



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 07:06 PM UTC

PDB ID : 7KZZ / pdb_00007kzz
EMDB ID : EMD-23093
Title : Cryo-EM structure of YiiP-Fab complex in Holo state
Authors : Lopez-Redondo, M.L.; Fan, S.; Koide, A.; Koide, S.; Beckstein, O.; Stokes, D.L.
Deposited on : 2020-12-10
Resolution : 3.42 Å(reported)
Based on initial model : 5VRF

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:

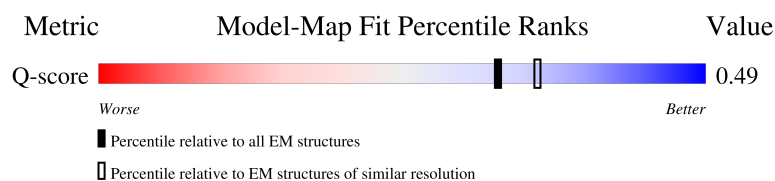
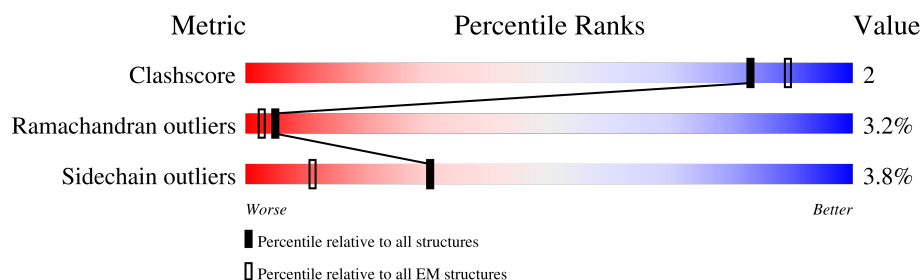
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.42 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	13959 (2.92 - 3.92)

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	296	12% 77% 17% • 5%
1	B	296	11% 79% 15% • 5%
2	C	216	69% 17% • 11%
2	E	216	69% 17% • 11%

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Mol	Chain	Length	Quality of chain
3	D	238	69% 15% • 12%
3	F	238	70% 14% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20864 atoms, of which 10404 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 Cadmium and zinc efflux pump FieF.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	281	Total	C	H	N	O	S	0	0
			4376	1396	2213	367	397	3		
1	A	281	Total	C	H	N	O	S	0	0
			4376	1396	2213	367	397	3		

- Molecule 2 is a protein called Fab2R light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	192	Total	C	H	N	O	S	0	0
			2915	926	1441	245	298	5		
2	C	192	Total	C	H	N	O	S	0	0
			2915	926	1441	245	298	5		

- Molecule 3 is a protein called Fab2R heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	209	Total	C	H	N	O	S	0	0
			3137	1012	1548	267	304	6		
3	D	209	Total	C	H	N	O	S	0	0
			3137	1012	1548	267	304	6		

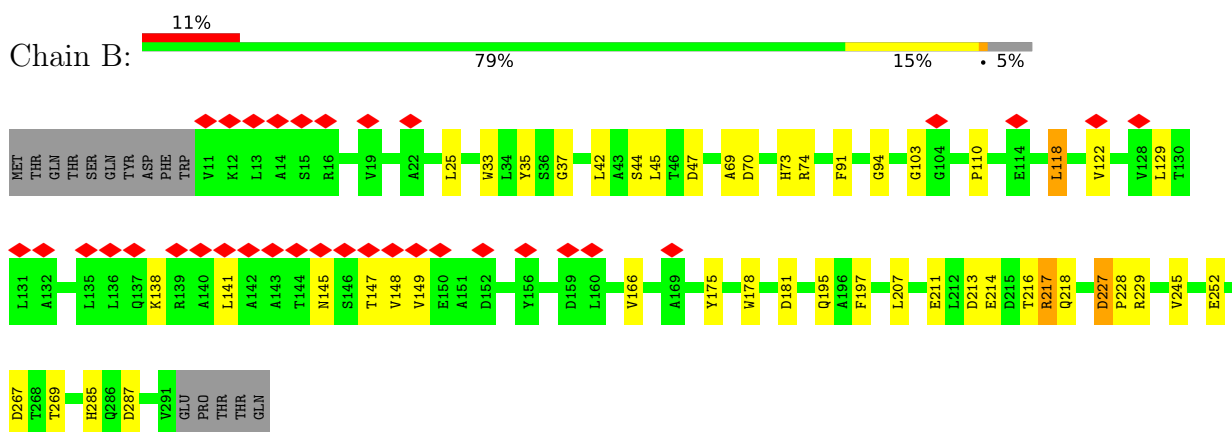
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	4	Total	Zn	0
			4	4	
4	A	4	Total	Zn	0
			4	4	

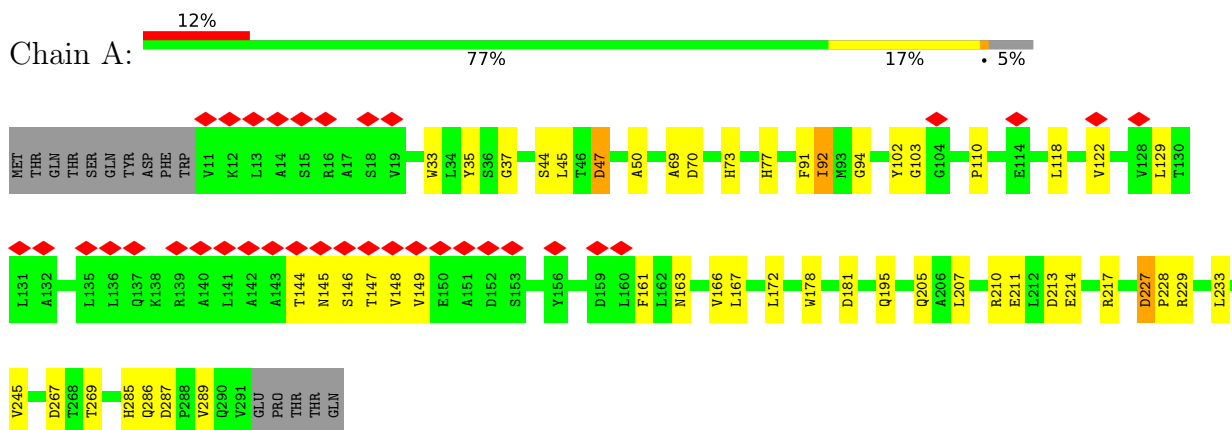
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

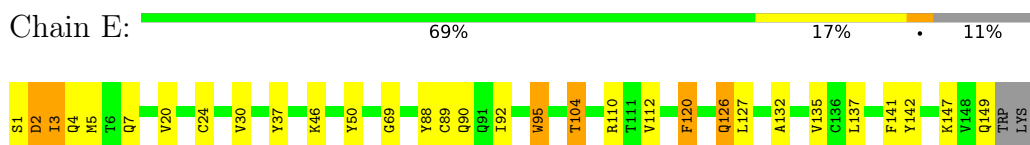
- Molecule 1: Cadmium and zinc efflux pump FieF

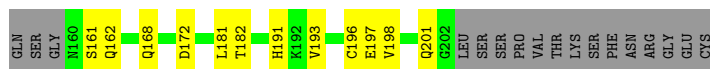


- Molecule 1: Cadmium and zinc efflux pump FieF



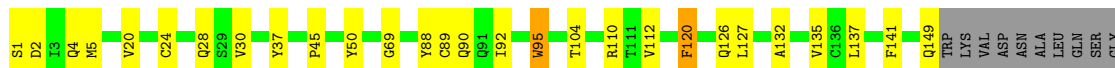
- Molecule 2: Fab2R light chain





• Molecule 2: Fab2R light chain

Chain C: 69% 17% 11%



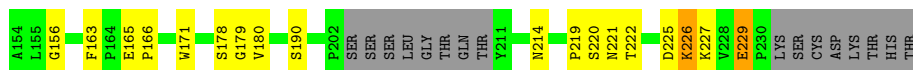
• Molecule 3: Fab2R heavy chain

Chain F: 70% 14% 12%



• Molecule 3: Fab2R heavy chain

Chain D: 69% 15% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	151898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.202	Depositor
Minimum map value	-2.487	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	345.84, 345.84, 345.84	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.86	0/2203	1.53	26/3001 (0.9%)
1	B	0.86	0/2203	1.53	21/3001 (0.7%)
2	C	1.02	1/1506 (0.1%)	1.56	10/2046 (0.5%)
2	E	1.02	0/1506	1.59	16/2046 (0.8%)
3	D	1.09	1/1631 (0.1%)	1.54	12/2222 (0.5%)
3	F	1.10	1/1631 (0.1%)	1.54	12/2222 (0.5%)
All	All	0.98	3/10680 (0.0%)	1.54	97/14538 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	6
2	C	0	11
2	E	0	10
3	D	0	15
3	F	0	16
All	All	0	63

