



## wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 11:55 PM JST

PDB ID : 5X5C  
EMDB ID : EMD-6706  
Title : Prefusion structure of MERS-CoV spike glycoprotein, conformation 1  
Authors : Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.  
Deposited on : 2017-02-15  
Resolution : 4.10 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](mailto: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>.

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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

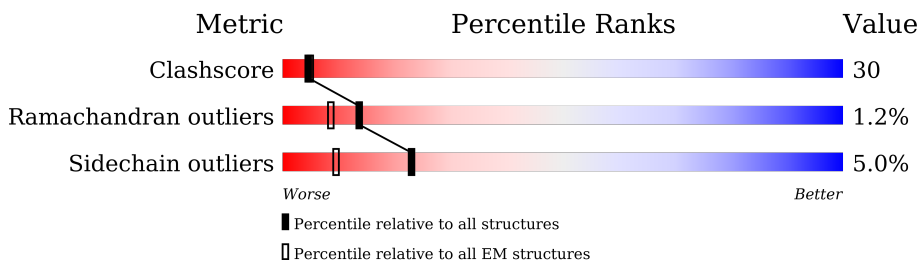
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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  $\geq 3$ , 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	1323	<div> <div>54%</div> <div>59%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
1	B	1323	<div> <div>53%</div> <div>57%</div> <div>24%</div> <div>5%</div> <div>•</div> <div>14%</div> </div>
1	C	1323	<div> <div>53%</div> <div>58%</div> <div>24%</div> <div>•</div> <div>14%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26418 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	B	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	C	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	751	SER	ARG	engineered mutation	UNP W6A028
A	1020	GLN	ARG	engineered mutation	UNP W6A028
A	1295	GLU	-	expression tag	UNP W6A028
A	1296	PHE	-	expression tag	UNP W6A028
A	1297	ARG	-	expression tag	UNP W6A028
A	1298	LEU	-	expression tag	UNP W6A028
A	1299	VAL	-	expression tag	UNP W6A028
A	1300	PRO	-	expression tag	UNP W6A028
A	1301	ARG	-	expression tag	UNP W6A028
A	1302	GLY	-	expression tag	UNP W6A028
A	1303	SER	-	expression tag	UNP W6A028
A	1304	PRO	-	expression tag	UNP W6A028
A	1305	GLY	-	expression tag	UNP W6A028
A	1306	SER	-	expression tag	UNP W6A028
A	1307	GLY	-	expression tag	UNP W6A028
A	1308	TYR	-	expression tag	UNP W6A028
A	1309	ILE	-	expression tag	UNP W6A028
A	1310	PRO	-	expression tag	UNP W6A028
A	1311	GLU	-	expression tag	UNP W6A028
A	1312	ALA	-	expression tag	UNP W6A028
A	1313	PRO	-	expression tag	UNP W6A028
A	1314	ARG	-	expression tag	UNP W6A028
A	1315	ASP	-	expression tag	UNP W6A028
A	1316	GLY	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1317	GLN	-	expression tag	UNP W6A028
A	1318	ALA	-	expression tag	UNP W6A028
A	1319	TYR	-	expression tag	UNP W6A028
A	1320	VAL	-	expression tag	UNP W6A028
A	1321	ARG	-	expression tag	UNP W6A028
A	1322	LYS	-	expression tag	UNP W6A028
A	1323	ASP	-	expression tag	UNP W6A028
A	1324	GLY	-	expression tag	UNP W6A028
A	1325	GLU	-	expression tag	UNP W6A028
A	1326	TRP	-	expression tag	UNP W6A028
A	1327	VAL	-	expression tag	UNP W6A028
A	1328	LEU	-	expression tag	UNP W6A028
A	1329	LEU	-	expression tag	UNP W6A028
A	1330	SER	-	expression tag	UNP W6A028
A	1331	THR	-	expression tag	UNP W6A028
A	1332	PHE	-	expression tag	UNP W6A028
A	1333	LEU	-	expression tag	UNP W6A028
A	1334	GLY	-	expression tag	UNP W6A028
A	1335	HIS	-	expression tag	UNP W6A028
A	1336	HIS	-	expression tag	UNP W6A028
A	1337	HIS	-	expression tag	UNP W6A028
A	1338	HIS	-	expression tag	UNP W6A028
A	1339	HIS	-	expression tag	UNP W6A028
A	1340	HIS	-	expression tag	UNP W6A028
B	751	SER	ARG	engineered mutation	UNP W6A028
B	1020	GLN	ARG	engineered mutation	UNP W6A028
B	1295	GLU	-	expression tag	UNP W6A028
B	1296	PHE	-	expression tag	UNP W6A028
B	1297	ARG	-	expression tag	UNP W6A028
B	1298	LEU	-	expression tag	UNP W6A028
B	1299	VAL	-	expression tag	UNP W6A028
B	1300	PRO	-	expression tag	UNP W6A028
B	1301	ARG	-	expression tag	UNP W6A028
B	1302	GLY	-	expression tag	UNP W6A028
B	1303	SER	-	expression tag	UNP W6A028
B	1304	PRO	-	expression tag	UNP W6A028
B	1305	GLY	-	expression tag	UNP W6A028
B	1306	SER	-	expression tag	UNP W6A028
B	1307	GLY	-	expression tag	UNP W6A028
B	1308	TYR	-	expression tag	UNP W6A028
B	1309	ILE	-	expression tag	UNP W6A028
B	1310	PRO	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1311	GLU	-	expression tag	UNP W6A028
B	1312	ALA	-	expression tag	UNP W6A028
B	1313	PRO	-	expression tag	UNP W6A028
B	1314	ARG	-	expression tag	UNP W6A028
B	1315	ASP	-	expression tag	UNP W6A028
B	1316	GLY	-	expression tag	UNP W6A028
B	1317	GLN	-	expression tag	UNP W6A028
B	1318	ALA	-	expression tag	UNP W6A028
B	1319	TYR	-	expression tag	UNP W6A028
B	1320	VAL	-	expression tag	UNP W6A028
B	1321	ARG	-	expression tag	UNP W6A028
B	1322	LYS	-	expression tag	UNP W6A028
B	1323	ASP	-	expression tag	UNP W6A028
B	1324	GLY	-	expression tag	UNP W6A028
B	1325	GLU	-	expression tag	UNP W6A028
B	1326	TRP	-	expression tag	UNP W6A028
B	1327	VAL	-	expression tag	UNP W6A028
B	1328	LEU	-	expression tag	UNP W6A028
B	1329	LEU	-	expression tag	UNP W6A028
B	1330	SER	-	expression tag	UNP W6A028
B	1331	THR	-	expression tag	UNP W6A028
B	1332	PHE	-	expression tag	UNP W6A028
B	1333	LEU	-	expression tag	UNP W6A028
B	1334	GLY	-	expression tag	UNP W6A028
B	1335	HIS	-	expression tag	UNP W6A028
B	1336	HIS	-	expression tag	UNP W6A028
B	1337	HIS	-	expression tag	UNP W6A028
B	1338	HIS	-	expression tag	UNP W6A028
B	1339	HIS	-	expression tag	UNP W6A028
B	1340	HIS	-	expression tag	UNP W6A028
C	751	SER	ARG	engineered mutation	UNP W6A028
C	1020	GLN	ARG	engineered mutation	UNP W6A028
C	1295	GLU	-	expression tag	UNP W6A028
C	1296	PHE	-	expression tag	UNP W6A028
C	1297	ARG	-	expression tag	UNP W6A028
C	1298	LEU	-	expression tag	UNP W6A028
C	1299	VAL	-	expression tag	UNP W6A028
C	1300	PRO	-	expression tag	UNP W6A028
C	1301	ARG	-	expression tag	UNP W6A028
C	1302	GLY	-	expression tag	UNP W6A028
C	1303	SER	-	expression tag	UNP W6A028
C	1304	PRO	-	expression tag	UNP W6A028

