



wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 07:37 PM EST

PDB ID : 8ZJK
EMDB ID : EMD-60148
Title : Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 3)
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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

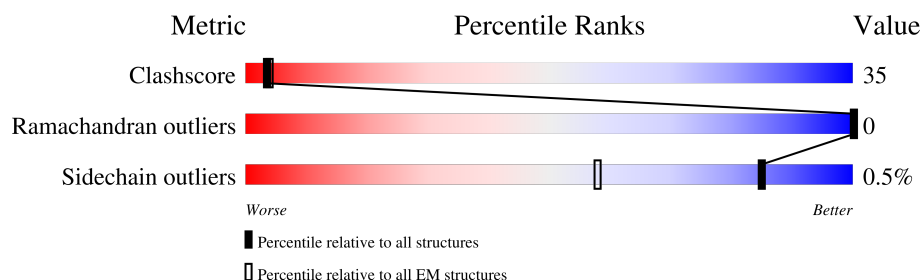
1 Overall quality at a glance

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	733	 11% 16% 73%
1	D	733	 11% 16% 73%
2	B	1648	 7% 41% 52%
2	E	1648	 6% 40% 54%
3	C	184	 34% 62% ..
3	F	184	 32% 64% ..

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

Continued on next page...

Continued from previous page...

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		

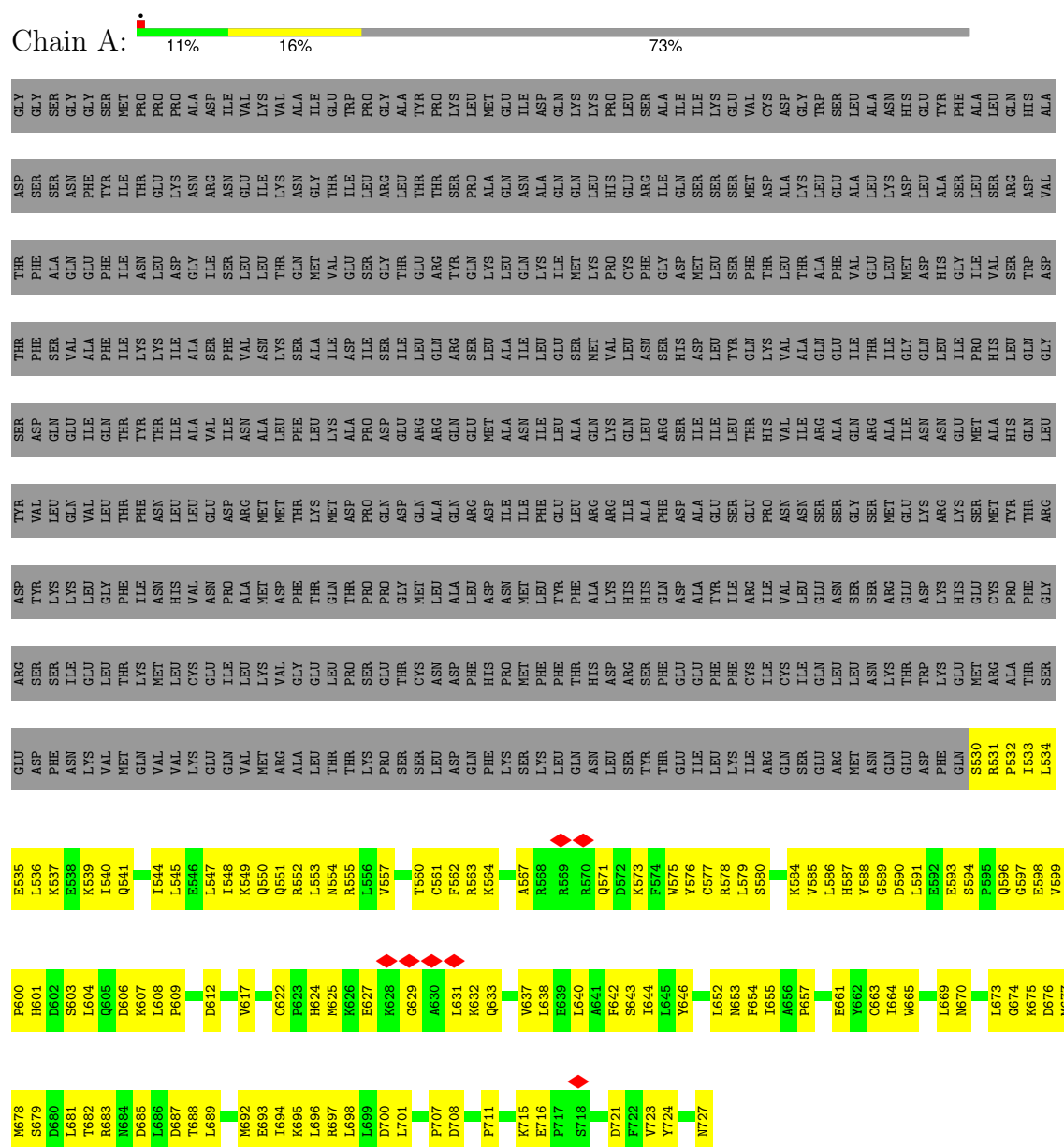
There are 16 discrepancies between the modelled and reference sequences:

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

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



Chain D:

11%

16%

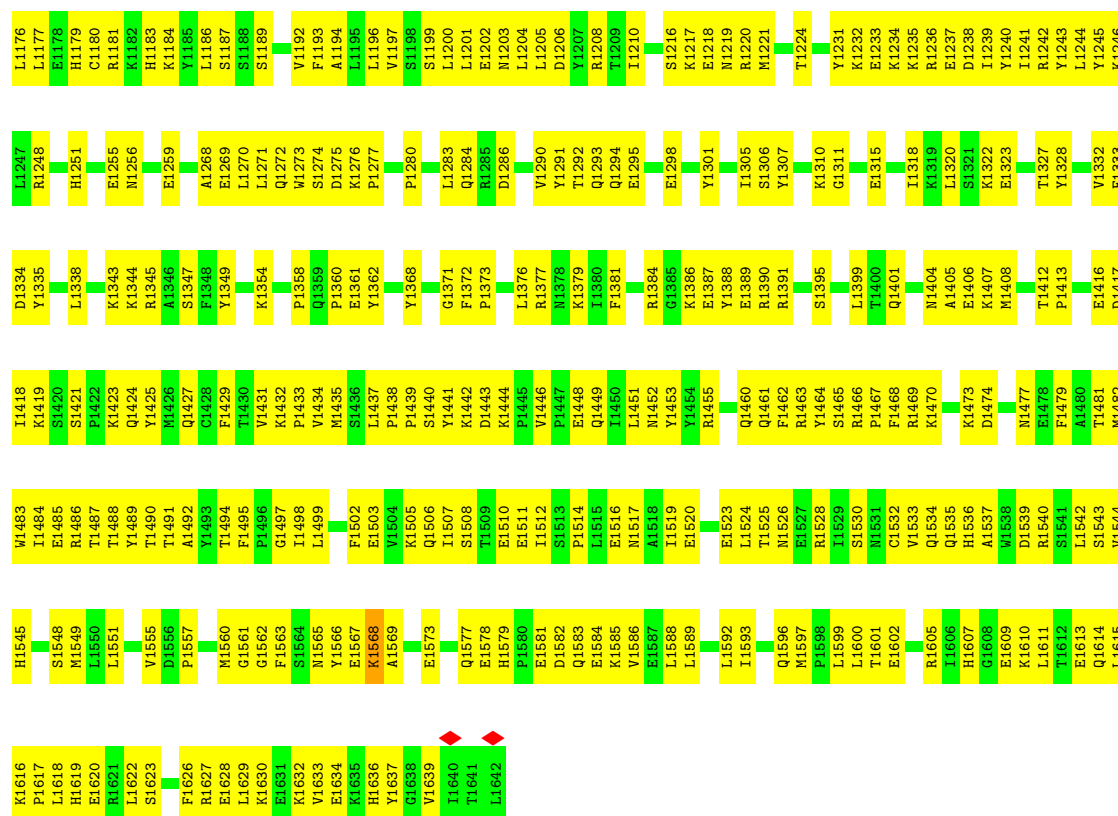
73%

Chain B:

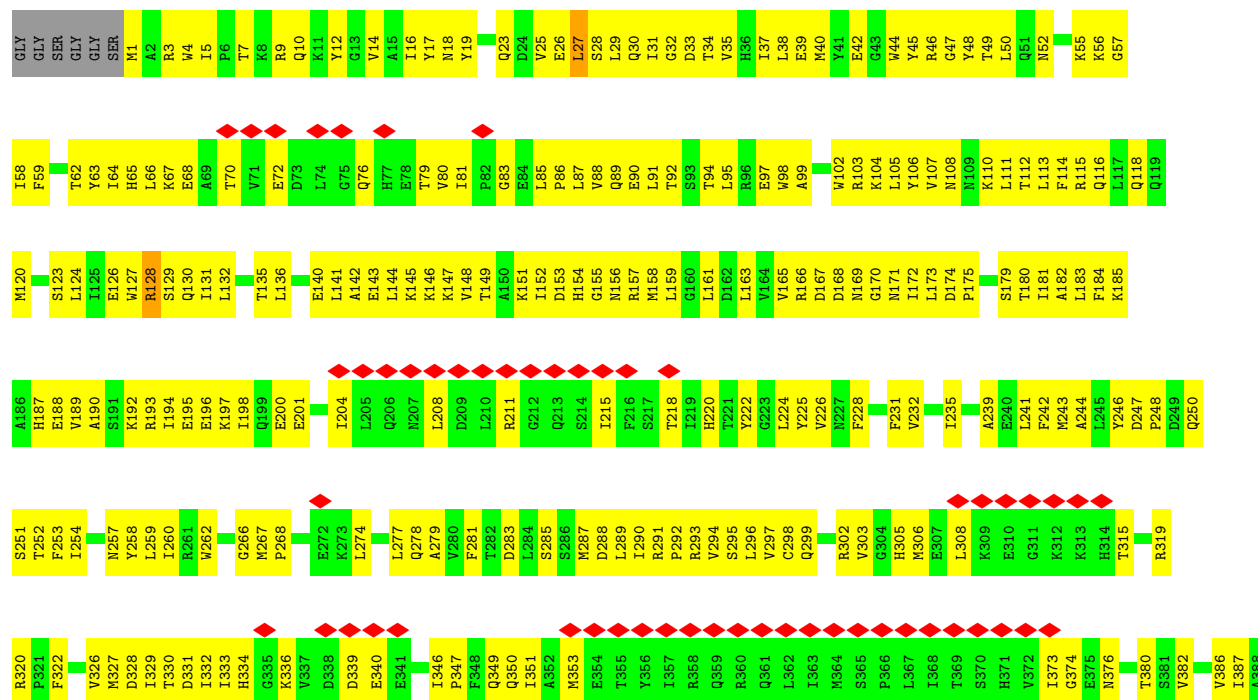
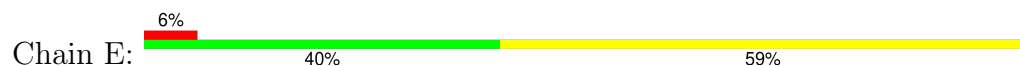
Residue	Category
GLY	Yellow
GLY	Yellow
SER	Yellow
GLY	Yellow
GLY	Yellow
SER	Yellow
M1	Green
A2	Yellow
R3	Yellow
K67	Yellow
W4	Yellow
I5	Yellow
P6	Yellow
T7	Yellow
K8	Green
R9	Yellow
K10	Yellow
Q11	Yellow
Y12	Yellow
G13	Yellow
V14	Yellow
A15	Green
I16	Yellow
Y17	Yellow
N18	Yellow
I19	Yellow
Q23	Yellow
D24	Green
L85	Yellow
V25	Yellow
E26	Yellow
L27	Orange
S28	Orange
L29	Yellow
Q30	Yellow
I31	Yellow
G32	Yellow
D33	Yellow
T34	Yellow
V35	Yellow
H36	Green
E97	Yellow
I37	Yellow
L38	Yellow
E39	Yellow
M40	Yellow
E41	Green
E42	Yellow
G43	Green
W44	Yellow
Y45	Yellow
R46	Yellow
G47	Yellow
Y48	Yellow
T49	Yellow
L50	Yellow

Residue	Category
I58	Yellow
F59	Green
T62	Yellow
Y63	Yellow
I64	Yellow
H65	Yellow
L66	Yellow
K67	Yellow
E68	Yellow
A69	Yellow
T70	Yellow
V71	Green
E72	Green
D73	Yellow
L74	Yellow
G75	Yellow
Q76	Yellow
H77	Green
E78	Yellow
T79	Yellow
W80	Yellow
I81	Yellow
P82	Green
G83	Yellow
E84	Yellow
L85	Yellow
P86	Yellow
L87	Yellow
V88	Orange
Q89	Yellow
E90	Yellow
L91	Yellow
T92	Yellow
S93	Green
T94	Yellow
L95	Yellow
R96	Yellow
E97	Yellow
I98	Yellow
A99	Yellow
W102	Yellow
R103	Yellow
K104	Yellow
L105	Yellow
Y106	Yellow
V107	Yellow
N108	Yellow
N109	Yellow
K110	Green
L111	Yellow
T112	Yellow

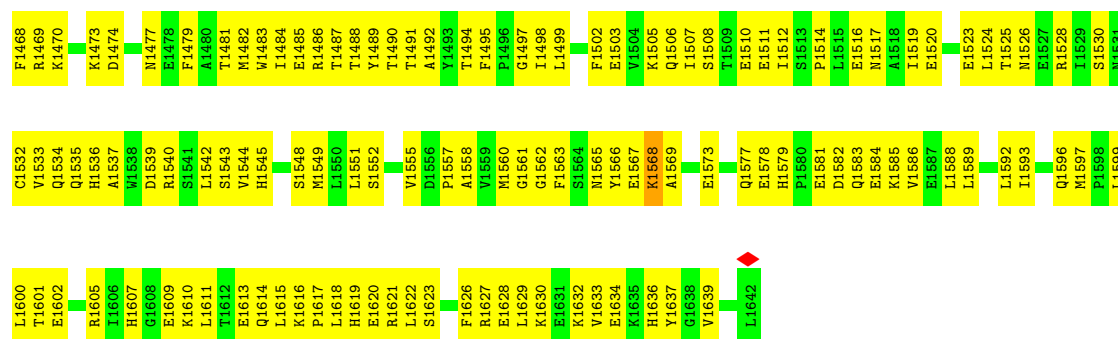
F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965	D892	H825	L760	M681	L606	Q537	P463	A389	P321	F253	F1108	D965</
-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	------	------	------	------	------	------	------	------	------	------	------	-------	--------