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	41	ARG	CA-C	-6.16	1.45	1.52
3	F	41	ARG	CA-C	-6.06	1.45	1.52
2	C	45	PRO	N-CD	-5.04	1.40	1.47

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	130	PHE	CA-CB-CG	9.59	123.39	113.80
3	D	130	PHE	CA-CB-CG	9.21	123.00	113.80
1	A	267	ASP	OD1-CG-OD2	-8.98	101.34	122.90
1	B	267	ASP	OD1-CG-OD2	-8.89	101.56	122.90
1	B	70	ASP	OD1-CG-OD2	-7.78	104.22	122.90
1	B	287	ASP	CA-CB-CG	7.66	120.26	112.60
2	E	120	PHE	CA-CB-CG	7.58	121.38	113.80
2	C	120	PHE	CA-CB-CG	7.57	121.37	113.80
1	A	287	ASP	CA-CB-CG	7.53	120.12	112.60
1	A	145	ASN	CA-CB-CG	7.40	120.00	112.60
1	B	145	ASN	CA-CB-CG	7.21	119.81	112.60
2	E	3	ILE	CA-CB-CG1	6.88	122.10	110.40
1	A	47	ASP	OD1-CG-OD2	-6.75	106.70	122.90
1	A	267	ASP	CA-CB-CG	6.67	119.27	112.60
2	E	90	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	B	267	ASP	CA-CB-CG	6.61	119.21	112.60
1	B	103	GLY	CA-C-N	6.56	127.21	120.00
1	B	103	GLY	C-N-CA	6.56	127.21	120.00
1	A	103	GLY	CA-C-N	6.52	127.17	120.00
1	A	103	GLY	C-N-CA	6.52	127.17	120.00
1	A	70	ASP	OD1-CG-OD2	-6.49	107.32	122.90
2	C	135	VAL	N-CA-C	6.47	117.13	108.27
1	B	47	ASP	OD1-CG-OD2	-6.46	107.41	122.90
2	E	135	VAL	N-CA-C	6.45	117.11	108.27
3	F	229	GLU	N-CA-C	6.45	115.56	108.14
3	D	112	HIS	CB-CG-CD2	-6.45	122.82	131.20
3	F	220	SER	CA-C-N	6.33	133.63	121.54
3	F	220	SER	C-N-CA	6.33	133.63	121.54
2	E	92	ILE	N-CA-CB	-6.32	105.26	112.21
3	D	229	GLU	N-CA-C	6.30	115.39	108.14
3	D	220	SER	CA-C-N	6.17	133.33	121.54
3	D	220	SER	C-N-CA	6.17	133.33	121.54
3	F	38	HIS	CB-CG-CD2	-6.16	123.20	131.20
3	D	38	HIS	CB-CG-CD2	-6.10	123.27	131.20
2	C	92	ILE	N-CA-CB	-6.06	105.54	112.21
3	F	76	ASP	CA-CB-CG	6.00	118.60	112.60
3	D	76	ASP	CA-CB-CG	5.93	118.53	112.60
3	F	112	HIS	CB-CG-CD2	-5.92	123.51	131.20
2	E	126	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	A	146	SER	CA-C-N	5.87	132.75	121.54
1	A	146	SER	C-N-CA	5.87	132.75	121.54
2	E	2	ASP	CA-C-N	5.82	132.44	121.97
2	E	2	ASP	C-N-CA	5.82	132.44	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ILE	CB-CA-C	-5.78	104.58	111.97
3	F	133	ILE	CB-CA-C	5.73	120.69	111.29
3	D	225	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	227	ASP	CA-CB-CG	5.63	118.23	112.60
3	D	133	ILE	CB-CA-C	5.61	120.49	111.29
1	B	195	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	B	229	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	118	LEU	CA-C-N	5.57	126.28	119.99
1	A	118	LEU	C-N-CA	5.57	126.28	119.99
1	B	197	PHE	CA-CB-CG	5.56	119.36	113.80
2	C	182	THR	N-CA-C	5.54	117.73	109.25
2	E	168	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	A	267	ASP	CB-CG-OD2	5.53	131.12	118.40
2	C	149	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	229	ARG	NE-CZ-NH1	-5.50	116.00	121.50
2	C	4	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	B	267	ASP	CB-CG-OD2	5.47	130.99	118.40
2	E	149	GLN	OE1-CD-NE2	-5.42	117.18	122.60
2	E	4	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	A	195	GLN	OE1-CD-NE2	-5.40	117.20	122.60
2	C	168	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	B	229	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	B	118	LEU	CA-C-N	5.27	125.94	119.99
1	B	118	LEU	C-N-CA	5.27	125.94	119.99
1	A	144	THR	CA-C-N	5.25	131.00	122.39
1	A	144	THR	C-N-CA	5.25	131.00	122.39
1	B	217	ARG	NE-CZ-NH2	-5.24	114.48	119.20
2	C	141	PHE	CA-CB-CG	5.22	119.03	113.80
3	F	219	PRO	CA-C-N	5.20	128.18	120.17
3	F	219	PRO	C-N-CA	5.20	128.18	120.17
1	B	227	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	229	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	B	73	HIS	CB-CG-CD2	-5.18	124.47	131.20
3	D	219	PRO	CA-C-N	5.17	128.13	120.17
3	D	219	PRO	C-N-CA	5.17	128.13	120.17
2	E	141	PHE	CA-CB-CG	5.16	118.95	113.80
2	E	172	ASP	CA-CB-CG	5.15	117.75	112.60
2	E	182	THR	N-CA-C	5.15	117.12	109.25
3	F	102	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	B	285	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
1	B	216	THR	CB-CA-C	5.12	119.83	110.36
2	E	201	GLN	OE1-CD-NE2	-5.12	117.48	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
1	A	286	GLN	OE1-CD-NE2	-5.09	117.51	122.60
2	C	201	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	205	GLN	OE1-CD-NE2	-5.07	117.53	122.60
3	D	214	ASN	CA-CB-CG	5.07	117.67	112.60
2	C	172	ASP	CA-CB-CG	5.06	117.66	112.60
2	E	162	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	218	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	285	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
3	F	225	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	73	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	A	161	PHE	CA-CB-CG	5.03	118.83	113.80

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	TYR	Sidechain
1	A	207	LEU	Peptide
1	A	210	ARG	Sidechain
1	A	211	GLU	Peptide
1	A	35	TYR	Peptide
1	B	175	TYR	Sidechain
1	B	207	LEU	Peptide
1	B	211	GLU	Peptide
1	B	217	ARG	Sidechain
1	B	35	TYR	Peptide
1	B	74	ARG	Sidechain
2	C	1	SER	Peptide
2	C	110	ARG	Sidechain
2	C	112	VAL	Peptide
2	C	120	PHE	Sidechain
2	C	196	CYS	Peptide
2	C	197	GLU	Peptide
2	C	199	THR	Peptide
2	C	30	VAL	Peptide
2	C	37	TYR	Sidechain
2	C	50	TYR	Sidechain
2	C	88	TYR	Sidechain
3	D	104	TYR	Sidechain
3	D	112	HIS	Sidechain
3	D	120	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	D	129	VAL	Peptide
3	D	163	PHE	Peptide
3	D	165	GLU	Peptide
3	D	18	GLY	Peptide
3	D	222	THR	Peptide
3	D	4	GLU	Sidechain
3	D	41	ARG	Sidechain
3	D	55	TYR	Sidechain
3	D	83	TYR	Sidechain
3	D	9	GLU	Peptide
3	D	97	TYR	Sidechain
3	D	98	TYR	Sidechain
2	E	1	SER	Peptide
2	E	110	ARG	Sidechain
2	E	112	VAL	Peptide
2	E	120	PHE	Sidechain
2	E	142	TYR	Sidechain
2	E	196	CYS	Peptide
2	E	30	VAL	Peptide
2	E	37	TYR	Sidechain
2	E	50	TYR	Sidechain
2	E	88	TYR	Sidechain
3	F	104	TYR	Sidechain
3	F	115	TYR	Sidechain
3	F	120	TYR	Sidechain
3	F	129	VAL	Peptide
3	F	163	PHE	Peptide
3	F	165	GLU	Peptide
3	F	18	GLY	Peptide
3	F	222	THR	Peptide
3	F	229	GLU	Peptide
3	F	4	GLU	Sidechain
3	F	41	ARG	Sidechain
3	F	55	TYR	Sidechain
3	F	83	TYR	Sidechain
3	F	9	GLU	Peptide
3	F	97	TYR	Sidechain
3	F	98	TYR	Sidechain

