



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:56 PM UTC

PDB ID : 9QK2 / pdb_00009qk2
EMDB ID : EMD-53217
Title : Structure of the Complement classical and lectin pathway C3 convertase in complex with substrate C3
Authors : De la O Becerra, K.I.; Brondijk, T.H.C.; Gros, P.
Deposited on : 2025-03-19
Resolution : 3.50 Å (reported)
Based on initial models : 7B2Q, 2A73, 2ODP, 5JTW

This is a Full wwPDB EM Validation 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:

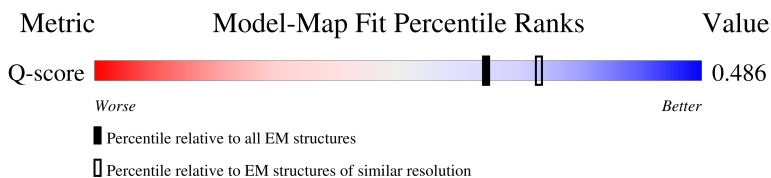
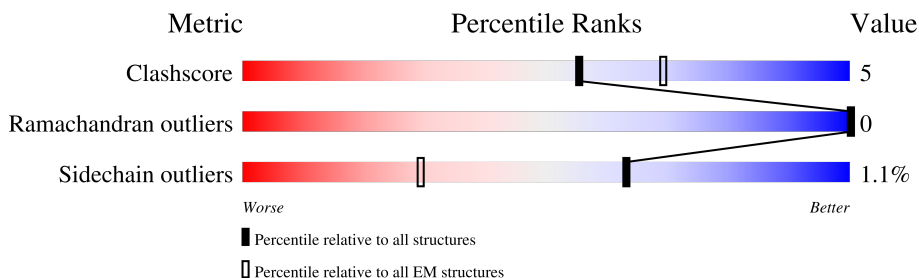
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.50 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	13950 (3.00 - 4.00)

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	1744	
1	B	1744	
1	C	1744	
2	E	752	

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Mol	Chain	Length	Quality of chain
3	D	120	13% 78% 18%
4	F	1663	34% 5% 62%
4	G	1663	51% 7% 41%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 29917 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 Complement C4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	651	Total	C	N	O	S	0	0
			5012	3185	872	939	16		
1	C	281	Total	C	N	O	S	0	0
			2241	1407	400	417	17		
1	B	618	Total	C	N	O	S	0	0
			4788	3034	829	911	14		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1201	SER	THR	variant	UNP P0C0L4
C	1201	SER	THR	variant	UNP P0C0L4
B	1201	SER	THR	variant	UNP P0C0L4

- Molecule 2 is a protein called Complement C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	507	Total	C	N	O	S	1	0
			4021	2527	715	752	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	679	ALA	SER	engineered mutation	UNP P06681

- Molecule 3 is a protein called Anti-C4b nanobody B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	116	Total	C	N	O	S	0	0
			908	566	159	177	6		

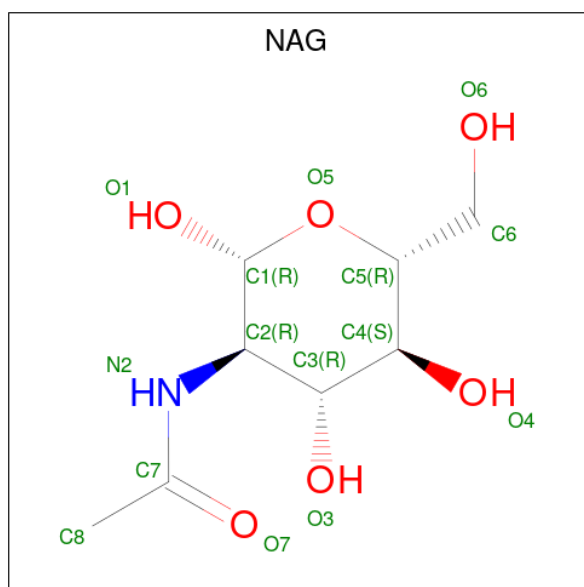
- Molecule 4 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	638	Total	C	N	O	S	0	0
			4976	3171	840	950	15		
4	G	982	Total	C	N	O	S	0	0
			7858	4964	1341	1507	46		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	314	LEU	PRO	variant	UNP P01024
G	314	LEU	PRO	variant	UNP P01024

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	E	1	Total	Mg	0
			1	1	

[illegible]

- Molecule 1: Complement C4-A

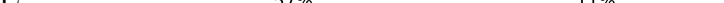
[illegible]

MET	ARG	LEU	LEU	TRP	GLY	LEU	ILE	TRP	ALA	SER	SER	PHE	THR	LEU	SER	LEU	LEU	GLN	LYS	PRO	ARG	LEU	LEU	PHE	SER	SER	PRO	VAL	VAL	HIS	LEU	GLY	VAL	VAL	PRO	LEU	SER	SER	GLY	VAL	GLN	LEU	GLN	ASP	VAL	VAL	PRO	ARG	GLY	VAL	GLN	VAL	LYS	GLY	SER	VAL	PHE	LEU	LEU	ARG	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

S1301	M1218	D1136	Q1068	N857	THR	LEU	GLY	LEU	PHE	ARG	ILE	TYR	SER	GLN	PHE	GLY	PHE	GLN	SER
D1304	A1219	E1137	F1069	Y858	LEU	SER	ALA	SER	TYR	PRO	GLN	THR	SER	THR	VAL	VAL	VAL	THR	SER
T1305	M1220	A1140	R1060	L859	ARG	GLN	GLN	GLN	PHE	ARG	GLN	SER	ARG	LEU	VAL	LEU	LEU	ARG	ASN
R1325	Q1221	L1149	A1062	L863	ARG	PRO	ASP	ASP	PHE	GLY	THR	TYR	THR	LEU	PRO	THR	THR	VAL	ASN
L1331	E1223	L1153	D1063	C876	LEU	SER	ALA	LEU	TYR	ASP	GLY	SER	SER	GLY	ASP	GLY	THR	VAL	ASN
N1337	THR	L1156	G1064	L877	PRO	CYS	ARG	PRO	TYR	THR	SER	GLY	LEU	GLN	GLY	GLY	GLY	GLY	ASN
K1340	ASP	Q1157	S1066	A878	GLY	GLY	ALA	ASP	HIS	ASP	LEU	LEU	LEU	VAL	VAL	TYR	TYR	VAL	ASN
S1341	N1227	D1158	A1067	P890	LEU	THR	LEU	PHE	GLY	GLY	GLY	SER	LEU	VAL	ILE	ILE	ILE	LEU	LEU
H1342	L1228	E1159	L1070	K929	THR	SER	LEU	SER	VAL	ARG	THR	PRO	THR	THR	THR	THR	THR	THR	PHE
M1348	Y1229	G1160	S1071	Y946	THR	THR	ARG	ARG	ALA	VAL	VAL	ALA	SER	SER	VAL	VAL	VAL	SER	THR
R1349	VAL	A1161	R1072	E947	ARG	CYS	HIS	THR	ALA	VAL	VAL	VAL	ASN	ILE	ILE	ILE	ILE	SER	SER
Q1350	THR	E1162	D1073	L948	LYS	GLN	LYS	LYS	LEU	GLY	GLY	THR	LEU	THR	THR	THR	THR	ARG	GLY
I1351	SER	P1163	S1074	R951	ARG	ASN	VAL	ASN	ARG	VAL	ALA	ALA	VAL	THR	PRO	GLN	GLN	GLY	GLY
L1354	GLN	K1165	S1087	D952	VAL	VAL	MET	VAL	ASP	THR	THR	THR	THR	THR	PRO	GLN	GLN	ASP	ASP
E1355	ASN	Q1166	G1094	H953	LEU	LEU	GLY	PHE	GLY	THR	SER	SER	GLY	GLY	GLY	GLY	GLY	LEU	LEU
E1356	ALA	R1167	G1095	R954	LYS	LYS	PHE	GLN	GLY	ALA	HIS	LEU	LEU	LEU	VAL	VAL	VAL	LEU	LEU
F1360	VAL	V1168	G1096	E959	SER	SER	ALA	ALA	ALA	ALA	TYR	LEU	LEU	LEU	LEU	LEU	LEU	ASP	ASP
K1365	PRO	E1169	P1097	N953	ARG	ARG	ILE	ASN	CYS	TYR	TYR	GLN	GLN	GLN	GLN	GLN	GLN	ASP	ASP
I1366	THR	A1170	E1098	L958	LYS	LYS	GLY	GLY	GLY	GLY	GLY	ALA	ALA	ALA	ALA	ALA	ALA	LEU	LEU
V1370	PRO	S1171	K1099	D971	GLY	GLY	ASN	ASN	LYS	LYS	LEU	LEU	LEU	LEU	LEU	LEU	LEU	PRO	PRO
N1373	ASN	I1172	L1100	Y977	GLY	GLY	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
T1383	PRO	S1173	E1102	D984	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
D1388	ASP	N1176	T1103	LEU	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
L1397	PRO	S1177	S1104	THR	ASP	THR	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Q1398	PRO	L1178	M1106	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
T1410	THR	G1180	L1107	GLY	LYS	LYS	LYS	LYS	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR
Y1417	THR	A1183	S1109	SER	CYS	CYS	CYS	CYS	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ASP	L1260	S1184	Q1110	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
TYR	H1276	A1185	Q1111	A994	ASP	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	GLY	G1186	Q1112	L995	GLY	VAL	VAL	VAL	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
K1278	GLY	L1187	A1113	S996	THR	THR	THR	THR	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
A1279	GLY	L1188	D1114	R1008	ARG	ARG	ARG	ARG	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
E1280	GLY	G1189	G1115	G1009	LEU	LEU	LEU	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
M1281	GLY	H1191	S1116	E1012	PRO	PRO	PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L1289	GLY	I1195	F1117	Q1010	MET	MET	MET	MET	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
Q1292	GLY	L1200	Q1118	G1011	THR	THR	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
G1293	GLY	S1201	D1119	E1013	ASP	ASP	ASP	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
S1294	GLY	T1202	P1120	Q1013	SER	SER	SER	SER	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
F1295	GLY	T1203	C1121	M1015	CYS	CYS	CYS	CYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
Q1296	GLY	K1204	F1122	E1032	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
F1299	PRO	P1206	L1124	I1049	ARG	ARG	ARG	ARG	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
R1300	ALA	V1207	D1126	R1055	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA

[illegible]

- Molecule 2: Complement C2

Chain E:  57% 11% 33%

[illegible]