• Molecule 2: Dedicator of cytokinesis protein 5

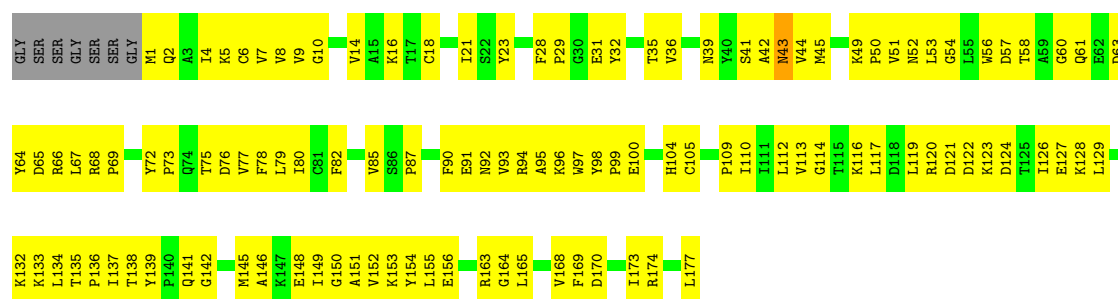


T1400	I1318	Y1240	Y1168	K1100	T1029	Q962	Q889	S822	F754	M881	V607	E538	K464	A389
Q1401	K1319	I1241	K1169	F1101	R1030	Q963	L890	I823	L757	E882	T608	T539	M465	K390
P1403	I1320	R1242	L1242	I1102	F1031	M964	D891	I824	L757	S886	F609	R540	V466	E391
M1404	S1321	L1243	L1171	V1106	F1032	D966	N892	N825	L760	D541	T610	D541	V468	V392
A1405	K1322	Y1245	L1172	G1107	D1034	S967	S884	D827	K761	Y689	P611	K542	T469	N393
E1406	E1323	K1246	L1175	P1108	Q1035	H963	N895	K828	K761	Y689	S612	S543	M470	H394
K1407	T1327	L1247	L1176	L1109	F1038	Y969	K896	K828	F764	L692	S613	E544	S471	Q397
M1408	Y1328	R1248	L1177	L1110	E1039	S970	H899	R830	R765	F694	K613	E544	V472	G398
T1412	H1251	H1251	E1178	E1111	L1040	H971	H899	F831	I767	F694	D614	F547	D474	L399
V1413	V1332	H1179	C1180	T1113	Q1041	I973	S902	P833	S770	L697	K617	F547	D474	V400
F1416	F1333	R1181	R1181	L1114	L1042	S974	S903	V834	S770	I700	F620	V549	G477	V401
D1417	D1334	K1182	K1182	T1115	M1043	T975	Q904	E835	R772	I701	Q621	A550	L479	S402
I1418	Y1335	H1183	H1183	P1116	W1043	T975	L905	I905	V771	I701	Q621	V551	L479	L403
K1419	E1260	A1260	K1184	E1117	M1045	F976	L906	L839	L773	L703	A623	K553	H485	K404
S1420	L1338	E1260	Y1185	V1118	N1045	R979	S907	F840	L775	I704	A623	L554	H485	Q412
S1421	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1422	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1423	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1424	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1425	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1426	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1427	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1428	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1429	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1430	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1431	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1432	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1433	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1434	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1435	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1436	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1437	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1438	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1439	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
S1440	L1186	E1260	Y1185	V1118	N1045	R979	N908	C841	R776	G705	A623	L554	H485	V413
Y1441	F1376	L1208	R1208	N1139	K1071	Y1002	E930	S866	F798	T727	R644	M579	K314	E435
P1437	G1371	Q1284	E1206	F1138	R1069	Y1002	E930	S866	F798	T727	R644	M579	K314	E435
P1439	F1372	R1285	D1206	F1138	R1069	Y1002	E930	S866	F798	T727	R644	M579	K314	E435
P1440	P1373	D1286	Y1207	S1139	K1071	Y1002	E930	S866	F798	T727	R644	M579	K314	E435
Y1441	F1376	L1208	R1208	N1139	K1071	Y1002	E930	S866	F798	T727	R644	M579	K314	E435
K1444	L1376	L1209	T1209	N1143	Y1076	V1008	R931	I867	N799	L728	S645	E580	V515	I436
E1448	I1378	V1290	I1210	H1145	G1077	M1009	L933	F869	M800	A729	S647	I517	S516	I436
Q1449	I1380	T1292	K1217	N1149	M1079	N1010	R934	R870	M802	V730	Q648	A518	I519	L437
I1450	F1381	Q1293	E1218	E1150	K1080	M1011	R935	S872	R804	V731	Q648	A518	I519	L437
L1451	R1384	K1294	N1219	L1151	K1081	T1012	R940	C874	L806	V736	H652	T522	V520	P439
M1452	G1385	E1295	R1220	T1152	I1082	R1015	I941	R875	L806	L737	N653	T523	G440	P439
Y1453	K1386	E1298	M1221	T1153	I1083	R1015	G942	E876	E808	N738	L654	G590	G440	P439
E1454	E1387	T1224	K1154	K1154	I1083	R1015	M943	V877	E808	F739	K655	T591	H526	G440
R1455	E1387	T1224	L1155	L1155	I1083	R1015	N944	L878	A809	V740	K655	K592	H526	I446
R1455	E1387	T1224	L1155	L1155	I1083	R1015	N944	L878	A809	V740	K655	K592	H526	I446
Q1460	I1388	Y1301	D1156	D1156	I1087	R1019	R945	L879	T812	V741	E659	M593	I527	T449
Q1461	I1388	Y1301	D1156	D1156	I1087	R1019	R945	L879	T812	V741	E659	M593	I527	T449
F1462	I1390	T1305	K1232	E1157	D1088	A1020	Q946	R880	K813	A742	V660	E594	I527	T449
F1462	I1391	S1306	E1233	Q1234	D1089	I1021	S947	L881	K813	A742	V660	E594	I527	T449
R1463	F1392	Y1307	K1234	V1159	M1090	Q1023	N1022	L882	G814	A744	D661	E596	T530	L451
R1463	D1393	K1235	K1235	R1163	G1095	Q1023	N1022	L882	G814	A744	D661	E596	T530	L451
Y1464	F1394	R1236	E1236	G1164	P1096	F1024	V954	Q885	K818	D745	I665	E599	R531	D456
S1465	S1395	D1238	D1238	G1165	H1097	A1025	V954	Q885	K818	D745	I665	E599	R531	D456
R1466	P1467	E1315	I1239	Q1167	K1098	I1027	I958	S887	Y819	K749	Q670	S535	R532	D456
P1467	L1399	E1315	I1239	Q1167	K1098	I1027	I958	S887	Y819	K749	Q670	S535	R532	D456



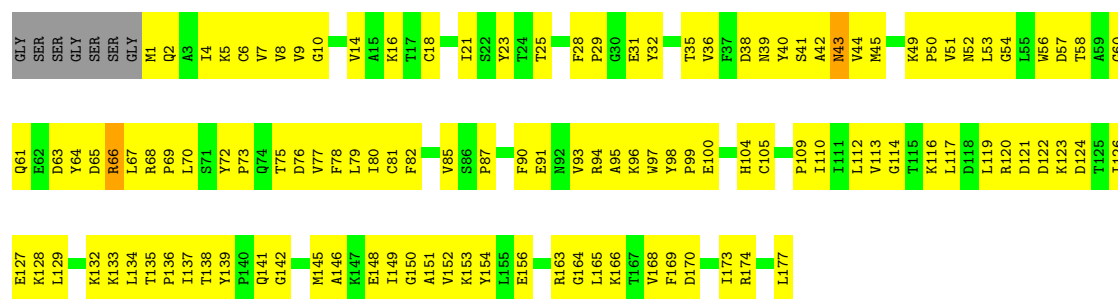
• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain C: 34% 62%



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

Chain F: 32% 64%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	120707	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	0.060	Depositor
Minimum map value	-0.022	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	0.30	0/1641	0.52	0/2218
1	D	0.30	0/1641	0.52	0/2218
2	B	0.37	1/13722 (0.0%)	0.54	5/18514 (0.0%)
2	E	0.37	1/13722 (0.0%)	0.54	5/18514 (0.0%)
3	C	0.34	0/1415	0.49	0/1924
3	F	0.34	0/1415	0.49	0/1924
All	All	0.36	2/33556 (0.0%)	0.53	10/45312 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	463	PRO	CG-CD	-14.33	1.03	1.50
2	B	463	PRO	CG-CD	-14.29	1.03	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	463	PRO	N-CD-CG	-17.32	77.21	103.20
2	E	463	PRO	N-CD-CG	-17.30	77.25	103.20
2	B	463	PRO	CA-CB-CG	-11.62	81.93	104.00
2	E	463	PRO	CA-CB-CG	-11.60	81.96	104.00
2	B	463	PRO	CA-N-CD	-7.71	100.70	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1608	0	1617	133	0
1	D	1608	0	1617	138	0
2	B	13436	0	13516	927	0
2	E	13436	0	13516	952	0
3	C	1385	0	1407	106	0
3	F	1385	0	1407	120	0
All	All	32858	0	33080	2301	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 35.