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	2163	2213	2212	13	0
1	B	2163	2213	2212	10	0
2	C	1474	1441	1440	10	0
2	E	1474	1441	1440	7	0
3	D	1589	1548	1546	11	0
3	F	1589	1548	1546	8	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
All	All	10460	10404	10396	49	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 2.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:MET:HE3	2:C:24:CYS:SG	2.30	0.71
2:E:5:MET:HE3	2:E:24:CYS:SG	2.31	0.70
2:E:127:LEU:HD13	2:E:132:ALA:HB2	1.81	0.62
1:B:228:PRO:HD3	2:E:95:TRP:CZ3	2.37	0.60
1:A:228:PRO:HD3	2:C:95:TRP:CZ3	2.37	0.59
2:C:127:LEU:HD13	2:C:132:ALA:HB2	1.85	0.58
1:A:44:SER:HB2	1:A:166:VAL:HG21	1.91	0.52
1:B:25:LEU:HD21	1:B:129:LEU:HD11	1.92	0.52
1:B:91:PHE:CE2	1:A:94:GLY:HA2	2.46	0.51
2:C:177:LEU:C	2:C:177:LEU:HD23	2.35	0.51
2:E:126:GLN:HA	3:F:139:PHE:CE1	2.47	0.49
1:A:163:ASN:O	1:A:167:LEU:HD13	2.13	0.48
1:B:44:SER:HB2	1:B:166:VAL:HG21	1.94	0.48
3:F:141:LEU:HD23	3:F:156:GLY:C	2.40	0.47
1:A:110:PRO:HA	1:A:178:TRP:CZ2	2.50	0.47
3:D:141:LEU:HD23	3:D:156:GLY:C	2.39	0.46
1:A:166:VAL:HB	1:A:167:LEU:HD12	1.96	0.46
2:C:200:HIS:CG	2:C:201:GLN:H	2.34	0.46
1:B:110:PRO:HA	1:B:178:TRP:CZ2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:95:TRP:CH2	3:F:55:TYR:CZ	3.04	0.46
1:A:217:ARG:HH11	1:A:217:ARG:HG2	1.81	0.46
1:B:94:GLY:HA2	1:A:91:PHE:CE2	2.52	0.45
3:F:180:VAL:HG13	3:F:180:VAL:O	2.17	0.45
2:C:95:TRP:CH2	3:D:55:TYR:CZ	3.04	0.45
1:A:50:ALA:HB1	1:A:92:ILE:CD1	2.47	0.45
3:D:180:VAL:O	3:D:180:VAL:HG13	2.17	0.44
3:F:60:SER:HB3	3:F:62:TYR:CE2	2.52	0.44
1:A:33:TRP:CD2	1:A:33:TRP:O	2.71	0.43
1:A:289:VAL:CG2	3:D:113:TRP:CD2	3.01	0.43
3:F:171:TRP:CD1	3:F:180:VAL:CG2	3.01	0.43
1:B:138:LYS:HE3	1:B:141:LEU:HD23	2.00	0.43
1:B:33:TRP:O	1:B:33:TRP:CD2	2.72	0.43
3:D:171:TRP:CD1	3:D:180:VAL:CG2	3.01	0.43
1:A:45:LEU:HD23	1:A:45:LEU:C	2.44	0.42
3:D:15:VAL:HG13	3:D:129:VAL:HG12	2.01	0.42
1:A:233:LEU:C	1:A:233:LEU:HD23	2.43	0.42
3:D:227:LYS:O	3:D:227:LYS:HE2	2.19	0.42
2:E:7:GLN:HE21	2:E:104:THR:HG23	1.84	0.42
3:D:25:CYS:HG	3:D:99:CYS:CB	2.32	0.42
3:D:140:PRO:HD3	3:D:226:LYS:HE3	2.01	0.42
3:F:140:PRO:HD3	3:F:226:LYS:HE3	2.02	0.41
2:C:200:HIS:CG	2:C:201:GLN:N	2.89	0.41
2:C:126:GLN:HA	3:D:139:PHE:CE1	2.56	0.41
1:B:129:LEU:HD12	1:B:129:LEU:C	2.45	0.41
2:E:5:MET:HE3	2:E:89:CYS:SG	2.60	0.41
2:C:90:GLN:HE22	3:D:118:MET:HE3	1.86	0.41
1:B:45:LEU:C	1:B:45:LEU:HD23	2.45	0.41
3:F:227:LYS:HE2	3:F:227:LYS:O	2.21	0.40
2:C:5:MET:HE3	2:C:89:CYS:SG	2.61	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	279/296 (94%)	248 (89%)	25 (9%)	6 (2%)	5	23
1	B	279/296 (94%)	245 (88%)	28 (10%)	6 (2%)	5	23
2	C	188/216 (87%)	155 (82%)	26 (14%)	7 (4%)	2	16
2	E	188/216 (87%)	153 (81%)	27 (14%)	8 (4%)	2	13
3	D	203/238 (85%)	167 (82%)	28 (14%)	8 (4%)	2	15
3	F	203/238 (85%)	167 (82%)	28 (14%)	8 (4%)	2	15
All	All	1340/1500 (89%)	1135 (85%)	162 (12%)	43 (3%)	5	18

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	ASP
2	E	3	ILE
2	E	95	TRP
3	F	130	PHE
3	F	166	PRO
3	F	221	ASN
1	A	213	ASP
2	C	95	TRP
3	D	130	PHE
3	D	166	PRO
3	D	221	ASN
1	B	37	GLY
1	B	147	THR
2	E	2	ASP
2	E	191	HIS
3	F	133	ILE
1	A	147	THR
2	C	197	GLU
2	E	197	GLU
3	F	111	ARG
2	C	2	ASP
2	C	191	HIS
3	D	111	ARG
3	D	133	ILE
1	B	69	ALA
2	E	69	GLY
3	F	178	SER

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Mol	Chain	Res	Type
3	F	190	SER
1	A	37	GLY
1	A	69	ALA
2	C	69	GLY
3	D	178	SER
3	D	190	SER
1	B	148	VAL
2	E	161	SER
1	A	149	VAL
2	C	161	SER
1	B	149	VAL
1	A	148	VAL
3	F	179	GLY
3	D	179	GLY
2	C	193	VAL
2	E	193	VAL

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	227/242 (94%)	218 (96%)	9 (4%)	28	52
1	B	227/242 (94%)	218 (96%)	9 (4%)	28	52
2	C	170/191 (89%)	163 (96%)	7 (4%)	27	52
2	E	170/191 (89%)	163 (96%)	7 (4%)	27	52
3	D	175/200 (88%)	169 (97%)	6 (3%)	32	56
3	F	175/200 (88%)	169 (97%)	6 (3%)	32	56
All	All	1144/1266 (90%)	1100 (96%)	44 (4%)	30	54

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	LEU
1	B	118	LEU

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Mol	Chain	Res	Type
1	B	122	VAL
1	B	181	ASP
1	B	214	GLU
1	B	227	ASP
1	B	245	VAL
1	B	252	GLU
1	B	269	THR
2	E	20	VAL
2	E	46	LYS
2	E	104	THR
2	E	137	LEU
2	E	147	LYS
2	E	181	LEU
2	E	198	VAL
3	F	4	GLU
3	F	38	HIS
3	F	65	ASP
3	F	104	TYR
3	F	226	LYS
3	F	229	GLU
1	A	47	ASP
1	A	122	VAL
1	A	129	LEU
1	A	172	LEU
1	A	181	ASP
1	A	214	GLU
1	A	227	ASP
1	A	245	VAL
1	A	269	THR
2	C	20	VAL
2	C	28	GLN
2	C	104	THR
2	C	137	LEU
2	C	177	LEU
2	C	181	LEU
2	C	198	VAL
3	D	4	GLU
3	D	65	ASP
3	D	104	TYR
3	D	132	GLN
3	D	226	LYS
3	D	229	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	58	ASN
1	B	145	ASN
1	B	248	GLN
1	B	286	GLN
2	E	7	GLN
2	E	39	GLN
2	E	191	HIS
3	F	42	GLN
1	A	58	ASN
1	A	145	ASN
1	A	174	GLN
1	A	218	GLN
1	A	248	GLN
2	C	39	GLN
2	C	139	ASN
3	D	42	GLN
3	D	181	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

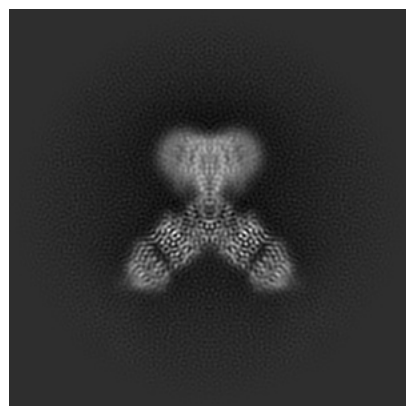
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23093. These allow visual inspection of the internal detail of the map and identification of artifacts.

