



wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 12:59 AM JST

PDB ID : 8ZJI
EMDB ID : EMD-60146
Title : Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 1)
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 : 4.23 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

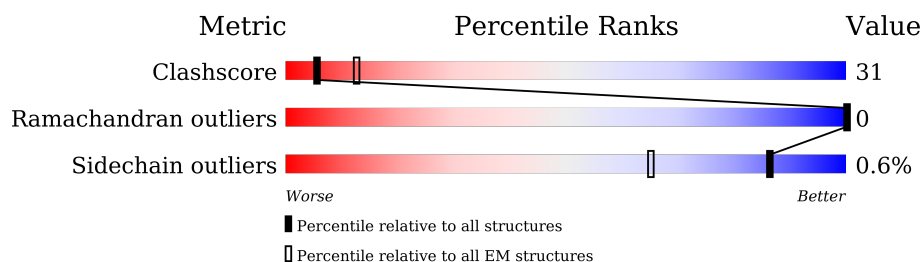
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.23 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	 13% 14% 73%
1	D	733	 12% 15% 73%
2	B	1648	 8% 43% 56%
2	E	1648	 8% 43% 56%
3	C	184	 49% 46% . .
3	F	184	 49% 46% . .

2 Entry composition

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
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
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
3	C	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
3	F	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
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

Chain D: 12% 15% 73%

Node	Node	Node	Node	Node	Node	Node	Node	Node	Node
K607	E595	L536	K539	L540	Q541	P542	E543	E544	L545
L608	L536	K539	L540	Q541	P542	E543	E544	L545	E546
P609	K539	L540	Q541	P542	E543	E544	L545	E546	L547
D612	L540	Q541	P542	E543	E544	L545	E546	L547	L548
F613	Q541	P542	E543	E544	L545	E546	L547	L548	K549
K614	P542	E543	E544	L545	E546	L547	L548	K549	Q550
L615	E543	E544	L545	E546	L547	L548	K549	Q550	Q551
E616	E544	L545	E546	L547	L548	K549	Q550	Q551	R552
K617	E545	L546	L547	L548	K549	Q550	Q551	R552	L553
L618	E546	L547	L548	K549	Q550	Q551	R552	L553	N554
E619	L547	L548	K549	Q550	Q551	R552	L553	N554	R555
K620	L548	K549	Q550	Q551	R552	L553	N554	R555	L556
L621	K549	Q550	Q551	R552	L553	N554	R555	L556	V557
E622	Q550	Q551	R552	L553	N554	R555	L556	V557	C561
K623	Q551	R552	L553	N554	R555	L556	V557	C561	F562
L624	R552	L553	N554	R555	L556	V557	C561	F562	R563
D700	R553	L554	R555	L556	V557	C561	F562	R563	Y646
E701	L554	R555	L556	V557	C561	F562	R563	Y646	D647
K702	L555	R556	L557	V558	C562	F563	R564	Y647	L665
L703	R556	L557	V558	C562	F563	R564	Y647	L665	S648
E704	L557	V558	C562	F563	R564	Y647	L665	S648	N649
K705	V558	C562	F563	R564	Y647	L665	S648	N649	R568
L706	C562	F563	R564	Y647	L665	S648	N649	R568	L569
E707	F563	R564	Y647	L665	S648	N649	R568	L569	C569
K708	R564	Y647	L665	S648	N649	R568	L569	C569	H660
L709	Y647	L665	S648	N649	R568	L569	C569	H660	E661
E710	L665	S648	N649	R568	L569	C569	H660	E661	Y662
K711	S648	N649	R568	L569	C569	H660	E661	Y662	C663
L712	N649	R568	L569	C569	H660	E661	Y662	C663	L664
E713	R568	L569	C569	H660	E661	Y662	C663	L664	Y665
K714	L569	C569	H660	E661	Y662	C663	L664	Y665	L666
L715	C569	H660	E661	Y662	C663	L664	Y665	L666	D667
E716	H660	E661	Y662	C663	L664	Y665	L666	D667	Y668
K717	E661	Y662	C663	L664	Y665	L666	D667	Y668	L669
L718	Y662	C663	L664	Y665	L666	D667	Y668	L669	M670
E719	C663	L664	Y665	L666	D667	Y668	L669	M670	L673
K720	L664	Y665	L666	D667	Y668	L669	M670	L673	K674
L721	Y665	L666	D667	Y668	L669	M670	L673	K674	G675
E722	L666	D667	Y668	L669	M670	L673	K674	G675	D676
K723	D667	Y668	L669	M670	L673	K674	G675	D676	M677
L724	Y668	L669	M670	L673	K674	G675	D676	M677	P678
E725	L669	M670	L673	K674	G675	D676	M677	P678	L681
K726	M670	L673	K674	G675	D676	M677	P678	L681	T682
L727	L673	K674	G675	D676	M677	P678	L681	T682	

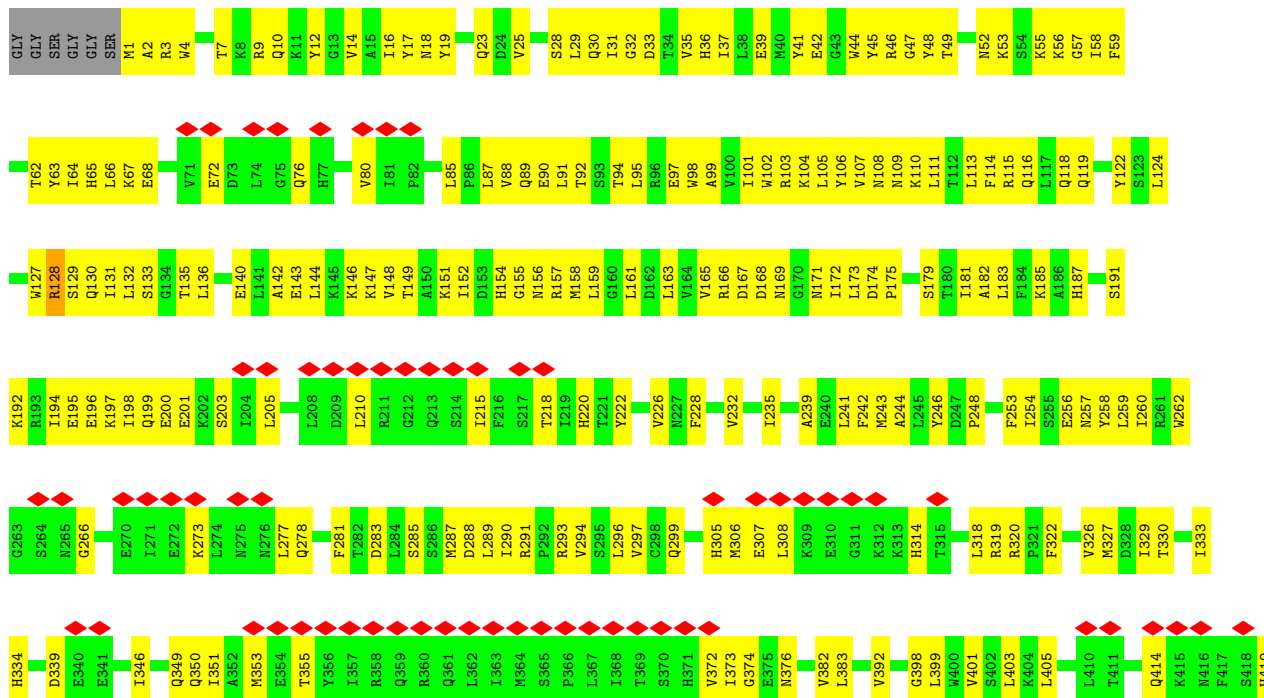
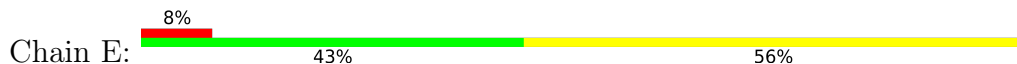
Chain B:

8% 43% 56%

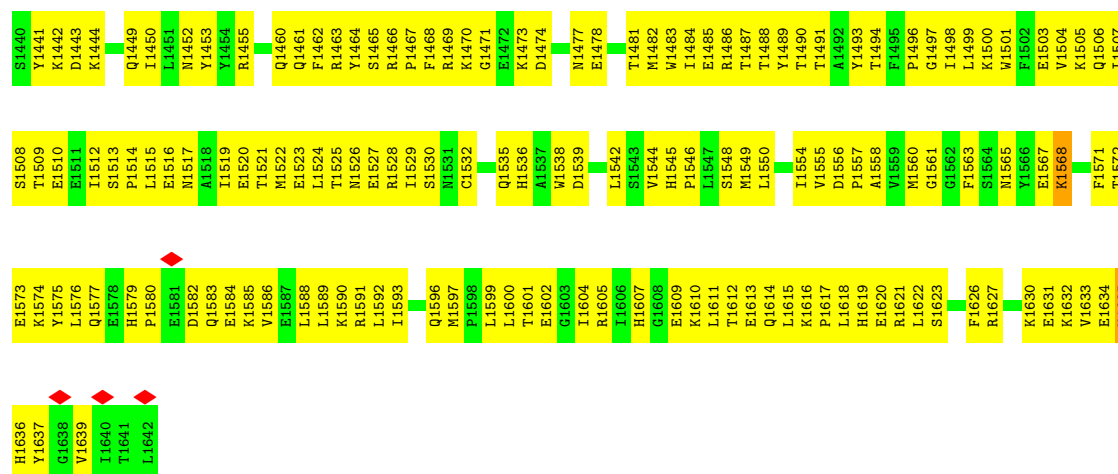
Residue	Category
GLY	Green
GLY	Green
SER	Green
GLY	Green
GLY	Green
SER	Green
M1	Yellow
A2	Yellow
R3	Yellow
W4	Yellow
T7	Yellow
K8	Green
R9	Yellow
Q10	Yellow
K11	Green
Y12	Yellow
G13	Green
V14	Yellow
A15	Yellow
I16	Yellow
Y17	Yellow
N18	Yellow
Y19	Yellow
Q23	Yellow
D24	Green
V25	Yellow
S28	Yellow
L29	Yellow
Q30	Yellow
I31	Yellow
G32	Yellow
D33	Yellow
T34	Yellow
V35	Yellow
H36	Yellow
I37	Yellow
L38	Green
E39	Yellow
M40	Yellow
Y41	Yellow
E42	Yellow
G43	Yellow
W44	Yellow
Y45	Yellow
R46	Yellow
G47	Yellow
Y48	Yellow
T49	Yellow
N52	Yellow
K53	Yellow
S54	Green
K55	Yellow
K56	Yellow
G57	Yellow
I58	Yellow
F59	Yellow
P60	Green
E61	Yellow
T62	Yellow
Y63	Yellow
I64	Yellow
H65	Yellow
L66	Yellow
K67	Yellow
E68	Yellow
V71	Green
E72	Yellow
D73	Green
L74	Yellow
G75	Yellow
Q76	Yellow
H77	Green
V80	Yellow
I81	Yellow
P82	Green
L85	Yellow
P86	Yellow
L87	Yellow
V88	Yellow
Q89	Yellow
E90	Yellow
L91	Yellow
T92	Yellow
S93	Green
T94	Yellow
L95	Yellow
R96	Green
E97	Yellow
W98	Yellow
A99	Yellow
I100	Yellow
V101	Yellow
M102	Yellow
R103	Yellow
K104	Green
L105	Yellow
G106	Yellow
Y107	Yellow
N108	Yellow
N109	Green
K110	Yellow
L111	Yellow
L112	Green
L113	Yellow
F114	Yellow
R115	Yellow
Q116	Yellow
L117	Yellow
Q118	Yellow
Q119	Yellow
L122	Yellow
T123	Yellow
L124	Yellow
W127	Yellow
S128	Green
Q130	Yellow
I131	Yellow
L132	Yellow
S133	Yellow
G134	Green
T135	Yellow
L136	Yellow
E140	Yellow
L141	Yellow
A142	Yellow
E143	Yellow
L144	Yellow
K145	Yellow
K146	Yellow
K147	Yellow
V148	Yellow
T149	Yellow
A150	Yellow
K151	Yellow
L152	Yellow
D153	Yellow
H154	Yellow
G155	Yellow
N156	Yellow
L157	Yellow
M158	Yellow
L159	Yellow
G160	Yellow
L161	Yellow
D162	Green
L163	Yellow
V164	Yellow
V165	Yellow
R166	Yellow
D167	Yellow
D168	Green
N171	Yellow
L172	Yellow
L173	Yellow
D174	Yellow
P175	Yellow
S179	Yellow
T180	Yellow
L181	Yellow
A182	Yellow
L183	Yellow
F184	Yellow
K185	Yellow
A186	Yellow
L187	Yellow
S191	Yellow