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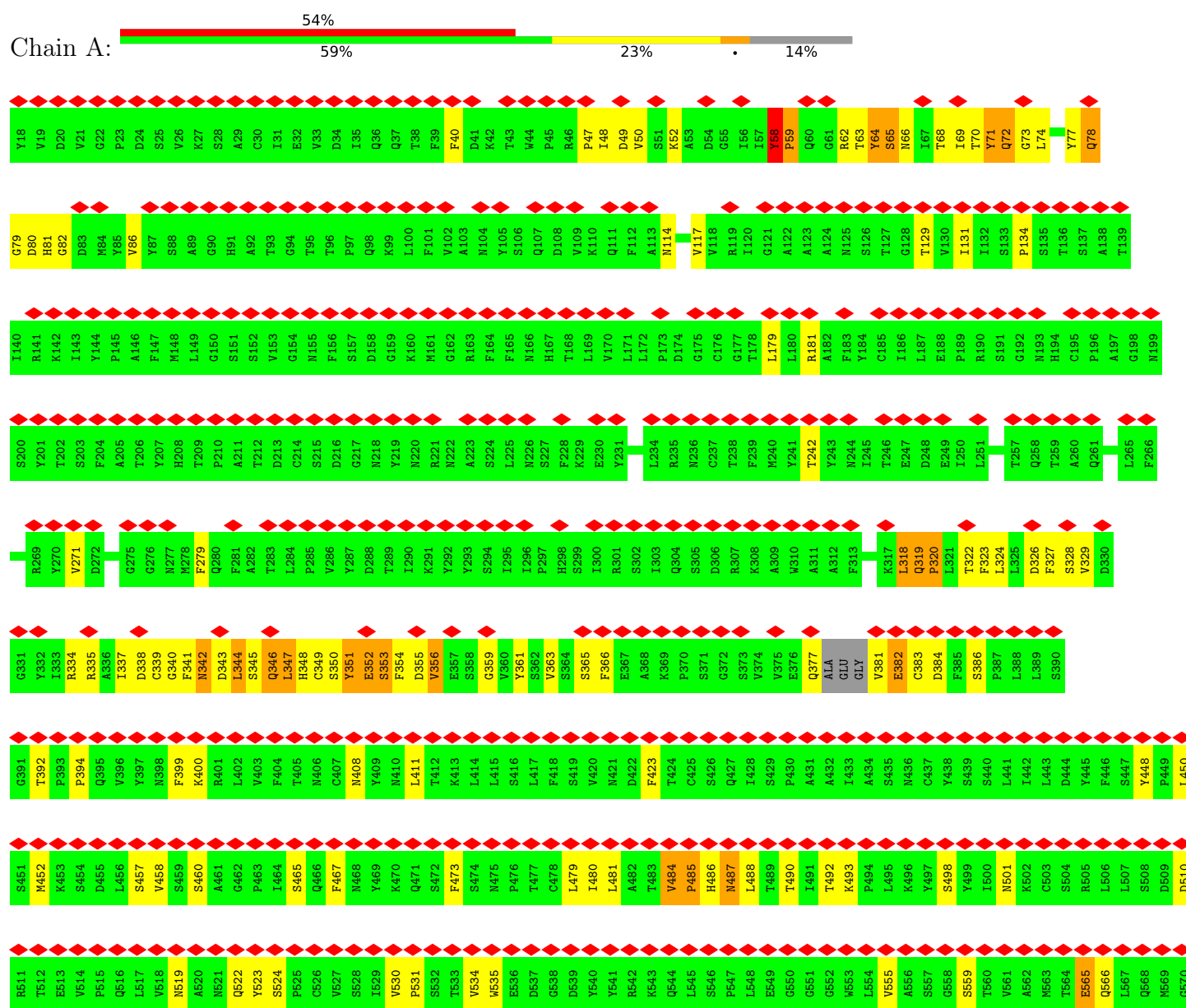
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1305	GLY	-	expression tag	UNP W6A028
C	1306	SER	-	expression tag	UNP W6A028
C	1307	GLY	-	expression tag	UNP W6A028
C	1308	TYR	-	expression tag	UNP W6A028
C	1309	ILE	-	expression tag	UNP W6A028
C	1310	PRO	-	expression tag	UNP W6A028
C	1311	GLU	-	expression tag	UNP W6A028
C	1312	ALA	-	expression tag	UNP W6A028
C	1313	PRO	-	expression tag	UNP W6A028
C	1314	ARG	-	expression tag	UNP W6A028
C	1315	ASP	-	expression tag	UNP W6A028
C	1316	GLY	-	expression tag	UNP W6A028
C	1317	GLN	-	expression tag	UNP W6A028
C	1318	ALA	-	expression tag	UNP W6A028
C	1319	TYR	-	expression tag	UNP W6A028
C	1320	VAL	-	expression tag	UNP W6A028
C	1321	ARG	-	expression tag	UNP W6A028
C	1322	LYS	-	expression tag	UNP W6A028
C	1323	ASP	-	expression tag	UNP W6A028
C	1324	GLY	-	expression tag	UNP W6A028
C	1325	GLU	-	expression tag	UNP W6A028
C	1326	TRP	-	expression tag	UNP W6A028
C	1327	VAL	-	expression tag	UNP W6A028
C	1328	LEU	-	expression tag	UNP W6A028
C	1329	LEU	-	expression tag	UNP W6A028
C	1330	SER	-	expression tag	UNP W6A028
C	1331	THR	-	expression tag	UNP W6A028
C	1332	PHE	-	expression tag	UNP W6A028
C	1333	LEU	-	expression tag	UNP W6A028
C	1334	GLY	-	expression tag	UNP W6A028
C	1335	HIS	-	expression tag	UNP W6A028
C	1336	HIS	-	expression tag	UNP W6A028
C	1337	HIS	-	expression tag	UNP W6A028
C	1338	HIS	-	expression tag	UNP W6A028
C	1339	HIS	-	expression tag	UNP W6A028
C	1340	HIS	-	expression tag	UNP W6A028

