



wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 01:03 AM JST

PDB ID : 8ZJ2
EMDB ID : EMD-60136
Title : Cryo-EM structure of the RhoG/DOCK5/ELMO1/Rac1 complex
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 : 2024-05-14
Resolution : 4.66 Å (reported)
Based on initial models : 7DPA, 6IE1, 7Y4A

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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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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

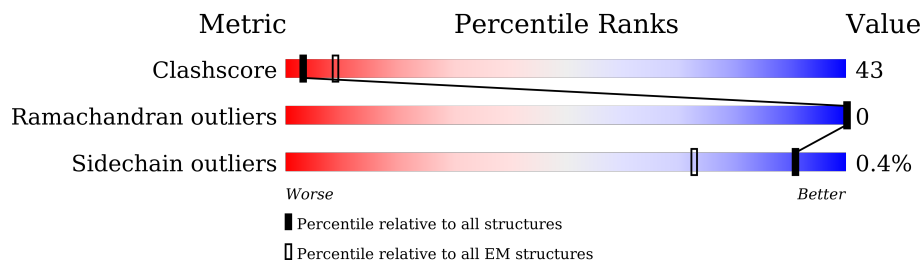
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.66 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	B	1648	
1	F	1648	
2	C	184	
2	G	184	
3	A	733	
3	E	733	
4	D	203	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38587 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 Dedicator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
1	F	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
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
F	-5	GLY	-	expression tag	UNP Q9H7D0
F	-4	GLY	-	expression tag	UNP Q9H7D0
F	-3	SER	-	expression tag	UNP Q9H7D0
F	-2	GLY	-	expression tag	UNP Q9H7D0
F	-1	GLY	-	expression tag	UNP Q9H7D0
F	0	SER	-	expression tag	UNP Q9H7D0
F	1285	ARG	LYS	variant	UNP Q9H7D0

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 1.

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

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
G	-6	GLY	-	expression tag	UNP P63000
G	-5	SER	-	expression tag	UNP P63000
G	-4	SER	-	expression tag	UNP P63000
G	-3	GLY	-	expression tag	UNP P63000
G	-2	SER	-	expression tag	UNP P63000
G	-1	SER	-	expression tag	UNP P63000
G	0	GLY	-	expression tag	UNP P63000
G	15	ALA	GLY	engineered mutation	UNP P63000

- Molecule 3 is a protein called Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	199	Total	C	N	O	S	0	0
			1617	1023	279	305	10		
3	A	727	Total	C	N	O	S	0	0
			5879	3721	1009	1108	41		

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Rho-related GTP-binding protein RhoG.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	181	Total	C	N	O	S	0	0
			1416	897	248	263	8		

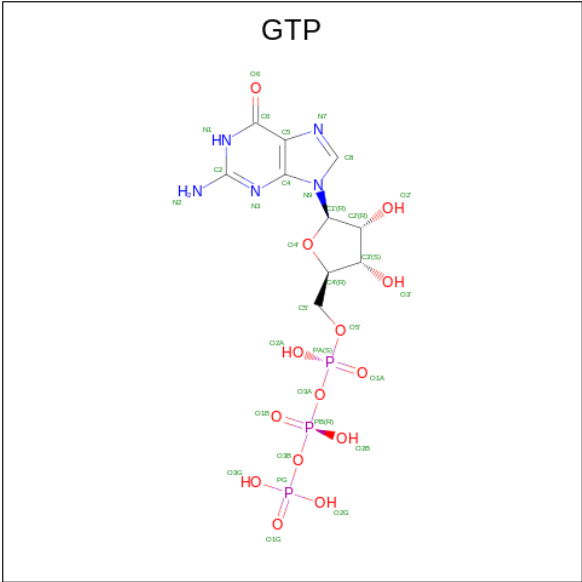
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP P84095
D	-5	SER	-	expression tag	UNP P84095
D	-4	SER	-	expression tag	UNP P84095
D	-3	GLY	-	expression tag	UNP P84095
D	-2	SER	-	expression tag	UNP P84095
D	-1	SER	-	expression tag	UNP P84095
D	0	GLY	-	expression tag	UNP P84095
D	61	LEU	GLN	engineered mutation	UNP P84095
D	185	SER	-	expression tag	UNP P84095
D	186	GLY	-	expression tag	UNP P84095
D	187	PRO	-	expression tag	UNP P84095
D	188	SER	-	expression tag	UNP P84095
D	189	SER	-	expression tag	UNP P84095
D	190	GLY	-	expression tag	UNP P84095
D	191	GLU	-	expression tag	UNP P84095
D	192	ASN	-	expression tag	UNP P84095
D	193	LEU	-	expression tag	UNP P84095
D	194	TYR	-	expression tag	UNP P84095
D	195	PHE	-	expression tag	UNP P84095
D	196	GLN	-	expression tag	UNP P84095

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Mg	0
			1	1	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			32	10	5	14	3	

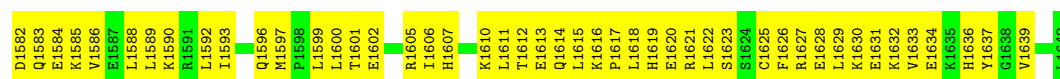
3 Residue-property plots

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.

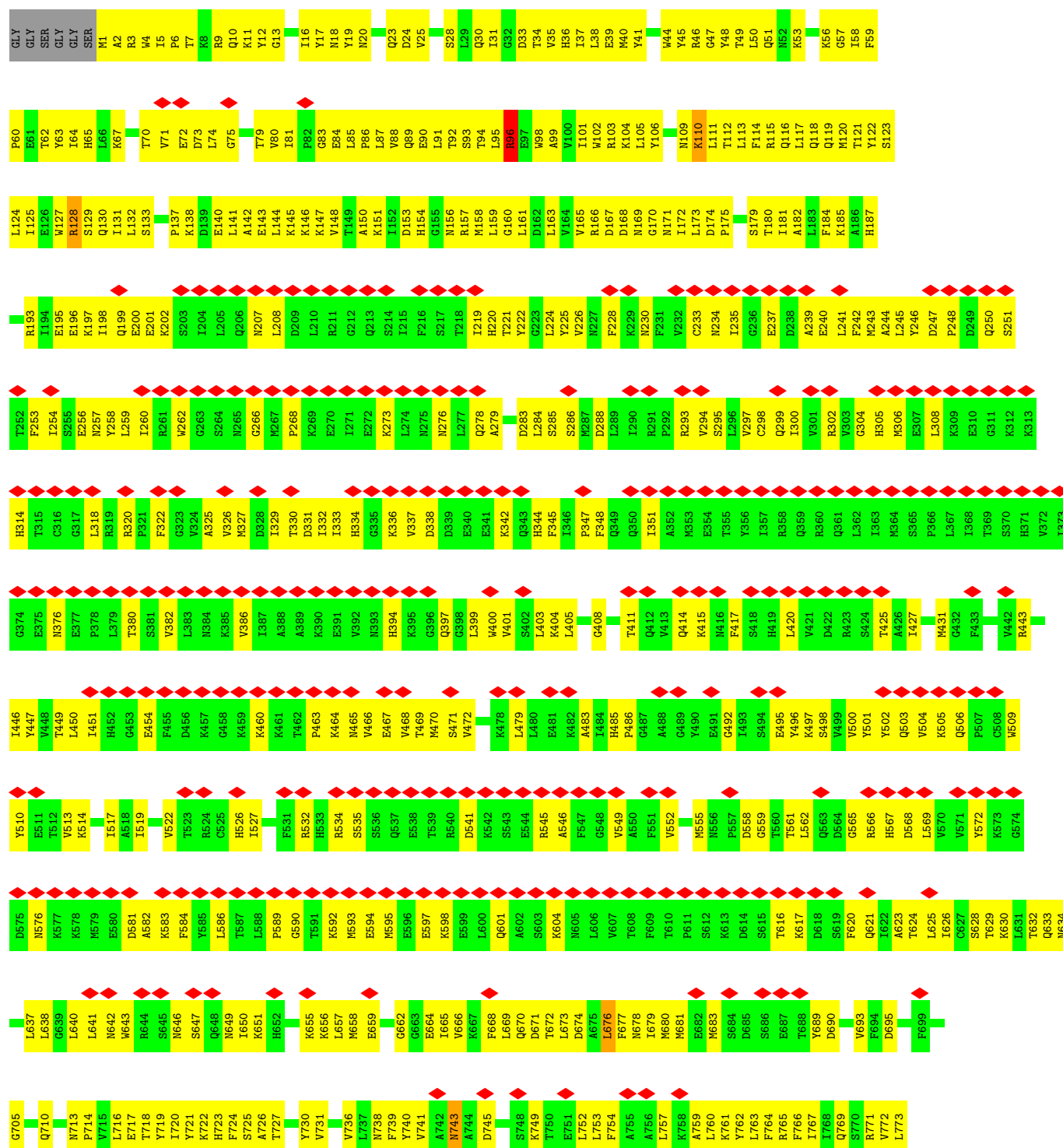
• Molecule 1: Deducator of cytokinesis protein 5