- Molecule 3: Anti-C4b nanobody B12

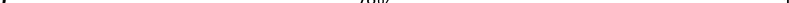
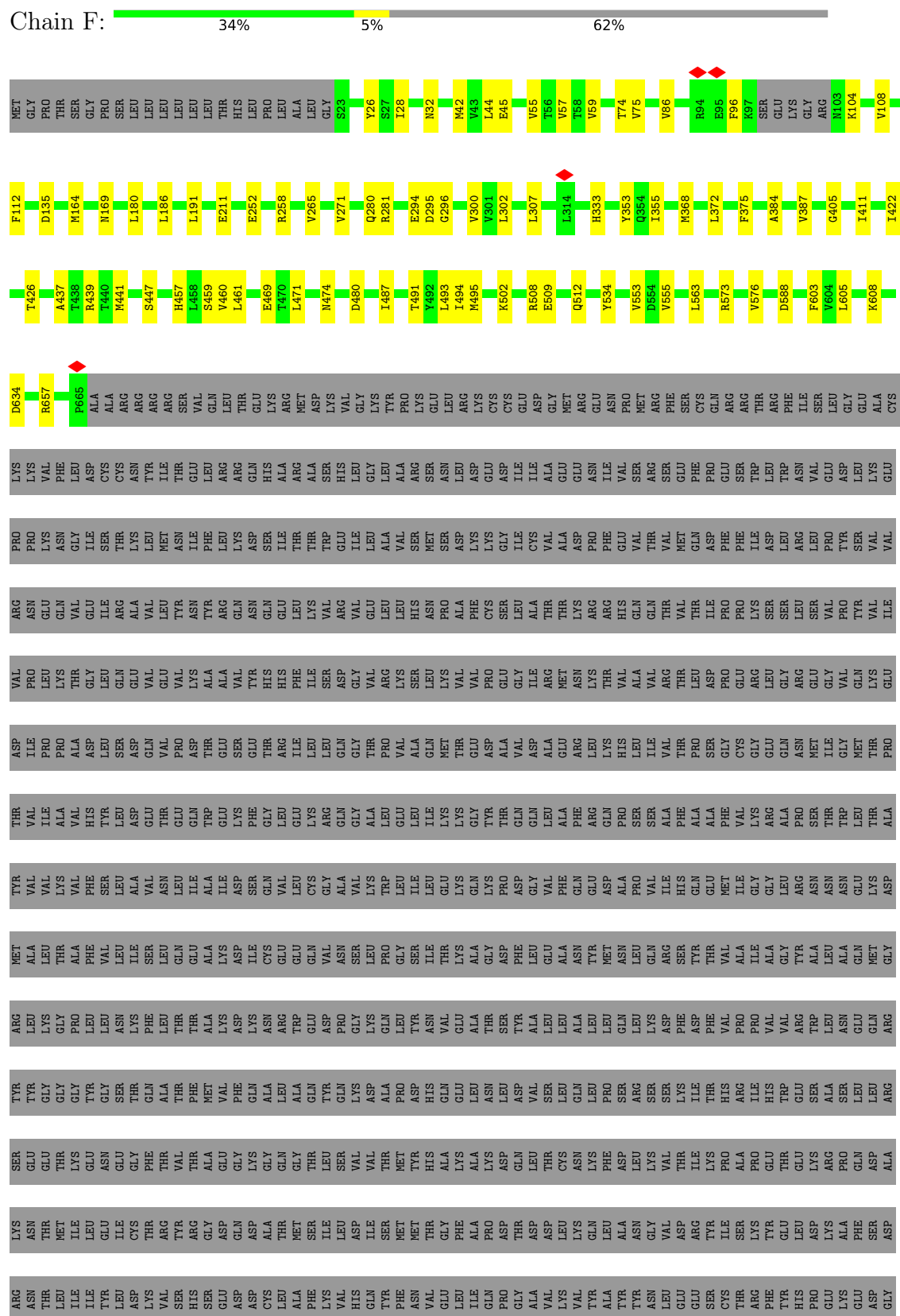
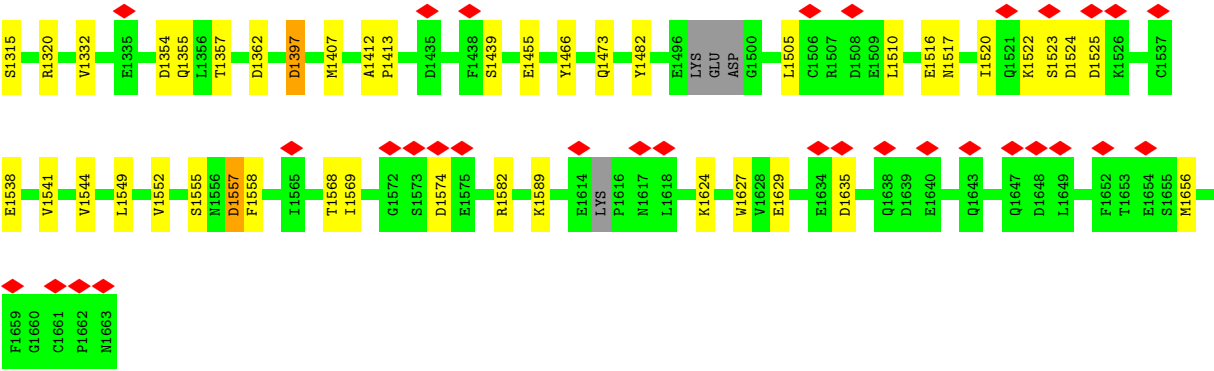
Chain D:  13% 78% 18% ..

Figure 1: A hierarchical tree diagram showing the classification of 140 protein families into 10 superfamilies. The tree is rooted at the top with 'S119' and 'S120' (green boxes). The first level branches into 'GLU' (grey box) and 'V2' (green box). 'GLU' branches into 'E6' (yellow box) and 'S7' (green box). 'V2' branches into 'G8' (yellow box) and 'GLY' (grey box). 'GLY' branches into 'LEU' (grey box) and 'V12' (green box). 'LEU' branches into 'Q13' (green box) and 'G16' (green box). 'Q13' branches into 'L20' (yellow box) and 'M30' (yellow box). 'M30' branches into 'A31' (yellow box) and 'A36' (green box). 'A36' branches into 'P37' (green box), 'G38' (green box), 'K39' (green box), and 'E40' (green box). 'E40' branches into 'F43' (orange box) and 'I47' (yellow box). 'F43' branches into 'A57' (green box). 'A57' branches into 'F64' (green box) and 'T65' (green box). 'T65' branches into 'R68' (yellow box) and 'A71' (green box). 'A71' branches into 'V75' (green box) and 'L77' (yellow box). 'L77' branches into 'Q78' (green box) and 'M79' (green box). 'M79' branches into 'N80' (green box) and 'S81' (green box). 'S81' branches into 'A94' (yellow box), 'D95' (yellow box), 'L96' (yellow box), 'R97' (yellow box), 'Q98' (green box), and 'R99' (yellow box). 'Q98' branches into 'E102' (yellow box) and 'R103' (yellow box). 'E102' branches into 'Y107' (yellow box) and 'T114' (yellow box). The diagram uses color coding: green for specific families, yellow for others, and grey for a subset. Red diamonds indicate specific relationships or annotations.

● Molecule 4: Complement C3







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	177801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.307	Depositor
Minimum map value	-2.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.199	Depositor
Map size ($\text{\AA}$)	395.19998, 395.19998, 395.19998	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.14	0/5128	0.29	0/6961
1	B	0.12	0/4883	0.29	0/6635
1	C	0.13	0/2288	0.32	0/3090
2	E	0.12	0/4104	0.31	0/5546
3	D	0.15	0/924	0.36	0/1247
4	F	0.14	0/5076	0.30	0/6898
4	G	0.12	0/8010	0.29	0/10828
All	All	0.13	0/30413	0.30	0/41205

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5012	0	5025	43	0
1	B	4788	0	4751	54	0
1	C	2241	0	2184	32	0
2	E	4021	0	3974	46	0
3	D	908	0	876	18	0
4	F	4976	0	5034	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	7858	0	7779	82	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	E	56	0	52	1	0
5	F	14	0	13	1	0
5	G	14	0	13	1	0
6	E	1	0	0	0	0
All	All	29917	0	29727	297	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 5.