The worst 5 of 2301 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:D:697:ARG:HH21	2:E:30:GLN:HB2	1.33	0.91
1:D:670:ASN:ND2	1:D:676:ASP:O	2.06	0.88
2:E:1579:HIS:HB3	2:E:1582:ASP:HB2	1.56	0.88
1:A:670:ASN:ND2	1:A:676:ASP:O	2.06	0.87
1:D:625:MET:HE1	1:D:638:LEU:HA	1.57	0.86

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%)	179 (91%)	17 (9%)	0	100	100
1	D	196/733 (27%)	179 (91%)	17 (9%)	0	100	100
2	B	1640/1648 (100%)	1512 (92%)	128 (8%)	0	100	100
2	E	1640/1648 (100%)	1512 (92%)	128 (8%)	0	100	100
3	C	175/184 (95%)	164 (94%)	11 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
All	All	4022/5130 (78%)	3711 (92%)	311 (8%)	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%)	183 (100%)	0	100	100
1	D	183/664 (28%)	183 (100%)	0	100	100
2	B	1495/1497 (100%)	1489 (100%)	6 (0%)	89	91
2	E	1495/1497 (100%)	1489 (100%)	6 (0%)	89	91
3	C	153/157 (98%)	150 (98%)	3 (2%)	50	69
3	F	153/157 (98%)	150 (98%)	3 (2%)	50	69
All	All	3662/4636 (79%)	3644 (100%)	18 (0%)	85	90

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	1568	LYS
3	F	123	LYS
3	F	66	ARG
3	C	123	LYS
2	E	1069	ARG

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

Mol	Chain	Res	Type
2	E	1203	ASN
2	E	1401	GLN
3	F	39	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1203	ASN
2	B	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

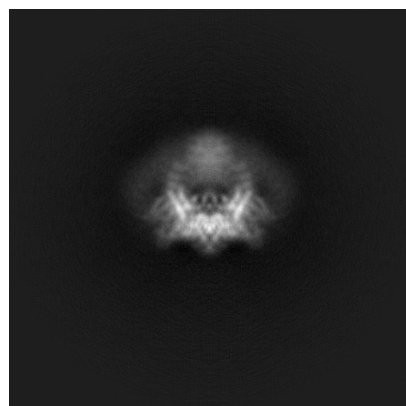
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60148. These allow visual inspection of the internal detail of the map and identification of artifacts.

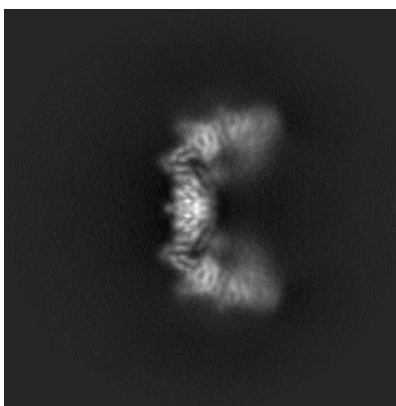
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

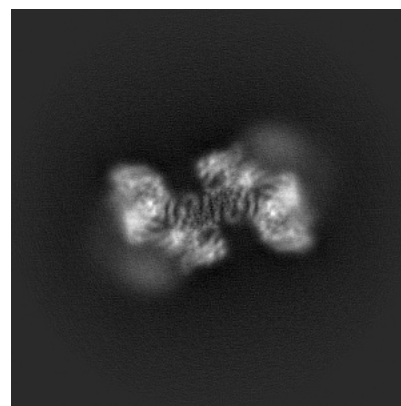
6.1.1 Primary map



X

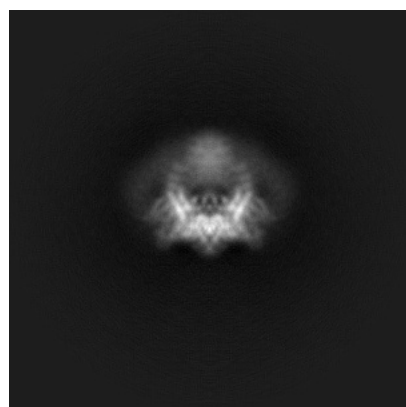


Y

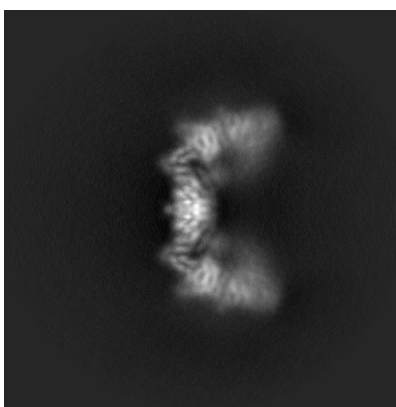


Z

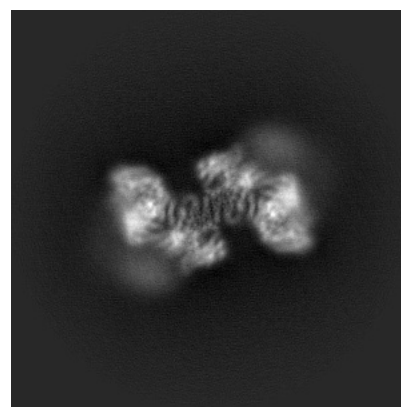
6.1.2 Raw map



X



Y

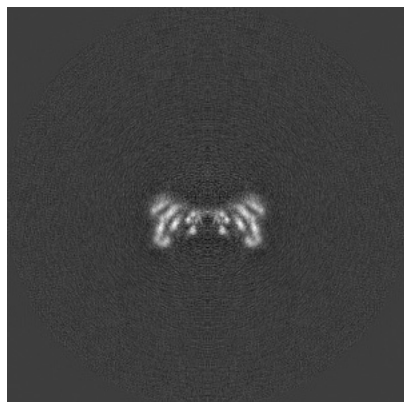


Z

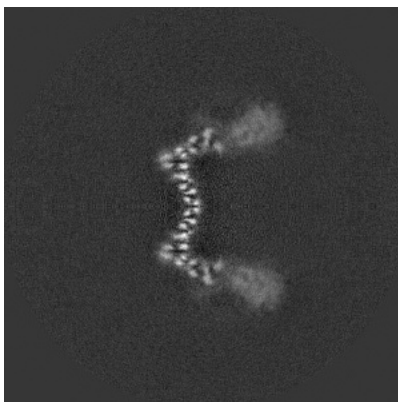
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

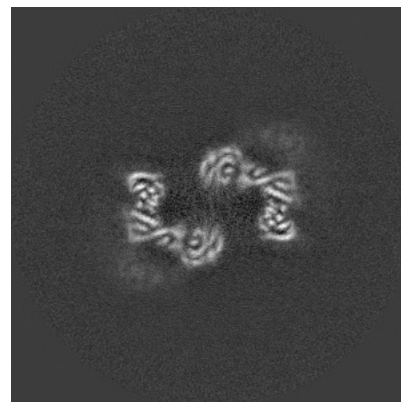
6.2.1 Primary map



X Index: 170

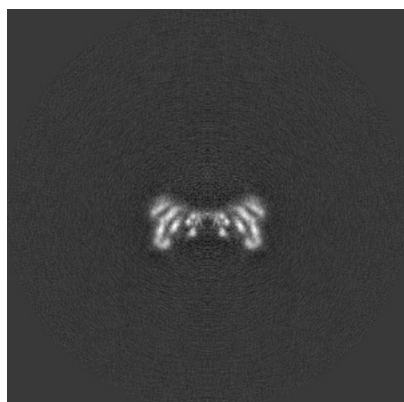


Y Index: 170

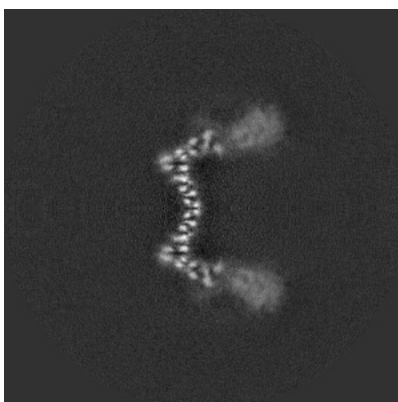


Z Index: 170

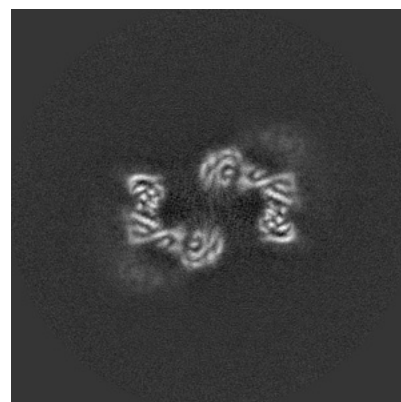
6.2.2 Raw map



X Index: 170



Y Index: 170

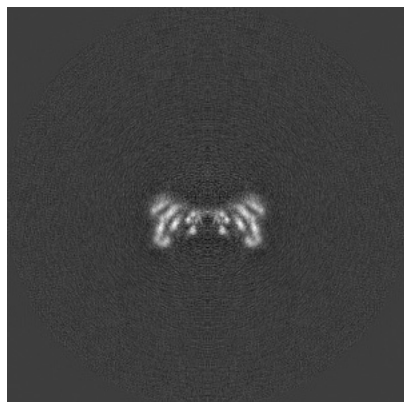


Z Index: 170

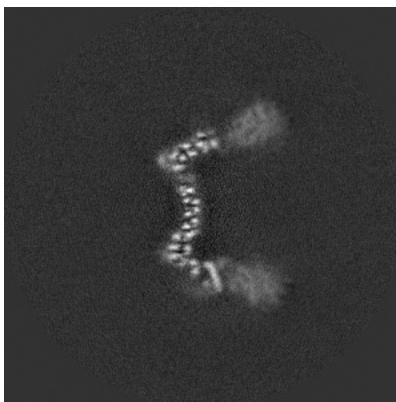
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

