



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:37 AM UTC

PDB ID : 8XM7 / pdb_00008xm7
EMDB ID : EMD-38466
Title : Cryo-EM structure of the RhoG/DOCK5/ELMO1/Rac1 complex:
RhoG/DOCK5/ELMO1 focused map
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 : 2023-12-27
Resolution : 4.91 Å(reported)
Based on initial models : 7DPA, 6IE1, 7Y4A

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

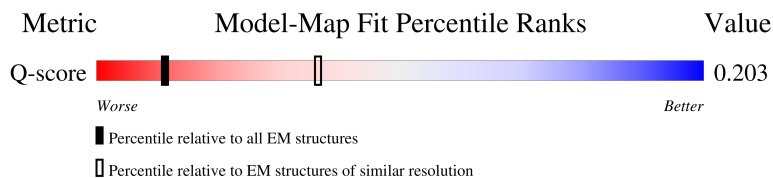
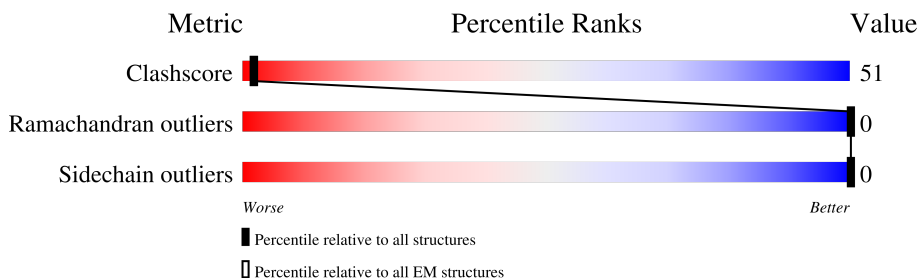
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

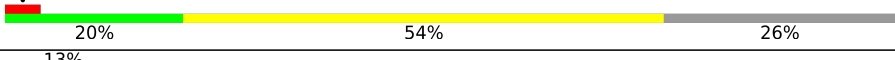
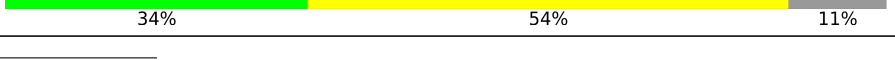
The reported resolution of this entry is 4.91 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1074 (4.41 - 5.41)

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	
2	B	1648	
3	D	203	

Validation Pipeline (wwPDB-VP) : 2.49

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GTP	D	202	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17190 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
1	A	727	Total	C	N	O	S	0	0
			5879	3721	1009	1108	41		

There are 6 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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1215	Total	C	N	O	S	0	0
			9862	6319	1669	1821	53		

There are 7 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

- Molecule 3 is a protein called Rho-related GTP-binding protein RhoG.

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

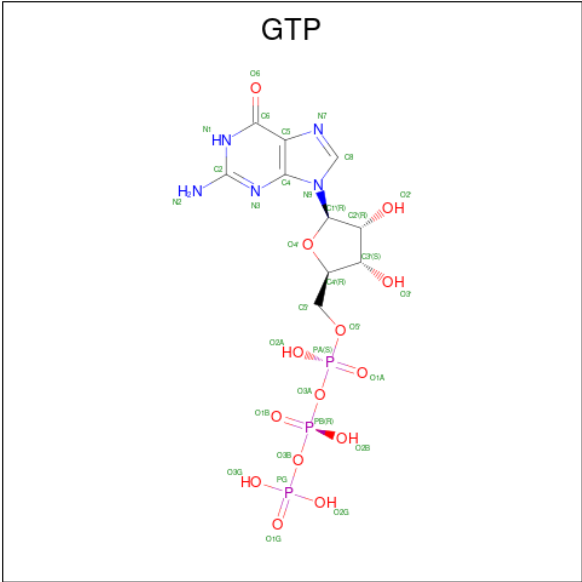
There are 20 discrepancies between the modelled and reference sequences:

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 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



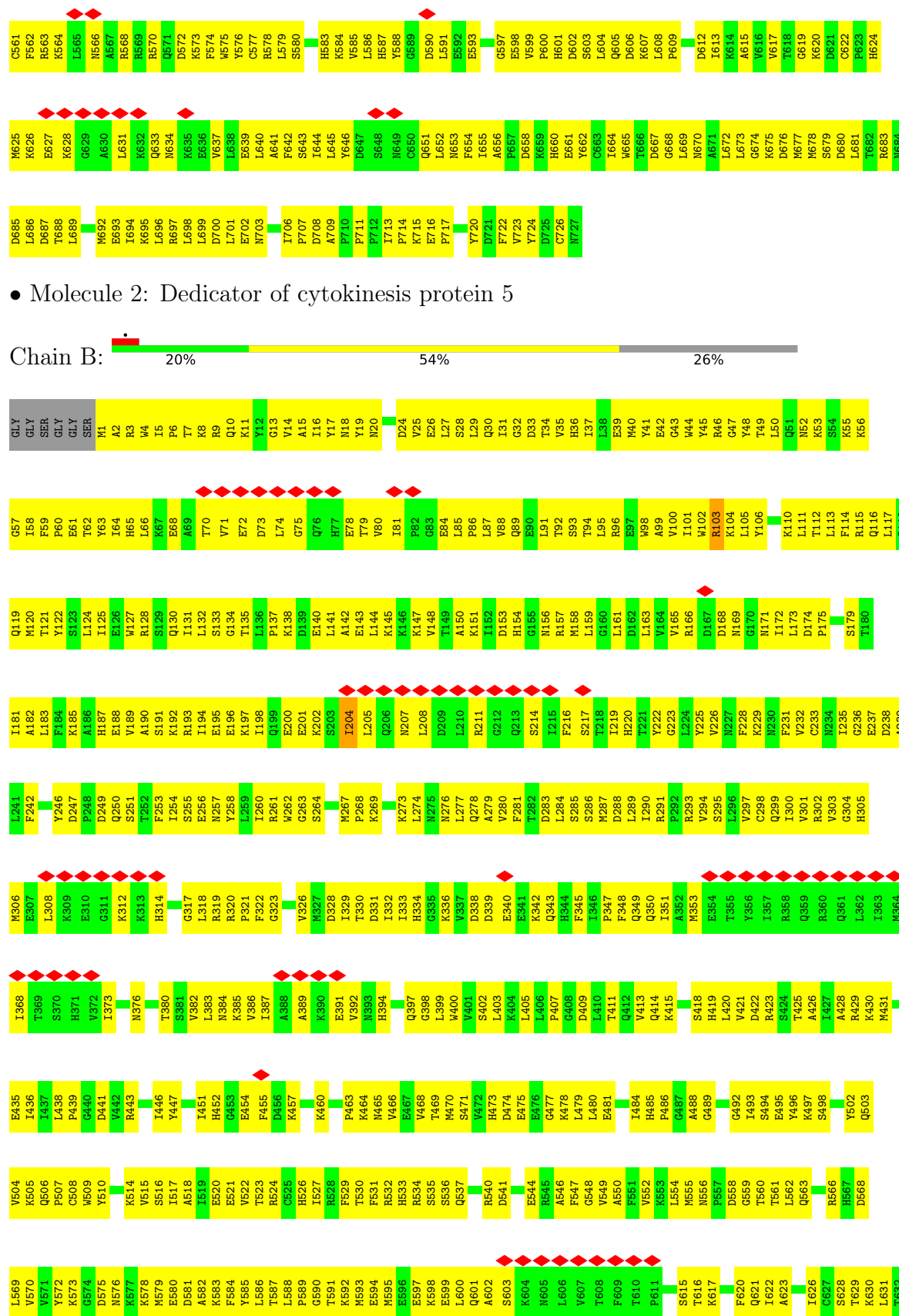
Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			32	10	5	14	3	