All (297) 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)
4:G:678:LYS:HE3	4:G:734:LEU:HD21	1.63	0.80
1:B:1299:PHE:HB3	1:B:1305:THR:HG22	1.68	0.76
2:E:338:ASN:HD22	2:E:341:ALA:HB2	1.50	0.74
4:G:1407:MET:HE1	4:G:1413:PRO:HD3	1.70	0.73
1:B:1331:LEU:HB3	1:B:1366:ILE:HD11	1.72	0.72
2:E:507:HIS:NE2	4:G:747:ALA:O	2.26	0.69
3:D:97:ARG:HD2	3:D:99:ARG:HH21	1.56	0.69
4:F:502:LYS:HA	5:F:1701:NAG:H83	1.76	0.68
4:F:45:GLU:OE1	4:F:534:TYR:OH	2.12	0.67
4:G:759:GLU:O	4:G:760:ASN:ND2	2.28	0.67
4:G:1555:SER:OG	4:G:1558:PHE:O	2.12	0.66
1:C:1620:TYR:HB3	1:C:1621:PRO:HD3	1.78	0.66
4:G:1574:ASP:OD2	4:G:1582:ARG:NH1	2.28	0.65
1:B:1014:THR:HG23	1:B:1015:MET:HE2	1.79	0.65
4:F:42:MET:HE1	4:F:108:VAL:HG11	1.79	0.65
1:A:481:ARG:NH1	4:F:469:GLU:OE1	2.30	0.65
2:E:675:CYS:SG	2:E:714:ARG:NH1	2.70	0.65
1:B:1105:ASN:OD1	1:B:1167:ARG:NH1	2.30	0.65
1:A:370:ASP:OD2	1:A:373:LYS:NZ	2.30	0.64
1:C:1495:HIS:ND1	1:C:1543:GLU:OE2	2.31	0.64
4:G:1505:LEU:HD13	4:G:1510:LEU:HD22	1.79	0.64
1:A:180:ASN:OD1	1:A:181:SER:N	2.31	0.63
1:B:837:LEU:O	1:B:929:LYS:NZ	2.32	0.62
1:A:421:ILE:HD13	1:A:435:ILE:HG22	1.82	0.62
4:F:44:LEU:HD13	4:F:55:VAL:HG11	1.80	0.62
3:D:6:GLU:N	3:D:6:GLU:OE1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1473:TRP:NE1	1:B:1398:GLN:OE1	2.33	0.61
2:E:655:VAL:HG13	2:E:656:ARG:HD2	1.83	0.61
1:A:223:LEU:HD21	1:B:1350:GLN:HB3	1.82	0.61
1:A:36:PRO:O	1:A:514:GLN:NE2	2.33	0.61
2:E:725:PRO:O	2:E:726:ARG:NH1	2.34	0.61
4:G:1516:GLU:OE1	4:G:1624:LYS:NZ	2.34	0.61
4:G:1111:LYS:NZ	4:G:1121:ASP:OD2	2.35	0.60
1:B:843:VAL:HG21	1:B:849:LEU:HD23	1.83	0.59
1:C:1582:LEU:HD22	1:C:1692:THR:HG21	1.85	0.59
2:E:601:ARG:O	2:E:605:ASN:ND2	2.35	0.59
4:G:1517:ASN:OD1	4:G:1589:LYS:NZ	2.35	0.59
1:A:147:GLN:NE2	1:A:154:GLN:OE1	2.36	0.59
1:C:1572:ALA:HB3	1:C:1575:LYS:HG2	1.84	0.58
1:A:104:ARG:NH2	1:B:1032:GLU:O	2.36	0.58
1:A:59:ARG:NH1	1:A:109:GLN:OE1	2.36	0.58
4:F:509:GLU:OE1	4:F:512:GLN:NE2	2.37	0.58
2:E:486:PRO:HA	2:E:518:TRP:CD1	2.38	0.57
4:G:1161:GLN:OE1	4:G:1161:GLN:N	2.37	0.57
4:G:1557:ASP:OD1	4:G:1557:ASP:N	2.34	0.57
1:C:1472:ILE:HD12	1:C:1529:VAL:HG12	1.86	0.57
4:F:135:ASP:OD1	4:F:135:ASP:N	2.38	0.57
3:D:68:ARG:HG2	3:D:75:VAL:HG12	1.87	0.57
2:E:483:THR:HG21	2:E:490:GLU:OE1	2.05	0.57
2:E:702:TYR:O	4:G:748:ARG:NH2	2.38	0.57
1:A:128:GLN:NE2	1:A:655:SER:O	2.38	0.56
1:A:300:GLU:OE2	1:C:1560:TYR:OH	2.17	0.56
1:B:1191:HIS:O	1:B:1195:ILE:HG22	2.05	0.56
2:E:511:ASP:N	2:E:511:ASP:OD1	2.39	0.56
1:B:1060:ARG:NH1	1:B:1066:TYR:OH	2.38	0.56
4:G:1520:ILE:HG23	4:G:1522:LYS:H	1.71	0.56
1:C:1533:ARG:NH2	1:C:1535:CYS:SG	2.79	0.56
4:F:480:ASP:OD1	4:F:480:ASP:N	2.37	0.56
3:D:30:MET:HA	3:D:94:ALA:HB2	1.87	0.55
4:F:252:GLU:OE1	4:F:252:GLU:N	2.39	0.55
2:E:265:VAL:O	2:E:328:TYR:OH	2.16	0.55
1:C:1487:ASP:OD1	1:C:1521:HIS:NE2	2.40	0.55
1:C:1678:GLU:OE1	1:C:1683:TYR:OH	2.24	0.55
4:F:447:SER:OG	4:F:634:ASP:OD1	2.25	0.55
4:G:995:VAL:HG21	4:G:1037:PHE:HZ	1.72	0.55
1:A:185:ARG:NH1	1:B:1356:GLU:OE2	2.41	0.54
1:A:605:ASP:OD1	1:A:606:THR:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:GLU:OE2	4:G:855:ARG:NH2	2.40	0.54
4:G:1295:ASP:OD1	4:G:1295:ASP:N	2.37	0.53
3:D:64:PHE:CE1	3:D:79:MET:HB3	2.43	0.53
1:A:69:SER:OG	1:A:88:GLN:O	2.25	0.53
1:C:1507:LEU:HD21	3:D:96:LEU:HB3	1.89	0.53
1:B:1009:GLY:O	1:B:1055:ARG:NH2	2.40	0.53
4:G:1312:HIS:O	4:G:1315:SER:OG	2.17	0.53
3:D:99:ARG:HH11	3:D:102:GLU:HG3	1.74	0.53
4:G:1355:GLN:NE2	4:G:1357:THR:O	2.40	0.53
2:E:350:MET:HG2	2:E:364:TRP:HH2	1.75	0.52
1:C:1465:ARG:HG2	1:C:1541:VAL:HG12	1.90	0.52
4:G:1412:ALA:HB3	4:G:1466:TYR:HE2	1.75	0.52
2:E:373:LEU:HD22	2:E:426:LEU:HD21	1.90	0.52
2:E:454:ASP:OD1	2:E:454:ASP:N	2.42	0.52
1:B:1301:SER:O	1:B:1305:THR:HG23	2.08	0.52
1:B:1158:ASP:N	1:B:1158:ASP:OD1	2.42	0.52
4:G:759:GLU:HG2	4:G:760:ASN:H	1.75	0.52
1:A:270:TYR:OH	1:A:346:GLU:OE2	2.13	0.52
2:E:467:ASN:HD22	5:E:803:NAG:H83	1.75	0.52
1:A:426:ASP:OD1	1:A:427:GLY:N	2.35	0.52
1:C:1474:ARG:HE	1:C:1529:VAL:HG23	1.75	0.51
4:G:1627:TRP:NE1	4:G:1629:GLU:HB2	2.24	0.51
3:D:43:PHE:CE1	3:D:103:ARG:HD2	2.44	0.51
4:F:355:ILE:HG23	4:F:439:ARG:HB2	1.92	0.51
4:G:1544:VAL:HG13	4:G:1569:ILE:HB	1.92	0.51
1:B:1190:ALA:HA	1:B:1220:MET:HE1	1.92	0.51
1:B:857:ASN:ND2	1:B:890:PRO:O	2.43	0.51
4:G:995:VAL:HG21	4:G:1037:PHE:CZ	2.46	0.51
4:G:744:LEU:HB2	4:G:747:ALA:HB2	1.92	0.51
4:G:1523:SER:OG	4:G:1525:ASP:OD1	2.26	0.51
1:A:207:ILE:HD12	1:B:1383:THR:HG21	1.93	0.51
4:F:26:TYR:HB3	4:F:112:PHE:CD2	2.46	0.51
2:E:703:ASN:OD1	4:G:748:ARG:NH1	2.43	0.50
4:F:302:LEU:HD21	4:F:307:LEU:HB2	1.94	0.50
1:A:299:LEU:HD23	1:A:314:LEU:HD21	1.93	0.50
4:F:487:ILE:O	4:F:508:ARG:NH1	2.45	0.50
4:G:971:VAL:O	4:G:974:THR:OG1	2.30	0.50
4:G:1257:ASN:OD1	4:G:1260:ARG:NH1	2.44	0.50
2:E:391:HIS:HA	2:E:394:GLU:HG2	1.94	0.50
4:F:461:LEU:HD22	4:F:471:LEU:HD13	1.94	0.50
4:G:839:VAL:HG13	4:G:931:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1112:GLN:NE2	1:B:1116:SER:OG	2.45	0.49
4:G:840:VAL:HG11	4:G:1473:GLN:HG3	1.95	0.49
1:A:41:VAL:HG11	1:A:74:PHE:CE2	2.48	0.49
2:E:259:LEU:HD23	2:E:273:PHE:HB3	1.94	0.49
4:F:280:GLN:N	4:F:280:GLN:OE1	2.45	0.49
1:C:1606:LEU:HD22	1:C:1612:TYR:OH	2.12	0.49
2:E:262:SER:OG	2:E:263:GLN:N	2.44	0.48
4:G:1455:GLU:N	4:G:1455:GLU:OE1	2.46	0.48
1:C:1583:CYS:HA	1:C:1588:CYS:HA	1.94	0.48
4:G:835:LEU:HD23	4:G:929:LEU:HD13	1.93	0.48
4:G:774:ASN:N	4:G:774:ASN:OD1	2.46	0.48
4:F:42:MET:HB3	4:F:86:VAL:HG13	1.96	0.48
2:E:498:SER:OG	2:E:499:ASP:N	2.46	0.48
3:D:31:ALA:HB3	3:D:107:TYR:HE2	1.78	0.48
1:A:247:PRO:HG3	1:A:357:LEU:HD21	1.94	0.48
4:G:1268:SER:OG	4:G:1482:TYR:O	2.30	0.48
2:E:244:LYS:N	2:E:433:GLU:OE2	2.46	0.48
1:C:1471:CYS:SG	1:C:1533:ARG:NH2	2.87	0.47
1:C:1608:ASP:OD1	1:C:1609:GLU:N	2.48	0.47
1:B:946:TYR:OH	1:B:959:GLU:O	2.27	0.47
4:F:59:VAL:HG12	4:F:108:VAL:HG22	1.95	0.47
1:A:207:ILE:HD11	1:B:977:TYR:CE1	2.49	0.47
4:G:1549:LEU:HD21	4:G:1552:VAL:HG23	1.96	0.47
1:C:1742:CYS:SG	2:E:380:ASN:HB3	2.54	0.47
1:B:948:LEU:HD11	1:B:1370:VAL:HG21	1.97	0.47
1:A:571:LEU:HD23	1:B:822:ALA:HB2	1.95	0.47
1:B:1153:LEU:HA	1:B:1156:PHE:HD2	1.80	0.47
4:F:281:ARG:NH1	4:G:759:GLU:OE2	2.47	0.47
1:B:1208:ASP:N	1:B:1208:ASP:OD1	2.47	0.47
4:F:28:ILE:HD11	4:F:42:MET:SD	2.54	0.47
1:C:1501:LEU:HD23	1:C:1504:LEU:HD12	1.96	0.47
4:G:1127:GLN:OE1	4:G:1185:ARG:NH1	2.48	0.47
1:B:775:ARG:HB3	1:B:801:ASP:HB3	1.97	0.47
1:C:1656:ASP:OD2	1:C:1701:TYR:OH	2.33	0.47
1:A:487:ASP:OD1	1:A:487:ASP:N	2.47	0.46
4:G:1538:GLU:O	4:G:1541:VAL:N	2.45	0.46
4:G:689:GLU:HG2	4:G:690:LEU:HD13	1.96	0.46
1:B:1348:ASN:O	1:B:1351:ILE:N	2.44	0.46
1:B:1136:ASP:OD1	1:B:1136:ASP:N	2.46	0.46
3:D:6:GLU:HG2	3:D:114:THR:HG23	1.98	0.46
1:A:253:LEU:HB2	1:A:260:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1611:GLY:HA2	1:C:1615:LYS:HB2	1.97	0.46
1:A:351:GLU:OE1	1:B:838:ARG:NH1	2.48	0.46
1:C:1582:LEU:HD11	1:C:1668:LEU:HD12	1.98	0.46
4:F:494:ILE:HD12	4:F:502:LYS:HG2	1.98	0.46
1:A:414:SER:OG	1:A:415:VAL:N	2.49	0.46
1:B:1373:ASN:OD1	1:B:1373:ASN:N	2.49	0.46
4:G:937:ARG:NH2	4:G:1439:SER:OG	2.49	0.46
4:G:1627:TRP:HE1	4:G:1629:GLU:HB2	1.81	0.46
4:F:169:ASN:OD1	4:F:169:ASN:N	2.44	0.46
4:F:180:LEU:HD11	4:F:191:LEU:HD11	1.97	0.46
1:B:1065:SER:HB3	1:B:1074:SER:HB2	1.98	0.46
3:D:77:LEU:HG	3:D:79:MET:SD	2.55	0.46
4:F:271:VAL:HG21	4:F:300:VAL:HG11	1.98	0.46
1:A:475:ILE:HG12	1:A:493:LEU:HD23	1.98	0.45
1:C:1465:ARG:NH2	1:C:1539:GLU:OE1	2.35	0.45
1:B:1342:HIS:CD2	1:B:1360:PHE:CZ	3.04	0.45
4:G:1219:ARG:NE	4:G:1221:GLU:OE1	2.36	0.45
1:A:134:PHE:CD1	1:A:134:PHE:C	2.95	0.45
1:A:573:LEU:HD22	1:A:591:LEU:HD22	1.98	0.45
2:E:510:ARG:HD2	4:G:744:LEU:HD11	1.97	0.45
2:E:675:CYS:HB3	2:E:705:CYS:HB2	1.73	0.45
4:G:1266:TYR:CZ	4:G:1275:VAL:HG11	2.52	0.45
1:A:384:PHE:HD2	1:A:435:ILE:HD11	1.81	0.45
3:D:8:GLY:HA3	3:D:20:LEU:HD13	1.98	0.45
1:C:1598:GLN:N	1:C:1598:GLN:OE1	2.50	0.45
4:F:294:GLU:C	4:F:296:GLY:H	2.24	0.45
1:C:1614:MET:HA	1:C:1614:MET:HE2	1.99	0.45
4:F:355:ILE:HD12	4:F:426:THR:HG23	1.98	0.45
1:C:1722:ARG:O	1:C:1722:ARG:NE	2.49	0.45
3:D:97:ARG:HD2	3:D:99:ARG:NH2	2.29	0.45
4:G:1311:ILE:HD11	4:G:1320:ARG:HG3	1.99	0.45
4:G:871:ALA:HB1	4:G:908:GLN:HE21	1.81	0.45
2:E:518:TRP:HE3	2:E:535:ILE:HD11	1.81	0.44
1:B:805:THR:HA	1:B:828:ARG:HA	1.99	0.44
4:F:96:PHE:CZ	4:F:104:LYS:HB2	2.52	0.44
1:C:1592:GLU:HG2	1:B:878:ALA:HA	1.98	0.44
4:F:368:MET:SD	4:F:457:HIS:HB2	2.57	0.44
4:G:1010:CYS:SG	4:G:1011:GLY:N	2.90	0.44
4:G:1036:LYS:HD3	4:G:1314:GLU:HA	1.99	0.44
4:F:42:MET:SD	4:F:57:VAL:HG21	2.57	0.44
4:G:958:GLN:NE2	4:G:960:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:675:LEU:O	4:G:679:ARG:HG3	2.18	0.44
4:G:1046:LEU:HD13	4:G:1093:ILE:HG22	1.99	0.44
2:E:721:LYS:CE	2:E:723:PRO:HD2	2.48	0.44
2:E:740:ARG:HE	2:E:749:PHE:HB3	1.82	0.44
4:F:460:VAL:HG13	4:F:471:LEU:HD11	1.99	0.44
2:E:249:ARG:HG3	2:E:460:ASP:OD2	2.17	0.44
2:E:249:ARG:NH2	2:E:462:ILE:HD12	2.33	0.44
2:E:608:LEU:HD23	2:E:613:VAL:HG21	2.00	0.44
4:G:811:ASP:OD1	4:G:811:ASP:N	2.45	0.44
1:C:1572:ALA:HB1	1:C:1573:PRO:HD2	1.99	0.44
1:B:1325:ARG:NH1	1:B:1373:ASN:O	2.50	0.44
1:B:1340:LYS:HG2	1:B:1342:HIS:NE2	2.33	0.44
1:B:1349:ARG:HG2	1:B:1354:LEU:HD22	1.99	0.44
1:B:1396:ASP:OD1	1:B:1396:ASP:N	2.42	0.43
4:F:563:LEU:HD22	4:G:808:SER:HB3	2.00	0.43
4:G:853:ASN:ND2	4:G:890:PRO:HA	2.33	0.43
1:A:665:LYS:HE3	1:A:665:LYS:HA	2.00	0.43
4:F:45:GLU:OE2	4:F:491:THR:HG21	2.18	0.43
4:F:603:PHE:HE2	4:G:805:LEU:HD21	1.83	0.43
1:B:1411:MET:SD	1:B:1411:MET:O	2.76	0.43
4:F:459:SER:OG	4:F:474:ASN:HB2	2.18	0.43
1:A:507:TYR:CZ	1:A:519:ASN:HB3	2.53	0.43
2:E:350:MET:HE1	2:E:392:ILE:HG23	2.00	0.43
4:F:32:ASN:ND2	4:F:657:ARG:HD3	2.34	0.43
4:F:605:LEU:O	4:F:608:LYS:NZ	2.51	0.43
4:G:1043:GLN:O	4:G:1047:GLU:HG2	2.19	0.43
4:G:1049:ILE:HG22	4:G:1093:ILE:HD13	1.99	0.43
2:E:356:LEU:HD23	2:E:357:LEU:N	2.34	0.43
1:B:946:TYR:CE2	1:B:958:LEU:HD13	2.53	0.43
3:D:95:ASP:OD2	3:D:99:ARG:NH2	2.51	0.43
3:D:97:ARG:HD2	3:D:99:ARG:HE	1.84	0.43
4:F:372:LEU:HD11	4:F:411:ILE:HG22	1.98	0.43
4:G:1522:LYS:HA	4:G:1522:LYS:HD2	1.88	0.43
2:E:722:VAL:HB	2:E:723:PRO:HD3	2.01	0.43
3:D:30:MET:HE2	3:D:75:VAL:HG13	2.01	0.43
3:D:47:ILE:HD13	3:D:68:ARG:HG3	1.99	0.43
4:G:937:ARG:HE	5:G:1701:NAG:H81	1.82	0.43
2:E:287:PHE:O	2:E:288:GLU:HG3	2.19	0.43
2:E:666:SER:OG	2:E:667:GLY:N	2.52	0.43
4:G:761:ILE:HD12	4:G:761:ILE:H	1.83	0.43
4:G:1218:ASN:ND2	4:G:1251:PRO:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:ILE:HD12	1:B:1049:ILE:HA	1.89	0.43
4:G:952:LEU:HD22	4:G:1254:ARG:HH22	1.83	0.43
4:G:844:GLN:HA	4:G:901:VAL:HG12	2.01	0.43
4:G:1505:LEU:HD12	4:G:1510:LEU:HB3	2.01	0.43
2:E:735:MET:HE3	2:E:735:MET:HB3	1.94	0.42
4:F:294:GLU:O	4:F:295:ASP:HB3	2.18	0.42
4:G:1262:TYR:CD1	4:G:1262:TYR:N	2.87	0.42
4:G:1522:LYS:HG3	4:G:1524:ASP:H	1.84	0.42
1:A:606:THR:OG1	1:B:805:THR:O	2.33	0.42
4:G:1397:ASP:OD1	4:G:1397:ASP:N	2.52	0.42
1:B:761:LEU:HD11	1:B:1410:THR:HG21	2.01	0.42
2:E:343:LEU:HB3	2:E:388:ALA:HB1	2.00	0.42
2:E:600:CYS:HA	2:E:603:HIS:HB2	2.02	0.42
4:G:960:GLU:HB2	4:G:1332:VAL:HB	2.01	0.42
2:E:479:PRO:HB2	2:E:578:ARG:H	1.85	0.42
1:B:958:LEU:HD23	1:B:958:LEU:HA	1.85	0.42
1:C:1488:VAL:HG12	1:C:1554:ALA:HB1	2.02	0.42
1:A:43:LEU:N	1:A:81:ASP:O	2.43	0.42
2:E:503:LEU:HD21	2:E:696:LEU:HD22	2.02	0.42
4:G:1148:LEU:HD12	4:G:1148:LEU:HA	1.84	0.42
1:C:1590:CYS:HB2	1:B:876:CYS:HB2	2.00	0.42
1:B:1289:LEU:HD23	1:B:1289:LEU:HA	1.91	0.42
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.89	0.41
1:A:629:ASN:OD1	1:A:629:ASN:C	2.63	0.41
4:F:74:THR:HG22	4:F:75:VAL:N	2.35	0.41
4:G:1015:MET:HG3	4:G:1081:TYR:CE2	2.55	0.41
1:B:963:ASN:OD1	1:B:963:ASN:N	2.47	0.41
4:G:1194:TYR:HA	4:G:1239:ALA:HB2	2.02	0.41
4:G:1635:ASP:N	4:G:1635:ASP:OD1	2.51	0.41
1:B:859:LEU:HD12	1:B:863:LEU:HD11	2.01	0.41
2:E:358:GLY:O	2:E:361:THR:OG1	2.37	0.41
4:F:258:ARG:HA	4:F:265:VAL:HG23	2.02	0.41
4:F:495:MET:HE3	4:F:495:MET:HB3	1.78	0.41
1:A:135:SER:OG	1:A:136:SER:N	2.53	0.41
1:C:1556:LEU:HD21	1:B:1397:LEU:HD22	2.02	0.41
1:B:1214:HIS:O	1:B:1218:MET:HG3	2.20	0.41
4:F:375:PHE:HA	4:F:405:GLY:O	2.21	0.41
1:A:99:LEU:HD22	1:A:134:PHE:CE2	2.55	0.41
1:C:1515:PHE:CD1	1:C:1515:PHE:C	2.98	0.41
4:G:1196:LEU:O	4:G:1200:GLY:N	2.53	0.41
1:B:1098:GLU:HA	1:B:1101:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:353:TYR:O	4:F:437:ALA:HB2	2.21	0.41
4:G:1004:ILE:HD12	4:G:1006:THR:OG1	2.20	0.41
2:E:252:HIS:NE2	2:E:292:SER:OG	2.49	0.41
4:G:765:SER:O	4:G:765:SER:OG	2.38	0.41
4:G:1018:MET:HE2	4:G:1018:MET:HB3	1.84	0.41
4:G:1141:MET:HE2	4:G:1141:MET:HB2	1.94	0.41
1:A:255:VAL:HG12	1:A:257:GLY:H	1.85	0.41
2:E:300:SER:OG	2:E:336:GLY:N	2.52	0.41
2:E:704:PRO:HB2	2:E:714:ARG:HG2	2.03	0.41
1:B:1153:LEU:HA	1:B:1156:PHE:CD2	2.54	0.41
1:B:1365:LYS:HD2	1:B:1365:LYS:HA	1.88	0.41
3:D:79:MET:SD	3:D:79:MET:N	2.93	0.41
4:F:164:MET:HE2	4:F:211:GLU:HG3	2.02	0.41
4:F:588:ASP:C	4:F:588:ASP:OD1	2.64	0.41
1:A:549:HIS:O	1:A:549:HIS:ND1	2.54	0.41
1:A:274:LYS:HD2	1:A:274:LYS:HA	1.95	0.40
2:E:284:ILE:HG12	2:E:449:PHE:HZ	1.86	0.40
4:G:920:PHE:O	4:G:920:PHE:CD1	2.74	0.40
1:A:280:ALA:HB2	1:A:305:LEU:HD11	2.03	0.40
4:G:776:GLU:N	4:G:776:GLU:OE1	2.54	0.40
4:G:1034:TRP:HB3	4:G:1039:LEU:HD13	2.04	0.40
4:G:1354:ASP:N	4:G:1354:ASP:OD1	2.54	0.40
4:F:384:ALA:HB1	4:F:387:VAL:HG21	2.04	0.40
2:E:519:ARG:HH12	2:E:534:LEU:HD21	1.86	0.40
1:B:1097:PRO:O	1:B:1101:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	649/1744 (37%)	623 (96%)	26 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	606/1744 (35%)	584 (96%)	22 (4%)	0	100	100
1	C	279/1744 (16%)	261 (94%)	18 (6%)	0	100	100
2	E	506/752 (67%)	484 (96%)	22 (4%)	0	100	100
3	D	112/120 (93%)	102 (91%)	10 (9%)	0	100	100
4	F	634/1663 (38%)	615 (97%)	19 (3%)	0	100	100
4	G	974/1663 (59%)	937 (96%)	37 (4%)	0	100	100
All	All	3760/9430 (40%)	3606 (96%)	154 (4%)	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	557/1480 (38%)	550 (99%)	7 (1%)	61	72
1	B	514/1480 (35%)	512 (100%)	2 (0%)	84	81
1	C	240/1480 (16%)	236 (98%)	4 (2%)	53	70
2	E	446/646 (69%)	443 (99%)	3 (1%)	76	78
3	D	96/98 (98%)	94 (98%)	2 (2%)	47	66
4	F	563/1468 (38%)	554 (98%)	9 (2%)	55	70
4	G	871/1468 (59%)	863 (99%)	8 (1%)	70	76
All	All	3287/8120 (40%)	3252 (99%)	35 (1%)	63	74