- Molecule 2: Dedicator of cytokinesis protein 5

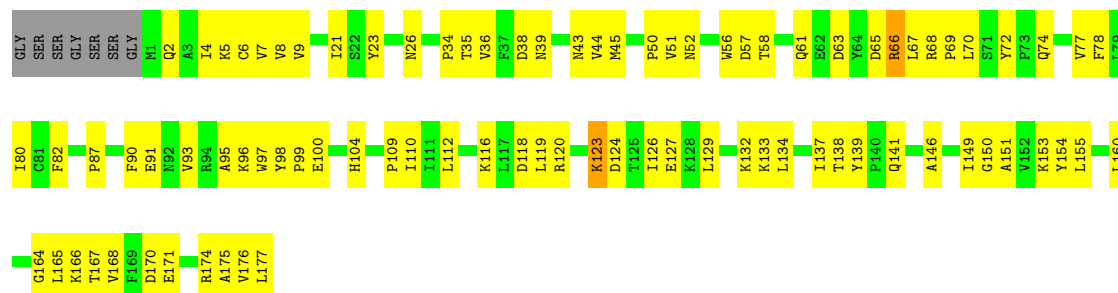


Y1362	Q1294	R1220	E1148	R1080	Y1002	R935	N858	F787	E717	G639	L562	G487	L420
Y1368	E1295	M1221	M1149	K1081	M1009	I936	C859	N788	T718	L640	L569	A488	V421
G1369	E1298	S1222	E1150	E1082	R1015	R937	M860	N789	Y719	N641	L569	G489	D422
Q1370	L1299	C1223	L1154	R1086	R1019	R938	T861	S790	T720	M642	Y572	Y490	R423
F1372	L1300	T1224	L1155	R1086	R1019	T939	I863	T791	K722	W643	T425	E495	S424
P1373	Y1301	V1227	D1156	D1089	R1019	V940	I862	R792	K722	R644	T426	Y496	T425
	Q1302		Q1157	M1090	G942	I941	E865	Q793	H723	S645	A126		A126
	E1303	Y1231	E1158	M1091	G942	G942	S866	L794	F724	N646	I427	V500	I427
	L1304	E1232	E1159	L1094	N944	N944	T867	L796	A726	S647	A428	Q503	A428
	I1305	E1233	V1160	L1094	R945	R945	Q1023	A726	T727	Q648	R429	Q503	R429
	S1306	K1234	E1160	L1094	Q946	Q946	F1024	F798	T727	N649	K430	Y510	K430
	Y1307	K1235	R1163	P1096	S947	S947	A1025	N799	A729	I650	M431	E511	M431
		R1236	G1164	H1097	I950	I950	E872	M800	Y730	K651	G432		G432
		E1237	D1165	K1098	I950	I950	S873	M802	V731	H579		K514	I436
	K1310	D1238	E1166	I1099	F953	F953	E873	L801	K732	D581		V515	I437
	G1311	E1239	E1166	G1107	R1035	R1035	C874	R804	V736	A582		S516	I437
	M1312	Y1240	Q1167	F1101	F1031	F1031	R875	R804	L737	K583		I517	L438
	E1313	I1241	Y1168	F1101	F1032	F1032	E876	P805	N738	F584		A518	F439
	E1315	R1242	K1169	I1102	M1033	M1033	E877	P805	F739	L586		I519	G440
	E1389	Y1243	L1172	M1105	D1034	D1034	L878	E808	N738	L657		E520	D441
	R1390	L1244	L1176	G1106	Q1035	Q1035	L879	A809	F739	H588		E521	V442
	R1391	Y1244	L1177	G1107	A1036	A1036	P880	V810	Y740	V660		E522	R443
	E1392	Y1245	E1178	I1109	S1037	S1037	L881	K812	A742	E664		T523	R444
	D1393	R1248	H1179	L1110	F1038	F1038	L882	K813	N743	K667		R524	M444
	F1394	D1249	C1180	E1111	E1039	E1039	L883	K813	A744	F668		C525	D445
	S1395	L1250	G1181	V1112	Q963	Q963	D884	A816	D745	Q670		R526	D446
	L1400	H1251	K1182	L1113	D965	D965	L890	Y819	S747	Q670		H527	L450
	Q1401	N1256	L1183	L1114	S967	S967	L890	L820	K749	L673		R528	I451
	N1404	E1259	Y1185	P1115	H968	H968	K896	P821	L753	L676		F529	F455
	A1405	A1260	L1186	E1117	Y969	Y969	L899	S922	L753	F677		F531	D456
	E1406	Y1262	S1187	V1118	S970	S970	H899	I823	L757	N600		R532	K457
	K1407	T1263	S1188	E1119	H871	H871	N825	N825	L757	L600		H533	G458
	M1408	L1264	S1189	L1120	Y972	Y972	L905	D826	A758	Q601		R534	K459
		L1264	V1192	K1122	I973	I973	L909	D827	L760	A602		S535	K460
		A1268	F1193	A1123	S974	S974	L910	K828	K761	S603		S536	K461
		L1271	L1196	I1125	T975	T975	E911	L829	L766	K604		Q537	T462
		Q1272	V1197	P1126	F976	F976	V912	V830	F766	N605		E538	R463
		W1273	S1198	I1127	T978	T978	R915	F831	I767	L606		T539	R464
		S1274	S1199	F1128	Q980	Q980	V918	P833	I768	V607		R540	M465
		D1275	L1200	F1129	D981	D981	T921	V834	Q769	F694		D541	V466
		K1276	M1130	S1065	E1062	E1062	V921	L839	S770	D695		K542	V468
		P1277	M1131	Q1066	F1064	F1064	A922	L839	V772	T610		S543	T469
		G1278	M1132	Q1067	Q1066	Q1066	V923	K842	L773	S611		E544	V472
		L1279	Q1133	K1068	R1069	R1069	H924	F843	Y774	S612		R545	H473
		P1280	C1134	R1069	R1069	R1069	I925	I844	L775	K613		A546	D474
		H1281	E1135	T989	R1069	R1069	Q926	Q845	L776	D614		F547	E475
		L1282	F1136	P990	K1071	K1071	L927	S946	I704	T700		G548	E476
		L1283	L1208	I991	I1072	I1072	I928	S946	I704	I701		V549	G477
		Q1284	S1139	M992	V1073	V1073	M929	L852	S781	F709		V552	L479
		R1285	K1074	F993	K1074	K1074	F930	V853	K782	Q627		N556	L480
		D1286	K1075	K994	K1075	K1075	R831	R854	D783	S628		P557	E481
		Y1291	Y1076	D985	R831	R831	L932	Q855	G784	T629		G559	A483
		T1292	G1077	L996	L932	L932	L933	Q856	G785	K630		T560	I484
		Q1293	M1079	I997	I997	I997	R934	L857	E786	L716		T561	H485
													P486



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

Chain C: 49% 46%



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

Chain F: 49% 46%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	133323	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	0.065	Depositor
Minimum map value	-0.020	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	0.50	0/2218
1	D	0.29	0/1641	0.50	0/2218
2	B	0.32	0/13722	0.50	0/18514
2	E	0.32	0/13722	0.50	0/18514
3	C	0.32	0/1415	0.50	0/1924
3	F	0.32	0/1415	0.50	0/1924
All	All	0.32	0/33556	0.50	0/45312

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	GLN	Peptide
1	D	541	GLN	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	1608	0	1617	101	0
1	D	1608	0	1617	107	0
2	B	13436	0	13516	857	0
2	E	13436	0	13516	860	0
3	C	1385	0	1407	80	0
3	F	1385	0	1407	87	0
All	All	32858	0	33080	2032	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 31.

The worst 5 of 2032 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:1346:ALA:HB2	2:E:1342:LEU:HD11	1.27	1.09
1:A:536:LEU:HD21	2:B:17:TYR:HB2	1.40	1.03
1:A:697:ARG:HB3	2:B:31:ILE:HB	1.53	0.89
3:F:93:VAL:HA	3:F:97:TRP:HB2	1.59	0.85
2:E:144:LEU:HD13	2:E:147:LYS:HE2	1.60	0.83

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%)	180 (92%)	16 (8%)	0	100	100
1	D	196/733 (27%)	180 (92%)	16 (8%)	0	100	100
2	B	1640/1648 (100%)	1539 (94%)	101 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	1640/1648 (100%)	1540 (94%)	100 (6%)	0	100	100
3	C	175/184 (95%)	163 (93%)	12 (7%)	0	100	100
3	F	175/184 (95%)	163 (93%)	12 (7%)	0	100	100
All	All	4022/5130 (78%)	3765 (94%)	257 (6%)	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	183/664 (28%)	182 (100%)	1 (0%)	88	93
1	D	183/664 (28%)	181 (99%)	2 (1%)	73	85
2	B	1495/1497 (100%)	1488 (100%)	7 (0%)	88	93
2	E	1495/1497 (100%)	1488 (100%)	7 (0%)	88	93
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%)	3641 (99%)	21 (1%)	86	92

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	651	LYS
2	E	1568	LYS
3	F	123	LYS
2	E	1635	LYS
2	E	1069	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1596	GLN
2	E	1517	ASN
2	E	119	GLN
2	E	1596	GLN
2	E	971	HIS

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.

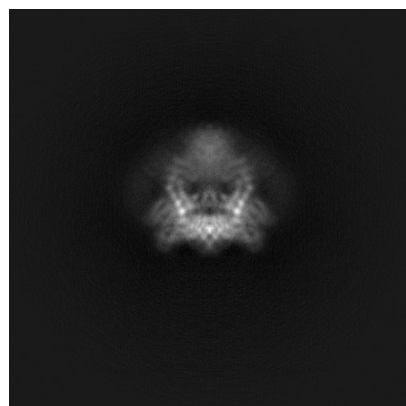
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60146. These allow visual inspection of the internal detail of the map and identification of artifacts.