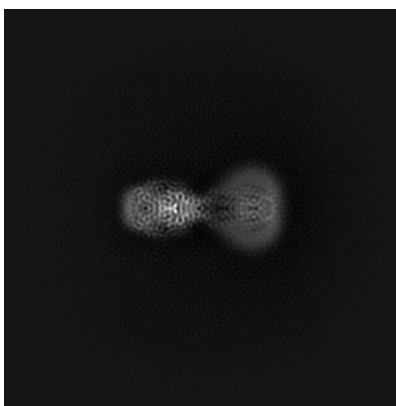
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

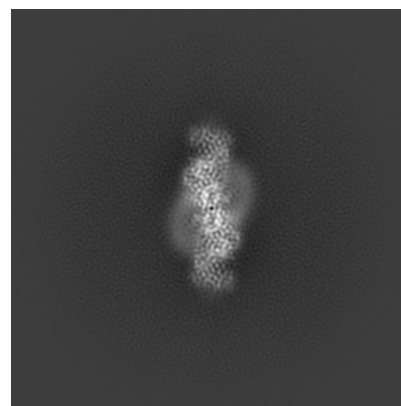
6.1.1 Primary map



X

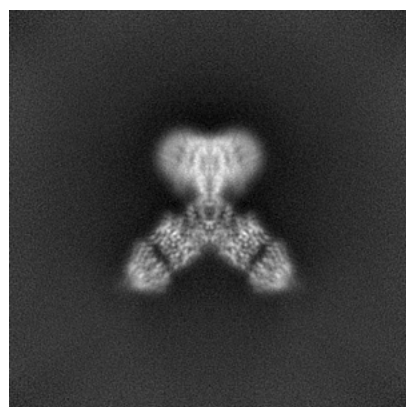


Y

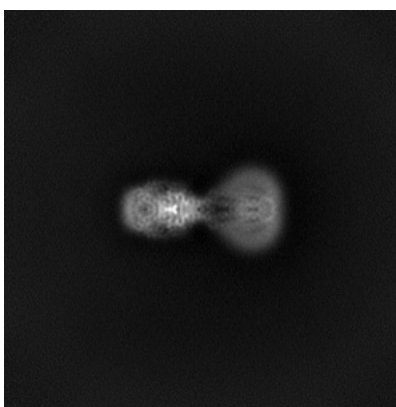


Z

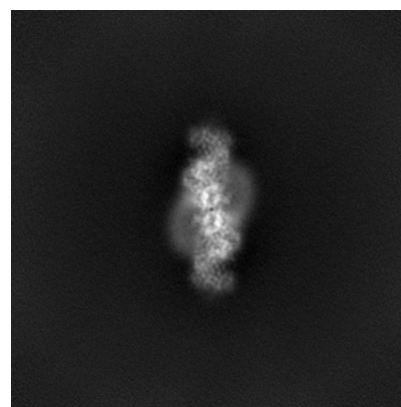
6.1.2 Raw map



X



Y

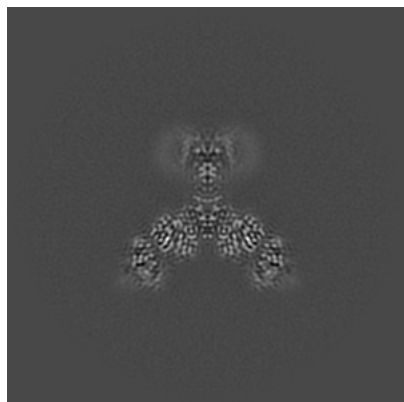


Z

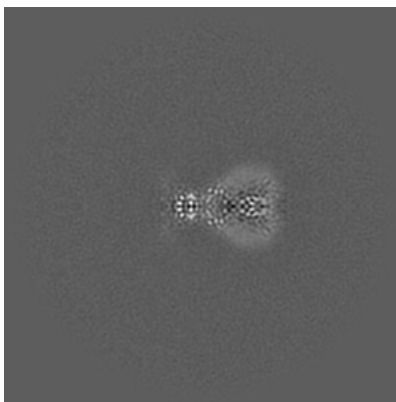
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

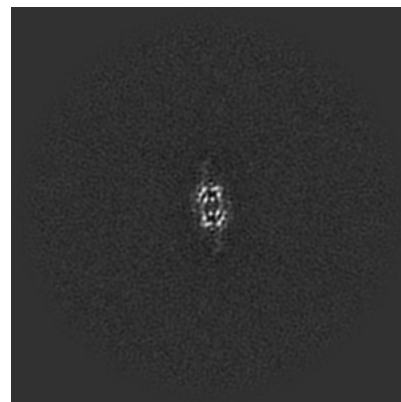
6.2.1 Primary map



X Index: 165

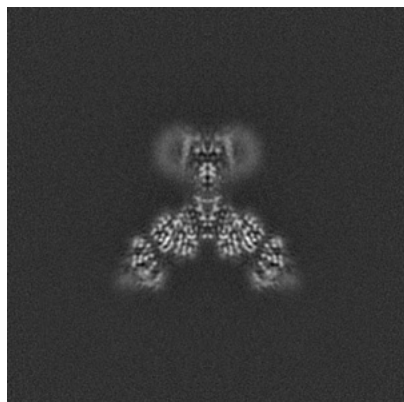


Y Index: 165

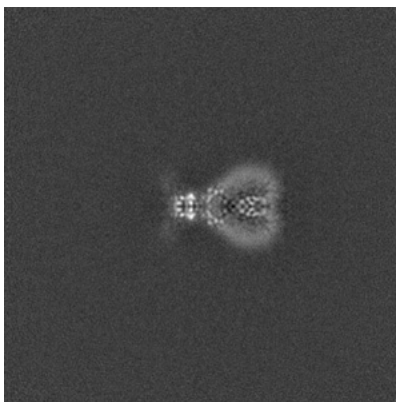


Z Index: 165

6.2.2 Raw map



X Index: 165



Y Index: 165

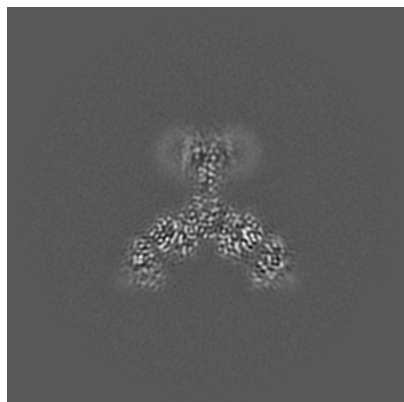


Z Index: 165

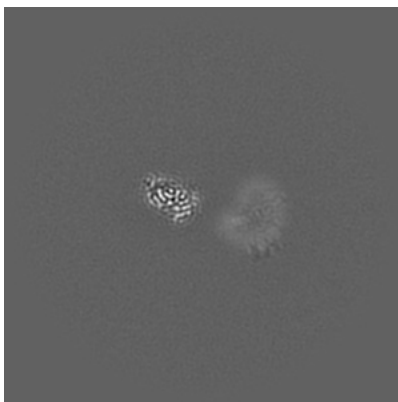
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

