



## wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 12:59 PM JST

PDB ID : 7V3L  
EMDB ID : EMD-31683  
Title : MERS S ectodomain trimer in complex with neutralizing antibody 6516  
Authors : Wang, X.; Zhao, J.; Wang, Z.; Wang, Y.; Zeng, J.  
Deposited on : 2021-08-10  
Resolution : 3.47 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

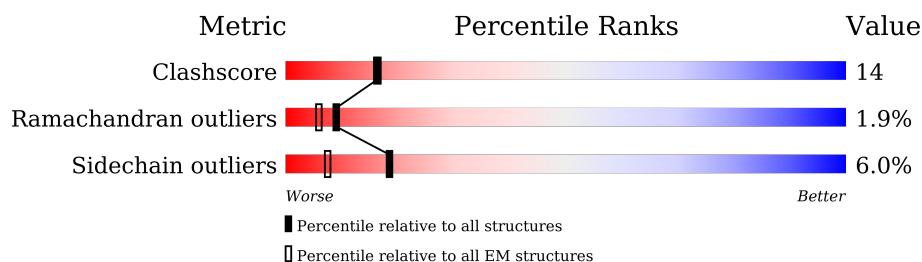
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.47 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	1290	
1	B	1290	
1	C	1290	
2	D	226	
2	F	226	
2	H	226	
3	E	215	
3	G	215	

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Mol	Chain	Length	Quality of chain
3	I	215	 79%18%..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36238 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	A	1131	Total	C	N	O	S	1	0
			8737	5550	1441	1695	51		
1	B	1135	Total	C	N	O	S	1	0
			8785	5579	1453	1702	51		
1	C	1126	Total	C	N	O	S	1	0
			8719	5536	1442	1690	51		

- Molecule 2 is a protein called antibody H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	226	Total	C	N	O	S	0	0
			1688	1063	279	337	9		
2	F	226	Total	C	N	O	S	0	0
			1688	1063	279	337	9		
2	H	226	Total	C	N	O	S	0	0
			1681	1057	279	336	9		

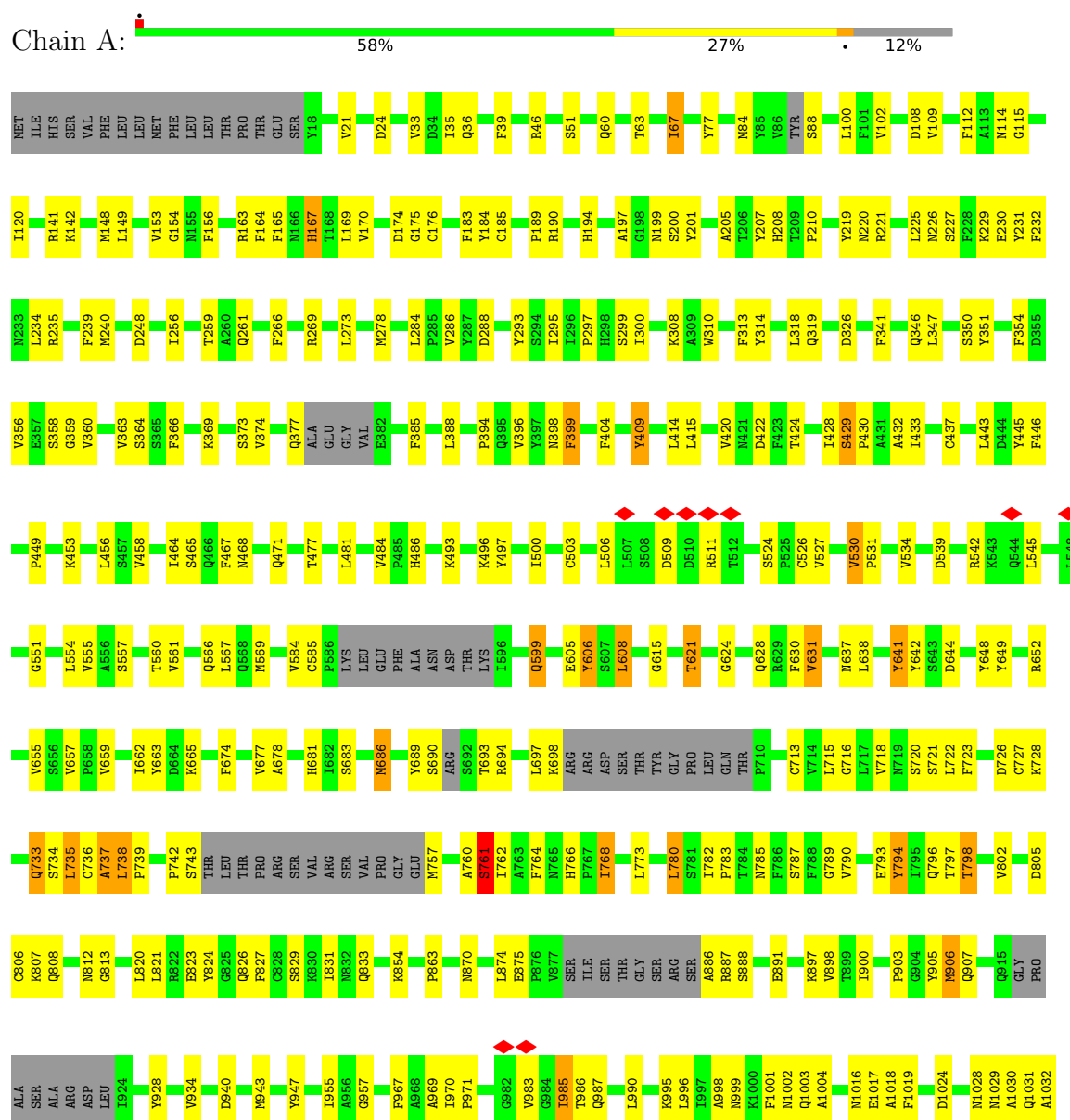
- Molecule 3 is a protein called antibody L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	214	Total	C	N	O	S	0	0
			1651	1037	277	332	5		
3	G	214	Total	C	N	O	S	0	0
			1651	1037	277	332	5		
3	I	212	Total	C	N	O	S	0	0
			1638	1030	275	328	5		

### 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



ASN	ILE	K1035	VAL	Y1142	Y1143	P1143	S1144	ASN	LEU	E1039	L1040	S1041	PRO	LEU	V1149	V1150	S1151	A1152	Y1153	G1154	LEU	GLY	D1157	A1158	A1159	N1160	P1161	T1162	ASN	ASP	P1167	VAL	N1169	G1170	Y1171	F1172	I1173	LYS	T1175	N1176	N1177	L1074	L1075	T1076	T1077	V1082	N1104	E1105	C1106	V1107	F1109	K1108	F1116	T1121	H1122	I1123	V1124	A1206	S1125	V1128	N1132	G1133
ASN	ILE	K1035	VAL	Y1142	Y1143	P1143	S1144	ASN	LEU	E1039	L1040	S1041	PRO	LEU	V1149	V1150	S1151	A1152	Y1153	G1154	LEU	GLY	D1157	A1158	A1159	N1160	P1161	T1162	ASN	ASP	P1167	VAL	N1169	G1170	Y1171	F1172	I1173	LYS	T1175	N1176	N1177	L1074	L1075	T1076	T1077	V1082	N1104	E1105	C1106	V1107	F1109	K1108	F1116	T1121	H1122	I1123	V1124	A1206	S1125	V1128	N1132	G1133
ASN	ILE	K1035	VAL	Y1142	Y1143	P1143	S1144	ASN	LEU	E1039	L1040	S1041	PRO	LEU	V1149	V1150	S1151	A1152	Y1153	G1154	LEU	GLY	D1157	A1158	A1159	N1160	P1161	T1162	ASN	ASP	P1167	VAL	N1169	G1170	Y1171	F1172	I1173	LYS	T1175	N1176	N1177	L1074	L1075	T1076	T1077	V1082	N1104	E1105	C1106	V1107	F1109	K1108	F1116	T1121	H1122	I1123	V1124	A1206	S1125	V1128	N1132	G1133
ASN	ILE	K1035	VAL	Y1142	Y1143	P1143	S1144	ASN	LEU	E1039	L1040	S1041	PRO	LEU	V1149	V1150	S1151	A1152	Y1153	G1154	LEU	GLY	D1157	A1158	A1159	N1160	P1161	T1162	ASN	ASP	P1167	VAL	N1169	G1170	Y1171	F1172	I1173	LYS	T1175	N1176	N1177	L1074	L1075	T1076	T1077	V1082	N1104	E1105	C1106	V1107	F1109	K1108	F1116	T1121	H1122	I1123	V1124	A1206	S1125	V1128	N1132	G1133