● Molecule 1: Dedicator of cytokinesis protein 5

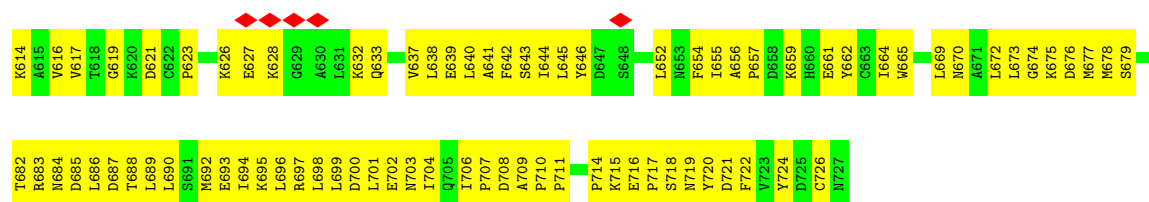


L1599	V1533	R1463	R1390	S1321	I1241	L1175	L1110	H968	Q904	S837	Y774
L1600	Q1534	Y1464	R1391	K1322	R1242	L1176	E1111	Y969	Q905	V838	L775
E1601	T1323	S1465	E1392	E1323	Y1243	L1177	V1112	S970	L906	E1039	L776
E1602	H1536	R1466	L1324	L1244	L1244	E1178	T1113	H971	S907	F840	F777
G1603	A1537	P1467	S1395	Y1245	Y1245	L1114	L1114	Y972	N908	C841	G778
R1605	V1538	F1468	E1326	R1248	R1248	R1181	PH116	Y973	I909	K842	K842
R1606	D1539	R1469	T1327	D1249	D1249	H1183	K1182	S974	L910	F843	F843
I1606	R1470	K1470	Y1328	L1250	L1250	H1184	K1184	T975	E911	I844	I844
H1607	S1541	K1473	E1329	R1252	R1252	Y1185	V1118	F976	V912	Q845	D783
G1608	L1542	G1473	Q1401	R1259	R1259	L1186	E1119	R979	L913	S846	D784
E1609	S1543	E1478	N1404	E1259	E1259	L1187	L1120	I982	D914	F1047	D785
K1610	H1544	T1481	A1405	Y1262	Y1262	S1187	R1121	I982	R915	K916	E786
L1611	H1545	M1482	E1406	Y1262	Y1262	S1188	K1122	I982	D917	T788	F787
T1612	P1546	M1483	K1407	Y1262	Y1262	E1191	A1123	I982	V918	N789	N789
E1613	L1547	L1482	K1407	Y1262	Y1262	V1192	T1124	F985	V918	S790	S790
Q1614	S1548	L1338	L1338	Y1262	Y1262	F1193	I1125	F986	Q855	Q855	I791
L1615	M1549	I1484	T1412	Q1272	Q1272	F1193	P1126	I986	T921	I791	I791
K1616	L1550	I1485	N1340	W1273	W1273	A1194	I1127	T989	A922	R792	R792
P1617	L1550	R1486	L1341	S1274	S1274	L1195	F1128	F990	V923	L857	Q793
L1618	D1556	T1487	L1342	D1275	D1275	L1196	F1129	T991	H924	H924	Q793
H1619	P1557	T1488	K1343	K1276	K1276	V1197	D1130	M992	R924	R924	I925
E1620	A1558	Y1489	K1344	P1277	P1277	S1198	M1131	F993	Q926	Q926	F795
R1621	V1559	T1490	R1345	C1278	C1278	S1199	M1132	F993	L927	L927	L796
L1622	M1560	T1491	A1346	V1279	V1279	L1200	Q1133	L996	I928	I928	A797
S1623	G1561	G1491	S1347	P1280	P1280	L1201	C1134	I997	M929	M929	F798
F1626	G1562	F1495	E1348	H1251	H1251	G1204	E1135	Y1002	E930	E930	N799
R1627	S1563	I1498	Y1349	L1252	L1252	L1205	M1137	I1002	R931	R931	M800
E1628	L1564	L1499	L1253	L1283	L1283	D1206	F1138	I1002	L932	L932	L801
L1629	V1565	L1499	K1284	Q1284	Q1284	Y1207	F1139	I1006	R933	R933	R804
K1630	Y1566	L1499	L1285	R1285	R1285	R1208	G1140	Y1006	R934	R934	P805
E1631	E1567	F1502	K1354	S1287	S1287	T1209	N1141	V1007	R935	R935	P805
E1632	K1568	E1503	Q1359	Y1288	Y1288	I1210	H1145	V1008	L806	L806	L806
V1633	F1571	K1505	P1360	Y1289	Y1289	I1211	H1146	M1009	E907	E907	E907
E1634	T1572	Q1506	L1437	V1290	V1290	M1212	M1146	M1010	E908	E908	E908
K1635	I1507	I1507	Y1361	Y1291	Y1291	M1212	F1147	T1012	A809	A809	V810
H1636	K1574	S1508	P1438	T1292	T1292	E1148	E1148	Q1013	C874	C874	V810
Y1637	Y1575	T1509	P1439	T1292	T1292	N1149	N1149	N1014	I941	I941	K811
G1638	L1576	E1510	S1440	Q1293	Q1293	E1150	E1150	N1014	G942	G942	I812
V1639	Q1577	E1511	Y1441	Q1294	Q1294	L1151	L1151	R1015	M943	M943	K813
L1640	E1578	I1512	K1442	E1296	E1296	I1152	I1152	F1017	R945	R945	G814
E1579	H1579	S1513	D1443	K1297	K1297	R1220	I1152	L1018	Q946	Q946	L817
P1580	P1580	P1514	P1445	E1298	E1298	M1221	D1156	R1019	S947	S947	K818
E1581	E1581	L1515	G1371	E1298	E1298	S1222	Q1157	R1087	P948	P948	Y819
E1582	D1582	E1516	F1372	Y1301	Y1301	C1223	E1158	R1088	L882	L882	L820
E1583	Q1583	E1517	F1372	Q1302	Q1302	T1224	V1159	D1089	T883	T883	P821
K1585	K1585	A1518	F1375	E1303	E1303	V1225	G1162	M1090	S822	S822	S822
V1586	V1586	I1519	L1376	I1304	I1304	M1229	R1163	Y1092	F953	F953	I823
E1587	E1587	M1522	R1377	I1305	I1305	F1230	R1163	F1024	V954	V954	I824
L1588	L1588	E1523	N1378	S1306	S1306	Y1231	G1164	E1026	A955	A955	N825
L1589	L1589	L1524	K1379	Y1307	Y1307	K1232	D1165	V1027	C956	C956	N826
K1590	T1525	T1525	I1380	Y1307	Y1307	E1233	E1166	L1028	Q889	Q889	V827
R1591	N1526	N1526	F1381	K1310	K1310	K1234	Q1167	T1029	L890	L890	K828
L1592	E1527	E1527	F1381	G1311	G1311	E1234	Y1168	K1100	I958	I958	L829
I1593	R1528	R1528	R1384	G1311	G1311	K1235	K1169	F1031	A959	A959	L829
E1593	E1528	E1528	G1385	K1316	K1316	K1236	V1170	F1032	L960	L960	V830
Q1596	I1529	I1529	K1386	K1317	K1317	E1237	L1171	M1033	K996	K996	F831
M1597	S1530	S1530	E1387	I1318	I1318	D1238	L1172	Q1034	D832	D832	D832
F1598	N1531	N1531	Y1388	K1319	K1319	I1239	E1173	D1035	P833	P833	P833
			E1389	L1320	L1320	Y1240	K1174	M964	V834	V834	V834
											L836

