



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:33 PM UTC

PDB ID : 5H0S / pdb_00005h0s
EMDB ID : EMD-9565
Title : EM Structure of VP1A and VP1B
Authors : Li, X.; Zhou, N.; Xu, B.; Chen, W.; Zhu, B.; Wang, X.; Wang, J.; Liu, H.;
Cheng, L.
Deposited on : 2016-10-06
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

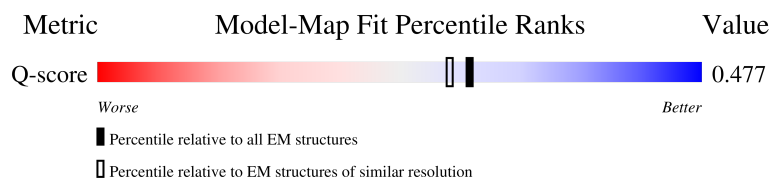
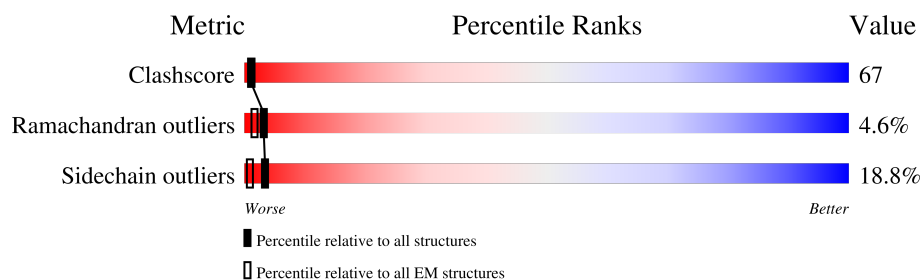
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	B	1333	
1	C	1333	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18885 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1148	Total	C	N	O	S	0	0
			9058	5731	1574	1718	35		
1	C	1247	Total	C	N	O	S	0	0
			9827	6202	1709	1878	38		



R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	
R848	M849	T850	T851	Y852	R853	Q854	Q855	L856	S857	H858	T859	R860	E861	R862	L863	R864	I865	T866	N867	V868	R869	S870	R871	R872	Y873	L874	R875	G876	A877	S878	T879	R880	R881	Q882	R883	Q888	T889	L885	S886	R887	Q888	Q889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	G904	S905	A906	R907	
T908	Y909	L910	R911	E912	R913	Q914	Q915	E914	V915	L916	V917	V918	M919	P920	D921	Y922	Y923	D924	V925	V926	S927	R928	D929	P930	R931	A932	I933	L934	Q935	S936	R937	R938	L939	D940	R941	R942	E943	S944	V945	V946	E947	I948	L949	R950	R951	R952	D953	Q954	A955	R956	R957	R958	D959	G960	V961	T962	N963	G964	S965	R966	R967
MET	GLU	E790	T791	T792	T793	T794	T795	T796	T797	T798	T799	L800	S801	Q802	L803	L804	S805	V806	A807	Q808	V809	L810	S811	K812	L813	T814	L815	T816	A817	R818	R819	R820	R821	R822	R823	L824	S825	G826	G827	R828	S829	R830	R831	R832	R833	T834	Q835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847		
F727	K728	P729	D730	T731	Y732	T733	T734	T735	T736	T737	E738	Y741	K742	T743	T744	T745	E746	T747	Q748	T749	E750	T751	V752	D753	T754	L755	T756	T757	T758	D759	T760	S761	T762	T763	T764	T765	T766	T767	T768	T769	C770	T771	Y772	T773	V774	ARG	GLN	SER	GLY	LYS	GLY	VAL	ASP	ALA	SER	ILE					
A667	V668	Q669	D670	D671	D672	D673	D674	D675	D676	D677	D678	D679	D680	D681	D682	Q683	L684	R685	H686	A687	E688	T689	Q690	F691	N692	L693	T694	A695	V696	A697	H698	T699	D700	H701	L702	S703	T704	V705	T706	A707	T708	T709	V710	T711	N712	T713	L714	T715	F716	GLY	T717	T718	T719	F720	L721	L722	L723	L724	A725	T726	
R605	L606	F607	T608	P609	Q610	Q611	L612	L613	R614	T615	A616	D617	L618	A619	L620	A621	N622	N623	F624	P625	R626	E627	A628	R629	N630	P631	Q632	T633	Y634	L635	V636	T637	T638	N639	Q640	R641	T642	G643	T644	T645	R646	E647	S648	P649	A650	L651	T652	T653	L654	L655	L656	A657	T658	L659	A660	N661	V662	V663	N664	E665	R666
P545	V546	E547	Y548	G549	L550	F551	L552	Q553	R554	G555	A556	T557	T558	T559	L560	N561	A562	A563	G564	F565	F566	E567	F568	S569	G570	R571	L572	E573	K574	L575	D576	Q577	L578	F579	Y580	L581	T582	E583	H584	F585	P586	A587	G588	D589	S590	L591	Q592	V593	L594	L595	A596	G597	N598	T599	L600	A601	I602	I603	M604		
E485	V486	Q487	P488	M489	M490	M491	M492	M493	M494	L495	L496	L497	L498	A499	E500	S501	F502	E503	D504	P505	S506	S507	L508	V509	V510	V511	L512	E513	F514	L515	L516	F517	A518	L519	F520	F521	P522	T523	E524	F525	N526	R527	L528	A529	K529	D530	L531	Q532	N533	V534	L535	L536	L537	L538	F539	F540	S541	R542	V543	Y544	
I425	I426	Q427	Q428	I429	I430	T431	G432	I433	V434	A435	A436	A437	I438	V439	I440	R441	P442	V443	S444	E445	K446	R447	Y448	F449	P450	E451	N452	N453	L454	Q455	N456	I457	N458	Q459	A460	R461	L462	V463	A464	A465	A466	K467	A468	R469	A470	S471	C472	L473	A474	L475	D476	S477	I478	H479	A480	A481	I482	A483	R484		
A364	L365	R366	E367	A368	N369	V370	T371	A372	D373	I374	R375	T376	K377	A378	L379	Q380	A381	H382	S383	I384	S385	S386	Q387	F388	F389	H390	G391	P392	N393	R394	G395	A396	L397	R398	P399	E400	L401	A402	F403	D404	H405	D406	H407	I408	I409	R410	C411	L412	M413	L414	A415	A416	A417	N418	R421	L422	Y423	E424			
R181	A182	S183	E184	A185	D186	N187	R188	I189	V190	T193	L196	F197	K198	Y199	G200	A201	A202	V203	V204	N205	I206	D207	L208	N209	R210	D211	F212	F213	D214	T215	A216	T217	G218	I219	D220	L221	T222	K223	G224	I225	P226	L227	V228	Q229	D230	L231	L232	V233	P234	I235	G236	N237	P238	L239	A240	E241	E242				
Q243	S244	A245	E246	Y247	V248	L249	L250	L251	L252	M253	V254	L255	F256	K257	V258	M259	D260	R261	R262	R263	L264	V265	I266	V267	G268	L269	G270	T271	T272	P273	M274	S275	N276	T277	L278	S279	T280	V281	V282	N283	N284	V285	L286	R287	T288	T289	Y290	H291	V294	G295	L296	N297	P298	A299	L300	R301	A302	G240	A241		
R304	T305	Q306	V307	N308	M309	L310	N311	R312	D313	I314	T315	N316	M317	L318	Q319	Q320	A321	G322	T323	K324	Y325	G326	L327	G328	L329	T330	E331	T332	R333	L334	D335	Y336	V337	R338	L339	V340	T341	T342	T343	V344	G345	A346	A347	L348	N349	T350	H351	H352	F353	A354	A355	S356	L357	L358	N359	I360	N361	L362	R363		

