Full wwPDB EM Validation Report ⓘ

Mar 17, 2025 – 08:29 AM EDT

PDB ID	:	9B13
EMDB ID	:	EMD-44064
Title	:	Cryo-EM structure of phospholipase Cepsilon PH-COOH in complex with an antigen-binding fragment (composite structure)
Authors	:	Samassekou, K.; Lyon, A.M.
Deposited on	:	2024-03-12
Resolution	:	3.90 Å(reported)

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:

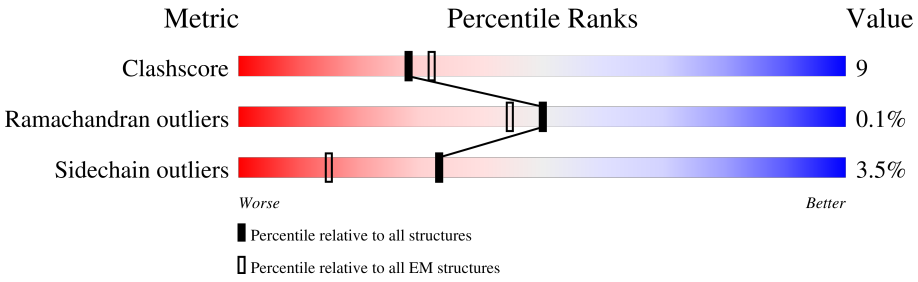
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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 <=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	1469	44% 12% 43%
2	H	264	9% 65% 19% 14%
3	L	238	21% 69% 17% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10013 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 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase epsilon-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	842	Total	C	N	O	S	0	0
			6745	4304	1154	1248	39		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	813	MET	-	initiating methionine	UNP Q99P84
A	814	HIS	-	expression tag	UNP Q99P84
A	815	HIS	-	expression tag	UNP Q99P84
A	816	HIS	-	expression tag	UNP Q99P84
A	817	HIS	-	expression tag	UNP Q99P84
A	818	HIS	-	expression tag	UNP Q99P84
A	819	HIS	-	expression tag	UNP Q99P84
A	820	SER	-	expression tag	UNP Q99P84
A	821	SER	-	expression tag	UNP Q99P84
A	822	GLY	-	expression tag	UNP Q99P84
A	823	VAL	-	expression tag	UNP Q99P84
A	824	ASP	-	expression tag	UNP Q99P84
A	825	LEU	-	expression tag	UNP Q99P84
A	826	GLY	-	expression tag	UNP Q99P84
A	827	THR	-	expression tag	UNP Q99P84
A	828	GLU	-	expression tag	UNP Q99P84
A	829	ASN	-	expression tag	UNP Q99P84
A	830	LEU	-	expression tag	UNP Q99P84
A	831	TYR	-	expression tag	UNP Q99P84
A	832	PHE	-	expression tag	UNP Q99P84
A	833	GLN	-	expression tag	UNP Q99P84
A	834	SER	-	expression tag	UNP Q99P84
A	835	ASN	-	expression tag	UNP Q99P84
A	836	ALA	-	expression tag	UNP Q99P84

- Molecule 2 is a protein called Antigen-binding fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	226	Total	C	N	O	S	0	0
			1697	1075	279	338	5		

- Molecule 3 is a protein called Antigen-binding fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	206	Total	C	N	O	S	0	0
			1570	979	266	320	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

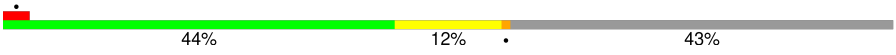
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

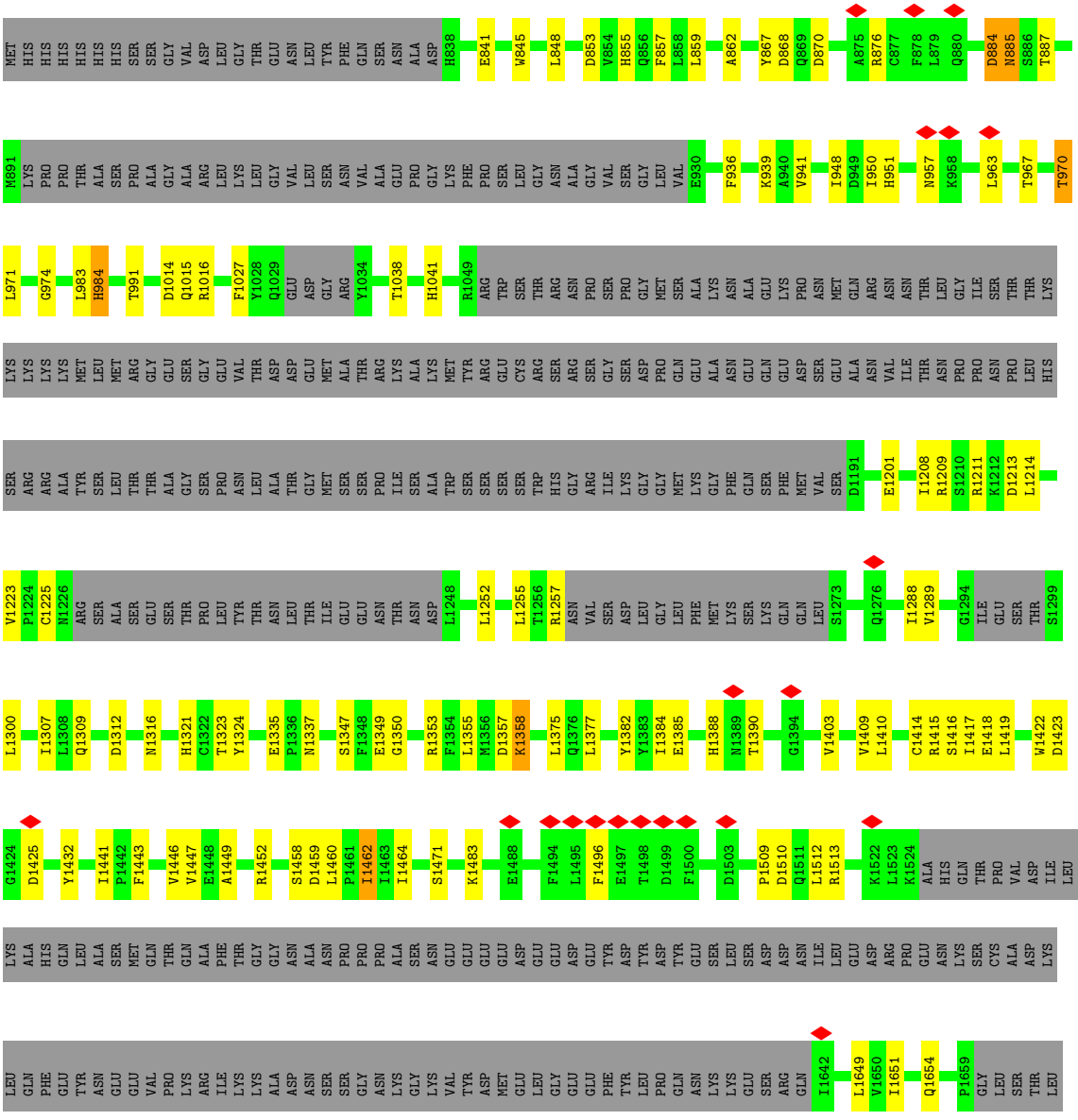
3 Residue-property plots (i)