• Molecule 1: Spike glycoprotein

Chain B:  57% 29% 12%

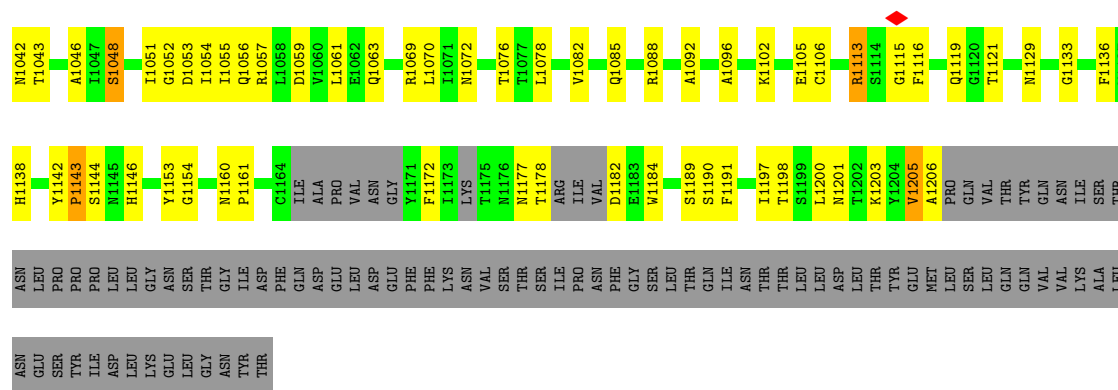
THR	N785	THR	F786	GLY	F617	LEU	W792	THR	F793	GLY	F623	LEU	W794	THR	F795	GLY	F627	LEU	W796	THR	F797	GLY	F628	LEU	W798	THR	F799	GLY	F629	LEU	W800	THR	F801	GLY	F630	LEU	W802	THR	F803	GLY	F631	LEU	W804	THR	F805	GLY	F632	LEU	W806	THR	F807	GLY	F633	LEU	W808	THR	F809	GLY	F634	LEU	W810	THR	F811	GLY	F635	LEU	W812	THR	F813	GLY	F636	LEU	W814	THR	F815	GLY	F637	LEU	W816	THR	F817	GLY	F638	LEU	W818	THR	F819	GLY	F639	LEU	W820	THR	F821	GLY	F640	LEU	W822	THR	F823	GLY	F641	LEU	W824	THR	F825	GLY	F642	LEU	W826	THR	F827	GLY	F643	LEU	W828	THR	F829	GLY	F644	LEU	W830	THR	F831	GLY	F645	LEU	W832	THR	F833	GLY	F646	LEU	W834	THR	F835	GLY	F647	LEU	W836	THR	F837	GLY	F648	LEU	W838	THR	F839	GLY	F649	LEU	W840	THR	F841	GLY	F650	LEU	W842	THR	F843	GLY	F651	LEU	W844	THR	F845	GLY	F652	LEU	W846	THR	F847	GLY	F653	LEU	W848	THR	F849	GLY	F654	LEU	W850	THR	F851	GLY	F655	LEU	W852	THR	F853	GLY	F656	LEU	W854	THR	F855	GLY	F657	LEU	W856	THR	F857	GLY	F658	LEU	W858	THR	F859	GLY	F659	LEU	W860	THR	F861	GLY	F660	LEU	W862	THR	F863	GLY	F661	LEU	W864	THR	F865	GLY	F662	LEU	W866	THR	F867	GLY	F663	LEU	W868	THR	F869	GLY	F664	LEU	W870	THR	F871	GLY	F665	LEU	W872	THR	F873	GLY	F666	LEU	W874	THR	F875	GLY	F667	LEU	W876	THR	F877	GLY	F668	LEU	W878	THR	F879	GLY	F669	LEU	W880	THR	F881	GLY	F670	LEU	W882	THR	F883	GLY	F671	LEU	W884	THR	F885	GLY	F672	LEU	W886	THR	F887	GLY	F673	LEU	W888	THR	F889	GLY	F674	LEU	W890	THR	F891	GLY	F675	LEU	W892	THR	F893	GLY	F676	LEU	W894	THR	F895	GLY	F677	LEU	W896	THR	F897	GLY	F678	LEU	W898	THR	F899	GLY	F679	LEU	W900	THR	F901	GLY	F680	LEU	W902	THR	F903	GLY	F681	LEU	W904	THR	F905	GLY	F682	LEU	W906	THR	F907	GLY	F683	LEU	W908	THR	F909	GLY	F684	LEU	W910	THR	F911	GLY	F685	LEU	W912	THR	F913	GLY	F686	LEU	W914	THR	F915	GLY	F687	LEU	W916	THR	F917	GLY	F688	LEU	W918	THR	F919	GLY	F689	LEU	W920	THR	F921	GLY	F690	LEU	W922	THR	F923	GLY	F691	LEU	W924	THR	F925	GLY	F692	LEU	W926	THR	F927	GLY	F693	LEU	W928	THR	F929	GLY	F694	LEU	W930	THR	F931	GLY	F695	LEU	W932	THR	F933	GLY	F696	LEU	W934	THR	F935	GLY	F697	LEU	W936	THR	F937	GLY	F698	LEU	W938	THR	F939	GLY	F699	LEU	W940	THR	F941	GLY	F700	LEU	W942	THR	F943	GLY	F701	LEU	W944	THR	F945	GLY	F702	LEU	W946	THR	F947	GLY	F703	LEU	W948	THR	F949	GLY	F704	LEU	W950	THR	F951	GLY	F705	LEU	W952	THR	F953	GLY	F706	LEU	W954	THR	F955	GLY	F707	LEU	W956	THR	F957	GLY	F708	LEU	W958	THR	F959	GLY	F709	LEU	W960	THR	F961	GLY	F710	LEU	W962	THR	F963	GLY	F711	LEU	W964	THR	F965	GLY	F712	LEU	W966	THR	F967	GLY	F713	LEU	W968	THR	F969	GLY	F714	LEU	W970	THR	F971	GLY	F715	LEU	W972	THR	F973	GLY	F716	LEU	W974	THR	F975	GLY	F717	LEU	W976	THR	F977	GLY	F718	LEU	W978	THR	F979	GLY	F719	LEU	W980	THR	F981	GLY	F720	LEU	W982	THR	F983	GLY	F721	LEU	W984	THR	F985	GLY	F722	LEU	W986	THR	F987	GLY	F723	LEU	W988	THR	F989	GLY	F724	LEU	W990	THR	F991	GLY	F725	LEU	W992	THR	F993	GLY	F726	LEU	W994	THR	F995	GLY	F727	LEU	W996	THR	F997	GLY	F728	LEU	W998	THR	F999	GLY	F729	LEU	W1000	THR	F1001	GLY	F730	LEU	W1002	THR	F1003	GLY	F731	LEU	W1004	THR	F1005	GLY	F732	LEU	W1006	THR	F1007	GLY	F733	LEU	W1008	THR	F1009	GLY	F734	LEU	W1010	THR	F1011	GLY	F735	LEU	W1012	THR	F1013	GLY	F736	LEU	W1014	THR	F1015	GLY	F737	LEU	W1016	THR	F1017	GLY	F738	LEU	W1018	THR	F1019	GLY	F739	LEU	W1020	THR	F1021	GLY	F740	LEU	W1022	THR	F1023	GLY	F741	LEU	W1024	THR	F1025	GLY	F742	LEU	W1026	THR	F1027	GLY	F743	LEU	W1028	THR	F1029	GLY	F744	LEU	W1030	THR	F1031	GLY	F745	LEU	W1032	THR	F1033	GLY	F746	LEU	W1034	THR	F1035	GLY	F747	LEU	W1036	THR	F1037	GLY	F748	LEU	W1038	THR	F1039	GLY	F749	LEU	W1040	THR	F1041	GLY	F750	LEU	W1042	THR	F1043	GLY	F751	LEU	W1044	THR	F1045	GLY	F752	LEU	W1046	THR	F1047	GLY	F753	LEU	W1048	THR	F1049	GLY	F754	LEU	W1050	THR	F1051	GLY	F755	LEU	W1052	THR	F1053	GLY	F756	LEU	W1054	THR	F1055	GLY	F757	LEU	W1056	THR	F1057	GLY	F758	LEU	W1058	THR	F1059	GLY	F759	LEU	W1060	THR	F1061	GLY	F760	LEU	W1062	THR	F1063	GLY	F761	LEU	W1064	THR	F1065	GLY	F762	LEU	W1066	THR	F1067	GLY	F763	LEU	W1068	THR	F1069	GLY	F764	LEU	W1070	THR	F1071	GLY	F765	LEU	W1072	THR	F1073	GLY	F766	LEU	W1074	THR	F1075	GLY	F767	LEU	W1076	THR	F1077	GLY	F768	LEU	W1078	THR	F1079	GLY	F769	LEU	W1080	THR	F1081	GLY	F770	LEU	W1082	THR	F1083	GLY	F771	LEU	W1084	THR	F1085	GLY	F772	LEU	W1086	THR	F1087	GLY	F773	LEU	W1088	THR	F1089	GLY	F774	LEU	W1090	THR	F1091	GLY	F775	LEU	W1092	THR	F1093	GLY	F776	LEU	W1094	THR	F1095	GLY	F777	LEU	W1096	THR	F1097	GLY	F778	LEU	W1098	THR	F1099	GLY	F779	LEU	