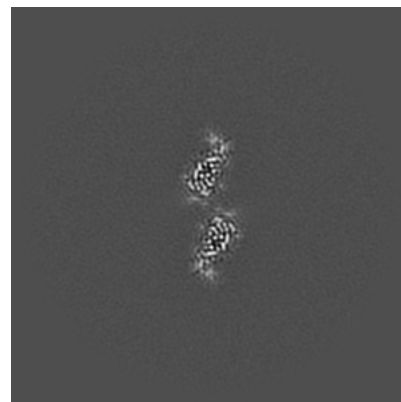
6.3.1 Primary map



X Index: 164

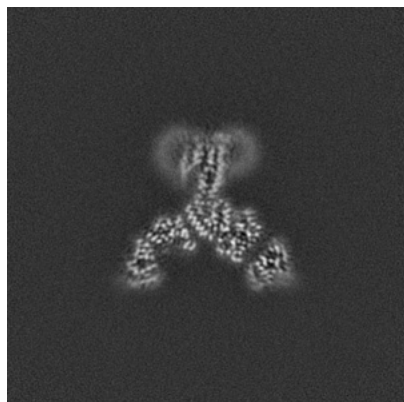


Y Index: 139

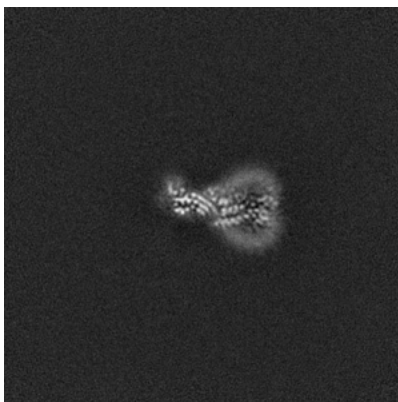


Z Index: 137

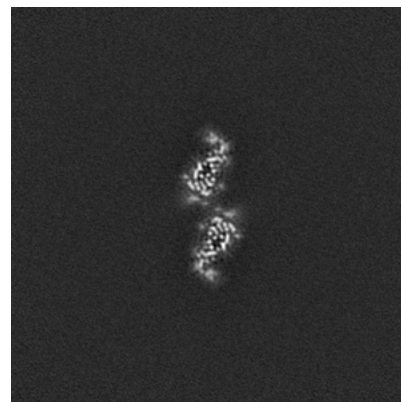
6.3.2 Raw map



X Index: 161



Y Index: 159

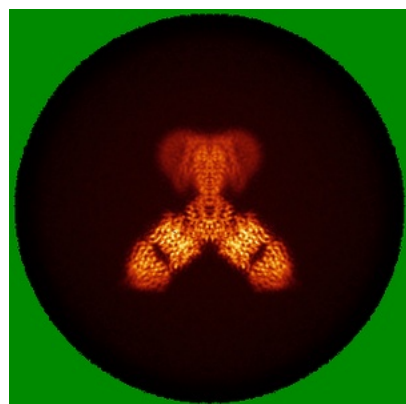


Z Index: 137

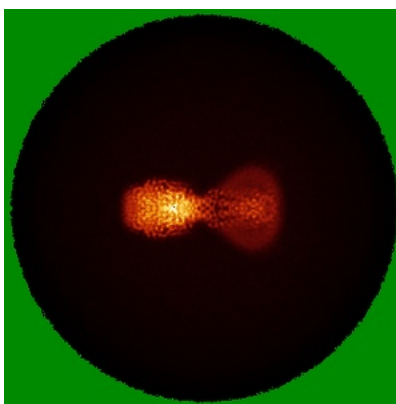
The images above show the largest variance slices of the map in three orthogonal directions.

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

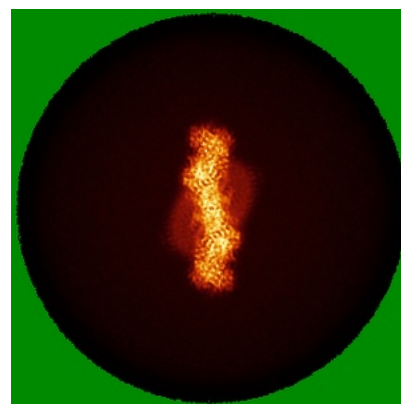
6.4.1 Primary map



X

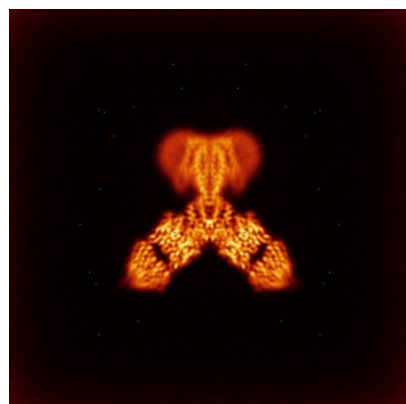


Y

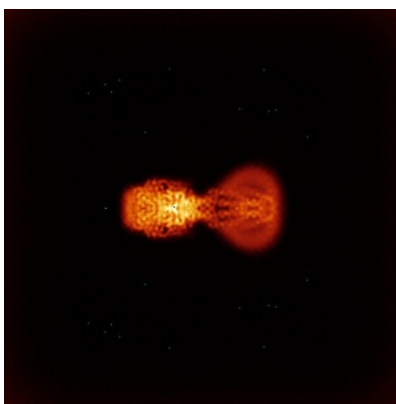


Z

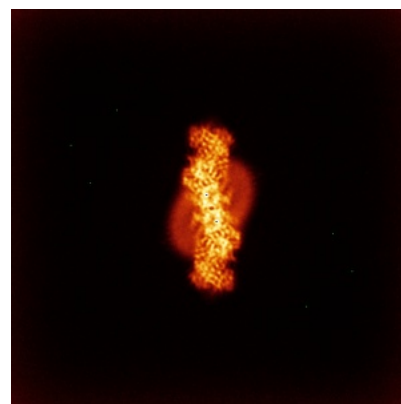
6.4.2 Raw map



X



Y

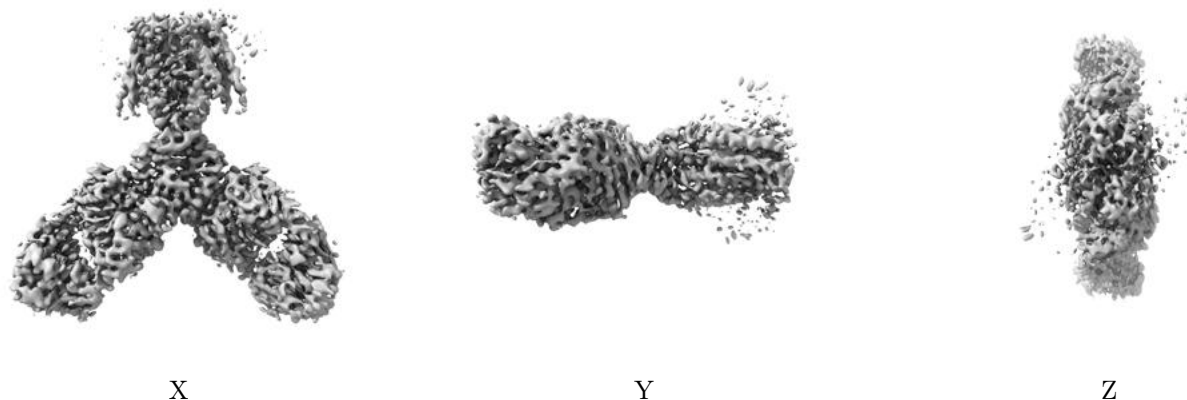


Z

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.

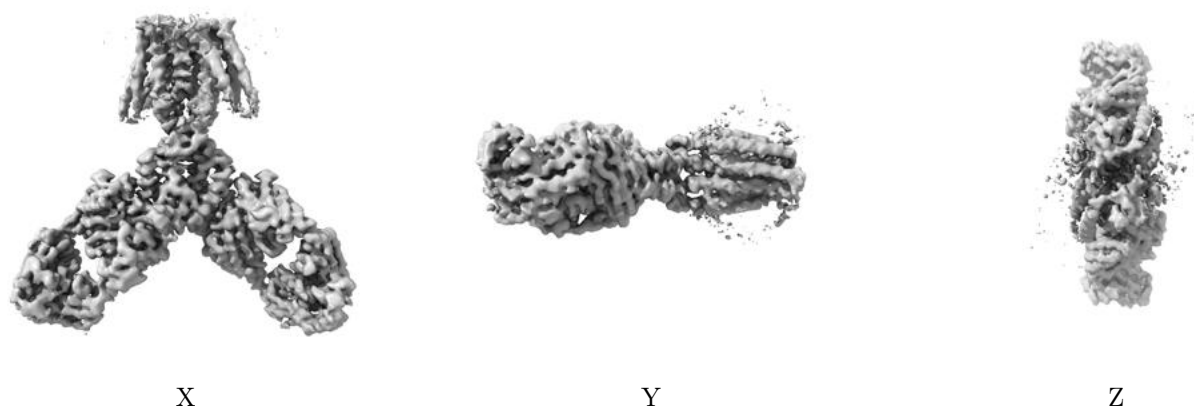
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

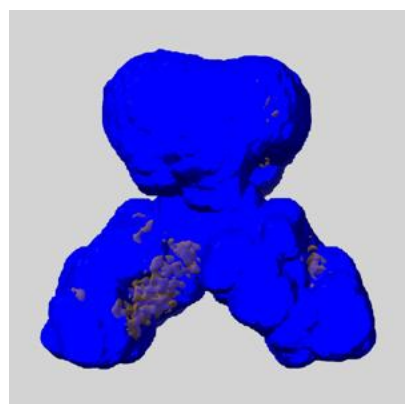
6.6 Mask visualisation [i](#)

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

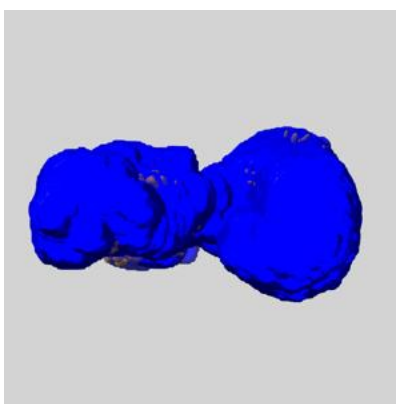
A mask typically either:

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

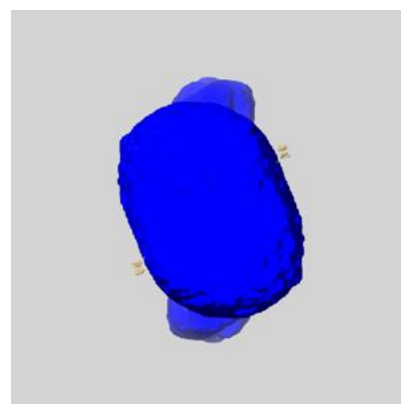
6.6.1 emd_23093_msk_1.map [i](#)



X



Y

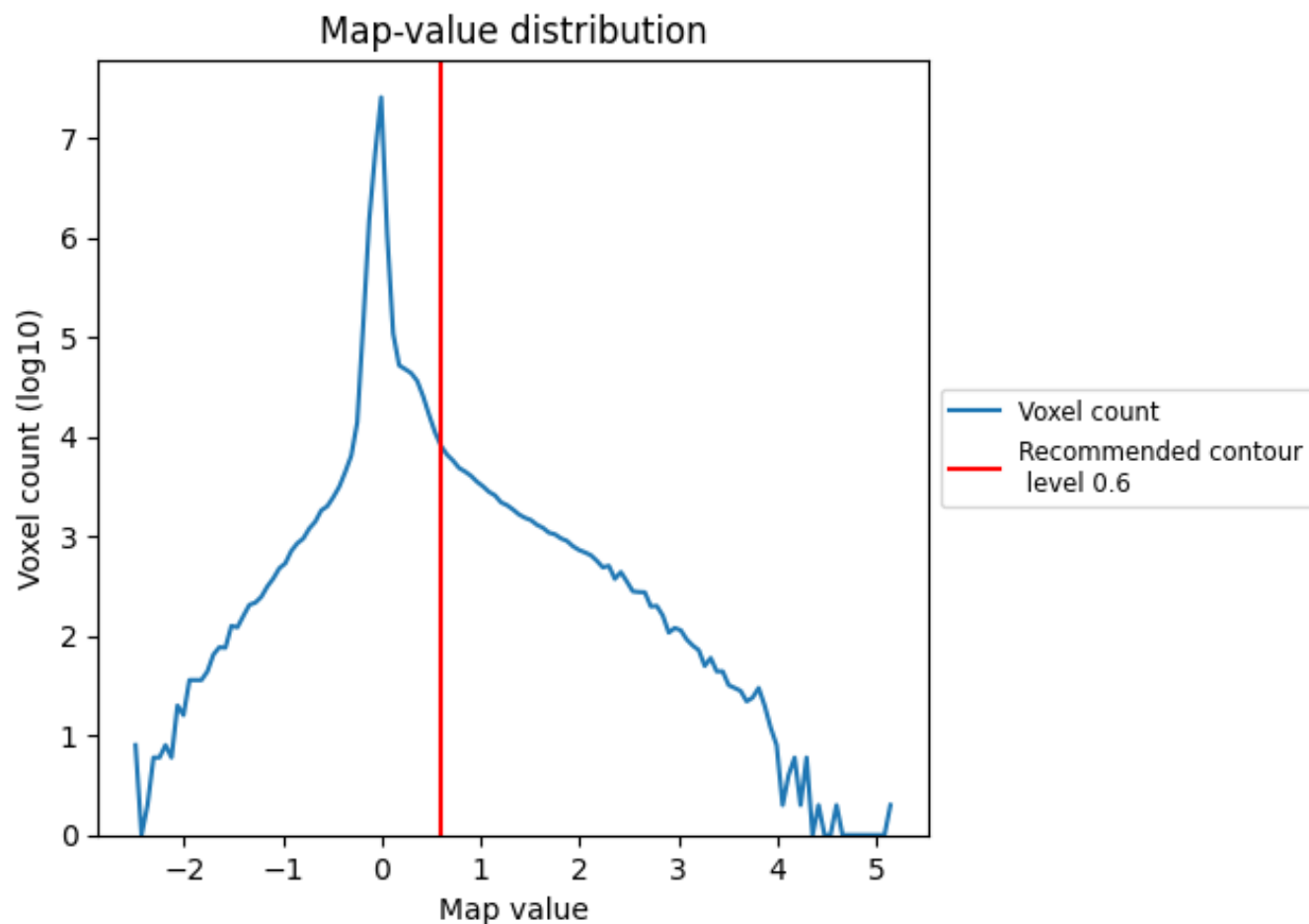


Z

7 Map analysis [i](#)

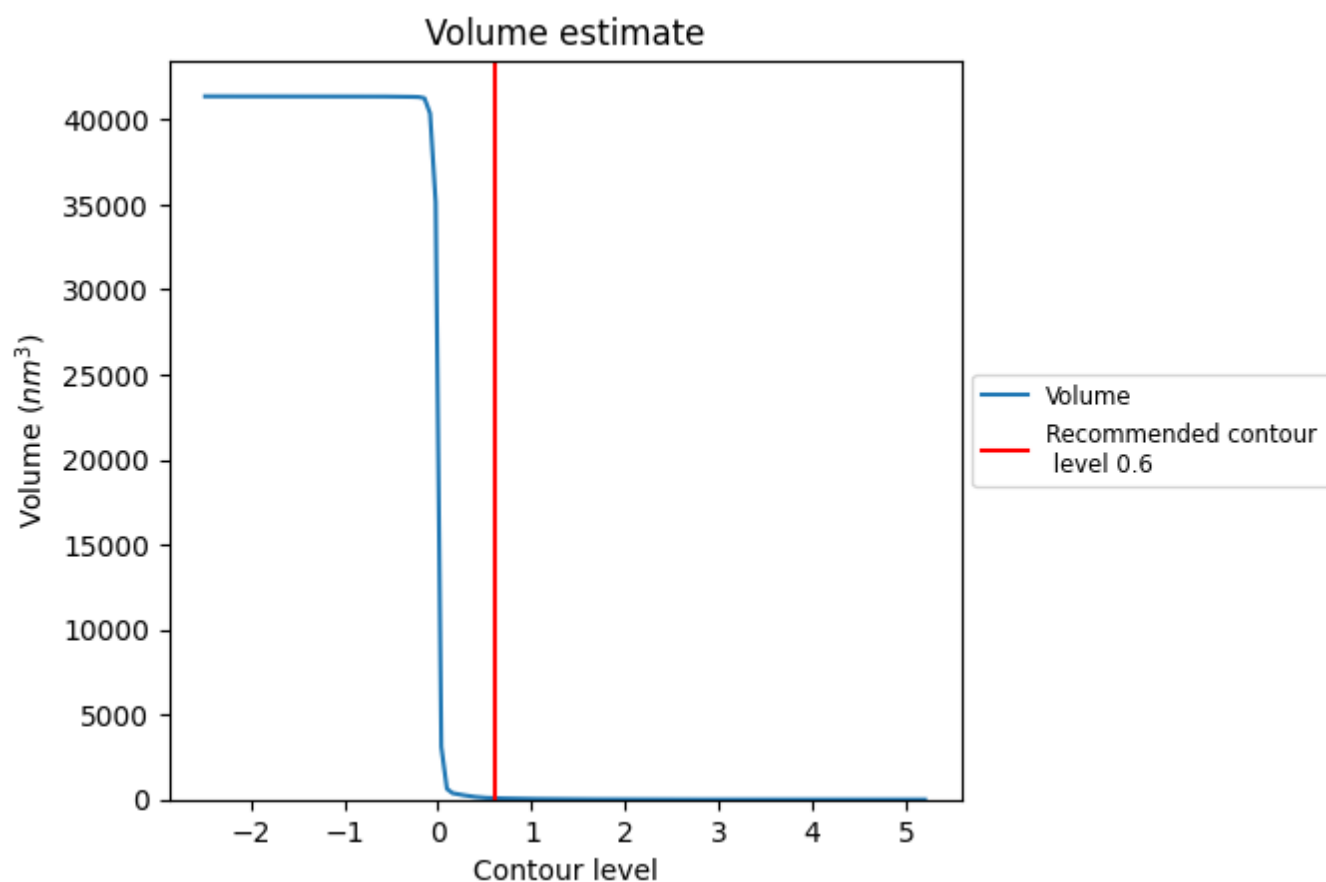
This section contains the results of statistical analysis of the map.

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.