G1274	D1275	L1276	L1277	Y1278	S1279	P1280	V1281	A1282	N1283	G1284	Q1285	V1286	G1287	I1288	P1289	K1290	L1291	E1292	V1293	D1294	H1295	I1296	S1297	P1298	S1299	N1300	V1301	V1302	S1303	M1304	M1305	T1306	A1307	N1308	I1309	R1310	T1311	G1312	D1313	D1314	M1315	A1316	V1317	E1318	R1319	V1320	M1321	P1322	D1323	G1324	V1325	R1326	A1327	I1328	N1329	I1330	R1331	M1332	A1333
L1211	R1212	P1213	E1214	P1215	D1219	P1220	P1221	A1222	S1223	G1224	E1225	D1226	M1227	R1228	L1229	I1230	Y1231	P1232	L1233	Q1234	P1235	T1236	S1237	V1238	A1239	R1240	S1241	M1242	R1243	A1244	I1245	V1246	M1247	H1248	N1249	E1250	V1251	D1252	R1253	P1254	A1257	V1258	A1259	P1260	S1261	S1262	Y1263	E1264	M1265	D1266	T1267	G1268	T1269	L1270	S1271	R1272	N1273		
L1150	V1151	A1152	D1153	M1154	I1155	I1156	A1157	S1158	V1159	L1160	K1161	S1162	N1163	W1164	V1165	V1166	D1167	I1168	H1169	D1170	I1171	E1172	Y1173	T1174	A1175	E1176	V1177	M1178	T1179	P1180	S1181	E1182	G1183	Y1184	T1185	Q1186	H1187	V1188	D1189	A1190	E1191	S1192	I1193	M1194	T1195	K1198	G1199	K1200	L1201	F1202	H1203	L1204	Q1205	F1206	M1207	D1208	G1209	L1210	
P1090	D1091	V1092	P1093	E1094	G1095	Y1096	V1097	A1098	V1099	Q1100	Y1101	A1102	H1103	R1104	L1105	F1106	S1107	S1108	S1109	L1110	A1111	N1112	K1113	R1114	N1115	R1116	V1117	T1118	Y1119	P1120	H1121	P1122	P1123	T1124	G1125	M1126	A1127	Y1128	P1129	S1130	P1131	T1132	G1133	R1134	P1135	H1136	V1137	H1138	M1139	T1140	I1141	N1142	E1143	R1144	A1145	G1146	M1147	S1148	K1149
L1029	L1030	Y1031	D1032	D1033	Q1034	I1035	D1036	I1037	E1038	A1039	F1040	R1041	W1042	S1043	R1044	Y1045	F1046	L1047	D1048	E1049	L1050	R1051	L1052	R1053	R1054	L1055	G1058	L1059	R1060	L1061	I1062	T1063	N1064	P1065	R1066	I1067	A1068	R1069	R1070	F1071	D1072	G1073	V1074	R1075	I1076	R1077	Y1078	L1079	T1080	D1081	D1082	P1084	D1085	P1086	D1087	F1088	V1089		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	53.433	Depositor
Minimum map value	-40.259	Depositor
Average map value	0.625	Depositor
Map value standard deviation	5.607	Depositor
Recommended contour level	17	Depositor
Map size (Å)	652.39996, 652.39996, 652.39996	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9319999, 0.9319999, 0.9319999	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	B	0.46	3/9244 (0.0%)	0.70	16/12582 (0.1%)
1	C	2.63	731/10028 (7.3%)	2.23	556/13653 (4.1%)
All	All	1.92	734/19272 (3.8%)	1.68	572/26235 (2.2%)