### 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.

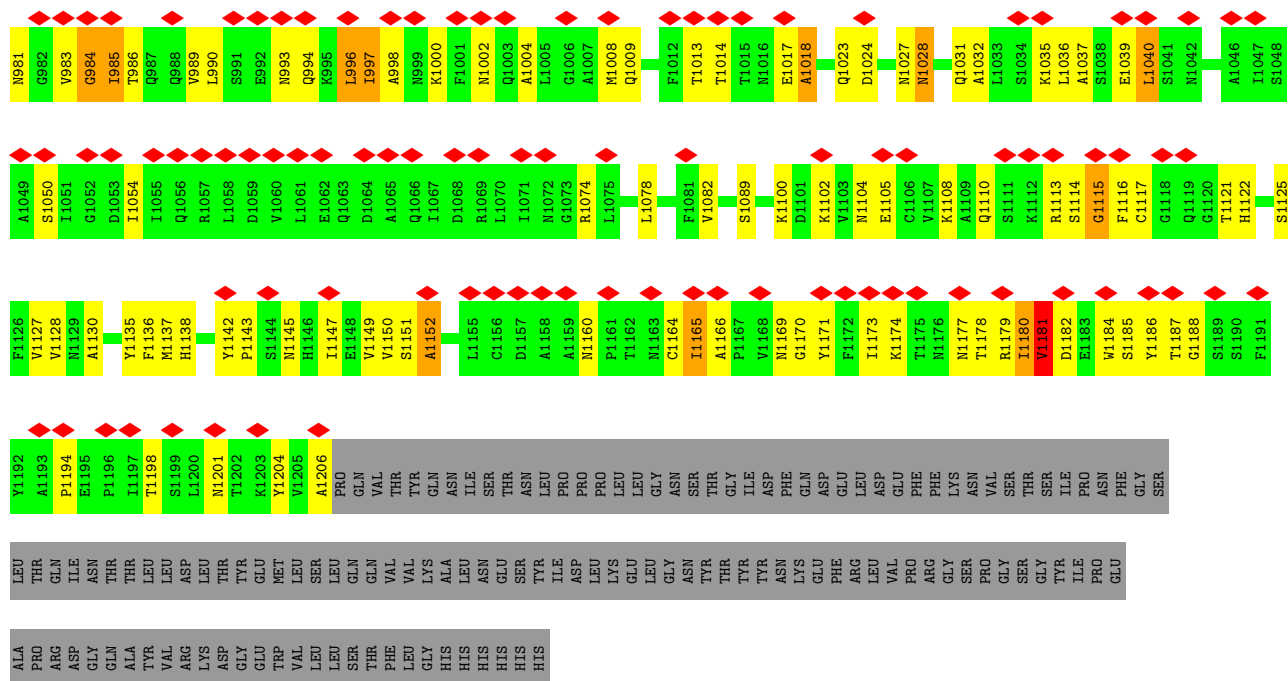
#### • Molecule 1: S protein



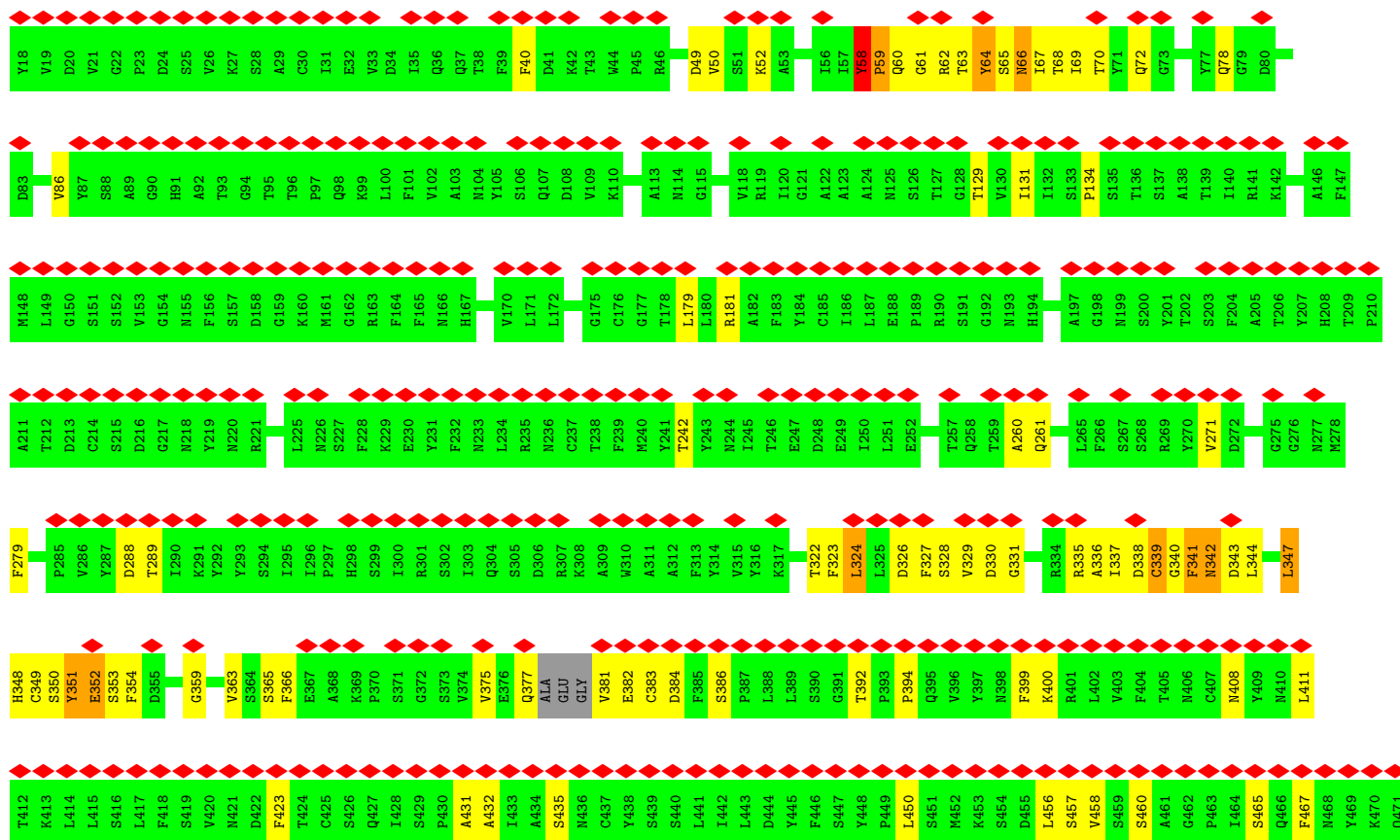




D911	C912	M913	Q914	Q915	GLY	PRO	ALA	SER	ALA	ARG	ASP	LEU	I924	A925	Q926	Q927	Y928	A930	Y932	K933	V934	L935	P936	D940	N941	N942	M943	A946	L951	L952	Q953	S954	G957	V958	G959	W960	T961	A962	Q963	L964	S965	S966	F967	A968	A969	I970	P971	I976	F977	Y978	R979	L980							
Q842	S845	V846	R847	N848	L849	V853	K854	S855	S856	Q857	I861	I862	P863	K864	F865	G866	G867	I868	K869	N870	L871	T872	L873	L874	E875	P876	V877	S878	I879	L880	N881	F882	K883	K884	S885	S886	D887	D888	F889	N890	F891	A892	L893	A894	A895	A896	A897	A898	A899	D890									
H81	G82	D83	V86	Y87	S88	A89	G90	H91	A92	T93	G94	T95	T96	P97	Q98	K99	L100	F101	V102	Y105	S106	Q107	D108	V109	K110	Q111	F112	A113	N114	R119	I120	G121	A122	A123	A124	N125	S126	T127	G128	T129	V130	I131	I132	S133	P134	S135	T136	S137	T139	R141	K142	I143	Y144						
P145	A146	F147	M148	L149	G150	S151	S152	V153	G154	N155	F156	S157	D158	G159	K160	M161	G162	R163	F164	F165	H167	T168	V169	V170	L171	L172	G175	C176	G177	T178	L179	R180	L181	A182	F183	Y184	C185	I186	L187	E188	P189	R190	S191	G192	N193	H194	C195	P196	A197	G198	N199	S200	T201	T202	S203	F204	A205		
T206	Y207	H208	T209	P210	A211	T212	D213	C214	S215	D216	G217	N218	Y219	N220	R221	N222	A223	S224	L225	N226	S227	F228	K229	E230	Y231	F232	N233	L234	R235	N236	C237	T238	F239	Y240	Y241	T242	Y243	N244	T245	T246	E247	D248	E249	I250	L251	E252	I256	T257	Q258	T259	A260	Q261	L265	K269	Y270	V271			
D272	L273	Y274	G275	G276	N277	F278	Q280	F281	A282	T283	L284	P285	V286	Y287	D288	T289	I290	K291	Y292	Y293	S294	I295	I296	P297	H298	S299	I300	R301	S302	I303	Q304	S305	D306	R307	K308	A309	W310	A311	Q319	L324	L325	D326	F327	S328	V329	D330	R334	R335	A336	I337	D338	C339	F341	N342					
D343	L344	Q345	Q346	L347	H348	C349	S350	S351	E352	S353	F354	D355	V356	G359	V360	Y361	S362	V363	S364	S365	F366	E367	A368	K369	P370	S371	G372	V375	E376	Q377	ALA	GLU	GLY	V381	E382	C383	D384	F385	S386	P387	L388	L389	S390	G391	T392	P393	P394	Q395	V396	Y397	N398	F399	K400	R401	L402	G403	F404		
T405	N406	C407	N408	Y409	N410	L411	T412	K413	L414	L415	S416	L417	F418	S419	V420	N421	D422	F423	T424	C425	Q427	I428	S429	P430	A431	A432	I433	A434	S435	N436	C437	Y438	S439	S440	L441	I442	L443	D444	Y445	F446	S447	Y448	P449	L450	S451	M452	K453	S454	D455	L456	S457	V458	S459	A460	A461	G462	P463	I464	
S465	Q466	F467	N468	Y469	K470	Q471	S472	F473	S474	N475	P476	T477	C478	L479	I480	L481	A482	T483	V484	P485	H486	N487	L488	T489	T490	I491	T492	K493	P494	L495	K496	Y497	S498	Y499	I500	N501	K502	C503	S504	R505	L506	L507	S508	D509	D510	R511	T512	E513	V514	P515	Q516	L517	V518	N519	A520	N521	Q522	Y523	S524
P525	C526	V527	S528	I529	V530	P531	S532	T533	V534	N535	E536	D537	G538	D539	Y540	Y541	B542	K543	O544	L545	S546	P547	L548	E549	G550	G551	G552	N553	L554	V555	A556	S557	G558	S559	T560	V561	A562	M563	T564	E565	O566	L567	O568	M569	L638	V639	S640	Y641	V642	S643	D644	D645	Y648						
C585	P586	K587	L588	GLU	PHE	ASN	ASP	THR	K595	I596	A597	S598	O599	L600	G601	N602	C603	V604	E605	L608	Y609	G610	G613	R614	F617	Q618	N619	C620	T621	A622	V623	G624	V625	R626	Q627	Q628	R629	F630	V631	Y632	D633	A634	V635	D636	N637	L638	V639	S640	Y641	V642	S643	D644	D645	Y648					
Y649	C650	N774	L651	R652	A653	C654	P658	V659	S660	V661	L662	Y663	D664	K665	E666	T667	K668	T669	H670	L671	T672	L673	F674	G675	S676	V677	A678	C679	E680	H681	T682	S683	S684	T685	M686	S687	G688	Q689	V690	G691	L692	A693	ARG	ARG	ASP	SER	THR	TYR	GLY	PRO	LEU	GLN	THR	P710					