W1100	THR	F1101	GLY	F780	LEU	W1102	THR	F1103	GLY	F781	LEU	W1104	THR	F1105	GLY	F782	LEU	W1106	THR	F1107	GLY	F783	LEU	W1108	THR	F1109	GLY	F784	LEU	W1110	THR	F1111	GLY	F785	LEU	W1112	THR	F1113	GLY	F786	LEU	W1114	THR	F1115	GLY	F787	LEU	W1116	THR	F1117	GLY	F788	LEU	W1118	THR	F1119	GLY	F789	LEU	W1120	THR	F1121	GLY	F790	LEU	W1122	THR	F1123	GLY	F791	LEU	W1124	THR	F1125	GLY	F792	LEU	W1126	THR	F1127	GLY	F793	LEU	W1128	THR	F1129	GLY	F794	LEU	W1130	THR	F1131	GLY	F795	LEU	W1132	THR	F1133	GLY	F796	LEU	W1134	THR	F1135	GLY	F797	LEU	W1136	THR	F1137	GLY	F798	LEU	W1138	THR	F1139	GLY	F799	LEU	W1140	THR	F1141	GLY	F800	LEU	W1142	THR	F1143	GLY	F801	LEU	W1144	THR	F1145	GLY	F802	LEU	W1146	THR	F1147	GLY	F803	LEU	W1148	THR	F1149	GLY	F804	LEU	W1150	THR	F1151	GLY	F805	LEU	W1152	THR	F1153	GLY	F806	LEU	W1154	THR	F1155	GLY	F807	LEU	W1156	THR	F1157	GLY	F808	LEU	W1158	THR	F1159	GLY	F809	LEU	W1160	THR	F1161	GLY	F810	LEU	W1162	THR	F1163	GLY	F811	LEU	W1164	THR	F1165	GLY	F812	LEU	W1166	THR	F1167	GLY	F813	LEU	W1168	THR	F1169	GLY	F814	LEU	W1170	THR	F1171	GLY	F815	LEU	W1172	THR	F1173	GLY	F816	LEU	W1174	THR	F1175	GLY	F817	LEU	W1176	THR	F1177	GLY	F818	LEU	W1178	THR	F1179	GLY	F819	LEU	W1180	THR	F1181	GLY	F820	LEU	W1182	THR	F1183	GLY	F821	LEU	W1184	THR	F1185	GLY	F822	LEU	W1186	THR	F1187	GLY	F823	LEU	W1188	THR	F1189	GLY	F824	LEU	W1190	THR	F1191	GLY	F825	LEU	W1192	THR	F1193	GLY	F826	LEU	W1194	THR	F1195	GLY	F827	LEU	W1196	THR	F1197	GLY	F828	LEU	W1198	THR	F1199	GLY	F829	LEU	W1200	THR	F1201	GLY	F830	LEU	W1202	THR	F1203	GLY	F831	LEU	W1204	THR	F1205	GLY	F832	LEU	W1206	THR	F1207	GLY	F833	LEU	W1208	THR	F1209	GLY	F834	LEU	W1210	THR	F1211	GLY	F835	LEU	W1212	THR	F1213	GLY	F836	LEU	W1214	THR	F1215	GLY	F837	LEU	W1216	THR	F1217	GLY	F838	LEU	W1218	THR	F1219	GLY	F839	LEU	W1220	THR	F1221	GLY	F840	LEU	W1222	THR	F1223	GLY	F841	LEU	W1224	THR	F1225	GLY	F842	LEU	W1226	THR	F1227	GLY	F843	LEU	W1228	THR	F1229	GLY	F844	LEU	W1230	THR	F1231	GLY	F845	LEU	W1232	THR	F1233	GLY	F846	LEU	W1234	THR	F1235	GLY	F847	LEU	W1236	THR	F1237	GLY	F848	LEU	W1238	THR	F1239	GLY	F849	LEU	W1240	THR	F1241	GLY	F850	LEU	W1242	THR	F1243	GLY	F851	LEU	W1244	THR	F1245	GLY	F852	LEU	W1246	THR	F1247	GLY	F853	LEU	W1248	THR	F1249	GLY	F854	LEU	W1250	THR	F1251	GLY	F855	LEU	W1252	THR	F1253	GLY	F856	LEU	W1254	THR	F1255	GLY	F857	LEU	W1256	THR	F1257	GLY	F858	LEU	W1258	THR	F1259	GLY	F859	LEU	W1260	THR	F1261	GLY	F860	LEU	W1262	THR	F1263	GLY	F861	LEU	W1264	THR	F1265	GLY	F862	LEU	W1266	THR	F1267	GLY	F863	LEU	W1268	THR	F1269	GLY	F864	LEU	W1270	THR	F1271	GLY	F865	LEU	W1272	THR	F1273	GLY	F866	LEU	W1274	THR	F1275	GLY	F867	LEU	W1276	THR	F1277	GLY	F868	LEU	W1278	THR	F1279	GLY	F869	LEU	W1280	THR	F1281	GLY	F870	LEU	W1282	THR	F1283	GLY	F871	LEU	W1284	THR	F1285	GLY	F872	LEU	W1286	THR	F1287	GLY	F873	LEU	W1288	THR	F1289	GLY	F874	LEU	W1290	THR	F1291	GLY	F875	LEU	W1292	THR	F1293	GLY	F876	LEU	W1294	THR	F1295	GLY	F877	LEU	W1296	THR	F1297	GLY	F878	LEU	W1298	THR	F1299	GLY	F879	LEU	W1300	THR	F1301	GLY	F880	LEU	W1302	THR	F1303	GLY	F881	LEU	W1304	THR	F1305	GLY	F882	LEU	W1306	THR	F1307	GLY	F883	LEU	W1308	THR	F1309	GLY	F884	LEU	W1310	THR	F1311	GLY	F885	LEU	W1312	THR	F1313	GLY	F886	LEU	W1314	THR	F1315	GLY	F887	LEU	W1316	THR	F1317	GLY	F888	LEU	W1318	THR	F1319	GLY	F889	LEU	W1320	THR	F1321	GLY	F890	LEU	W1322	THR	F1323	GLY	F891	LEU	W1324	THR	F1325	GLY	F89
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L996	G1115	A1206	MET
L997	F1116	PRO	LEU
A998	C1117	GLN	SER
	G1118	VAL	SER
	Q1119	THR	GLN
	G1120	TYR	GLN
	T1121	GLN	VAL
	H1122	ASN	VAL
F1019	I1123	ILE	LYS
Q1020	V1124	SER	ALA
K1021	S1125	THR	LEU
		ASN	ASN
H1027	A1130	LEU	GLU
H1028	P1131	PRO	SER
H1029	M1132	PRO	TYR
A1030	G1133	PRO	ILE
Q1031	L1134	LEU	GLU
A1032	L1135	LEU	ASP
L1033	Y1136	GLY	LEU
S1034	M1137	ASN	LYS
K1035	H1138	GLY	GLU
	Y1141	SER	LEU
L1040	Y1142	GLY	ASN
T1043	P1143	ILE	TYR
PHE	S1144	PHE	THR
G1045		GLN	
	Y1153	ASP	
S1050	G1154	GLU	D34
I1051		LEU	I35
G1052	M1160	ASP	Q36
D1053	P1161	GLU	Q37
I1054		PHE	F40
Q1055	C1164	PHE	S137
L1055	I1165	LYS	W44
Q1056	A1166	ASN	P45
R1057	P1167	VAL	B46
L1058	P1168	SER	
	M1169	THR	V50
E1062	G1170	SER	
Q1063		ILE	I56
	R1179	PRO	I57
I1067		ASN	Y58
	V1180		P59
R1074	V1181	PHE	Q60
L1075	D1182	GLY	S61
T1076	E1183	SER	B62
T1077	W1184	LEU	T63
L1078	S1185	THR	Y64
	Y1186	GLN	S65
A1092		ILE	B66
	Y1192	ASN	I67
		THR	Y71
N1104	P1196	THR	Q78
		LEU	L77
K1108	S1199	LEU	L72
A1109	I1200	ASP	P173
Q1110	N1201	LEU	D174
S1111		TYR	
K1112	Y1204	THR	
R1113		TYR	
S1114		GLU	

