



wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 12:38 AM JST

PDB ID : 8ZJL
EMDB ID : EMD-60149
Title : Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 4)
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Mishima-Tsumagari, C.; Yonemochi, M.; Inoue, M.; Nakagawa, R.; Kaushik, R.; Zhang, K.Y.J.; Shirouzu, M.
Deposited on : 2024-05-15
Resolution : 4.31 Å (reported)
Based on initial model : 7DPA

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:

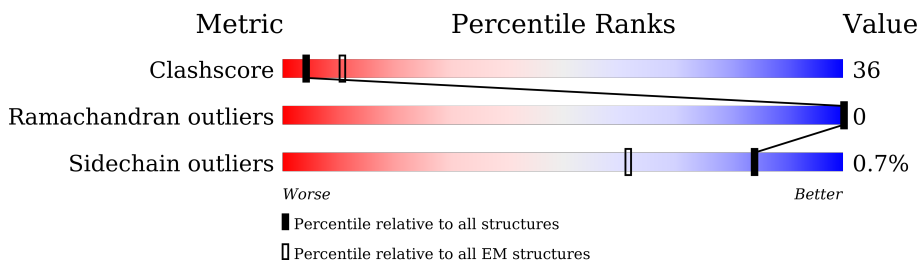
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.31 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	733	 11% 16% 73%
1	D	733	 11% 15% 73%
2	B	1648	 7% 39% 60%
2	E	1648	 7% 38% 61%
3	C	184	 40% 56%
3	F	184	 38% 58%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32858 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 Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		
1	D	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q92556
A	-4	GLY	-	expression tag	UNP Q92556
A	-3	SER	-	expression tag	UNP Q92556
A	-2	GLY	-	expression tag	UNP Q92556
A	-1	GLY	-	expression tag	UNP Q92556
A	0	SER	-	expression tag	UNP Q92556
D	-5	GLY	-	expression tag	UNP Q92556
D	-4	GLY	-	expression tag	UNP Q92556
D	-3	SER	-	expression tag	UNP Q92556
D	-2	GLY	-	expression tag	UNP Q92556
D	-1	GLY	-	expression tag	UNP Q92556
D	0	SER	-	expression tag	UNP Q92556

- Molecule 2 is a protein called Deducator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
2	E	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9H7D0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q9H7D0
B	-3	SER	-	expression tag	UNP Q9H7D0
B	-2	GLY	-	expression tag	UNP Q9H7D0
B	-1	GLY	-	expression tag	UNP Q9H7D0
B	0	SER	-	expression tag	UNP Q9H7D0
B	1285	ARG	LYS	variant	UNP Q9H7D0
E	-5	GLY	-	expression tag	UNP Q9H7D0
E	-4	GLY	-	expression tag	UNP Q9H7D0
E	-3	SER	-	expression tag	UNP Q9H7D0
E	-2	GLY	-	expression tag	UNP Q9H7D0
E	-1	GLY	-	expression tag	UNP Q9H7D0
E	0	SER	-	expression tag	UNP Q9H7D0
E	1285	ARG	LYS	variant	UNP Q9H7D0

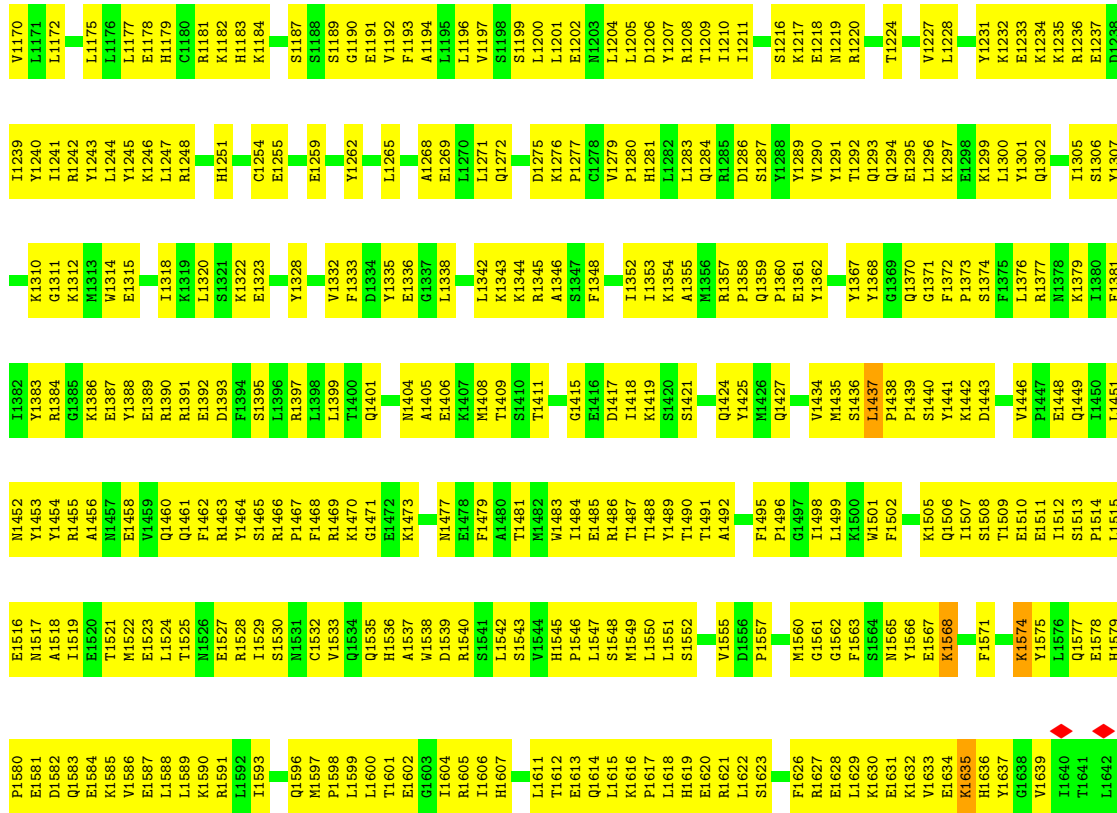
- Molecule 3 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	177	1385	890	228	259	8	0	0
3	F	177	1385	890	228	259	8	0	0

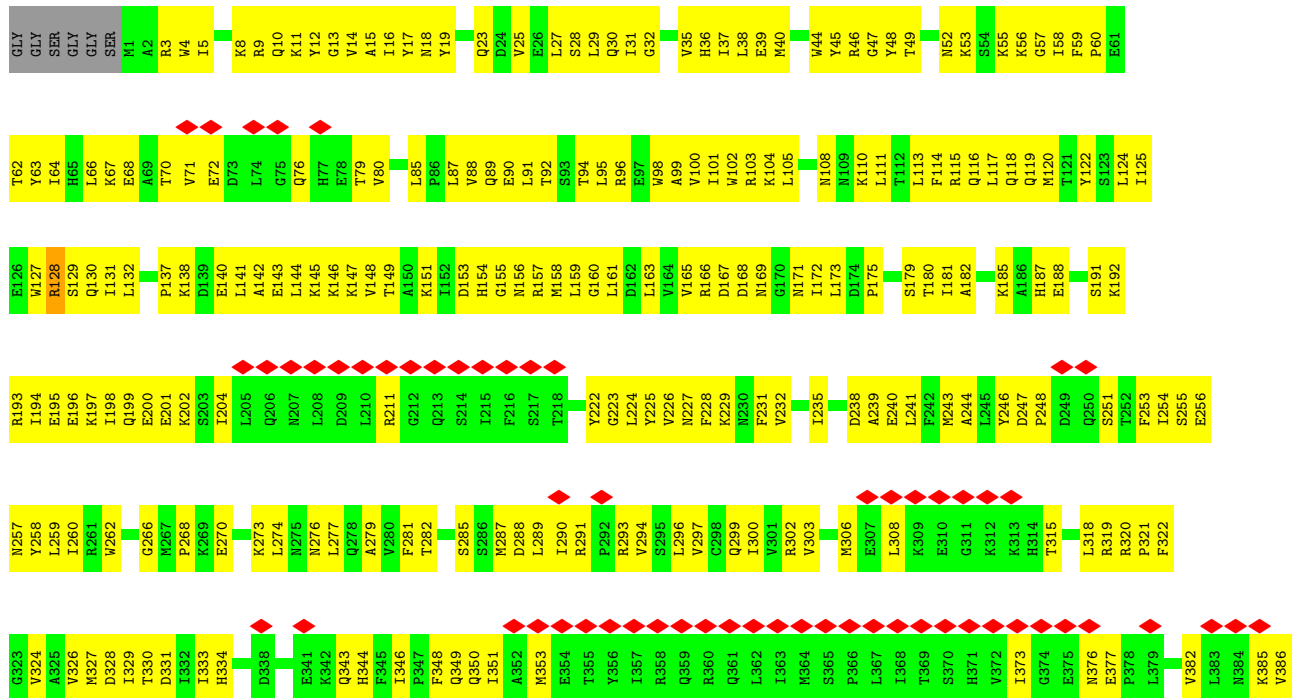
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP P63000
C	-5	SER	-	expression tag	UNP P63000
C	-4	SER	-	expression tag	UNP P63000
C	-3	GLY	-	expression tag	UNP P63000
C	-2	SER	-	expression tag	UNP P63000
C	-1	SER	-	expression tag	UNP P63000
C	0	GLY	-	expression tag	UNP P63000
C	15	ALA	GLY	engineered mutation	UNP P63000
F	-6	GLY	-	expression tag	UNP P63000
F	-5	SER	-	expression tag	UNP P63000
F	-4	SER	-	expression tag	UNP P63000
F	-3	GLY	-	expression tag	UNP P63000
F	-2	SER	-	expression tag	UNP P63000
F	-1	SER	-	expression tag	UNP P63000
F	0	GLY	-	expression tag	UNP P63000
F	15	ALA	GLY	engineered mutation	UNP P63000

