	G225
			P1070	L923	N846	A771	Y701	Y628	S542	T450	S380	N302	N226
			W1071	G924	G847	S772	G629	I630	Q543	I452	K382	L227	L227
			E1075	T925	S848	P773	I630	P633	E544	T455	Y383	G303	G228
			N1076	N926	V850	A776	G705	P634	P645	T456	T384	F307	L230
			V1077	G927	G851	S777	Y706	P635	M546	E459	V387	N313	Y235
			V1078	T928	S852	L778	S707	S635	Q547	I460	Y388	T315	Y236
			K1079		N853	P779	N708	I636	M549	S461	E389	T316	H237
			Q1080	W931	I854	S780	F709	S637	N550	I462	N550	T318	P238
			P1081	S932	L855	S781	N710	S637	N551	T463	G391	A319	V239
			N1013	P934	L856	S782	A714	I636	N552	G464	G392	I240	I240
			S1015	N935	T857	S783	V715	P641	L553	S465		W241	W241
			L1016	Y858	T859		T716	N642	T554	S466	G395	G242	G242
			L1017	T859		F787	T717	Y643	E555	T467	T396	R243	R243
			S1018	D862		M788	F718	Q644	V556	I468	T397	P326	A244
			V1019	Y863		Y789	T719	N645		T469	I398	S327	L245
			T1020	A864		L790	Y720	F646		A470	T399	P561	I246
			Q1089	V865		P792			A560	Q471	L400	N829	N247
			F1090	L866		S793	Q723		P561		T401	F330	T248
			D1023	F867		A794	S724		F562		G402	T331	T249
			Y1024	Y869		A795	G725		Y652		T477	T332	L250
			T1026	N870			S728		V653				

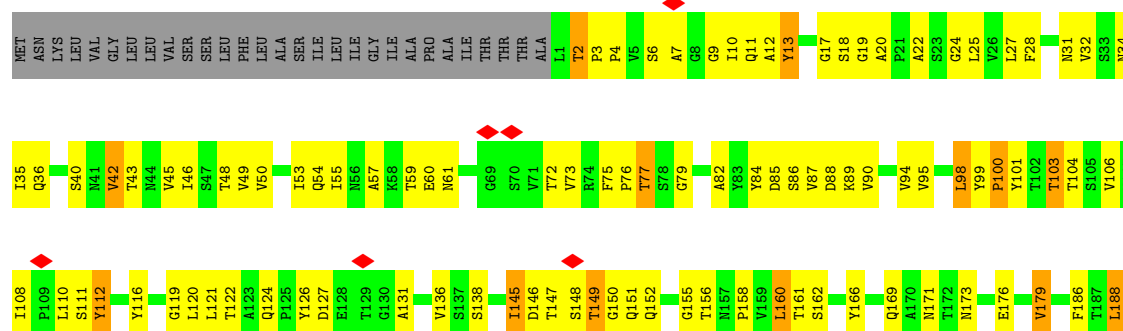


• Molecule 1: S-layer protein A





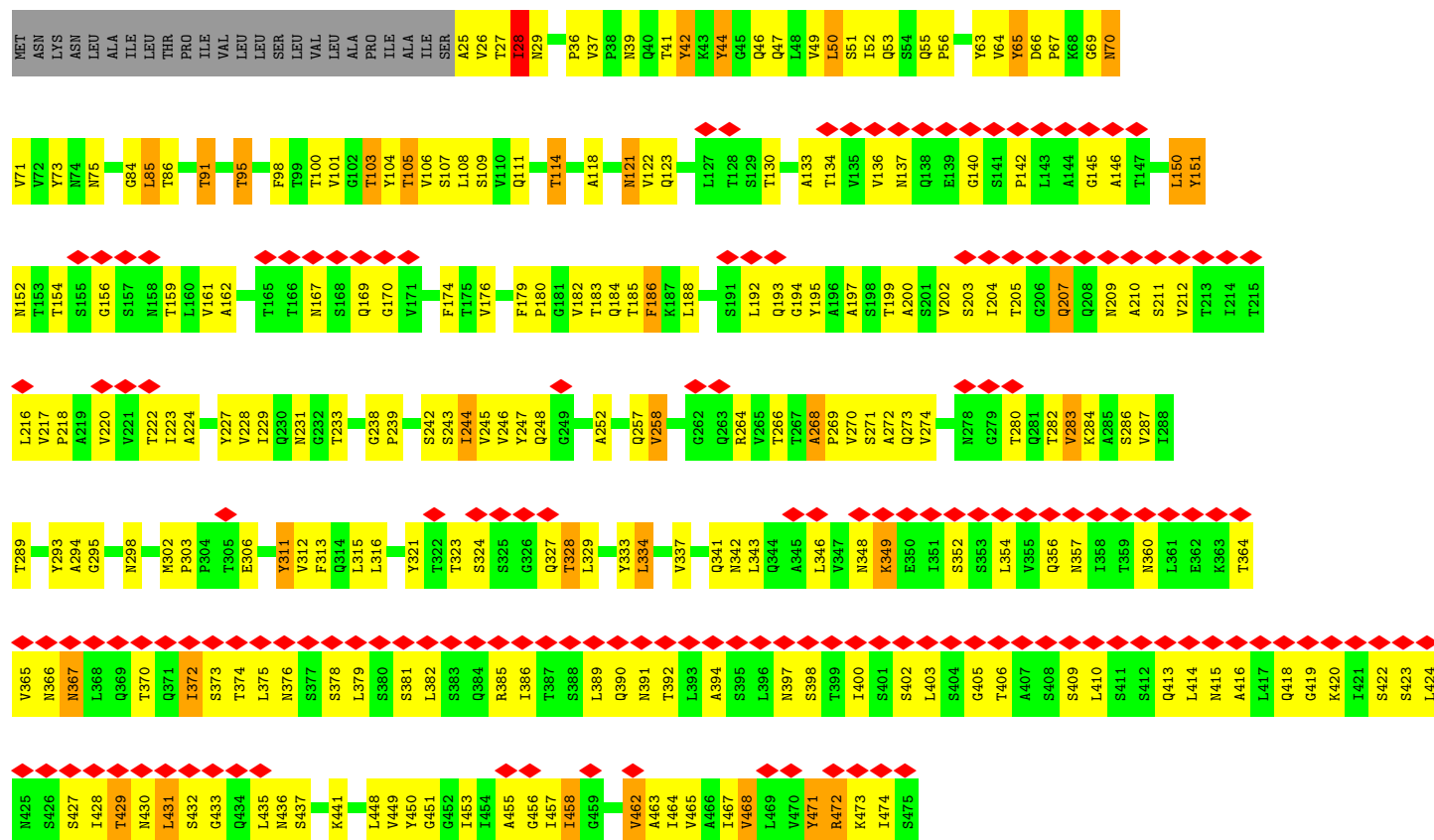
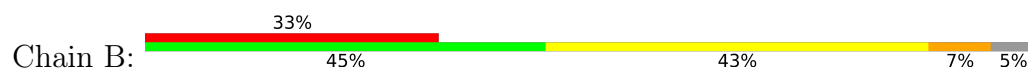
• Molecule 1: S-layer protein A