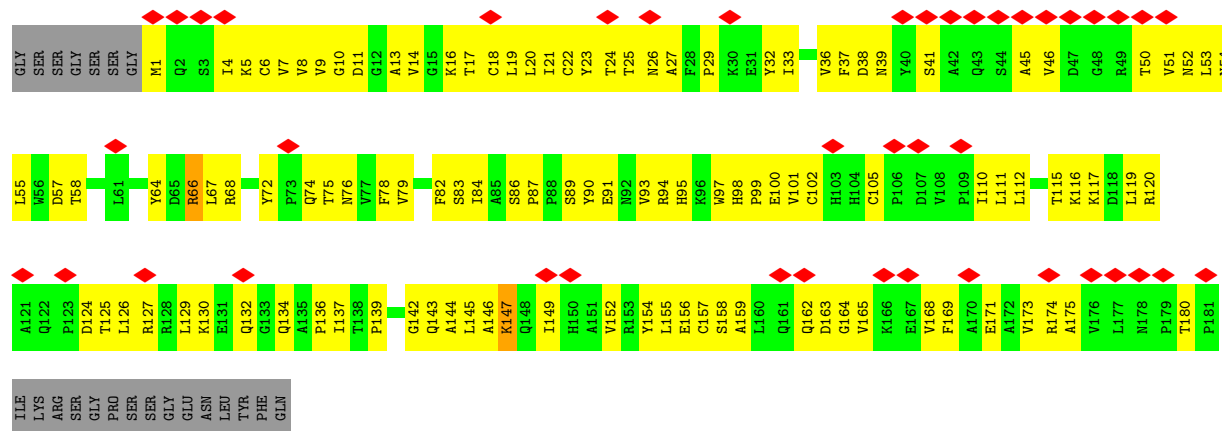
● Molecule 2: Ras-related C3 botulinum toxin substrate 1

Chain C:  33% 63%





• Molecule 4: Rho-related GTP-binding protein RhoG



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169096	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	0.062	Depositor
Minimum map value	-0.021	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP

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	0.41	0/13722	0.58	1/18514 (0.0%)
1	F	0.34	0/13722	0.55	2/18514 (0.0%)
2	C	0.36	0/1415	0.55	0/1924
2	G	0.34	0/1415	0.54	0/1924
3	A	0.30	0/5992	0.55	0/8086
3	E	0.30	0/1650	0.56	0/2230
4	D	0.30	0/1449	0.51	0/1977
All	All	0.36	0/39365	0.56	3/53169 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	676	LEU	CA-CB-CG	6.09	129.30	115.30
1	B	992	MET	CA-CB-CG	-5.47	104.00	113.30
1	F	96	ARG	CB-CG-CD	5.10	124.86	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	LYS	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	13436	0	13516	1324	0
1	F	13436	0	13516	1068	0
2	C	1385	0	1407	117	0
2	G	1385	0	1407	139	0
3	A	5879	0	5902	479	0
3	E	1617	0	1625	159	0
4	D	1416	0	1413	123	0
5	D	1	0	0	0	0
6	D	32	0	12	4	0
All	All	38587	0	38798	3295	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 43.

The worst 5 of 3295 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:F:1028:LEU:O	1:F:1032:PHE:HB2	1.63	0.98
1:F:1217:LYS:HA	1:F:1220:ARG:HE	1.31	0.94
3:A:302:PHE:HB3	3:A:431:GLY:H	1.31	0.94
1:B:1462:PHE:HB2	1:B:1489:TYR:HB2	1.46	0.94
1:F:740:TYR:HA	1:F:749:LYS:HD3	1.47	0.94

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	1640/1648 (100%)	1416 (86%)	224 (14%)	0	100	100
1	F	1640/1648 (100%)	1466 (89%)	174 (11%)	0	100	100
2	C	175/184 (95%)	156 (89%)	19 (11%)	0	100	100
2	G	175/184 (95%)	157 (90%)	18 (10%)	0	100	100
3	A	725/733 (99%)	657 (91%)	68 (9%)	0	100	100
3	E	197/733 (27%)	162 (82%)	35 (18%)	0	100	100
4	D	179/203 (88%)	161 (90%)	18 (10%)	0	100	100
All	All	4731/5333 (89%)	4175 (88%)	556 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1495/1497 (100%)	1490 (100%)	5 (0%)	92	95
1	F	1495/1497 (100%)	1489 (100%)	6 (0%)	91	94
2	C	153/157 (98%)	153 (100%)	0	100	100
2	G	153/157 (98%)	151 (99%)	2 (1%)	69	82
3	A	662/664 (100%)	659 (100%)	3 (0%)	88	93
3	E	184/664 (28%)	183 (100%)	1 (0%)	88	93
4	D	157/174 (90%)	155 (99%)	2 (1%)	69	82
All	All	4299/4810 (89%)	4280 (100%)	19 (0%)	91	94

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	218	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	66	ARG
4	D	147	LYS
3	A	516	LYS
1	F	743	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	793	GLN
1	F	1526	ASN
3	A	703	ASN
1	F	799	ASN
1	F	1035	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GTP	D	202	5,4	26,34,34	1.11	2 (7%)	32,54,54	1.70	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GTP	D	202	5,4	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	202	GTP	C5-C6	-3.95	1.39	1.47
6	D	202	GTP	C2-N3	2.15	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	202	GTP	PA-O3A-PB	-5.03	115.55	132.83
6	D	202	GTP	PB-O3B-PG	-3.40	121.15	132.83
6	D	202	GTP	C5-C6-N1	3.20	119.61	113.95
6	D	202	GTP	C3'-C2'-C1'	2.95	105.42	100.98
6	D	202	GTP	C8-N7-C5	2.88	108.48	102.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	202	GTP	PB-O3B-PG-O3G
6	D	202	GTP	PB-O3B-PG-O1G

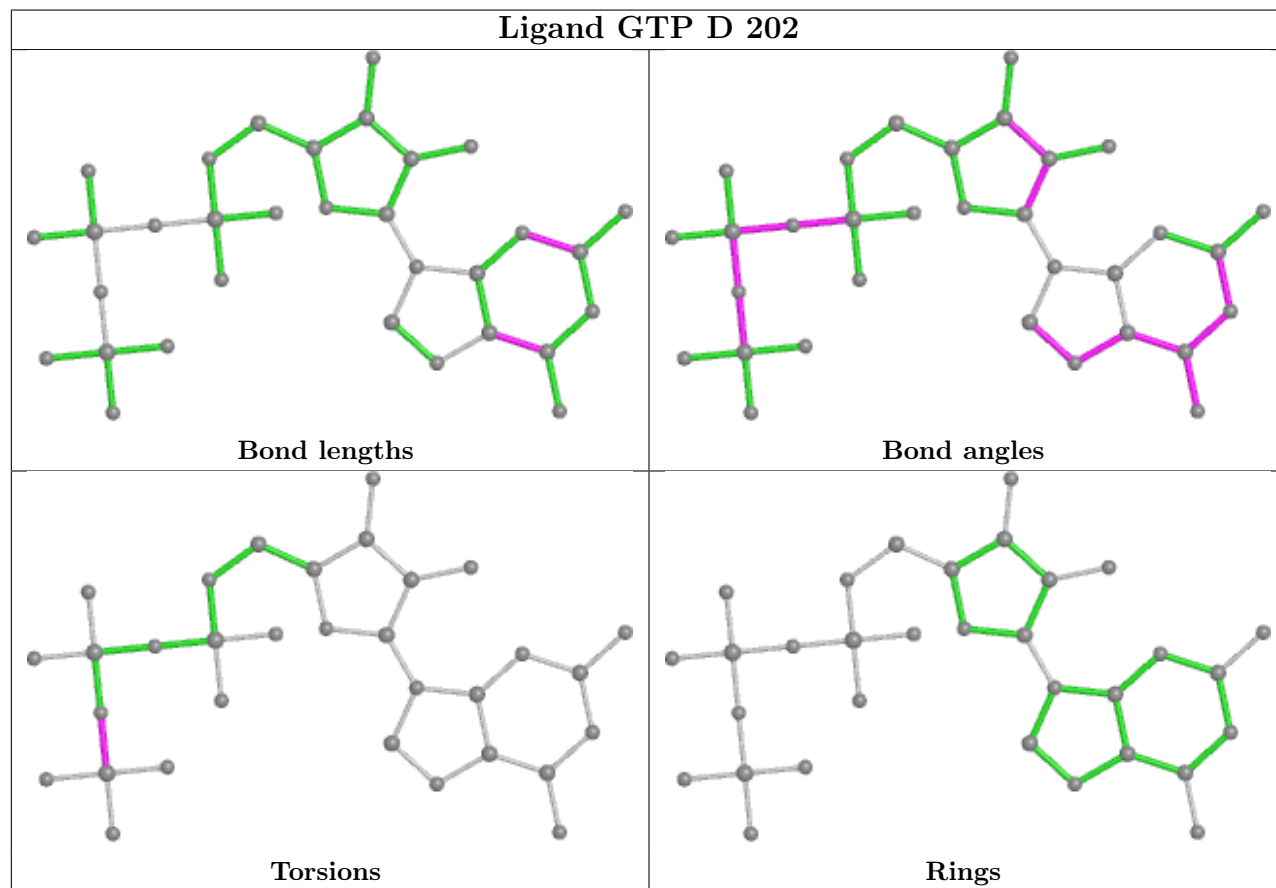
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	202	GTP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