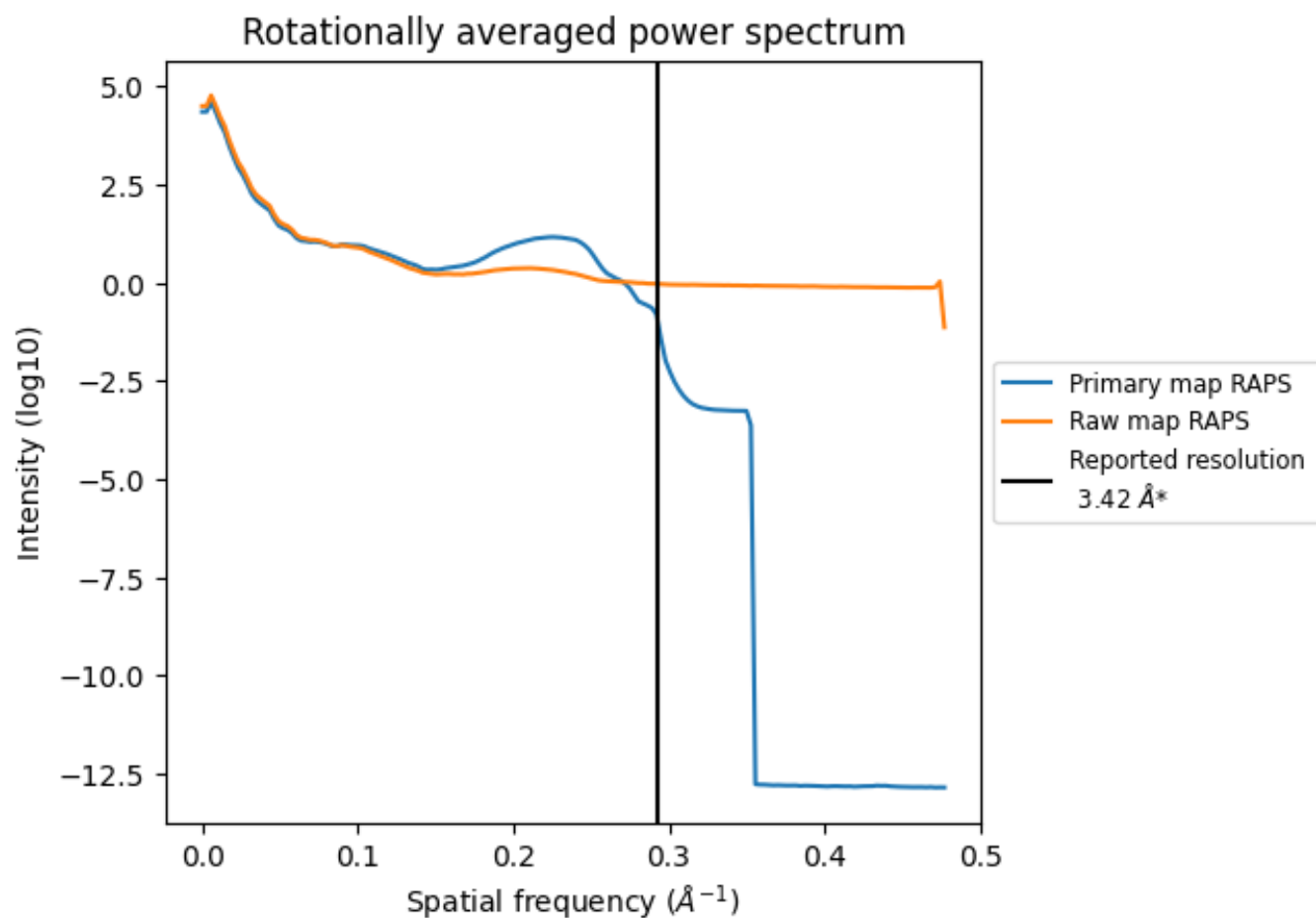
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm^3 ; this corresponds to an approximate mass of 74 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 ⓘ

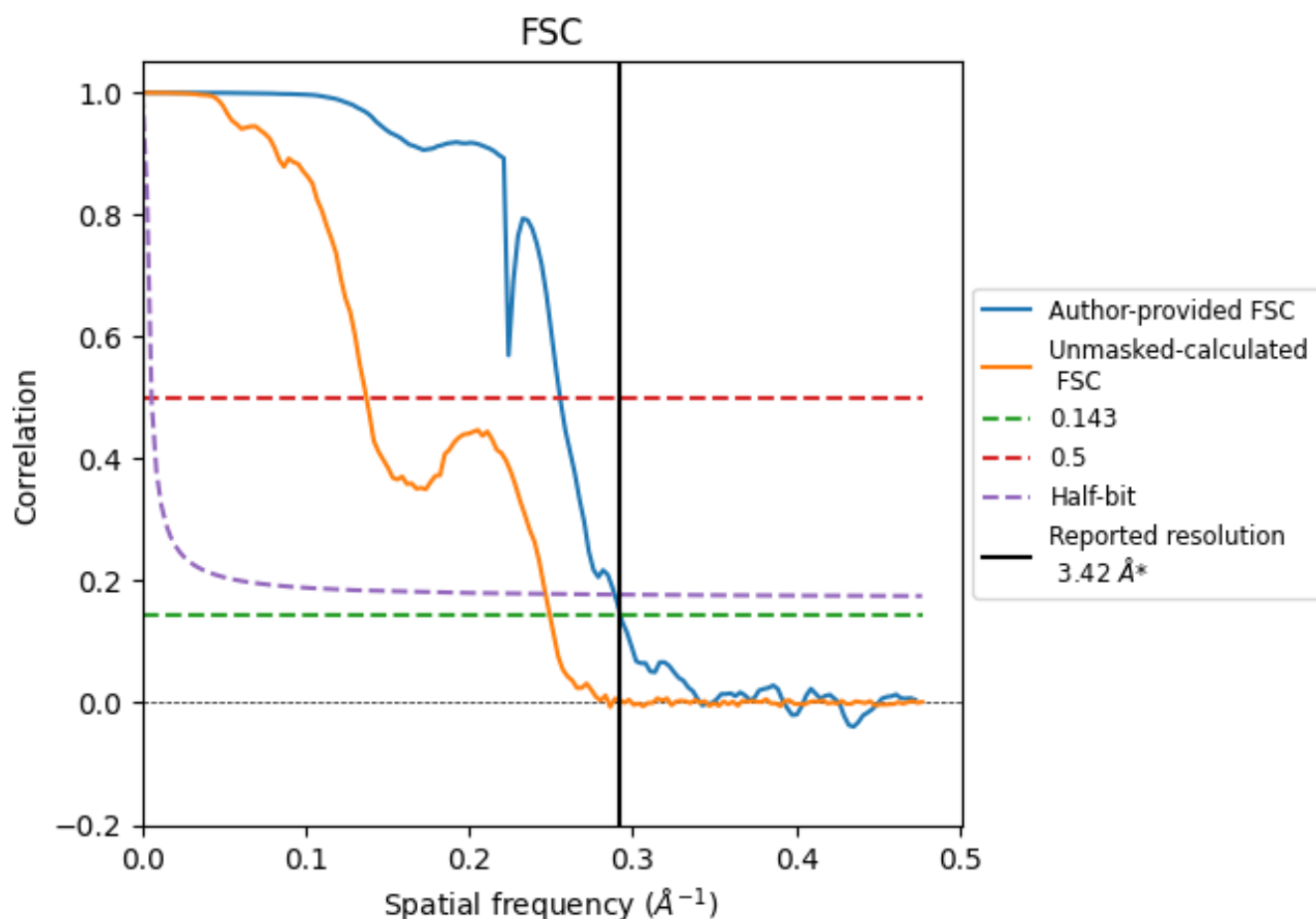


*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

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 0.292 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

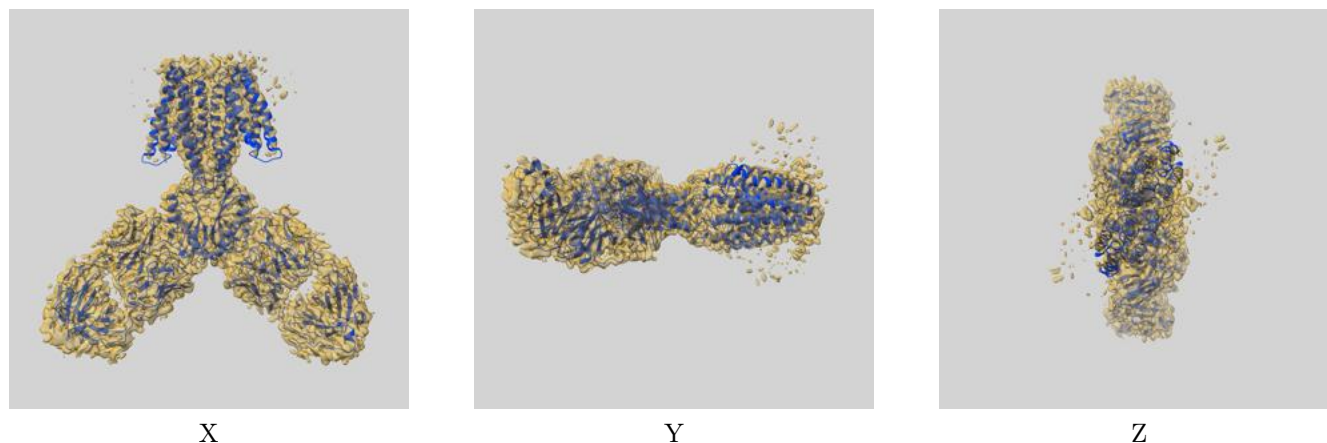
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	3.91	3.46
Unmasked-calculated*	4.01	7.29	4.05