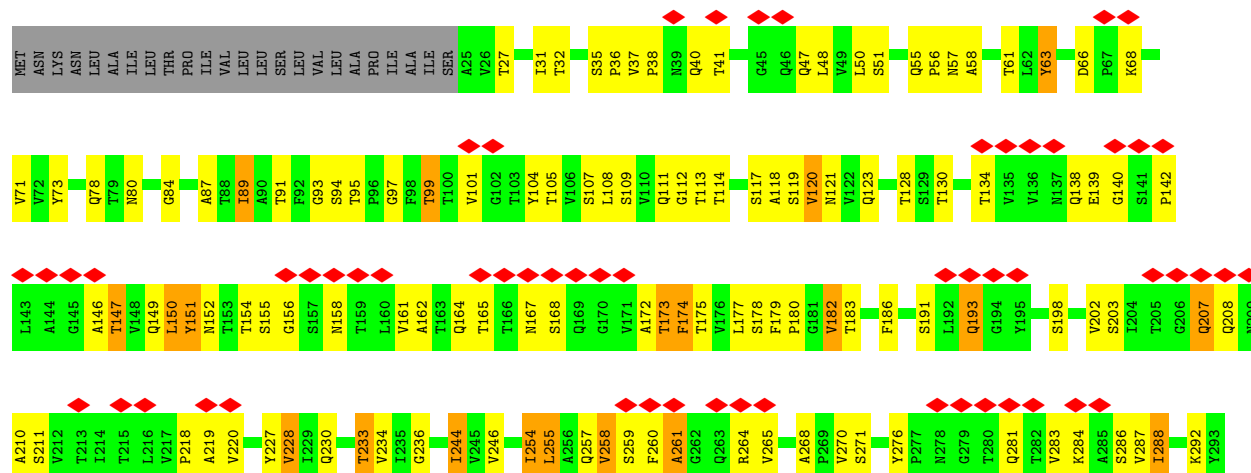


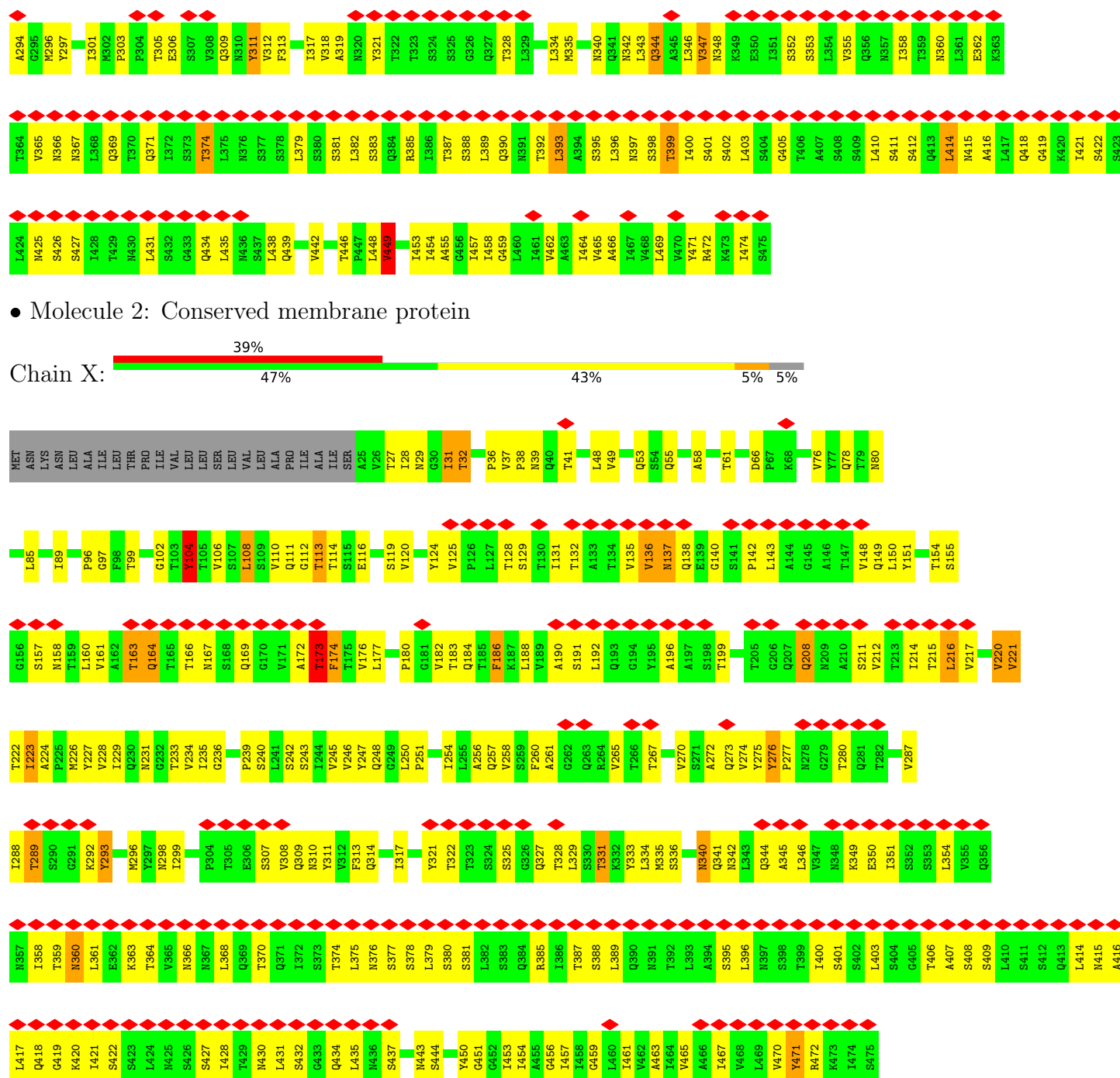


• Molecule 2: Conserved membrane protein



• Molecule 2: Conserved membrane protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	2771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, TFS TALOS	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	83, 83	Depositor
Minimum defocus (nm)	4000, 4000	Depositor
Maximum defocus (nm)	6000, 6000	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	TFS FALCON 4i (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00509	Depositor
Map size ($\text{\AA}$)	700.0, 700.0, 700.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	3.5, 3.5, 3.5	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	2.27	397/10749 (3.7%)	2.38	672/14803 (4.5%)
1	V	2.27	385/10749 (3.6%)	2.35	649/14803 (4.4%)
1	W	2.26	389/10749 (3.6%)	2.35	617/14803 (4.2%)
1	Z	2.22	360/10749 (3.3%)	2.37	623/14803 (4.2%)
2	B	2.28	127/3359 (3.8%)	2.39	208/4606 (4.5%)
2	C	2.26	118/3359 (3.5%)	2.37	185/4606 (4.0%)
2	X	2.29	133/3359 (4.0%)	2.40	197/4606 (4.3%)
All	All	2.26	1909/53073 (3.6%)	2.37	3151/73030 (4.3%)

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	A	0	60
1	V	0	40
1	W	0	47
1	Z	0	53
2	B	0	11
2	C	0	8
2	X	0	7
All	All	0	226

The worst 5 of 1909 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	464	GLY	CA-C	-14.41	1.37	1.51
1	Z	526	GLY	CA-C	-13.23	1.42	1.52
1	A	108	ILE	N-CA	-11.28	1.32	1.46
1	V	526	GLY	CA-C	-11.02	1.44	1.52
1	V	688	GLY	N-CA	10.92	1.53	1.44

The worst 5 of 3151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	1258	VAL	CA-C-O	-13.23	111.34	119.15
2	X	55	GLN	CA-C-N	13.18	133.34	119.90
2	X	55	GLN	C-N-CA	13.18	133.34	119.90
1	V	92	PHE	CA-CB-CG	13.01	126.81	113.80
1	W	861	THR	N-CA-C	-12.74	96.40	114.12

There are no chirality outliers.

