



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 10:26 PM EDT

PDB ID : 9Y3P / pdb_00009y3p
EMDB ID : EMD-72462
Title : Eukaryotic translation initiation factor 2-B in its apo form (active-state)
Authors : Dalwadi, U.; Croll, T.; Subramanian, A.; Lee, D.J.; Arthur, C.; Walter, P.; Frost, A.
Deposited on : 2025-09-02
Resolution : 2.90 Å(reported)
Based on initial model : 7L7G

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

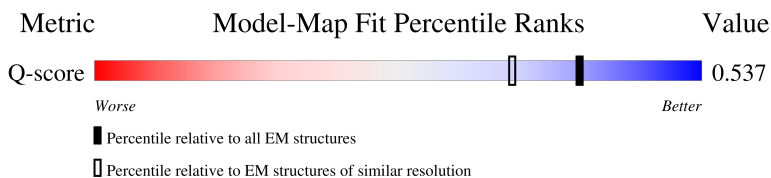
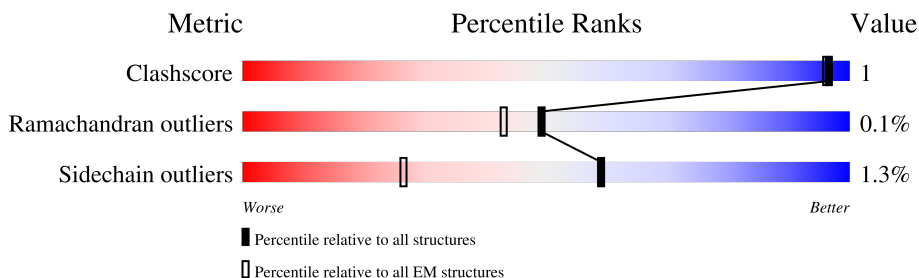
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	461	
1	B	461	
2	C	344	
2	D	344	

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Mol	Chain	Length	Quality of chain
3	E	357	<div><div></div><div>94%</div><div>5% •</div></div>
4	F	356	<div><div></div><div>93%</div><div>7%</div></div>
5	G	305	<div><div>9%</div><div>92%</div><div>5% •</div></div>
5	H	305	<div><div>6%</div><div>92%</div><div>5% • •</div></div>
6	I	443	<div><div>20%</div><div>91%</div><div>• 5%</div></div>
6	J	443	<div><div>18%</div><div>91%</div><div>• • 5%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28946 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 Translation initiation factor eIF2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	437	Total	C	N	O	S	0	0
			3423	2167	606	635	15		
1	B	437	Total	C	N	O	S	0	0
			3423	2167	606	635	15		

- Molecule 2 is a protein called Translation initiation factor eIF2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	344	Total	C	N	O	S	0	0
			2693	1695	473	510	15		
2	D	344	Total	C	N	O	S	0	0
			2693	1695	473	510	15		

- Molecule 3 is a protein called Translation initiation factor eIF2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	357	Total	C	N	O	S	0	0
			2779	1756	495	514	14		

- Molecule 4 is a protein called Translation initiation factor eIF2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	356	Total	C	N	O	S	0	0
			2770	1751	493	512	14		

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	296	Total	C	N	O	S	0	0
			2302	1477	381	432	12		
5	H	296	Total	C	N	O	S	0	0
			2302	1477	381	432	12		