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: Engulfment and cell motility protein 1

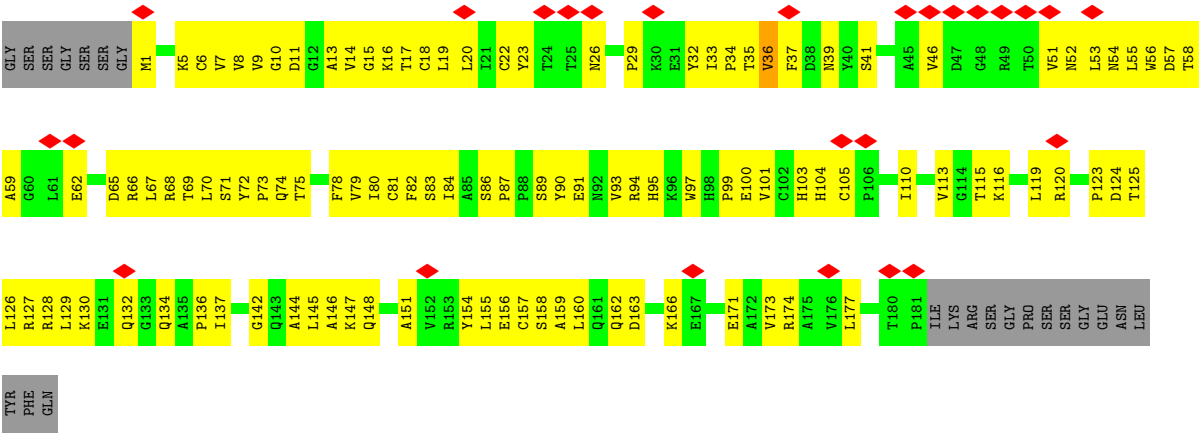




• Molecule 2: Dedicator of cytokinesis protein 5

ARG	GLU	LYS	ALA	THR	GLY	ILE	PRO	GLU	THR	HIS	Y1207	H1145	K1081	R1019	C956	K896	E835	I768	I703	Q633
LEU	LEU	LEU	LEU	GLY	GLU	THR	GLN	TYR	GLY	ALA	R1208	M1146	E1062	A1020	M957	P897	L836	Q769	I704	M634
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	T1209	E1147	G1084	I1021	A959	H899	L839	S770	G705	V635
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	I1211	E1148	G1083	I1022	A959	H899	L839	S770	G706	D636
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	M1212	E1150	F1086	F1024	L961	A901	C841	V772	I707	L637
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	Q1213	L1151	R1087	A1025	Q962	S902	K842	L775	F709	G639
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	D1214	T1152	I1088	E1026	Q963	S903	F843	K776	Q710	L640
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	E1215	T1153	D1089	V1027	M964	Q904	I844		H711	L641
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	SER	K1154	M1090	L1028	D965	L905	Q845	S781	F712	W643
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	LYS	L1155	W1091	T1029	D966	L906	Q846	D783	N713	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	GLU	L1156	W1092	R1030	S967	S907	I847	F714	F715	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	ASN	Q1157	N1093	R1031	H968	N908	P848	G784	G785	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	E1158	L1094	F1032	Y969	I909	D849	L716	L717	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	W1159		M1033	S970	L910	N850	E786	E718	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	GLN	G1162	K1098	D1034	H971	E911	Q851	F787	F719	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	THR	R1163	I1099	Q1035	I973	L913	L852	N788	I720	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	G1164	K1100	A1036	I974	D914	R854	S790	K721	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	D1165	F1101	S1037	T975	R915	Q855	I791	K722	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	E1166	I1102	F976	R916	K916	L857	Q793	H723	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	Y1167		R979	D917	G919	N858	L794	F724	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	Q1168	M1105	Q980	R979	G919	C859	F795	T727	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	K1169	G1107	Q981	I882	T921	M860	L796	A729	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1171	P1108	I883	I922	K862	T881	A737	F730	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	E1172	I1109	R983	N923	K863	R862	F798	K731	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	K1173	L1110	D984	I924	R864	N799	M800	K732	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1174	E1111	F985	I925	E865	F864	L801	K733	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1175	I1112	R986	I926	E866	N789	L801	K734	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1176	T1113	Q926	Q926	S866	N789	L801	K735	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1177	I1114	E988	I927	T867	R804	L737	L737	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	E1178	T1115	R989	I928	L868	P805	N738	N738	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	H1179	P1116	F990	M929	R869	L806	F739	N739	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	C1180	E1117	I991	E930	R870	L806	Q670	Q670	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	R1181	V1118	M992	R931	Q871	A809	V741	L673	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	K1182	E1119	L932	L932	L932	V810	A742	A742	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	H1183	L1120	L996	L996	L996	K811	N743	L876	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	K1184	L1121	Q997	Q997	Q997	I812	A744	L876	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	Y1185	K1122	K998	K998	K998	K813	D745	I679	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1186	A1123	N1000	N1000	N1000	G814	D746	M680	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	S1187	T1124	V1001	V1001	V1001	A815	S747	M681	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	S1188	I1125	Y1002	Y1002	Y1002	A816	S748	E682	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	S1189	P1126	I1003	I1003	I1003	L817	K749	M683	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	G1190	I1127	A1004	A1004	A1004	K818	T760	E687	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	E1191	F1128	D1006	D1006	D1006	Y819	L752	T688	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	F1192	F1129	K1004	K1004	K1004	L820	L753	L753	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	F1193	D1130	M1007	M1007	M1007	P821	L757	F691	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	A1194	M1131	V1008	V1008	V1008	S822	K758	L693	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1195	M1132	M1009	M1009	M1009	I823	L759	V693	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1196	Q1133	I1010	I1010	I1010	I824	K760	F694	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	V1197	C1134	M1011	M1011	M1011	N825	L761	D695	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	S1198	F1136	T1012	T1012	T1012	D826	K761	D695	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	S1199	N1137	Q1013	Q1013	Q1013	V827	V762	A696	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1200	N1137	L890	L890	L890	K828	L763	L697	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1201	F1138	N1014	N1014	N1014	L829	F764	L697	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	E1202	S1139	R1015	R1015	R1015	D892	F765	L700	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	M1203	N1143	F1016	F1016	F1016	N893	F766	I701	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL	L1204	F1144	I1018	I1018	I1018	S894	F766	S702	
VAL	GLY	THR	ASN	LEU	LEU	ILE	ASN	ASP	LEU	LEU	VAL			R1080	L1018	A955	N895	I767	S702	

- Molecule 3: 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	181978	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	0.061	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	319.2, 319.2, 319.2	wwPDB
Map dimensions	240, 240, 240	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](#)

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	A	0.25	0/5992	0.58	2/8086 (0.0%)
2	B	0.38	0/10057	0.63	3/13569 (0.0%)
3	D	0.24	0/1449	0.53	0/1977
All	All	0.33	0/17498	0.61	5/23632 (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
2	B	0	1
3	D	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	204	ILE	N-CA-C	-6.92	106.75	113.53
1	A	253	LYS	CA-C-N	-6.91	110.18	120.68
1	A	253	LYS	C-N-CA	-6.91	110.18	120.68
2	B	103	ARG	CA-C-N	-5.54	113.62	122.66
2	B	103	ARG	C-N-CA	-5.54	113.62	122.66

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	870	ARG	Peptide
3	D	36	VAL	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	A	5879	0	5902	585	0
2	B	9862	0	9968	1107	0
3	D	1416	0	1413	130	0
4	D	1	0	0	0	0
5	D	32	0	12	12	0
All	All	17190	0	17295	1765	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 51.