5 of 226 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	TYR	Sidechain
1	A	55	ILE	Peptide
1	A	75	PHE	Sidechain
1	A	84	TYR	Sidechain
1	A	97	PHE	Sidechain

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	10478	0	10402	47	0
1	V	10478	0	10402	30	0
1	W	10478	0	10402	42	0
1	Z	10478	0	10402	52	0
2	B	3312	0	3388	9	0
2	C	3312	0	3388	15	0
2	X	3312	0	3388	17	0
All	All	51848	0	51772	206	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 2.

The worst 5 of 206 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:V:255:ALA:HB2	1:V:617:ASN:HD21	1.59	0.66
2:C:344:GLN:H	2:C:344:GLN:HE21	1.43	0.65
1:V:1215:TYR:CD1	1:V:1371:VAL:HG13	2.33	0.64
2:X:288:ILE:HD12	2:X:296:MET:HB2	1.80	0.63
1:V:1010:GLN:HE22	1:V:1039:LEU:HD23	1.62	0.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	1189/1212 (98%)	1103 (93%)	86 (7%)	13	35
1	V	1189/1212 (98%)	1122 (94%)	67 (6%)	19	40
1	W	1189/1212 (98%)	1110 (93%)	79 (7%)	15	37
1	Z	1189/1212 (98%)	1124 (94%)	65 (6%)	19	41
2	B	386/407 (95%)	358 (93%)	28 (7%)	13	34
2	C	386/407 (95%)	363 (94%)	23 (6%)	17	39
2	X	386/407 (95%)	371 (96%)	15 (4%)	28	49
All	All	5914/6069 (97%)	5551 (94%)	363 (6%)	19	38

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	413	ILE
2	X	114	THR
1	W	556	VAL

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Mol	Chain	Res	Type
1	W	991	THR
1	Z	103	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 183 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	708	ASN
2	X	310	ASN
1	W	755	GLN
1	W	1094	ASN
1	Z	52	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.

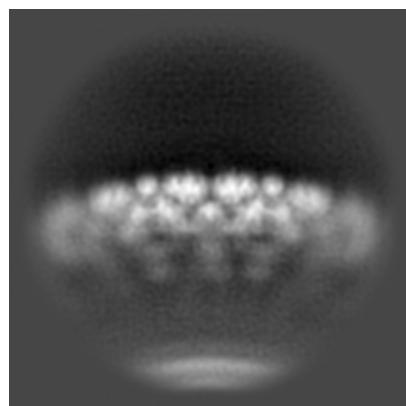
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18127. These allow visual inspection of the internal detail of the map and identification of artifacts.

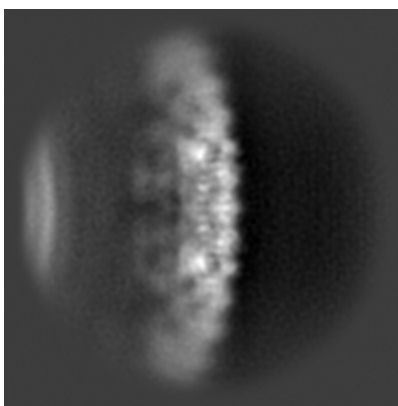
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

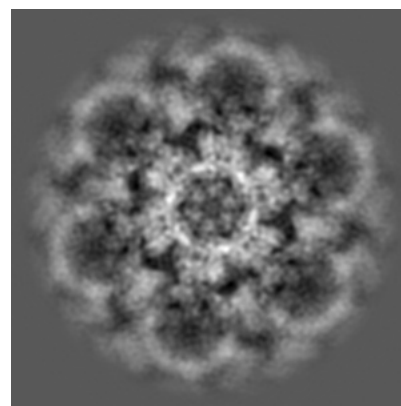
6.1.1 Primary map



X

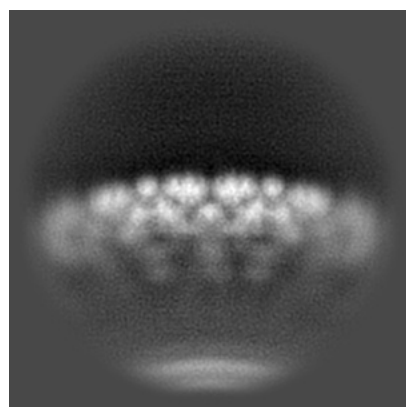


Y

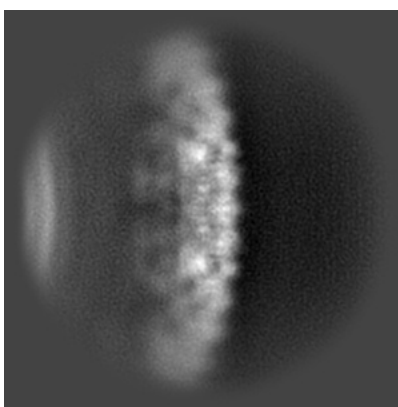


Z

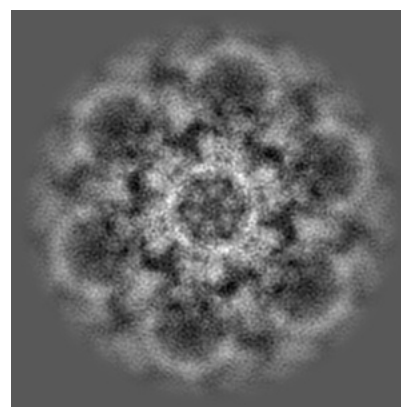
6.1.2 Raw map



X



Y

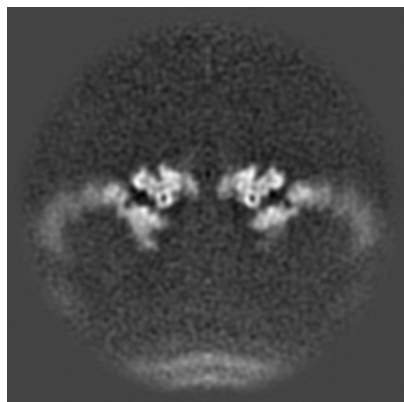


Z

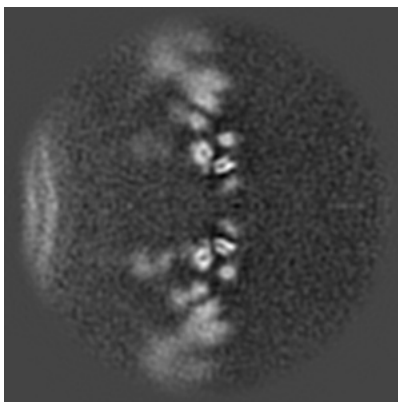
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