V711	G712	C713	V714	L715	G716	L717	V718	H719	S720	G721	L722	F723	V724	E725	D726	C727	K728	L729	V730	L731	G732	Q733	S734	L735	C736	A737	L738	P739	D740	S743	LEU	THR	PRO	ARG	ARG	VAL	SER	SER	SER	VAL	PRO	GLY	GLU	M757	R758	L759	A760	S761	I762	A763	F764	N765	H766	P767	I768	D771	Q772		
L773	N774	S775	V776	Y777	F778	S781	I782	P783	T784	N785	F786	S787	F788	G789	V790	T791	Q792	E793	Y794	I795	Q796	T797	T798	T799	Q800	T803	H804	K807	Q808	Y809	V810	C811	N812	G813	F814	K815	K816	C817	E818	L821	R822	F823	Y824	G825	Q826	F827	K830	I831	N832	Q833	N839	L840	R841						
Q842	S845	V846	R847	N848	L849	V853	K854	S855	S856	Q857	I861	I862	P863	K864	F865	G866	G867	I868	K869	N870	L871	T872	L873	L874	E875	P876	V877	S878	I879	L880	N881	F882	K883	K884	S885	S886	D887	D888	F889	N890	F891	A892	L893	A894	A895	A896	A897	A898	A899	D890									



• Molecule 1: S protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	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 ( $e^-/\text{\AA}^2$ )	8	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	0.213	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0618	Depositor
Map size (Å)	233.99998, 233.99998, 233.99998	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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	0.52	2/9006 (0.0%)	0.79	24/12245 (0.2%)
1	B	0.52	2/9006 (0.0%)	0.79	24/12245 (0.2%)
1	C	0.51	1/9006 (0.0%)	0.78	22/12245 (0.2%)
All	All	0.51	5/27018 (0.0%)	0.79	70/36735 (0.2%)

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	20
1	B	0	19
1	C	0	18
All	All	0	57

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	PRO	N-CD	5.48	1.55	1.47
1	C	59	PRO	N-CD	5.20	1.55	1.47
1	B	59	PRO	N-CD	5.17	1.55	1.47
1	A	59	PRO	N-CD	5.17	1.55	1.47
1	A	320	PRO	N-CD	5.07	1.54	1.47

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	735	LEU	CA-CB-CG	11.57	141.92	115.30
1	B	735	LEU	CA-CB-CG	11.55	141.87	115.30
1	A	735	LEU	CA-CB-CG	11.55	141.86	115.30
1	C	1040	LEU	CA-CB-CG	7.83	133.30	115.30
1	A	1040	LEU	CA-CB-CG	7.83	133.30	115.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	TYR	Peptide
1	A	639	VAL	Peptide
1	A	642	TYR	Peptide
1	A	65	SER	Peptide
1	A	733	GLN	Peptide

## 5.2 Too-close contacts

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	8806	0	8508	532	0
1	B	8806	0	8506	697	0
1	C	8806	0	8505	624	0
All	All	26418	0	25519	1569	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 30.

The worst 5 of 1569 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:B:439:SER:CB	1:B:582:ASN:CA	1.76	1.62
1:B:344:LEU:HD22	1:B:670:HIS:CB	1.16	1.61
1:A:623:VAL:CG1	1:B:65:SER:HB2	1.31	1.60
1:C:335:ARG:HB3	1:C:354:PHE:CE2	1.32	1.60
1:C:324:LEU:HD11	1:C:354:PHE:CD1	1.37	1.59

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1128/1323 (85%)	966 (86%)	149 (13%)	13 (1%)	11	44
1	B	1128/1323 (85%)	964 (86%)	149 (13%)	15 (1%)	10	42
1	C	1128/1323 (85%)	966 (86%)	149 (13%)	13 (1%)	11	44
All	All	3384/3969 (85%)	2896 (86%)	447 (13%)	41 (1%)	14	44

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	596	ILE
1	A	597	ALA
1	A	797	THR
1	B	66	ASN
1	B	350	SER

### 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	973/1143 (85%)	929 (96%)	44 (4%)	23	47
1	B	973/1143 (85%)	917 (94%)	56 (6%)	17	40
1	C	973/1143 (85%)	928 (95%)	45 (5%)	23	46
All	All	2919/3429 (85%)	2774 (95%)	145 (5%)	23	44

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	479	LEU
1	C	1165	ILE
1	C	488	LEU
1	C	722	LEU
1	B	335	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	800	GLN
1	C	1009	GLN
1	B	1009	GLN
1	C	870	ASN
1	C	1104	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.