The worst 5 of 1765 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:B:238:ASP:HB2	2:B:303:VAL:O	1.61	1.01
1:A:376:PRO:HB2	1:A:379:LEU:HB3	1.40	0.99
2:B:46:ARG:HA	2:B:57:GLY:O	1.71	0.91
2:B:330:THR:O	2:B:334:HIS:ND1	2.03	0.91
2:B:37:ILE:HA	2:B:47:GLY:HA3	1.50	0.90

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	725/733 (99%)	658 (91%)	67 (9%)	0	100	100
2	B	1213/1648 (74%)	1055 (87%)	158 (13%)	0	100	100
3	D	179/203 (88%)	168 (94%)	11 (6%)	0	100	100
All	All	2117/2584 (82%)	1881 (89%)	236 (11%)	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	A	662/664 (100%)	662 (100%)	0	100	100
2	B	1101/1497 (74%)	1101 (100%)	0	100	100
3	D	157/174 (90%)	157 (100%)	0	100	100
All	All	1920/2335 (82%)	1920 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	924	HIS
3	D	148	GLN
2	B	1013	GLN
2	B	1133	GLN
1	A	624	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	GTP	D	202	4	33,34,34	0.91	0	50,54,54	1.52	8 (16%)

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
5	GTP	D	202	4	-	3/22/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	202	GTP	C5-C4-N3	-4.88	120.62	128.39
5	D	202	GTP	C2-N3-C4	4.56	120.15	112.30
5	D	202	GTP	N9-C4-N3	3.03	132.01	125.95
5	D	202	GTP	C2-N1-C6	-2.65	120.31	125.11
5	D	202	GTP	C5-C6-N1	2.39	119.35	113.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

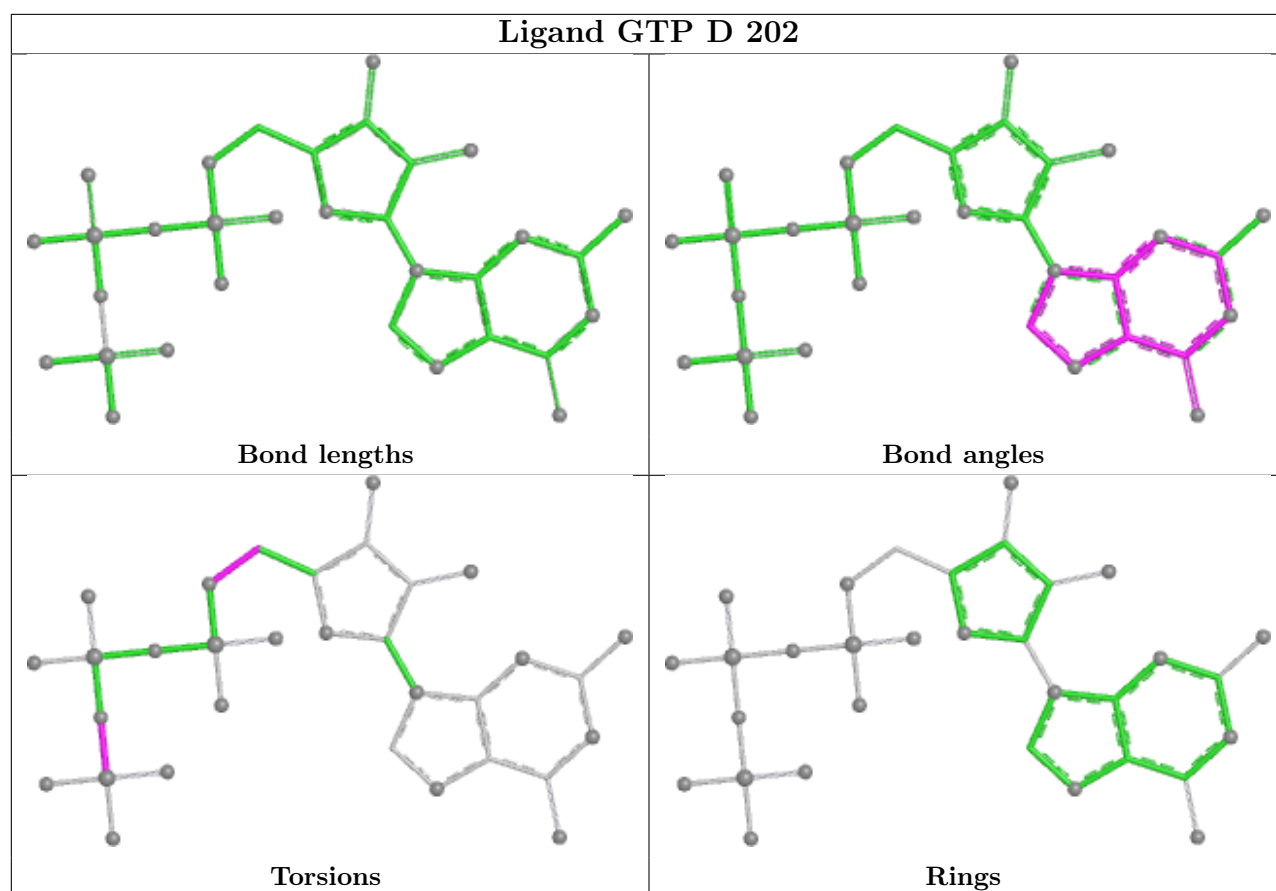
Mol	Chain	Res	Type	Atoms
5	D	202	GTP	PB-O3B-PG-O3G
5	D	202	GTP	PB-O3B-PG-O1G
5	D	202	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	202	GTP	12	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.

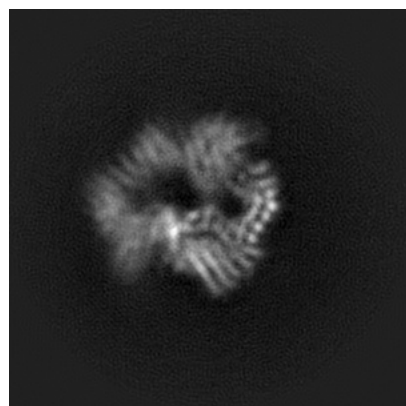
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38466. These allow visual inspection of the internal detail of the map and identification of artifacts.

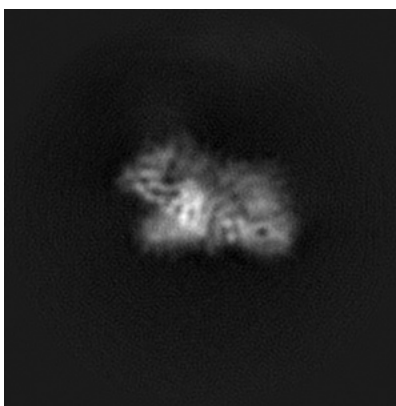
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