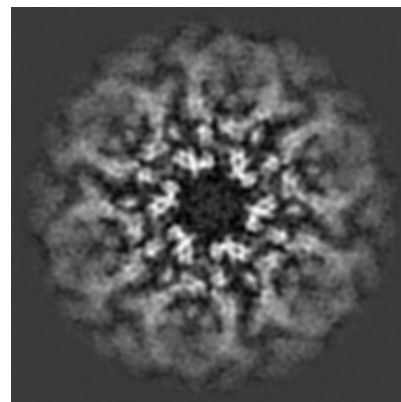
6.2.1 Primary map



X Index: 100

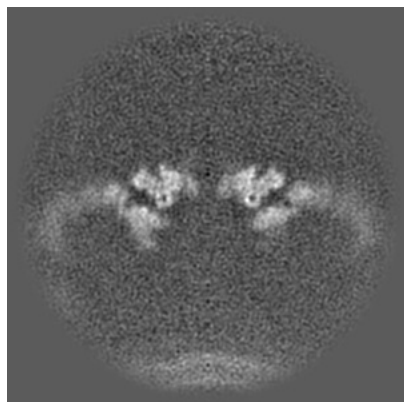


Y Index: 100

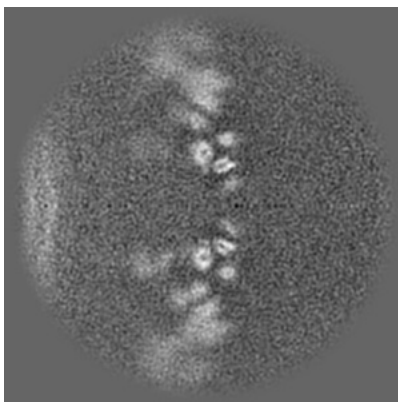


Z Index: 100

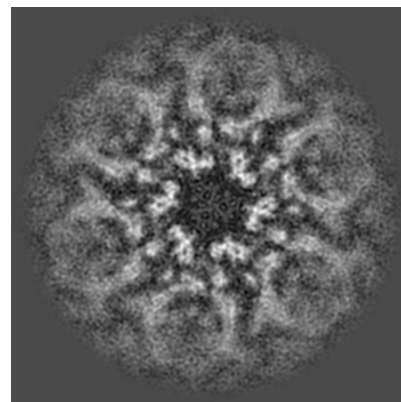
6.2.2 Raw map



X Index: 100



Y Index: 100

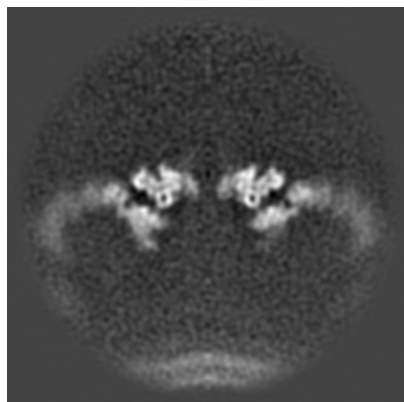


Z Index: 100

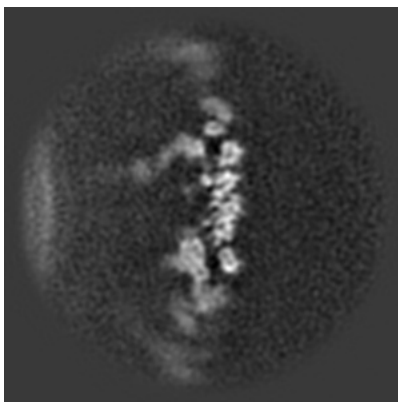
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

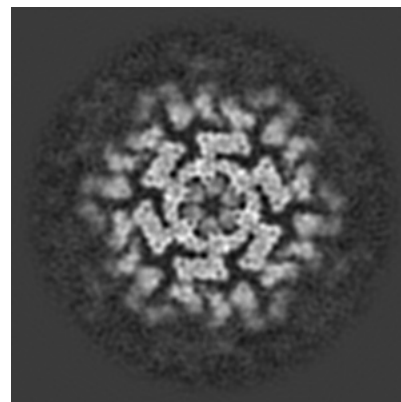
6.3.1 Primary map



X Index: 100

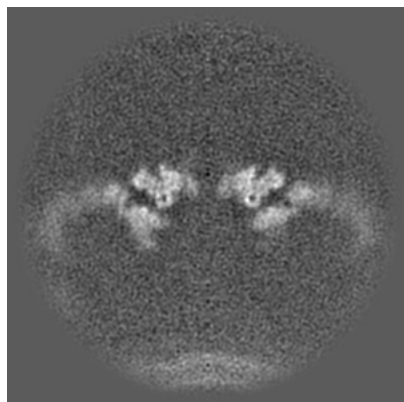


Y Index: 117

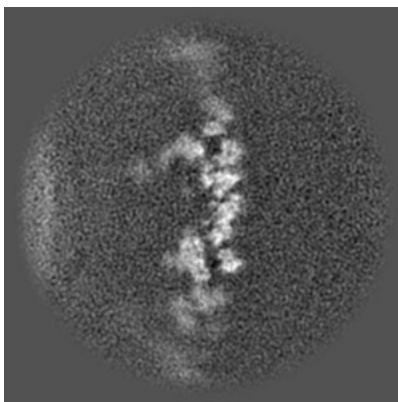


Z Index: 110

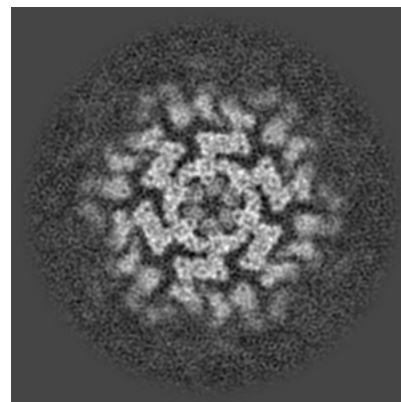
6.3.2 Raw map



X Index: 100



Y Index: 116

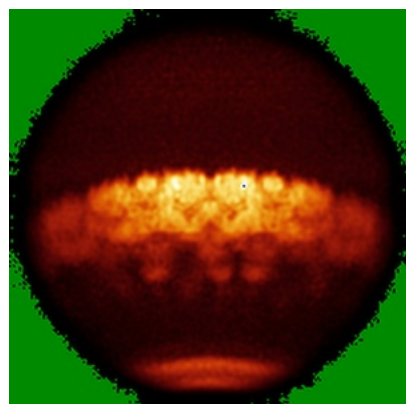


Z Index: 110

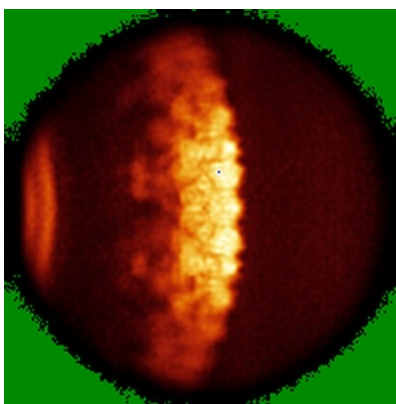
The images above show the largest variance slices of the map in three orthogonal directions.