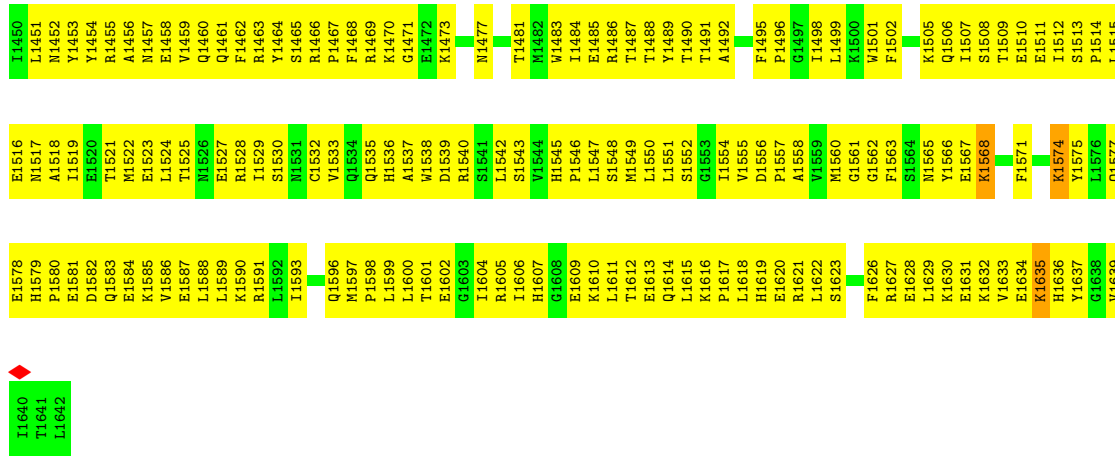
M1105	Q1035	Q962	Q889	I823	L753	L673	A602	1527	K461	A389	F522	N957	R193	E126
V1106	A1036	Q963	L890	I824	F754	L767	S603	R828	T462	K390	G523	Y258	I194	M127
G1107	S1037	M964	D891	M825	F677	F676	S604	F529	F463	E391	V324	L259	E195	R128
P1108	F1038	D965	D892	N826	N878	N879	R604	T530	V464	V392	M327	I260	K196	S129
L1109	E1039	D966	N893	N827	L879	L878	N605	F531	N465	N393	V326	R261	K197	S130
E1111	Q1041	H968	S894	L828	L760	M880	L606	F534	V466	H394	D328	V262	I198	I131
V1112	H1042	H969	N895	L829	K761	M881	V607	R535	V467	K395	I329	N265	Q199	L132
T1113	M1043	S970	K996	V830	Y762	E882	T608	S536	V468	G396	T330	G266	E201	P137
L1114	N1044	H971	V831	P833	L763	M883	F609	Q537	T469	G398	I332	M267	K138	K138
T1115	N1045	H972	H899	V834	F764	S684	T610	E538	M470	G399	I333	P268	D139	D139
P1116	N1046	S973	H900	E835	R765	S685	P611	S471	S472	G399	I333	K269	E140	E140
E1117	H1048	S974	Q904	L836	F766	L692	P612	V470	V471	G399	I333	K269	L141	L141
V1118	H1048	T975	Q904	S837	I767	V693	S612	H473	H473	G399	I333	K269	A142	A142
E1119	V1051	F976	F976	V838	I768	F694	D541	D474	D474	M400	H334	E270	L204	L204
L1120	A1052	S907	S907	L839	I769	F695	K613	G477	G477	S402	E341	K273	L205	L205
R1121	F1053	N908	N908	F940	Q769	D695	D614	K478	K478	V401	K342	L274	Q206	Q206
K1122	L1054	N909	N909	S770	A696	L697	S615	L479	L479	S402	K342	L274	N207	N207
A1123	T1055	L910	L910	R842	L697	L697	T616	L480	L480	K403	Q343	N275	L208	L208
T1124	H1056	E911	E911	F843	L773	I700	K617	L481	L481	L405	H344	N276	L209	L209
L1125	V1057	S912	S912	F844	L774	I701	D618	E481	E481	L406	P347	Q278	L210	L210
F1126	S1058	L913	L913	Q845	L775	S702	L619	K482	K482	D409	F348	V280	G212	G212
T1127	L1059	M992	M992	S846	R776	L703	S619	L554	L554	L410	Q349	F281	Q213	Q213
F1128	Q1060	F993	F993	I847	R776	I704	F620	N556	N556	T411	Q350	T282	Q214	Q214
V1129	L1061	K994	V918	I847	S781	I704	Q621	P857	P857	Q412	I351	S285	S214	S214
D1130	E1062	D995	V918	P848	K782	I707	Q621	D558	D558	V413	I351	S285	L215	L215
M1131	F1063	L996	T921	Q851	D783	K782	T624	G559	G559	Q414	A352	S286	F216	F216
M1132	T1064	L997	A922	L852	F784	F784	L625	A488	A488	H419	M353	M287	S117	S117
E1135	S1065	V923	V923	R853	D785	Q710	T626	G489	G489	H420	E354	L289	T218	T218
F1138	A1003	H924	H924	R854	E786	L715	C627	L561	L561	L420	T355	I290	Y222	Y222
S1139	K1004	K856	K856	Q855	F787	L716	S628	L562	L562	V421	T355	I290	G223	G223
F1144	D1005	K856	K856	K856	N788	L716	T629	D564	D564	D422	T356	R291	L224	L224
H1145	D1006	L857	L857	K856	N788	E717	K630	D564	D564	R423	T357	P292	Y222	Y222
L1146	M1007	M1007	M1007	M858	S790	I718	T632	G497	G497	S424	R358	R293	L224	L224
F1147	M1008	R931	R931	R859	S790	I719	L631	V496	V496	R429	R358	R293	Y222	Y222
E1148	M1009	L932	L932	M860	R792	I720	Q633	S498	S498	K430	Q359	V294	Y222	Y222
M1149	M1010	T933	T933	T861	Q793	I721	N634	V499	V499	R439	Q360	S295	N227	N227
L1150	M1011	L933	L933	K862	L794	K722	N634	V500	V500	M431	Q361	L296	F228	F228
F1151	T1012	R934	R934	L863	F795	H723	L637	V501	V501	M431	Q361	L296	F229	F229
L1152	Q1013	R935	R935	S866	L796	H723	L638	Y502	Y502	E435	L362	C298	K230	K230
T1153	N1014	I936	I936	T867	N799	L727	L639	G574	G574	I436	L363	Q299	F231	F231
L1154	R1015	L936	L936	L868	N799	L728	L640	D575	D575	I437	L363	I300	V232	V232
E1155	V1016	T939	T939	F869	N804	A729	N642	N576	N576	L438	M364	V301	V232	V232
L1156	L1018	M943	M943	R870	P805	V730	N643	N579	N579	G440	P366	V303	I235	I235
F1157	L1019	R944	R944	Q871	P805	V731	R644	E580	E580	D442	L367	V303	D338	D338
R1086	M1022	R945	R945	S872	E807	L733	R644	E580	E580	V442	L367	V303	A239	A239
V1081	Q1023	Q946	Q946	E873	E808	S734	N646	L586	L586	R443	L368	E307	A240	A240
L1094	F1024	S947	S947	C874	A809	K735	N646	P889	P889	M444	T369	E307	L241	L241
G1161	A1025	T950	T950	R875	V810	K735	L650	E589	E589	D445	S370	K309	F242	F242
F1162	E1026	E876	E876	E876	K611	N738	N653	G590	G590	I446	H371	E310	M243	M243
R1163	V1027	L878	L878	L878	R813	F739	L654	T591	T591	Y447	G311	E310	A244	A244
G1164	L1028	L879	L879	L879	V741	V740	L657	K514	K514	L450	I373	G311	M243	M243
L1098	T1029	P880	P880	A742	A742	A742	L657	V515	V515	L450	I373	G311	L245	L245
E1166	H1030	K818	K818	N743	N743	N743	L657	V516	V516	I451	G374	K312	Y246	Y246
L1099	F1031	L882	L882	A744	A744	A744	V660	A518	A518	E454	G374	K313	D247	D247
V1168	P1032	T883	T883	D745	D745	D745	E664	E521	E521	F455	N375	K313	P248	P248
K1169	D1034	Q885	Q885	K749	K749	K749	E664	E521	E521	D456	E377	T315	D249	D249