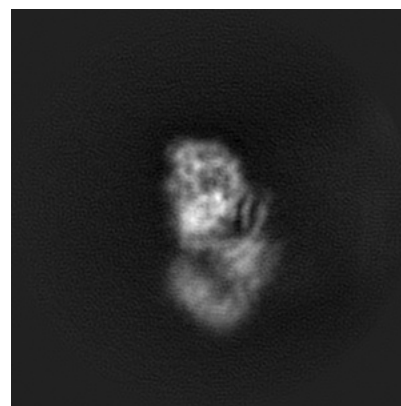
6.1.1 Primary map



X

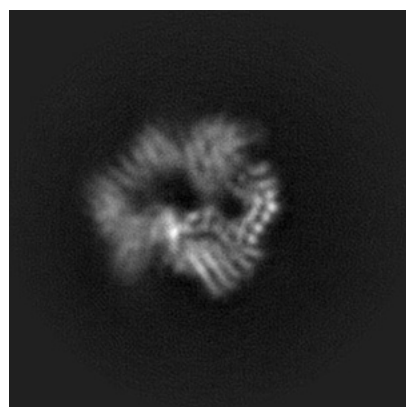


Y

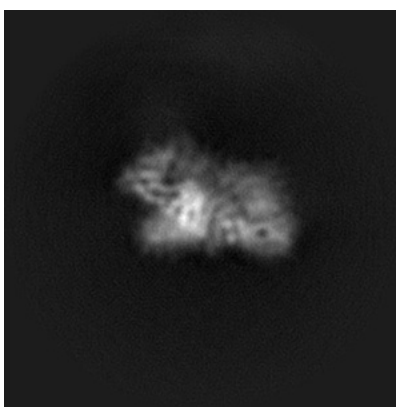


Z

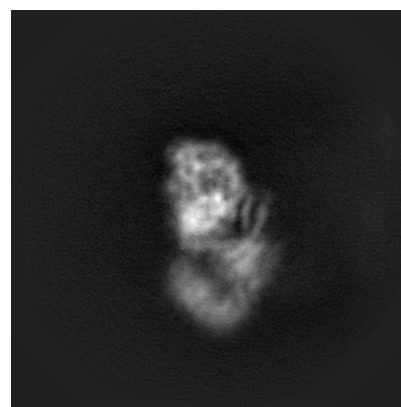
6.1.2 Raw map



X



Y

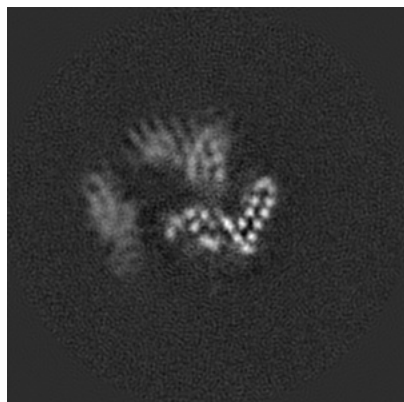


Z

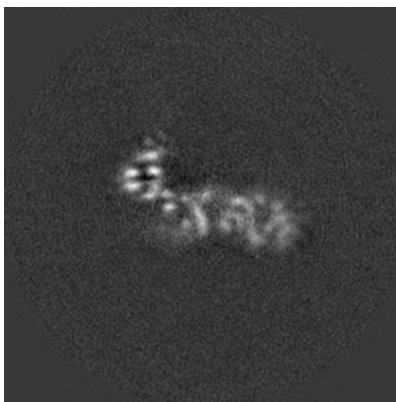
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

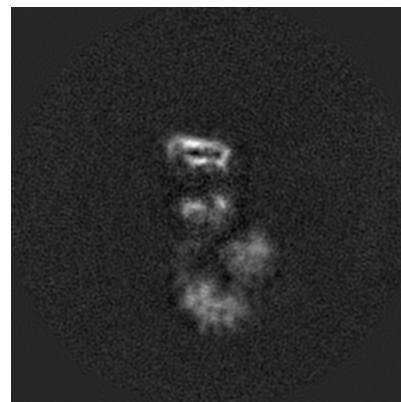
6.2.1 Primary map



X Index: 120

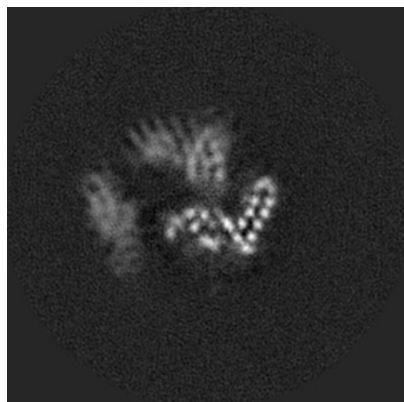


Y Index: 120

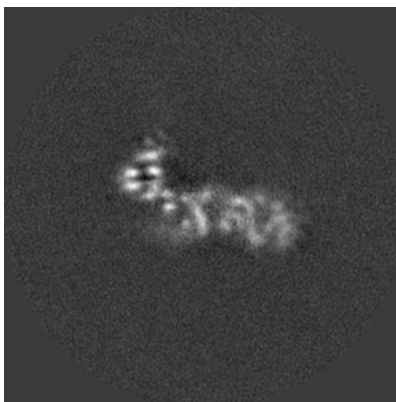


Z Index: 120

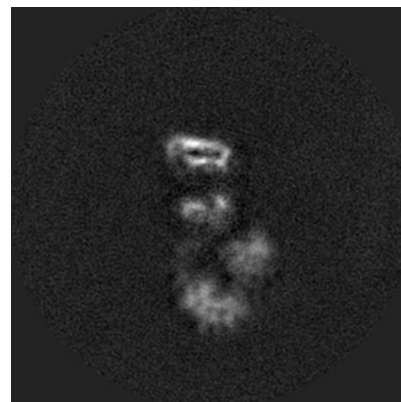
6.2.2 Raw map



X Index: 120



Y Index: 120

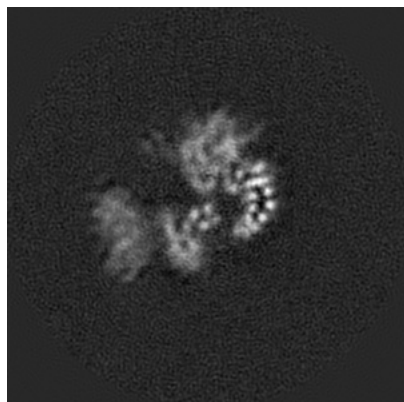


Z Index: 120

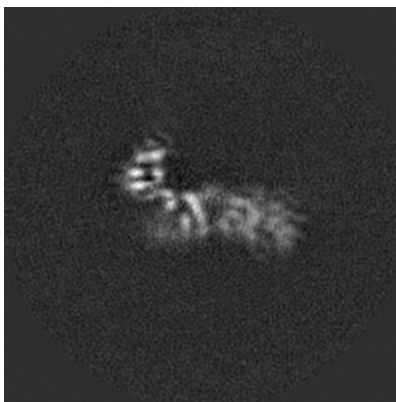
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 110

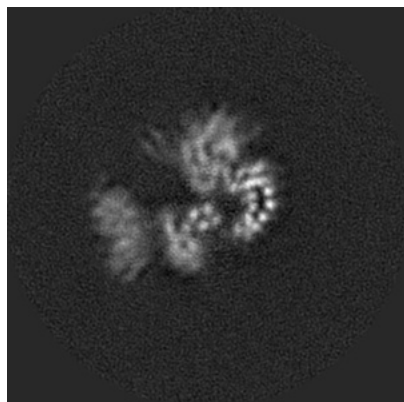


Y Index: 118

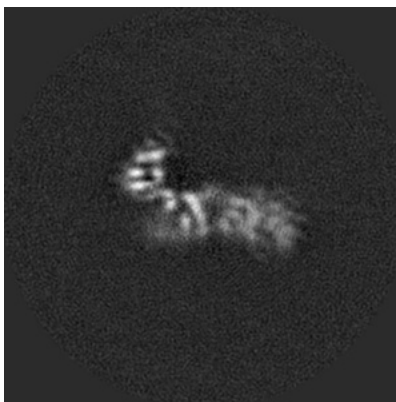


Z Index: 108

6.3.2 Raw map



X Index: 111



Y Index: 118

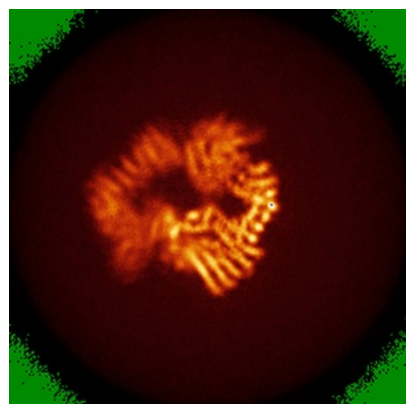


Z Index: 108

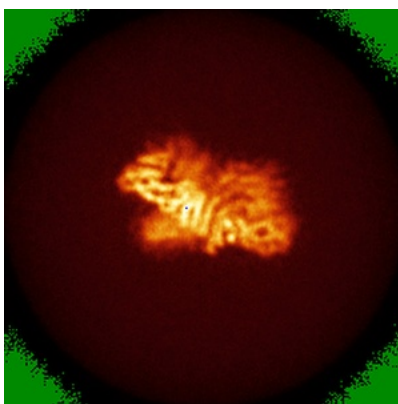
The images above show the largest variance slices of the map in three orthogonal directions.