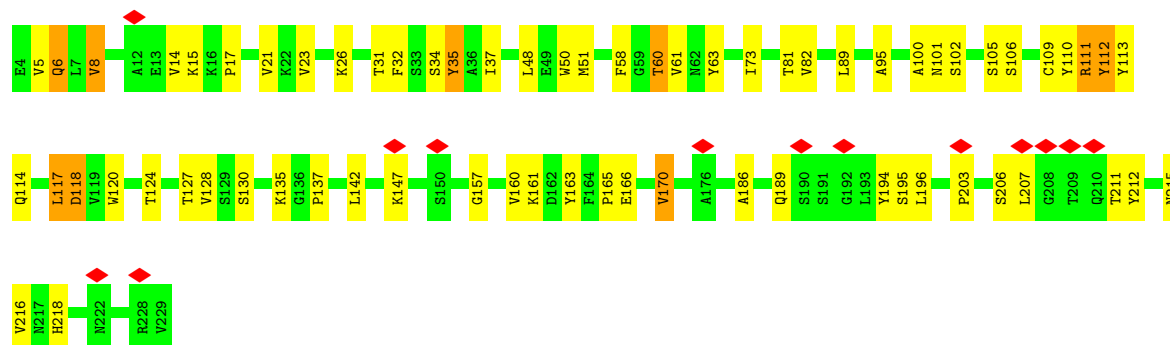
• Molecule 1: Spike glycoprotein

Chain C:  54% 31% 13%

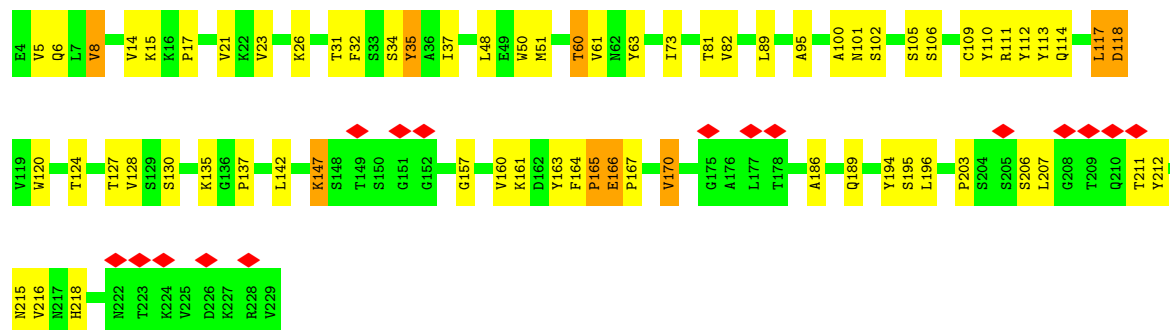
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ILE	V86	L180	Q258	GLY	A482	C585	T741	Q819	PRO
HIS	TYR	R181	T259	VAL	T483	P586	T744	Q822	ALA
SER	S88	A182	H264	F385	V484	LEU	THR	I831	ALA
VAL	A89	F183	L265	L388	P485	GLU	PRO	Q842	ARG
GLN	G90	Y184	F266	V385	H486	PHE	ARG	I849	ASP
LEU	H91	C185	S268	P394	T490	ALA	THR	Q849	LEU
VAL	A92	E188	R269	Q395	T491	ASN	ASP	V846	
LEU	T95	P189	D272	V396	T492	THR	THR	V846	
LEU	P97	R190	M278	V397	T493	K595	SER	L849	
THR	Q98	S191	G278	N398	Y497	L596	PRO	V853	
PRO	K99	G192	K291	F399	Y497	A597	GLY	V853	
THR	F101	N193	Y292	F404	Y497	S598	VAL	I861	
GLY	Y105	C195	Y293	Y409	Y497	Q599	ARG	I862	
TYR	K110	A197	G198	L414	Y497	G603	ASP	R865	
	I120	G198	Y201	L415	Y497	T604	THR	G866	
	A123	F204	T202	L415	Y497	R614	THR	F869	
	S126	A205	S203	V420	Y497	G615	THR	T872	
	T129	T206	D306	T424	Y497	G616	THR	E875	
	I130	Y207	R307	L428	Y497	F617	THR	P876	
	I131	P210	K308	S429	Y497	Q618	THR	G877	
	I132	A211	A309	P430	Y497	N619	THR	I878	
	T136	T212	V310	A431	Y497	T621	THR	G879	
	S137	S215	G331	A432	Y497	A622	THR	W881	
	A138	N218	R334	L433	Y497	R626	THR	A882	
	I140	Y219	L337	L443	Y497	R629	THR	S885	
	R141	R220	D338	D444	Y497	F630	THR	A886	
	K142	R221	C339	Y445	Y497	G631	THR	R887	
	F40	N222	F341	F446	Y497	D633	THR	I888	
	I56	L225	Q346	P449	Y497	Y635	THR	A889	
	I57	L226	E357	K453	Y497	L638	THR	Q891	
	P59	S227	S358	L456	Y497	V639	THR	D892	
	Q60	E230	V363	S457	Y497	G640	THR	Q796	
	B62	Y231	S364	V458	Y497	Y641	THR	T798	
	Y64	F232	S365	T464	Y497	D644	THR	V802	
	S65	L234	F366	S465	Y497	D644	THR	T803	
	B66	R235	K369	Q466	Y497	Y648	THR	V804	
	I67	Y240	V373	F467	Y497	Y649	THR	D805	
	Y71	T245	Y375	N468	Y497	C650	THR	Y905	
	Q78	E249	Q377	Q471	Y497	L651	THR	Q907	
	H81	T250	ALA	T477	Y497	R652	THR	V810	
	M84			L480	Y497	A653	THR	L735	
					Y497	S656	THR	C736	
					Y497	V659	THR	Q914	
					Y497		THR	L1033	



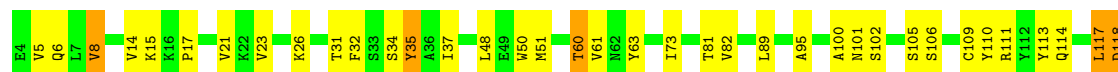
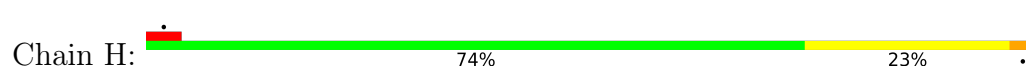
• Molecule 2: antibody H



• Molecule 2: antibody H



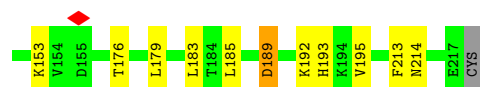
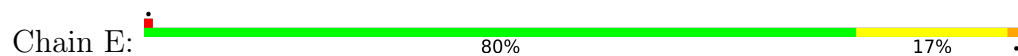
• Molecule 2: antibody H



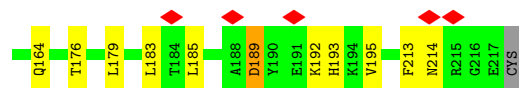
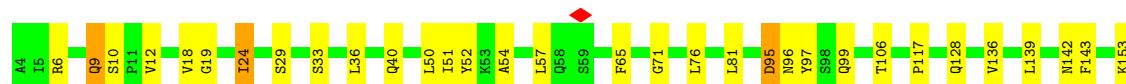
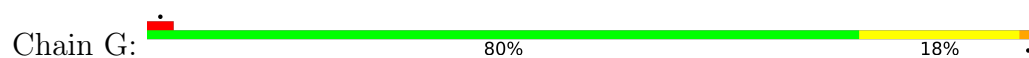




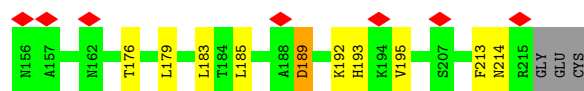
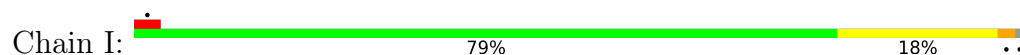
- Molecule 3: antibody L