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

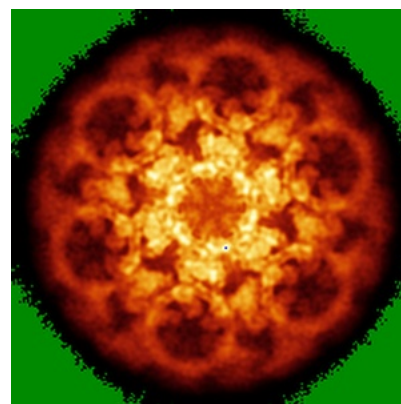
6.4.1 Primary map



X

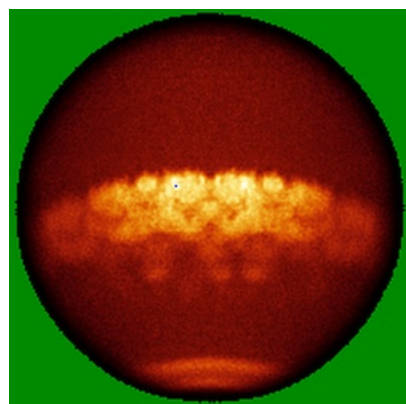


Y

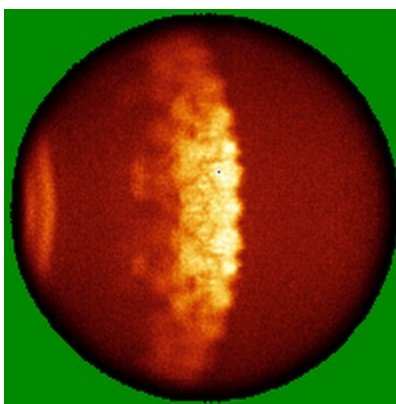


Z

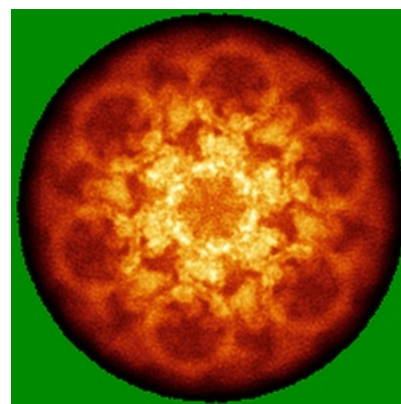
6.4.2 Raw map



X



Y

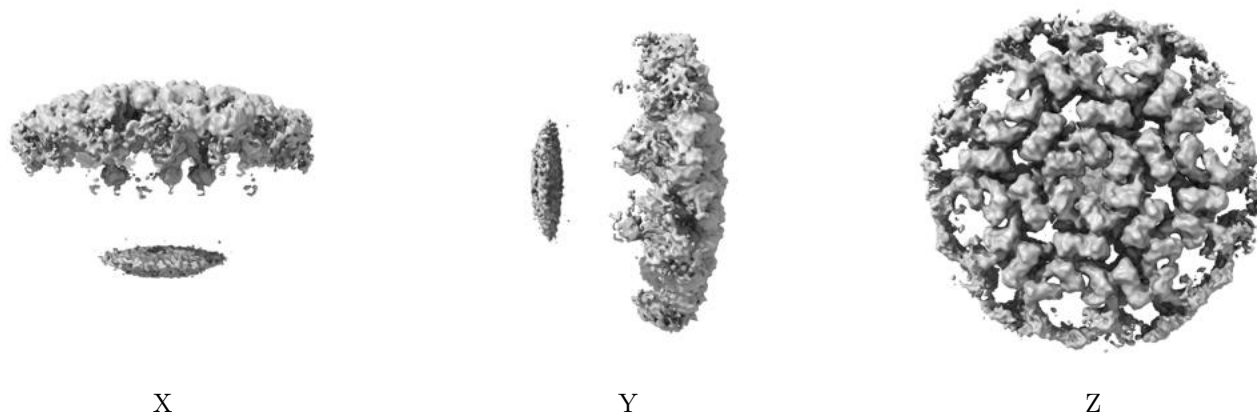


Z

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.

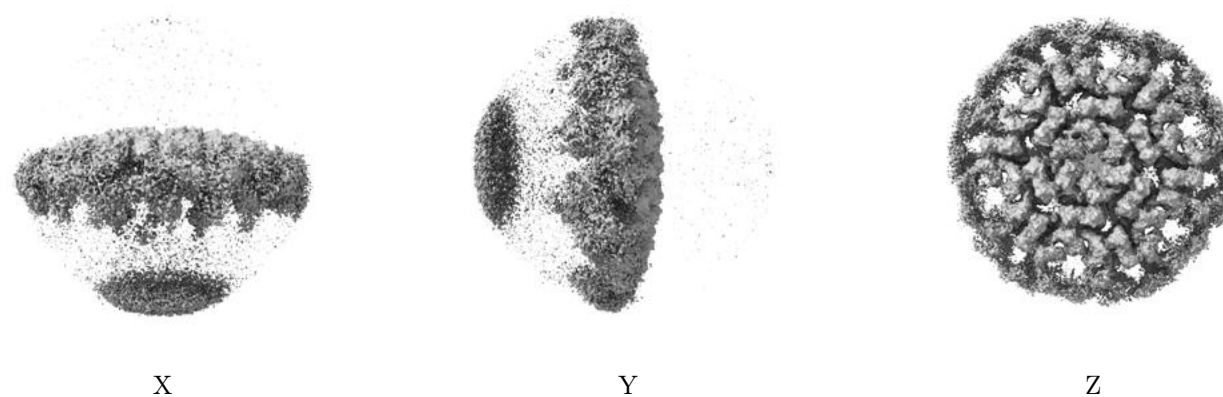
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00509. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