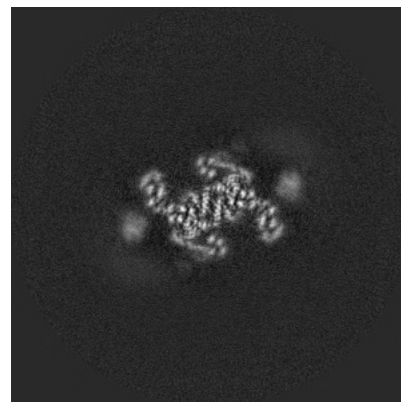
6.3.1 Primary map



X Index: 170

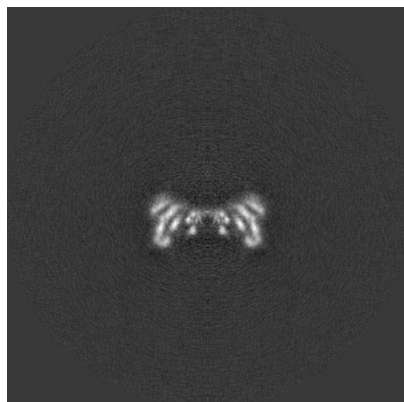


Y Index: 166

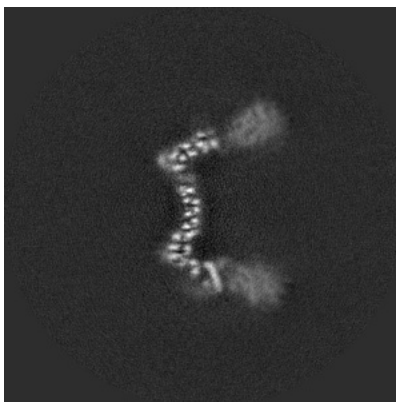


Z Index: 155

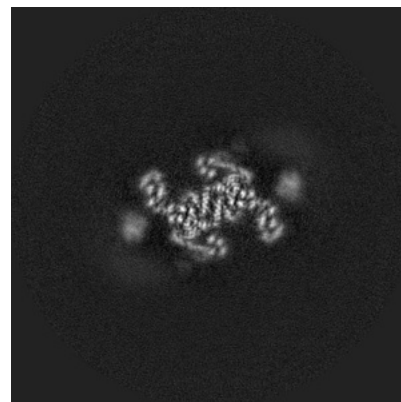
6.3.2 Raw map



X Index: 170



Y Index: 166

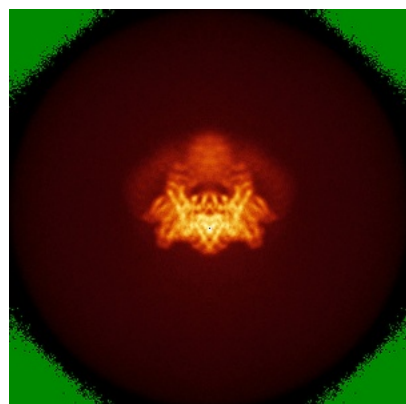


Z Index: 155

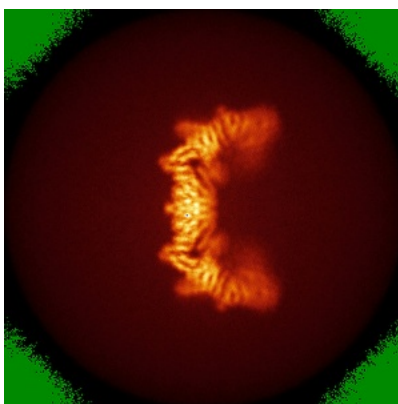
The images above show the largest variance slices of the map in three orthogonal directions.

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

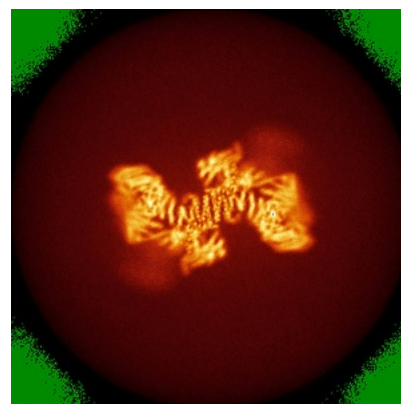
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

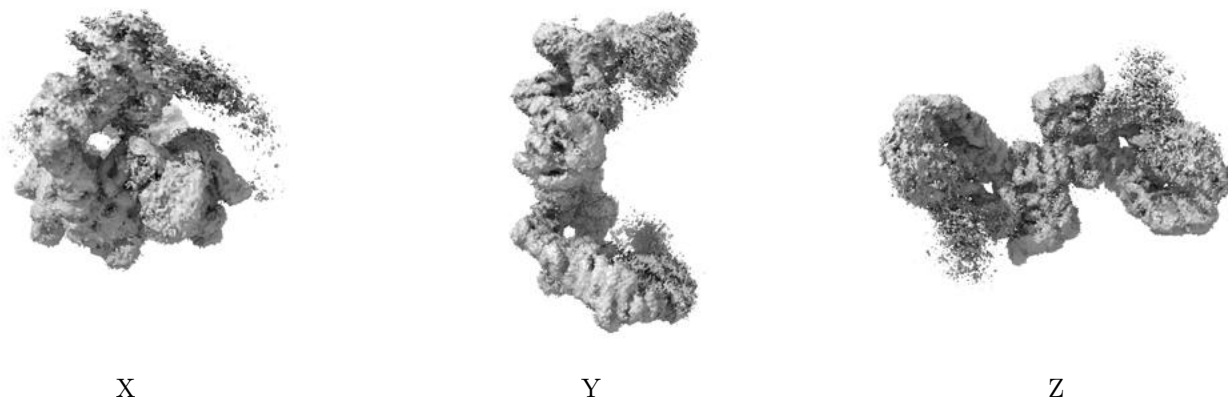


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

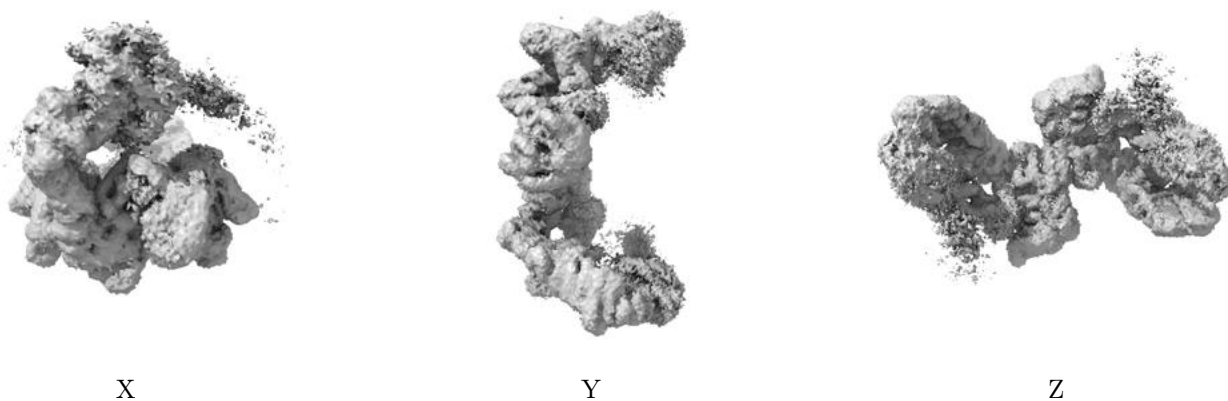
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

