Full wwPDB EM Validation Report ⓘ

May 8, 2025 – 01:17 pm BST

PDB ID	:	9FNS / pdb_00009fns
EMDB ID	:	EMD-50609
Title	:	Cryo-EM structure of the P domain of the Hepatitis E Virus ORF2 protein in complex with Fab ES1.327
Authors	:	Baquero, E.; Molinos, L.; Mouquet, H.
Deposited on	:	2024-06-11
Resolution	:	3.50 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:

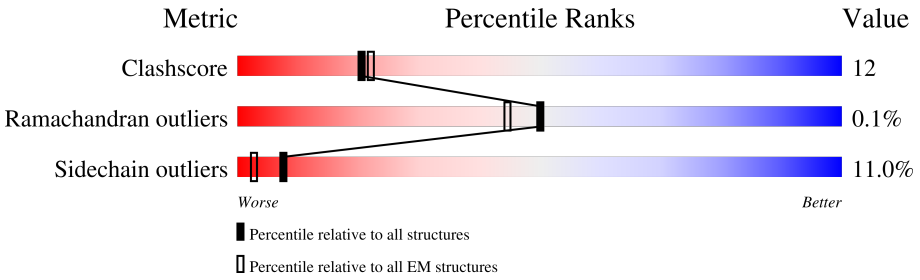
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.50 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)
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	486	19% 8% · 71%
1	B	486	19% 8% · 71%
2	C	233	39% 11% · 48%
2	E	233	38% 12% 48%
3	D	207	36% 11% · 52%
3	F	207	37% 10% · 52%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5542 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 Secreted protein ORF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	143	Total	C	N	O	S	0	0
			1074	685	173	215	1		
1	B	143	Total	C	N	O	S	0	0
			1080	688	176	215	1		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	THR	ALA	conflict	UNP Q9YLQ9
A	500	PHE	LEU	conflict	UNP Q9YLQ9
A	551	SER	GLY	conflict	UNP Q9YLQ9
A	602	HIS	-	expression tag	UNP Q9YLQ9
A	603	HIS	-	expression tag	UNP Q9YLQ9
A	604	HIS	-	expression tag	UNP Q9YLQ9
A	605	HIS	-	expression tag	UNP Q9YLQ9
A	606	HIS	-	expression tag	UNP Q9YLQ9
A	607	HIS	-	expression tag	UNP Q9YLQ9
A	608	HIS	-	expression tag	UNP Q9YLQ9
A	609	HIS	-	expression tag	UNP Q9YLQ9
A	610	HIS	-	expression tag	UNP Q9YLQ9
A	611	HIS	-	expression tag	UNP Q9YLQ9
B	356	THR	ALA	conflict	UNP Q9YLQ9
B	500	PHE	LEU	conflict	UNP Q9YLQ9
B	551	SER	GLY	conflict	UNP Q9YLQ9
B	602	HIS	-	expression tag	UNP Q9YLQ9
B	603	HIS	-	expression tag	UNP Q9YLQ9
B	604	HIS	-	expression tag	UNP Q9YLQ9
B	605	HIS	-	expression tag	UNP Q9YLQ9
B	606	HIS	-	expression tag	UNP Q9YLQ9
B	607	HIS	-	expression tag	UNP Q9YLQ9
B	608	HIS	-	expression tag	UNP Q9YLQ9
B	609	HIS	-	expression tag	UNP Q9YLQ9
B	610	HIS	-	expression tag	UNP Q9YLQ9
B	611	HIS	-	expression tag	UNP Q9YLQ9

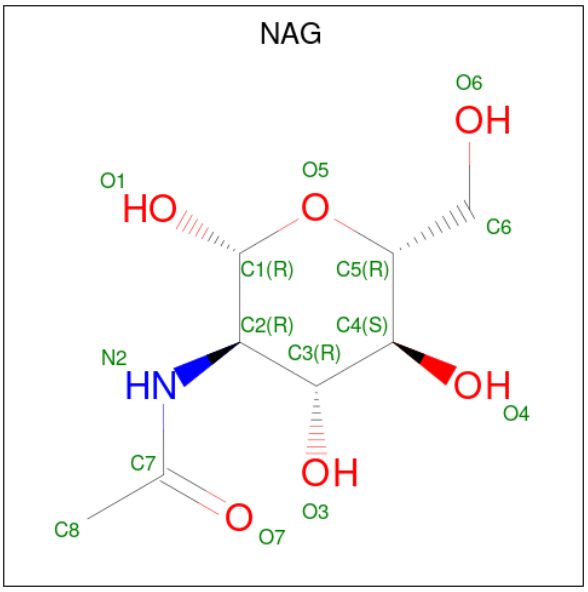
- Molecule 2 is a protein called human IgG antibody ES1.327 - Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	121	Total	C	N	O	S	0	0
			946	593	164	185	4		
2	E	120	Total	C	N	O	S	0	0
			930	583	163	180	4		

- Molecule 3 is a protein called human IgG antibody ES1.327 - Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	100	Total	C	N	O	S	0	0
			738	465	122	149	2		
3	F	100	Total	C	N	O	S	0	0
			746	470	123	151	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



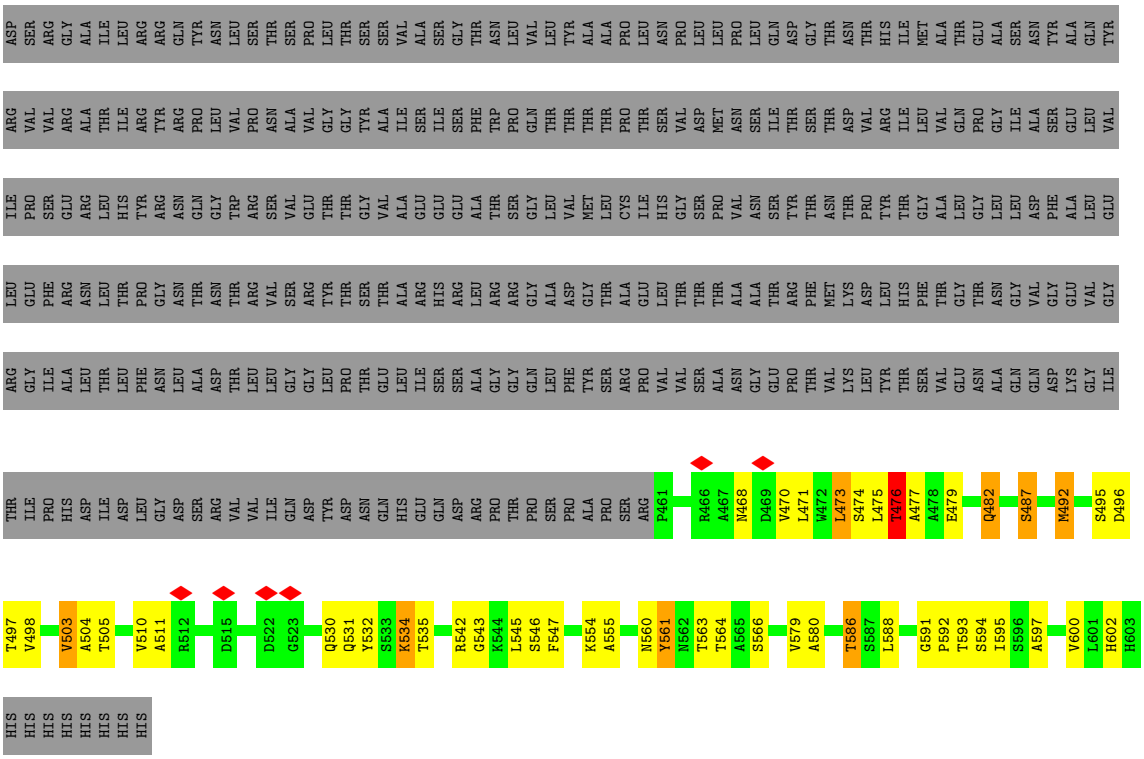
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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.

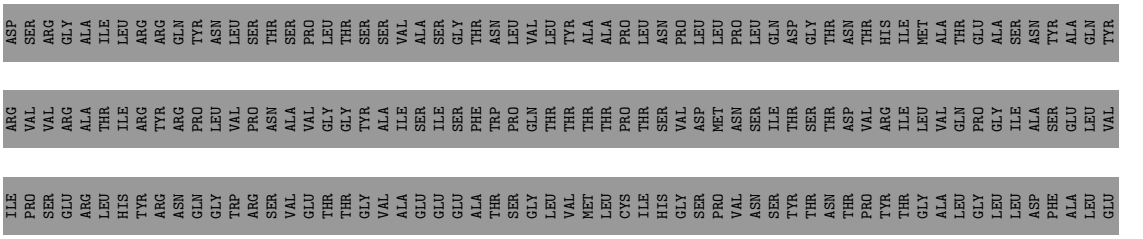
• Molecule 1: Secreted protein ORF2

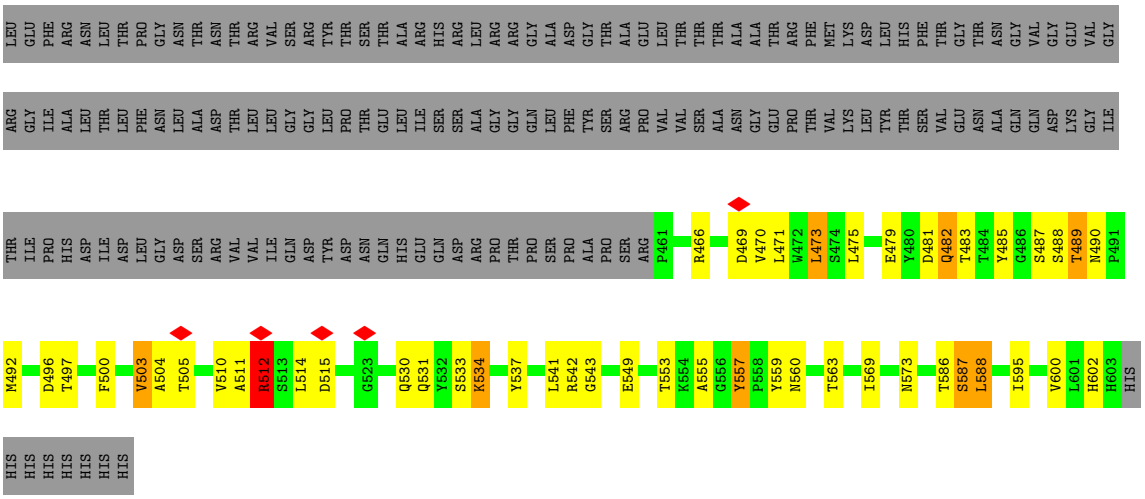
Chain A:



• Molecule 1: Secreted protein ORF2

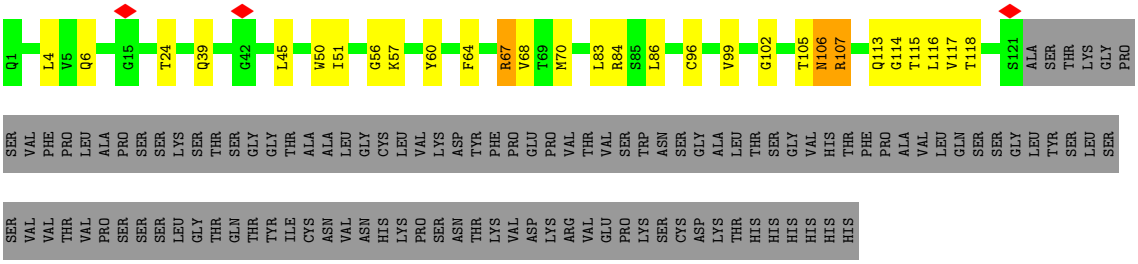
Chain B:





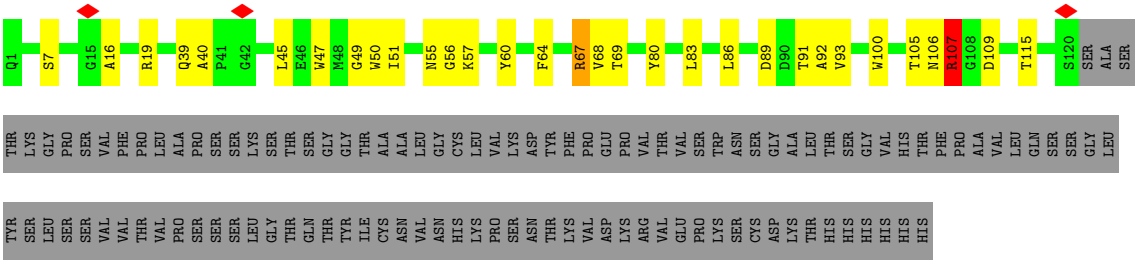
• Molecule 2: human IgG antibody ES1.327 - Fab heavy chain

Chain C:



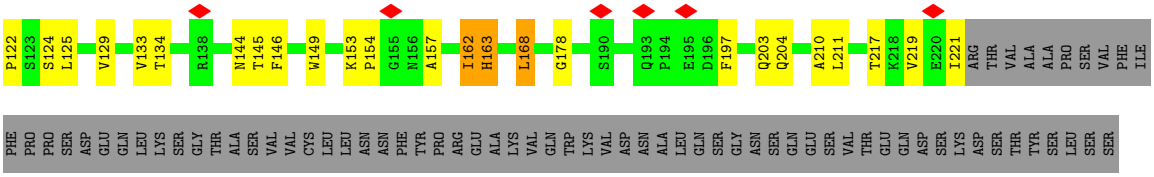
• Molecule 2: human IgG antibody ES1.327 - Fab heavy chain

Chain E:

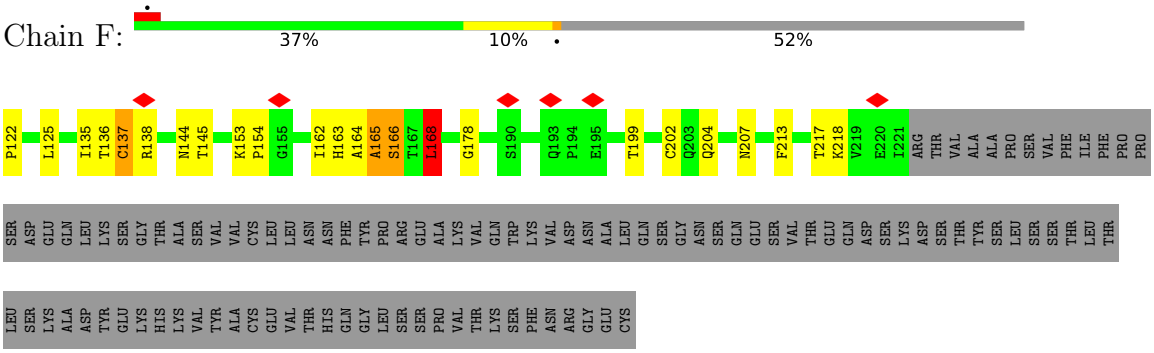


• Molecule 3: human IgG antibody ES1.327 - Fab Light chain

Chain D:



• Molecule 3: human IgG antibody ES1.327 - Fab Light chain



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106903	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.480	Depositor
Minimum map value	-0.847	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	240.8, 240.8, 240.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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

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	0.69	0/1100	1.22	11/1512 (0.7%)
1	B	0.78	0/1106	1.28	12/1519 (0.8%)
2	C	0.42	0/969	0.80	3/1319 (0.2%)
2	E	0.44	0/953	0.76	0/1300
3	D	0.63	0/755	1.09	8/1029 (0.8%)
3	F	0.72	0/763	1.23	6/1038 (0.6%)
All	All	0.63	0/5646	1.09	40/7717 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	E	0	2
3	F	0	1
All	All	0	4

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	561	TYR	N-CA-C	-8.50	102.09	111.36
3	D	157	ALA	CA-C-N	8.29	128.79	119.92
3	D	157	ALA	C-N-CA	8.29	128.79	119.92
1	A	534	LYS	N-CA-CB	-8.06	98.12	110.77
1	A	564	THR	N-CA-C	-7.69	99.99	110.68
1	B	482	GLN	N-CA-CB	7.56	121.31	110.88
1	B	482	GLN	N-CA-C	-7.34	103.92	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	165	ALA	CB-CA-C	7.28	122.50	110.92
3	F	165	ALA	N-CA-C	-7.09	102.37	111.02
1	B	531	GLN	N-CA-C	-7.08	99.53	108.45
1	A	482	GLN	N-CA-C	-6.97	103.89	112.88
1	B	482	GLN	CB-CA-C	6.85	120.89	109.38
3	F	218	LYS	N-CA-C	-6.78	97.85	108.90
3	D	145	THR	N-CA-C	-6.55	105.25	112.72
3	F	137	CYS	CB-CA-C	6.41	120.39	110.14
1	B	504	ALA	CB-CA-C	6.32	120.80	109.29
1	A	547	PHE	CA-CB-CG	6.27	120.07	113.80
2	C	106	ASN	N-CA-CB	-6.23	101.25	111.66
1	B	489	THR	CB-CA-C	6.21	119.98	109.55
1	B	587	SER	N-CA-C	-6.21	104.14	111.03
1	A	504	ALA	CB-CA-C	5.96	120.14	109.29
3	D	134	THR	N-CA-CB	-5.78	101.16	110.69
1	A	476	THR	N-CA-C	5.72	117.51	111.28
1	B	481	ASP	N-CA-C	-5.71	98.78	108.26
1	A	505	THR	N-CA-CB	-5.58	102.22	111.49
3	F	144	ASN	N-CA-C	5.50	116.67	108.31
3	D	144	ASN	N-CA-C	5.49	116.66	108.31
3	D	219	VAL	CB-CA-C	5.46	117.56	110.96
3	F	168	LEU	N-CA-C	-5.42	101.64	110.20
2	C	56	GLY	N-CA-C	5.41	122.27	114.10
1	B	485	TYR	N-CA-C	-5.40	107.34	114.31
1	B	481	ASP	CB-CA-C	5.28	118.26	110.14
1	A	535	THR	N-CA-CB	-5.26	101.85	110.21
1	A	532	TYR	CB-CA-C	-5.24	104.02	112.09
1	B	490	ASN	N-CA-CB	-5.23	103.42	110.74
1	A	482	GLN	CB-CA-C	-5.18	101.96	110.72
1	B	512	ARG	N-CA-C	-5.18	105.71	111.36
3	D	219	VAL	N-CA-C	-5.14	100.37	108.23
2	C	115	THR	CB-CA-C	-5.08	101.73	110.16
3	D	146	PHE	N-CA-C	5.04	116.82	108.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	512	ARG	Sidechain
2	E	107	ARG	Sidechain
2	E	67	ARG	Sidechain
3	F	138	ARG	Sidechain

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	1074	0	1031	31	0
1	B	1080	0	1042	34	0
2	C	946	0	898	29	0
2	E	930	0	872	24	0
3	D	738	0	693	16	0
3	F	746	0	708	8	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
All	All	5542	0	5270	129	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 12.