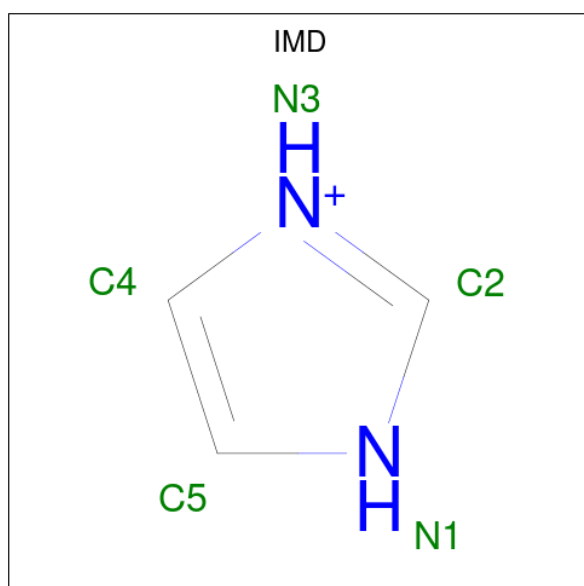
- Molecule 6 is a protein called Translation initiation factor eIF2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	421	Total	C	N	O	S	0	0
			3269	2068	561	614	26		
6	J	421	Total	C	N	O	S	0	0
			3269	2068	561	614	26		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Cl	0
			1	1	
7	B	1	Total	Cl	0
			1	1	
7	C	1	Total	Cl	0
			1	1	
7	D	1	Total	Cl	0
			1	1	
7	E	4	Total	Cl	0
			4	4	
7	F	3	Total	Cl	0
			3	3	

- Molecule 8 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			AltConf
8	E	1	Total	C	N	0
			5	3	2	

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Mol	Chain	Residues	Atoms			AltConf
8	F	1	Total	C	N	0
			5	3	2	

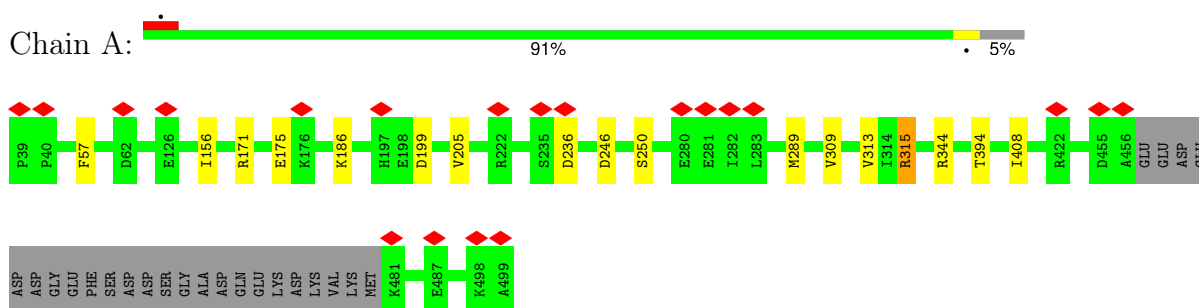
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	E	1	Total	Zn	0
			1	1	
9	F	1	Total	Zn	0
			1	1	

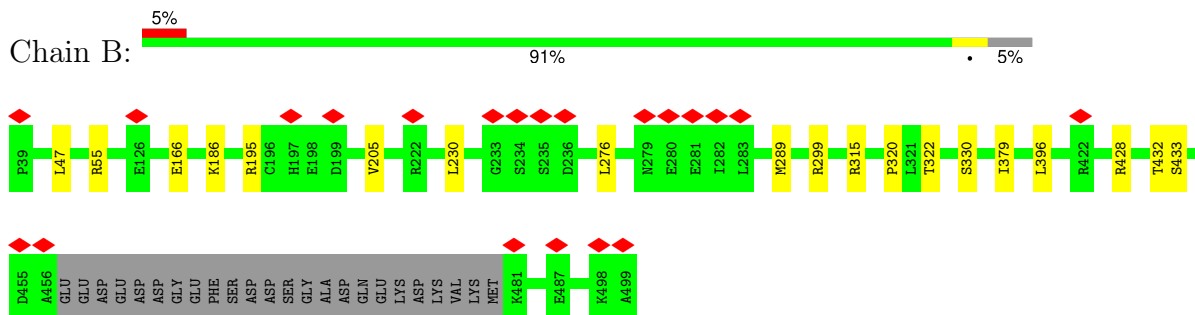
3 Residue-property plots [i](#)

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.