- Molecule 3: antibody L



- Molecule 3: antibody L



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1289518	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size ( $\text{\AA}$ )	343.74402, 343.74402, 343.74402	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0742, 1.0742, 1.0742	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	0.60	0/8931	0.69	2/12136 (0.0%)
1	B	0.59	0/8981	0.70	3/12206 (0.0%)
1	C	0.59	0/8912	0.69	3/12105 (0.0%)
2	D	0.68	1/1729 (0.1%)	0.71	1/2357 (0.0%)
2	F	0.66	0/1729	0.70	1/2357 (0.0%)
2	H	0.66	0/1721	0.69	0/2346
3	E	0.65	0/1687	0.70	0/2291
3	G	0.65	0/1687	0.70	0/2291
3	I	0.65	0/1674	0.70	0/2274
All	All	0.61	1/37051 (0.0%)	0.69	10/50363 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	111	ARG	C-N	6.06	1.48	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	SER	N-CA-C	6.42	128.33	111.00
1	C	788	PHE	CB-CA-C	-6.16	98.08	110.40
1	A	641	TYR	CB-CA-C	-5.65	99.09	110.40
2	D	111	ARG	O-C-N	5.61	131.67	122.70
1	C	642	TYR	CB-CA-C	5.15	120.70	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51[A]	SER	Mainchain
1	A	51[B]	SER	Mainchain

## 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	8737	0	8422	264	0
1	B	8785	0	8501	302	0
1	C	8719	0	8414	311	0
2	D	1688	0	1636	39	0
2	F	1688	0	1636	39	0
2	H	1681	0	1629	35	0
3	E	1651	0	1615	26	0
3	G	1651	0	1615	24	0
3	I	1638	0	1606	23	0
All	All	36238	0	35074	999	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 999 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:985:ILE:H	1:A:1181:VAL:HG21	1.50	0.77
1:B:189:PRO:HB2	1:B:197:ALA:HB2	1.66	0.77
1:A:683:SER:H	1:A:686:MET:HG2	1.50	0.77
1:C:990:LEU:HD21	1:C:1184:TRP:HB2	1.67	0.76
1:B:1040:LEU:HD22	1:B:1077:THR:HB	1.67	0.76

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	1108/1290 (86%)	977 (88%)	117 (11%)	14 (1%)	10	41
1	B	1118/1290 (87%)	957 (86%)	132 (12%)	29 (3%)	4	28
1	C	1103/1290 (86%)	938 (85%)	135 (12%)	30 (3%)	4	28
2	D	224/226 (99%)	203 (91%)	18 (8%)	3 (1%)	10	41
2	F	224/226 (99%)	202 (90%)	18 (8%)	4 (2%)	7	35
2	H	224/226 (99%)	206 (92%)	15 (7%)	3 (1%)	10	41
3	E	212/215 (99%)	198 (93%)	13 (6%)	1 (0%)	25	59
3	G	212/215 (99%)	198 (93%)	13 (6%)	1 (0%)	25	59
3	I	210/215 (98%)	196 (93%)	12 (6%)	2 (1%)	13	46
All	All	4635/5193 (89%)	4075 (88%)	473 (10%)	87 (2%)	9	34

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	737	ALA
1	A	995	LYS
1	A	1153	TYR
1	A	1181	VAL
1	B	731	LEU

### 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	970/1118 (87%)	908 (94%)	62 (6%)	14	42
1	B	978/1118 (88%)	924 (94%)	54 (6%)	18	46
1	C	969/1118 (87%)	928 (96%)	41 (4%)	25	54
2	D	191/191 (100%)	175 (92%)	16 (8%)	9	32
2	F	191/191 (100%)	174 (91%)	17 (9%)	8	31
2	H	190/191 (100%)	174 (92%)	16 (8%)	9	32
3	E	188/189 (100%)	175 (93%)	13 (7%)	13	39
3	G	188/189 (100%)	176 (94%)	12 (6%)	14	42
3	I	187/189 (99%)	175 (94%)	12 (6%)	14	42
All	All	4052/4494 (90%)	3809 (94%)	243 (6%)	18	43

5 of 243 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1186	TYR
2	H	48	LEU
1	C	862	ILE
2	H	31	THR
3	I	97	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	346	GLN
3	I	93	GLN
1	C	1023	GLN
2	H	210	GLN
3	G	96	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

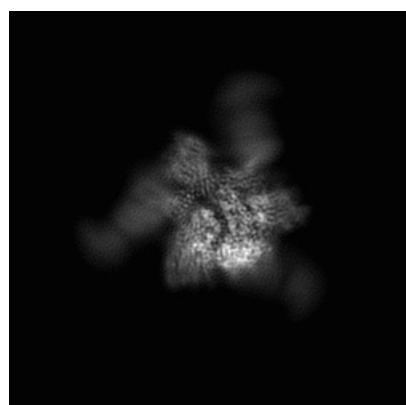
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31683. These allow visual inspection of the internal detail of the map and identification of artifacts.

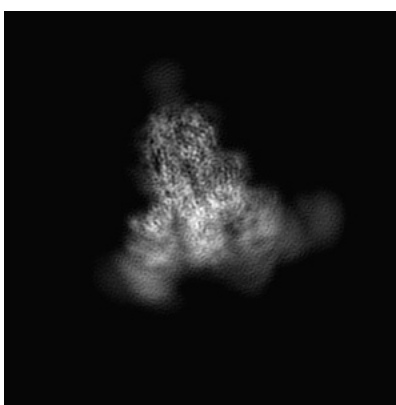
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

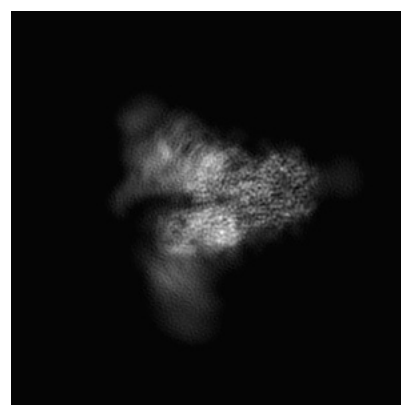
#### 6.1.1 Primary map



X



Y

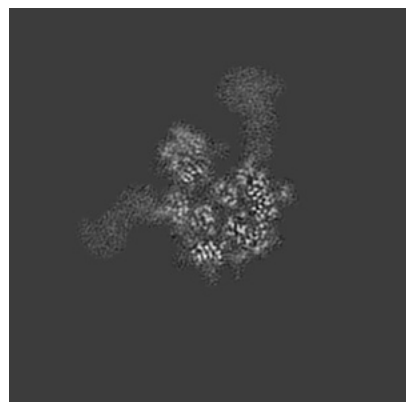


Z

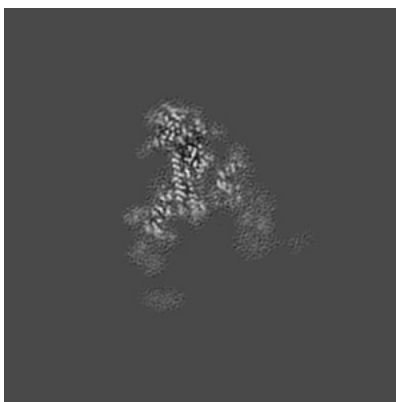
The images above show the map projected in three orthogonal directions.

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

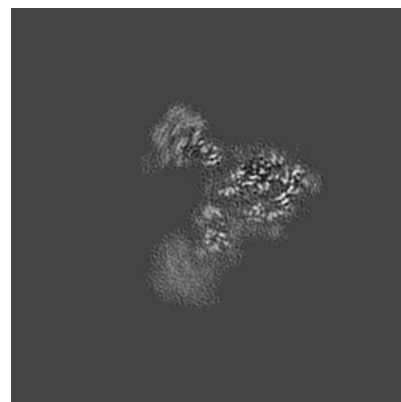
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



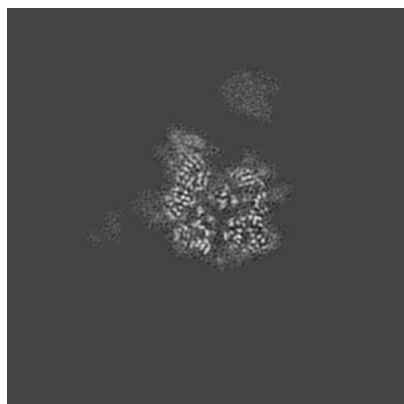
Z Index: 160



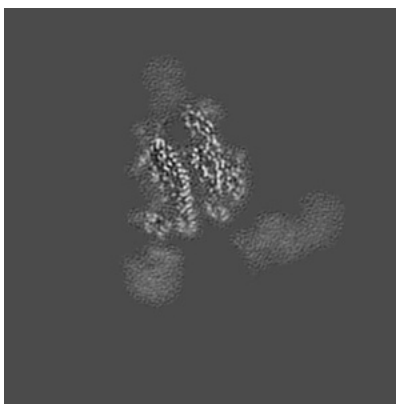
The images above show central slices of the map in three orthogonal directions.