All (129) 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:B:515:ASP:O	1:B:515:ASP:OD1	1.55	1.19
1:A:543:GLY:HA2	1:B:555:ALA:CB	1.79	1.12
1:A:543:GLY:HA2	1:B:555:ALA:HB2	1.31	1.12
1:A:475:LEU:HD12	1:A:595:ILE:HG13	1.39	1.03
1:B:466:ARG:HG3	1:B:469:ASP:OD2	1.66	0.95
2:E:39:GLN:O	2:E:92:ALA:HB1	1.67	0.93
3:D:124:SER:O	3:D:125:LEU:HD12	1.69	0.93
1:A:477:ALA:HA	1:A:593:THR:O	1.69	0.91
2:C:116:LEU:C	2:C:116:LEU:HD23	1.95	0.91
1:B:466:ARG:CG	1:B:469:ASP:OD2	2.21	0.88
1:B:466:ARG:HG3	1:B:469:ASP:CG	1.99	0.86
2:E:83:LEU:HD23	2:E:86:LEU:CD1	2.10	0.81
2:C:116:LEU:HD21	2:C:118:THR:OG1	1.80	0.81
2:C:84:ARG:HB3	2:C:84:ARG:NH1	1.98	0.78
2:C:107:ARG:HD2	3:D:163:HIS:HD2	1.49	0.78
3:D:197:PHE:CZ	3:D:221:ILE:HD12	2.21	0.76
2:E:83:LEU:HD23	2:E:86:LEU:HD12	1.68	0.74
1:B:515:ASP:OD1	1:B:515:ASP:C	2.30	0.74
1:A:470:VAL:HG21	1:B:503:VAL:HG11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:THR:HG1	1:A:497:THR:HG1	1.33	0.72
2:C:116:LEU:HD23	2:C:117:VAL:N	2.04	0.72
1:A:476:THR:OG1	1:A:497:THR:OG1	2.09	0.70
1:A:555:ALA:HB2	1:B:543:GLY:HA2	1.73	0.70
1:A:475:LEU:HD12	1:A:595:ILE:CG1	2.20	0.70
2:C:6:GLN:NE2	2:C:96:CYS:H	1.88	0.70
1:A:545:LEU:HD22	1:A:597:ALA:HB1	1.75	0.67
1:B:514:LEU:HD12	1:B:515:ASP:H	1.59	0.67
1:A:510:VAL:HG12	1:A:511:ALA:N	2.10	0.67
1:A:555:ALA:CB	1:B:543:GLY:HA2	2.26	0.66
2:C:64:PHE:O	2:C:68:VAL:HG22	1.95	0.66
2:C:107:ARG:HD2	3:D:163:HIS:CD2	2.31	0.66
2:E:39:GLN:C	2:E:92:ALA:HB1	2.21	0.66
3:D:124:SER:C	3:D:125:LEU:HD12	2.22	0.65
3:D:197:PHE:CE2	3:D:221:ILE:CD1	2.81	0.64
2:E:83:LEU:HD23	2:E:86:LEU:HD11	1.80	0.63
2:C:116:LEU:C	2:C:116:LEU:CD2	2.69	0.62
3:F:199:THR:HG23	3:F:217:THR:O	1.99	0.62
3:D:204:GLN:NE2	3:D:210:ALA:O	2.32	0.62
1:A:498:VAL:HG21	1:A:579:VAL:HB	1.83	0.61
2:E:115:THR:O	2:E:115:THR:HG23	2.00	0.61
2:C:84:ARG:HB3	2:C:84:ARG:HH11	1.65	0.60
1:A:542:ARG:HG2	1:A:602:HIS:HB2	1.82	0.60
2:E:16:ALA:O	2:E:86:LEU:HB2	2.02	0.60
1:A:470:VAL:HG12	1:A:470:VAL:O	2.01	0.60
1:B:473:LEU:HD11	1:B:569:ILE:HD13	1.83	0.59
2:E:40:ALA:HA	2:E:92:ALA:HB2	1.83	0.59
2:E:91:THR:HG23	2:E:91:THR:O	2.03	0.59
1:B:515:ASP:O	1:B:515:ASP:CG	2.44	0.58
2:C:84:ARG:HH11	2:C:84:ARG:CB	2.17	0.58
1:A:510:VAL:CG1	1:A:511:ALA:N	2.67	0.57
2:C:6:GLN:HE22	2:C:96:CYS:H	1.51	0.57
2:C:51:ILE:HG13	2:C:57:LYS:O	2.05	0.57
1:B:557:TYR:N	1:B:557:TYR:CD1	2.72	0.57
3:D:149:TRP:HD1	3:D:162:ILE:HG21	1.70	0.57
3:F:166:SER:HB3	3:F:178:GLY:O	2.06	0.56
3:D:122:PRO:O	3:D:217:THR:OG1	2.24	0.55
1:A:543:GLY:CA	1:B:555:ALA:HB2	2.22	0.55
2:C:6:GLN:OE1	2:C:114:GLY:HA2	2.06	0.55
1:A:468:ASN:HA	1:A:600:VAL:HG13	1.88	0.54
2:E:89:ASP:O	2:E:89:ASP:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:LEU:HG	2:C:24:THR:HG22	1.90	0.54
2:C:60:TYR:CE1	2:C:68:VAL:HG23	2.43	0.53
1:B:514:LEU:HD12	1:B:515:ASP:N	2.21	0.53
1:B:466:ARG:HG3	1:B:469:ASP:OD1	2.08	0.53
2:C:83:LEU:O	2:C:86:LEU:CD1	2.56	0.52
2:E:64:PHE:O	2:E:68:VAL:HG22	2.10	0.52
2:C:50:TRP:O	2:C:50:TRP:CD1	2.63	0.52
2:C:50:TRP:CD1	2:C:50:TRP:C	2.88	0.52
1:A:477:ALA:CA	1:A:593:THR:O	2.51	0.51
3:F:164:ALA:O	3:F:165:ALA:C	2.52	0.51
2:C:60:TYR:CD1	2:C:68:VAL:HG23	2.46	0.50
3:D:197:PHE:CE2	3:D:221:ILE:HD12	2.43	0.50
1:B:466:ARG:HG2	1:B:469:ASP:OD2	2.10	0.50
2:C:84:ARG:NH1	2:C:84:ARG:CB	2.73	0.50
1:B:533:SER:O	1:B:534:LYS:HB2	2.12	0.49
2:E:50:TRP:C	2:E:50:TRP:CD1	2.91	0.48
1:B:475:LEU:HD12	1:B:595:ILE:HD11	1.95	0.48
2:C:67:ARG:O	2:C:84:ARG:HG2	2.14	0.47
2:E:19:ARG:NH1	2:E:80:TYR:CG	2.82	0.47
3:F:153:LYS:HB3	3:F:154:PRO:HD2	1.95	0.47
1:B:542:ARG:HG3	1:B:602:HIS:HB2	1.95	0.47
1:A:593:THR:HG22	1:A:594:SER:H	1.79	0.47
1:A:470:VAL:O	1:A:503:VAL:HB	2.15	0.47
1:A:487:SER:HA	2:C:102:GLY:HA2	1.96	0.47
2:E:60:TYR:CE1	2:E:68:VAL:HG23	2.50	0.47
3:D:197:PHE:CE2	3:D:221:ILE:HD13	2.49	0.46
2:E:19:ARG:NH1	2:E:80:TYR:CD1	2.83	0.46
2:E:68:VAL:HG12	2:E:83:LEU:HD12	1.97	0.46
2:C:39:GLN:HB2	2:C:45:LEU:HD23	1.95	0.46
1:B:473:LEU:HD22	1:B:500:PHE:CD2	2.51	0.46
1:A:510:VAL:CG1	1:A:511:ALA:H	2.28	0.45
2:E:100:TRP:HE3	2:E:107:ARG:HG3	1.81	0.45
1:A:477:ALA:O	1:A:495:SER:HB2	2.15	0.45
2:E:55:ASN:OD1	2:E:56:GLY:N	2.50	0.45
3:F:168:LEU:HD12	3:F:168:LEU:HA	1.69	0.45
1:A:470:VAL:HG11	1:B:470:VAL:HG11	1.98	0.45
3:D:153:LYS:HB3	3:D:154:PRO:HD2	1.98	0.45
2:C:50:TRP:HE3	2:C:99:VAL:HG21	1.82	0.45
2:E:51:ILE:HG13	2:E:57:LYS:O	2.17	0.44
1:A:586:THR:O	1:A:586:THR:HG23	2.18	0.44
1:B:489:THR:O	1:B:559:TYR:CE2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:122:PRO:CB	3:F:125:LEU:HD21	2.47	0.44
2:E:50:TRP:CD1	2:E:50:TRP:O	2.71	0.44
1:B:541:LEU:HG	1:B:600:VAL:O	2.18	0.43
2:C:50:TRP:CE3	2:C:99:VAL:HG21	2.53	0.43
3:D:162:ILE:HD11	3:D:178:GLY:HA3	2.00	0.43
1:A:471:LEU:HD23	1:A:473:LEU:CD2	2.49	0.43
1:A:591:GLY:O	1:A:592:PRO:C	2.61	0.43
1:B:473:LEU:N	1:B:473:LEU:HD23	2.34	0.43
1:A:492:MET:HG2	1:A:580:ALA:HB1	1.99	0.43
2:E:40:ALA:HA	2:E:92:ALA:CB	2.47	0.43
1:B:470:VAL:O	1:B:503:VAL:HG23	2.19	0.42
3:D:168:LEU:HD23	3:D:168:LEU:HA	1.77	0.42
2:C:106:ASN:HD21	3:D:211:LEU:HD21	1.85	0.42
1:B:483:THR:HG23	3:F:207:ASN:HD22	1.84	0.42
1:B:510:VAL:HG12	1:B:511:ALA:N	2.35	0.42
1:B:573:ASN:OD1	1:B:573:ASN:C	2.63	0.41
1:A:588:LEU:HD23	1:A:588:LEU:HA	1.78	0.41
1:B:510:VAL:HG12	1:B:511:ALA:H	1.85	0.41
1:B:549:GLU:HB2	1:B:588:LEU:HD22	2.02	0.41
2:E:39:GLN:HB2	2:E:45:LEU:HD23	2.02	0.41
2:C:50:TRP:O	2:C:50:TRP:HD1	2.03	0.41
1:B:483:THR:HG23	3:F:207:ASN:ND2	2.36	0.41
1:A:496:ASP:OD1	1:A:496:ASP:C	2.63	0.40
1:B:537:TYR:CE2	1:B:573:ASN:HB2	2.56	0.40
2:E:7:SER:O	2:E:115:THR:HB	2.21	0.40
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.57	0.40
3:D:203:GLN:HE21	3:D:211:LEU:HB3	1.86	0.40
2:C:60:TYR:OH	2:C:70:MET:N	2.47	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	141/486 (29%)	136 (96%)	5 (4%)	0	100 100
1	B	141/486 (29%)	137 (97%)	3 (2%)	1 (1%)	19 53
2	C	119/233 (51%)	118 (99%)	1 (1%)	0	100 100
2	E	118/233 (51%)	116 (98%)	2 (2%)	0	100 100
3	D	98/207 (47%)	95 (97%)	3 (3%)	0	100 100
3	F	98/207 (47%)	94 (96%)	4 (4%)	0	100 100
All	All	715/1852 (39%)	696 (97%)	18 (2%)	1 (0%)	50 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	534	LYS