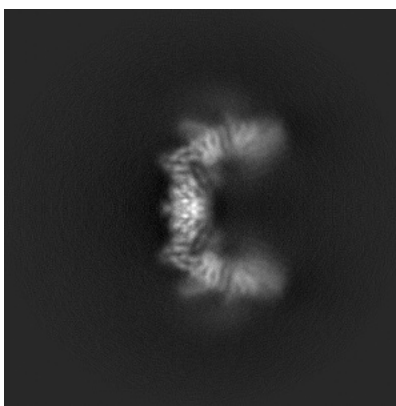
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

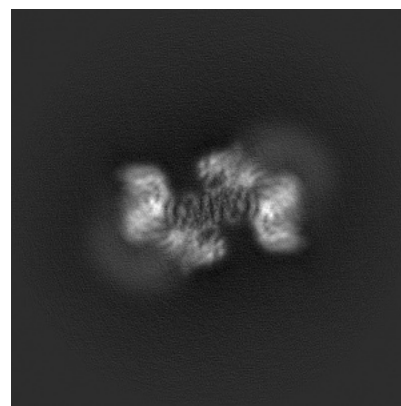
6.1.1 Primary map



X

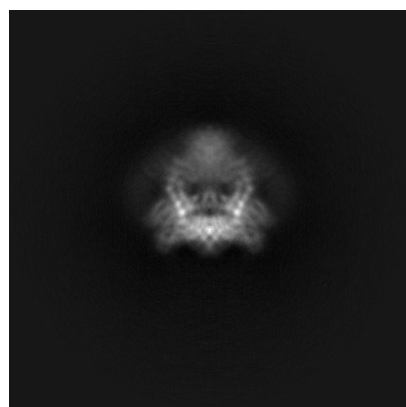


Y

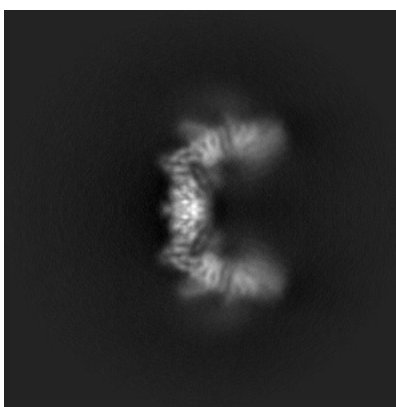


Z

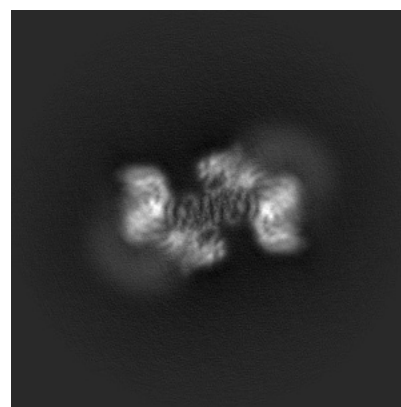
6.1.2 Raw map



X



Y

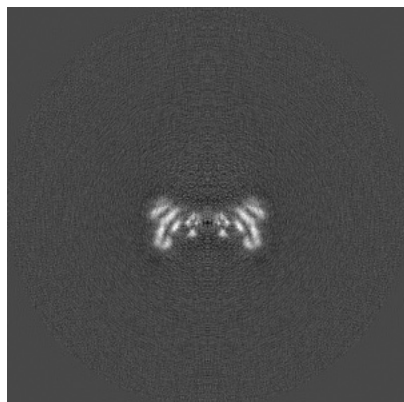


Z

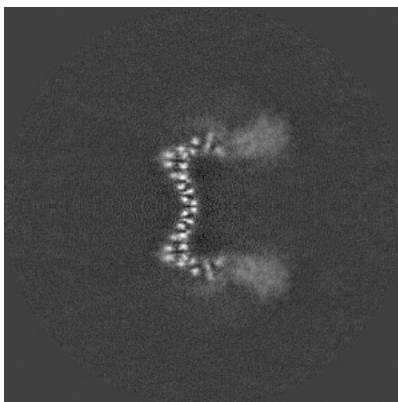
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

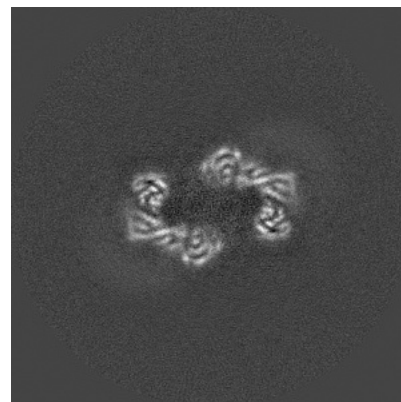
6.2.1 Primary map



X Index: 170

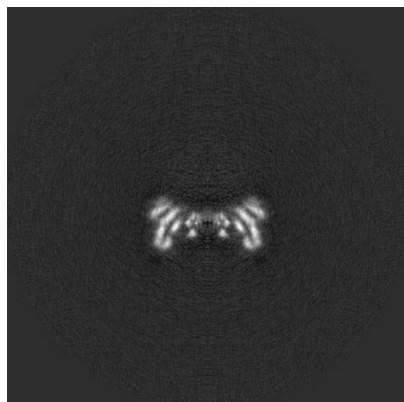


Y Index: 170

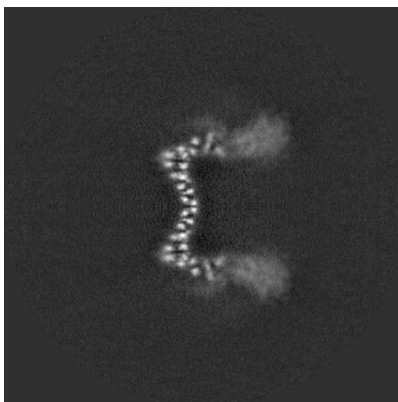


Z Index: 170

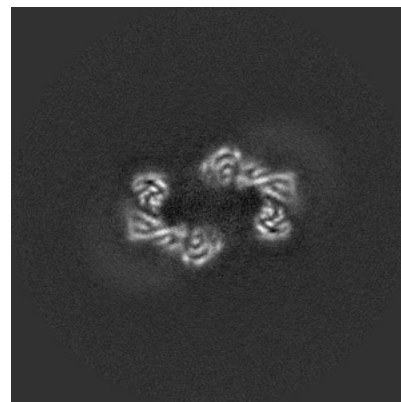
6.2.2 Raw map



X Index: 170



Y Index: 170

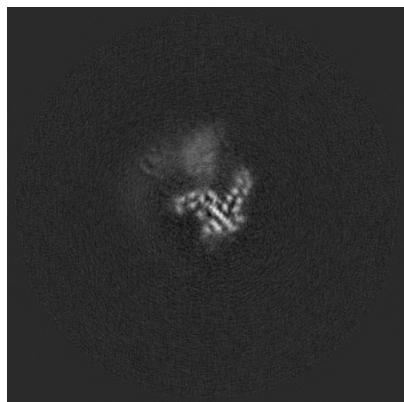


Z Index: 170

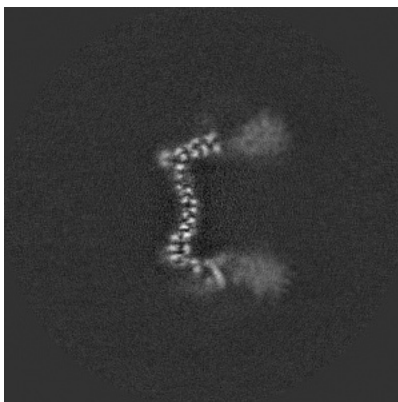
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