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

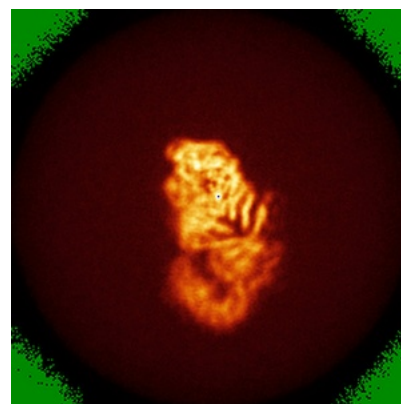
6.4.1 Primary map



X



Y

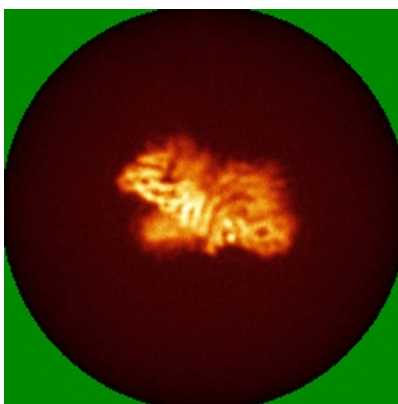


Z

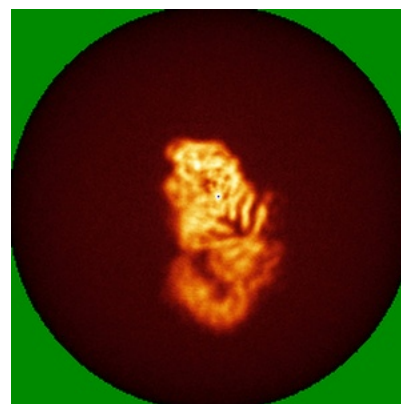
6.4.2 Raw map



X



Y

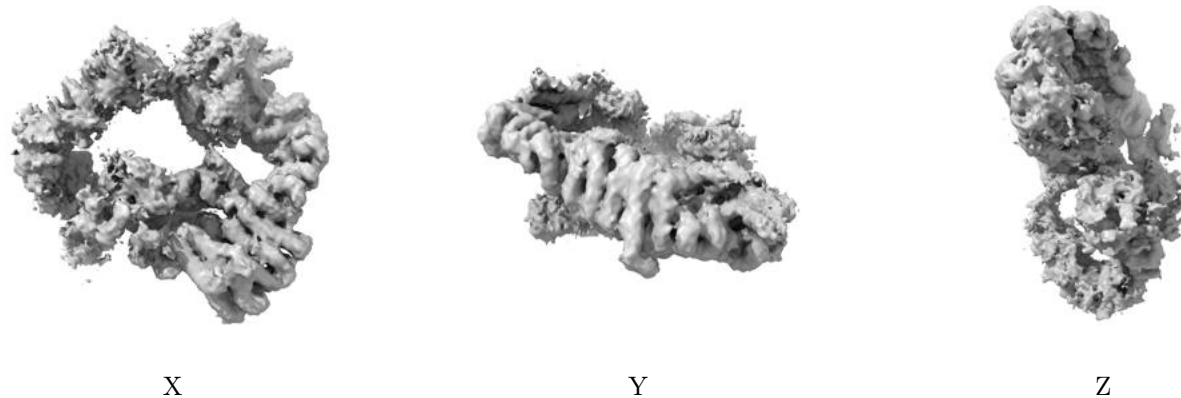


Z

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.

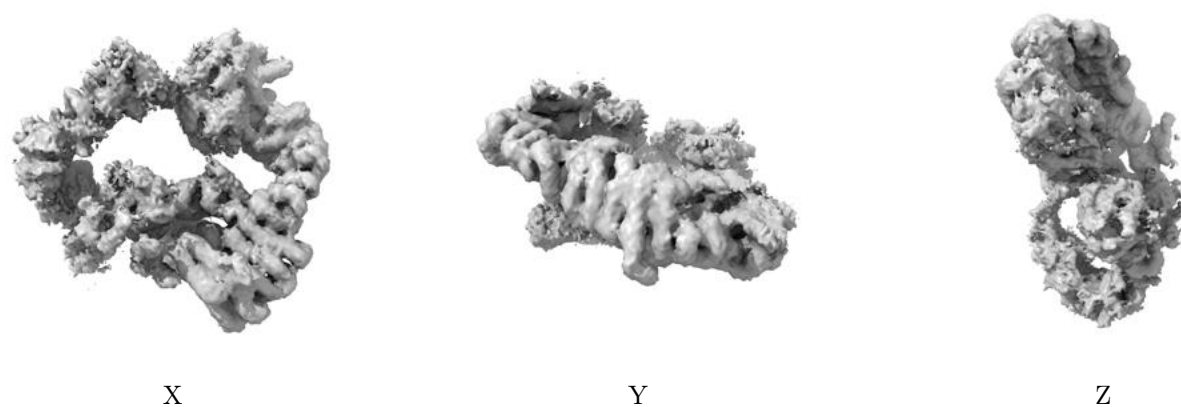
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