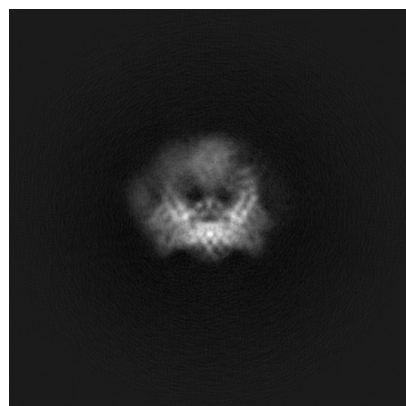
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60136. These allow visual inspection of the internal detail of the map and identification of artifacts.

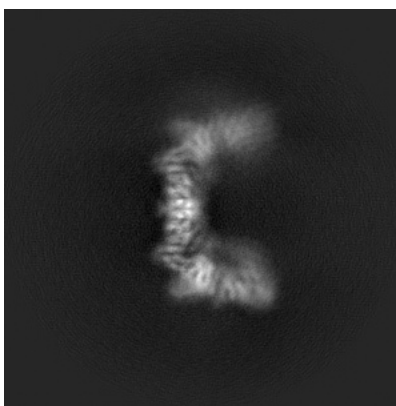
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

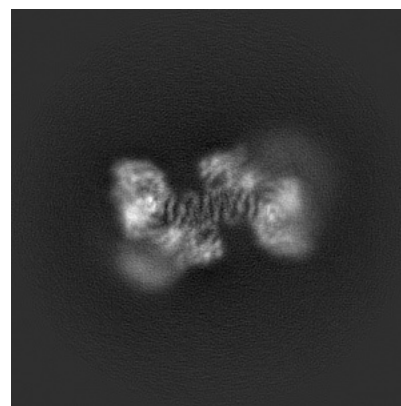
6.1.1 Primary map



X

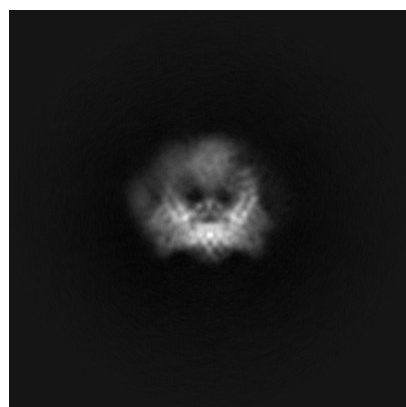


Y

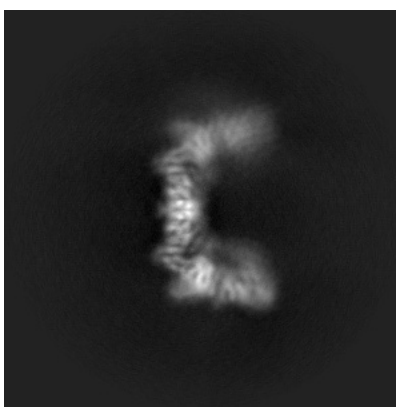


Z

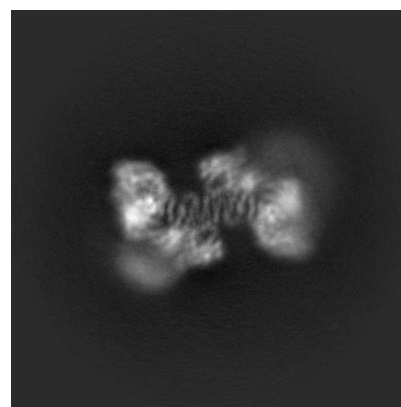
6.1.2 Raw map



X



Y

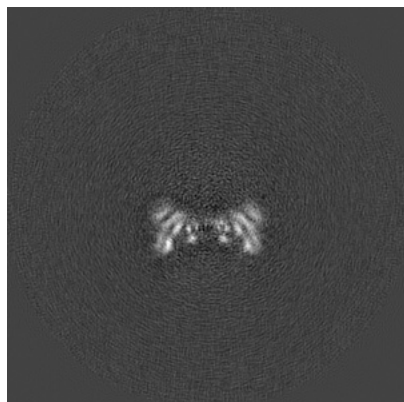


Z

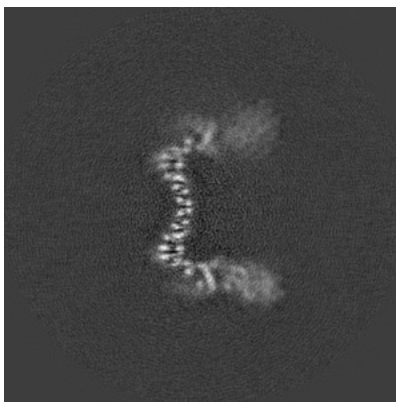
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

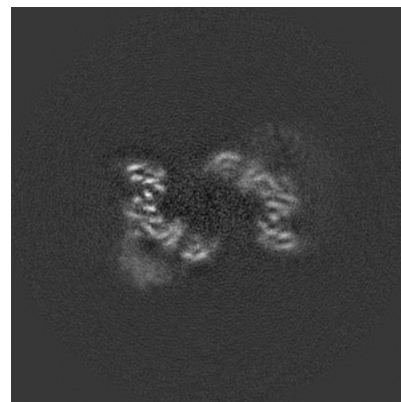
6.2.1 Primary map



X Index: 170

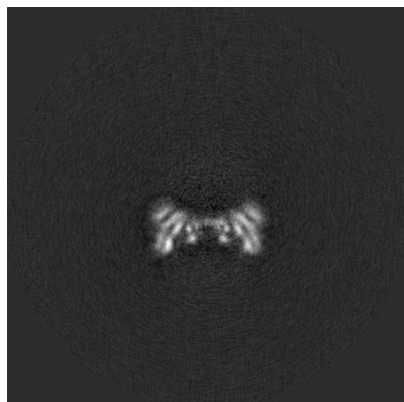


Y Index: 170

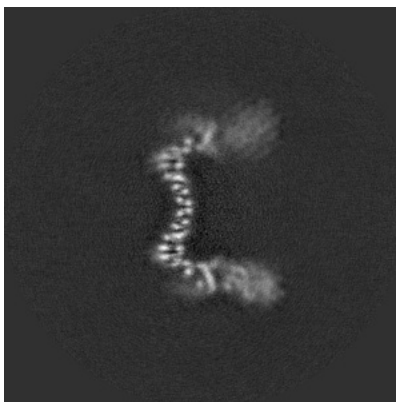


Z Index: 170

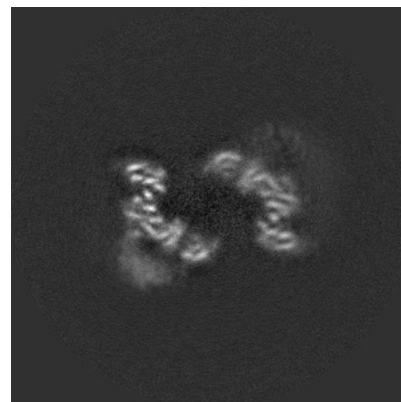
6.2.2 Raw map



X Index: 170



Y Index: 170

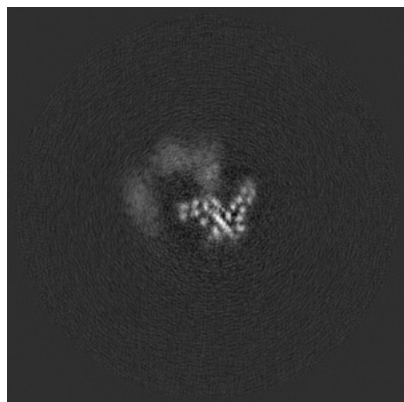


Z Index: 170

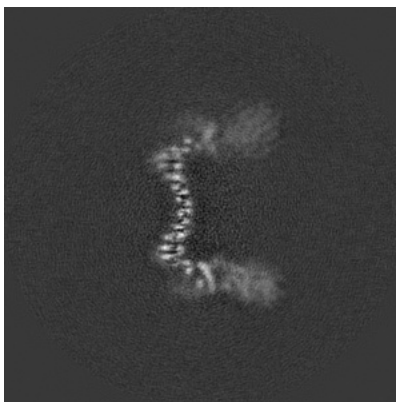
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