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	CYS
1	A	130	ILE
1	A	344	ILE
1	A	352	MET
1	A	360	TRP

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Mol	Chain	Res	Type
1	A	487	ASP
1	A	509	ILE
1	C	1475	ASN
1	C	1602	LEU
1	C	1666	ASN
1	C	1723	GLN
2	E	514	ASP
2	E	649	PHE
2	E	727	ASP
1	B	758	LEU
1	B	1049	ILE
3	D	43	PHE
3	D	65	THR
4	F	186	LEU
4	F	333	HIS
4	F	422	ILE
4	F	441	MET
4	F	493	LEU
4	F	553	VAL
4	F	555	VAL
4	F	573	ARG
4	F	576	VAL
4	G	707	CYS
4	G	856	GLN
4	G	911	GLU
4	G	1362	ASP
4	G	1397	ASP
4	G	1557	ASP
4	G	1568	THR
4	G	1656	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	302	GLN
1	A	454	HIS
2	E	312	ASN
2	E	489	GLN
1	B	1013	GLN
1	B	1157	GLN
1	B	1348	ASN

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Mol	Chain	Res	Type
4	F	184	ASN
4	F	378	ASN
4	F	457	HIS
4	F	652	GLN
4	G	884	GLN
4	G	1055	GLN
4	G	1242	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](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	NAG	E	804	2	14,14,15	0.72	0	17,19,21	0.81	0
5	NAG	A	1801	1	14,14,15	0.76	0	17,19,21	1.02	1 (5%)
5	NAG	E	803	2	14,14,15	0.77	0	17,19,21	1.33	2 (11%)
5	NAG	F	1701	4	14,14,15	0.70	0	17,19,21	1.18	2 (11%)
5	NAG	G	1701	4	14,14,15	0.70	0	17,19,21	2.13	2 (11%)
5	NAG	E	805	2	14,14,15	0.73	0	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	802	2	14,14,15	0.69	0	17,19,21	1.37	1 (5%)
5	NAG	B	1801	1	14,14,15	0.97	1 (7%)	17,19,21	2.71	5 (29%)