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	B	0	9
1	C	0	30
All	All	0	39

The worst 5 of 734 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	278	LEU	C-N	16.35	1.57	1.33
1	C	227	LEU	C-N	14.79	1.53	1.33
1	C	585	PHE	C-O	13.48	1.34	1.24
1	C	244	SER	C-N	13.37	1.52	1.33
1	C	521	PHE	C-O	-12.05	1.11	1.24

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	VAL	O-C-N	27.50	151.47	122.04
1	C	172	ASP	CA-C-N	-20.92	92.00	123.17
1	C	172	ASP	C-N-CA	-20.92	92.00	123.17
1	C	1307	ALA	N-CA-C	-20.83	88.36	113.15
1	C	398	ARG	N-CA-C	20.81	140.24	112.35

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	261	ASP	Peptide
1	B	506	SER	Peptide
1	B	717	THR	Peptide
1	B	825	SER	Peptide
1	B	875	THR	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	B	9058	0	8964	546	0
1	C	9827	0	9719	2017	0
All	All	18885	0	18683	2518	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 67.

The worst 5 of 2518 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:835:TYR:CE1	1:C:942:HIS:HB3	1.27	1.68
1:C:1278:TYR:CD2	1:C:1288:ILE:HG13	1.23	1.64
1:C:910:LEU:HD23	1:C:915:VAL:CG2	1.27	1.63
1:C:233:VAL:CG2	1:C:234:PRO:HD2	1.28	1.62
1:C:1093:PRO:HG2	1:C:1096:TYR:CE1	1.30	1.61

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	B	1132/1333 (85%)	999 (88%)	121 (11%)	12 (1%)	11	39
1	C	1243/1333 (93%)	937 (75%)	209 (17%)	97 (8%)	1	5
All	All	2375/2666 (89%)	1936 (82%)	330 (14%)	109 (5%)	3	13

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	120	VAL
1	C	121	PHE
1	C	122	ASN
1	C	129	ALA
1	C	144	ASN

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	B	1000/1155 (87%)	987 (99%)	13 (1%)	61	74
1	C	1087/1155 (94%)	707 (65%)	380 (35%)	0	1
All	All	2087/2310 (90%)	1694 (81%)	393 (19%)	3	7

5 of 393 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	866	THR
1	C	1049	GLU
1	C	894	VAL
1	C	958	ILE
1	C	1079	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	693	ASN
1	C	1121	HIS
1	C	748	GLN
1	C	903	ASN
1	C	1205	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

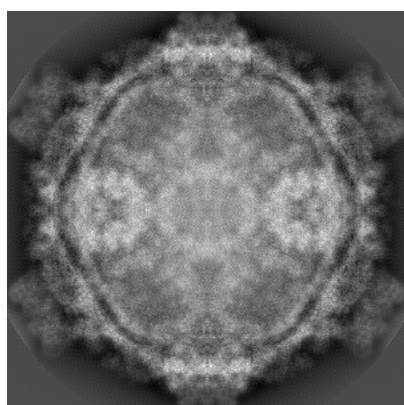
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9565. These allow visual inspection of the internal detail of the map and identification of artifacts.

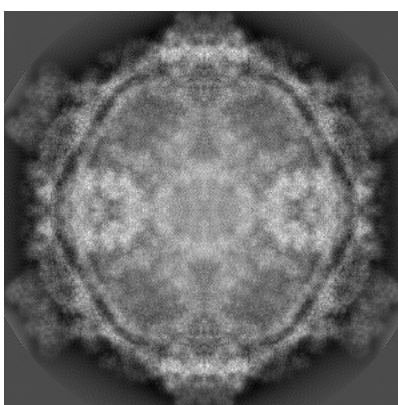
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