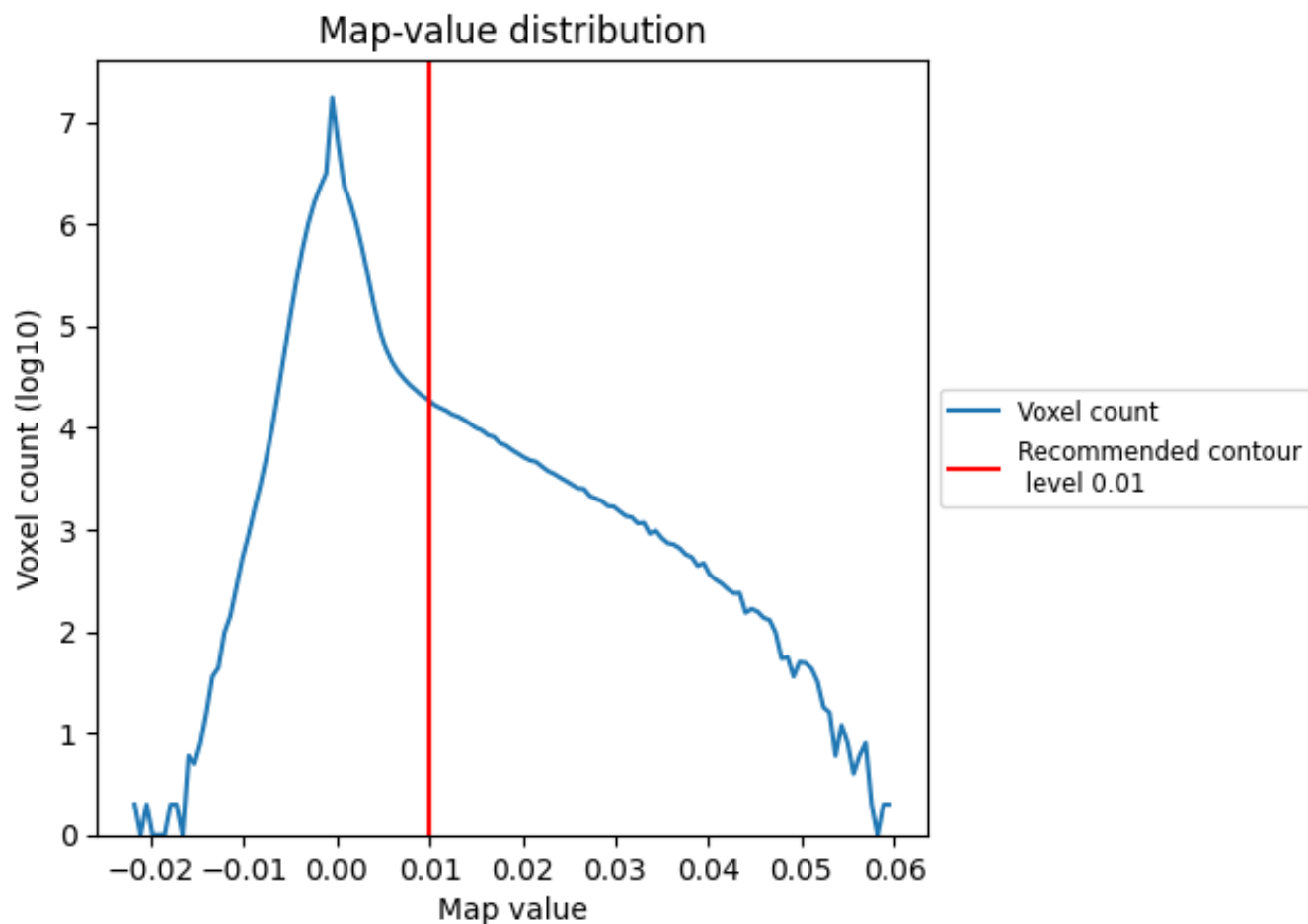
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

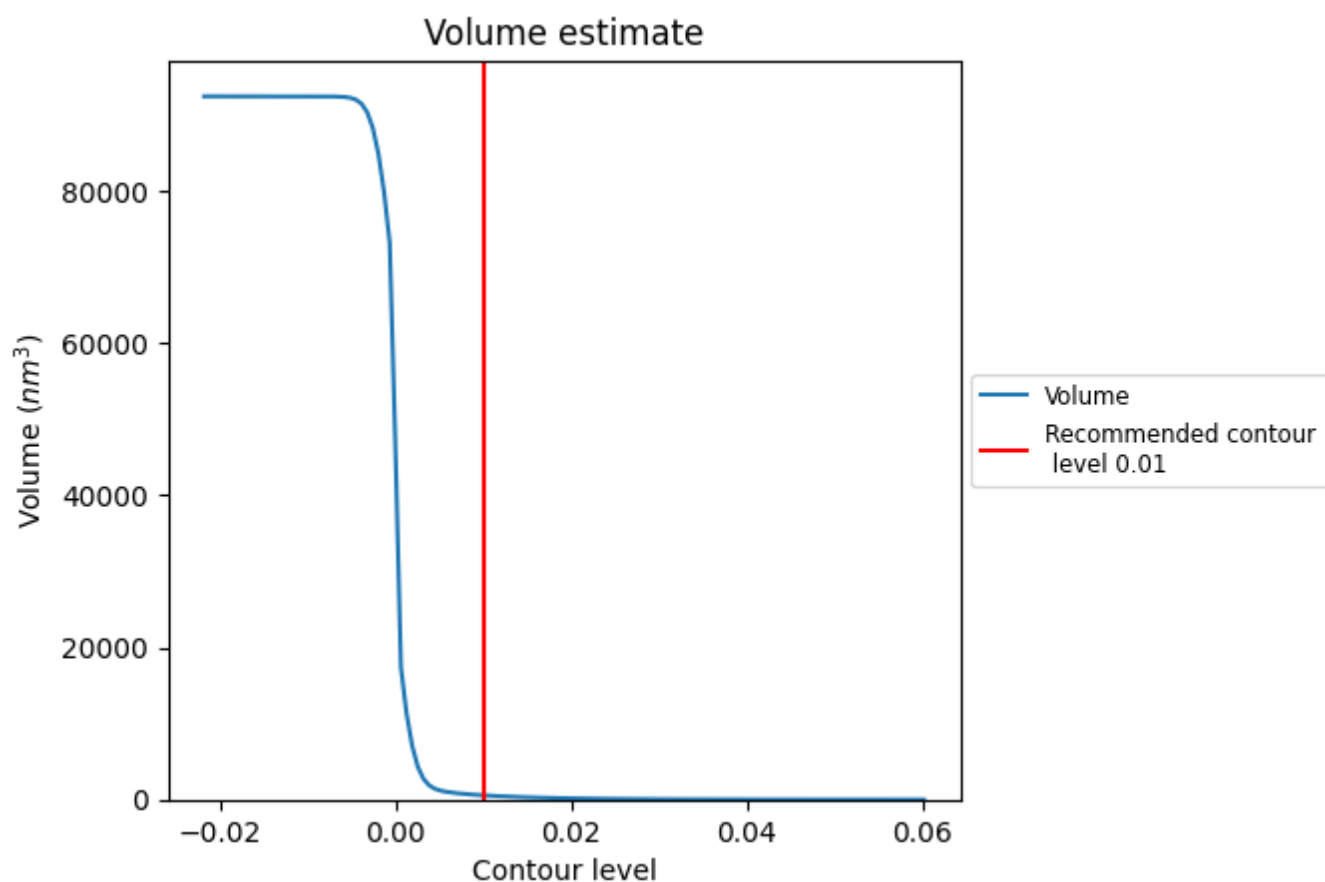
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