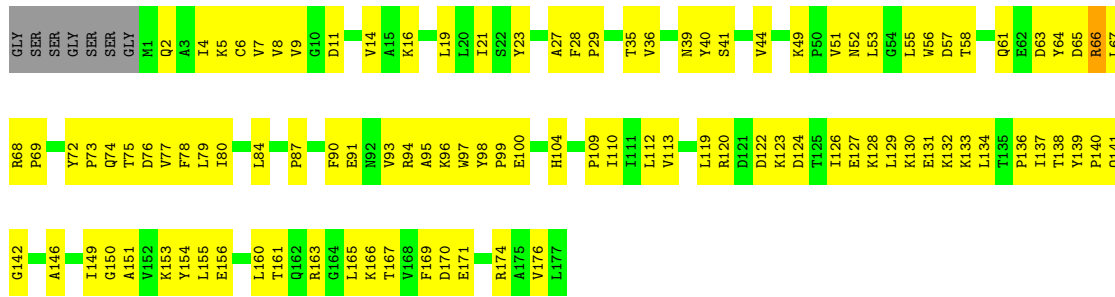
• Molecule 2: Dedicator of cytokinesis protein 5



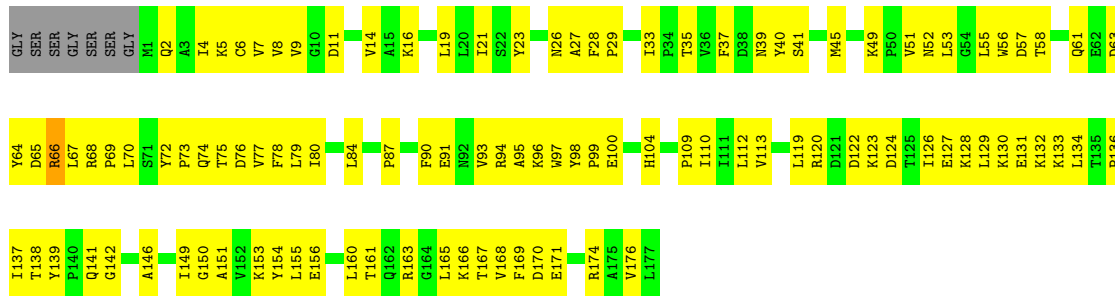
R1377	R1378	K1379	I1380	F1381	G1311	K1312	M1313	W1314	E1315	F1387	Y1388	R1389	G1385	K1386	E1387	Y1388	R1389	R1391	E1392	D1393	F1394	S1395	L1386	R1397	L1398	L1399	L1400	Q1401	M1404	A1405	E1406	K1407	M1408	G1415	E1416	D1417	I1418	K1419	S1420	S1421	Q1424	Y1425	A1436	L1437	P1438	P1439	S1440	K1442	D1443	V1446	R1447	E1448	Q1449	I1305	S1306	Y1307	K1310	I1239	G1311	K1312	M1313	W1314	E1315	F1387	Y1388	R1389	G1385	K1386	E1387	Y1388	R1389	R1391	E1392	D1393	F1394	S1395	L1386	R1397	L1398	L1399	L1400	Q1401	M1404	A1405	E1406	K1407	M1408	G1415	E1416	D1417	I1418	K1419	S1420	S1421	Q1424	Y1425	A1436	L1437	P1438	P1439	S1440	K1442	D1443	V1446	R1447	E1448	Q1449	K1235	R1236	D1238	I1239	Y1240	I1241	R1242	L1243	W1244	E1245	F1246	K1247	R1248	H1251	G1254	E1255	E1259	Y1262	T1263	L1264	L1265	A1268	E1269	L1270	L1271	Q1272	D1275	K1276	P1277	G1278	V1279	P1280	H1281	L1282	L1283	A1355	M1356	Q1284	E1285	D1286	V1290	Y1291	T1292	Q1293	Q1294	E1295	L1296	K1297	K1299	E1298	L1299	G1370	G1371	F1372	P1373	S1374	E1375	L1376	Q1167	Y1168	K1169	V1170	L1171	L1172	L1173	L1174	L1175	P1116	E1117	E1118	K1184	Y1185	S1186	L1187	S1188	S1189	G1190	E1191	V1192	F1193	A1194	L1195	F1129	D1130	M1131	M1132	E1135	F1138	S1139	F1144	H1145	M1146	F1147	E1148	M1149	E1150	L1151	T1152	T1153	K1154	L1155	D1156	Q1157	E1158	V1159	E1160	G1161	G1162	G1163	E1164	D1165	K1233	K1234	K1235	R1236	D1238	I1239	Y1240	I1241	R1242	L1243	W1244	E1245	F1246	K1247	R1248	H1251	G1254	E1255	E1259	Y1262	T1263	L1264	L1265	A1268	E1269	L1270	L1271	Q1272	D1275	K1276	P1277	G1278	V1279	P1280	H1281	L1282	L1283	A1355	M1356	Q1284	E1285	D1286	V1290	Y1291	T1292	Q1293	Q1294	E1295	L1296	K1297	K1299	E1298	L1299	G1370	G1371	F1372	P1373	S1374	E1375	L1376	Q1167	Y1168	K1169	V1170	L1171	L1172	L1173	L1174	L1175	P1116	E1117	E1118	K1184	Y1185	S1186	L1187	S1188	S1189	G1190	E1191	V1192	F1193	A1194	L1195	F1129	D1130	M1131	M1132	E1135	F1138	S1139	F1144	H1145	M1146	F1147	E1148	M1149	E1150	L1151	T1152	T1153	K1154	L1155	D1156	Q1157	E1158	V1159	E1160	G1161	G1162	G1163	E1164	D1165	K1233	K1234	K1235	R1236	D1238	I1239	Y1240	I1241	R1242	L1243	W1244	E1245	F1246	K1247	R1248	H1251	G1254	E1255	E1259	Y1262	T1263	L1264	L1265	A1268	E1269	L1270	L1271	Q1272	D1275	K1276	P1277	G1278	V1279	P1280	H1281	L1282	L1283	A1355	M1356	Q1284	E1285	D1286	V1290	Y1291	T1292	Q1293	Q1294	E1295	L1296	K1297	K1299	E1298	L1299	G1370	G1371	F1372	P1373	S1374	E1375	L1376	H526	I527	F528	R529	F530	F531	R534	Q537	E538	T539	R540	D541	V549	A550	F551	V552	K553	L554	M555	M556	D558	G559	S560	T561	L562	Q563	D564	G565	R566	L569	V570	V571	G574	D575	N576	M579	E580	L586	P589	G590	T591	K592	M593	E594	M595	E596	E597	K598	E599	L600	Q601	A602	S603	K604	N605	L606	V607	T608	F609	T610	P611	S612	K613	D614	S615	T616	K617	D618	L625	I626	G627	S628	L716	T629	K630	L631	T632	Q633	N634	L637	L638	G639	L640	L641	L642	W643	R644	N645	N646	I650	N653	L654	L657	L658	V660	E664	I665	V666	K667	F668	L669	L673	L676	F677	M678	I679	M681	E682	M683	S684	L692	V693	L697	I700	S702	L703	I704	I707	K708	F709	Q710	H711	D781	D782	D783	G784	D785	E786	F787	N788	N789	S790	K722	I791	R792	H723	F724	S725	A726	T727	L728	A729	Y730	V731	K732	L733	S734	K735	N738	F739	Y740	I812	K813	L817	K818	Y819	L820	S747	L821	D884	S822	I823	I824	N825	L826	V827	K828	L829	V830	P833	E834	E835	L836	S837	Q838	I839	F840	C841	R842	F843	I844	Q845	S846	P848	Q851	L852	V853	R854	Q855	K856	R857	N858	C859	M860	T861	R862	S866	T867	L868	F869	Q870	R871	S872	E873	C874	R875	E876	I877	L878	L879	V854	L881	L882	T883	D884	Q885	Q889	L890	D891	S892	N893	S894	H895	S896	Q897	S903	I904	S907	N908	I909	L910	E911	L912	L913	D917	V918	T921	A922	V923	H924	I925	Q926	I927	I928	R931	L932	L933	R934	R935	I936	T939	M943	N944	R945	Q946	S947	I950	V877	E953	V954	L957	M957	I958	A959	L961	Q962	L963	N964	D965	D966	S967	H968	V969	S970	H971	Y972	I973	S974	T975	F976	R979	E988	T989	F990	I991	M992	F993	K994	D995	L996	I997	A1003	K1004	D1005	M1006	M1007	V1008	M1009	N1010	M1011	T1012	Q1013	N1014	I936	L1015	V1016	F1017	L1018	R1019	M1022	F1023	F1024	A1025	E1026	V1027	L1028	T1029	F1030	R1031	F1032	M1033	D1034	Q1035	A1036	S1037	E1038	E1039	L1040	W1043	M1044	M1045	H1048	V1051	A1052	F1053	L1054	T1055	H1056	E1057	S1058	L1059	Q1060	L1061	E1062	T1063	F1064	S1065	Q1066	A1067	K1068	R1069	K1071	I1072	K1075	Y1076	G1077	D1078	M1079	K1080	K1081	E1082	D1089	M1090	W1091	L1094	V1027	G1095	F1096	H1097	K1098	I1099	L1102	M1105	V1106	G1107	F1108	L1109	L1110	E1111	V1112	L1114	T1115	P1116	E1117	E1118	K1184	Y1185	S1186	L1187	S1188	S1189	G1190	E1191	V1192	F1193	A1194	L1195	F1129	D1130	M1131	M1132	E1135	F1138	S1139	F1144	H1145	M1146	F1147	E1148	M1149	E1150	L1151	T1152	T1153	K1154	L1155	D1156	Q1157	E1158	V1159	E1160	G1161	G1162	G1163	E1164	D1165	K1233	K1234	K1235	R1236	D1238	I1239	Y1240	I1241	R1242	L1243	W1244	E1245	F1246	K1247	R1248	H1251	G1254	E1255	E1259	Y1262	T1263	L1264	L1265	A1268	E1269	L1270	L1271	Q1272	D1275	K1276	P1277	G1278	V1279	P1280	H1281	L1282	L1283	A1355	M1356	Q1284	E1285	D1286	V1290	Y1291	T1292	Q1293	Q1294	E1295	L1296	K1297	K1299	E1298	L1299	G1370	G1371	F1372	P1373	S1374	E1375	L1376	I457	K460	K461	T462	P463	K464	E467	V468	T469	M470	S471	V472	H473	D474	G477	K478	L479	L480	E481	K482	A483	I484	H485	V486	G487	A488	C489	Y490	S494	E495	Y496	K497	S498	V499	V500	Y501	Y502	Q503	V504	K505	Q506	C508	V509	Y510	E511	K514	V515	S516	I517	A518	I519	E520	E521	E454	F455	D456	I387	A388	A389	K390	E391	V392	N393	H394	K395	G396	G397	G398	L399	W400	I401	S402	L403	K404	L405	L406	D409	L410	T411	Q412	V413	Q414	H419	L420	V421	D422	R423	S424	T425	R429	K430	M431	E435	L436	I437	L438	P439	G440	V441	V442	R443	M444	D445	I446	Y447	L450	I451	E454	F455	D456
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● Molecule 3: Ras-related C3 botulinum toxin substrate 1