5.3.2 Protein sidechains (i)

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	115/409 (28%)	97 (84%)	18 (16%)	2 13
1	B	116/409 (28%)	96 (83%)	20 (17%)	1 9
2	C	101/200 (50%)	97 (96%)	4 (4%)	27 56
2	E	97/200 (48%)	90 (93%)	7 (7%)	12 37
3	D	80/180 (44%)	75 (94%)	5 (6%)	15 42
3	F	82/180 (46%)	71 (87%)	11 (13%)	3 18
All	All	591/1578 (38%)	526 (89%)	65 (11%)	7 24

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	473	LEU
1	A	474	SER
1	A	476	THR
1	A	479	GLU

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Mol	Chain	Res	Type
1	A	482	GLN
1	A	487	SER
1	A	492	MET
1	A	503	VAL
1	A	530	GLN
1	A	531	GLN
1	A	534	LYS
1	A	546	SER
1	A	554	LYS
1	A	560	ASN
1	A	561	TYR
1	A	563	THR
1	A	566	SER
1	A	586	THR
1	B	471	LEU
1	B	473	LEU
1	B	479	GLU
1	B	482	GLN
1	B	487	SER
1	B	488	SER
1	B	492	MET
1	B	496	ASP
1	B	497	THR
1	B	503	VAL
1	B	505	THR
1	B	512	ARG
1	B	530	GLN
1	B	553	THR
1	B	557	TYR
1	B	560	ASN
1	B	563	THR
1	B	586	THR
1	B	587	SER
1	B	588	LEU
2	C	67	ARG
2	C	105	THR
2	C	107	ARG
2	C	113	GLN
3	D	129	VAL
3	D	133	VAL
3	D	162	ILE
3	D	163	HIS

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Mol	Chain	Res	Type
3	D	168	LEU
2	E	67	ARG
2	E	69	THR
2	E	93	VAL
2	E	105	THR
2	E	106	ASN
2	E	107	ARG
2	E	109	ASP
3	F	135	ILE
3	F	136	THR
3	F	137	CYS
3	F	145	THR
3	F	162	ILE
3	F	163	HIS
3	F	166	SER
3	F	168	LEU
3	F	202	CYS
3	F	204	GLN
3	F	213	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	482	GLN
1	A	531	GLN
1	A	560	ASN
1	A	577	HIS
2	C	6	GLN
2	C	113	GLN
3	D	151	GLN
3	D	163	HIS
3	D	203	GLN
2	E	65	GLN
3	F	203	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)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	NAG	B	1000	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	A	1000	1	14,14,15	0.53	0	17,19,21	1.26	3 (17%)

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
4	NAG	B	1000	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1000	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1000	NAG	O5-C1-C2	-2.63	107.14	111.29
4	A	1000	NAG	C2-N2-C7	-2.62	119.18	122.90
4	A	1000	NAG	C6-C5-C4	-2.00	108.32	113.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1000	NAG	C8-C7-N2-C2
4	B	1000	NAG	O7-C7-N2-C2
4	A	1000	NAG	C4-C5-C6-O6
4	A	1000	NAG	O5-C5-C6-O6

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)

There are no chain breaks in this entry.

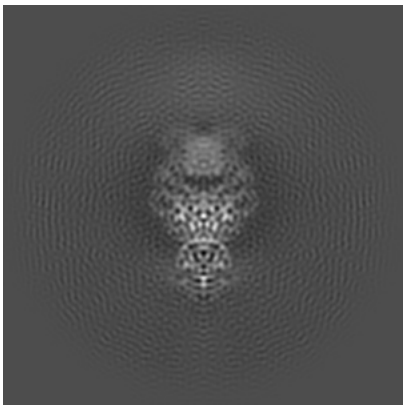
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50609. These allow visual inspection of the internal detail of the map and identification of artifacts.

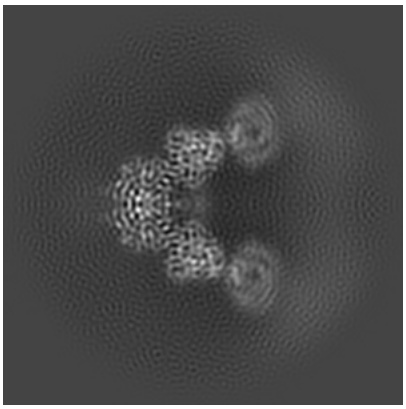
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

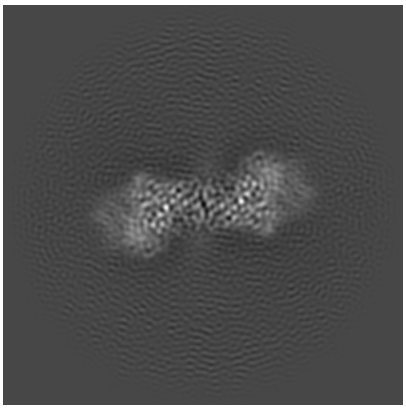
6.1.1 Primary map



X

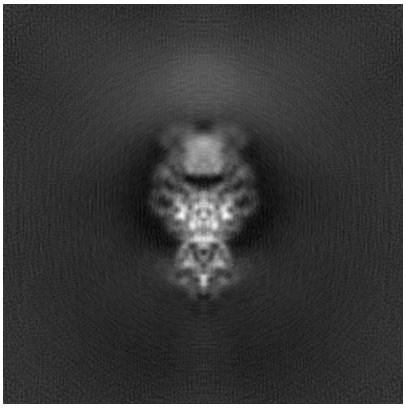


Y

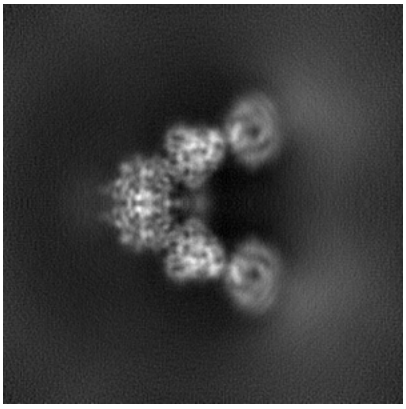


Z

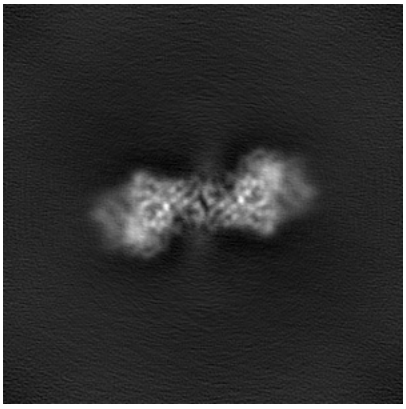
6.1.2 Raw map



X



Y

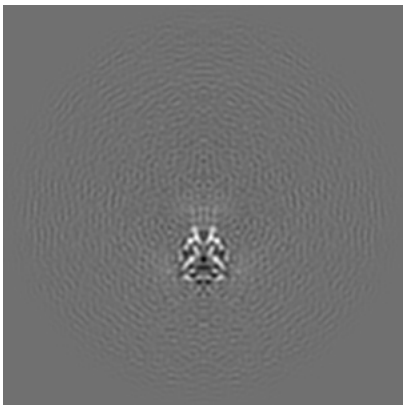


Z

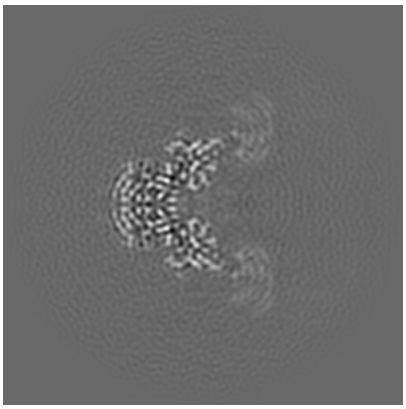
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