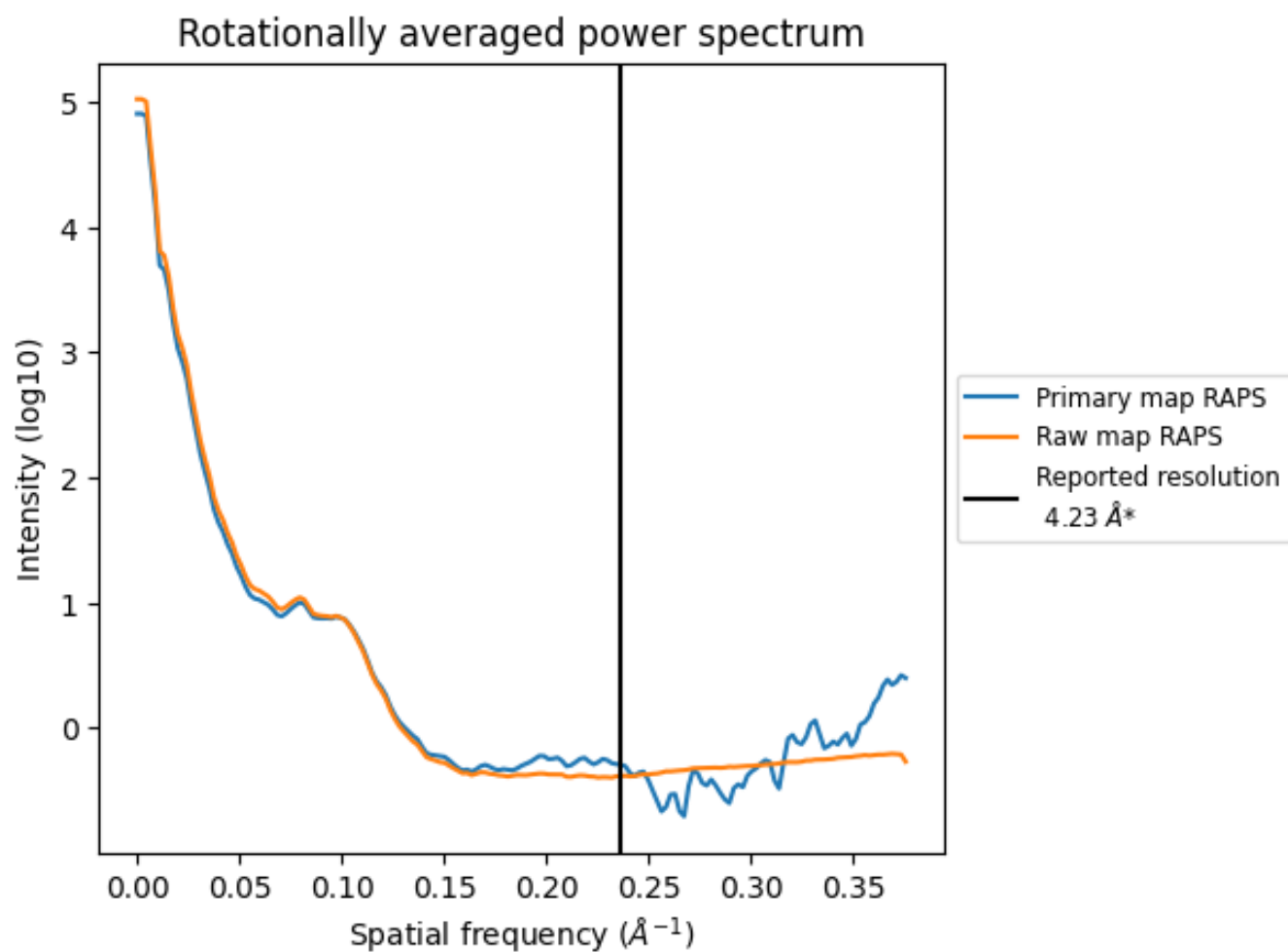
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 558 nm³; this corresponds to an approximate mass of 504 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 ⓘ

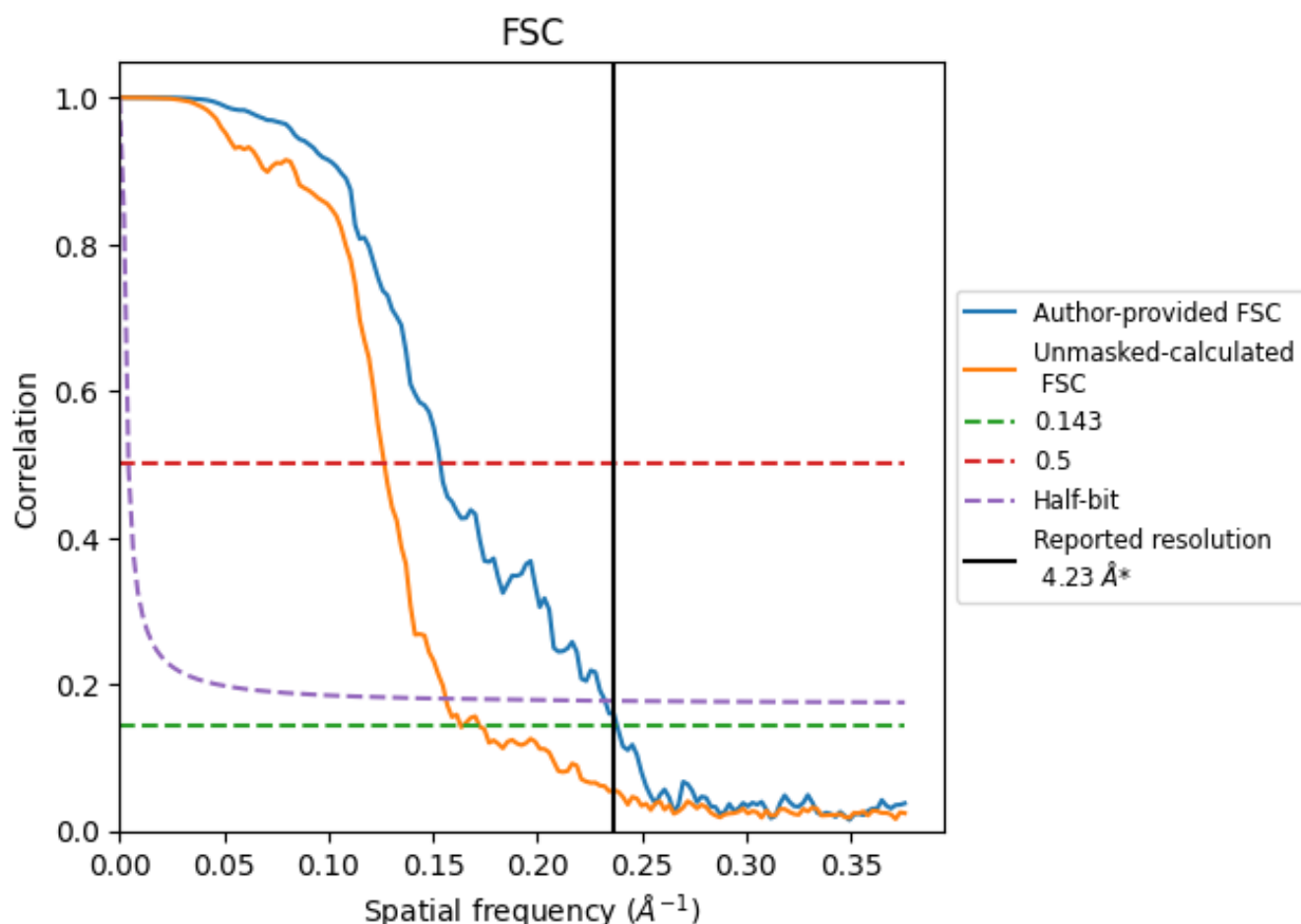


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

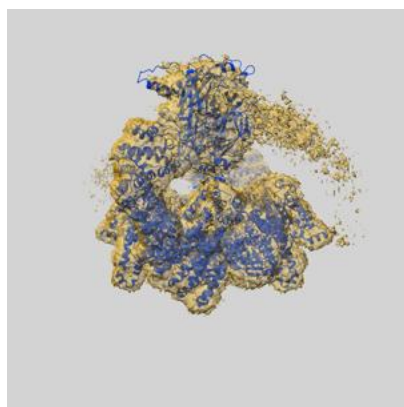
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.20	6.51	4.30
Unmasked-calculated*	6.12	7.89	6.40

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

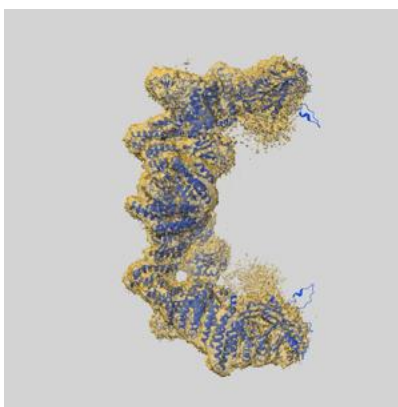
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60148 and PDB model 8ZJK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