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

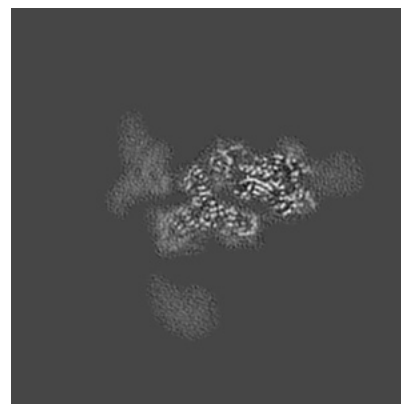
### 6.3.1 Primary map



X Index: 167



Y Index: 179

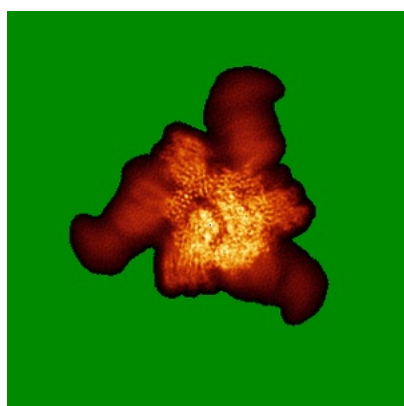


Z Index: 127

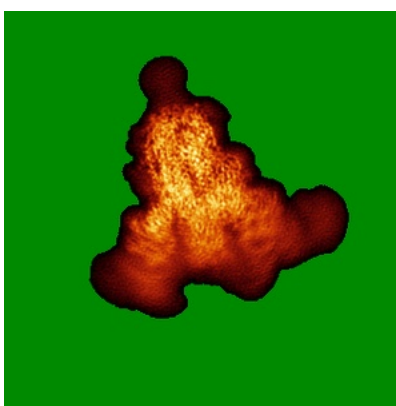
The images above show the largest variance slices of the map in three orthogonal directions.

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

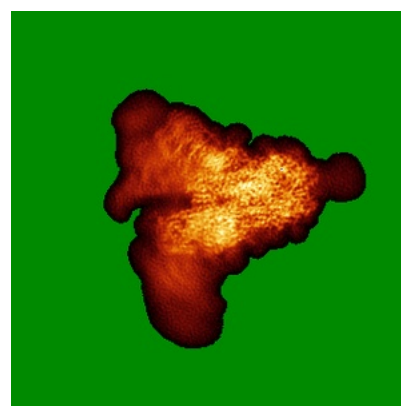
### 6.4.1 Primary map



X



Y

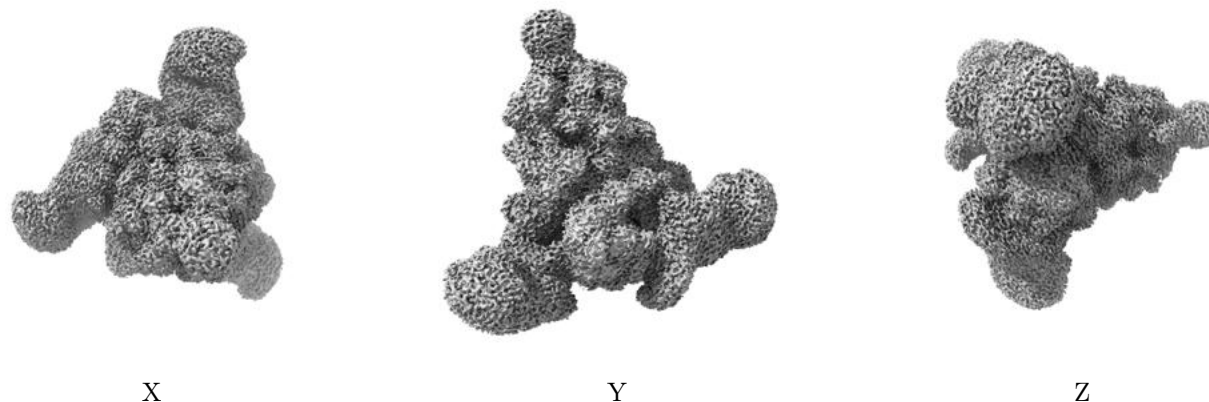


Z

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

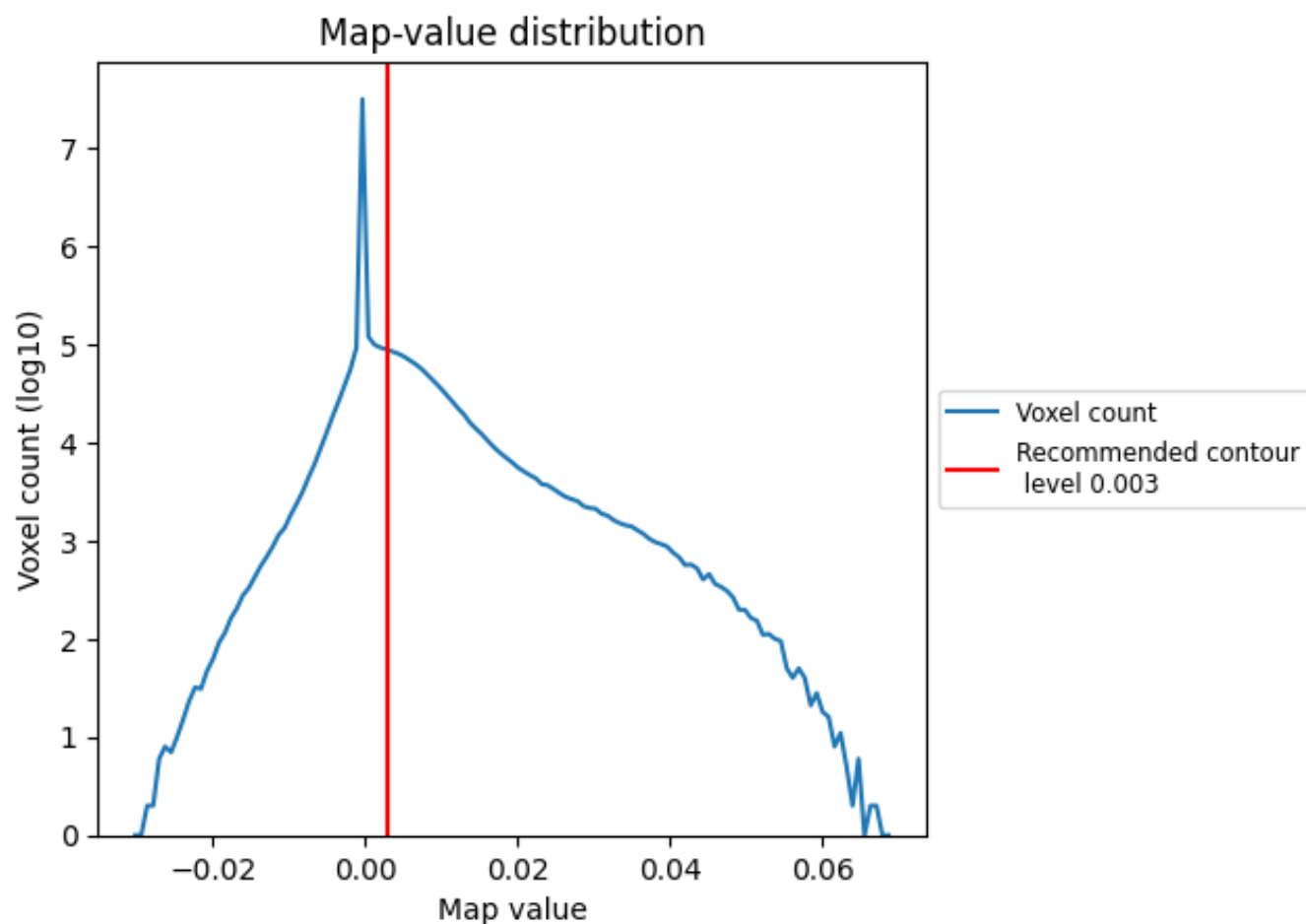
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