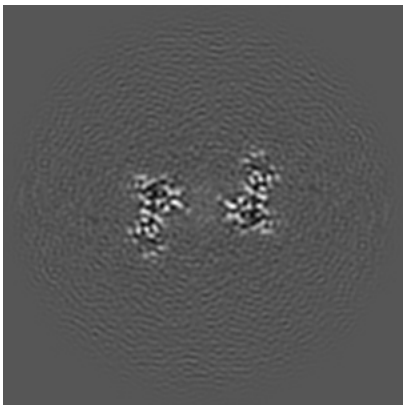
6.2.1 Primary map



X Index: 140

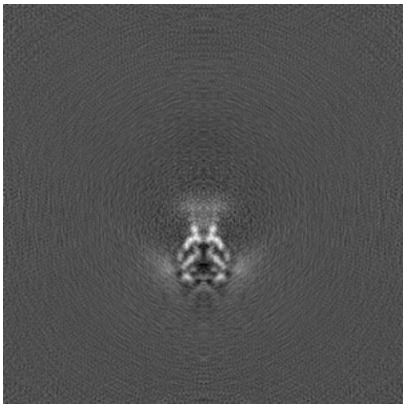


Y Index: 140

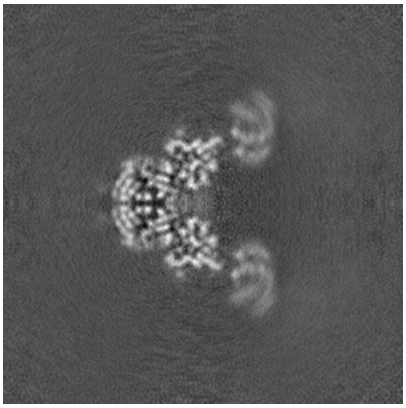


Z Index: 140

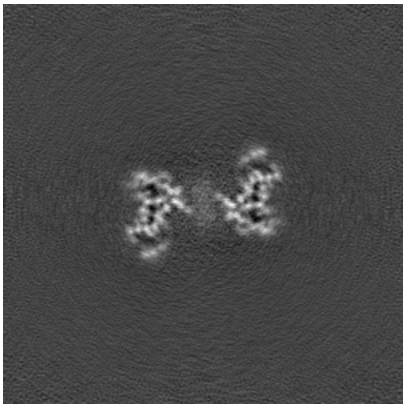
6.2.2 Raw map



X Index: 140



Y Index: 140

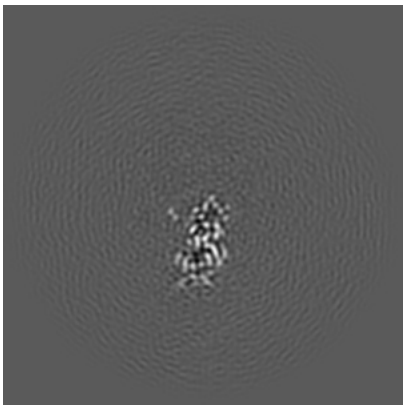


Z Index: 140

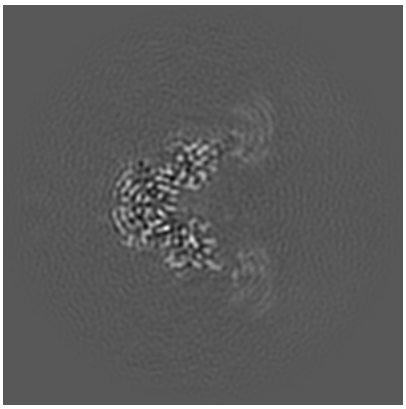
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

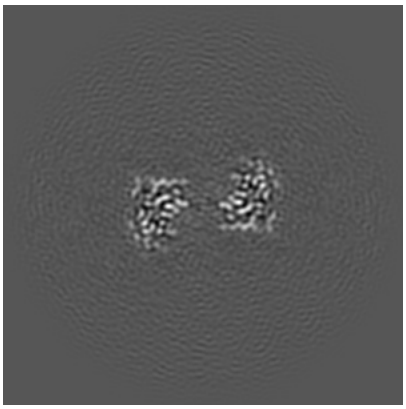
6.3.1 Primary map



X Index: 118

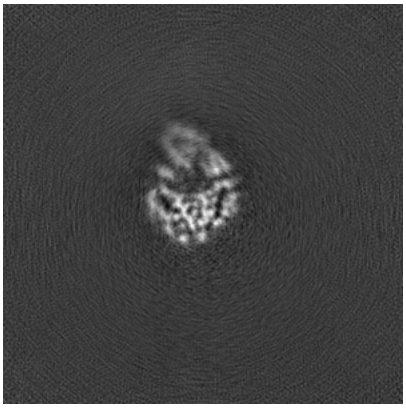


Y Index: 139

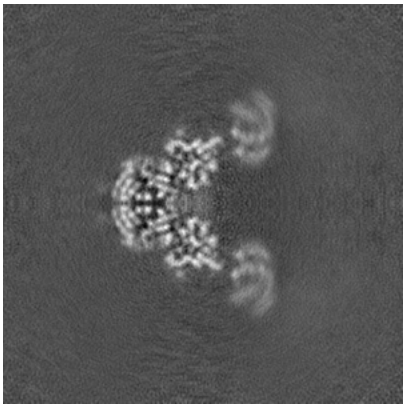


Z Index: 131

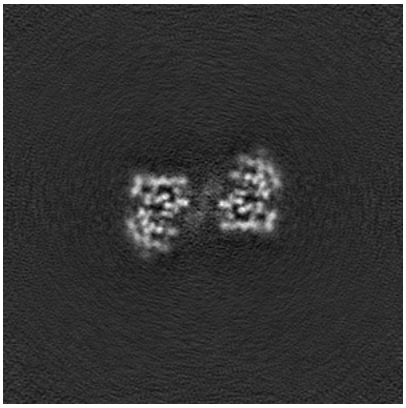
6.3.2 Raw map



X Index: 100



Y Index: 140

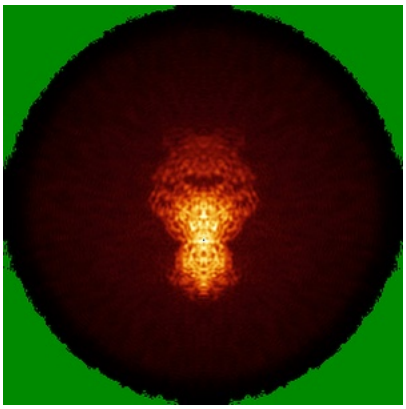


Z Index: 131

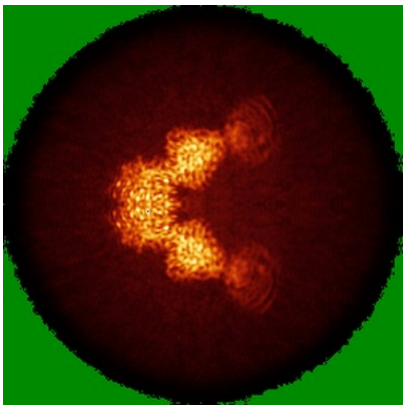
The images above show the largest variance slices of the map in three orthogonal directions.