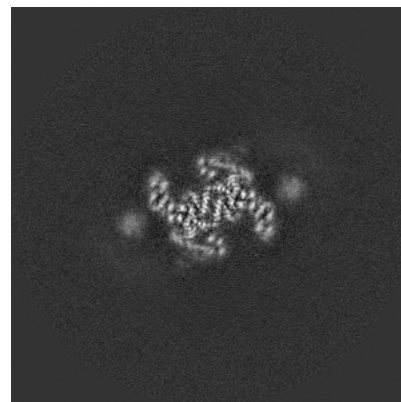
6.3.1 Primary map



X Index: 120

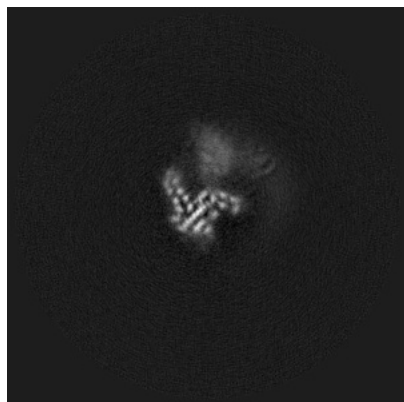


Y Index: 167

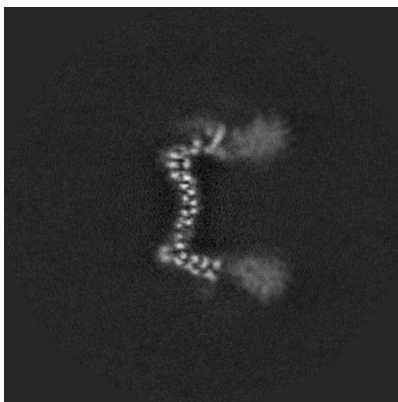


Z Index: 153

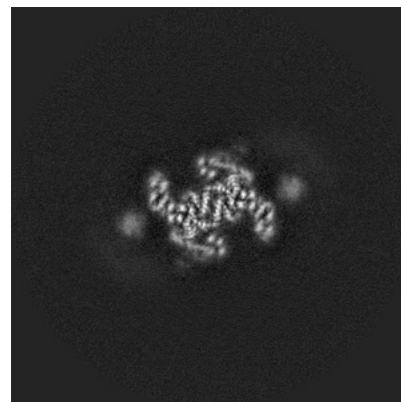
6.3.2 Raw map



X Index: 220



Y Index: 173

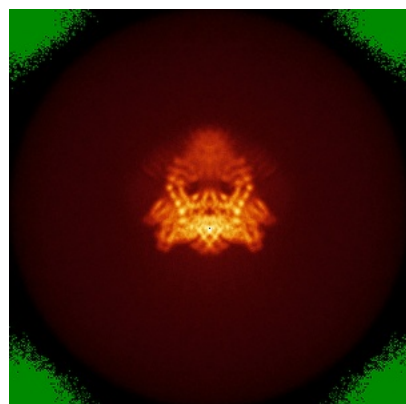


Z Index: 153

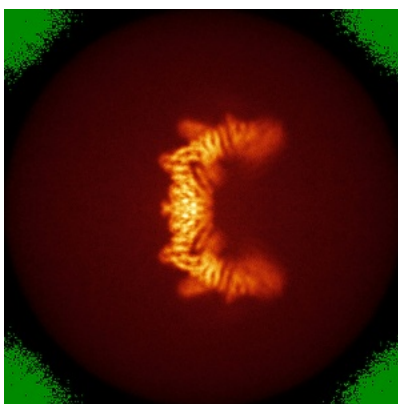
The images above show the largest variance slices of the map in three orthogonal directions.

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

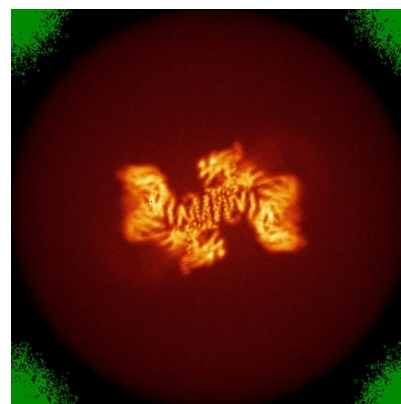
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

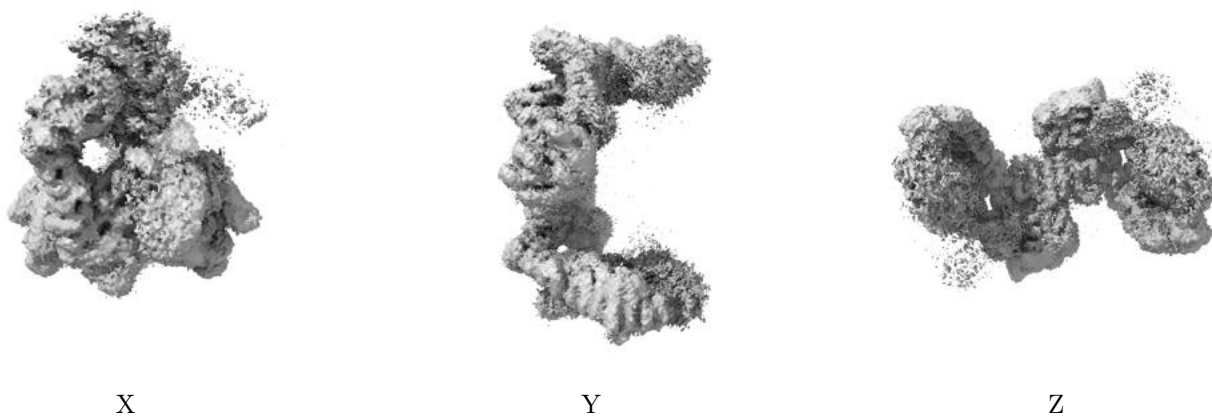


Z

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.

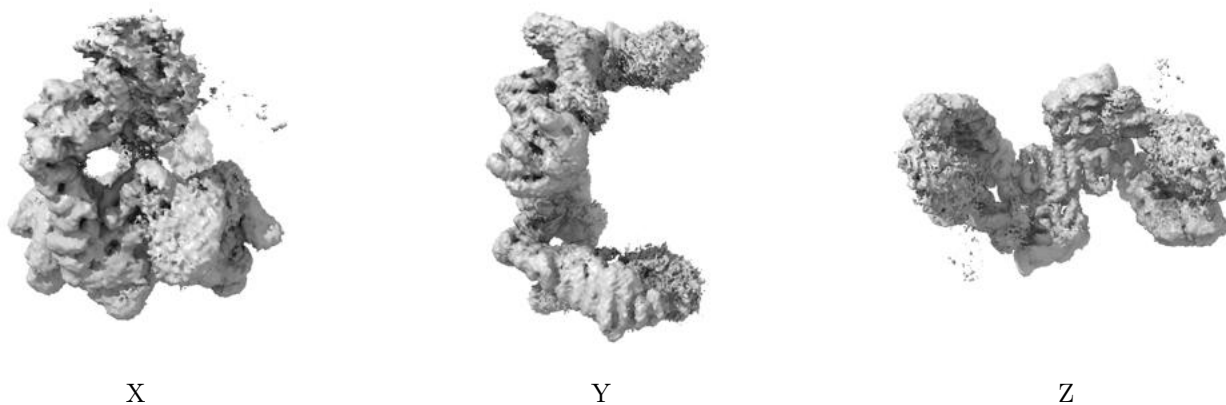
6.5 Orthogonal surface views [i](#)

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.