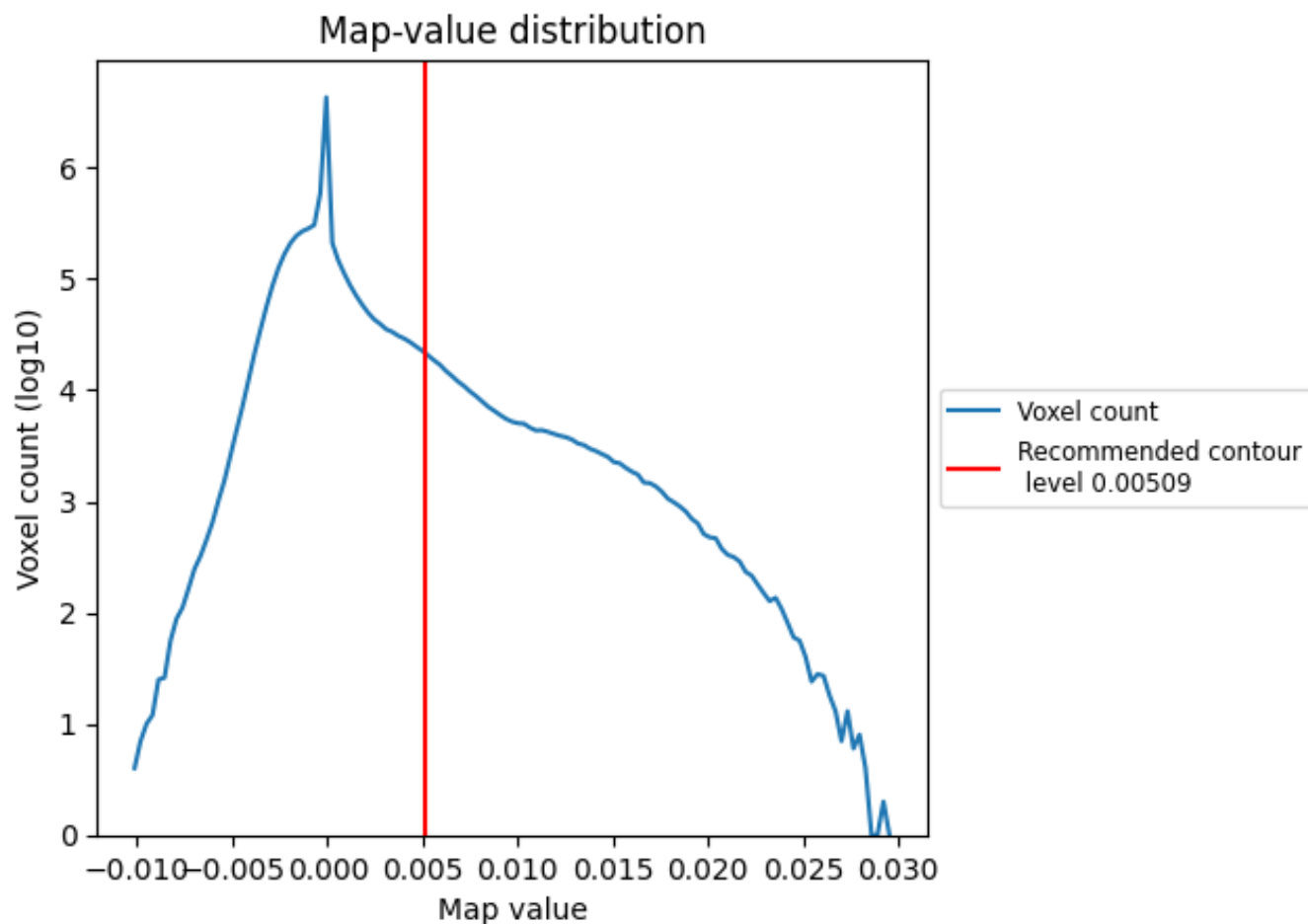
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

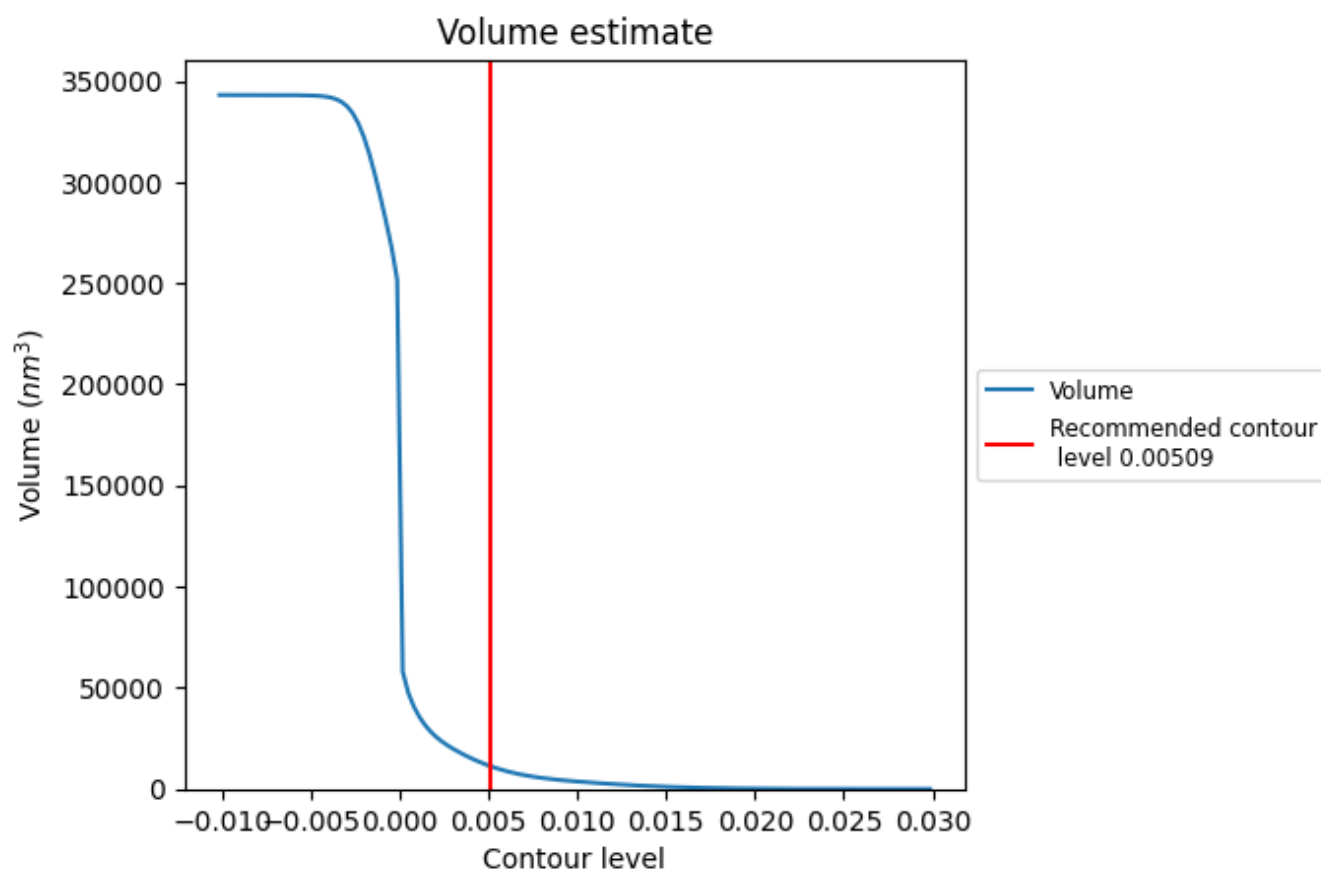
This section contains the results of statistical analysis of the map.

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.