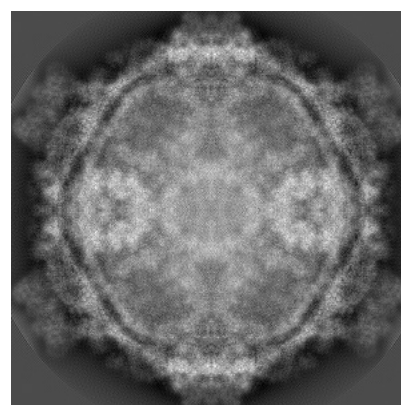
6.1.1 Primary map



X



Y

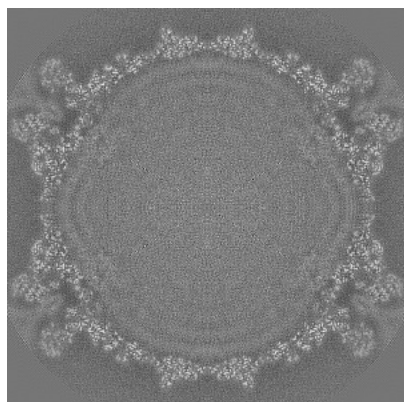


Z

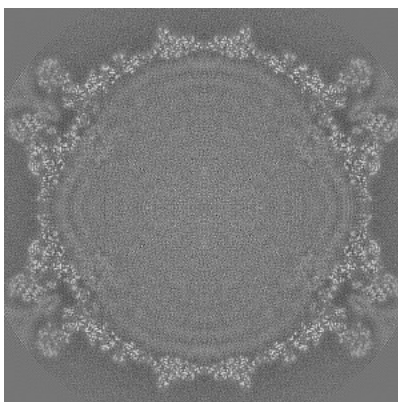
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

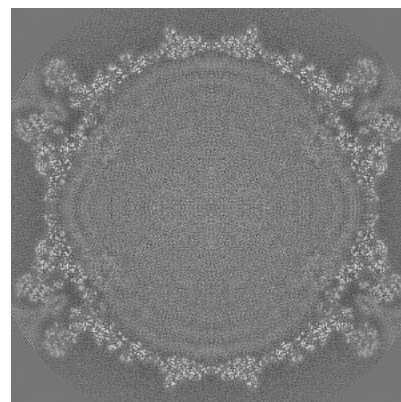
6.2.1 Primary map



X Index: 350



Y Index: 350

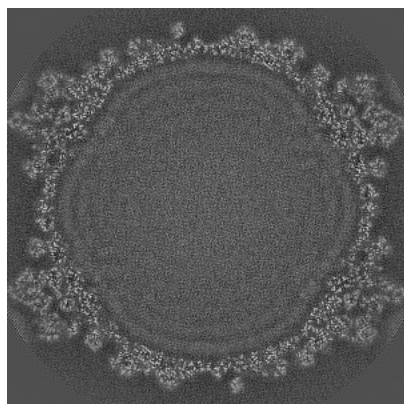


Z Index: 350

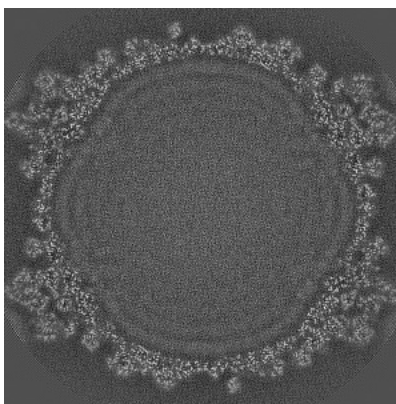
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

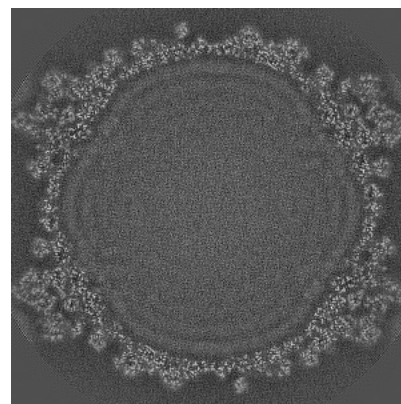
6.3.1 Primary map



X Index: 320



Y Index: 320

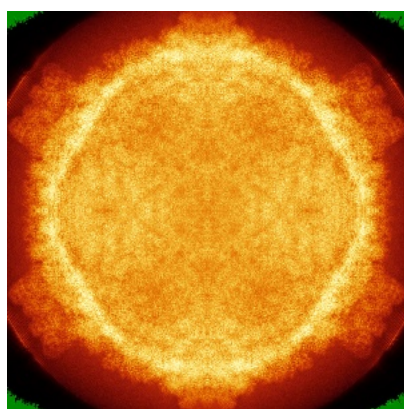


Z Index: 320

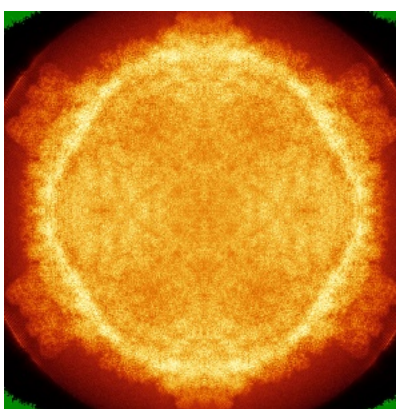
The images above show the largest variance slices of the map in three orthogonal directions.