● Molecule 3: Ras-related C3 botulinum toxin substrate 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	123816	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	452.2, 452.2, 452.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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	0.29	0/1641	0.52	1/2218 (0.0%)
1	D	0.29	0/1641	0.52	1/2218 (0.0%)
2	B	0.34	0/13722	0.51	1/18514 (0.0%)
2	E	0.33	0/13722	0.51	1/18514 (0.0%)
3	C	0.33	0/1415	0.49	0/1924
3	F	0.33	0/1415	0.49	0/1924
All	All	0.33	0/33556	0.51	4/45312 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	536	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	A	536	LEU	CB-CG-CD2	-5.40	101.81	111.00
2	E	1437	LEU	CA-CB-CG	5.25	127.36	115.30
2	B	1437	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1608	0	1617	127	0
1	D	1608	0	1617	123	0
2	B	13436	0	13516	987	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	13436	0	13516	1003	0
3	C	1385	0	1407	106	0
3	F	1385	0	1407	111	0
All	All	32858	0	33080	2381	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 36.

The worst 5 of 2381 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)
2:E:1217:LYS:HA	2:E:1220:ARG:HE	1.30	0.96
2:B:1217:LYS:HA	2:B:1220:ARG:HE	1.30	0.95
2:B:46:ARG:HB3	2:B:58:ILE:HG13	1.54	0.89
2:E:4:TRP:HB3	2:E:39:GLU:HB3	1.55	0.88
3:F:9:VAL:HG22	3:F:78:PHE:HZ	1.39	0.88

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	196/733 (27%)	174 (89%)	22 (11%)	0	100	100
1	D	196/733 (27%)	174 (89%)	22 (11%)	0	100	100
2	B	1640/1648 (100%)	1493 (91%)	147 (9%)	0	100	100
2	E	1640/1648 (100%)	1493 (91%)	147 (9%)	0	100	100
3	C	175/184 (95%)	164 (94%)	11 (6%)	0	100	100
3	F	175/184 (95%)	164 (94%)	11 (6%)	0	100	100
All	All	4022/5130 (78%)	3662 (91%)	360 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	183/664 (28%)	181 (99%)	2 (1%)	73	85
1	D	183/664 (28%)	181 (99%)	2 (1%)	73	85
2	B	1495/1497 (100%)	1486 (99%)	9 (1%)	86	92
2	E	1495/1497 (100%)	1486 (99%)	9 (1%)	86	92
3	C	153/157 (98%)	151 (99%)	2 (1%)	69	82
3	F	153/157 (98%)	151 (99%)	2 (1%)	69	82
All	All	3662/4636 (79%)	3636 (99%)	26 (1%)	84	90

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	570	ARG
2	E	854	ARG
3	F	66	ARG
2	E	644	ARG
2	E	935	ARG

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

Mol	Chain	Res	Type
2	E	1359	GLN
2	E	1401	GLN
3	F	2	GLN
2	B	1401	GLN
2	B	1359	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 monosaccharides 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.

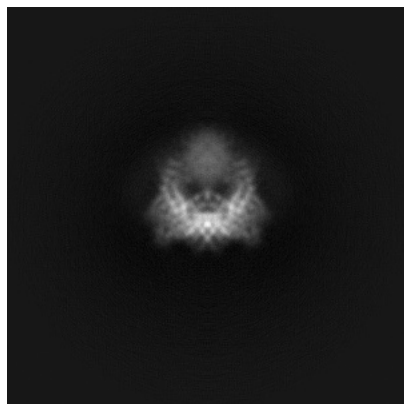
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60149. These allow visual inspection of the internal detail of the map and identification of artifacts.

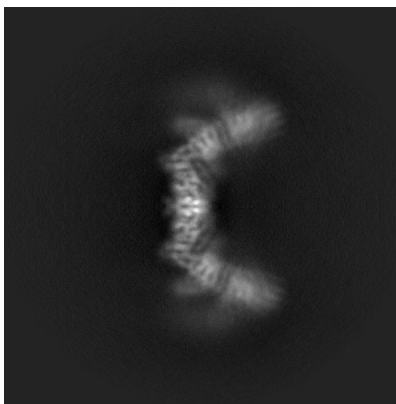
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

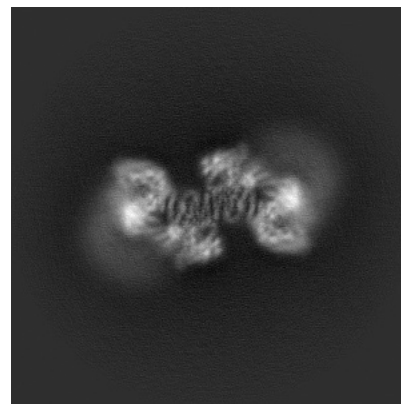
6.1.1 Primary map



X

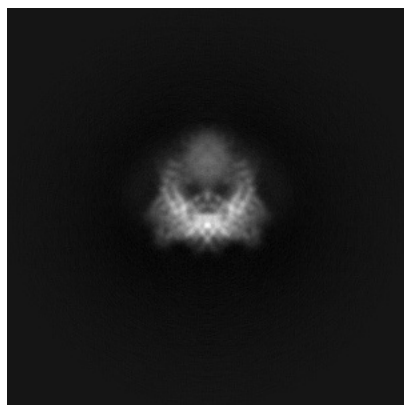


Y

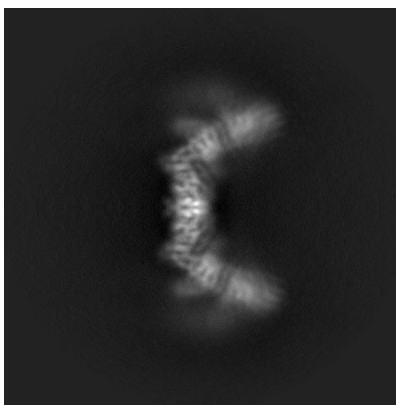


Z

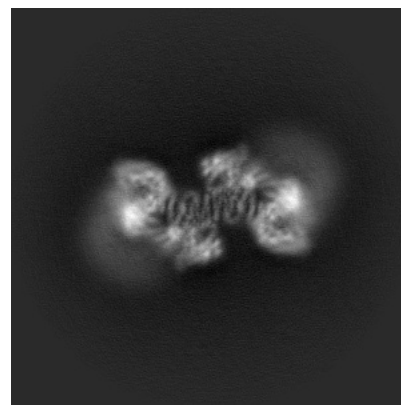
6.1.2 Raw map



X



Y

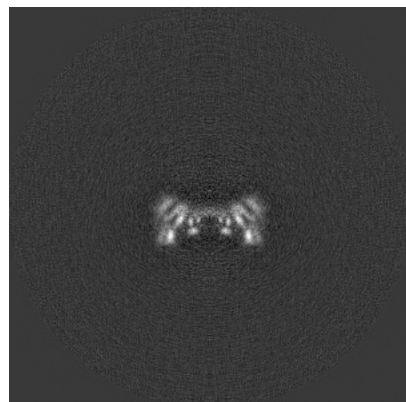


Z

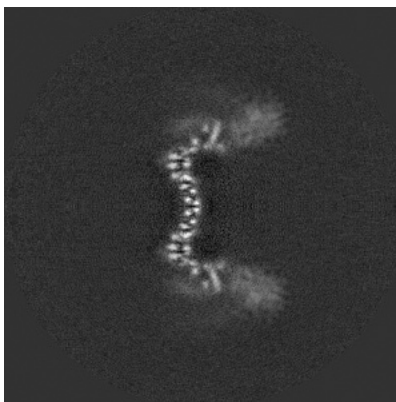
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