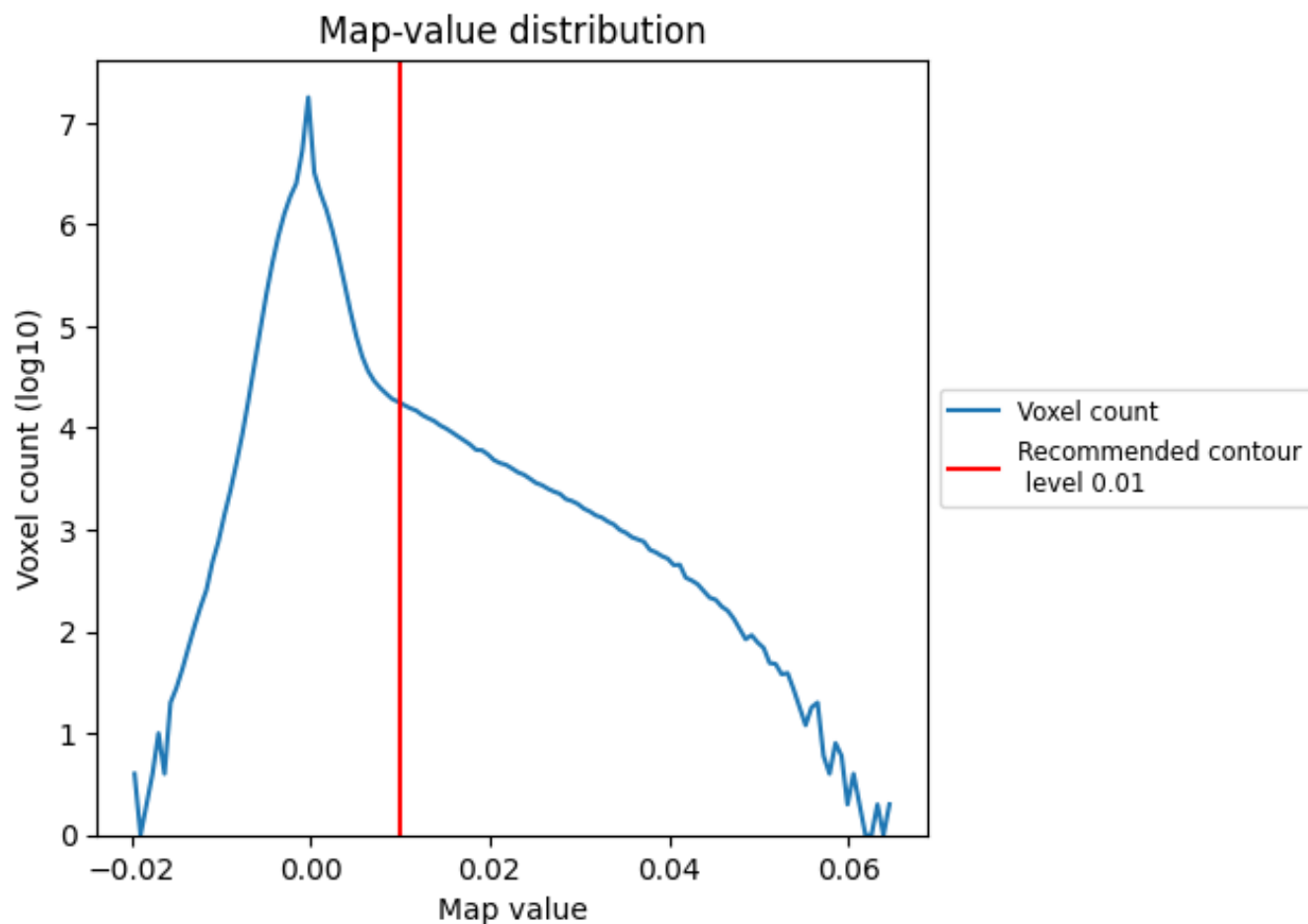
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

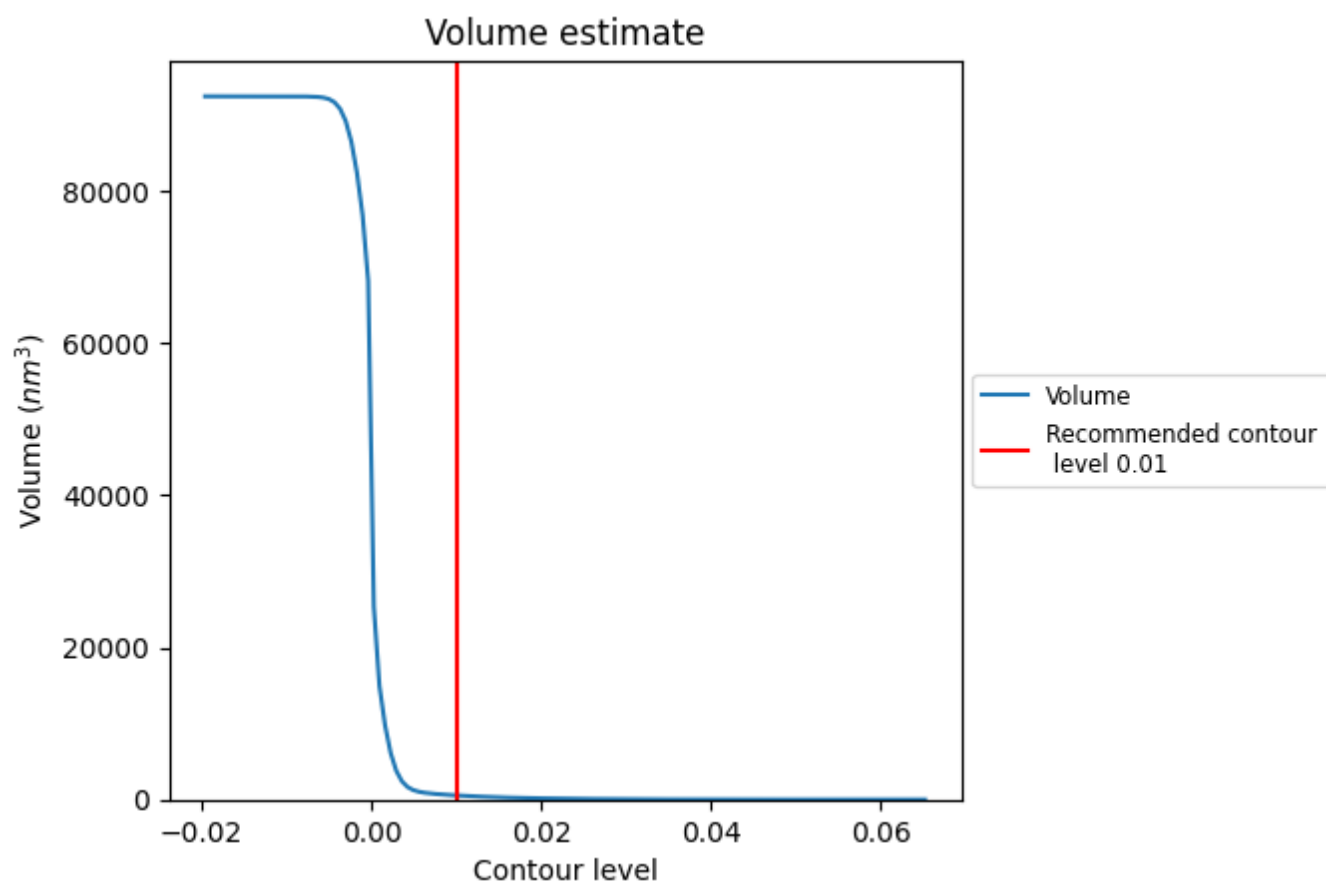
This section contains the results of statistical analysis of the map.

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.