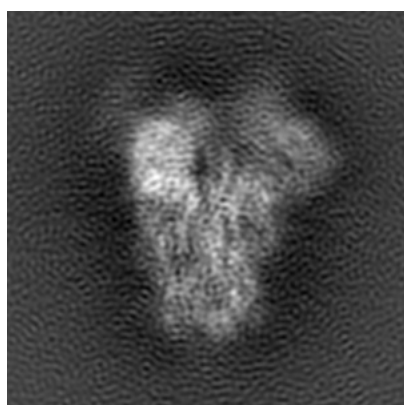
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6706. These allow visual inspection of the internal detail of the map and identification of artifacts.

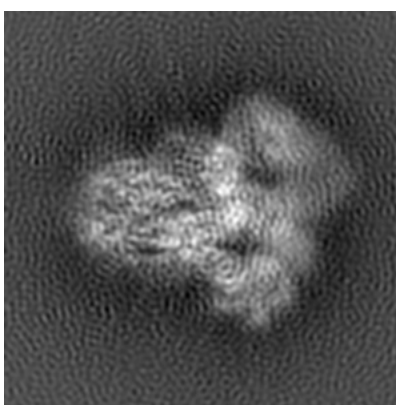
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

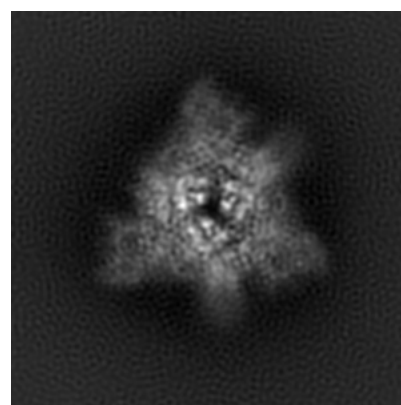
#### 6.1.1 Primary map



X



Y

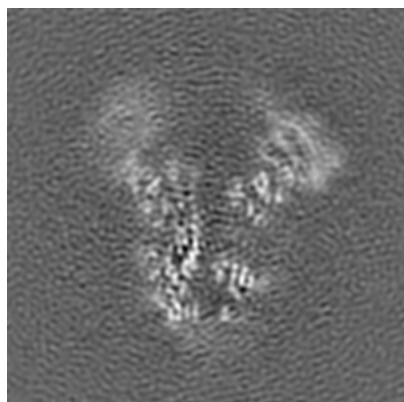


Z

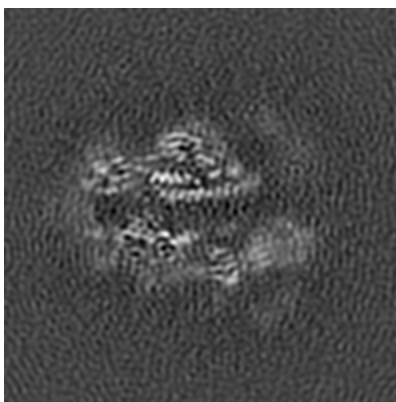
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

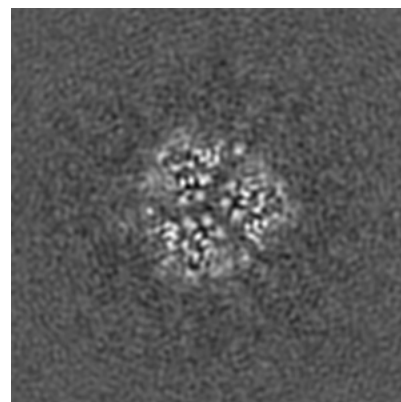
#### 6.2.1 Primary map



X Index: 90



Y Index: 90

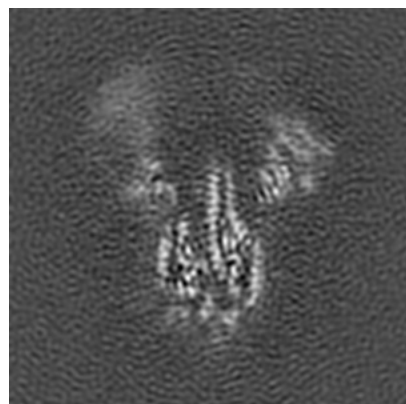


Z Index: 90

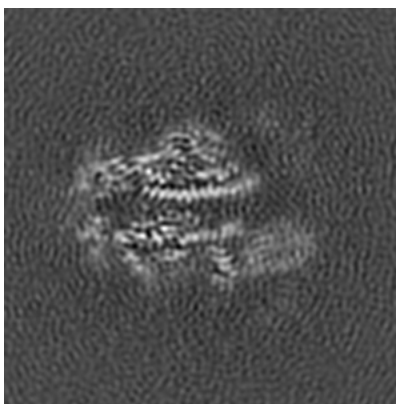
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

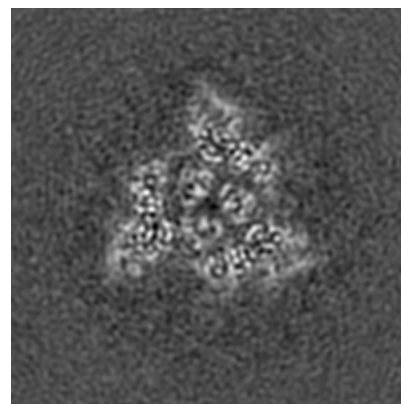
### 6.3.1 Primary map



X Index: 97



Y Index: 92

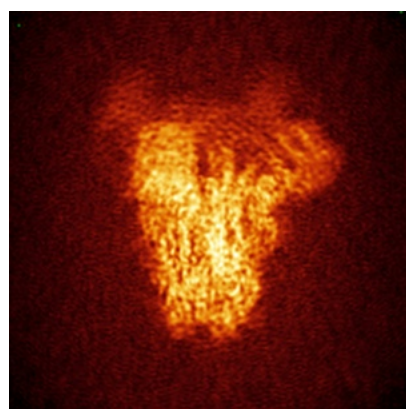


Z Index: 100

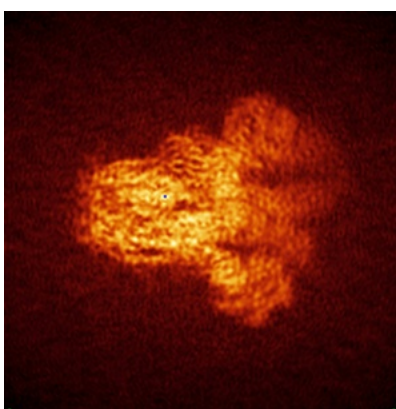
The images above show the largest variance slices of the map in three orthogonal directions.