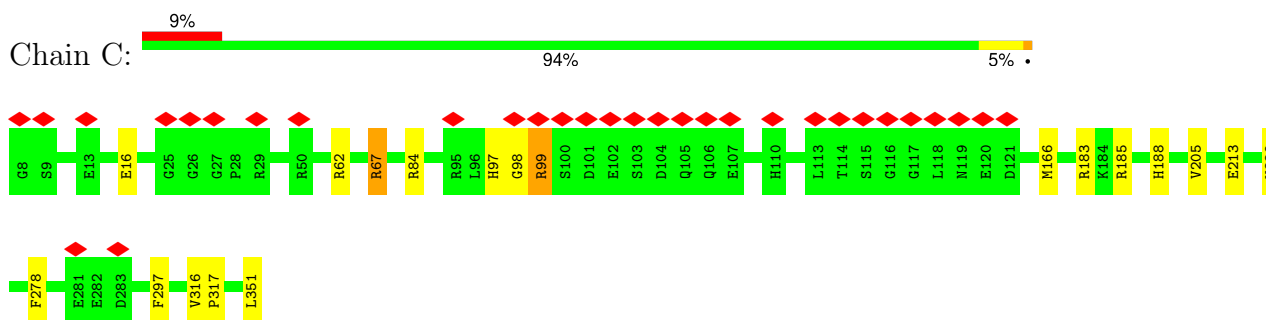
- Molecule 1: Translation initiation factor eIF2B subunit epsilon



- Molecule 1: Translation initiation factor eIF2B subunit epsilon

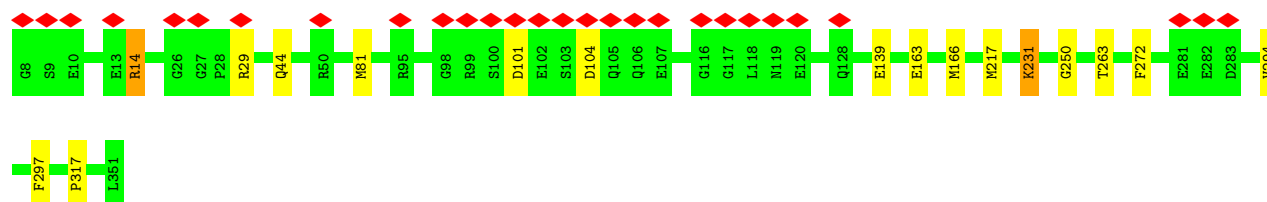


- Molecule 2: Translation initiation factor eIF2B subunit beta



- Molecule 2: Translation initiation factor eIF2B subunit beta





- Molecule 3: Translation initiation factor eIF2B subunit delta

Chain E: 94% 5%



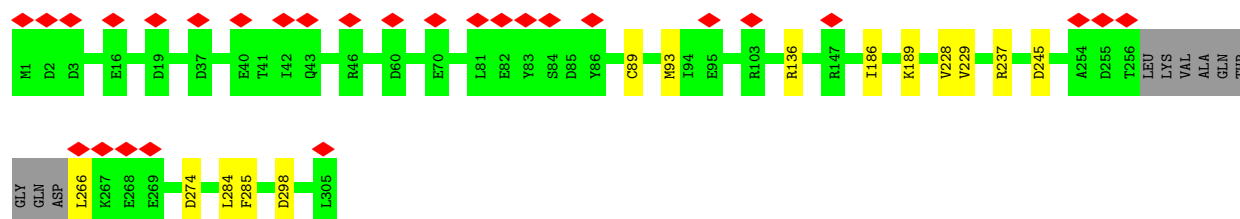
- Molecule 4: Translation initiation factor eIF2B subunit delta

Chain F: 93% 7%



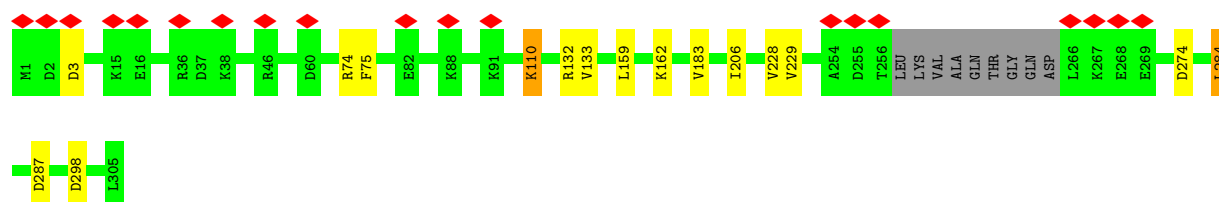
- Molecule 5: Translation initiation factor eIF-2B subunit alpha