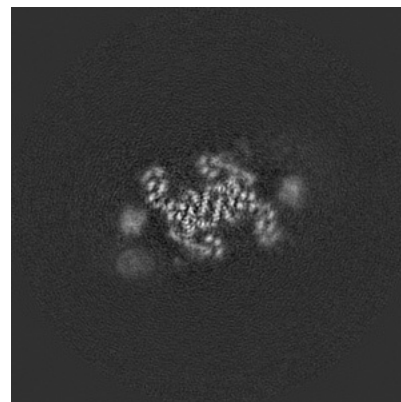
6.3.1 Primary map



X Index: 118

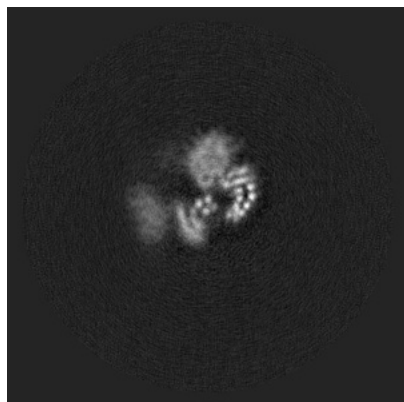


Y Index: 169

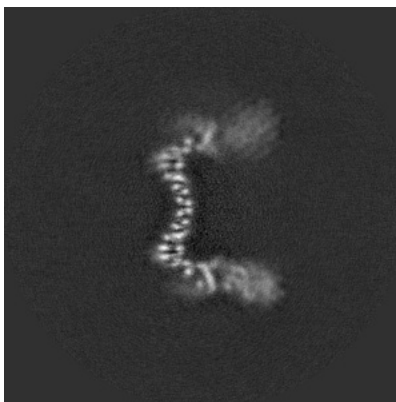


Z Index: 149

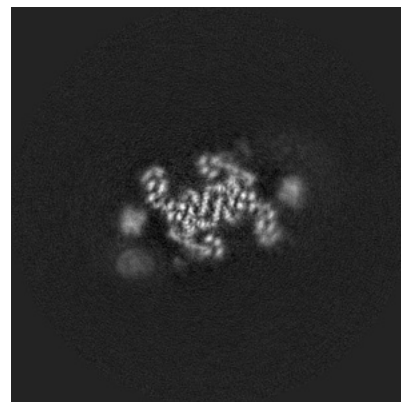
6.3.2 Raw map



X Index: 104



Y Index: 170

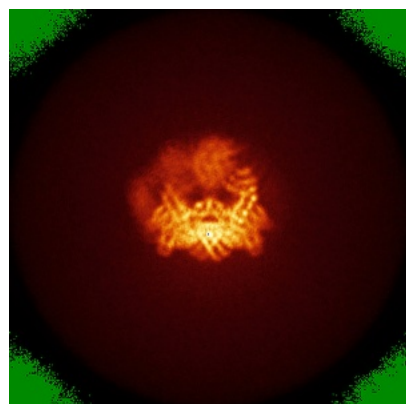


Z Index: 149

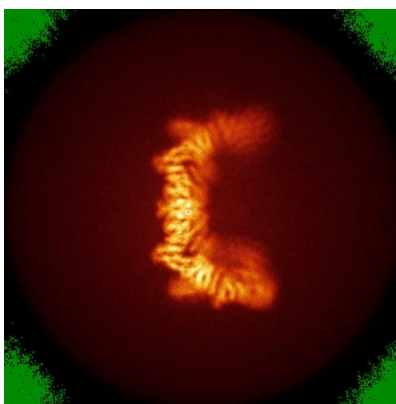
The images above show the largest variance slices of the map in three orthogonal directions.

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

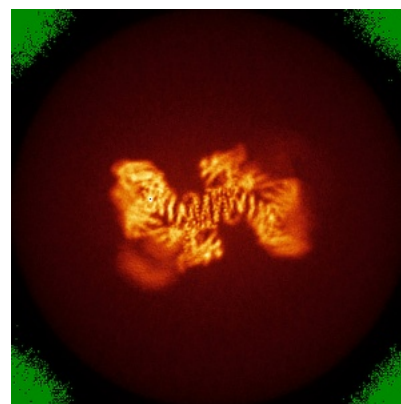
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

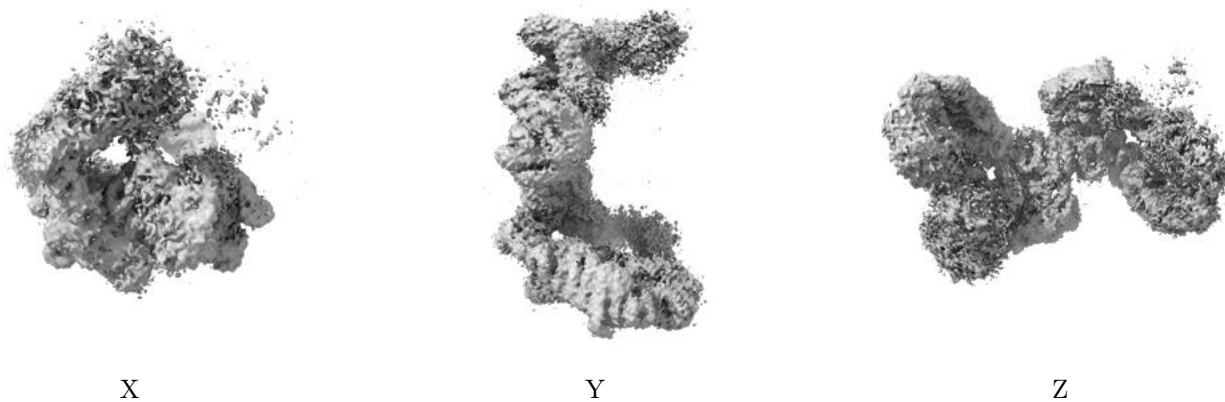


Z

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.

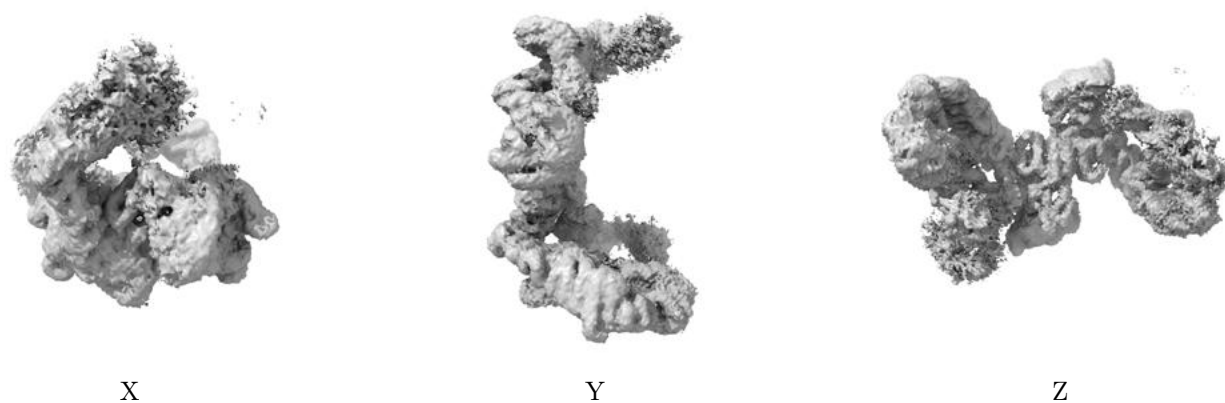
6.5 Orthogonal surface views [i](#)

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.