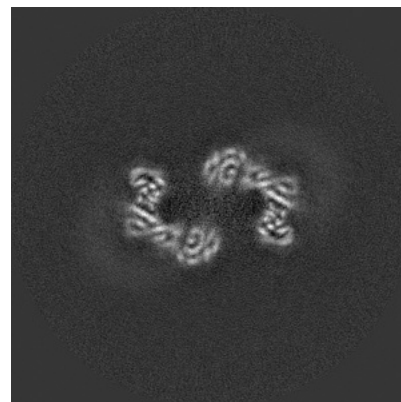
6.2.1 Primary map



X Index: 170

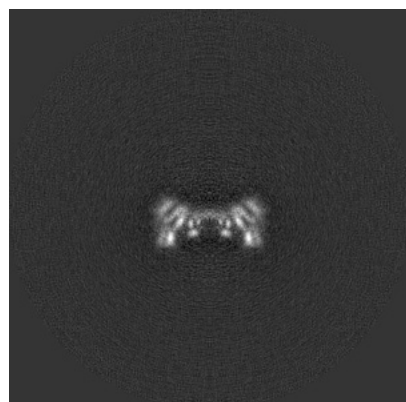


Y Index: 170

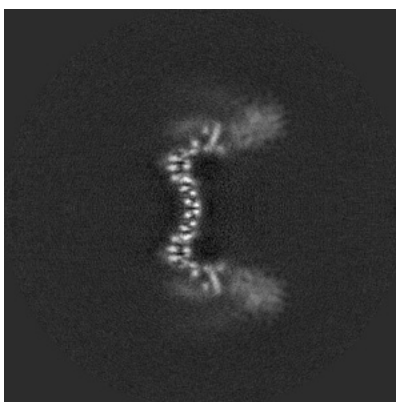


Z Index: 170

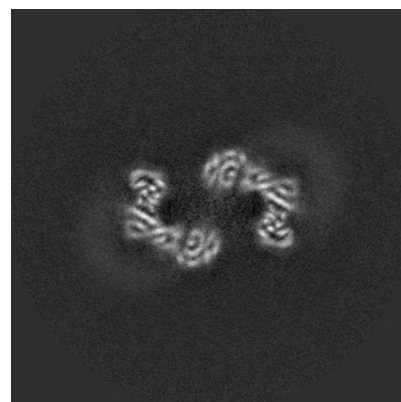
6.2.2 Raw map



X Index: 170



Y Index: 170

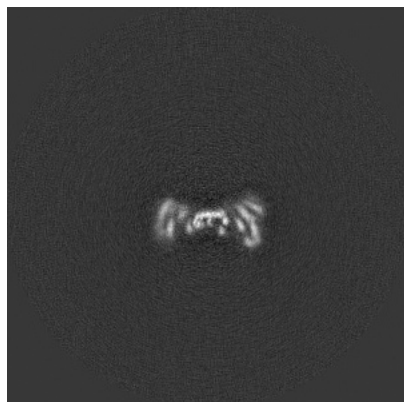


Z Index: 170

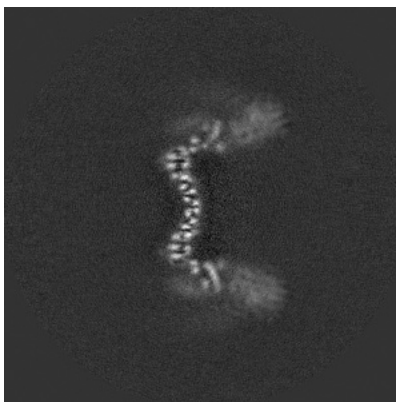
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

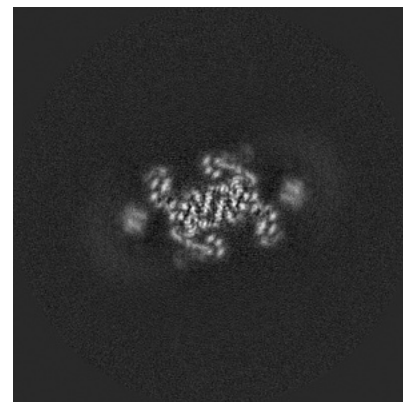
6.3.1 Primary map



X Index: 173

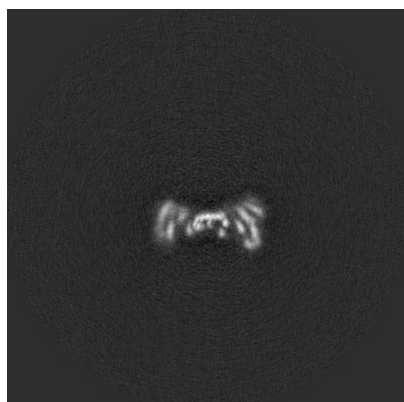


Y Index: 169

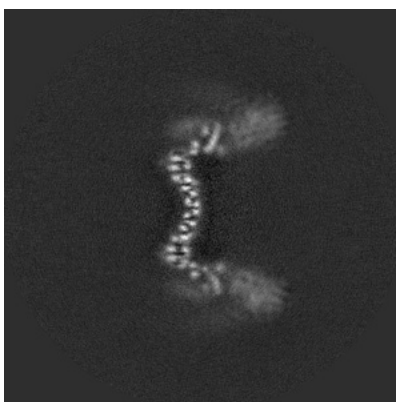


Z Index: 155

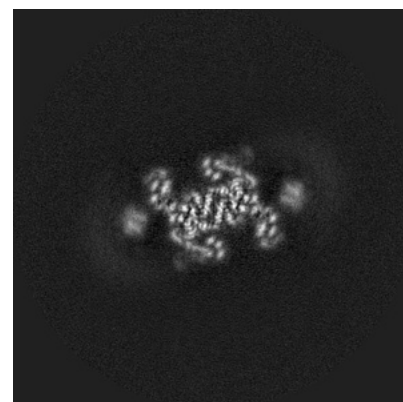
6.3.2 Raw map



X Index: 173



Y Index: 171

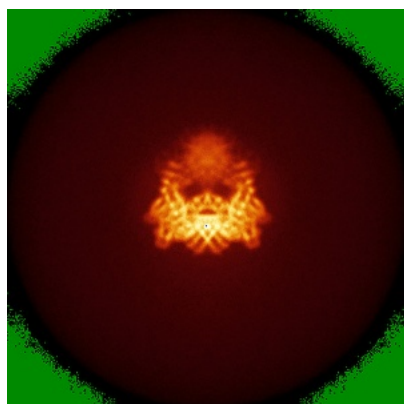


Z Index: 155

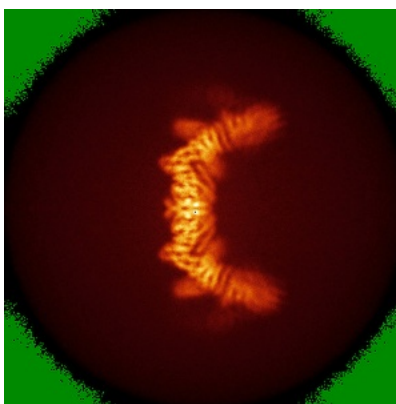
The images above show the largest variance slices of the map in three orthogonal directions.

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

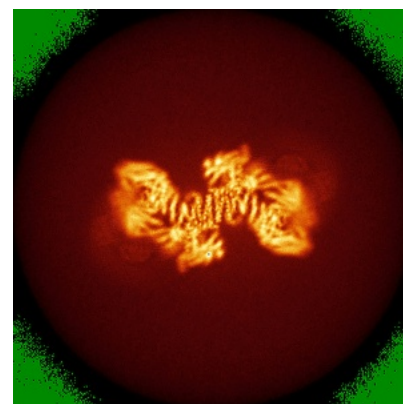
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

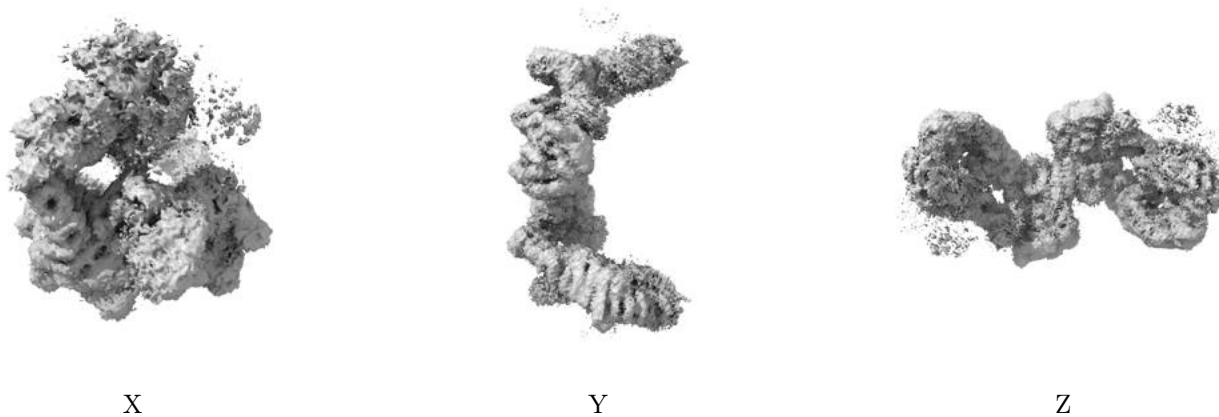


Z

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.