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

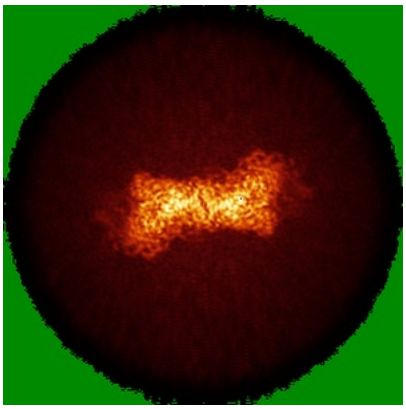
6.4.1 Primary map



X

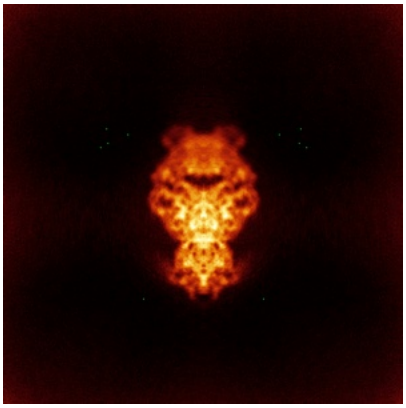


Y

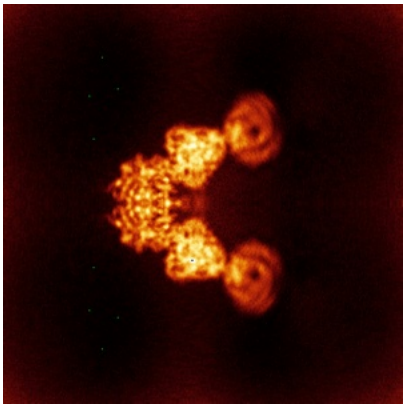


Z

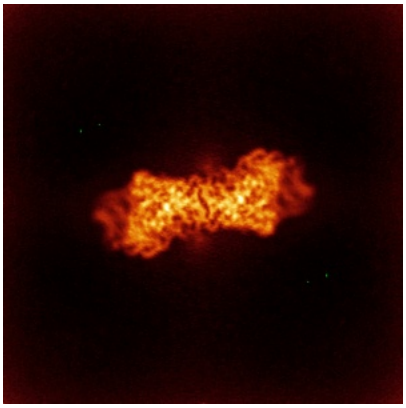
6.4.2 Raw map



X



Y

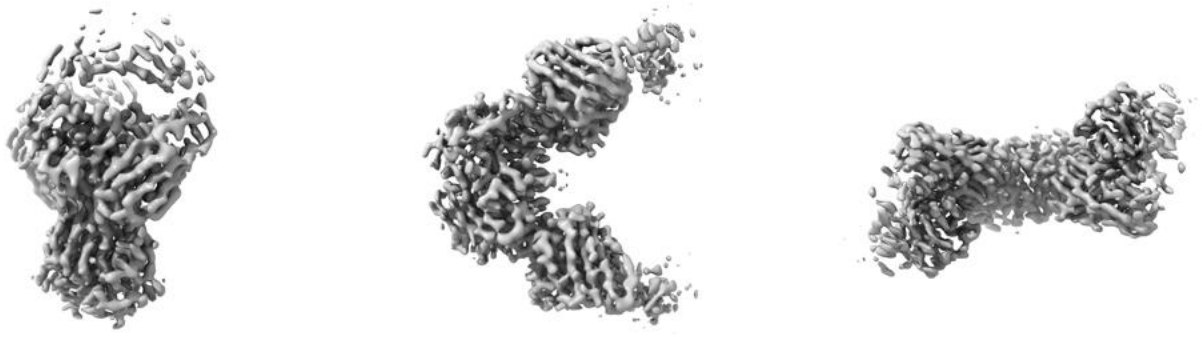


Z

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)

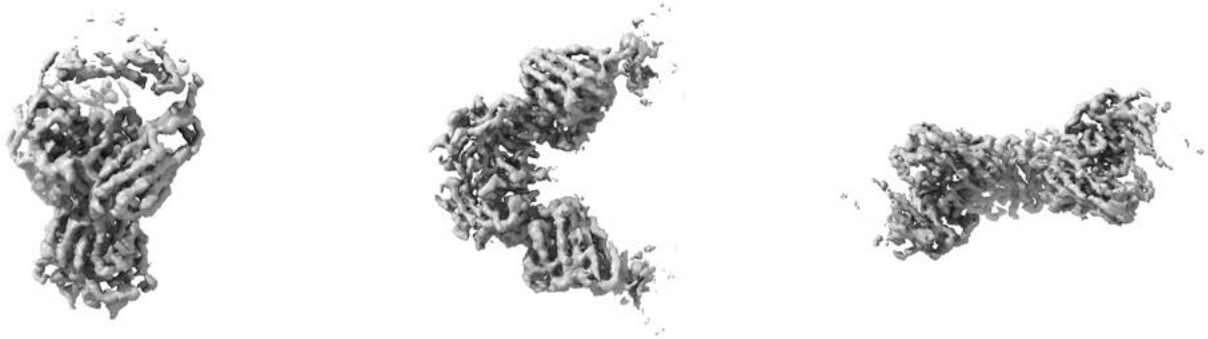
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

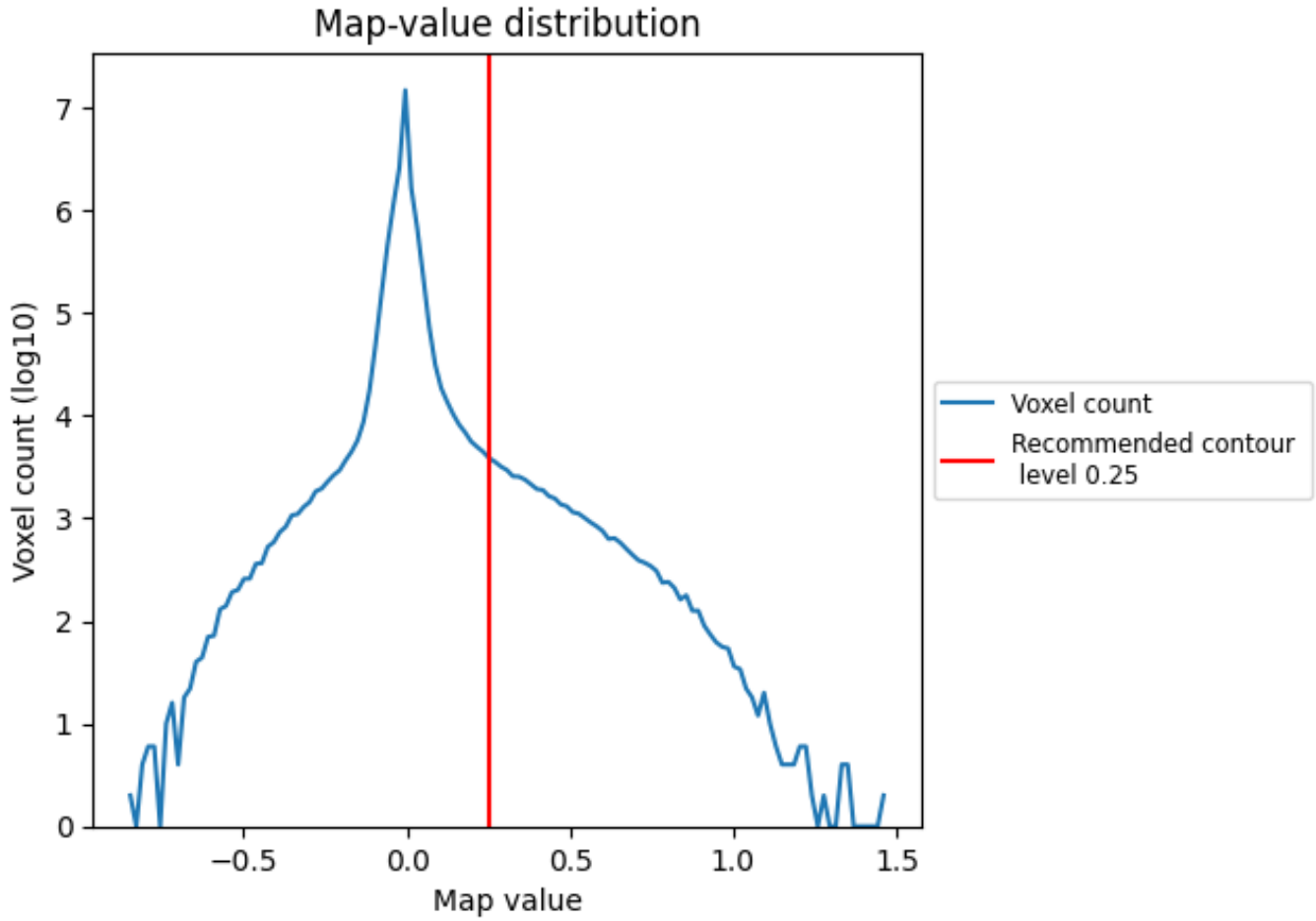
6.6 Mask visualisation (i)