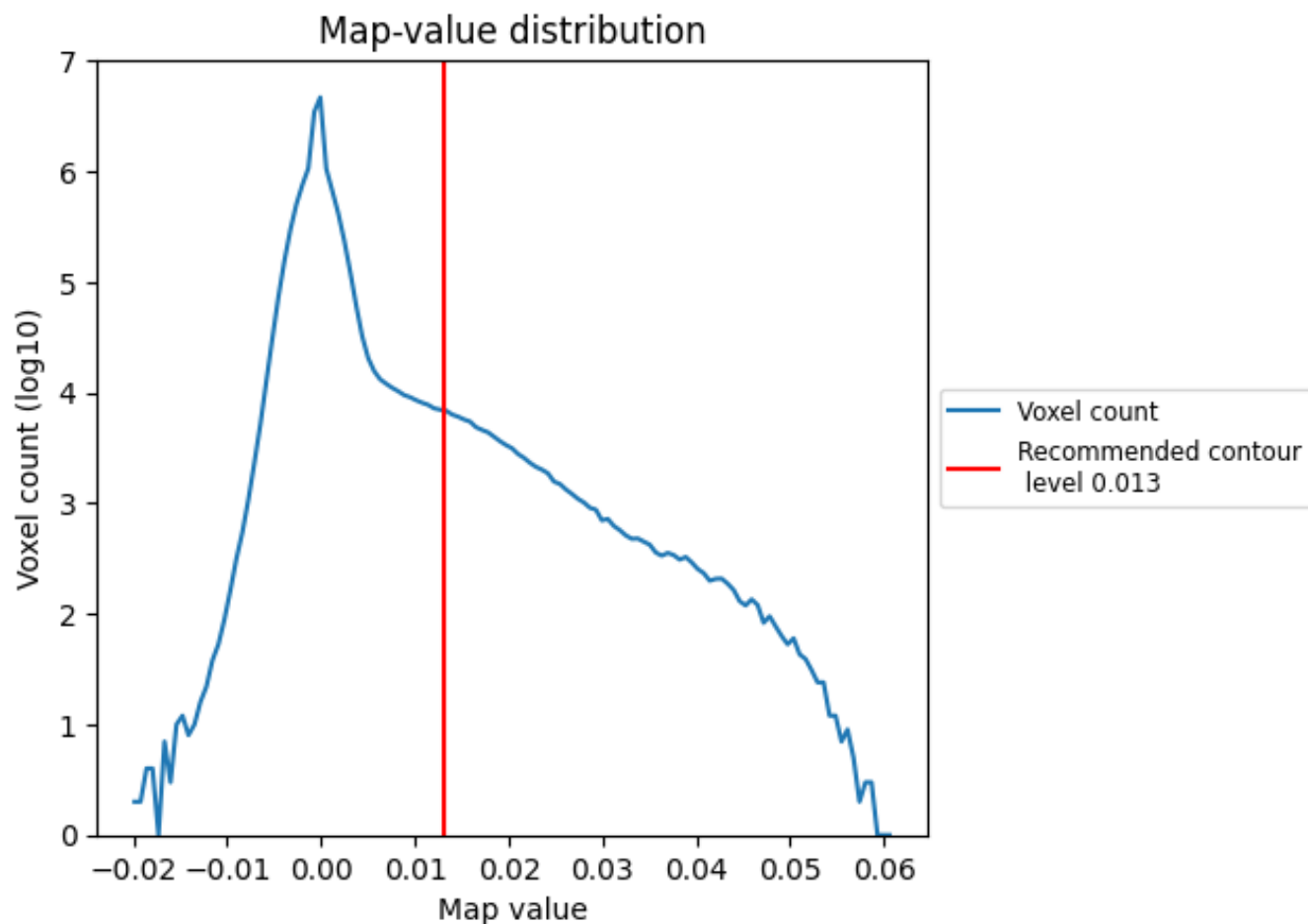
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

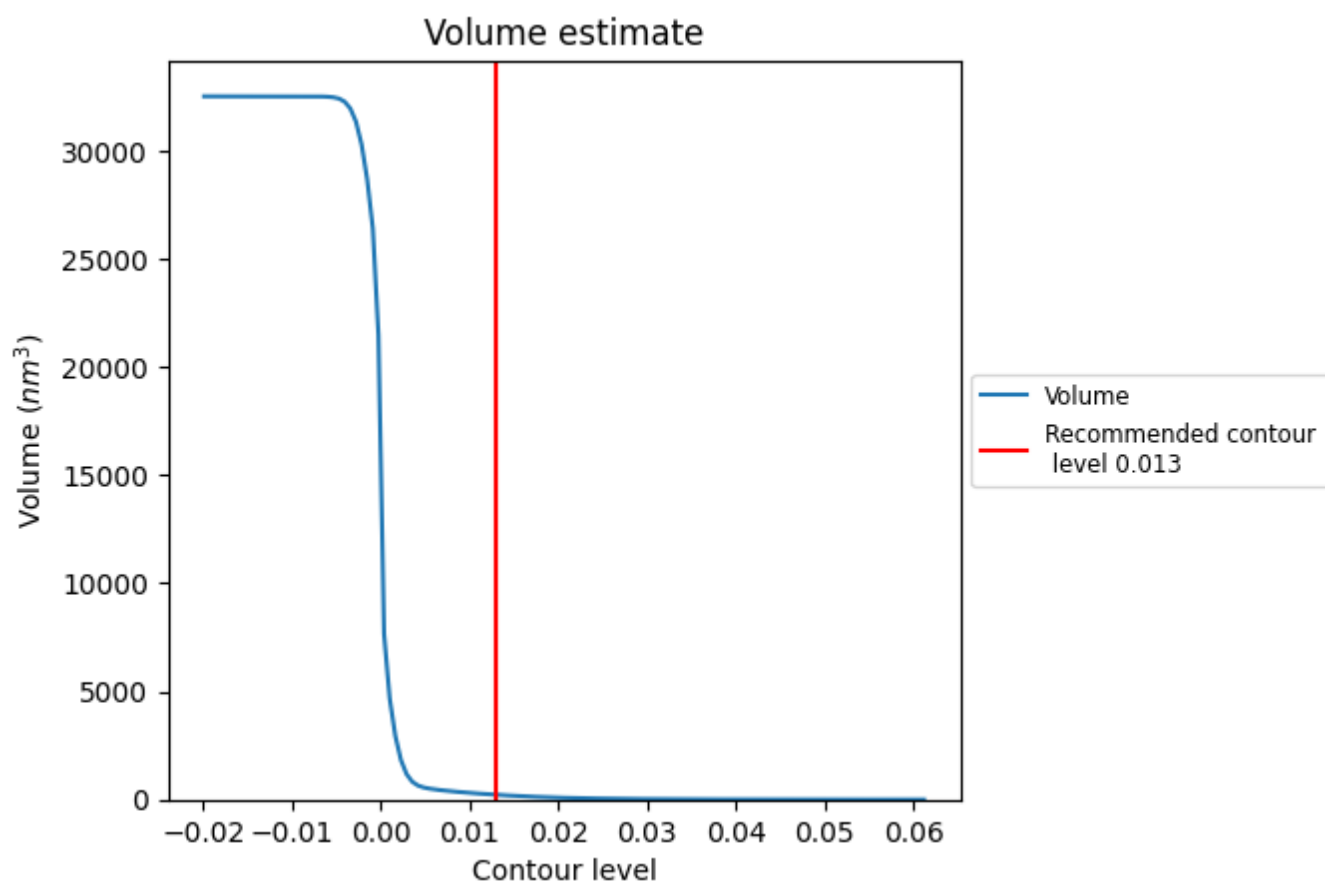
This section contains the results of statistical analysis of the map.

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.