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

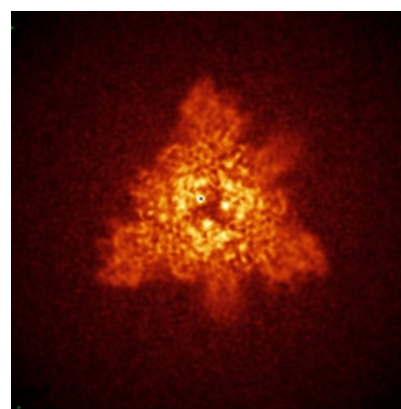
### 6.4.1 Primary map



X



Y

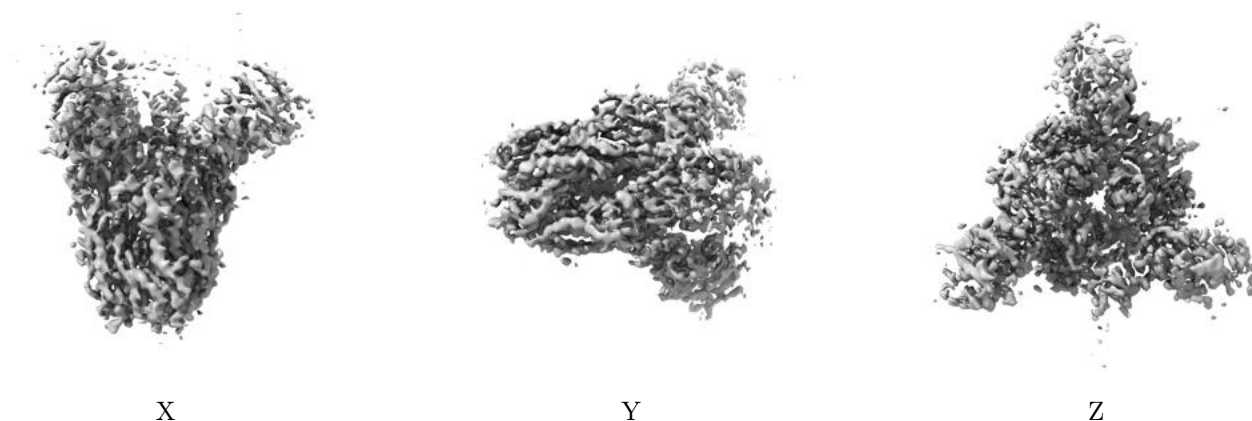


Z

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 0.0618. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

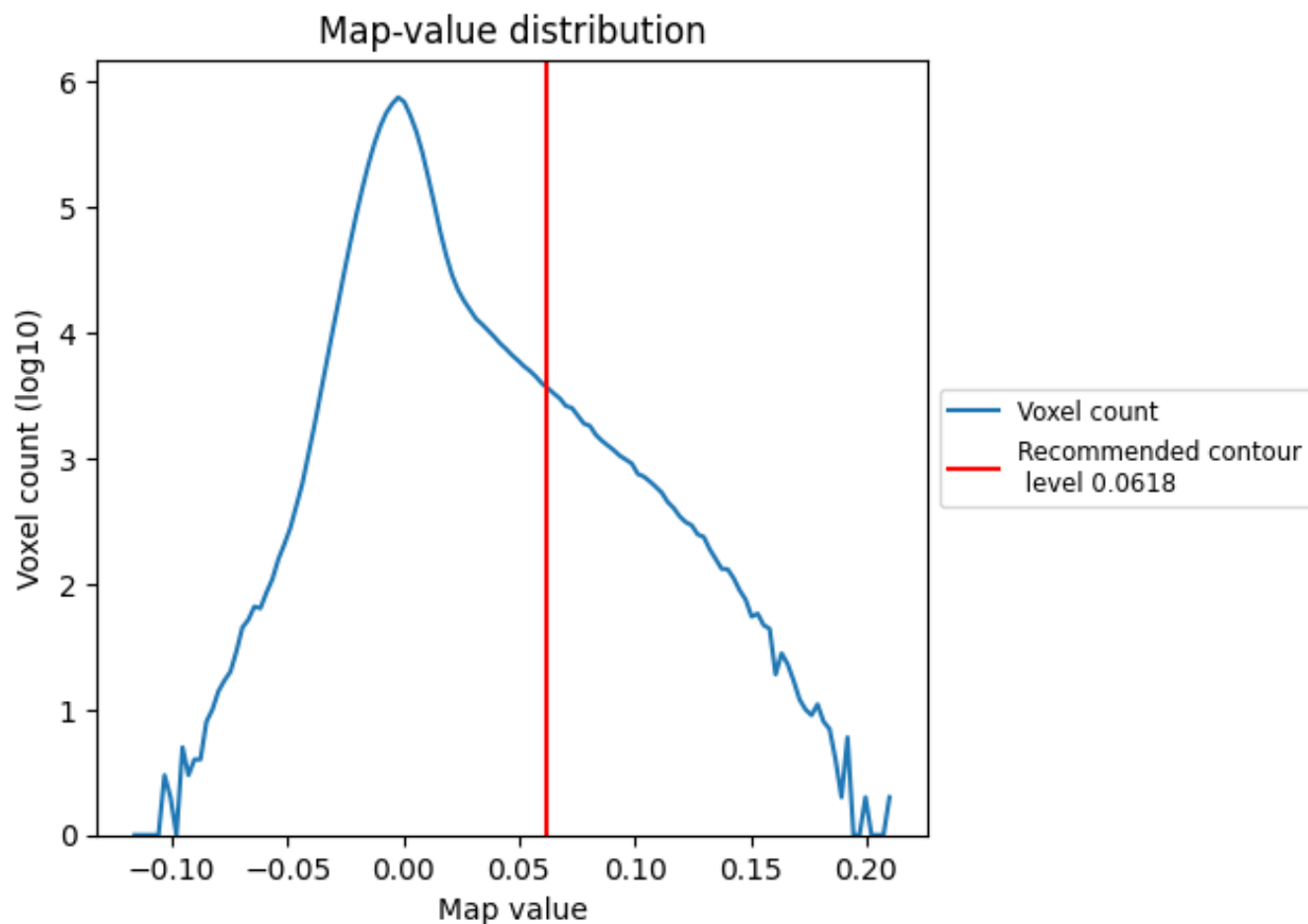
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

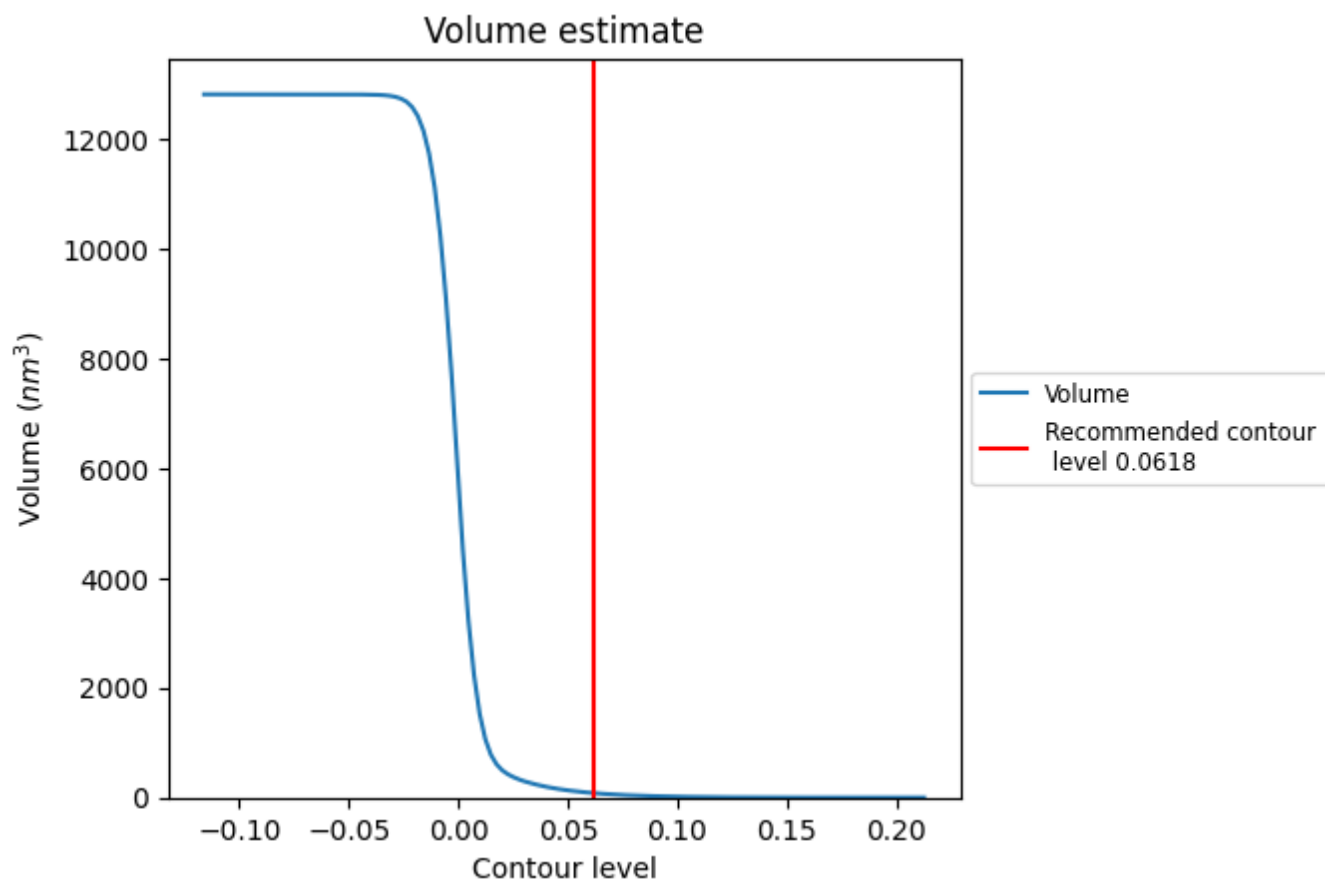
This section contains the results of statistical analysis of the map.