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

7 Map analysis

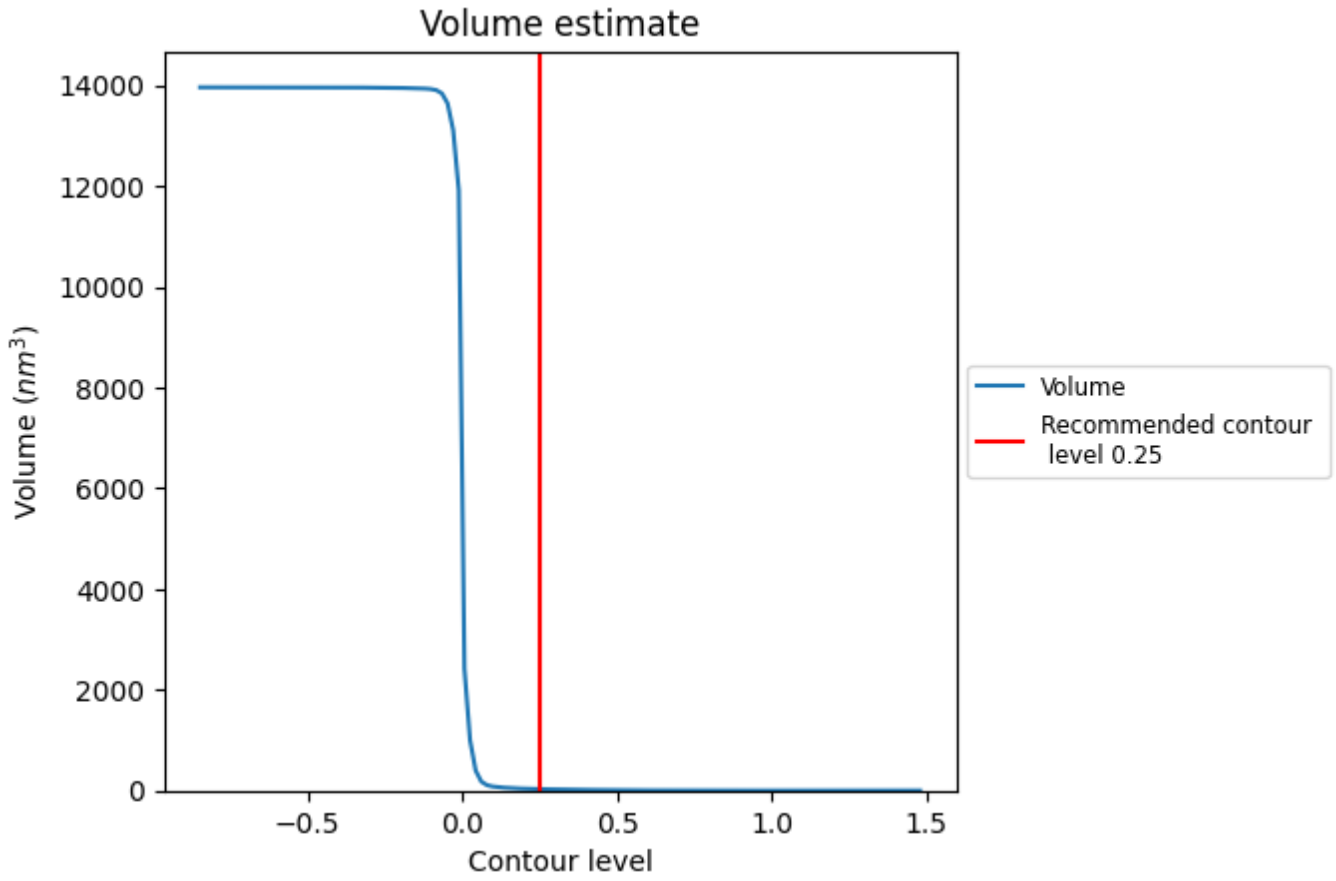
This section contains the results of statistical analysis of the map.

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.

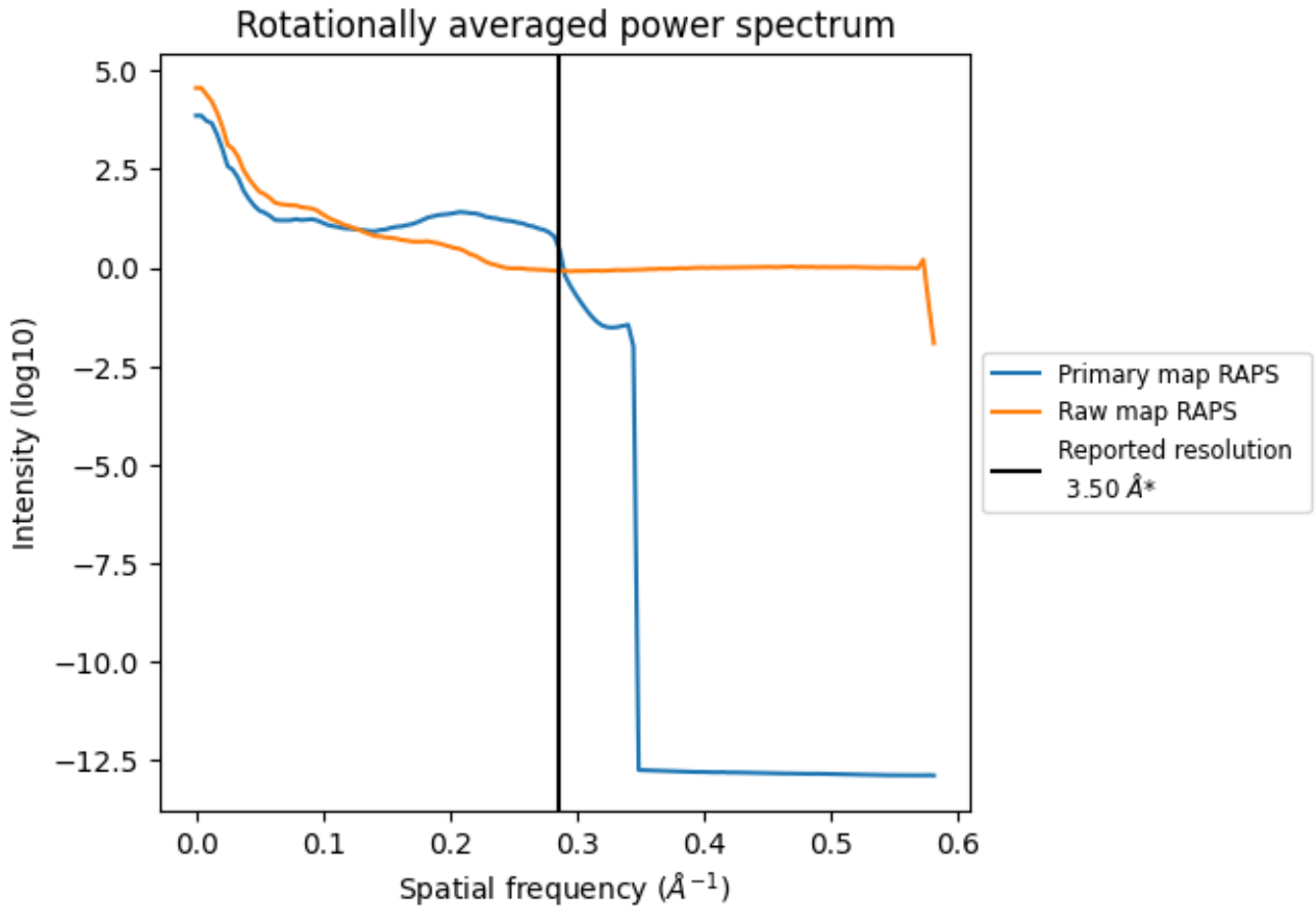
7.2 Volume estimate



The volume at the recommended contour level is 29 nm^3; this corresponds to an approximate mass of 26 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)

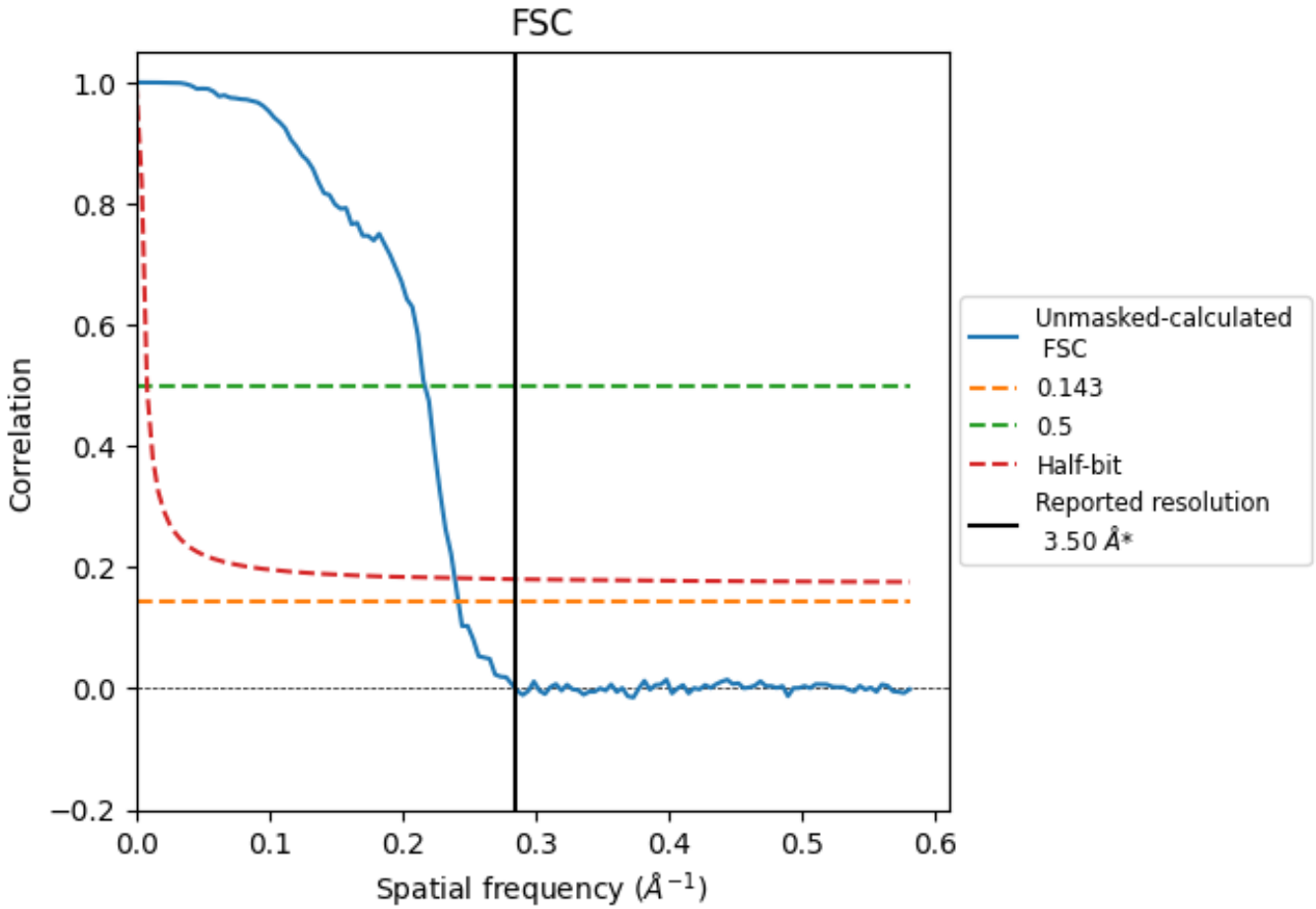


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

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 0.286 $Å^{-1}$

8.2 Resolution estimates (i)

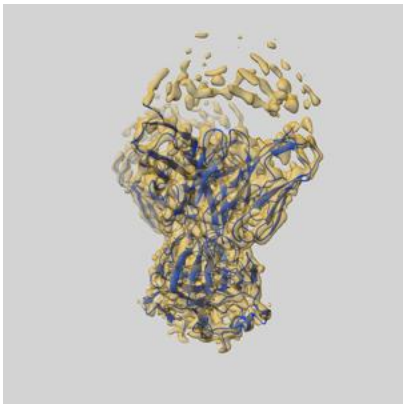
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	4.61	4.18