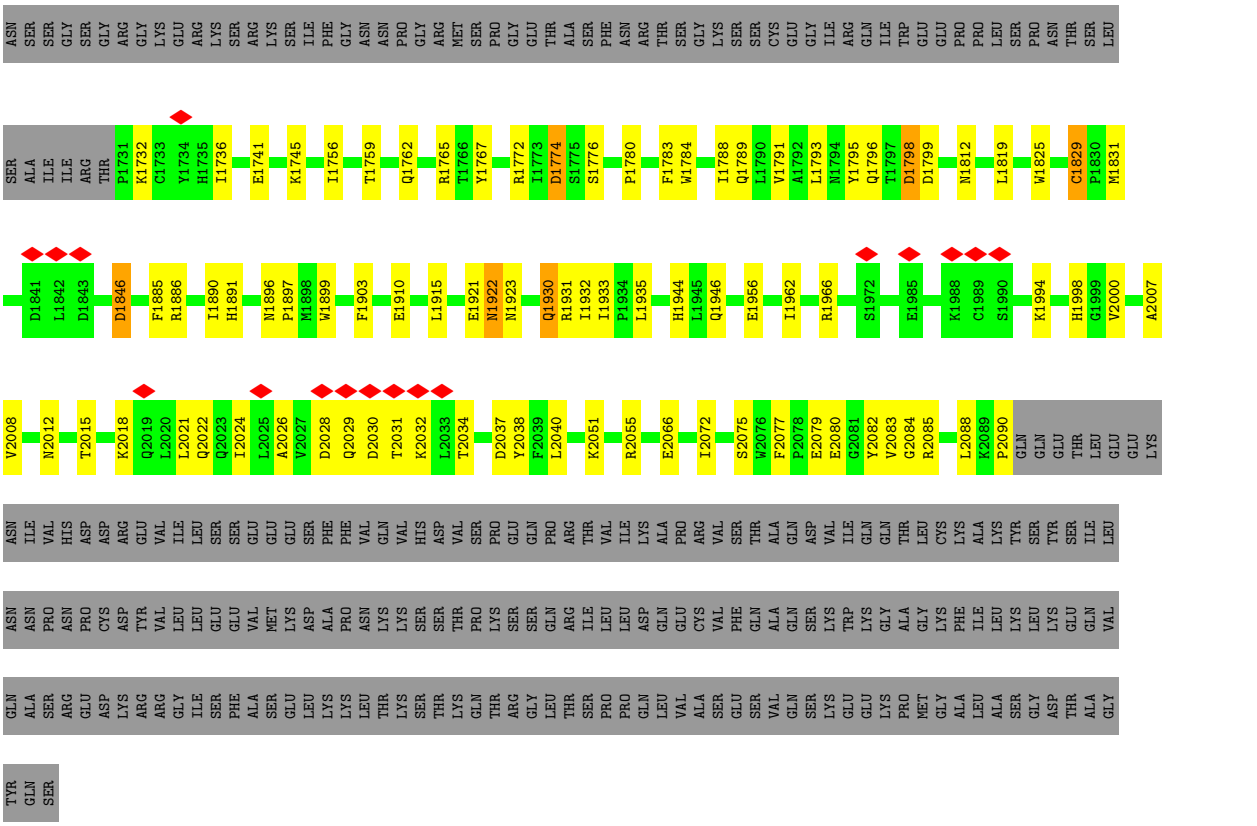
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase epsilon-1

Chain A:

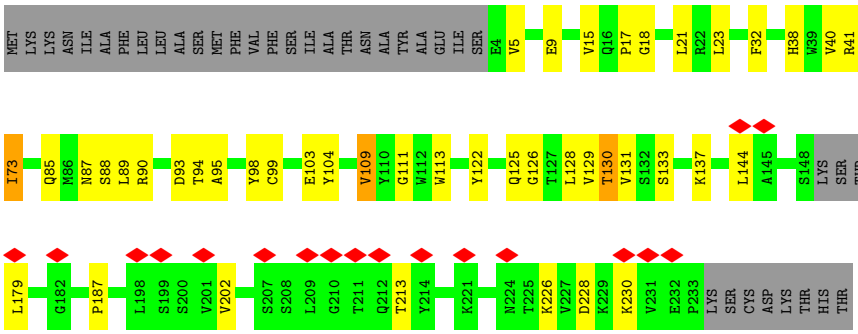






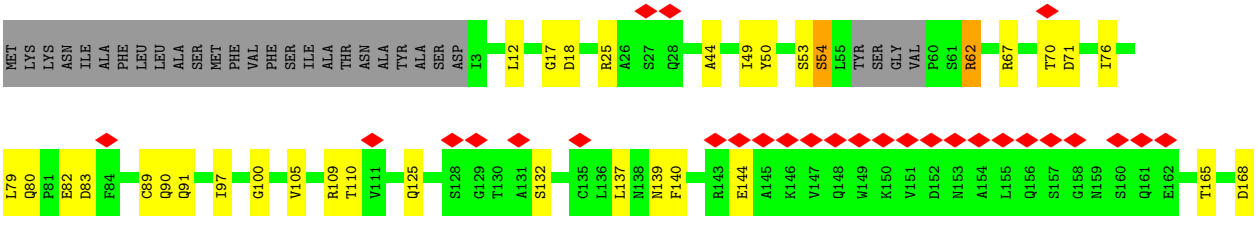
• Molecule 2: Antigen-binding fragment heavy chain

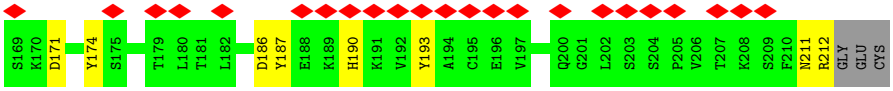
Chain H:



• Molecule 3: Antigen-binding fragment light chain

Chain L:




S169
K170
D171
Y174
S175
T179
L180
T181
L182
D186
Y187
E188
K189
H190
K191
V192
Y193
A194
C195
E196
V197
Q200
G201
L202
S203
S204
P205
V206
T207
K208
S209
F210
N211
R212
GLY
GLU
CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	147120	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 ($e^-/Å^2$)	53.75	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	51.275	Depositor
Minimum map value	-36.569	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.967	Depositor
Recommended contour level	5.34	Depositor
Map size (Å)	275.968, 275.968, 275.968	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.539, 0.539, 0.539	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/6895	0.48	0/9329
2	H	0.32	0/1742	0.47	0/2377
3	L	0.27	0/1600	0.48	0/2168
All	All	0.30	0/10237	0.48	0/13874

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	6745	0	6705	121	0
2	H	1697	0	1619	42	0
3	L	1570	0	1544	31	0
4	A	1	0	0	0	0
All	All	10013	0	9868	187	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 9.