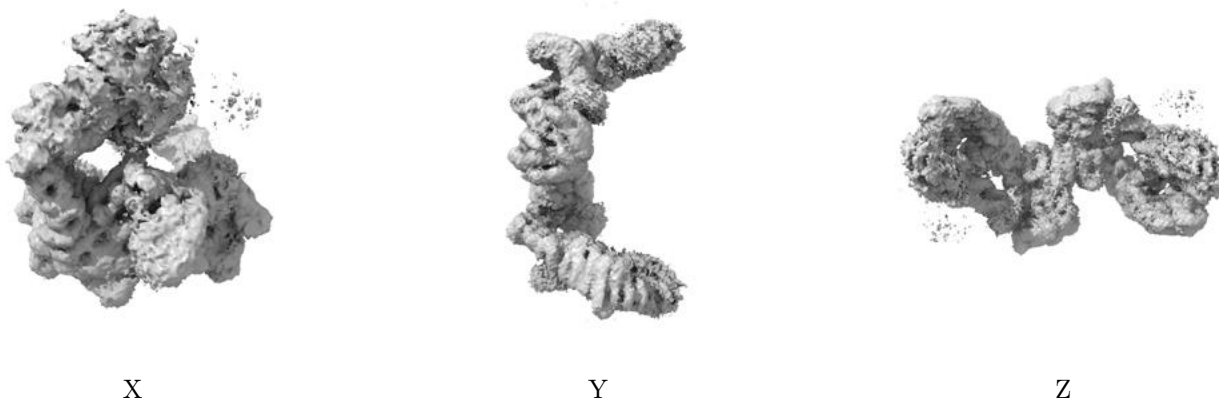
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

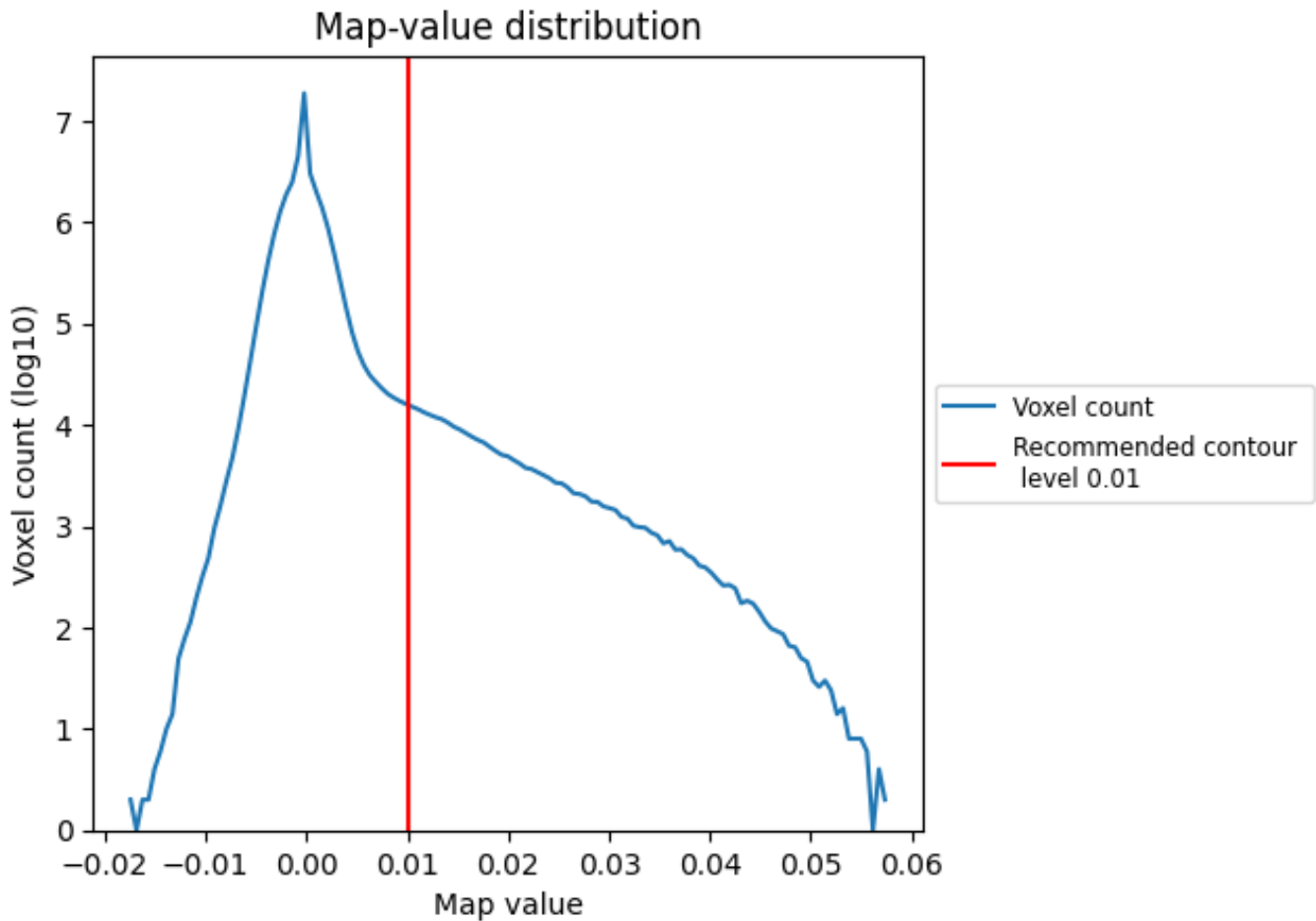
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

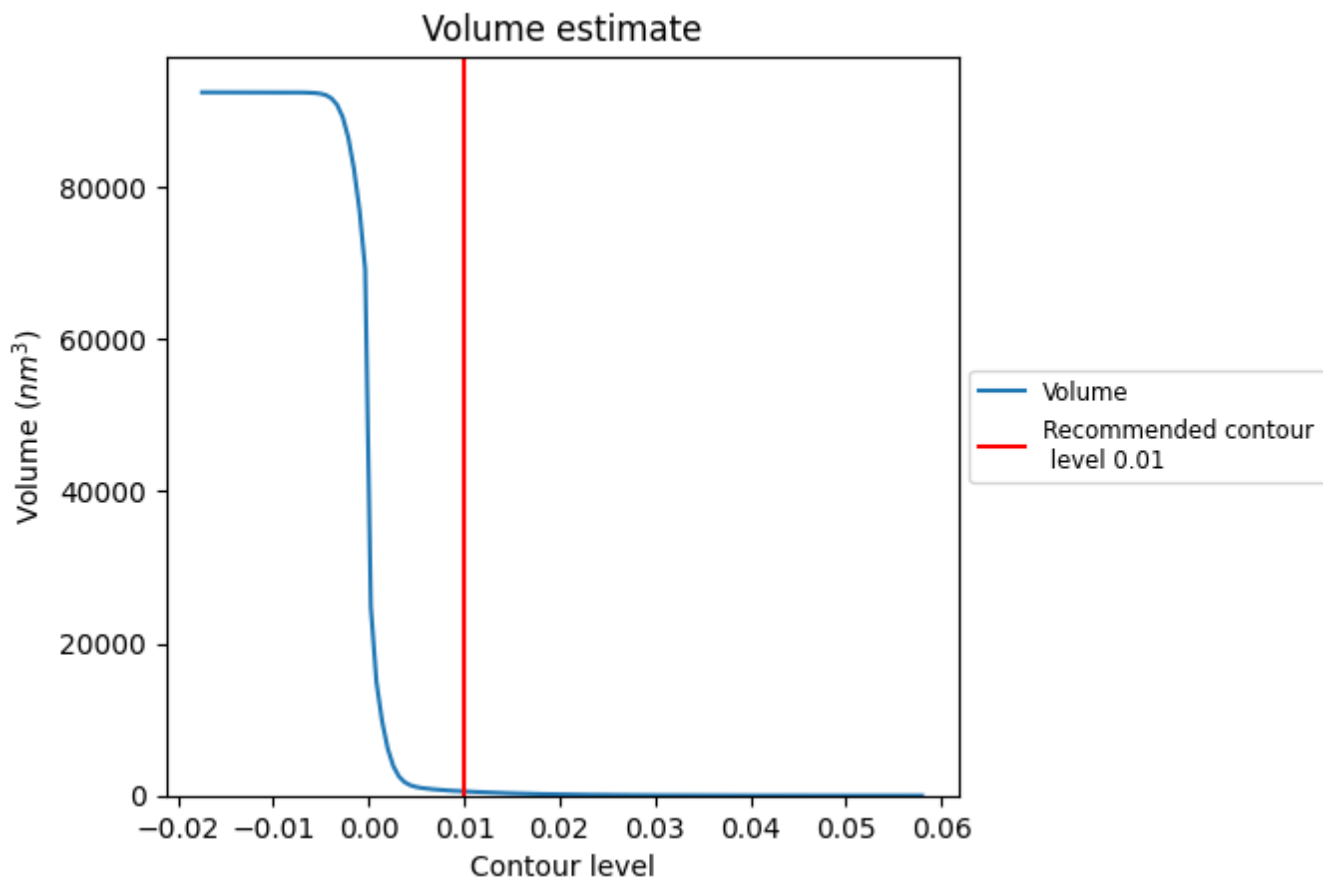
This section contains the results of statistical analysis of the map.