### 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.

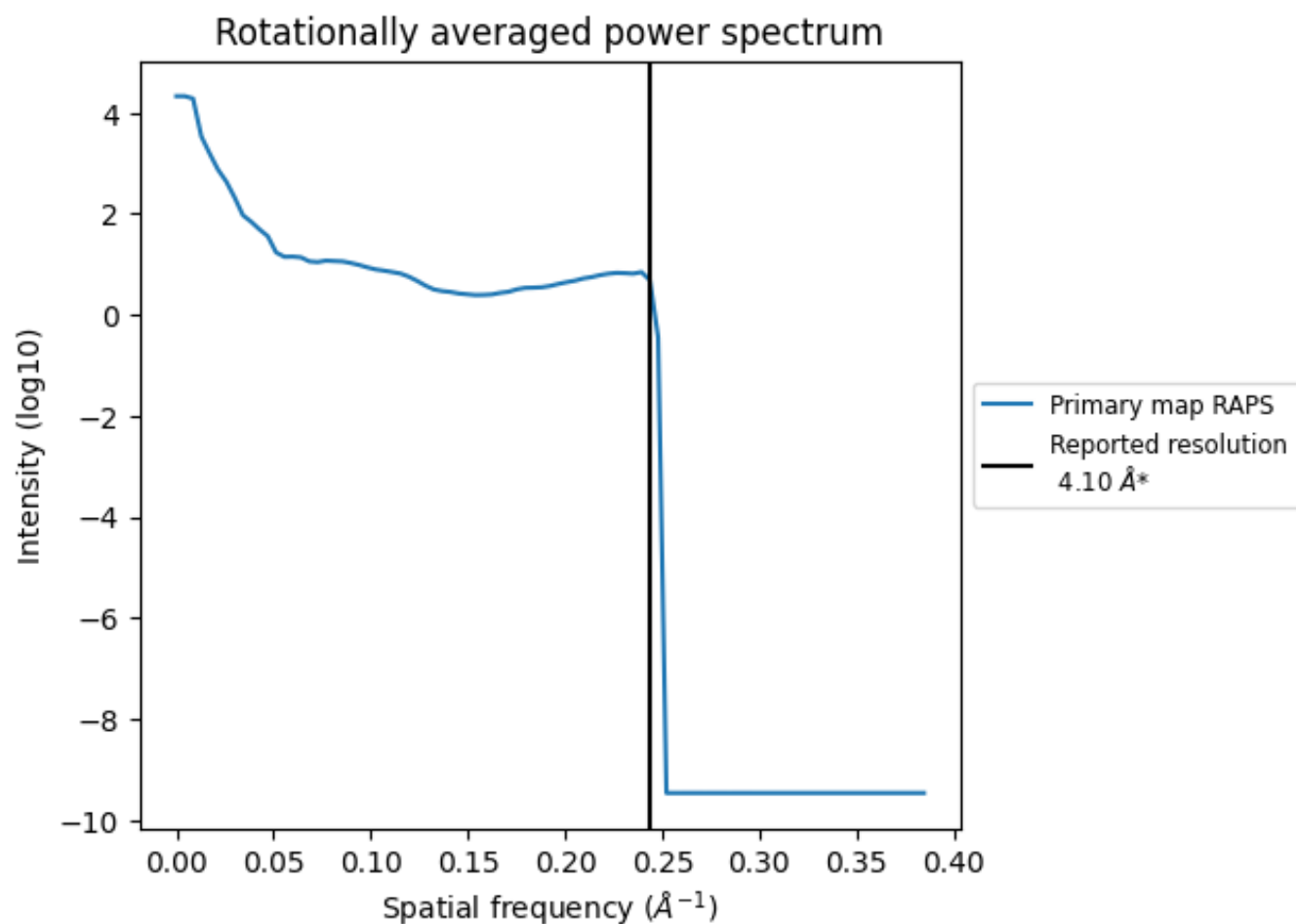
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm<sup>3</sup>; this corresponds to an approximate mass of 74 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 0.244  $\text{\AA}^{-1}$

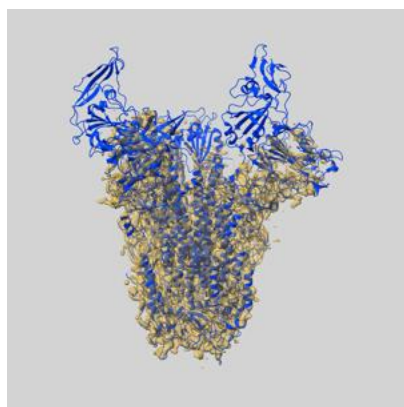
## 8 Fourier-Shell correlation

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

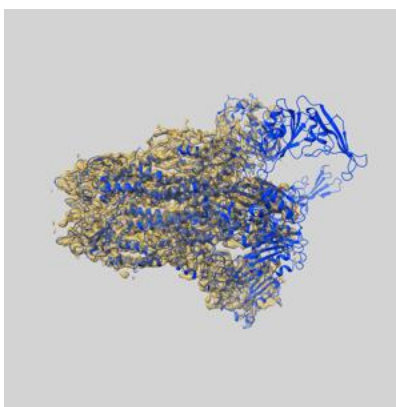
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6706 and PDB model 5X5C. Per-residue inclusion information can be found in section [3](#) on page [7](#).