All (187) 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:A:1225:CYS:SG	2:H:58:SER:OG	2.22	0.87
2:H:226:LYS:NZ	2:H:228:ASP:OD1	2.10	0.84
1:A:1014:ASP:OD2	1:A:1016:ARG:NH1	2.12	0.83
1:A:1335:GLU:OE2	1:A:1337:ASN:N	2.12	0.83
1:A:1316:ASN:OD1	1:A:2084:GLY:N	2.10	0.83
1:A:1796:GLN:N	1:A:1796:GLN:OE1	2.11	0.82
1:A:1772:ARG:NE	1:A:1776:SER:O	2.13	0.81
1:A:876:ARG:NH1	1:A:957:ASN:OD1	2.15	0.80
1:A:1309:GLN:N	1:A:1309:GLN:OE1	2.16	0.78
1:A:1654:GLN:N	1:A:1654:GLN:OE1	2.16	0.78
1:A:1510:ASP:OD1	1:A:1513:ARG:NE	2.15	0.78
1:A:841:GLU:OE1	1:A:845:TRP:N	2.18	0.76
1:A:1789:GLN:N	1:A:1789:GLN:OE1	2.20	0.74
1:A:2080:GLU:N	1:A:2080:GLU:OE1	2.20	0.74
2:H:41:ARG:NE	2:H:49:GLU:OE1	2.20	0.74
2:H:90:ARG:N	2:H:93:ASP:OD2	2.22	0.72
1:A:1423:ASP:OD1	1:A:1471:SER:N	2.22	0.72
1:A:2055:ARG:NH2	2:H:103:GLU:OE2	2.24	0.71
3:L:82:GLU:N	3:L:82:GLU:OE1	2.24	0.71
2:H:9:GLU:OE2	2:H:125:GLN:N	2.24	0.70
1:A:1930:GLN:OE1	1:A:1931:ARG:N	2.25	0.70
3:L:187:TYR:O	3:L:193:TYR:OH	2.10	0.69
1:A:1910:GLU:OE2	1:A:1966:ARG:NH2	2.24	0.69
3:L:49:ILE:HD12	3:L:53:SER:HA	1.75	0.69
3:L:125:GLN:OE1	3:L:132:SER:N	2.25	0.69
2:H:17:PRO:CD	2:H:133:SER:HB3	2.23	0.69
1:A:1946:GLN:NE2	1:A:1956:GLU:O	2.24	0.68
1:A:2000:VAL:HG21	1:A:2007:ALA:HB3	1.75	0.68
1:A:2012:ASN:OD1	1:A:2015:THR:OG1	2.08	0.68
1:A:867:TYR:CD2	1:A:948:ILE:HG23	2.28	0.68
3:L:140:PHE:O	3:L:174:TYR:N	2.28	0.67
1:A:1651:ILE:O	1:A:1654:GLN:NE2	2.28	0.66
1:A:1774:ASP:OD1	1:A:1774:ASP:N	2.23	0.66
2:H:50:TRP:CD1	3:L:97:ILE:HD12	2.31	0.66
1:A:2021:LEU:HD23	1:A:2024:ILE:HD12	1.78	0.66
3:L:144:GLU:N	3:L:144:GLU:OE1	2.28	0.65
1:A:1819:LEU:HD11	1:A:1825:TRP:CZ2	2.32	0.65
2:H:15:VAL:HG11	2:H:89:LEU:HD12	1.79	0.64
2:H:63:TYR:OH	2:H:73:ILE:N	2.30	0.64
2:H:72:THR:O	2:H:85:GLN:N	2.29	0.64
2:H:9:GLU:OE2	2:H:126:GLY:N	2.31	0.64
2:H:94:THR:OG1	2:H:131:VAL:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:ARG:NH2	1:A:1349:GLU:OE2	2.31	0.64
1:A:1357:ASP:OD1	1:A:1358:LYS:N	2.32	0.63
1:A:884:ASP:OD1	1:A:884:ASP:N	2.31	0.63
1:A:1732:LYS:O	1:A:1762:GLN:NE2	2.30	0.63
1:A:1388:HIS:N	1:A:1793:LEU:O	2.32	0.63
1:A:1038:THR:OG1	1:A:1041:HIS:ND1	2.32	0.62
1:A:1896:ASN:N	1:A:1896:ASN:OD1	2.33	0.62
1:A:2021:LEU:HD21	1:A:2040:LEU:HG	1.82	0.62
1:A:1312:ASP:OD2	1:A:2085:ARG:NH2	2.31	0.61
2:H:40:VAL:HG13	2:H:49:GLU:O	2.00	0.61
1:A:2038:TYR:HB3	1:A:2088:LEU:HD11	1.82	0.60
1:A:963:LEU:O	1:A:967:THR:OG1	2.07	0.60
2:H:9:GLU:N	2:H:9:GLU:OE1	2.35	0.60
3:L:168:ASP:OD2	3:L:171:ASP:N	2.33	0.60
1:A:2024:ILE:HG21	1:A:2088:LEU:HD22	1.85	0.59
1:A:867:TYR:CE2	1:A:948:ILE:HG23	2.38	0.59
1:A:941:VAL:HG13	1:A:970:THR:O	2.03	0.59
1:A:1890:ILE:HD11	1:A:1899:TRP:CD1	2.38	0.58
2:H:70:ARG:NH1	2:H:88:SER:O	2.37	0.57
1:A:1223:VAL:HG11	1:A:1309:GLN:HE21	1.69	0.57
1:A:1307:ILE:HG21	1:A:1324:TYR:CE1	2.40	0.57
2:H:95:ALA:O	2:H:128:LEU:HD12	2.06	0.56
2:H:179:LEU:HD21	2:H:202:VAL:HG21	1.87	0.56
1:A:1307:ILE:O	1:A:1307:ILE:HG22	2.04	0.56
1:A:1458:SER:OG	1:A:1459:ASP:N	2.38	0.56
1:A:2022:GLN:O	1:A:2026:ALA:N	2.37	0.55
1:A:2037:ASP:O	1:A:2090:PRO:HB3	2.06	0.55
1:A:1410:LEU:O	1:A:1415:ARG:NH2	2.40	0.55
1:A:1460:LEU:HD22	1:A:1509:PRO:HB2	1.88	0.55
2:H:137:LYS:NZ	2:H:164:ASP:O	2.37	0.55
2:H:38:HIS:CE1	3:L:97:ILE:HD11	2.43	0.54
3:L:89:CYS:O	3:L:100:GLY:N	2.40	0.54
1:A:857:PHE:CZ	1:A:862:ALA:HB2	2.42	0.54
1:A:2018:LYS:NZ	1:A:2066:GLU:OE2	2.32	0.54
2:H:21:LEU:HB3	2:H:89:LEU:HD11	1.88	0.54
1:A:1214:LEU:HD22	1:A:1355:LEU:HD12	1.91	0.53
3:L:62:ARG:HG2	3:L:76:ILE:HG23	1.90	0.53
1:A:1922:ASN:O	1:A:1923:ASN:ND2	2.42	0.53
1:A:1257:ARG:NH1	1:A:1357:ASP:OD2	2.43	0.52
1:A:1799:ASP:N	1:A:1799:ASP:OD1	2.43	0.52
2:H:50:TRP:HZ2	2:H:53:SER:HG	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1483:LYS:HE2	1:A:1649:LEU:HD21	1.91	0.52
1:A:1414:CYS:O	1:A:1415:ARG:NE	2.43	0.52
1:A:1798:ASP:N	1:A:1798:ASP:OD1	2.43	0.51
1:A:1377:LEU:N	1:A:1382:TYR:OH	2.44	0.51
1:A:1403:VAL:HG13	1:A:1446:VAL:HG22	1.91	0.51
1:A:1915:LEU:HD21	1:A:1935:LEU:HD13	1.92	0.51
1:A:1422:TRP:NE1	1:A:1432:TYR:O	2.43	0.51
1:A:885:ASN:N	1:A:885:ASN:OD1	2.44	0.51
1:A:1795:TYR:N	1:A:1796:GLN:OE1	2.44	0.50
1:A:1213:ASP:N	1:A:1213:ASP:OD1	2.44	0.50
2:H:5:VAL:HG21	2:H:122:TYR:CE2	2.47	0.50
1:A:1014:ASP:OD1	1:A:1015:GLN:N	2.45	0.50
1:A:1890:ILE:HG22	1:A:1891:HIS:H	1.76	0.49
1:A:1921:GLU:OE1	1:A:1923:ASN:N	2.39	0.49
2:H:17:PRO:HD3	2:H:133:SER:HB3	1.93	0.49
3:L:25:ARG:NH1	3:L:70:THR:OG1	2.45	0.49
1:A:2077:PHE:O	1:A:2079:GLU:N	2.44	0.49
2:H:85:GLN:NE2	2:H:87:ASN:OD1	2.44	0.49
1:A:848:LEU:HD11	1:A:885:ASN:HD22	1.78	0.49
1:A:2034:THR:O	1:A:2034:THR:HG23	2.12	0.49
2:H:50:TRP:NE1	2:H:52:ALA:O	2.37	0.48
1:A:1890:ILE:HD11	1:A:1899:TRP:HD1	1.78	0.48
2:H:5:VAL:HB	2:H:122:TYR:CE1	2.49	0.48
1:A:862:ALA:HB1	1:A:991:THR:HG23	1.96	0.48
1:A:1886:ARG:NH2	1:A:1922:ASN:OD1	2.46	0.48
1:A:2030:ASP:OD1	1:A:2031:THR:N	2.46	0.48
3:L:137:LEU:HD12	3:L:137:LEU:N	2.29	0.48
1:A:1416:SER:O	1:A:1417:ILE:HG23	2.14	0.47
2:H:15:VAL:HG11	2:H:89:LEU:CD1	2.43	0.47
1:A:1419:LEU:HD13	1:A:1464:ILE:CG2	2.45	0.47
1:A:1347:SER:O	1:A:1350:GLY:N	2.49	0.47
1:A:1780:PRO:O	1:A:1783:PHE:N	2.46	0.47
3:L:12:LEU:HD12	3:L:12:LEU:C	2.36	0.46
1:A:868:ASP:OD1	1:A:870:ASP:N	2.46	0.46
1:A:853:ASP:N	1:A:853:ASP:OD1	2.49	0.46
3:L:12:LEU:HD11	3:L:105:VAL:HG22	1.98	0.46
1:A:1384:ILE:HG22	1:A:1385:GLU:O	2.16	0.46
1:A:855:HIS:CE1	1:A:859:LEU:HD11	2.51	0.46
1:A:1449:ALA:HA	1:A:1452:ARG:HE	1.81	0.46
1:A:1288:ILE:HG22	1:A:1289:VAL:N	2.31	0.46
1:A:2072:ILE:O	1:A:2075:SER:OG	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:ILE:HD11	1:A:1353:ARG:CG	2.46	0.46
1:A:1208:ILE:HD11	1:A:1353:ARG:HG2	1.97	0.46
2:H:17:PRO:CG	2:H:133:SER:HB3	2.46	0.45
3:L:49:ILE:HD13	3:L:54:SER:O	2.16	0.45
2:H:128:LEU:HD12	2:H:129:VAL:N	2.31	0.45
1:A:1741:GLU:OE2	1:A:1745:LYS:NZ	2.49	0.45
2:H:23:LEU:N	2:H:23:LEU:HD22	2.32	0.45
1:A:1829:CYS:SG	1:A:1831:MET:N	2.84	0.45
3:L:12:LEU:HD11	3:L:105:VAL:HG13	1.99	0.45
3:L:17:GLY:N	3:L:79:LEU:O	2.47	0.45
3:L:49:ILE:HG23	3:L:53:SER:O	2.17	0.44
1:A:948:ILE:HD11	1:A:984:HIS:CG	2.52	0.44
1:A:1415:ARG:HD3	1:A:1462:ILE:HG22	1.99	0.44
3:L:25:ARG:NH2	3:L:71:ASP:OD2	2.50	0.44
1:A:939:LYS:NZ	1:A:974:GLY:O	2.51	0.43
1:A:1441:ILE:HD12	1:A:1446:VAL:HG21	2.00	0.43
1:A:1741:GLU:OE1	1:A:1772:ARG:NH1	2.51	0.43
1:A:1418:GLU:OE2	1:A:1765:ARG:NH2	2.51	0.43
2:H:187:PRO:HD3	3:L:165:THR:HG22	2.00	0.43
3:L:109:ARG:NH2	3:L:110:THR:OG1	2.47	0.43
1:A:855:HIS:ND1	1:A:859:LEU:HD11	2.34	0.43
1:A:2051:LYS:HB2	2:H:113:TRP:CZ3	2.53	0.43
2:H:70:ARG:HB3	2:H:87:ASN:O	2.19	0.43
3:L:18:ASP:O	3:L:79:LEU:N	2.51	0.43
1:A:950:ILE:HG23	1:A:951:HIS:N	2.34	0.43
2:H:213:THR:HG23	2:H:230:LYS:HE3	2.00	0.43
2:H:94:THR:HA	2:H:130:THR:HA	2.00	0.43
1:A:948:ILE:HD11	1:A:984:HIS:CB	2.49	0.43
1:A:1335:GLU:OE1	1:A:1347:SER:OG	2.36	0.43
2:H:144:LEU:N	2:H:159:GLY:O	2.48	0.43
1:A:1409:VAL:HG12	1:A:1414:CYS:HB3	2.01	0.42
1:A:1885:PHE:HB3	1:A:1903:PHE:CE1	2.54	0.42
1:A:1409:VAL:O	1:A:1414:CYS:HB3	2.19	0.42
1:A:1496:PHE:HE2	1:A:1512:LEU:HD21	1.84	0.42
1:A:1897:PRO:HB2	1:A:1899:TRP:CZ2	2.54	0.42
1:A:1323:THR:HG22	1:A:2008:VAL:CG2	2.50	0.42
1:A:1932:ILE:HG22	1:A:1933:ILE:N	2.35	0.42
1:A:2028:ASP:OD1	1:A:2029:GLN:N	2.53	0.42
3:L:53:SER:O	3:L:54:SER:CB	2.67	0.42
3:L:211:ASN:O	3:L:212:ARG:HB2	2.20	0.42
1:A:1211:ARG:HB2	1:A:1214:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:PHE:CZ	1:A:1447:VAL:HG21	2.54	0.42
2:H:95:ALA:N	2:H:129:VAL:O	2.49	0.42
1:A:1784:TRP:CD1	1:A:1791:VAL:HG21	2.55	0.42
1:A:1390:THR:HG23	1:A:1409:VAL:HG21	2.02	0.41
1:A:971:LEU:N	1:A:983:LEU:O	2.47	0.41
1:A:1321:HIS:HB2	1:A:1994:LYS:CD	2.51	0.41
3:L:80:GLN:N	3:L:83:ASP:OD2	2.46	0.41
1:A:1783:PHE:HB3	1:A:1788:ILE:HD12	2.01	0.41
1:A:1756:ILE:O	1:A:1759:THR:OG1	2.30	0.41
2:H:18:GLY:N	2:H:89:LEU:O	2.33	0.41
3:L:139:ASN:ND2	3:L:171:ASP:OD2	2.52	0.41
3:L:186:ASP:O	3:L:190:HIS:ND1	2.45	0.41
1:A:1252:LEU:H	1:A:1252:LEU:HD12	1.86	0.41
1:A:1846:ASP:OD1	1:A:1846:ASP:N	2.54	0.41
3:L:109:ARG:HD2	3:L:171:ASP:O	2.20	0.41
1:A:1375:LEU:HD13	1:A:1460:LEU:HD11	2.03	0.40
2:H:98:TYR:CE1	3:L:44:ALA:HB2	2.56	0.40
1:A:2024:ILE:HG21	1:A:2088:LEU:CD2	2.50	0.40
2:H:109:VAL:O	2:H:111:GLY:N	2.54	0.40
3:L:18:ASP:N	3:L:18:ASP:OD1	2.54	0.40
2:H:94:THR:HG23	2:H:130:THR:HA	2.04	0.40
1:A:1414:CYS:C	1:A:1415:ARG:HE	2.25	0.40