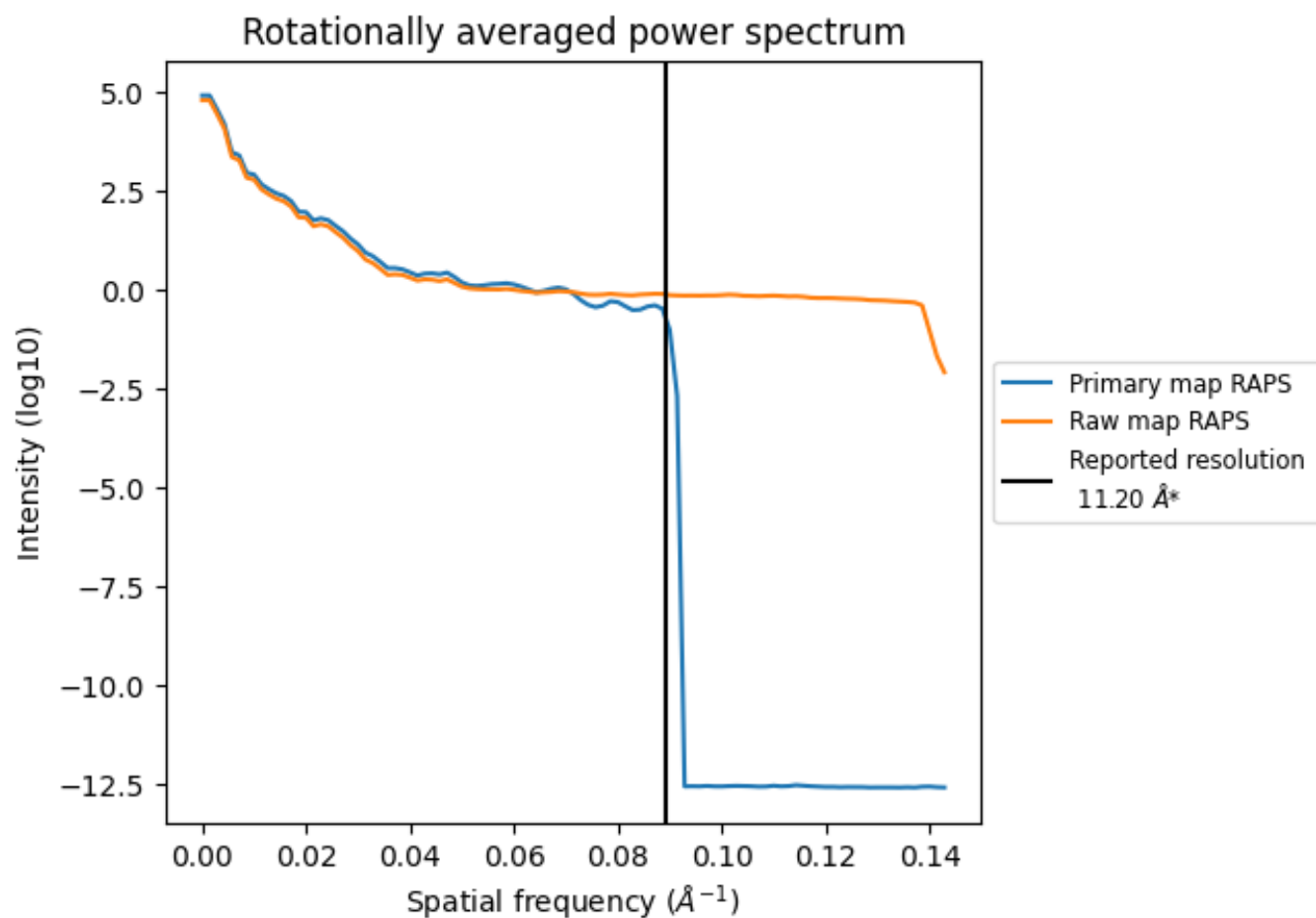
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11315 nm^3 ; this corresponds to an approximate mass of 10221 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 ⓘ

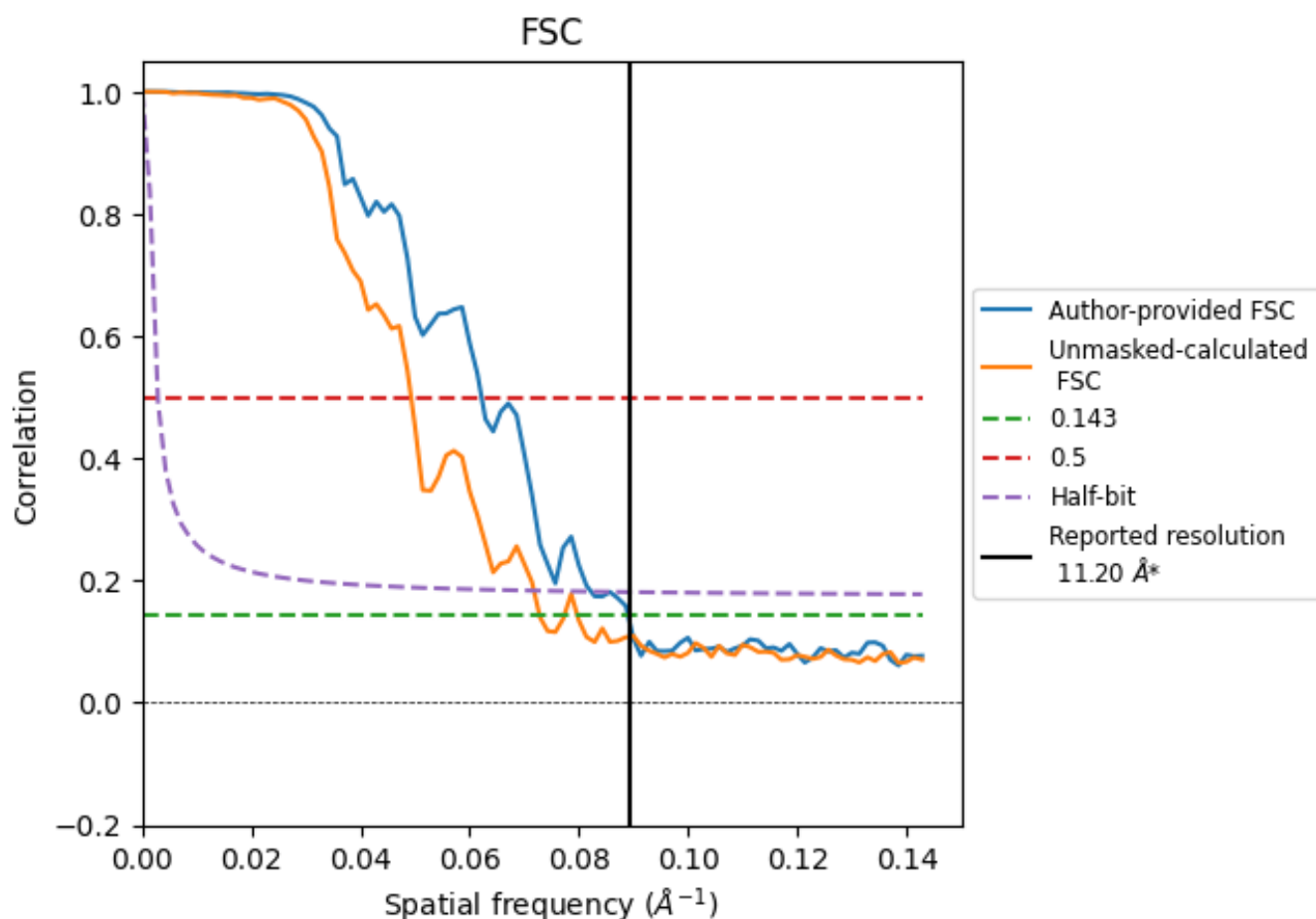


*Reported resolution corresponds to spatial frequency of 0.089 Å⁻¹

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 $0.089 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.20	-	-
Author-provided FSC curve	11.24	16.08	12.17
Unmasked-calculated*	13.74	20.33	13.93

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.74 differs from the reported value 11.2 by more than 10 %