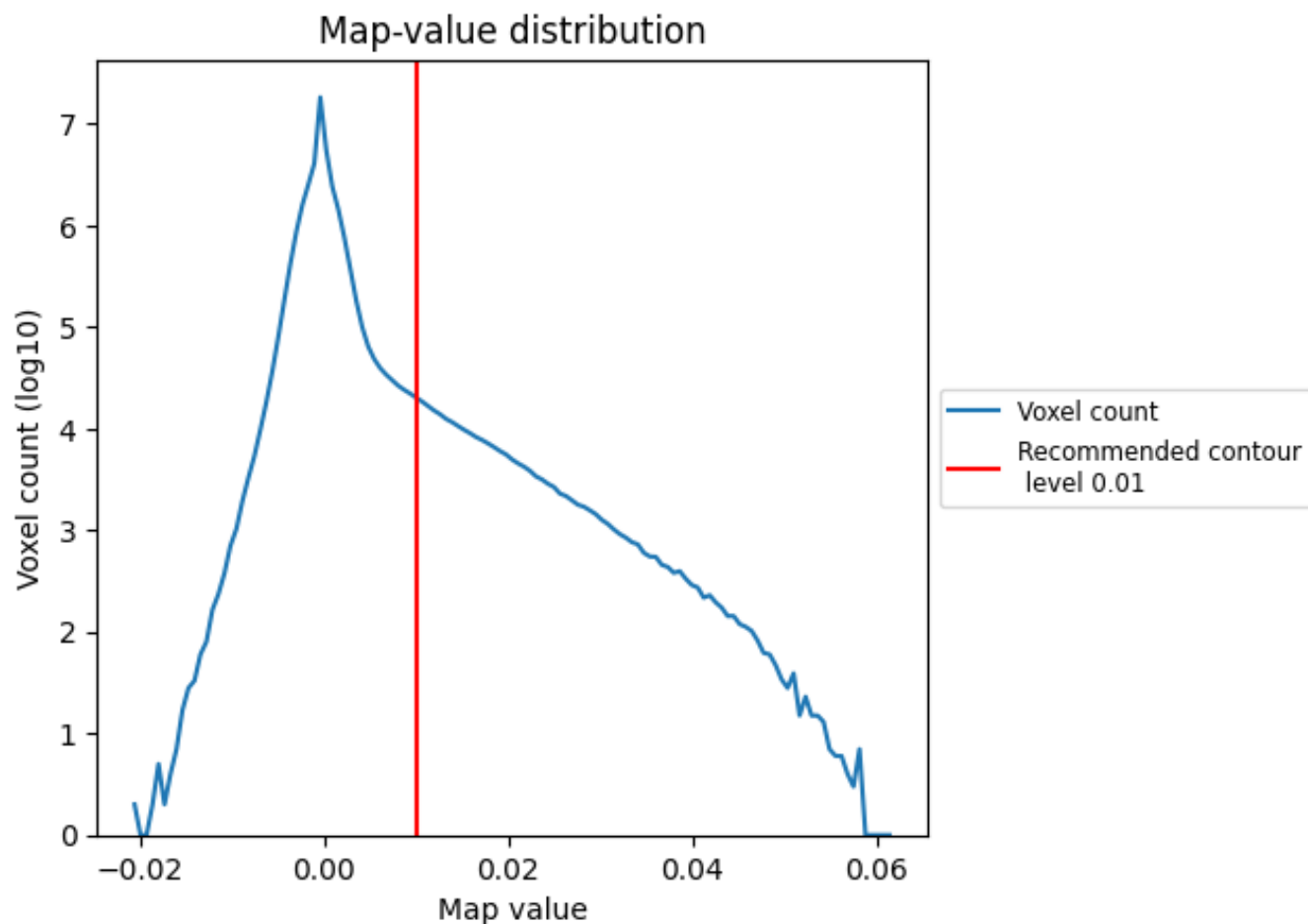
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

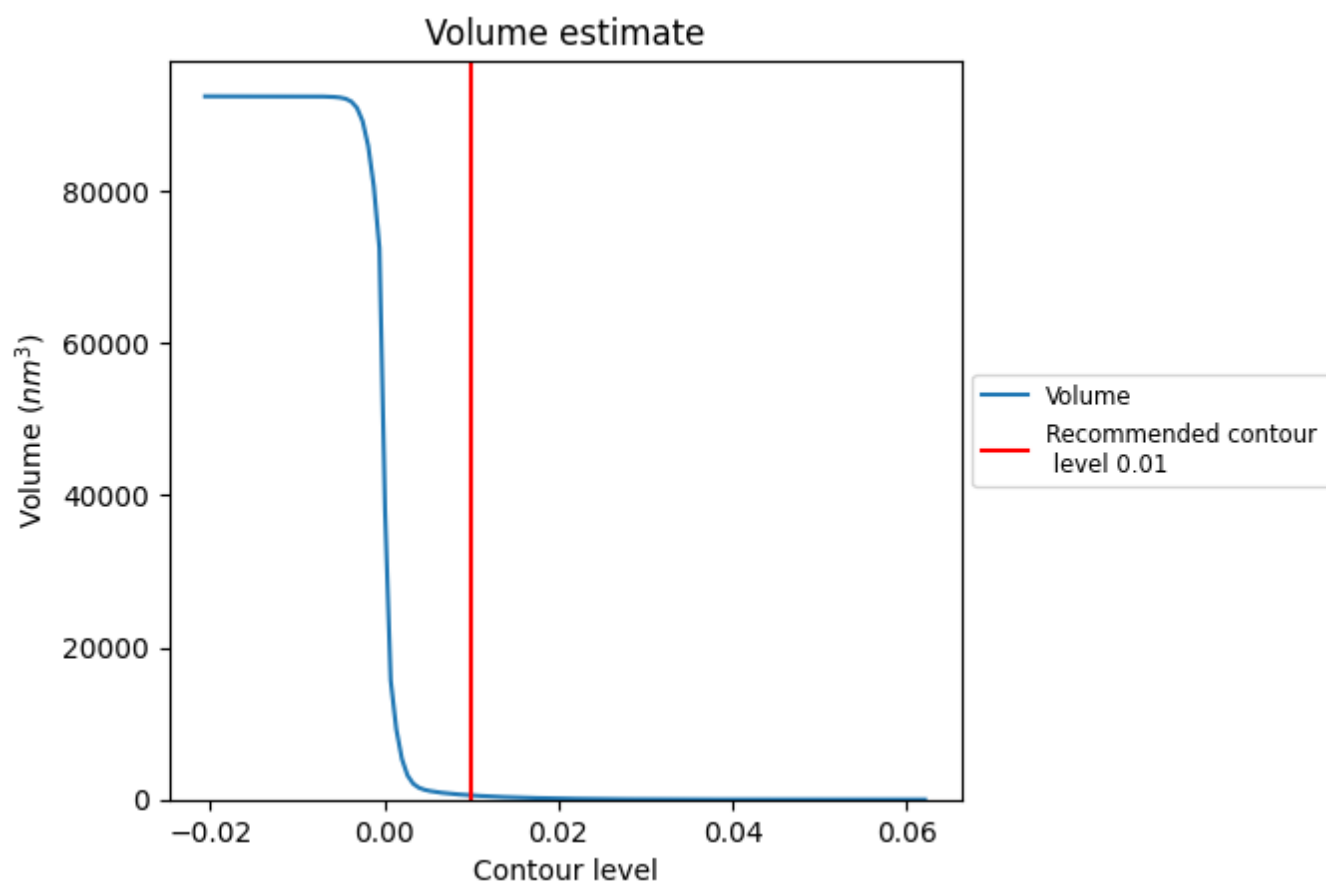
This section contains the results of statistical analysis of the map.

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.