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.

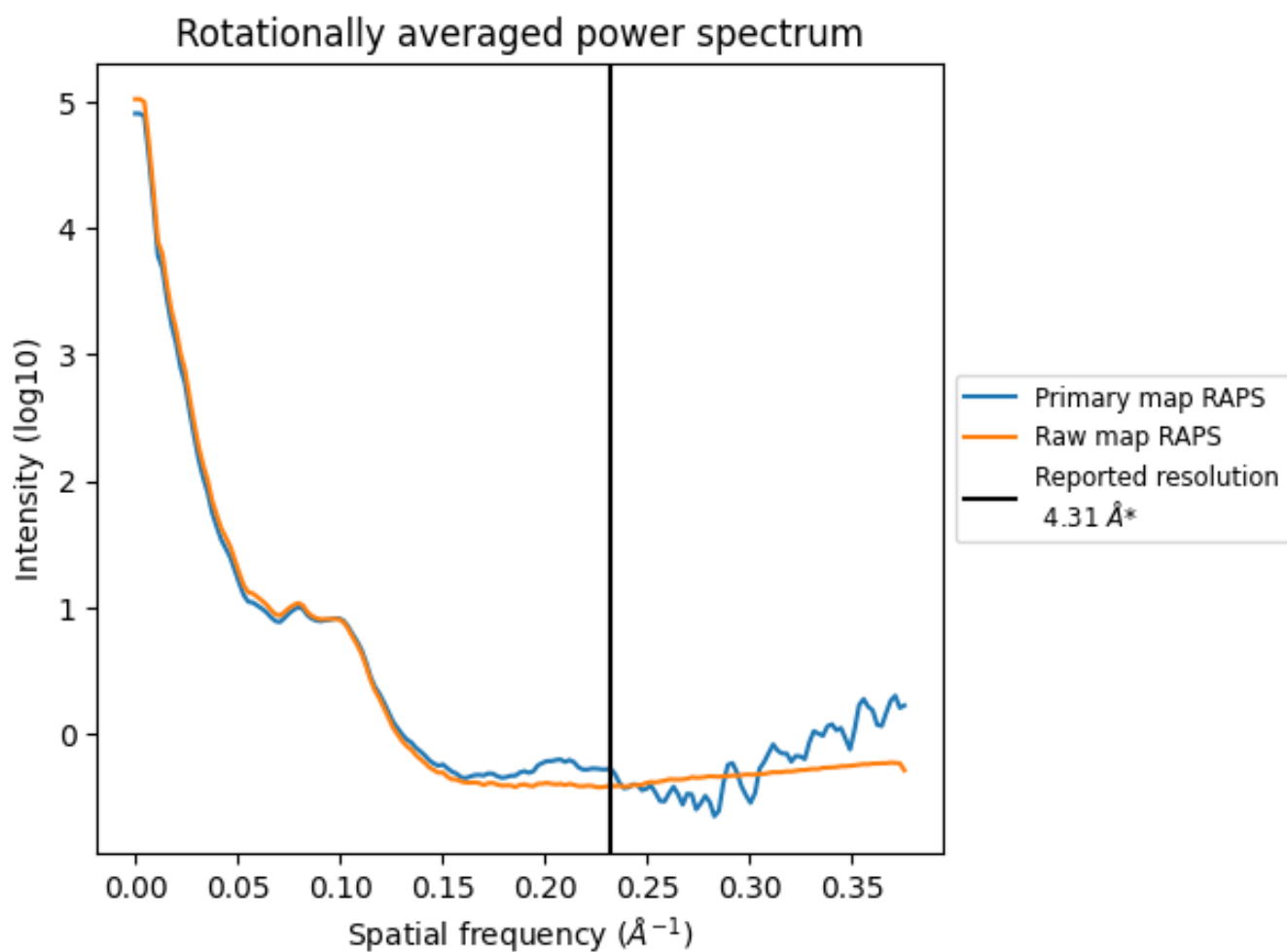
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 550 nm³; this corresponds to an approximate mass of 497 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 [i](#)