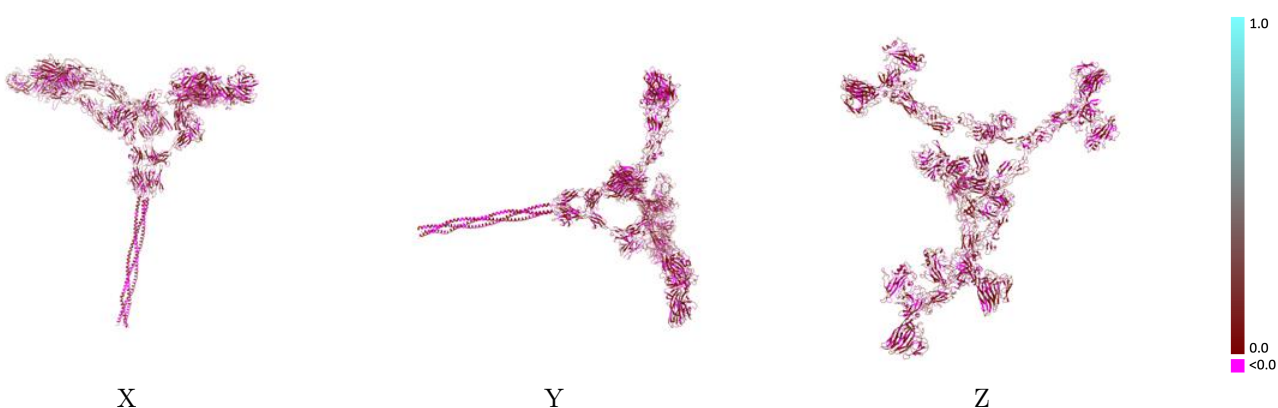
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18127 and PDB model 8QOX. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

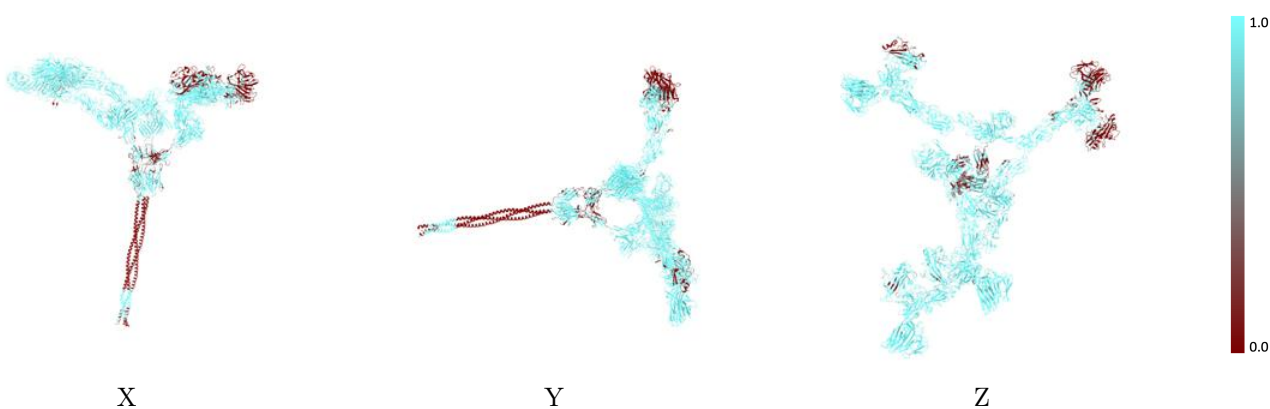
This section was not generated.

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



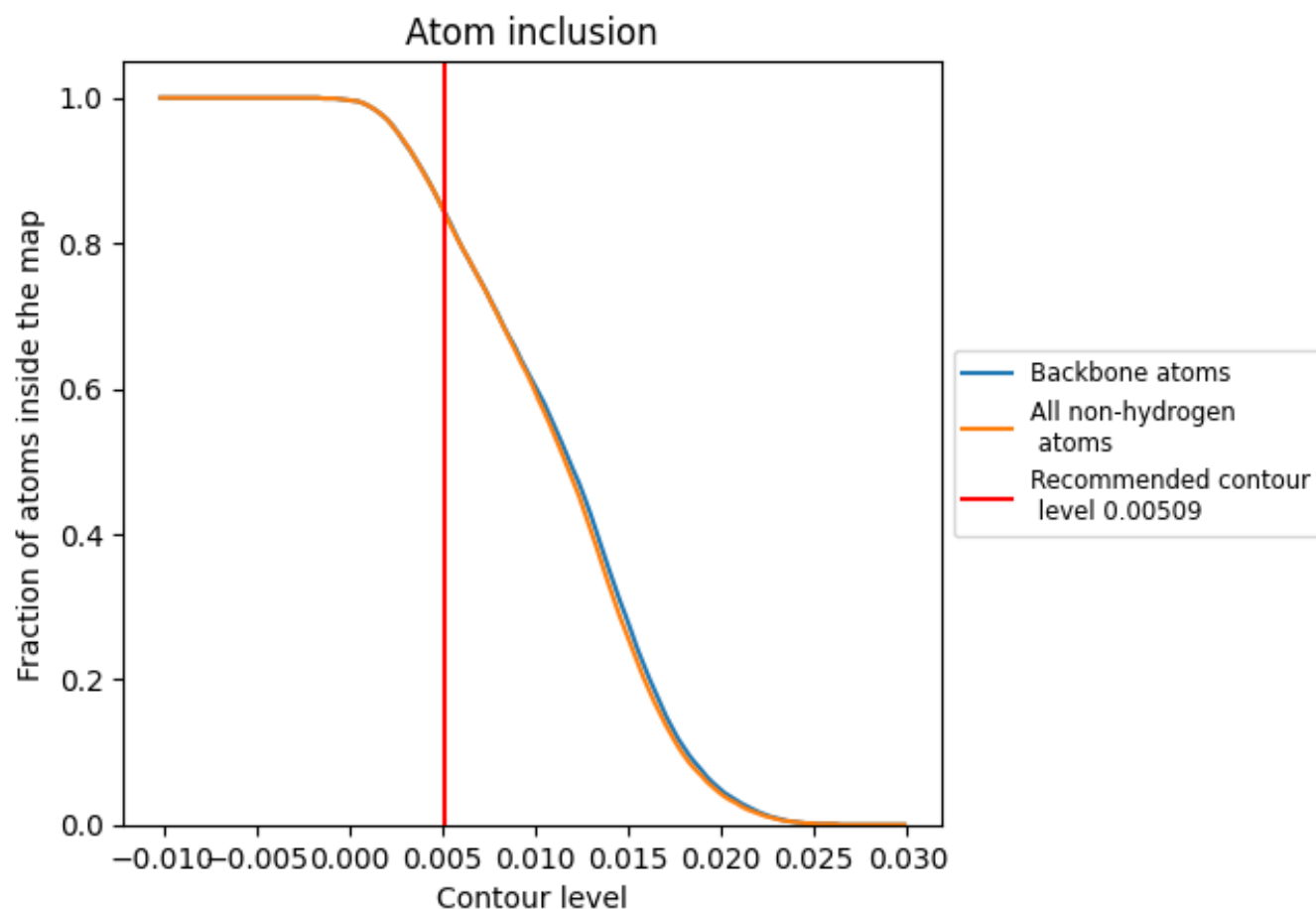
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00509).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.00509) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.0660
A	0.9780	0.0790
B	0.6270	0.0550
C	0.6100	0.0560
V	0.9390	0.0660
W	0.6970	0.0510
X	0.5710	0.0460
Z	0.9890	0.0810

1.0

0.0

<0.0