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

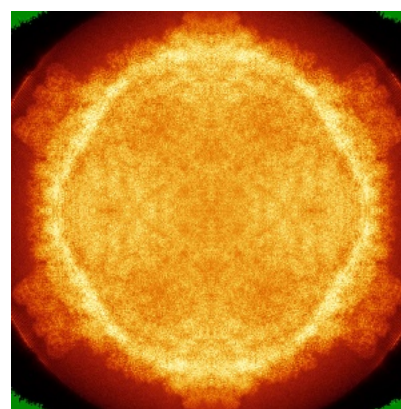
6.4.1 Primary map



X



Y

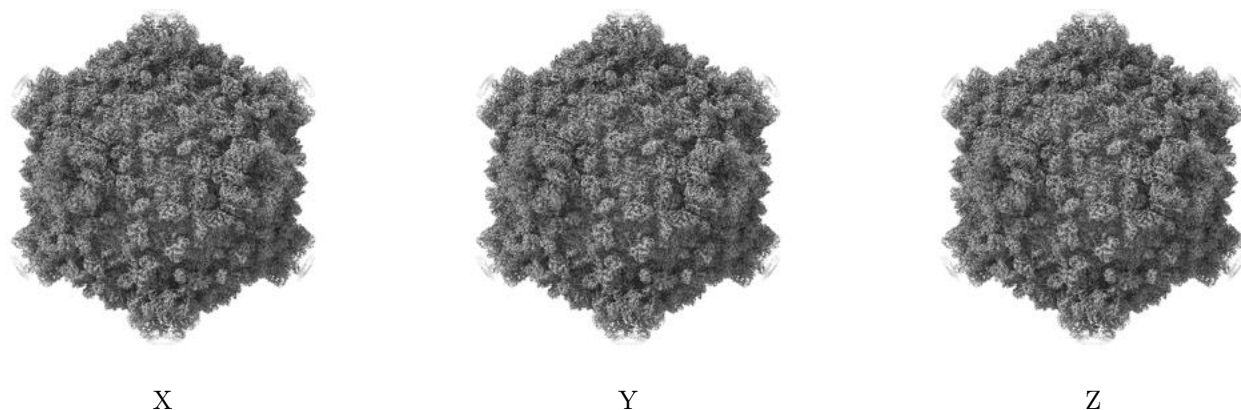


Z

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

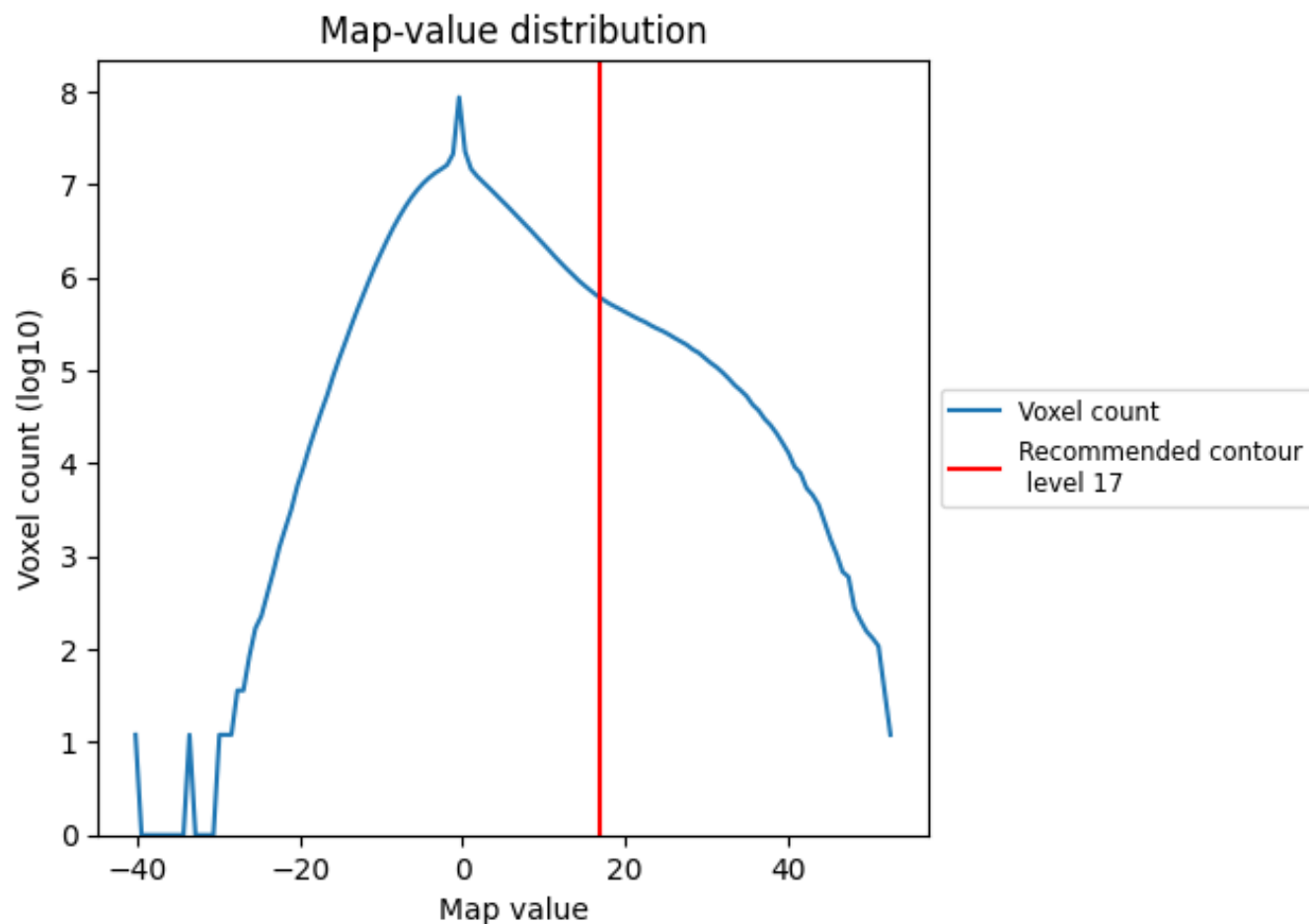
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