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	NAG	E	804	2	-	0/6/23/26	0/1/1/1
5	NAG	A	1801	1	-	2/6/23/26	0/1/1/1
5	NAG	E	803	2	-	2/6/23/26	0/1/1/1
5	NAG	F	1701	4	-	1/6/23/26	0/1/1/1
5	NAG	G	1701	4	-	1/6/23/26	0/1/1/1
5	NAG	E	805	2	-	3/6/23/26	0/1/1/1
5	NAG	E	802	2	-	1/6/23/26	0/1/1/1
5	NAG	B	1801	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1801	NAG	C1-C2	2.83	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1801	NAG	C2-N2-C7	8.15	133.82	122.90
5	G	1701	NAG	C2-N2-C7	7.33	132.73	122.90
5	B	1801	NAG	C1-O5-C5	5.33	119.33	112.19
5	E	802	NAG	C2-N2-C7	3.78	127.96	122.90
5	E	803	NAG	C1-O5-C5	3.50	116.88	112.19
5	B	1801	NAG	C1-C2-N2	3.08	115.29	110.43
5	G	1701	NAG	O7-C7-N2	2.89	127.09	121.98
5	B	1801	NAG	C8-C7-N2	2.73	120.64	116.12
5	E	803	NAG	C2-N2-C7	2.72	126.54	122.90
5	F	1701	NAG	O5-C1-C2	-2.44	107.51	111.29
5	F	1701	NAG	C1-C2-N2	-2.34	106.75	110.43
5	A	1801	NAG	C1-O5-C5	2.30	115.26	112.19
5	E	805	NAG	C2-N2-C7	2.15	125.78	122.90
5	B	1801	NAG	O7-C7-C8	-2.04	118.42	122.05

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	802	NAG	C1-C2-N2-C7
5	G	1701	NAG	C3-C2-N2-C7
5	A	1801	NAG	C8-C7-N2-C2
5	A	1801	NAG	O7-C7-N2-C2
5	E	803	NAG	C8-C7-N2-C2
5	E	803	NAG	O7-C7-N2-C2
5	E	805	NAG	C8-C7-N2-C2
5	E	805	NAG	O7-C7-N2-C2
5	B	1801	NAG	C8-C7-N2-C2
5	B	1801	NAG	O7-C7-N2-C2
5	E	805	NAG	O5-C5-C6-O6
5	F	1701	NAG	O5-C5-C6-O6
5	B	1801	NAG	C3-C2-N2-C7
5	B	1801	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	803	NAG	1	0
5	F	1701	NAG	1	0
5	G	1701	NAG	1	0

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.

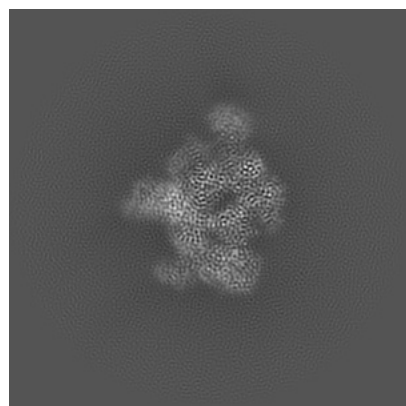
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53217. These allow visual inspection of the internal detail of the map and identification of artifacts.

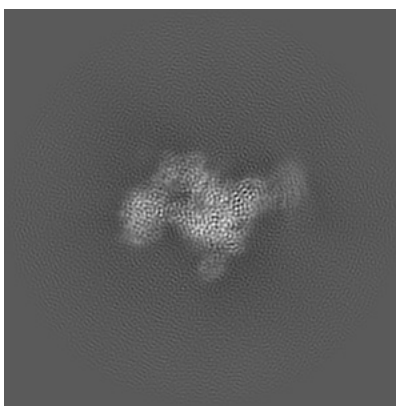
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

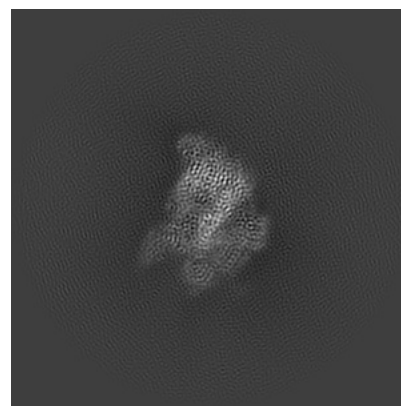
6.1.1 Primary map



X

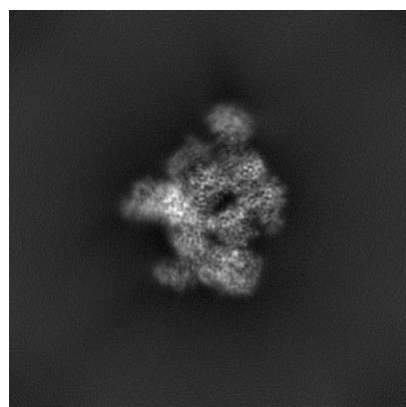


Y

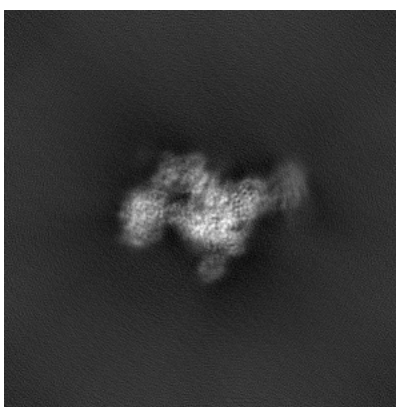


Z

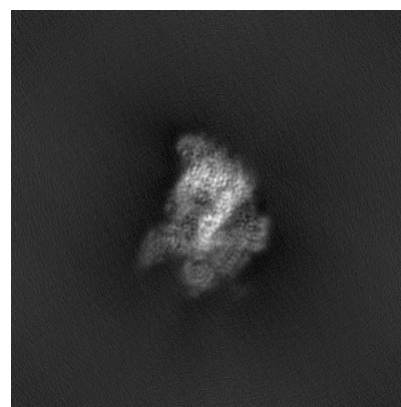
6.1.2 Raw map



X



Y

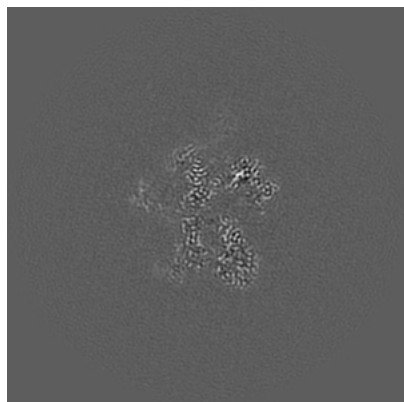


Z

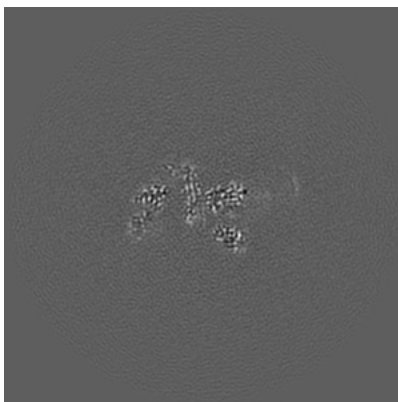
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

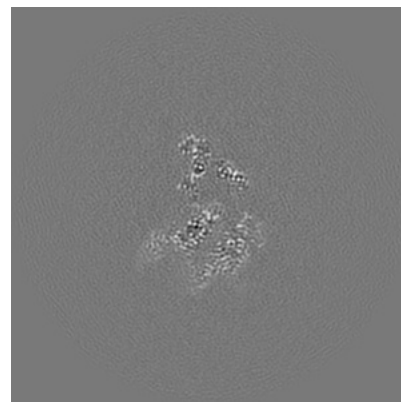
6.2.1 Primary map



X Index: 190

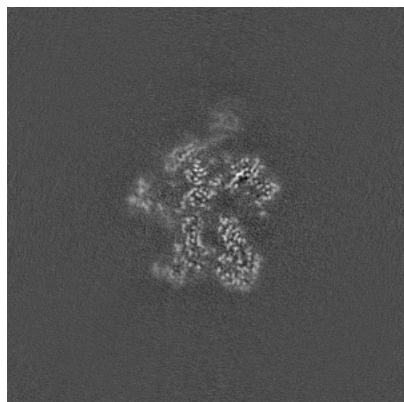


Y Index: 190

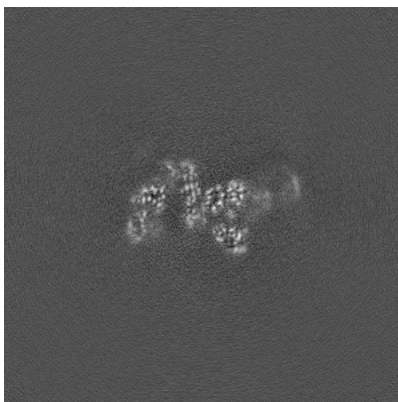


Z Index: 190

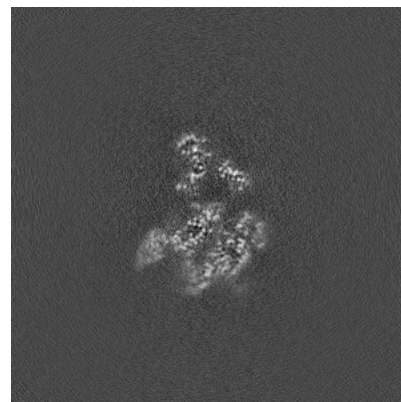
6.2.2 Raw map



X Index: 190



Y Index: 190

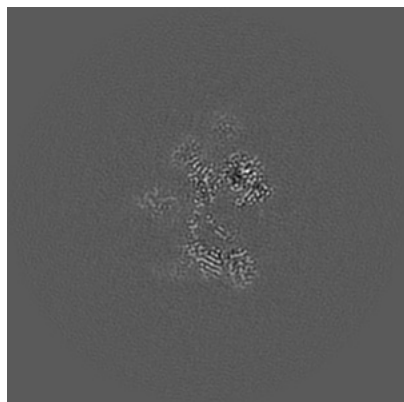


Z Index: 190

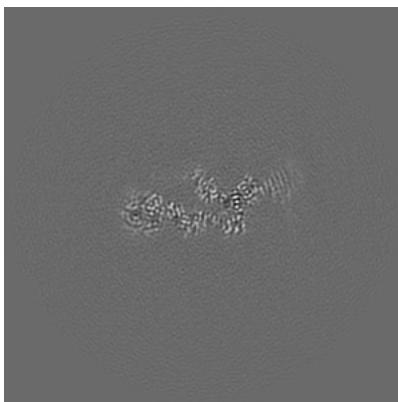
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