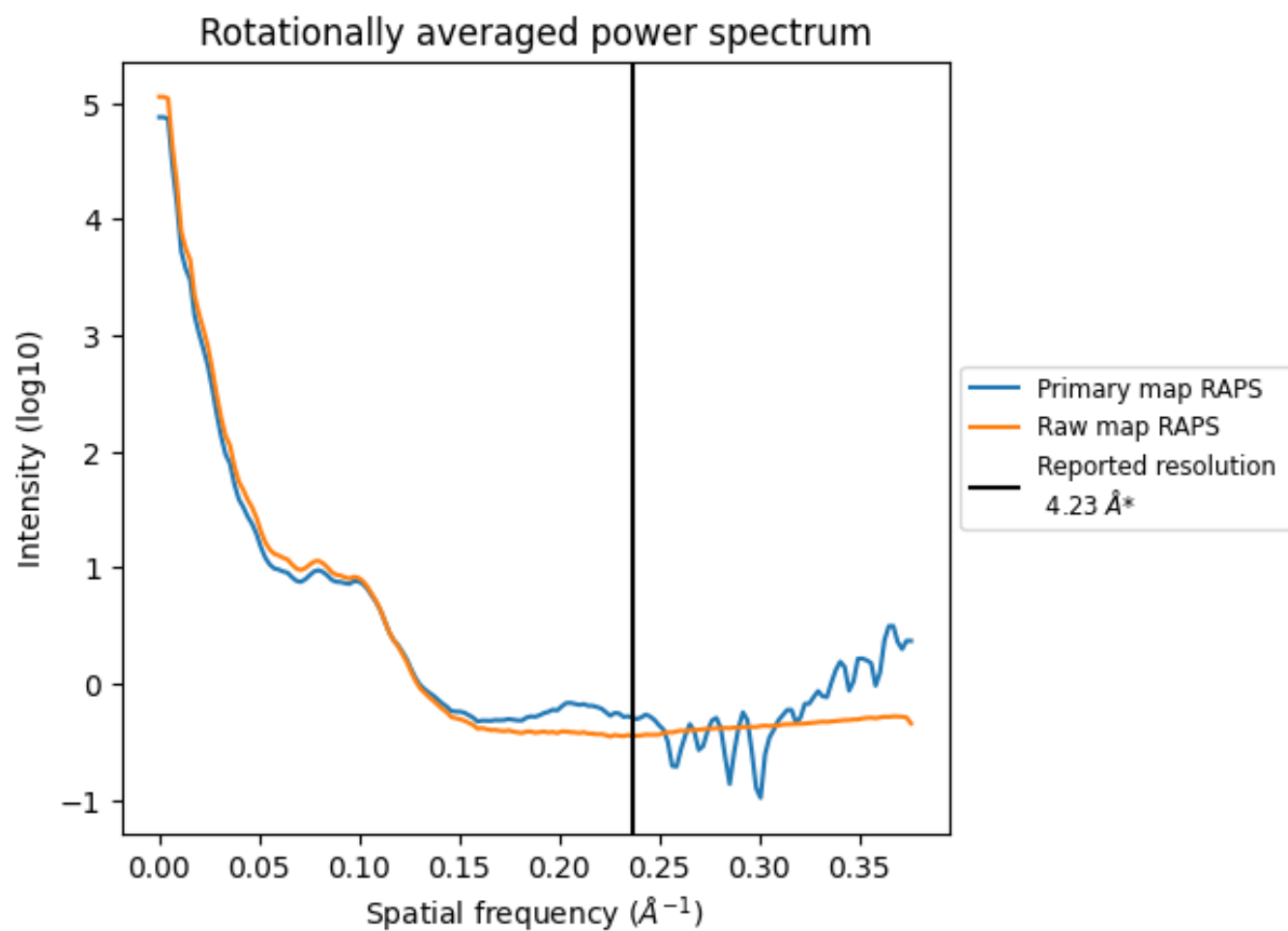
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 546 nm³; this corresponds to an approximate mass of 494 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 ⓘ

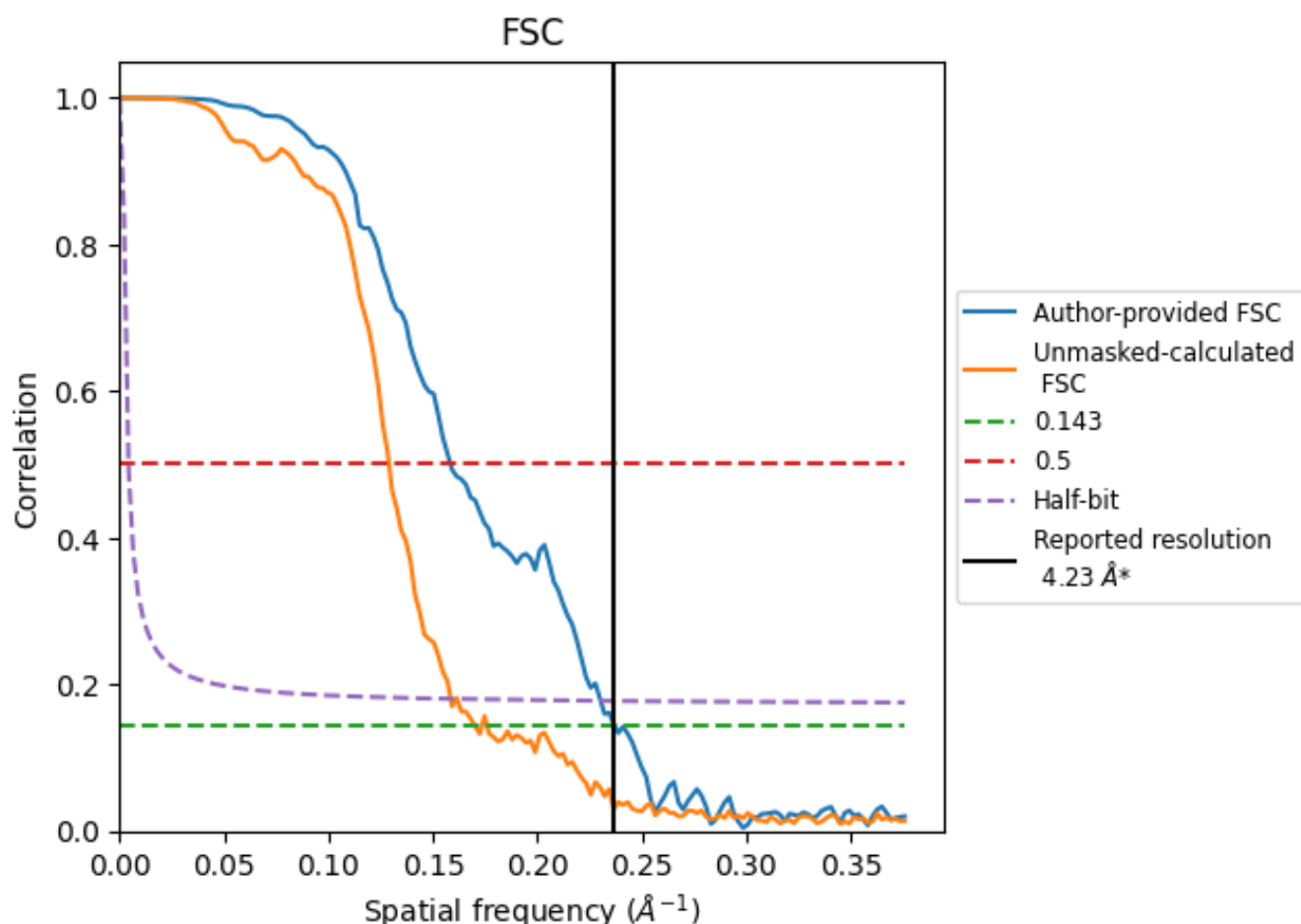


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

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 0.236 Å⁻¹

8.2 Resolution estimates [i](#)

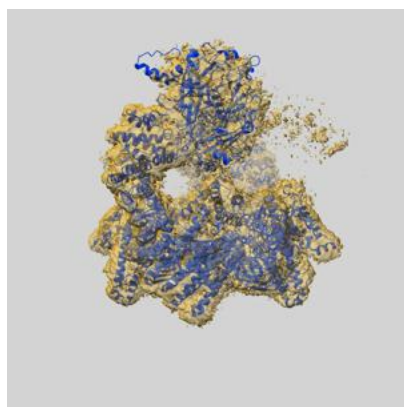
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.22	6.31	4.34
Unmasked-calculated*	5.88	7.75	6.31