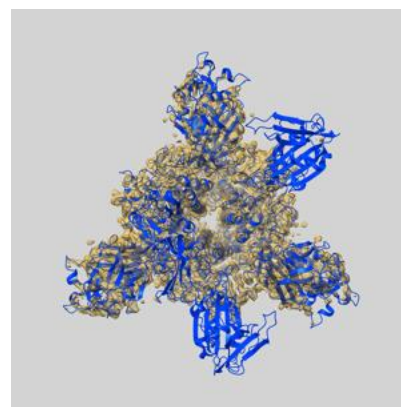
### 9.1 Map-model overlay [i](#)



X



Y

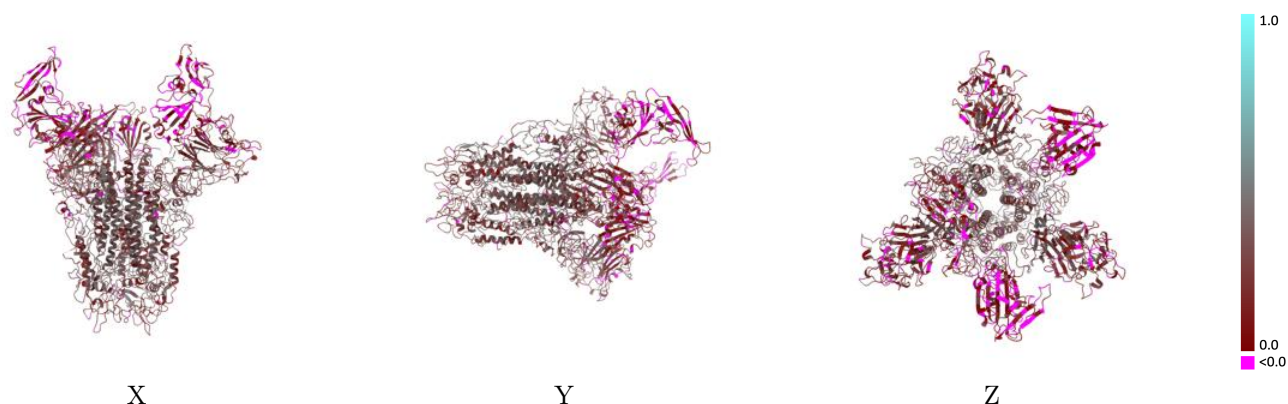


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0618 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.

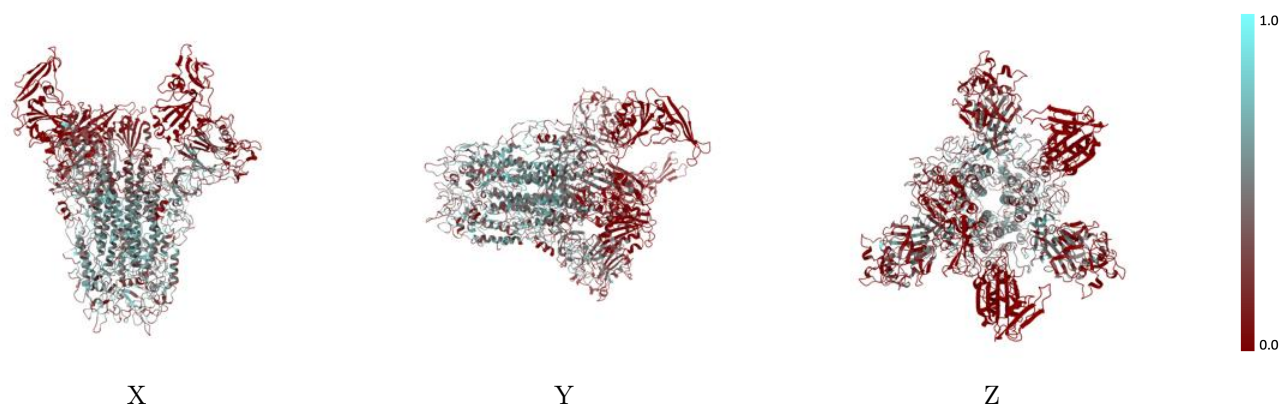


## 9.2 Q-score mapped to coordinate model [i](#)



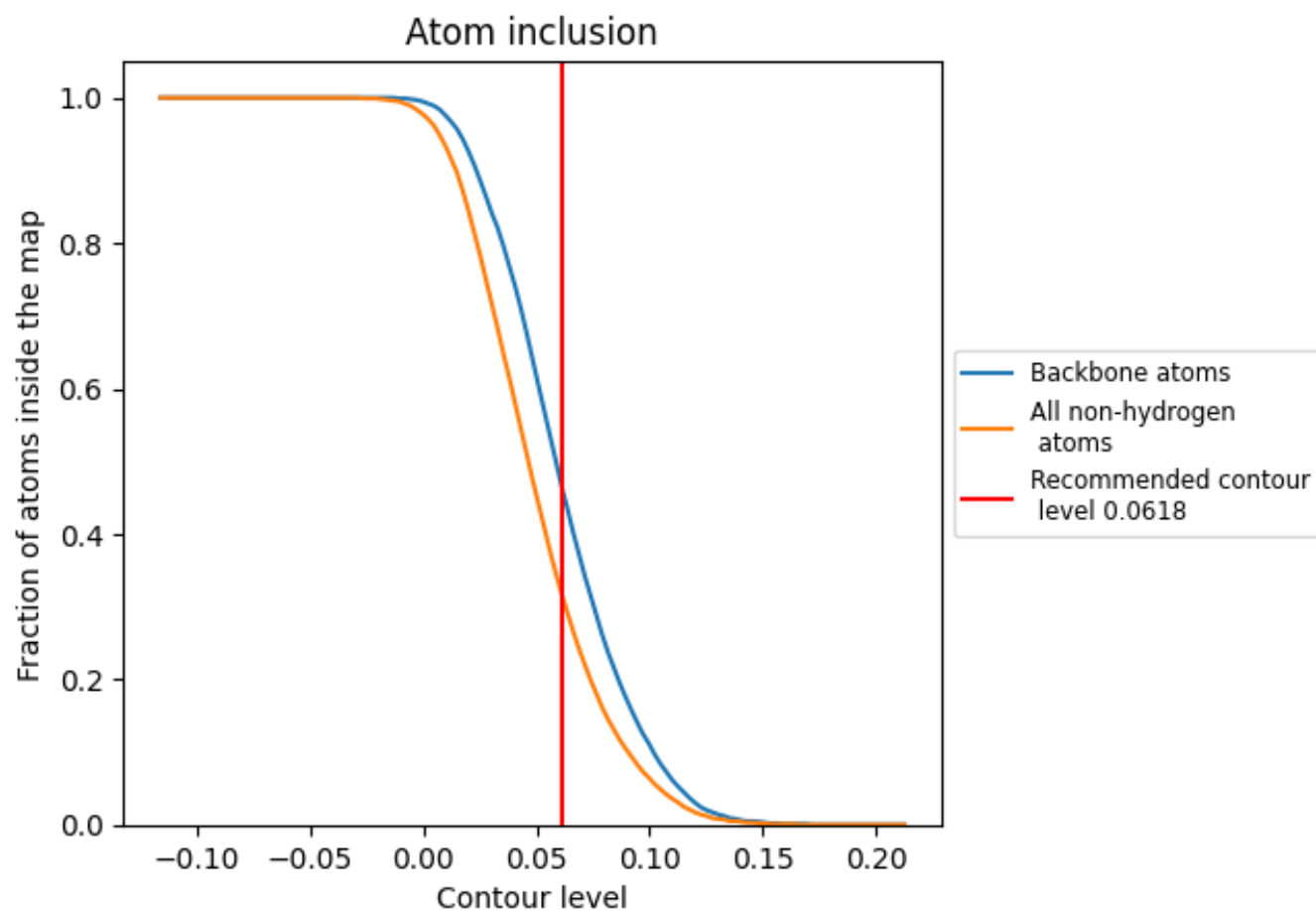
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0618).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 31% 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 (0.0618) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3110	<div></div> 0.2350
A	<div></div> 0.3100	<div></div> 0.2390
B	<div></div> 0.3110	<div></div> 0.2420
C	<div></div> 0.3130	<div></div> 0.2250