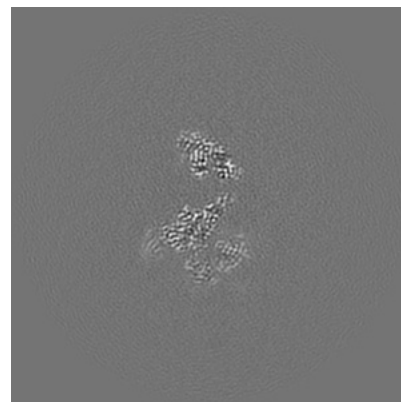
6.3.1 Primary map



X Index: 196

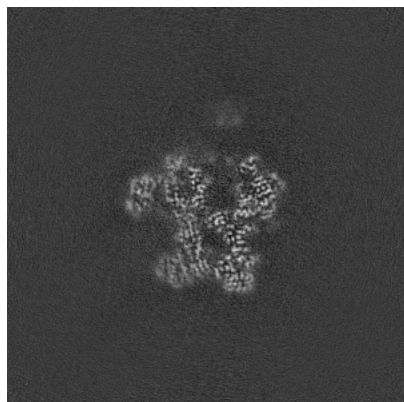


Y Index: 220



Z Index: 199

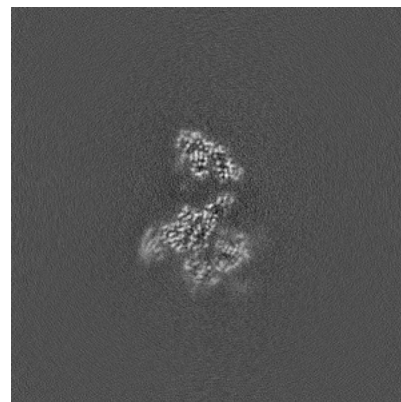
6.3.2 Raw map



X Index: 183



Y Index: 215

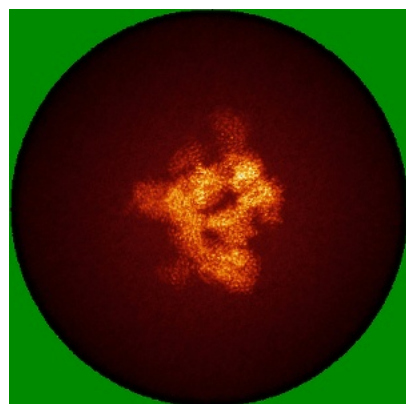


Z Index: 199

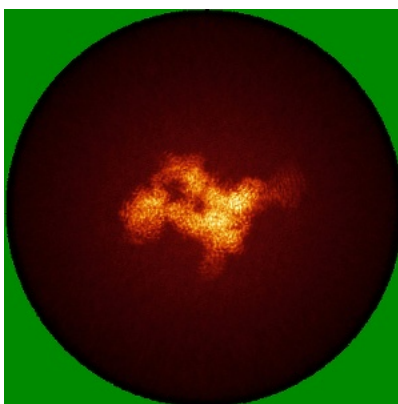
The images above show the largest variance slices of the map in three orthogonal directions.

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

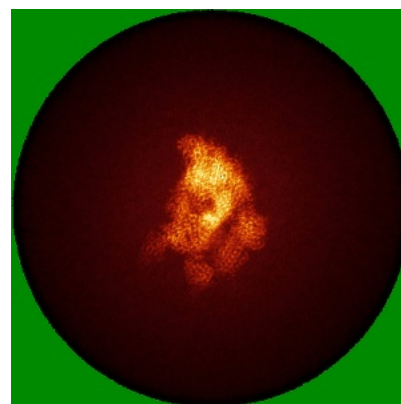
6.4.1 Primary map



X

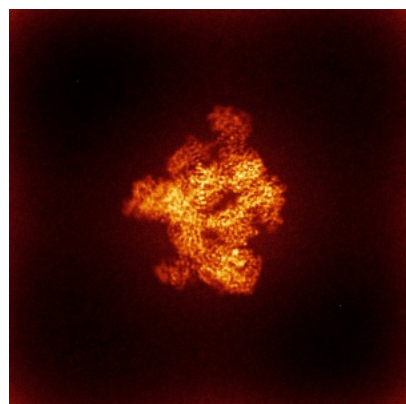


Y

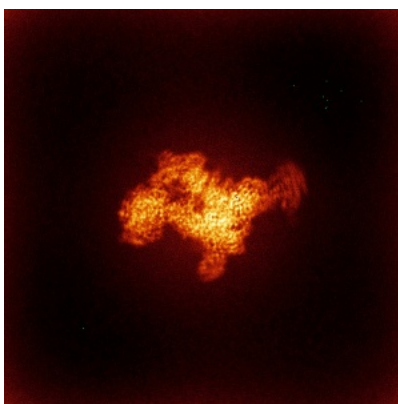


Z

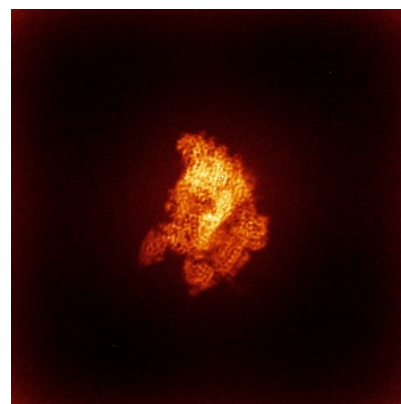
6.4.2 Raw map



X



Y

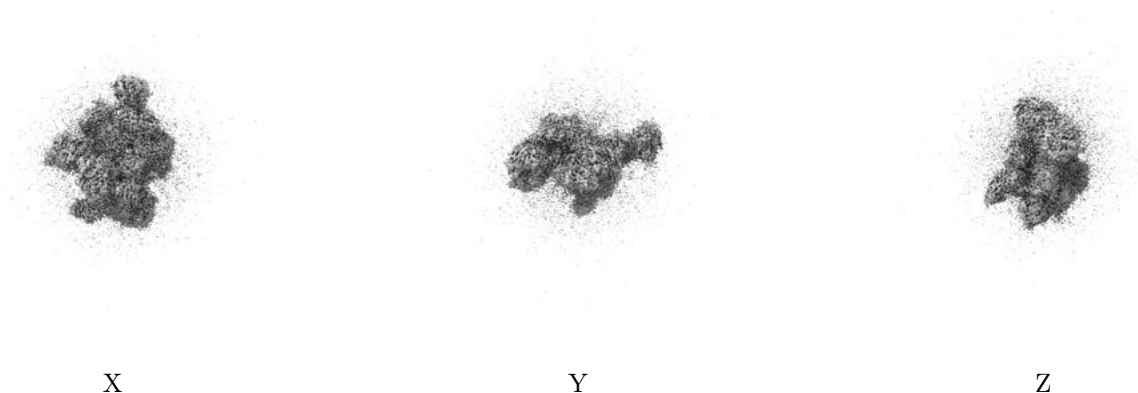


Z

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.

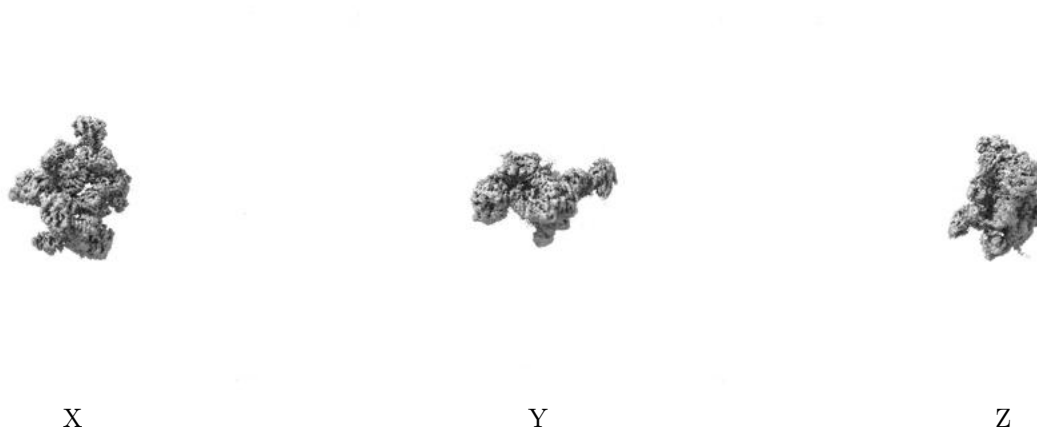
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.199. 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.

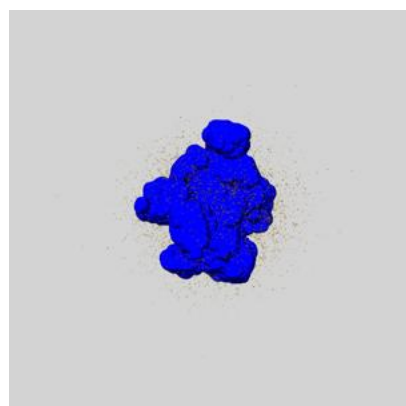
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

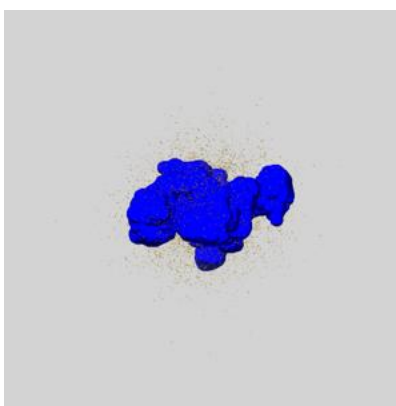
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

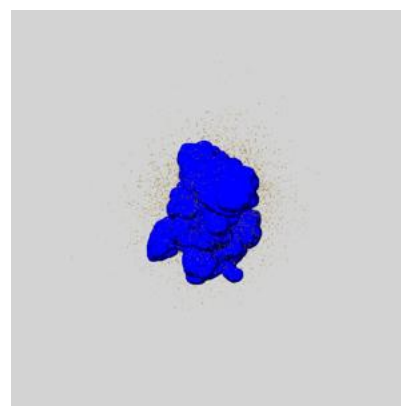
6.6.1 emd_53217_msk_1.map [i](#)



X

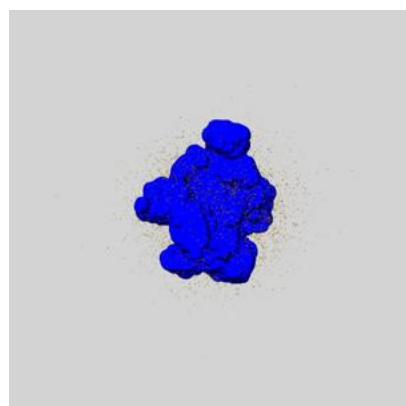


Y

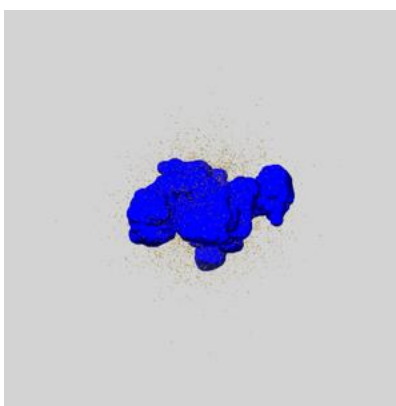


Z

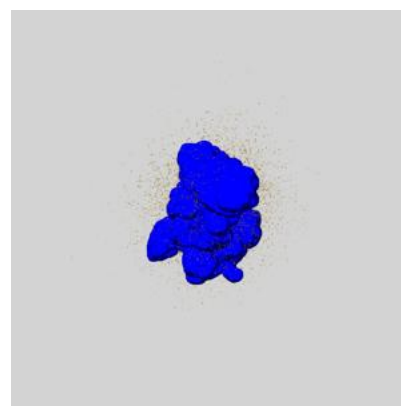
6.6.2 emd_53217_msk_2.map [i](#)