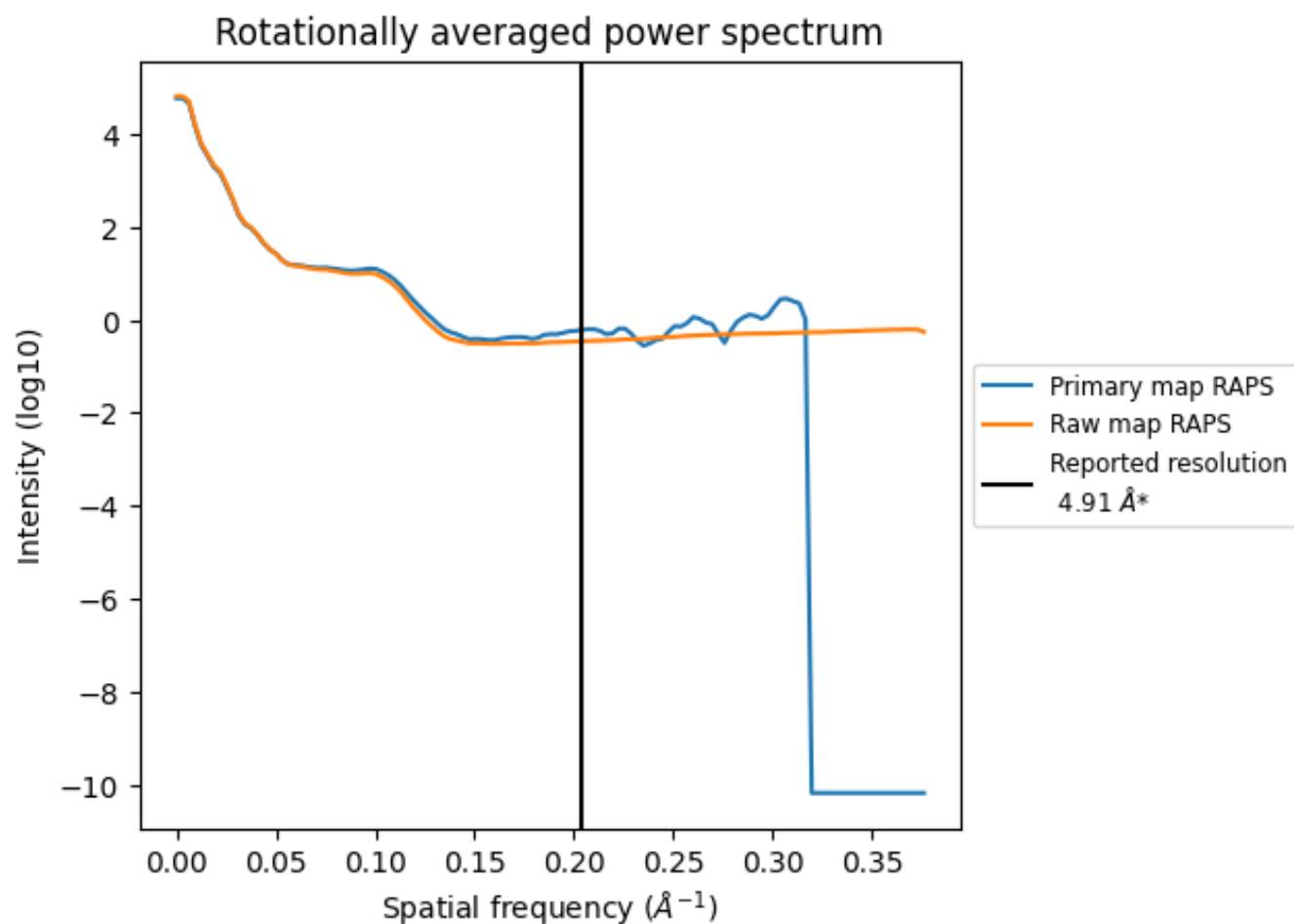
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 202 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 ⓘ

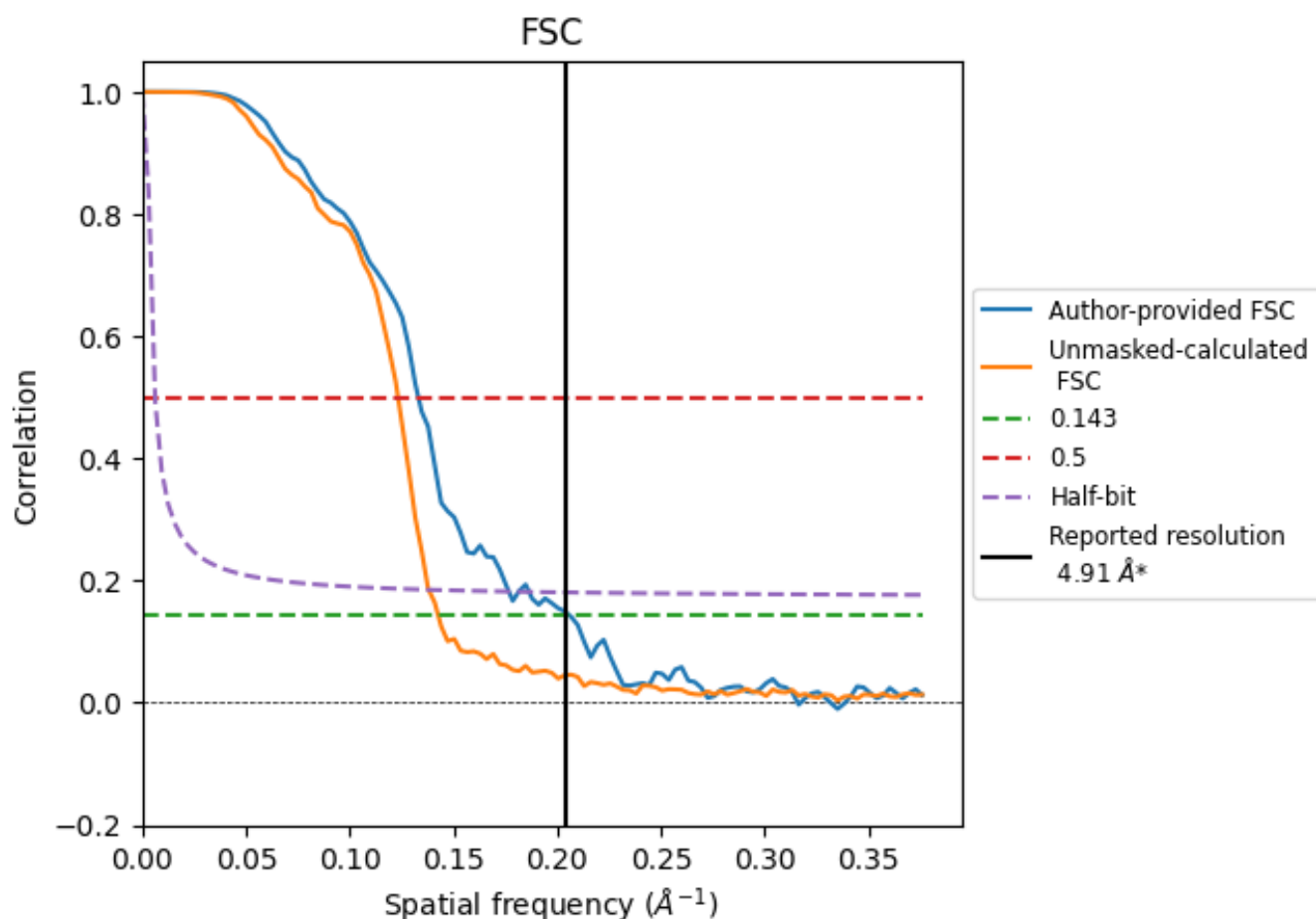


*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

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 $0.204 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

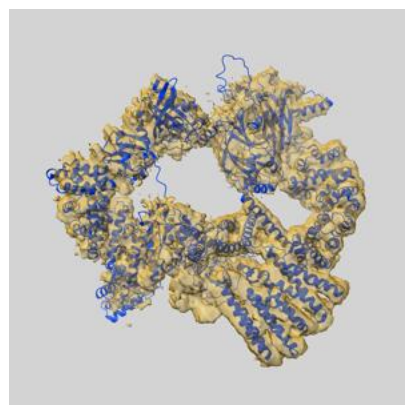
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.91	-	-
Author-provided FSC curve	4.86	7.51	5.66
Unmasked-calculated*	7.01	8.11	7.24

*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 7.01 differs from the reported value 4.91 by more than 10 %

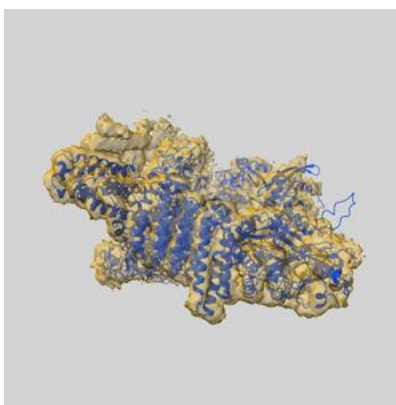
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38466 and PDB model 8XM7. Per-residue inclusion information can be found in section 3 on page 7.