Chain G: 9% 92% 5%



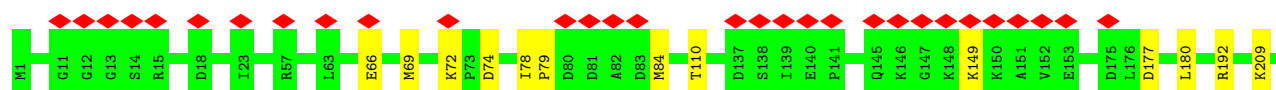
- Molecule 5: Translation initiation factor eIF-2B subunit alpha

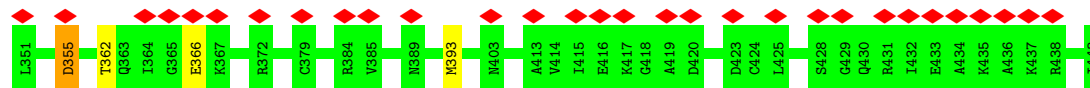
Chain H: 6% 92% 5%



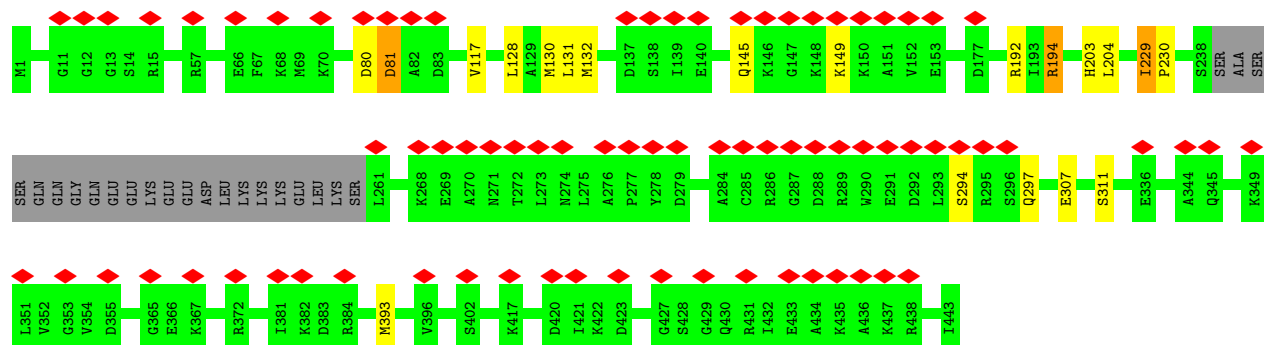
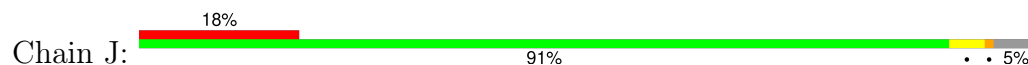
- Molecule 6: Translation initiation factor eIF2B subunit gamma

Chain I: 20% 91% 5%





- Molecule 6: Translation initiation factor eIF2B subunit gamma



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	4.361	Depositor
Minimum map value	-1.753	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	1.05	Depositor
Map size (Å)	457.52002, 457.52002, 457.52002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1438, 1.1438, 1.1438	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: CL, ZN, IMD

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	0.64	0/3497	1.09	5/4758 (0.1%)
1	B	0.65	0/3497	1.11	3/4758 (0.1%)
2	C	0.69	0/2744	1.18	7/3709 (0.2%)
2	D	0.69	0/2744	1.20	8/3709 (0.2%)
3	E	0.72	0/2831	1.17	6/3847 (0.2%)
4	F	0.72	0/2822	1.19	11/3835 (0.3%)
5	G	0.62	0/2338	1.10	3/3155 (0.1%)
5	H	0.62	0/2338	1.10	4/3155 (0.1%)
6	I	0.60	0/3319	1.04	5/4481 (0.1%)
6	J	0.61	0/3319	1.05	4/4481 (0.1%)
All	All	0.66	0/29449	1.12	56/39888 (0.1%)