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	824/1469 (56%)	755 (92%)	68 (8%)	1 (0%)	48 80
2	H	220/264 (83%)	201 (91%)	19 (9%)	0	100 100
3	L	202/238 (85%)	184 (91%)	18 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1246/1971 (63%)	1140 (92%)	105 (8%)	1 (0%)	50 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1300	LEU

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	758/1304 (58%)	731 (96%)	27 (4%)	30 54
2	H	188/221 (85%)	182 (97%)	6 (3%)	34 56
3	L	183/208 (88%)	177 (97%)	6 (3%)	33 56
All	All	1129/1733 (65%)	1090 (96%)	39 (4%)	33 54

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	884	ASP
1	A	885	ASN
1	A	887	THR
1	A	936	PHE
1	A	970	THR
1	A	984	HIS
1	A	1027	PHE
1	A	1201	GLU
1	A	1255	LEU
1	A	1358	LYS
1	A	1425	ASP
1	A	1462	ILE
1	A	1736	ILE
1	A	1767	TYR
1	A	1774	ASP

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Mol	Chain	Res	Type
1	A	1798	ASP
1	A	1812	ASN
1	A	1829	CYS
1	A	1846	ASP
1	A	1922	ASN
1	A	1930	GLN
1	A	1944	HIS
1	A	1962	ILE
1	A	1998	HIS
1	A	2032	LYS
1	A	2082	TYR
1	A	2083	VAL
2	H	32	PHE
2	H	73	ILE
2	H	99	CYS
2	H	104	TYR
2	H	109	VAL
2	H	130	THR
3	L	50	TYR
3	L	54	SER
3	L	62	ARG
3	L	67	ARG
3	L	90	GLN
3	L	91	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	980	ASN
1	A	1408	GLN
1	A	1794	ASN

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	133:SER	C	134:ALA	N	3.05

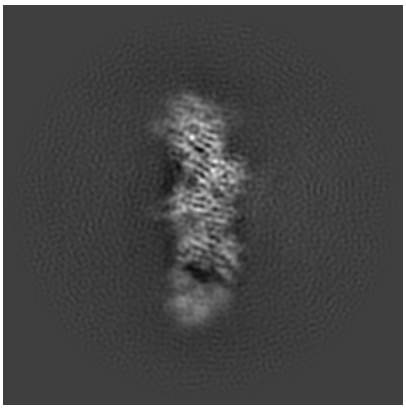
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44064. These allow visual inspection of the internal detail of the map and identification of artifacts.

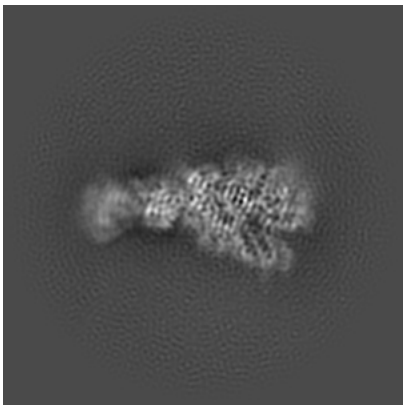
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