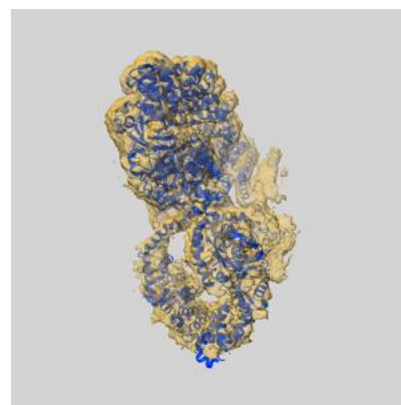
9.1 Map-model overlay [i](#)



X



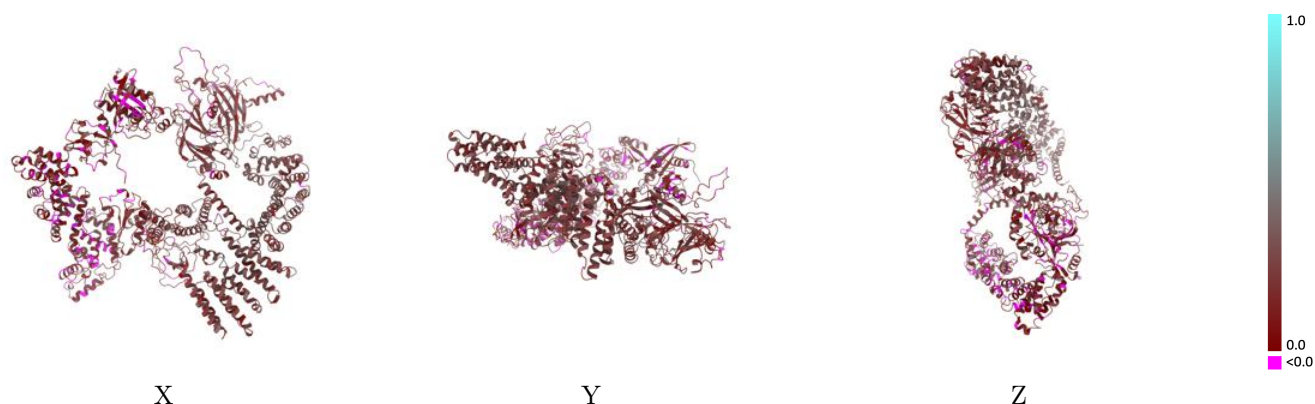
Y



Z

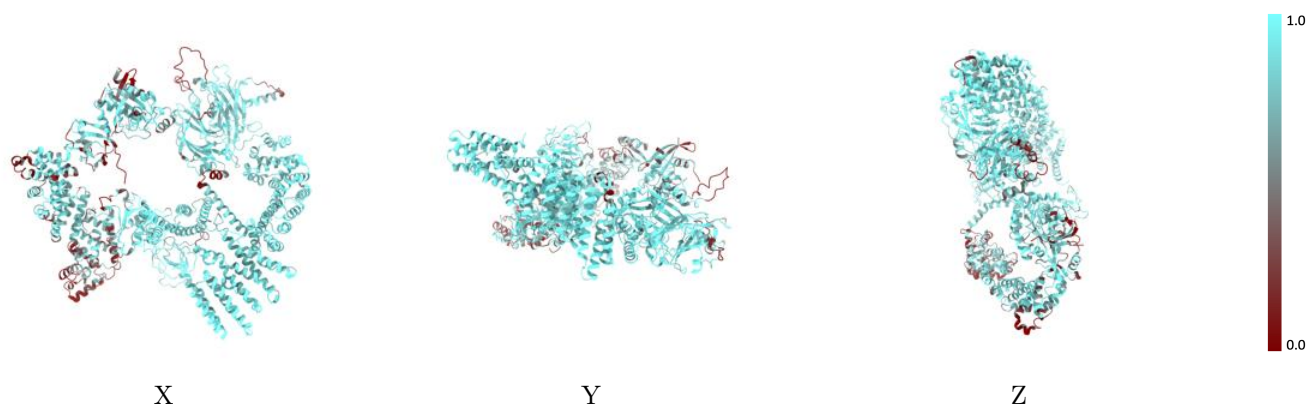
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



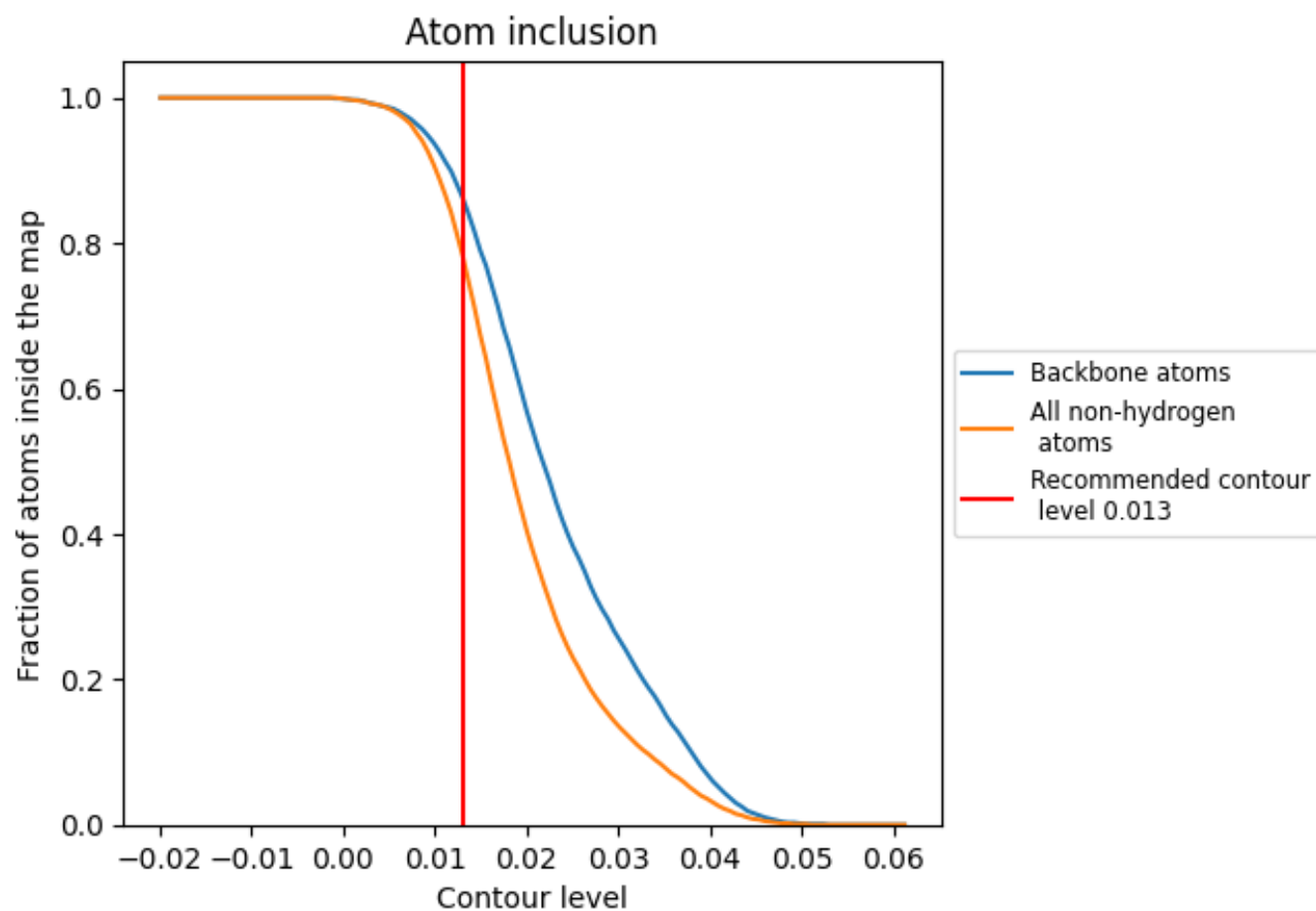
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7860	0.2030
A	0.6730	0.1600
B	0.8610	0.2350
D	0.7340	0.1670