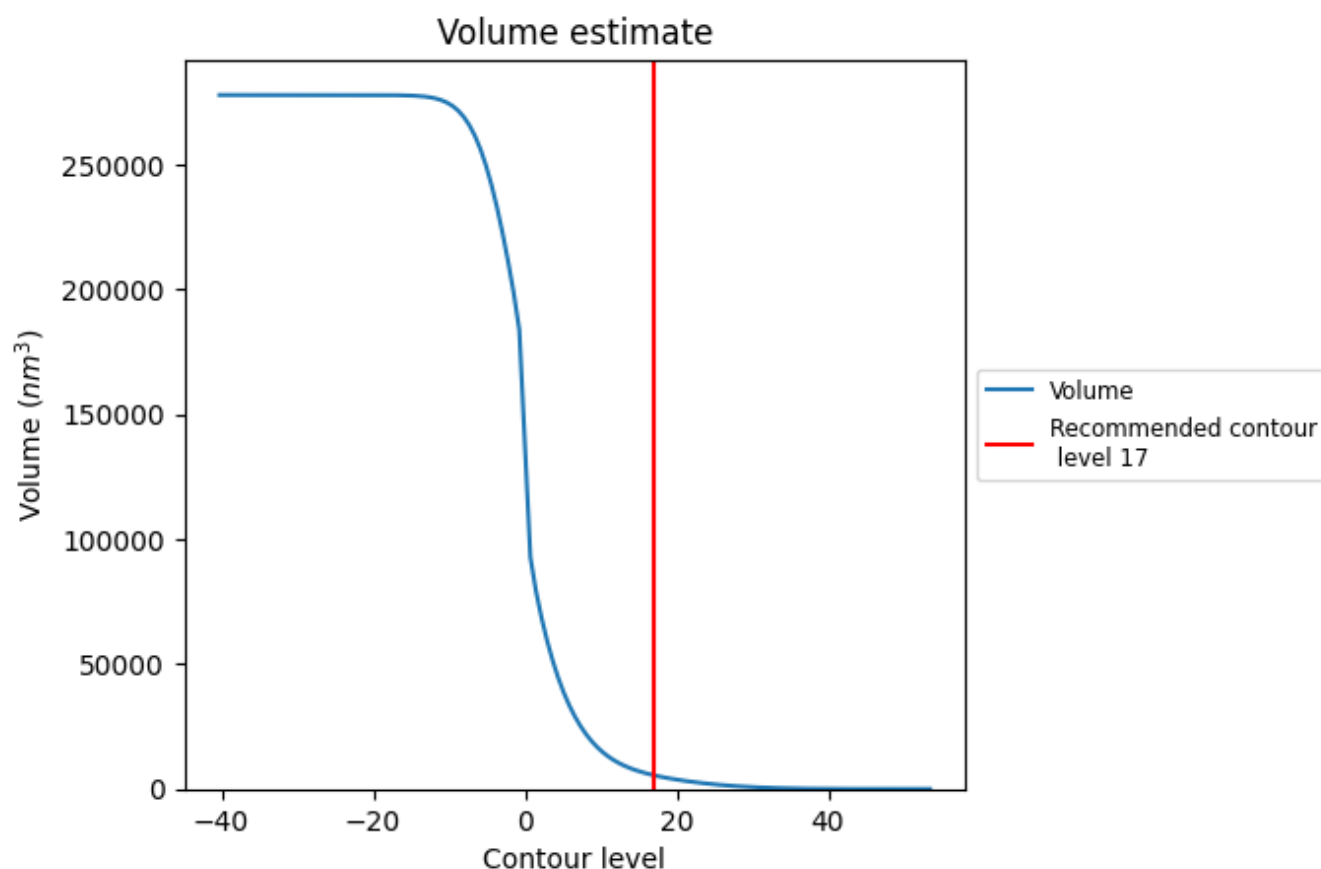
This section contains the results of statistical analysis of the map.

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.