*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 4.01 differs from the reported value 3.42 by more than 10 %

9 Map-model fit [i](#)

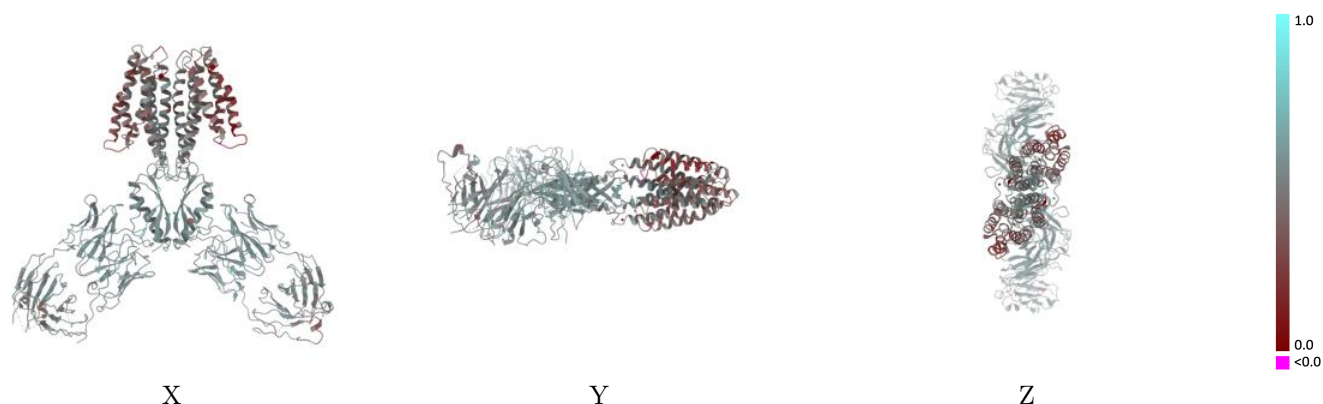
This section contains information regarding the fit between EMDB map EMD-23093 and PDB model 7KZZ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



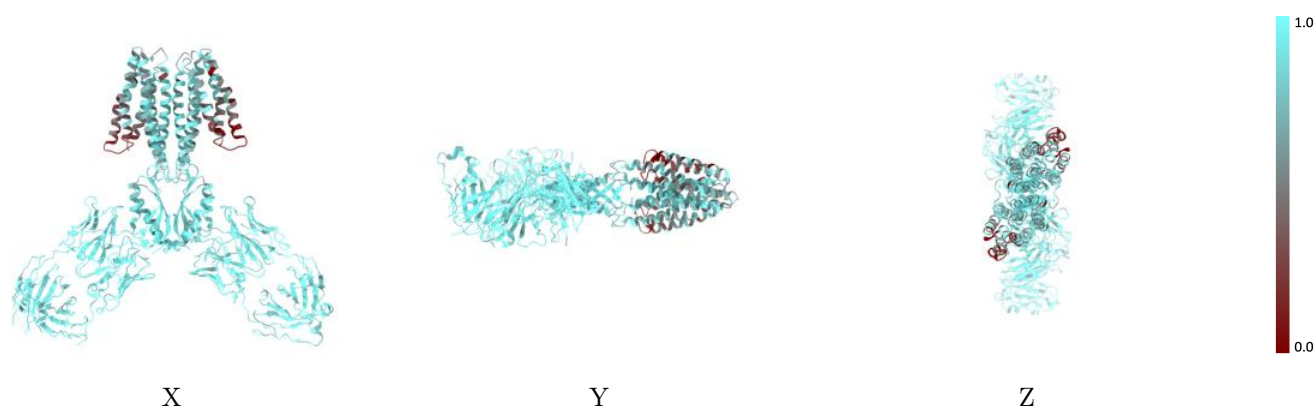
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



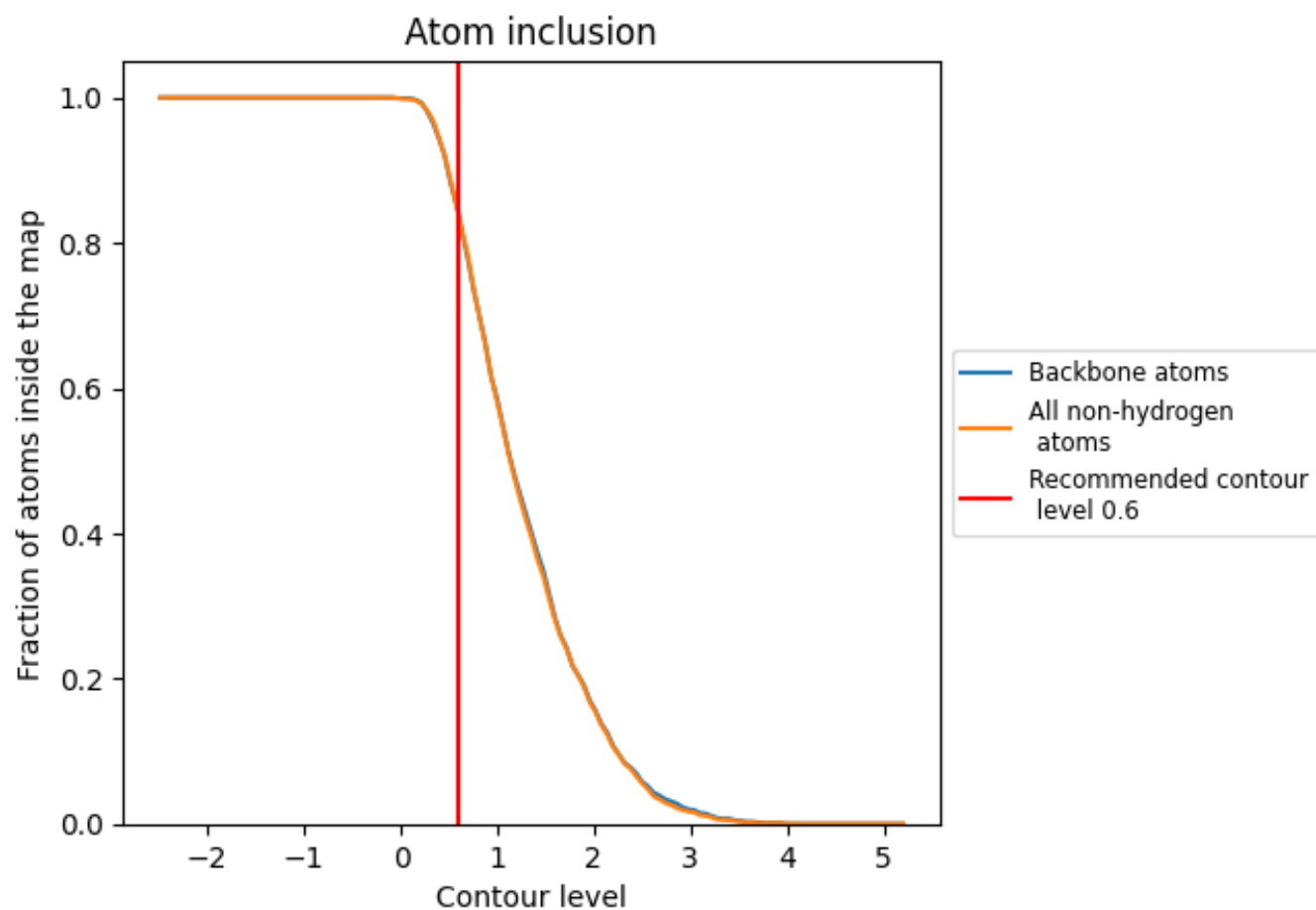
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.4900
A	0.7390	0.4430
B	0.7350	0.4390
C	0.9060	0.5170
D	0.9300	0.5320
E	0.9100	0.5180
F	0.9270	0.5310

1.0

0.0

<0.0