*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 5.88 differs from the reported value 4.23 by more than 10 %

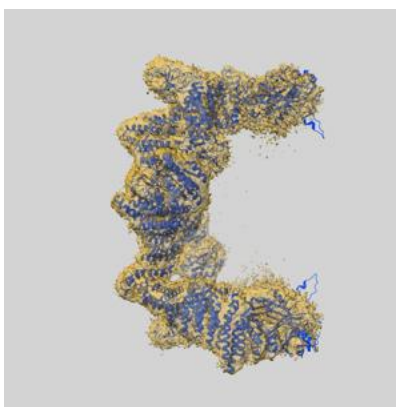
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60146 and PDB model 8ZJI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

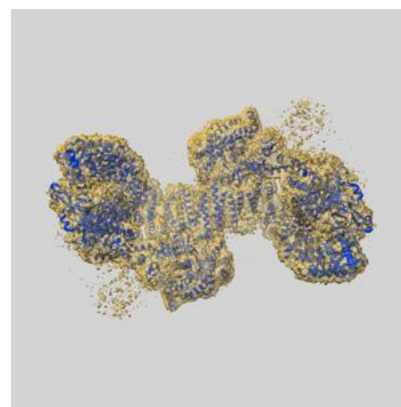
9.1 Map-model overlay [i](#)



X



Y



Z

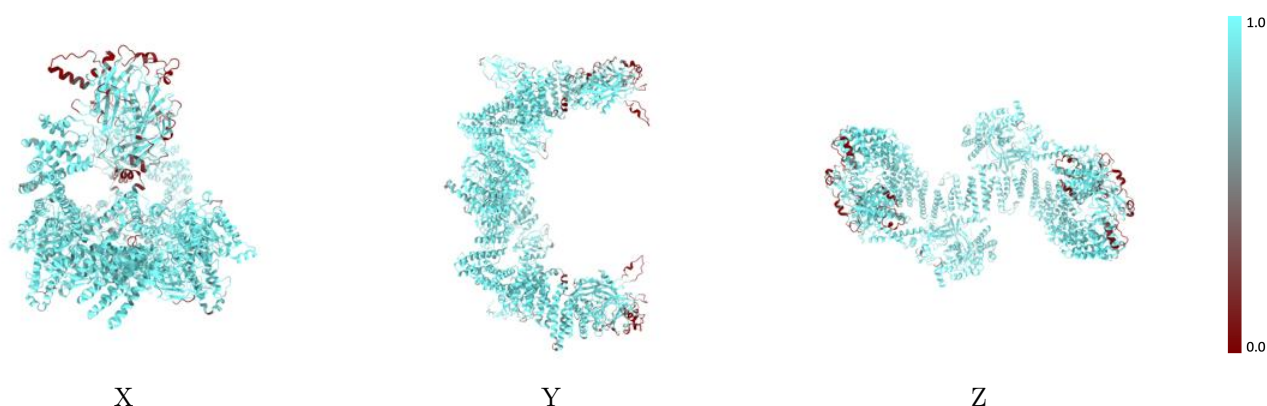
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



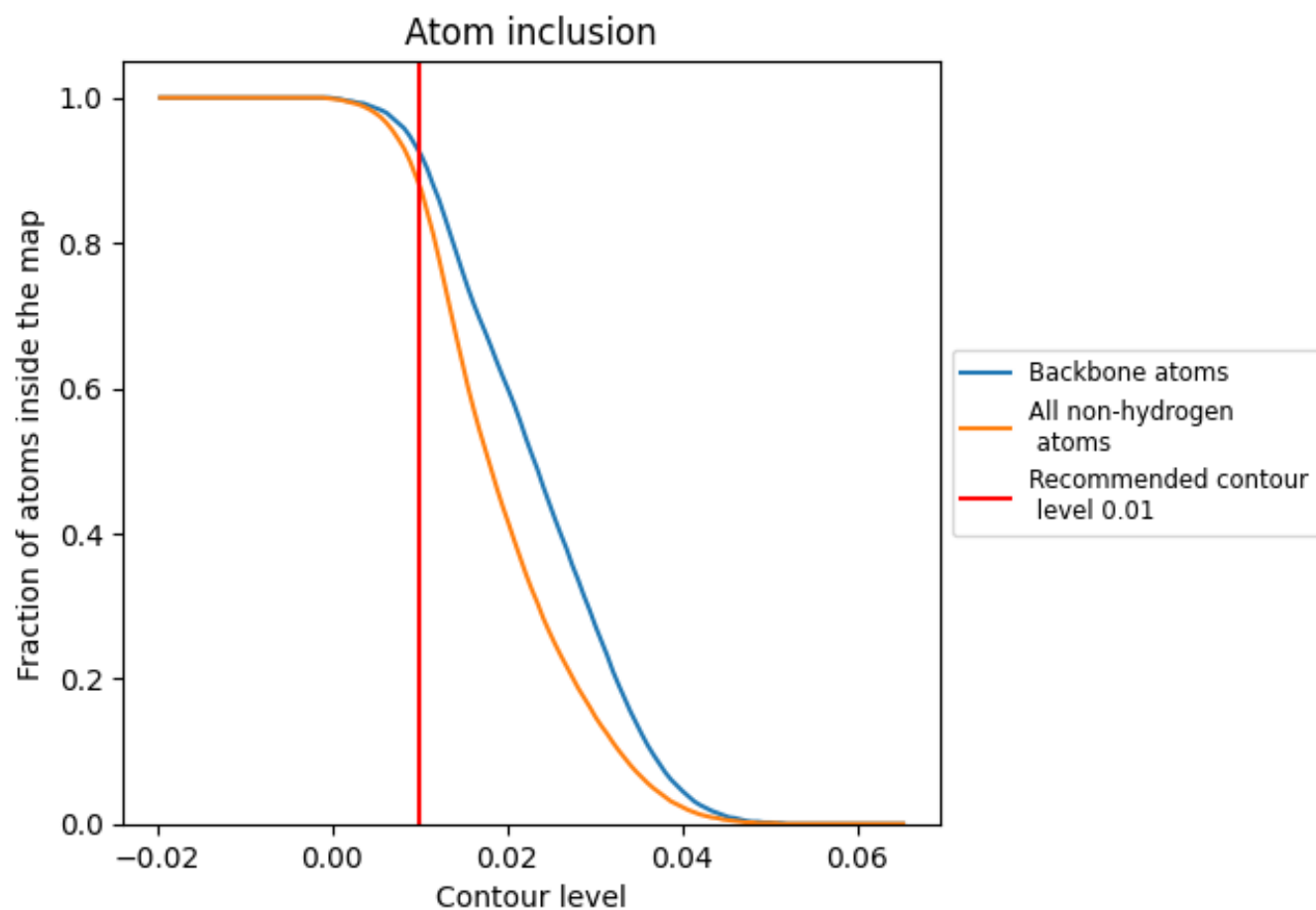
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 92% of all backbone atoms, 88% 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></div>0.8790</div>	<div><div></div>0.1920</div>
A	<div><div></div>0.9060</div>	<div><div></div>0.1590</div>
B	<div><div></div>0.8680</div>	<div><div></div>0.1910</div>
C	<div><div></div>0.9700</div>	<div><div></div>0.2480</div>
D	<div><div></div>0.9130</div>	<div><div></div>0.1580</div>
E	<div><div></div>0.8650</div>	<div><div></div>0.1900</div>
F	<div><div></div>0.9720</div>	<div><div></div>0.2490</div>

1.0

0.0

<0.0