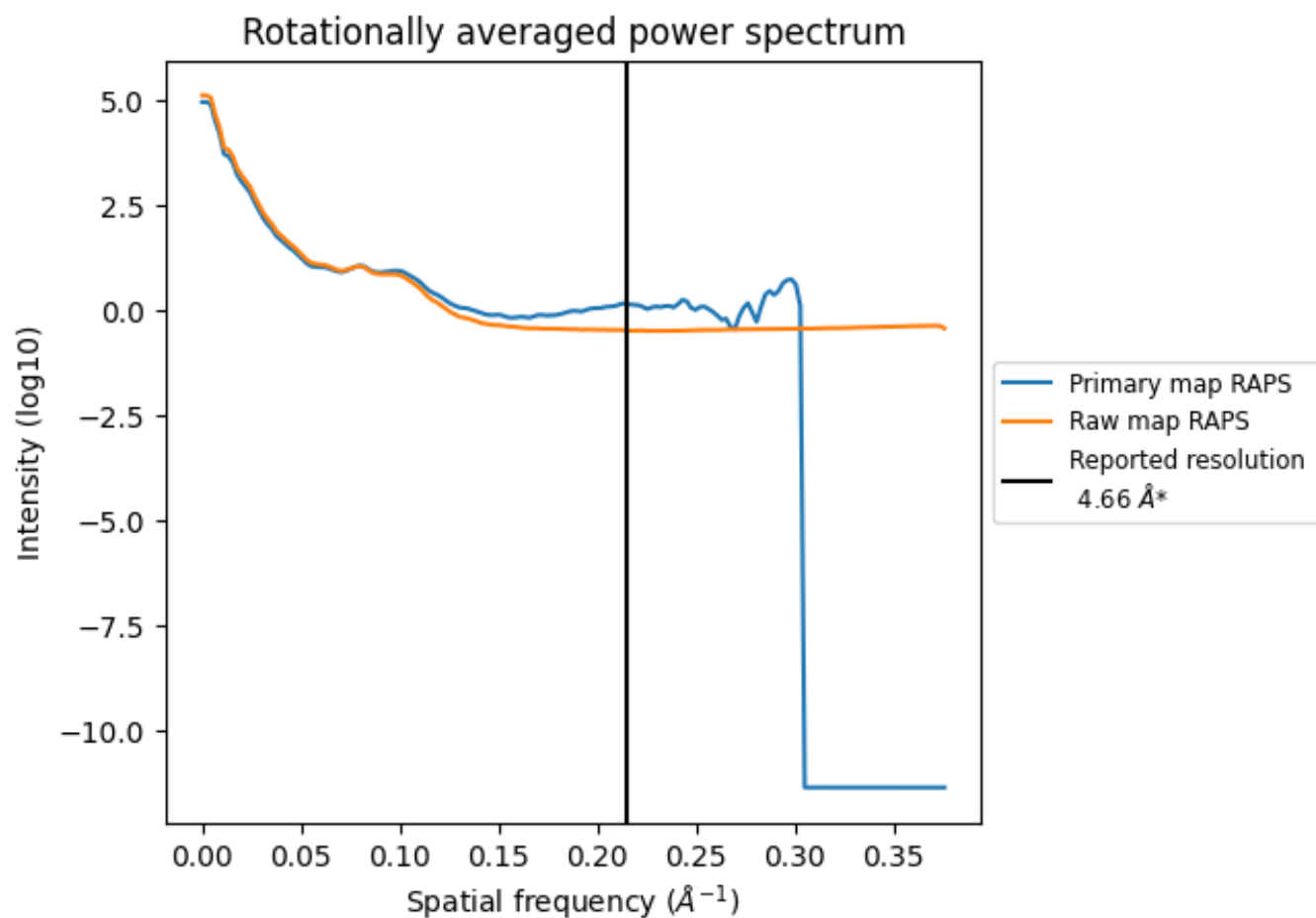
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 551 nm³; this corresponds to an approximate mass of 498 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 ⓘ

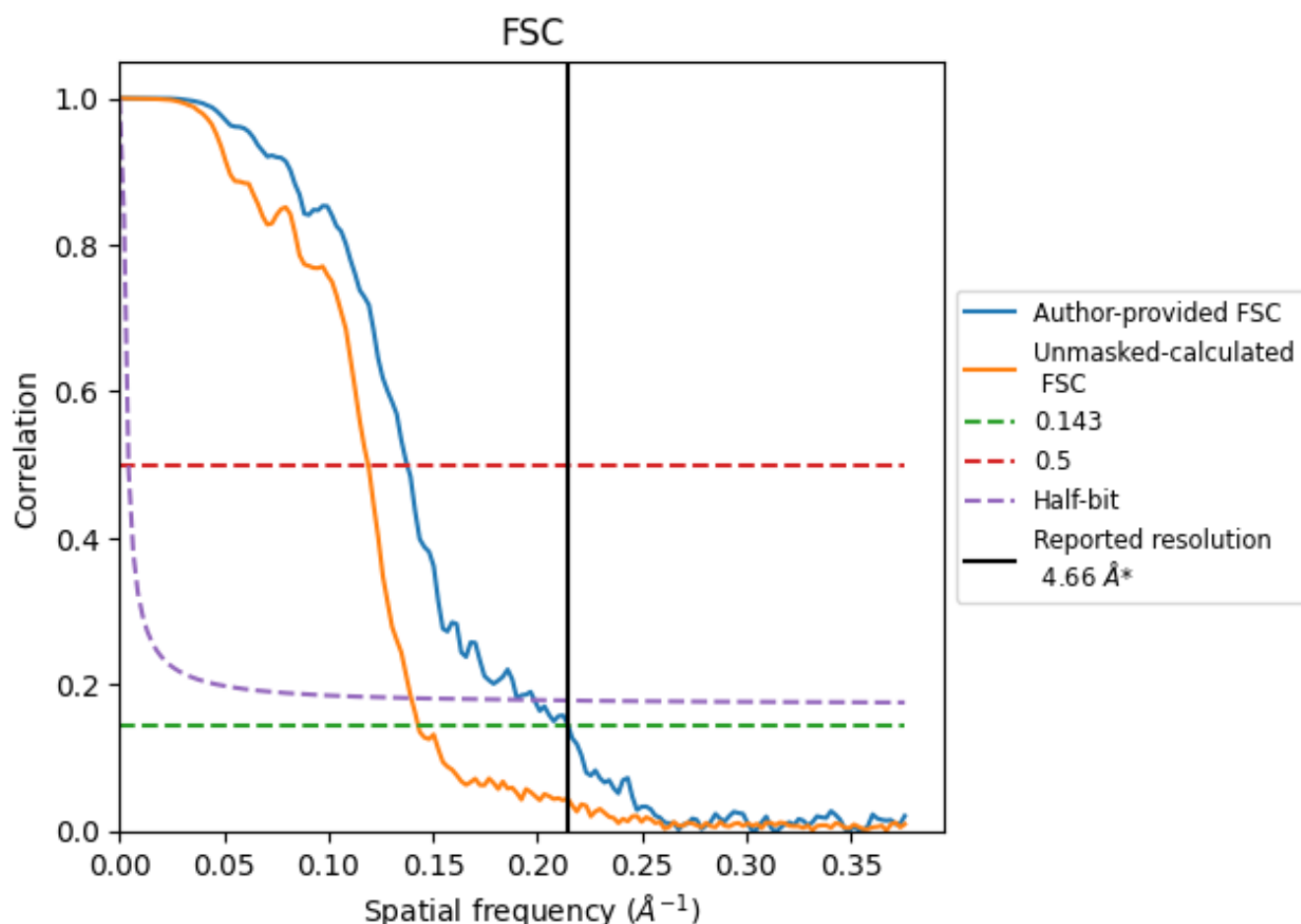


*Reported resolution corresponds to spatial frequency of 0.215 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.215 \AA^{-1}

8.2 Resolution estimates [i](#)

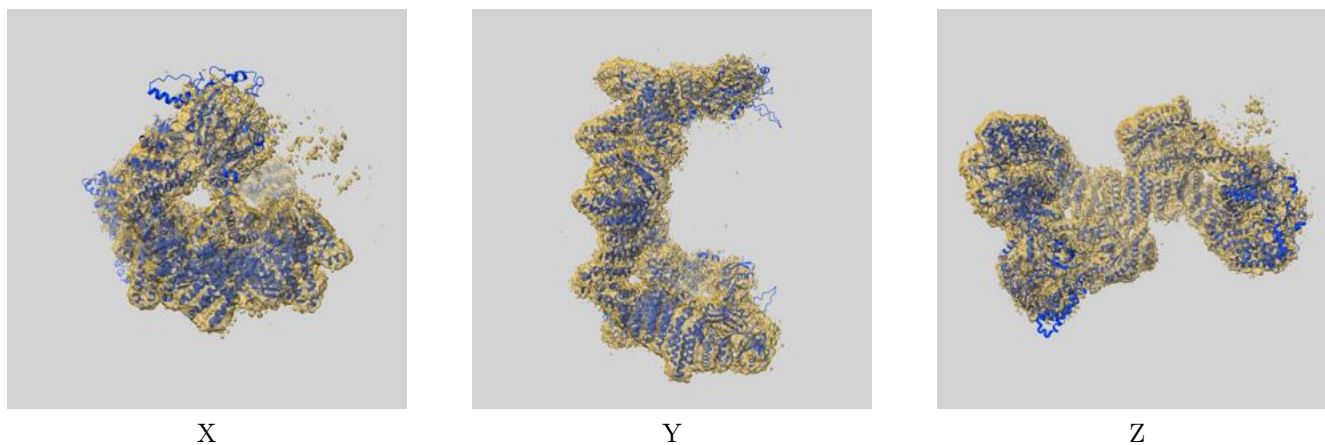
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.66	-	-
Author-provided FSC curve	4.65	7.27	5.03
Unmasked-calculated*	6.99	8.40	7.16