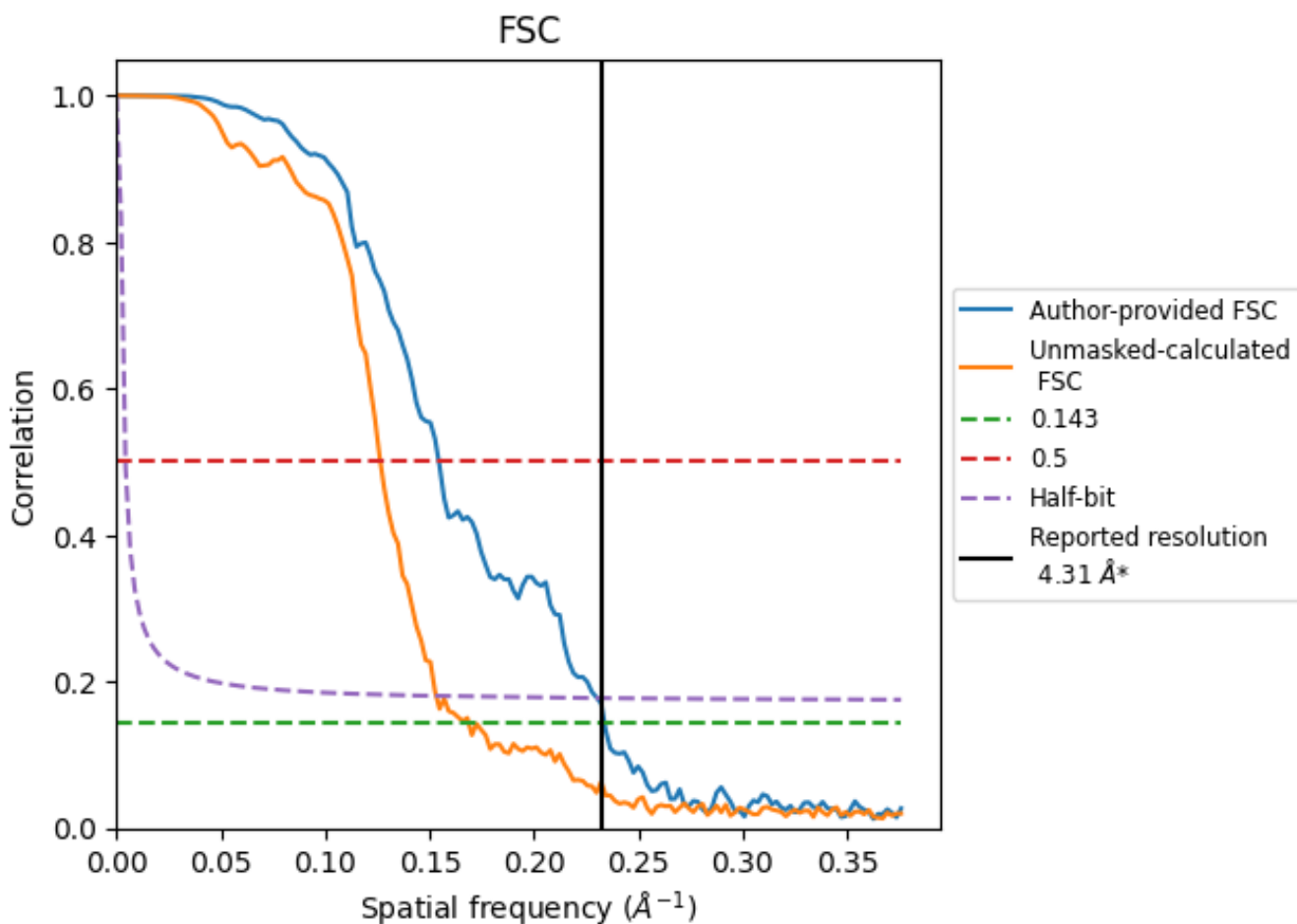


*Reported resolution corresponds to spatial frequency of 0.232 \AA^{-1}

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 0.232 Å⁻¹

8.2 Resolution estimates [i](#)

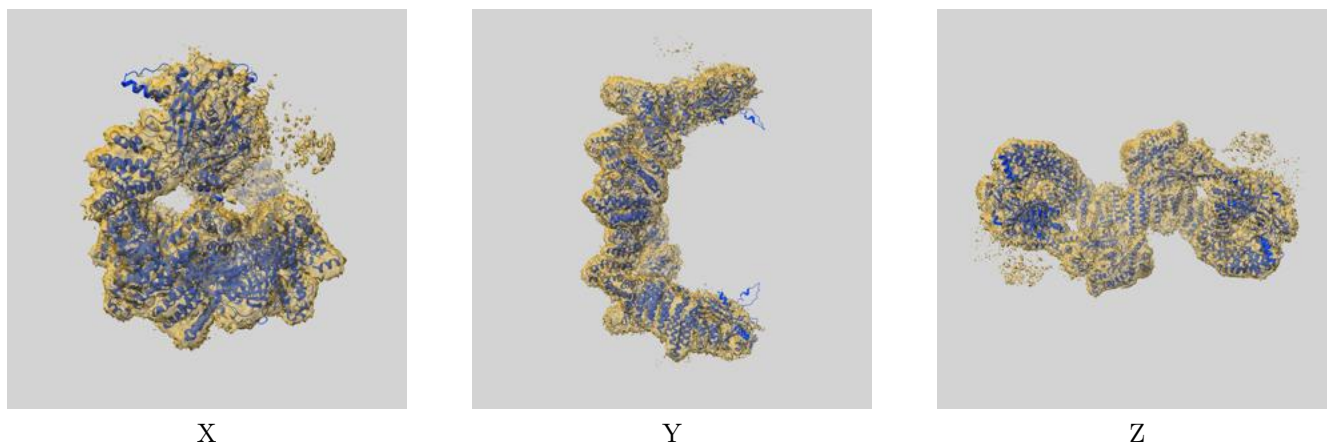
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.31	-	-
Author-provided FSC curve	4.28	6.47	4.34
Unmasked-calculated*	5.93	7.91	6.53

*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 5.93 differs from the reported value 4.31 by more than 10 %

9 Map-model fit [i](#)

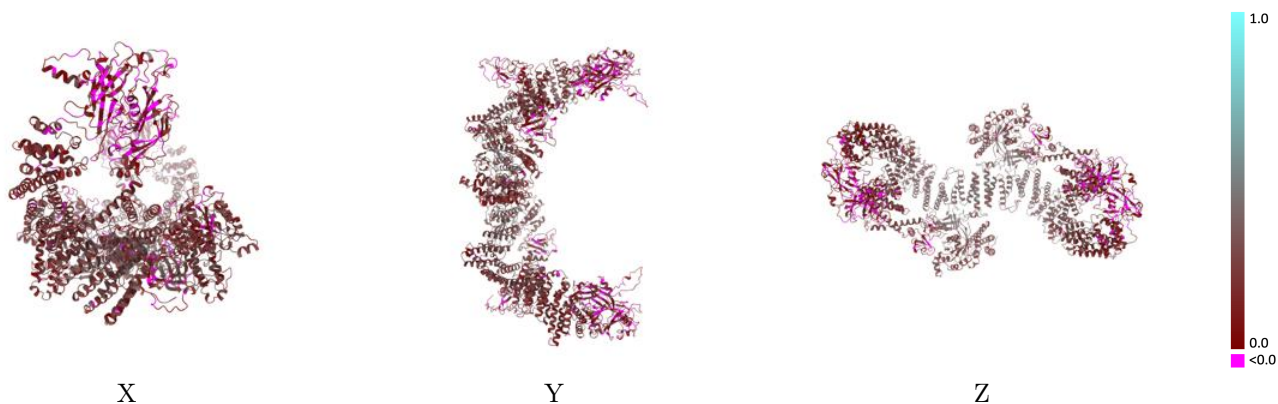
This section contains information regarding the fit between EMDB map EMD-60149 and PDB model 8ZJL. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



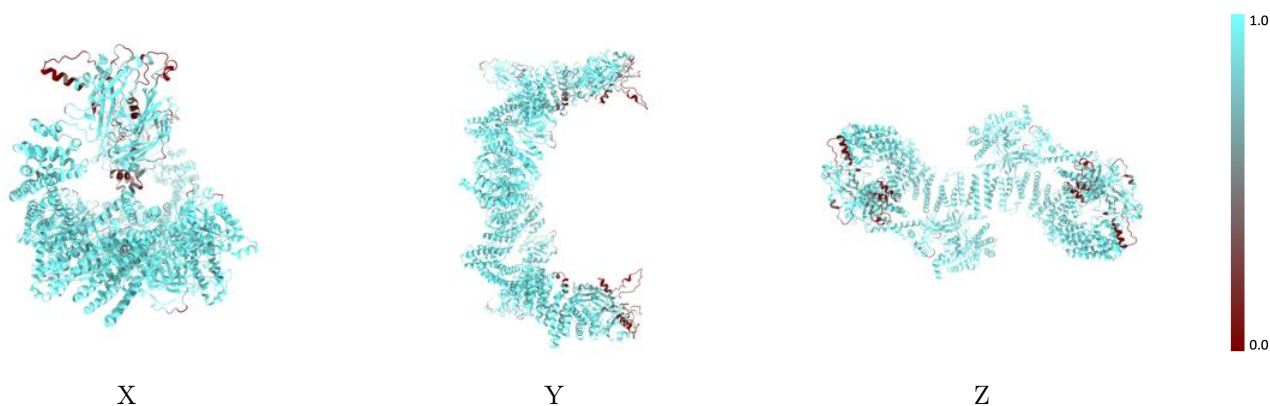
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



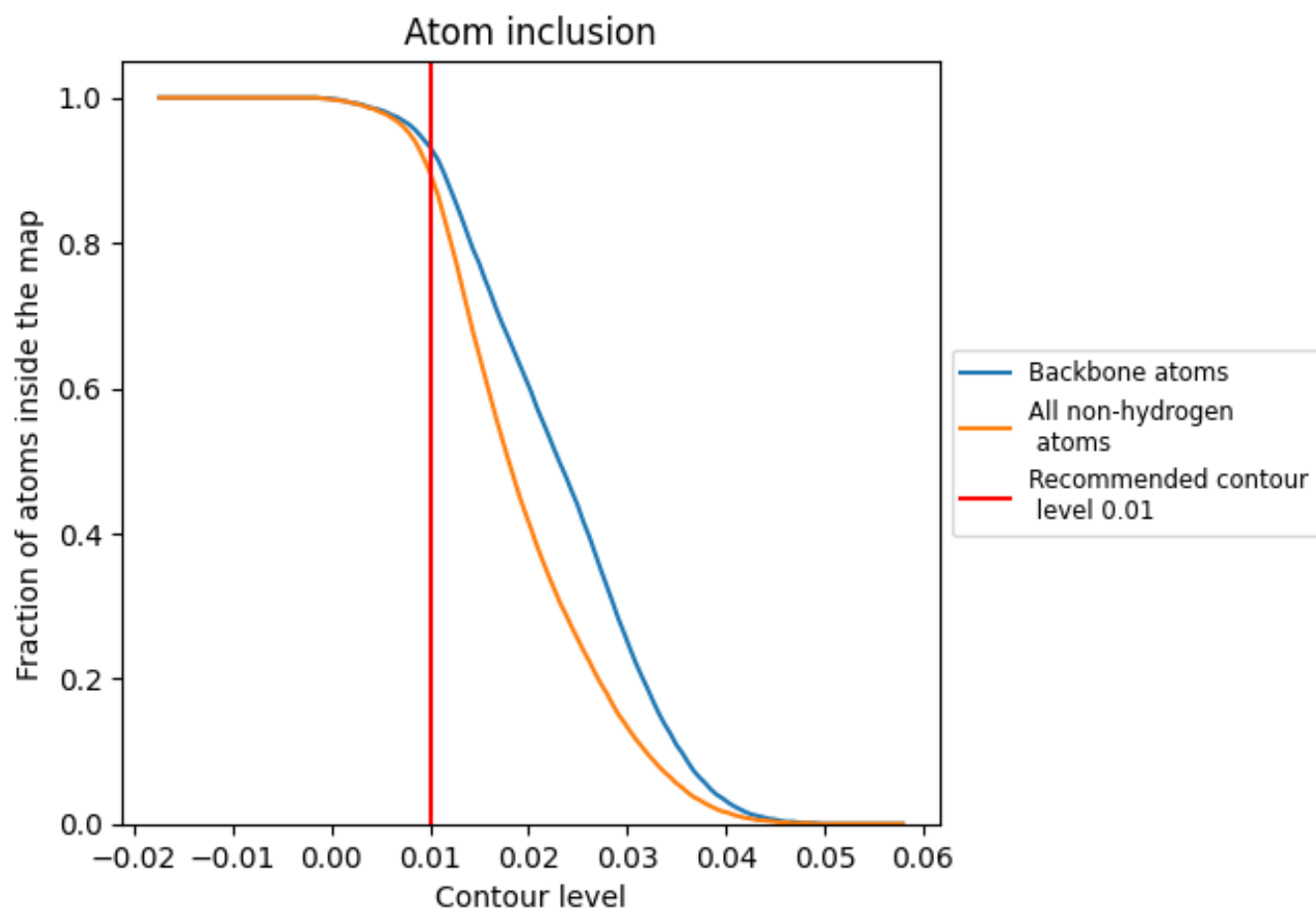
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).















9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.2110
A	 0.9040	 0.1550
B	 0.8860	 0.2130
C	 0.9740	 0.2670
D	 0.9080	 0.1620
E	 0.8890	 0.2090
F	 0.9750	 0.2690