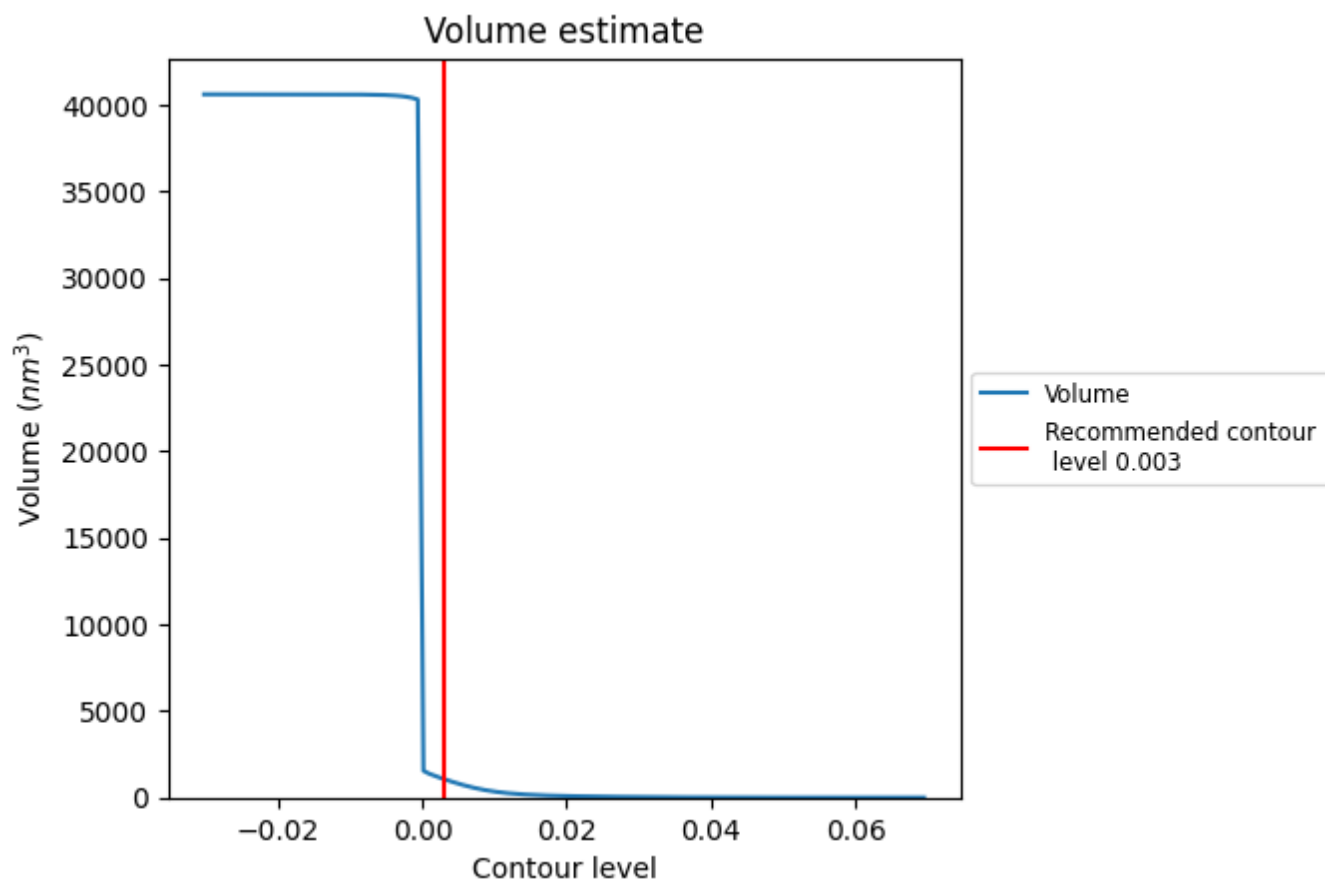
This section contains the results of statistical analysis of the map.

### 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.

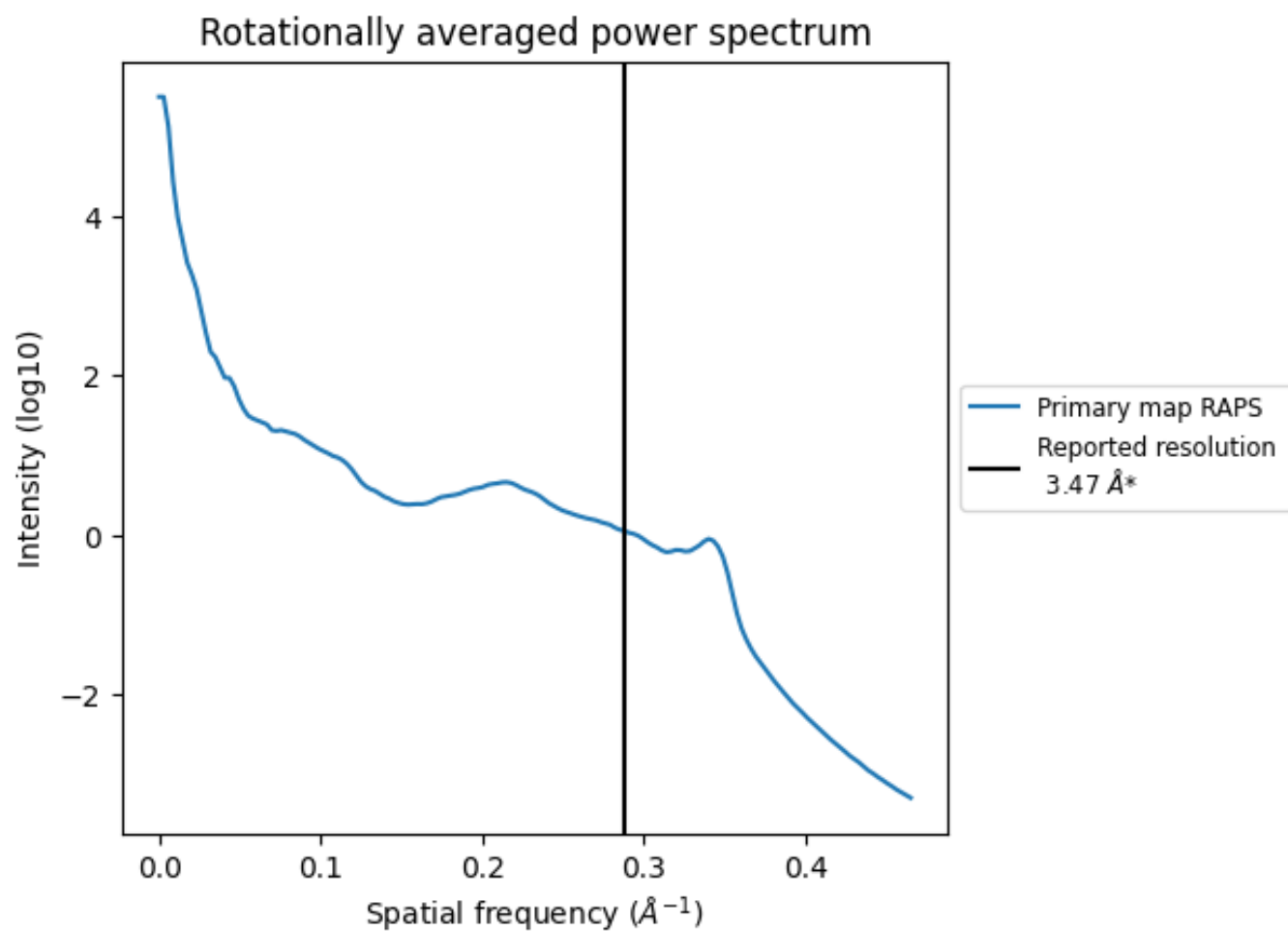
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1070  $\text{nm}^3$ ; this corresponds to an approximate mass of 967 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 0.288 Å<sup>-1</sup>