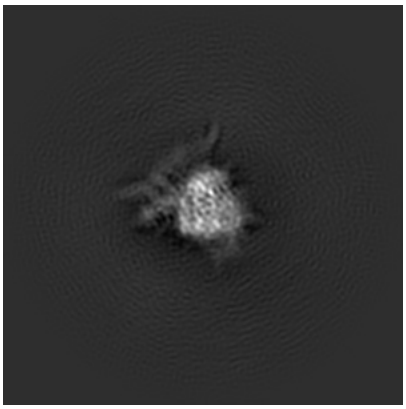
6.1.1 Primary map



X

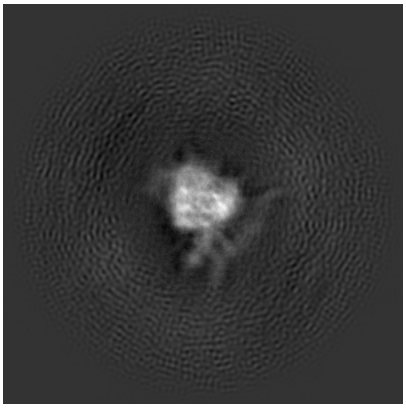


Y

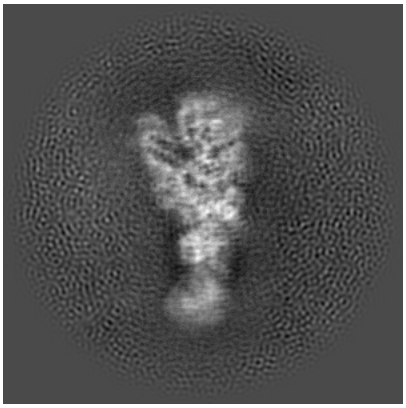


Z

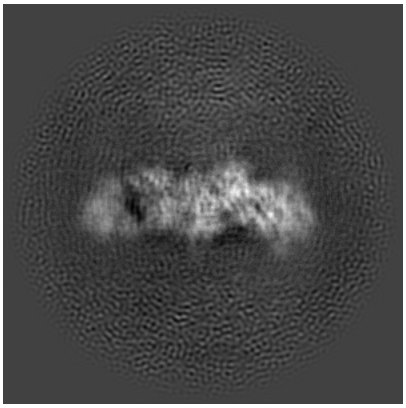
6.1.2 Raw map



X



Y

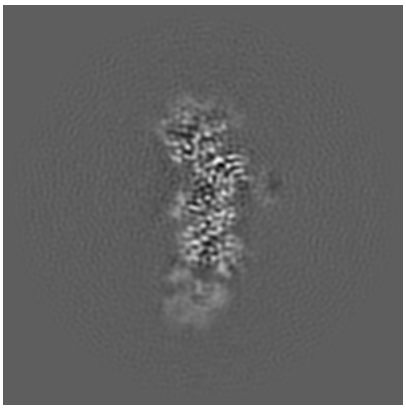


Z

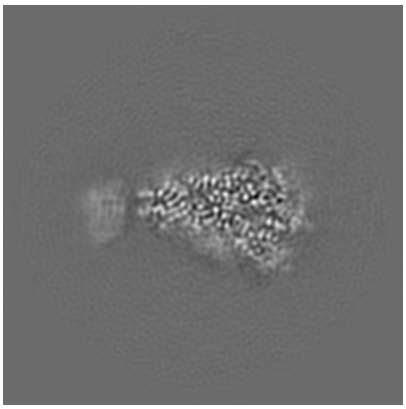
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

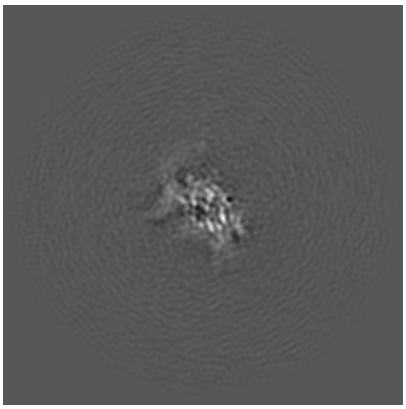
6.2.1 Primary map



X Index: 256

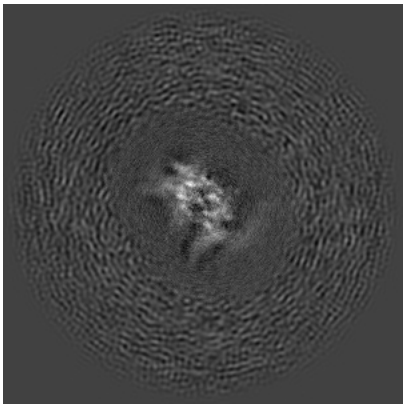


Y Index: 256

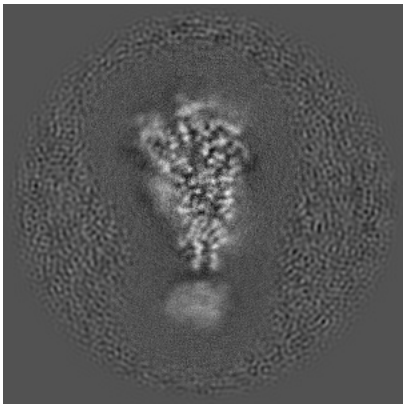


Z Index: 256

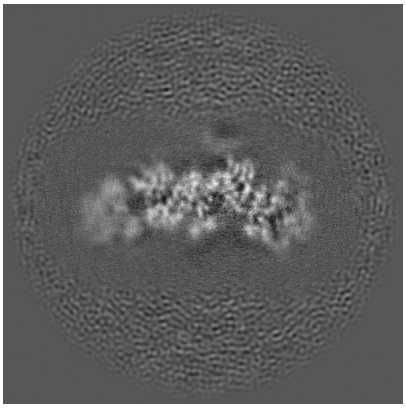
6.2.2 Raw map



X Index: 256



Y Index: 256

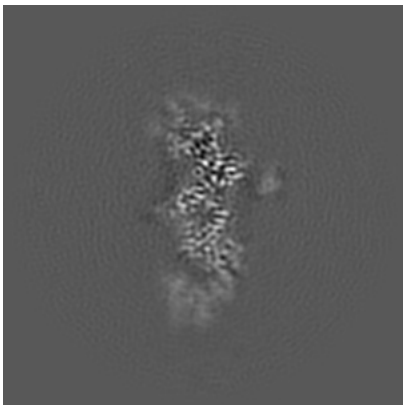


Z Index: 256

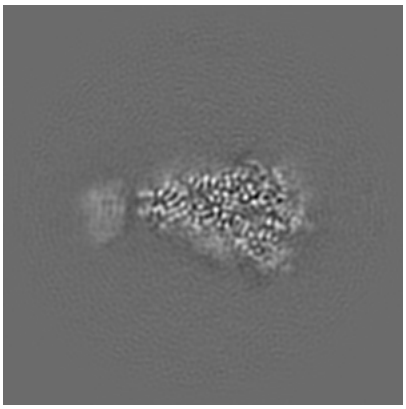
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

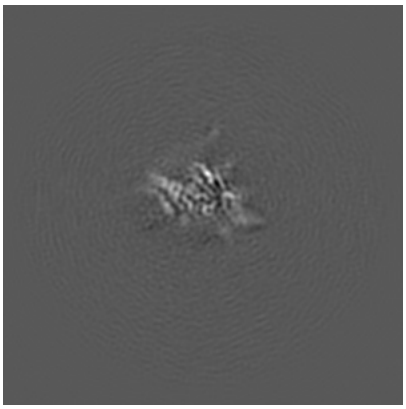
6.3.1 Primary map



X Index: 265

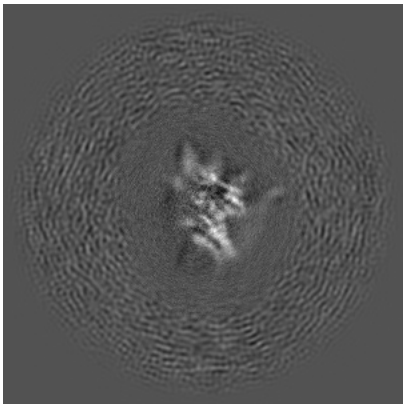


Y Index: 256

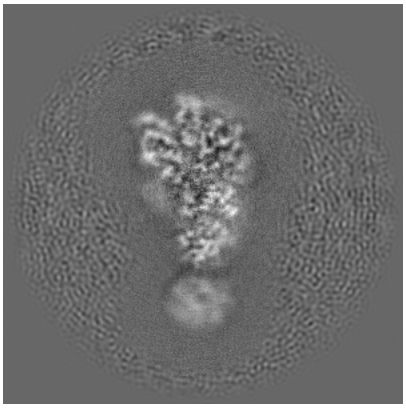


Z Index: 300

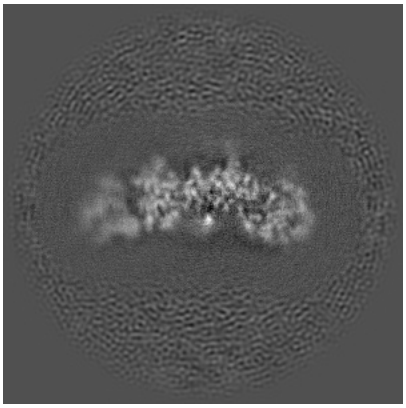
6.3.2 Raw map



X Index: 299



Y Index: 248

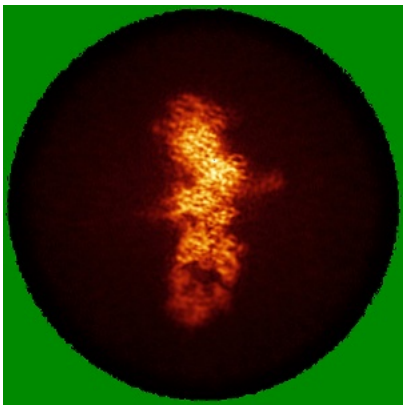


Z Index: 249

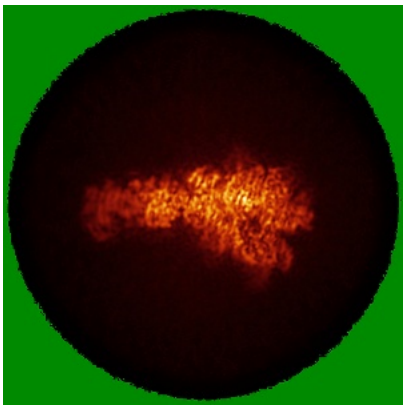
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