X



Y

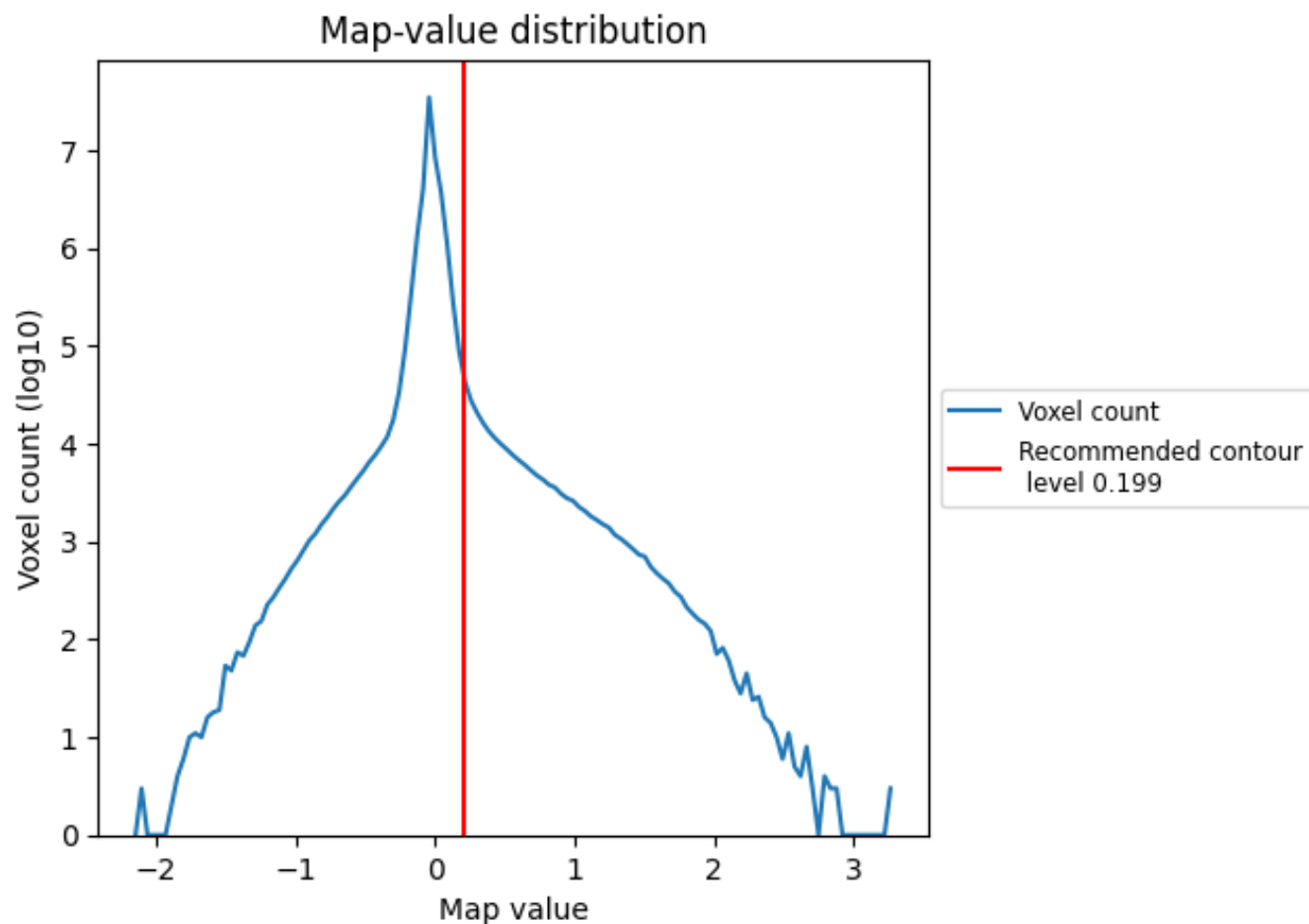


Z

7 Map analysis [i](#)

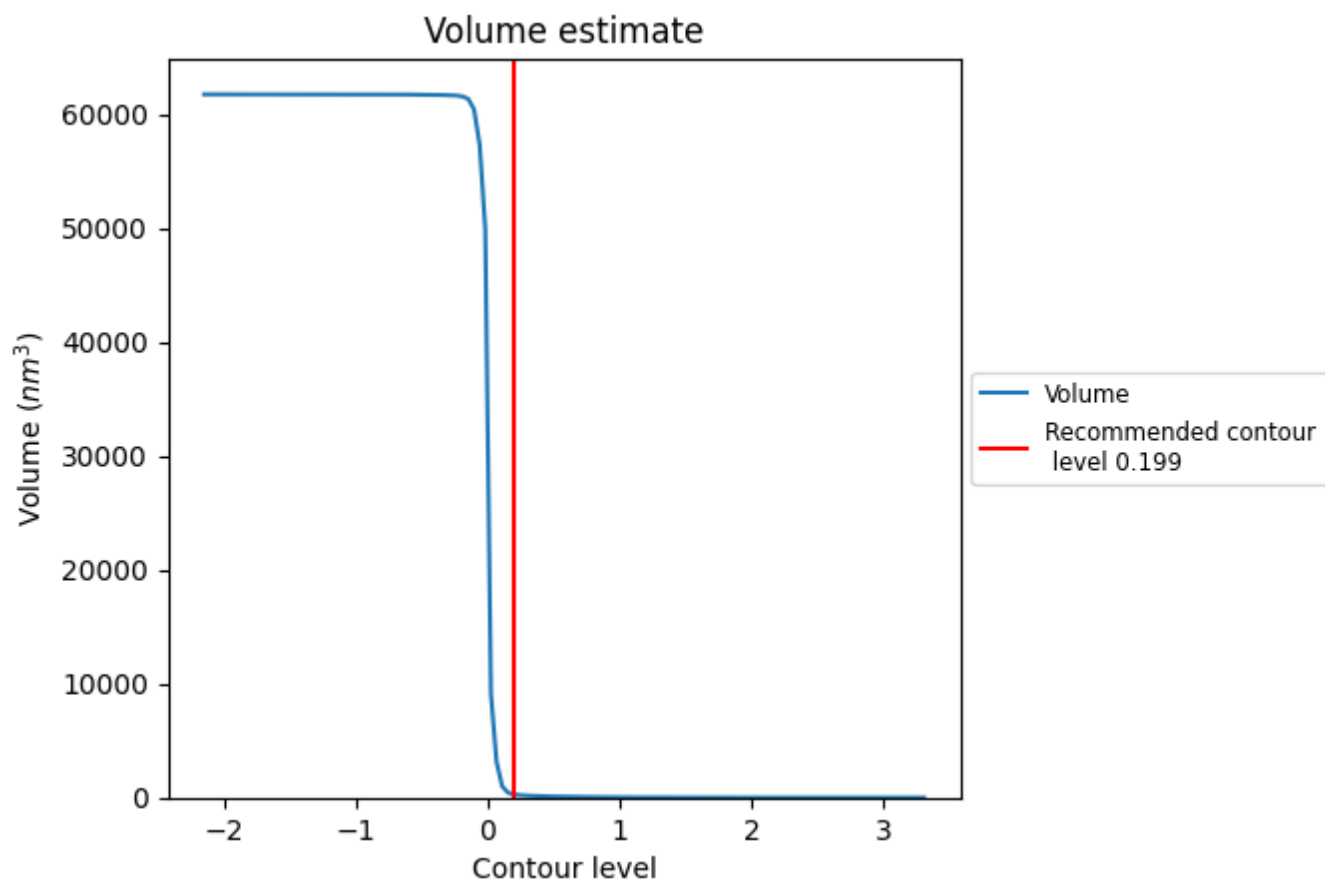
This section contains the results of statistical analysis of the map.

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.

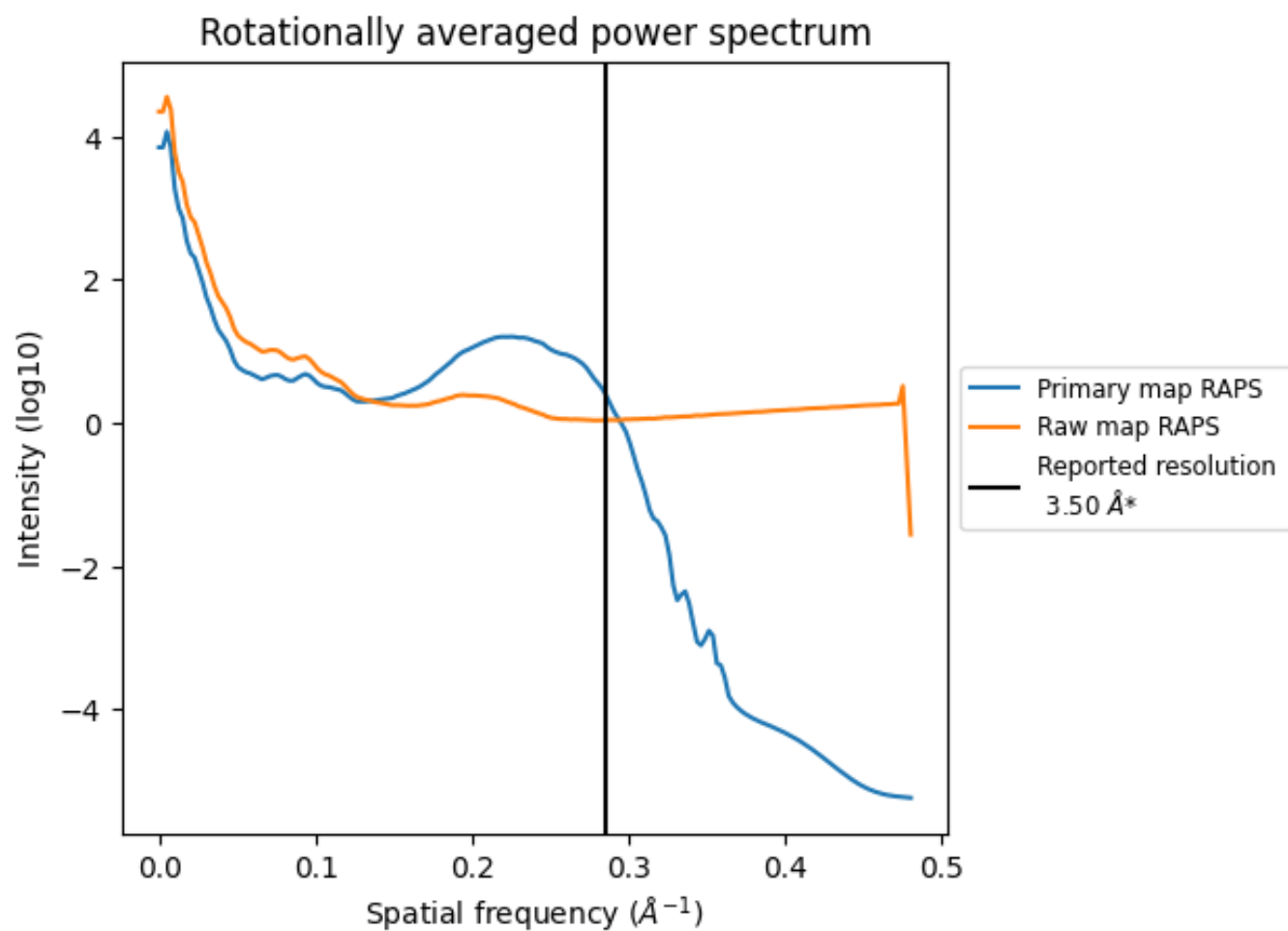
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 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 ⓘ