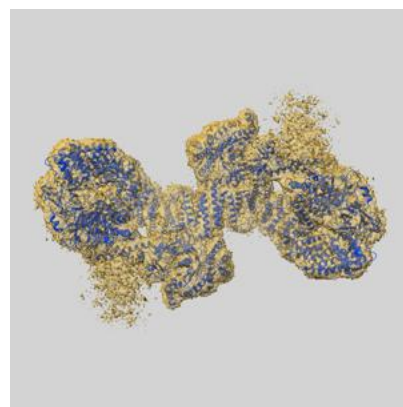
9.1 Map-model overlay [i](#)



X



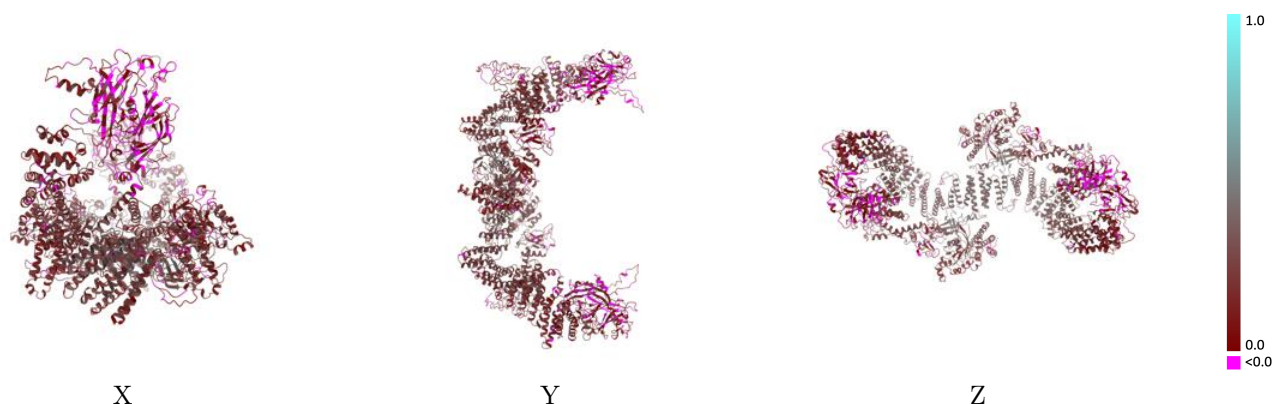
Y



Z

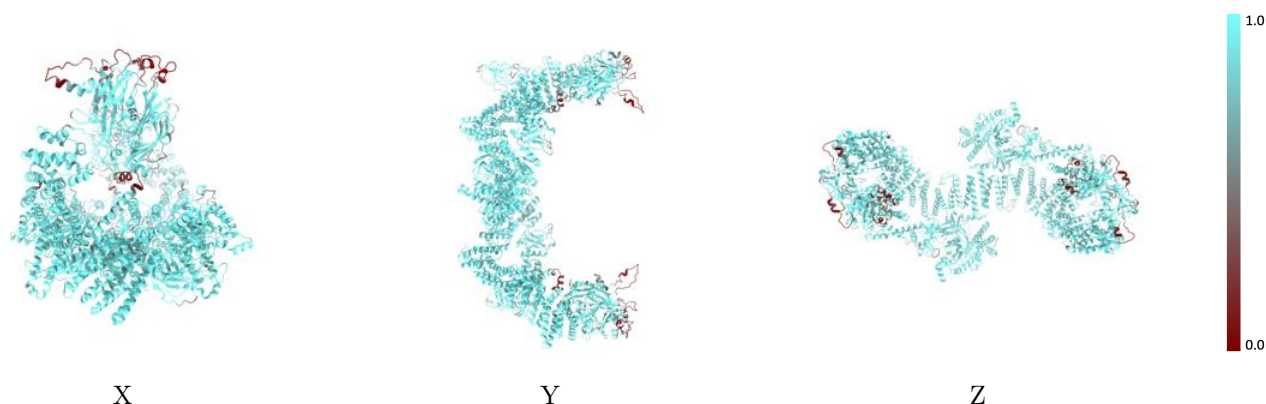
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



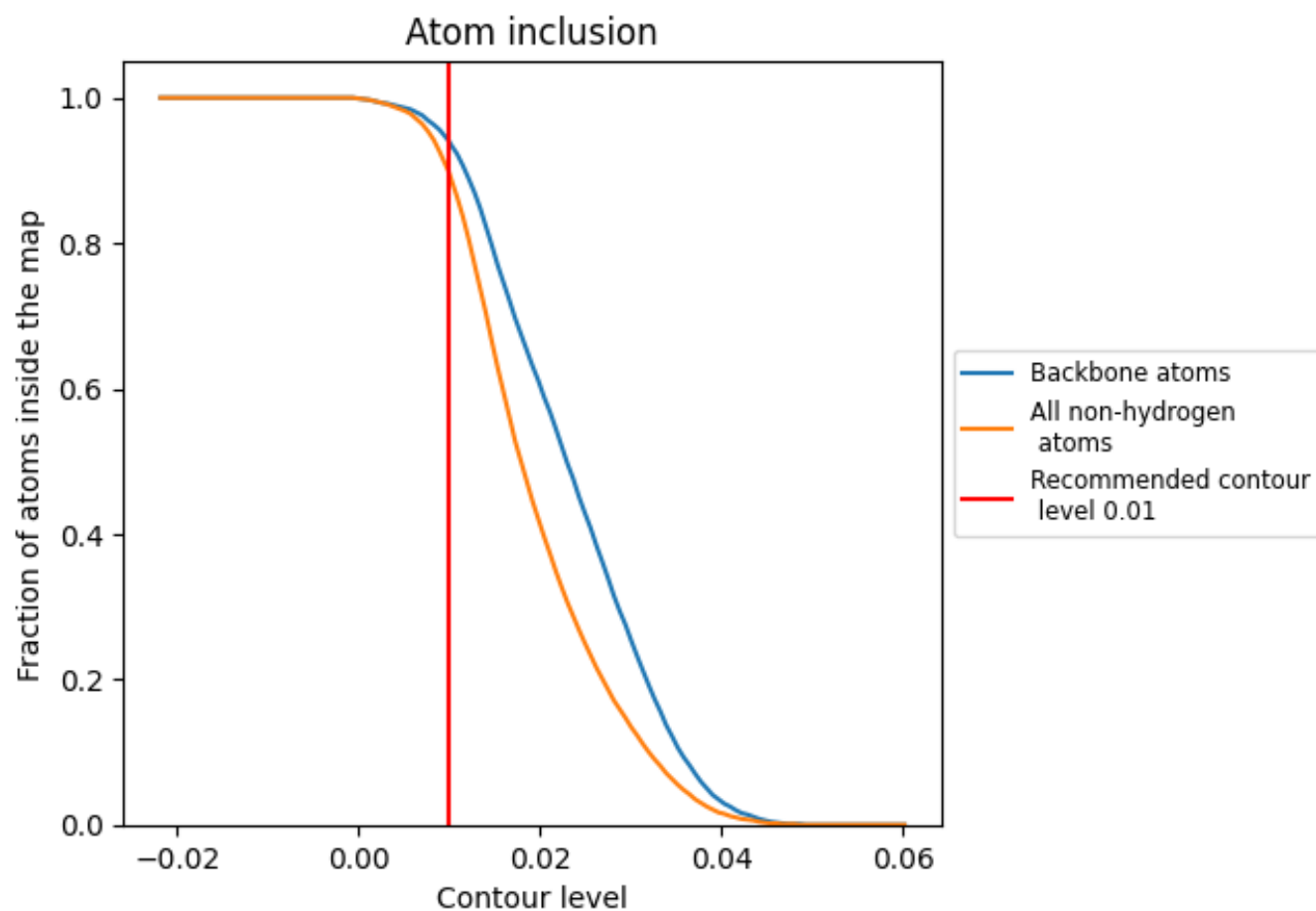
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 94% of all backbone atoms, 90% 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>0.8970</div>	<div><div></div>0.2030</div>
A	<div><div></div>0.8970</div>	<div><div></div>0.1680</div>
B	<div><div></div>0.8870</div>	<div><div></div>0.2030</div>
C	<div><div></div>0.9560</div>	<div><div></div>0.2450</div>
D	<div><div></div>0.9070</div>	<div><div></div>0.1610</div>
E	<div><div></div>0.8930</div>	<div><div></div>0.2040</div>
F	<div><div></div>0.9600</div>	<div><div></div>0.2420</div>

1.0

0.0

<0.0