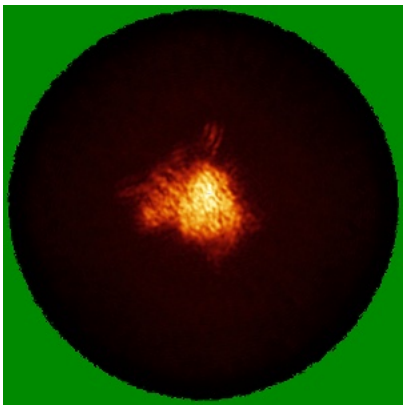
6.4.1 Primary map



X

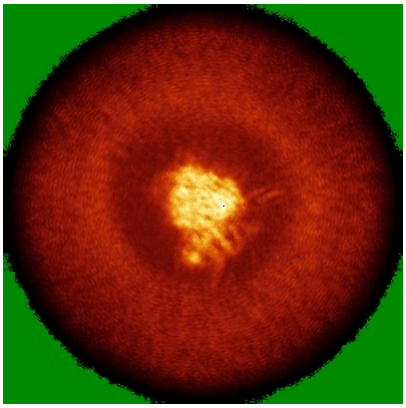


Y

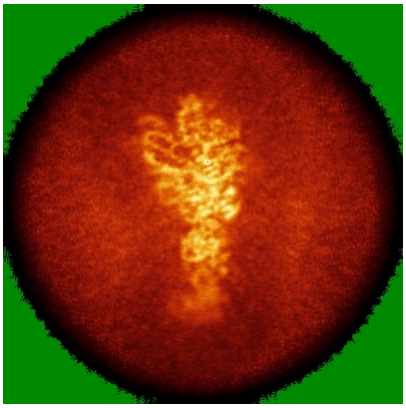


Z

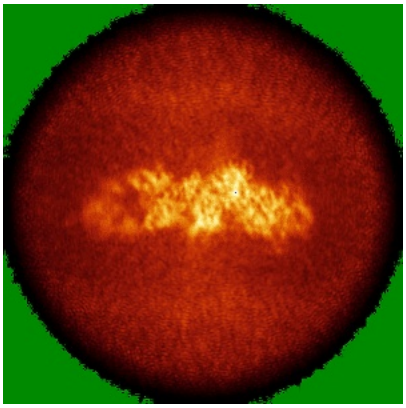
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.34. 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

X Y Z

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.

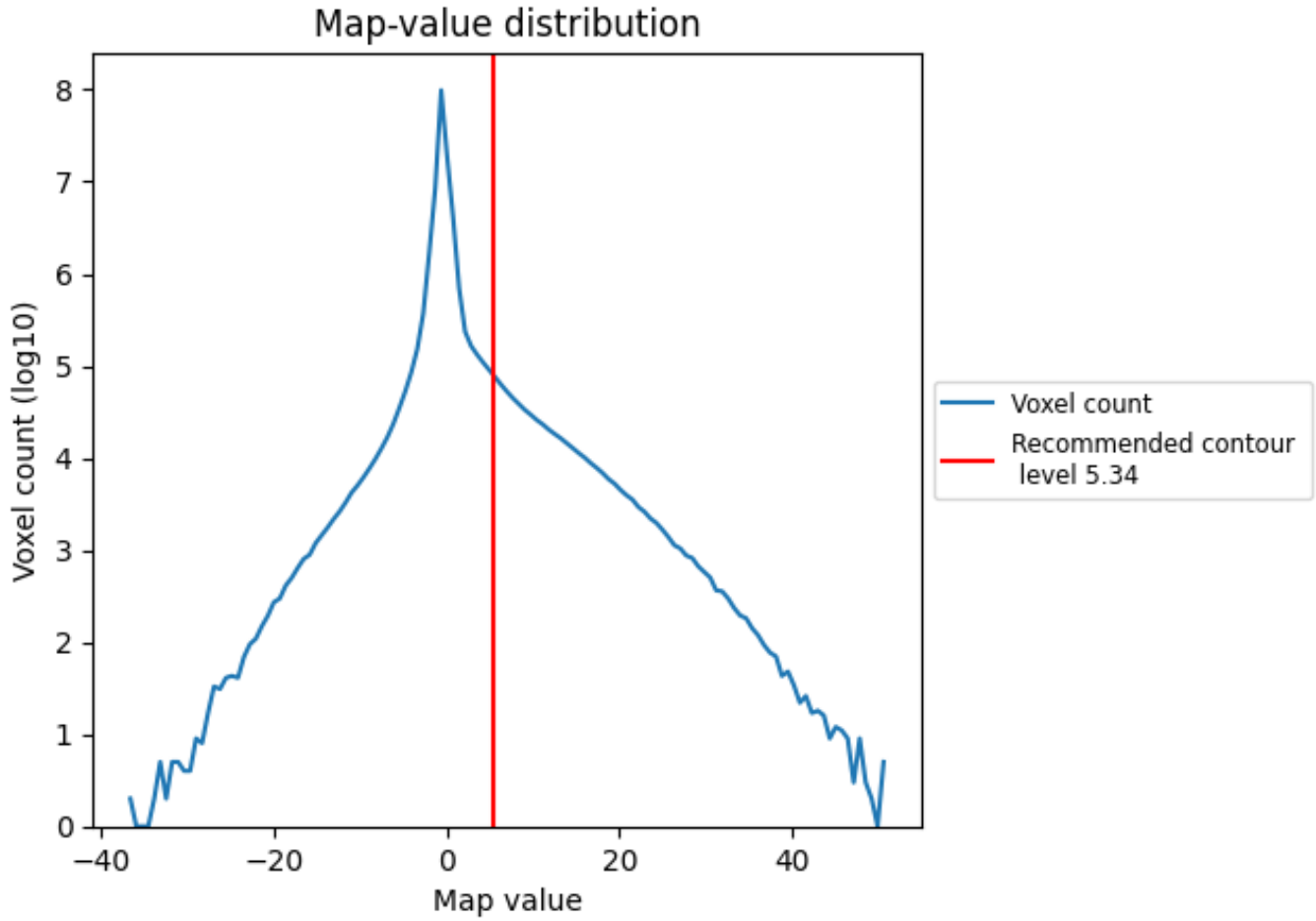
6.6 Mask visualisation (i)

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

7 Map analysis

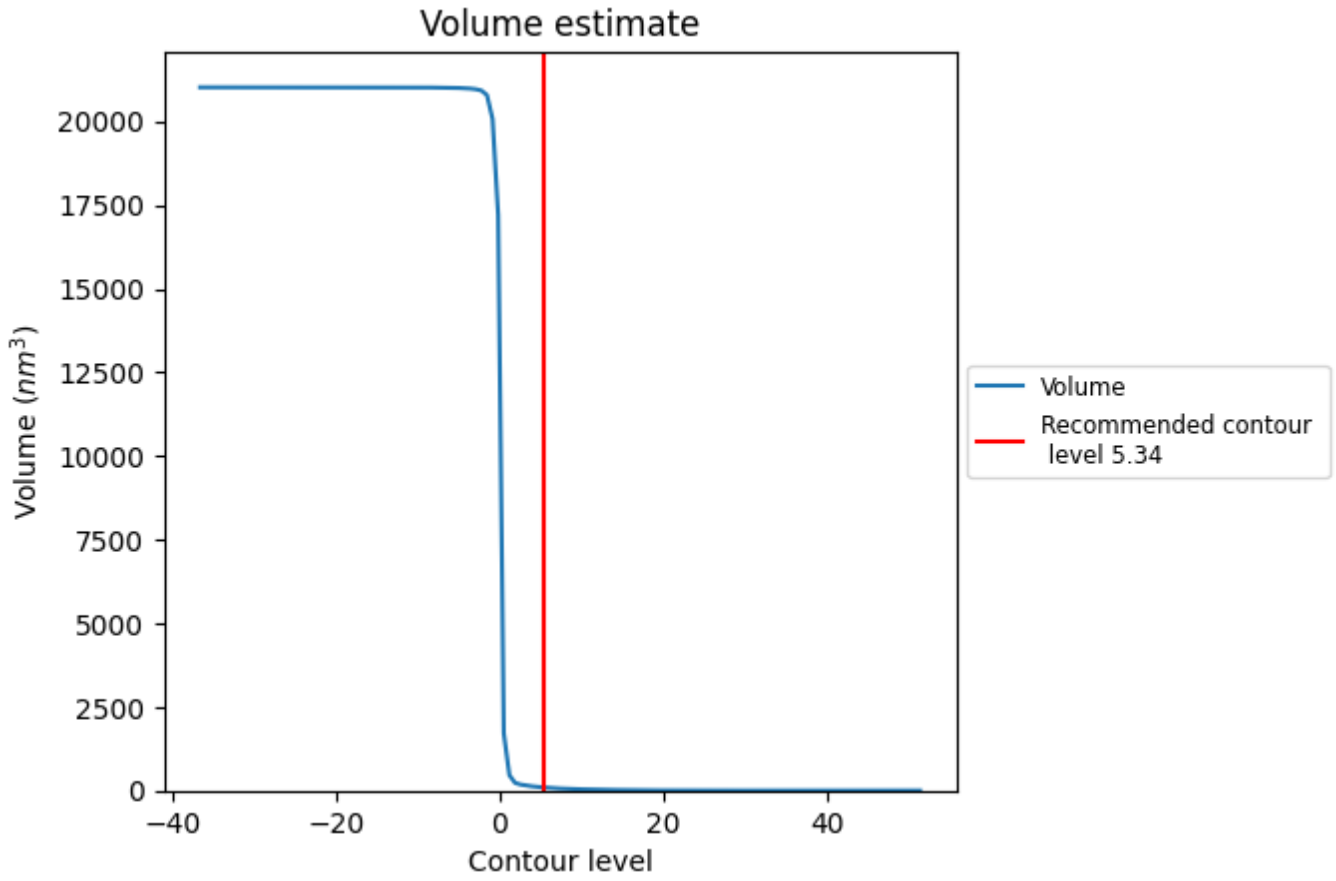
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