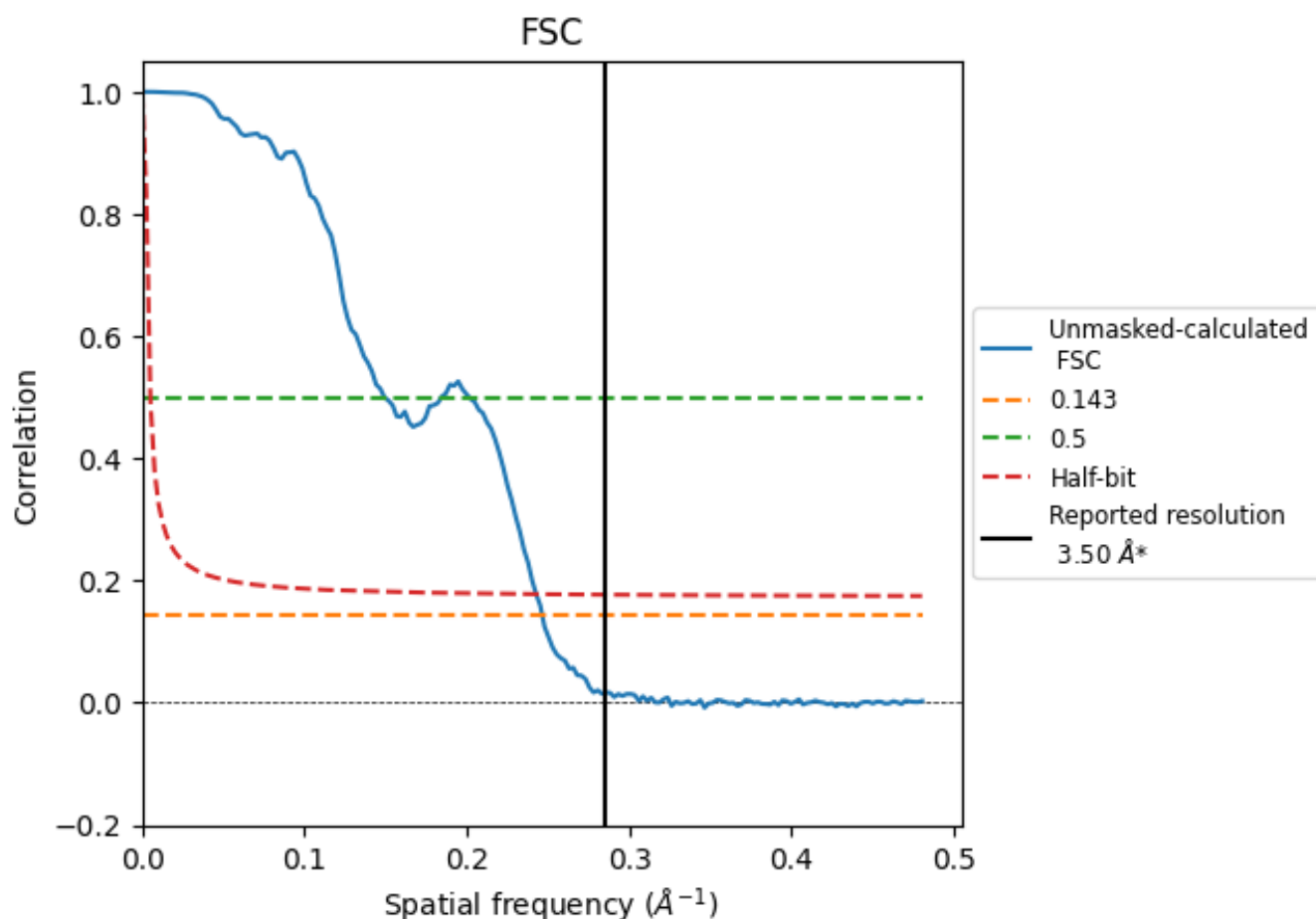


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

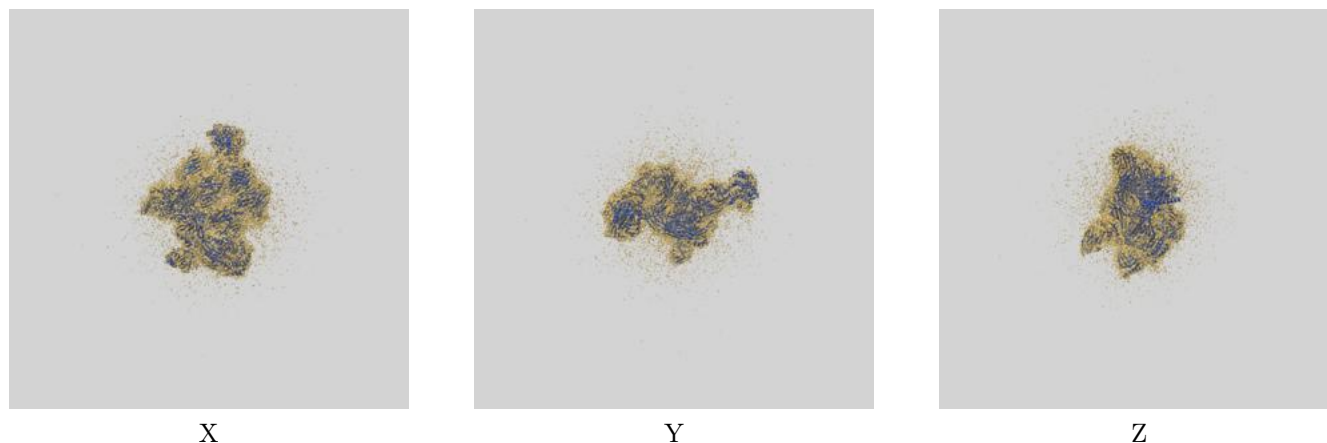
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	6.70	4.12

*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 4.06 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

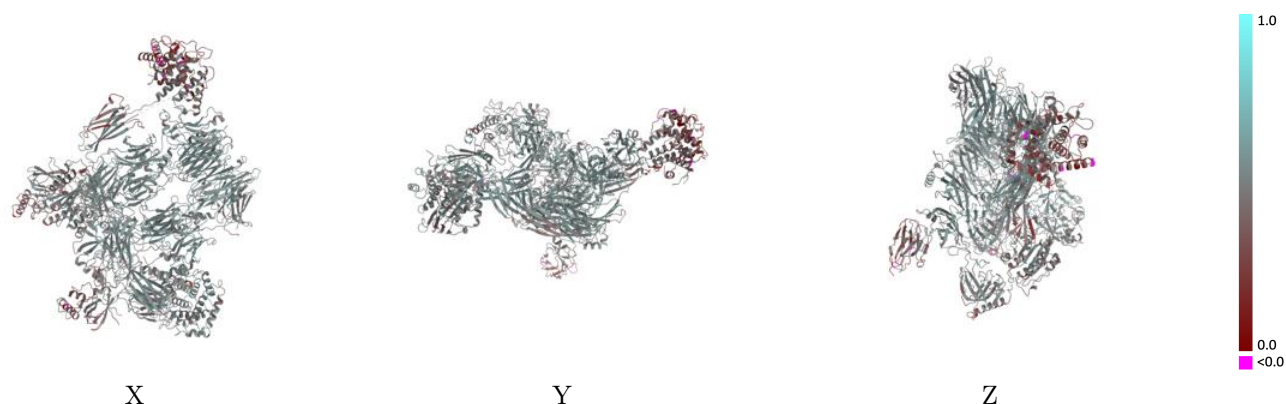
This section contains information regarding the fit between EMDB map EMD-53217 and PDB model 9QK2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



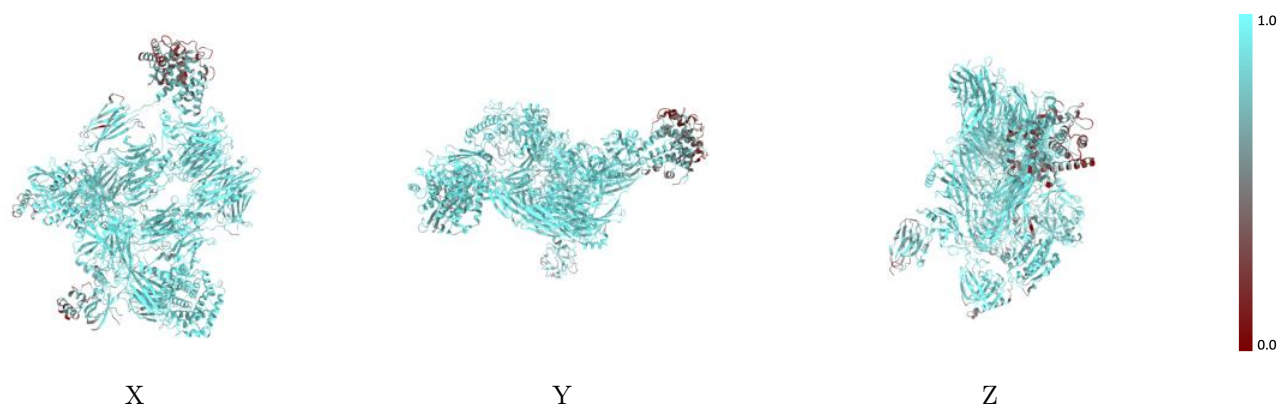
The images above show the 3D surface view of the map at the recommended contour level 0.199 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



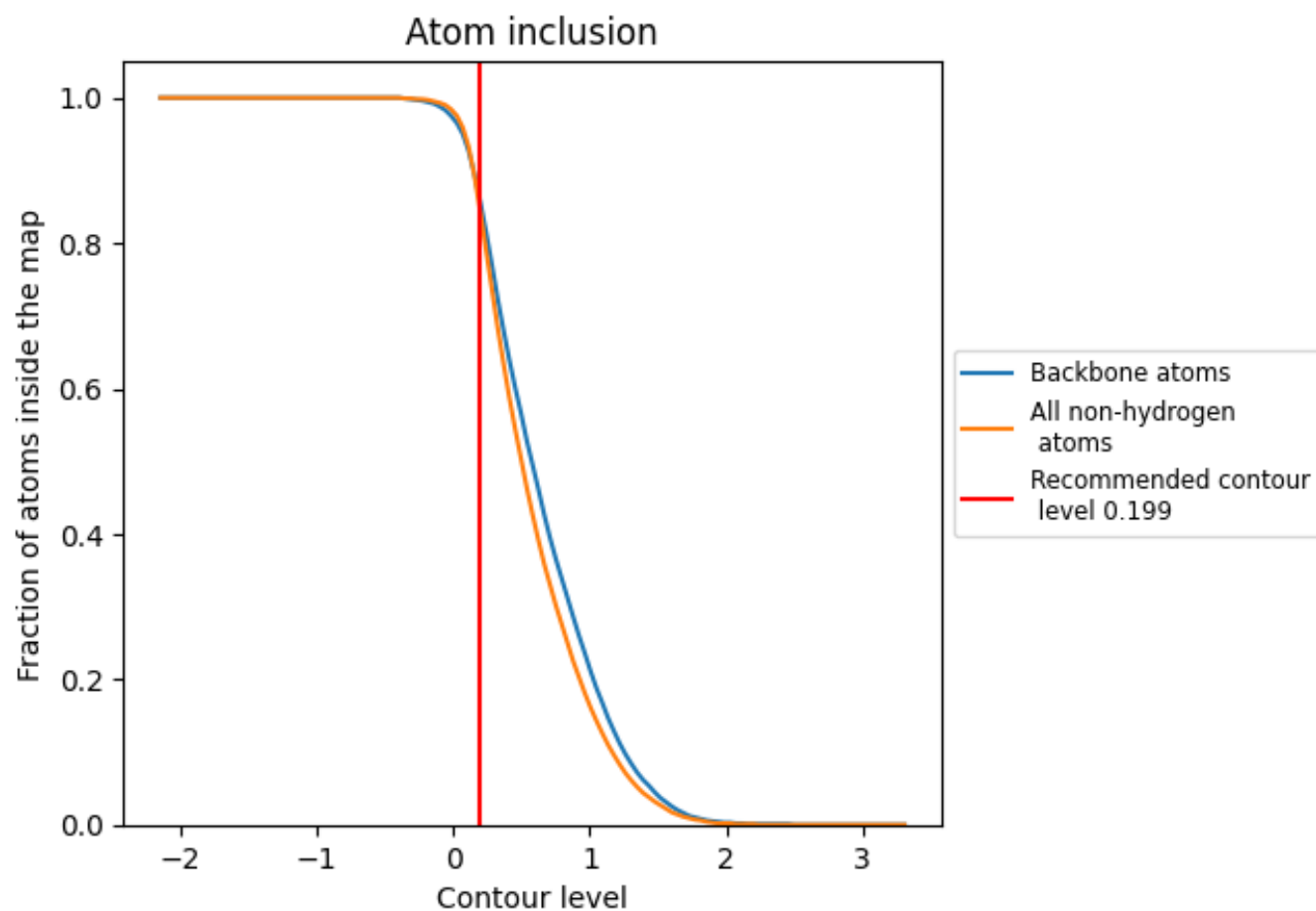
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.199).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.199) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8410	0.4860
A	0.9130	0.5310
B	0.7220	0.4260
C	0.8500	0.4810
D	0.6650	0.3280
E	0.8630	0.4890
F	0.8980	0.5260
G	0.8370	0.4860

1.0

0.0

<0.0