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	3
1	B	0	5
2	C	0	2
2	D	0	1
3	E	0	2
4	F	0	1
5	G	0	2
5	H	0	2
6	I	0	2
6	J	0	1
All	All	0	21

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	LEU	N-CA-CB	-8.97	96.40	110.22
2	D	317	PRO	CB-CA-C	-7.55	104.29	111.39
2	C	317	PRO	CB-CA-C	-7.42	104.42	111.39
6	I	72	LYS	CB-CA-C	6.92	116.67	110.44
6	J	81	ASP	CA-CB-CG	6.61	119.21	112.60
4	F	428	ARG	CG-CD-NE	6.56	126.44	112.00
6	I	180	LEU	N-CA-CB	-6.49	100.38	110.57
1	A	246	ASP	CA-CB-CG	6.38	118.98	112.60
6	I	355	ASP	CA-CB-CG	6.37	118.97	112.60
2	D	294	VAL	N-CA-CB	-6.36	106.43	111.64
4	F	169	THR	CA-CB-OG1	-6.36	100.07	109.60
5	H	274	ASP	CA-CB-CG	6.35	118.95	112.60
3	E	433	PRO	CB-CA-C	-6.08	103.61	111.46
6	J	229	ILE	N-CA-CB	5.93	115.08	110.45
6	J	192	ARG	CB-CA-C	-5.81	99.18	109.70
1	B	166	GLU	CB-CA-C	-5.81	101.52	110.81
3	E	310	GLU	CB-CA-C	-5.75	102.04	110.95
4	F	173	TYR	CB-CA-C	-5.71	99.27	109.71
2	C	185	ARG	N-CA-CB	-5.64	101.00	110.99
5	G	245	ASP	CA-CB-CG	5.56	118.16	112.60
5	G	274	ASP	CA-CB-CG	5.55	118.15	112.60
3	E	418	VAL	O-C-N	-5.55	116.45	121.89
5	G	298	ASP	CA-CB-CG	5.53	118.13	112.60
5	H	298	ASP	CA-CB-CG	5.47	118.07	112.60
4	F	378	HIS	CA-CB-CG	-5.44	108.36	113.80
3	E	487	LEU	N-CA-CB	-5.43	101.85	110.06
6	I	192	ARG	CB-CA-C	-5.43	99.77	109.71
4	F	351	THR	CA-CB-OG1	-5.43	101.46	109.60
4	F	370	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	A	313	VAL	N-CA-CB	5.41	116.88	110.55
4	F	428	ARG	CD-NE-CZ	5.41	131.97	124.40
6	I	74	ASP	CA-CB-CG	5.39	117.99	112.60
2	C	316	VAL	CA-C-N	5.25	123.49	119.66
2	C	316	VAL	C-N-CA	5.25	123.49	119.66
2	D	139	GLU	CB-CA-C	-5.21	102.69	110.88
3	E	244	PRO	CB-CA-C	5.21	117.81	110.98
1	B	289	MET	CB-CA-C	-5.21	100.34	109.71
2	D	101	ASP	CA-CB-CG	5.20	117.80	112.60
2	C	278	PHE	CA-CB-CG	-5.18	108.62	113.80
2	D	231	LYS	CB-CA-C	-5.13	99.41	110.45
6	J	194	ARG	N-CA-CB	-5.13	102.07	110.43
5	H	110	LYS	CB-CA-C	-5.13	102.28	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	84	ARG	NE-CZ-NH2	5.12	123.81	119.20
4	F	278	LYS	CB-CA-C	-5.11	101.99	110.68
4	F	522	ASP	CA-CB-CG	5.11	117.70	112.60
1	A	171	ARG	N-CA-CB	-5.08	102.39	110.22
2	D	104	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	315	ARG	NE-CZ-NH2	5.07	123.76	119.20
2	D	272	PHE	N-CA-CB	5.06	119.33	110.42
2	D	250	GLY	N-CA-C	-5.06	108.67	114.69
3	E	282	LYS	N-CA-CB	5.06	117.34	110.01
1	A	236	ASP	CA-CB-CG	5.05	117.65	112.60
4	F	433	PRO	CB-CA-C	-5.04	104.96	111.46
4	F	208	VAL	N-CA-CB	5.03	117.00	110.57
2	C	67	ARG	CB-CA-C	-5.01	103.01	110.88
5	H	229	VAL	N-CA-CB	-5.00	105.01	111.82