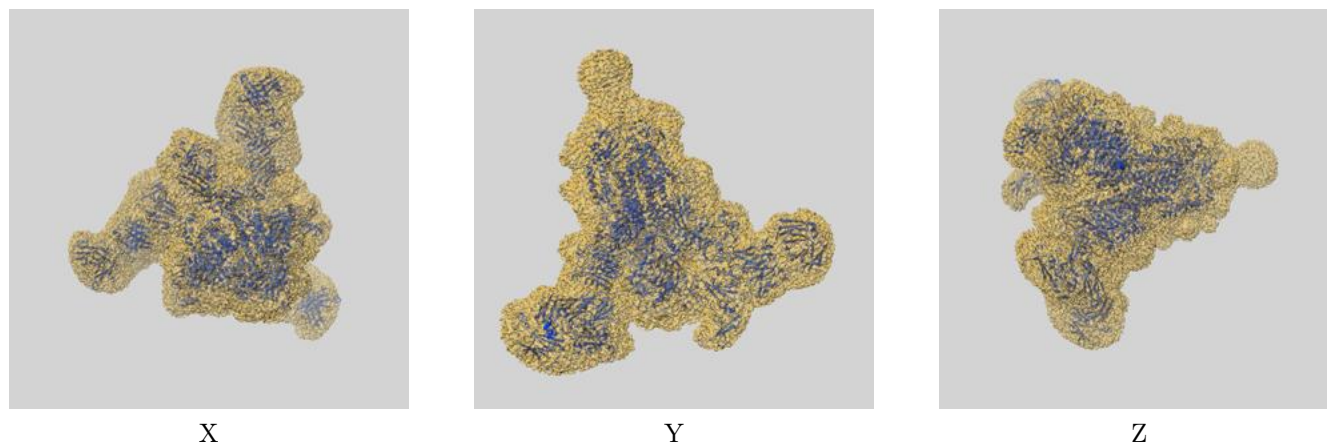
## 8 Fourier-Shell correlation

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

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

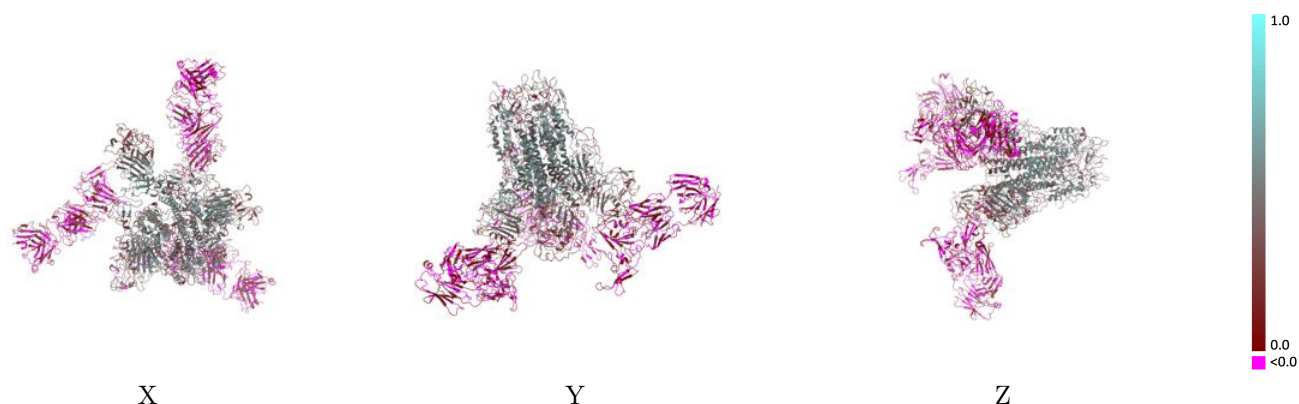
This section contains information regarding the fit between EMDB map EMD-31683 and PDB model 7V3L. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



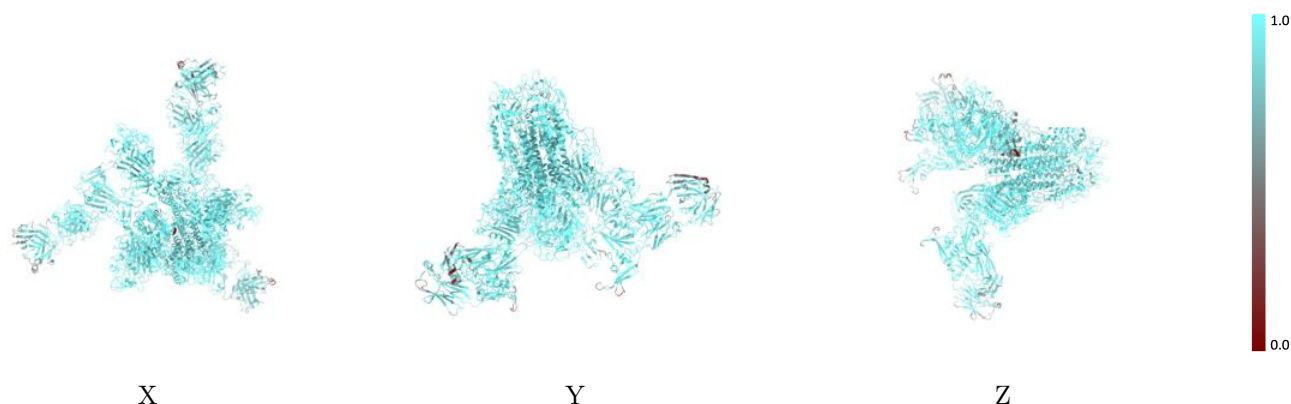
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

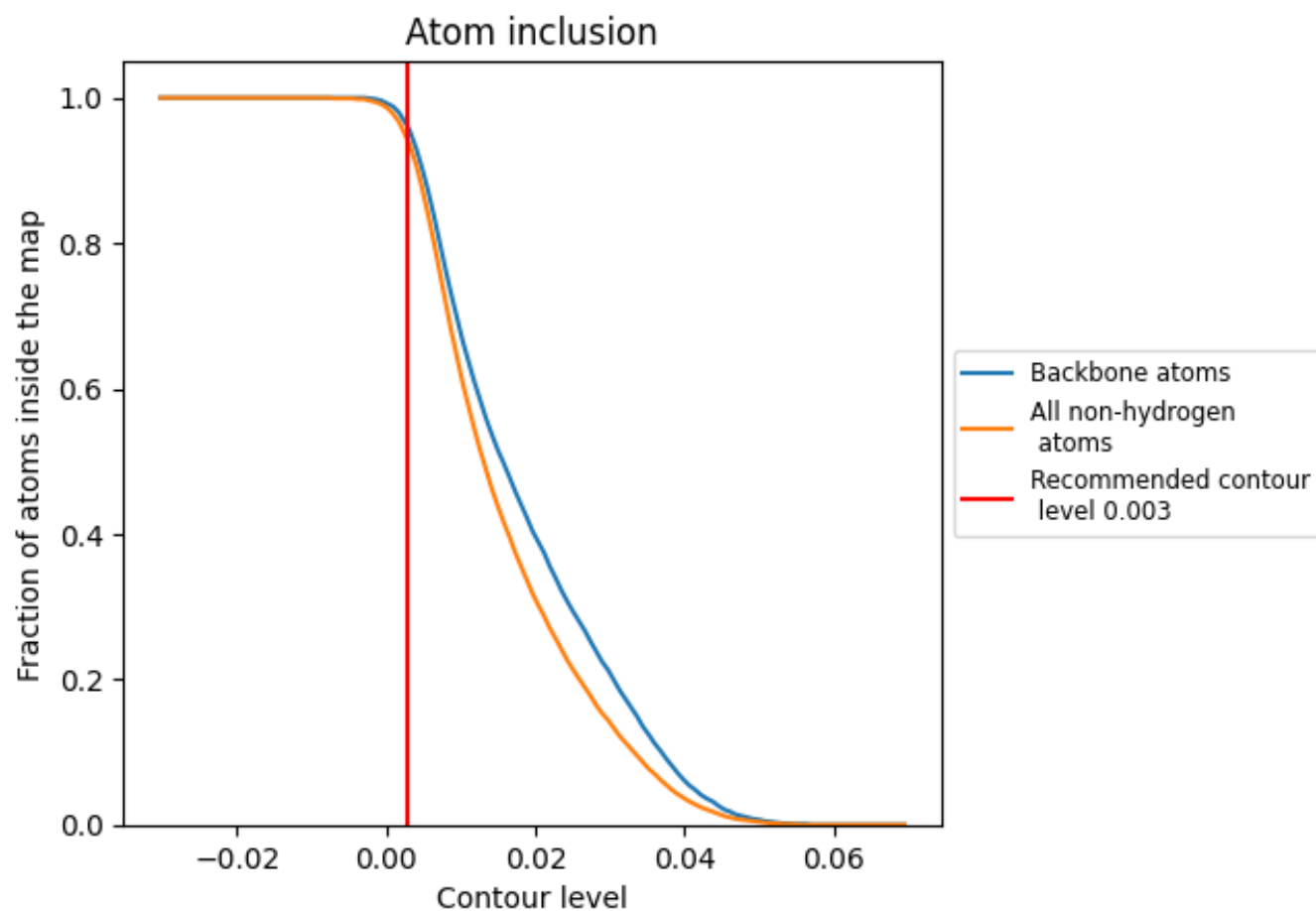
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.003).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9400	<div></div> 0.2560
A	<div></div> 0.9640	<div></div> 0.3380
B	<div></div> 0.9630	<div></div> 0.3520
C	<div></div> 0.9680	<div></div> 0.3390
D	<div></div> 0.8610	<div></div> 0.0170
E	<div></div> 0.8950	<div></div> 0.0350
F	<div></div> 0.8510	<div></div> 0.0400
G	<div></div> 0.8600	<div></div> 0.0300
H	<div></div> 0.9060	<div></div> 0.0200
I	<div></div> 0.8800	<div></div> 0.0120

1.0

0.0

<0.0