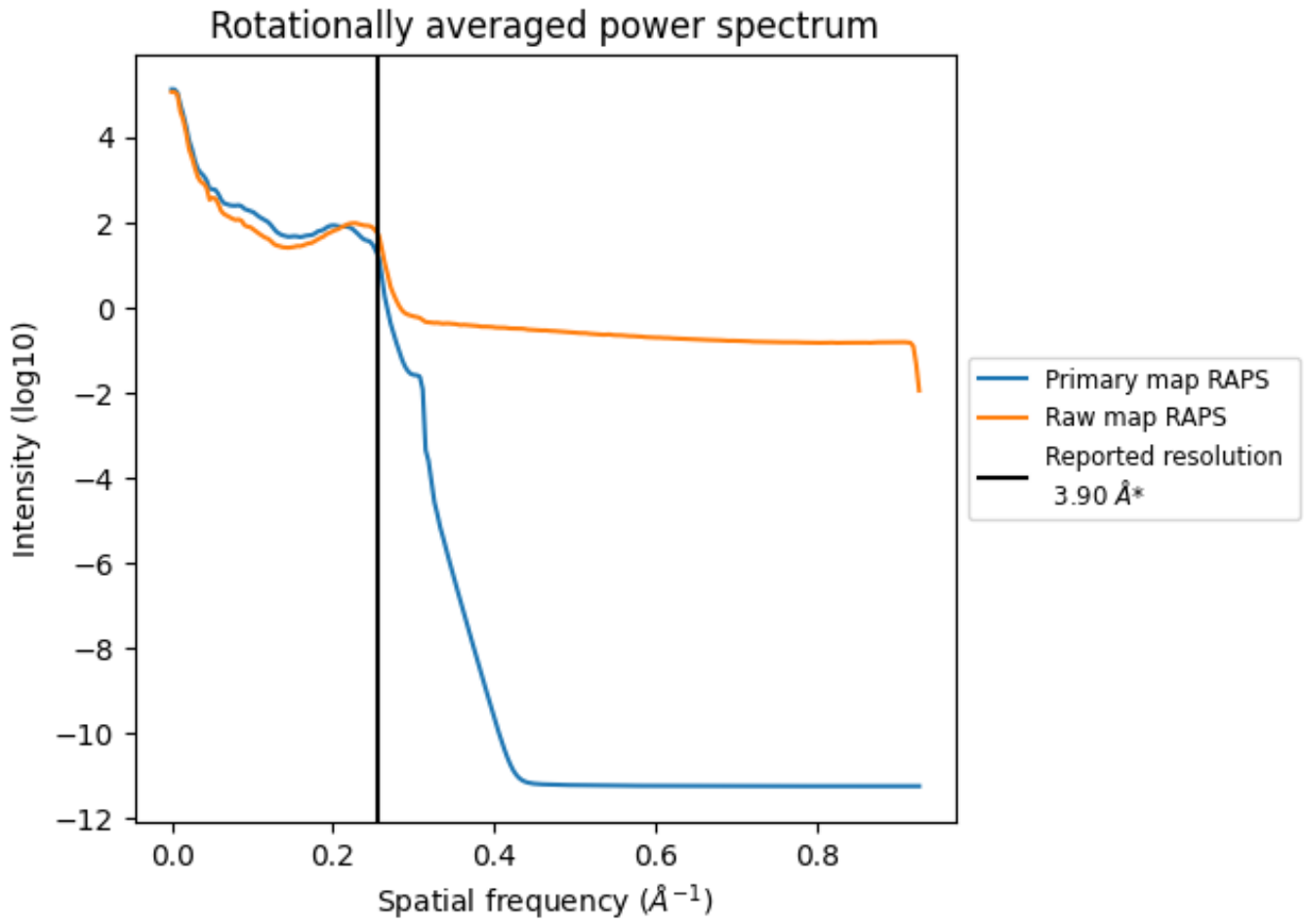
7.2 Volume estimate



The volume at the recommended contour level is 93 nm^3; this corresponds to an approximate mass of 84 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 (i)

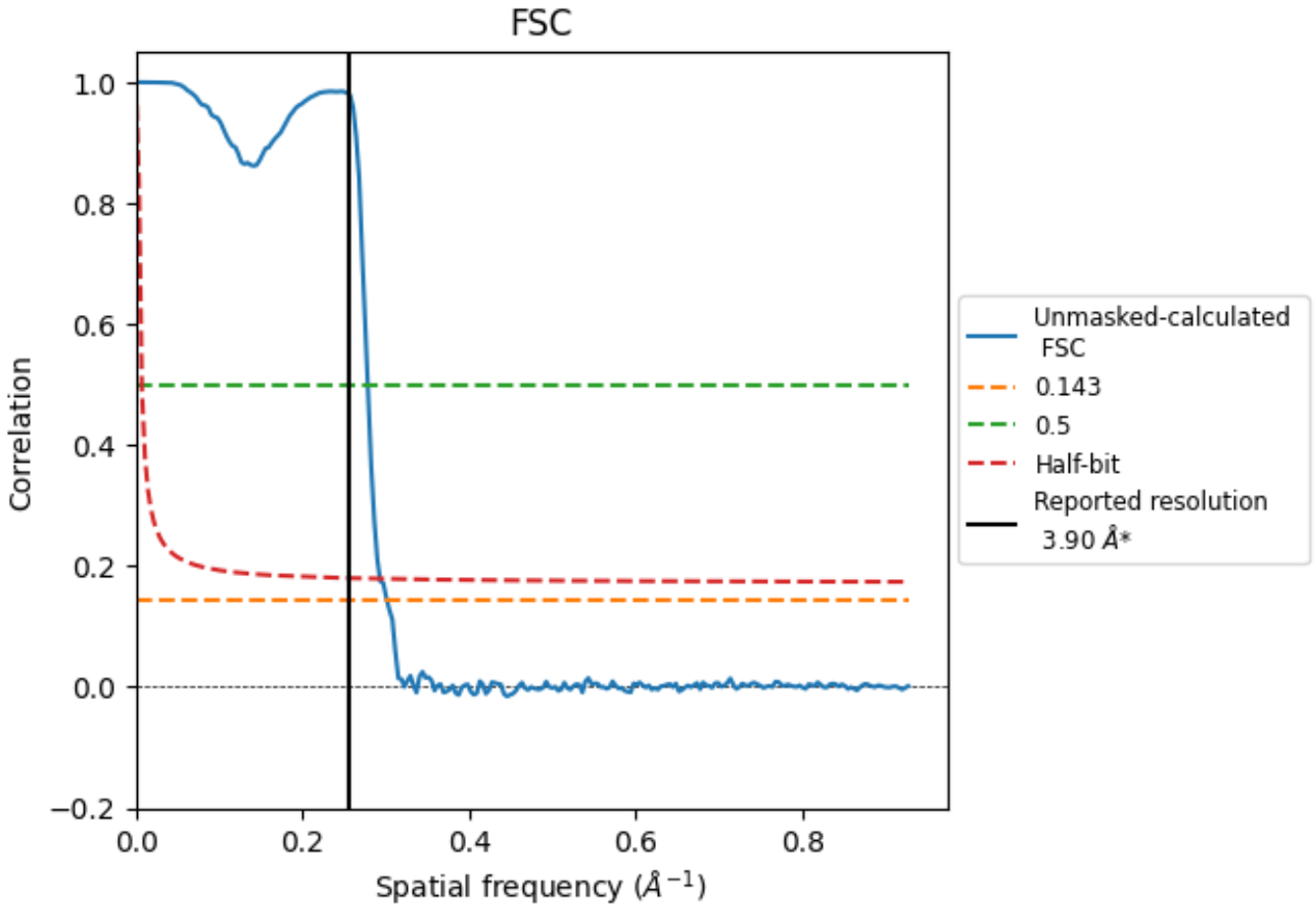


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

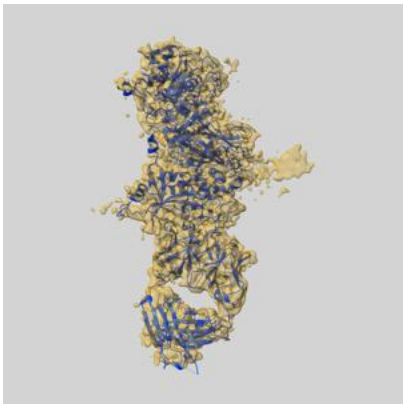
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.32	3.59	3.41

*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 3.32 differs from the reported value 3.9 by more than 10 %

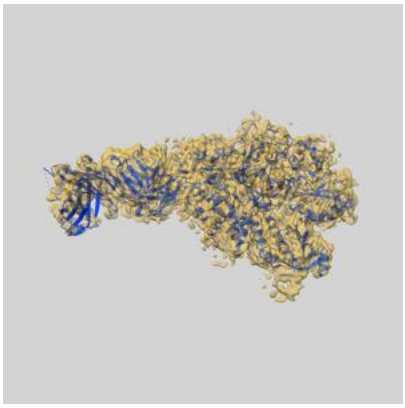
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44064 and PDB model 9B13. Per-residue inclusion information can be found in section 3 on page 5.