*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 6.99 differs from the reported value 4.66 by more than 10 %

9 Map-model fit [i](#)

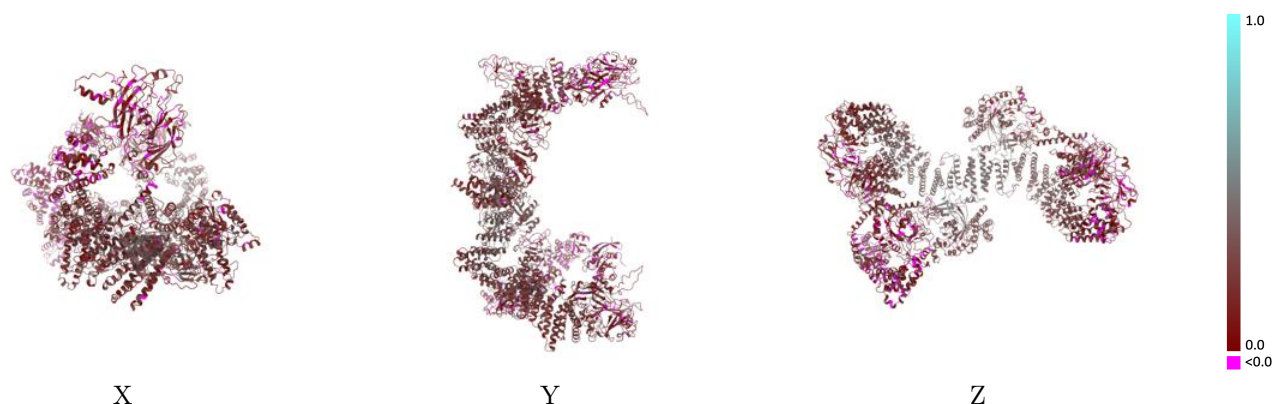
This section contains information regarding the fit between EMDB map EMD-60136 and PDB model 8ZJ2. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



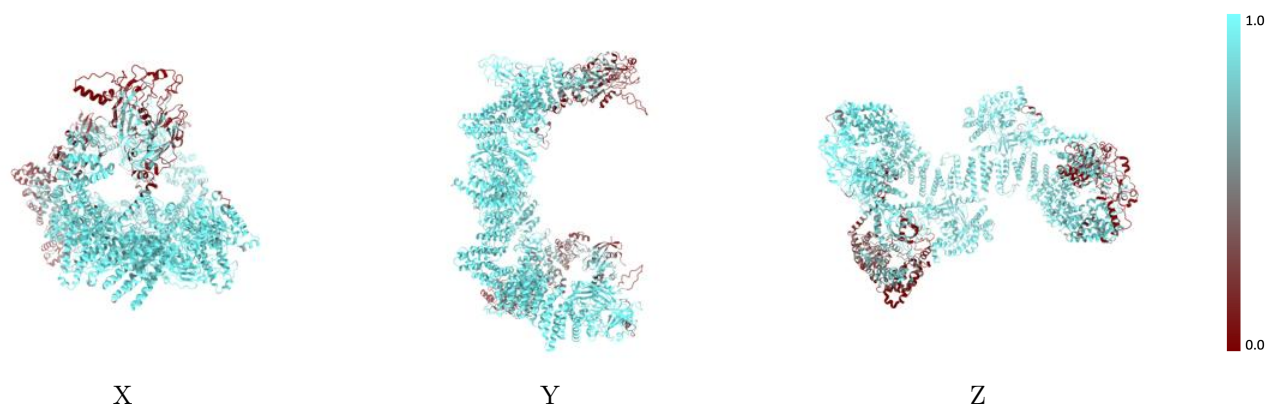
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



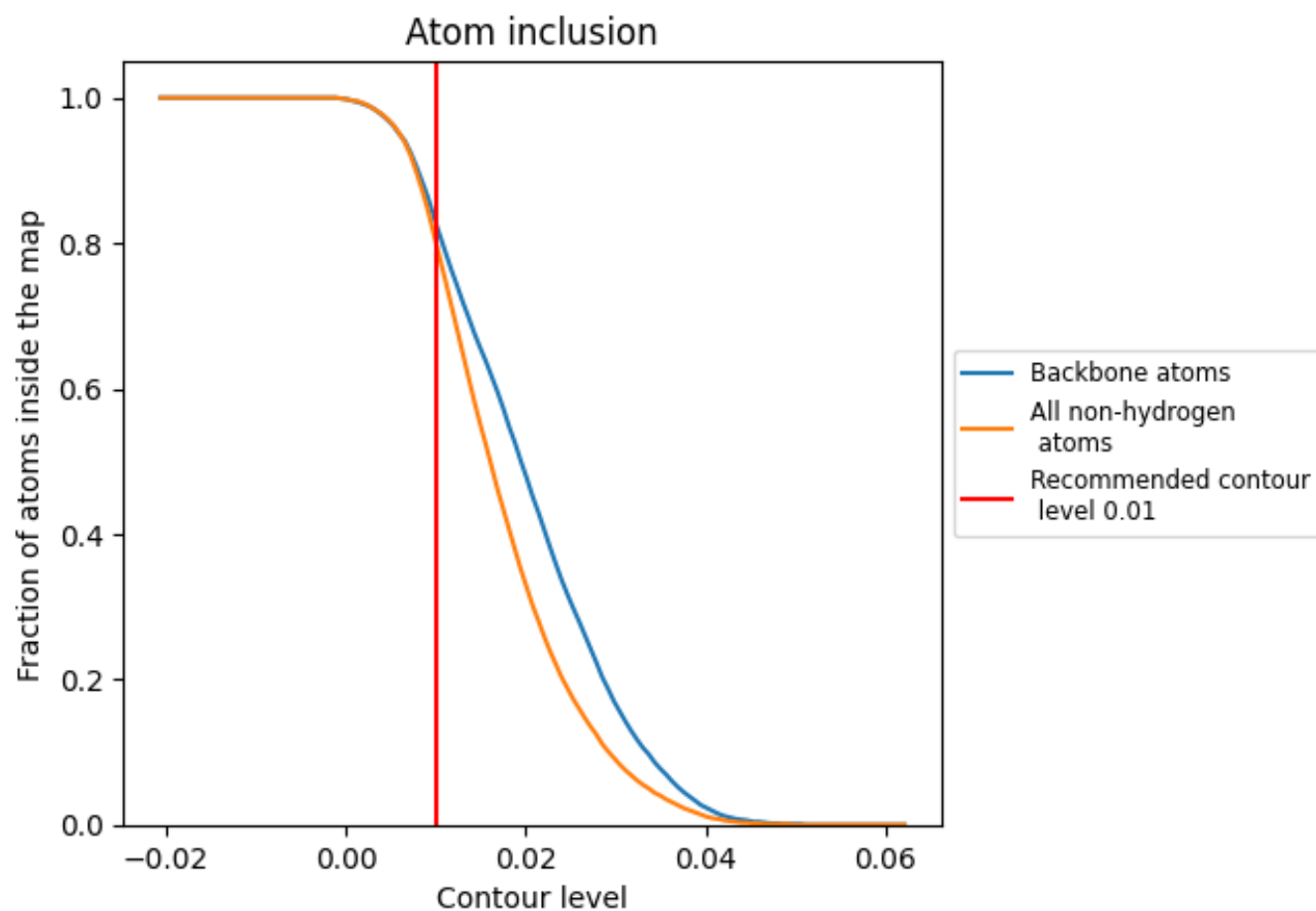
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 80% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8010	<div></div> 0.2310
A	<div></div> 0.4950	<div></div> 0.1540
B	<div></div> 0.9400	<div></div> 0.2700
C	<div></div> 0.9660	<div></div> 0.3030
D	<div></div> 0.6550	<div></div> 0.1510
E	<div></div> 0.8810	<div></div> 0.2070
F	<div></div> 0.7700	<div></div> 0.2260
G	<div></div> 0.9550	<div></div> 0.2650

1.0

0.0

<0.0