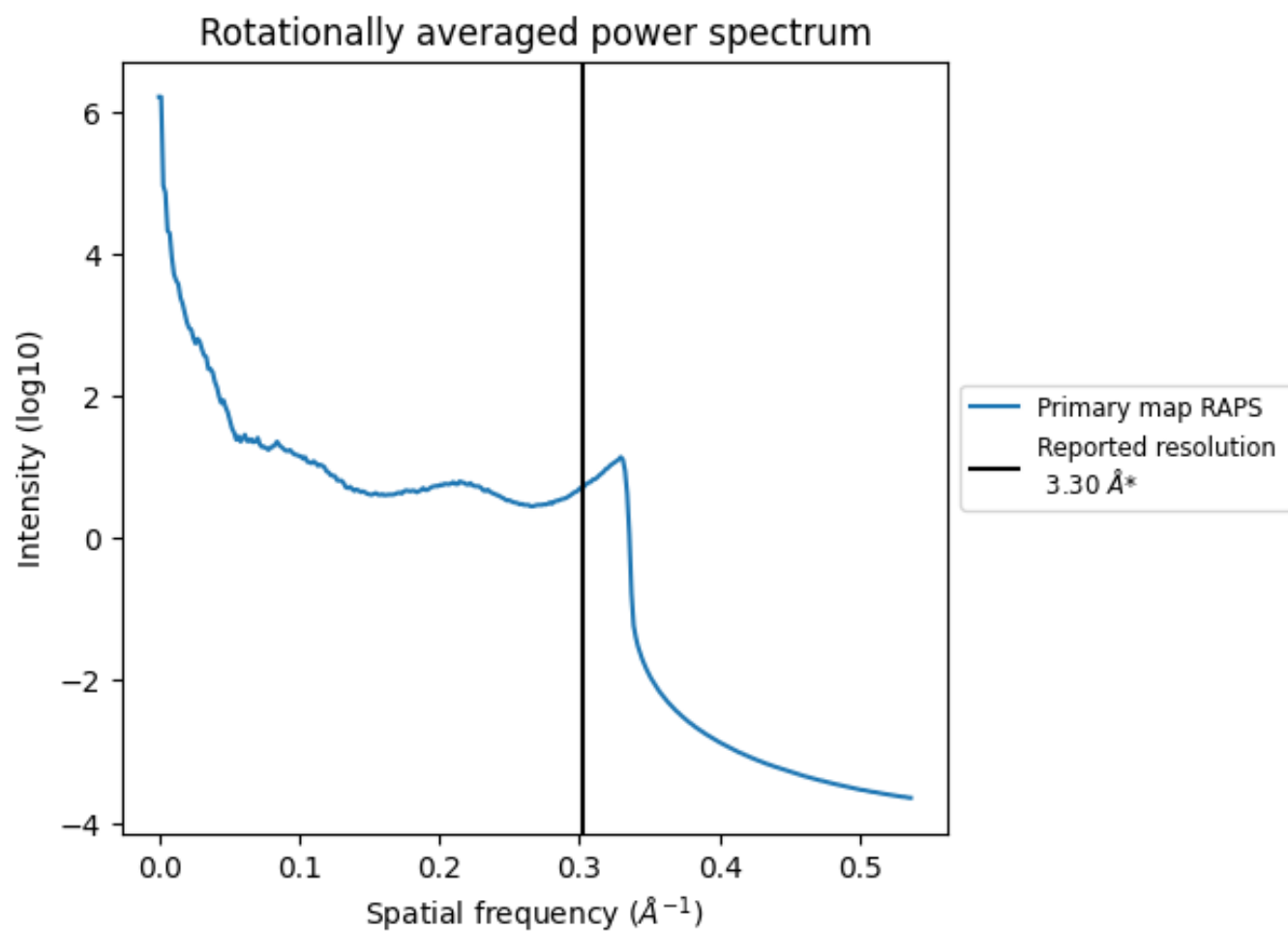
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5491 nm^3 ; this corresponds to an approximate mass of 4961 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 0.303 Å⁻¹

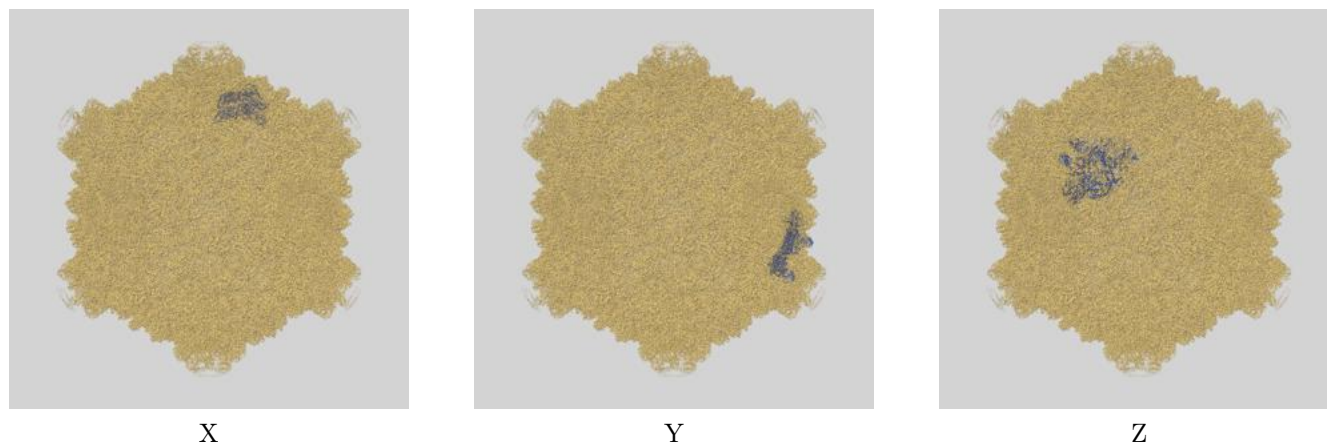
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