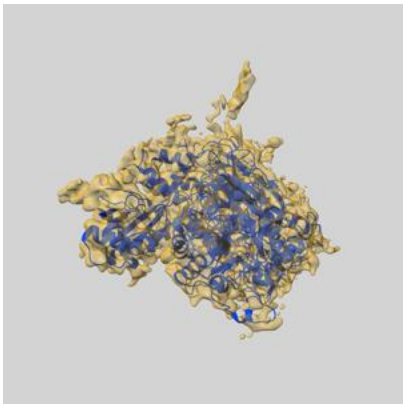
9.1 Map-model overlay



X



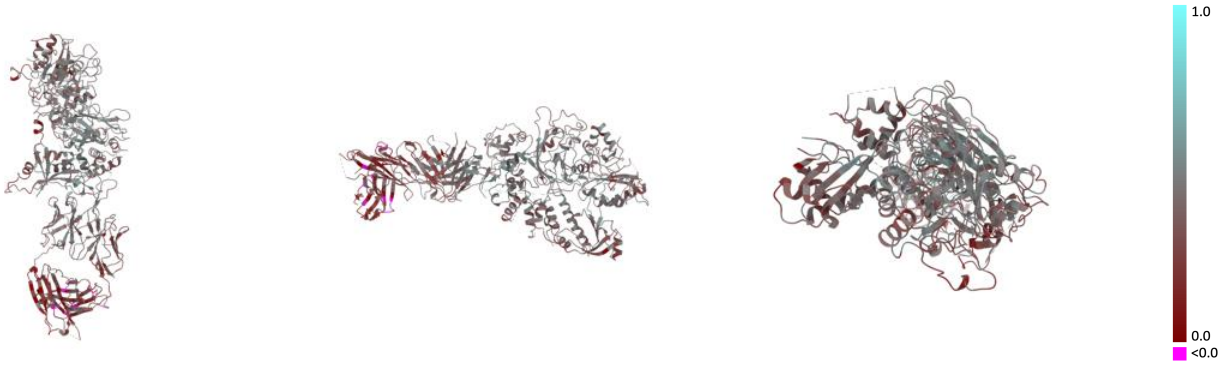
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.34 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.

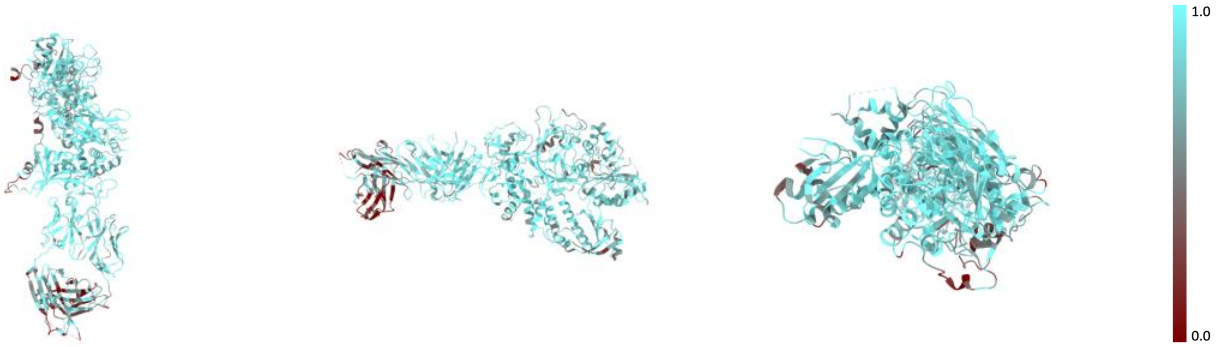
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

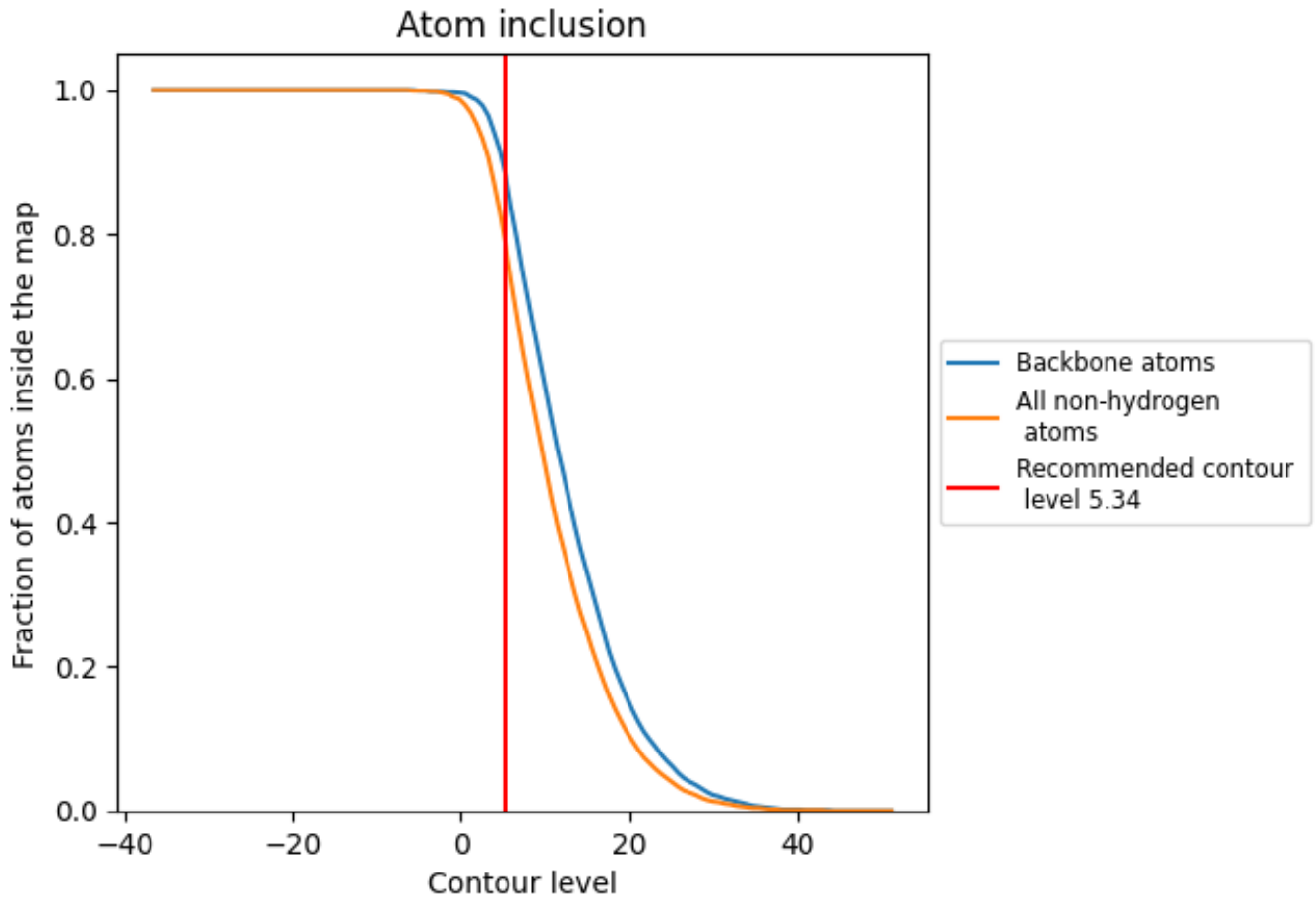
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (5.34).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (5.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.3890
A	0.8180	0.4220
H	0.7930	0.3470
L	0.6260	0.2930