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

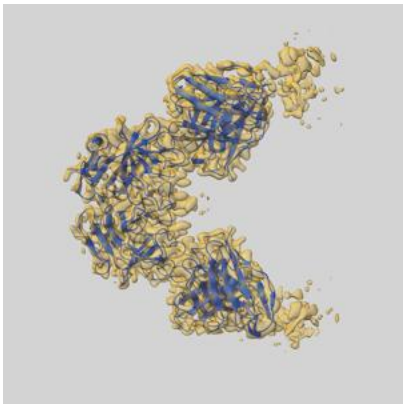
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50609 and PDB model 9FNS. Per-residue inclusion information can be found in section 3 on page 5.

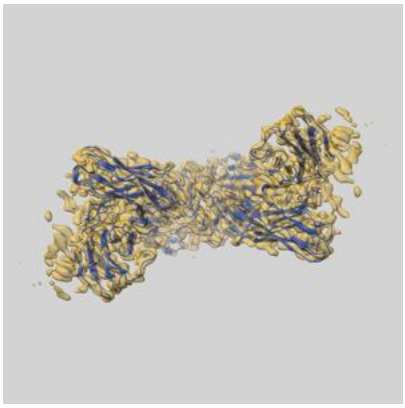
9.1 Map-model overlay



X



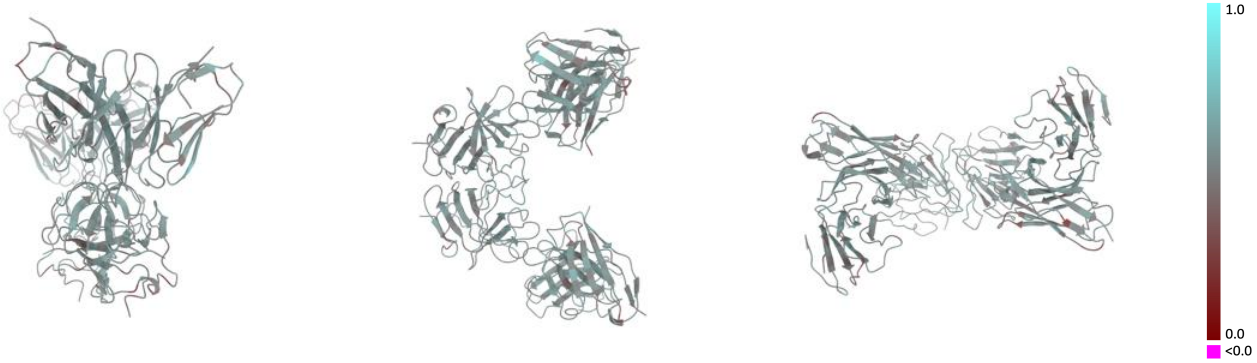
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

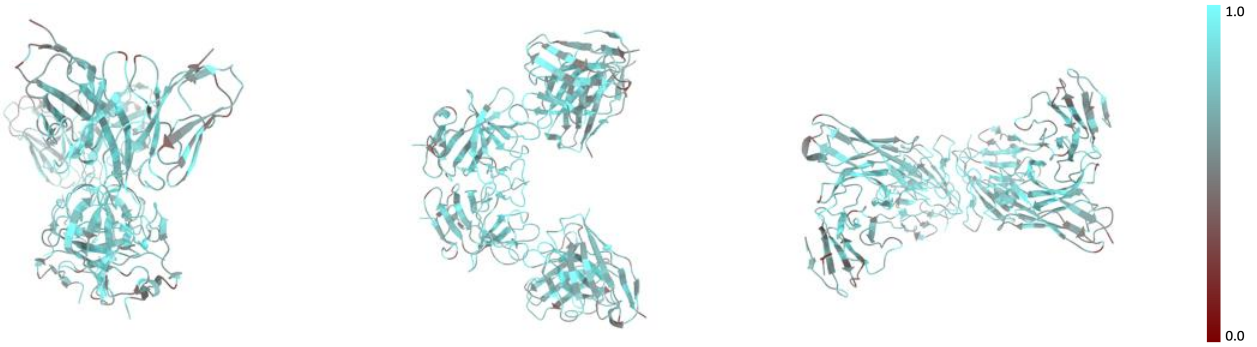
9.2 Q-score mapped to coordinate model (i)



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.

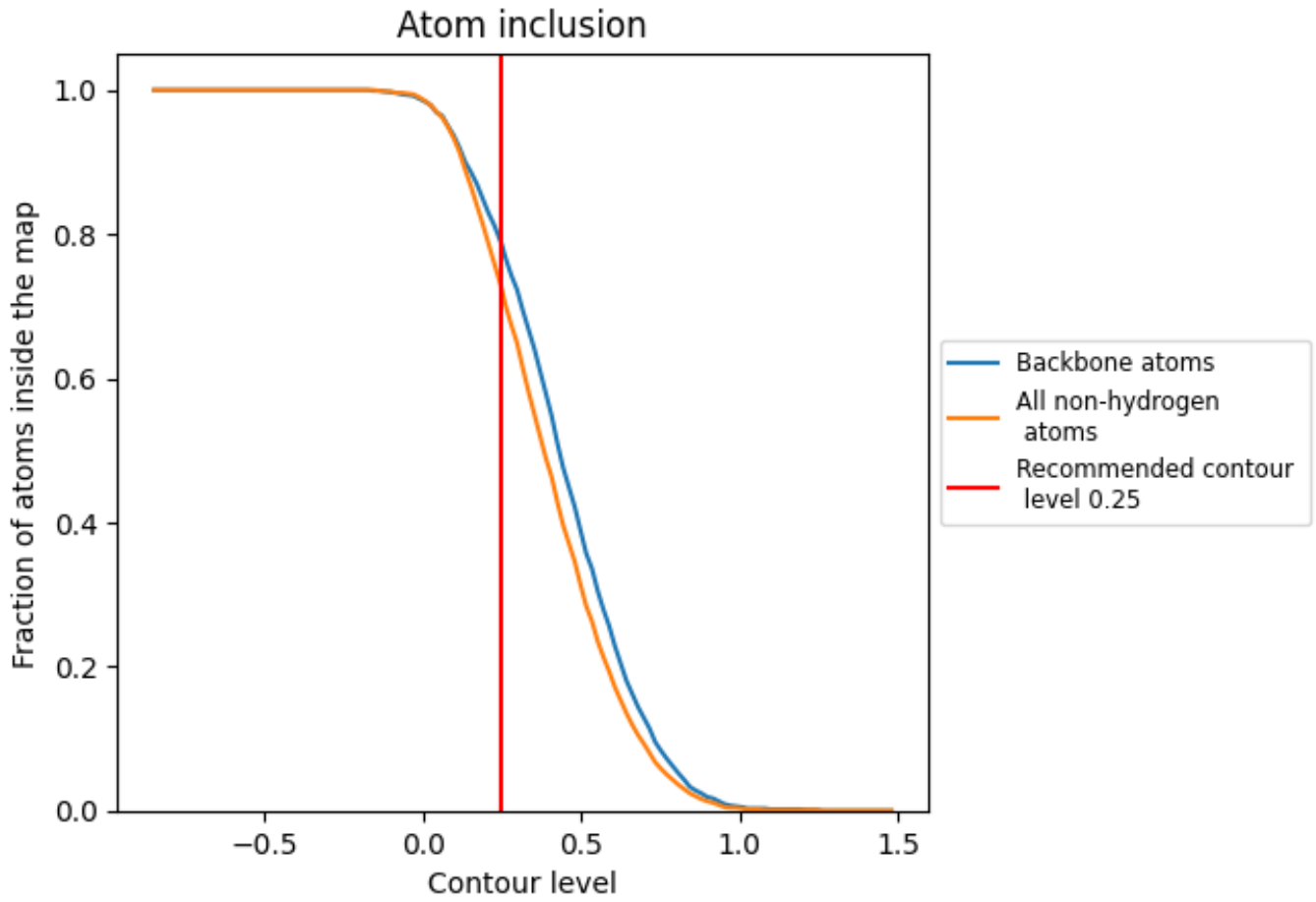
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.5220
A	0.7490	0.5210
B	0.7370	0.5210
C	0.7310	0.5240
D	0.6750	0.5150
E	0.7400	0.5290
F	0.6820	0.5150