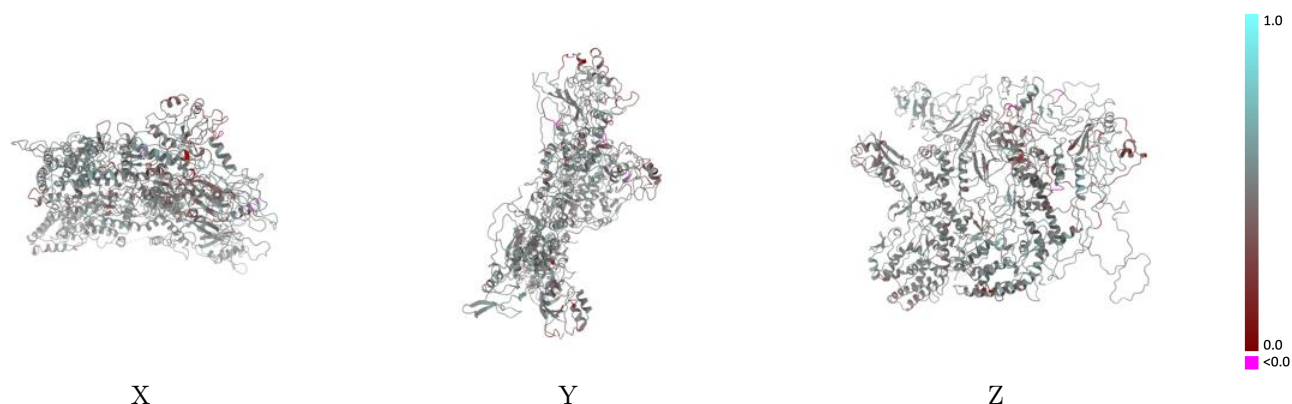
This section contains information regarding the fit between EMDB map EMD-9565 and PDB model 5H0S. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 17.0 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](#)

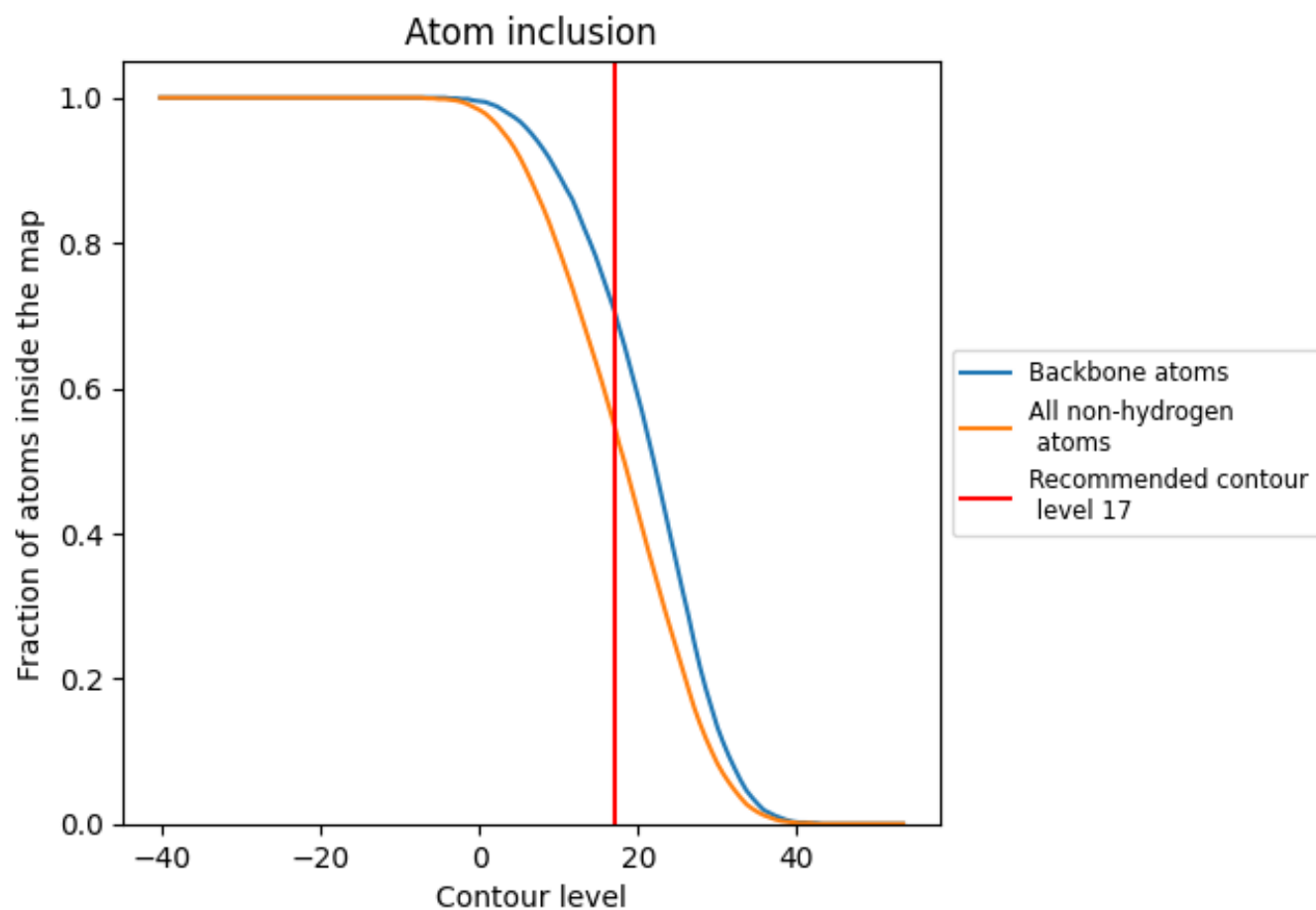


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 55% 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 (17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5490	0.4770
B	0.5460	0.4780
C	0.5520	0.4760