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	GLU	Peptide
1	A	315	ARG	Sidechain
1	A	344	ARG	Sidechain
1	B	195	ARG	Sidechain
1	B	299	ARG	Sidechain
1	B	315	ARG	Sidechain
1	B	428	ARG	Sidechain
1	B	55	ARG	Sidechain
2	C	183	ARG	Sidechain
2	C	99	ARG	Peptide
2	D	14	ARG	Sidechain
3	E	306	ARG	Sidechain
3	E	374	ARG	Sidechain
4	F	321	ARG	Sidechain
5	G	136	ARG	Sidechain
5	G	237	ARG	Sidechain
5	H	132	ARG	Sidechain
5	H	74	ARG	Sidechain
6	I	66	GLU	Peptide
6	I	79	PRO	Peptide
6	J	194	ARG	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	3423	0	3419	3	0
1	B	3423	0	3419	6	0
2	C	2693	0	2686	6	0
2	D	2693	0	2686	5	0
3	E	2779	0	2837	5	0
4	F	2770	0	2829	6	0
5	G	2302	0	2378	4	0
5	H	2302	0	2378	4	0
6	I	3269	0	3368	2	0
6	J	3269	0	3368	7	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	4	0	0	0	0
7	F	3	0	0	0	0
8	E	5	0	5	0	0
8	F	5	0	5	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
All	All	28946	0	29378	46	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 1.

All (46) 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)
3:E:269:LEU:HD22	3:E:273:MET:HE2	1.74	0.69
6:J:130:MET:HE2	6:J:132:MET:HE2	1.73	0.69
6:I:231:TYR:OH	6:I:262:ASP:OD1	2.15	0.64
2:C:166:MET:HE3	2:C:229:VAL:HG21	1.84	0.59
1:B:47:LEU:C	1:B:47:LEU:HD23	2.30	0.57
2:D:163:GLU:OE2	2:D:231:LYS:HG3	2.05	0.56
4:F:499:LEU:HD11	4:F:506:MET:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:THR:HG22	1:B:433:SER:H	1.73	0.53
4:F:512:VAL:N	4:F:513:PRO:HD2	2.25	0.51
3:E:291:LYS:NZ	3:E:299:GLU:OE2	2.43	0.50
6:J:203:HIS:O	6:J:203:HIS:ND1	2.44	0.50
3:E:512:VAL:N	3:E:513:PRO:HD2	2.26	0.50
1:B:186:LYS:HE3	2:C:297:PHE:CD2	2.47	0.49
4:F:319:ILE:HD13	4:F:341:LEU:HD21	1.97	0.47
1:A:156:ILE:HG13	1:A:309:VAL:HG11	1.97	0.47
3:E:499:LEU:HD11	3:E:506:MET:HB3	1.97	0.47
2:C:62:ARG:NH2	2:C:351:LEU:O	2.47	0.46
6:J:229:ILE:HB	6:J:230:PRO:HD3	1.97	0.46
4:F:204:HIS:CG	4:F:205:PRO:HD2	2.50	0.46
6:J:130:MET:CE	6:J:132:MET:HE2	2.43	0.46
5:H:206:ILE:HG21	5:H:228:VAL:HG11	1.98	0.46
1:B:320:PRO:O	1:B:322:THR:N	2.50	0.45
1:A:186:LYS:HE3	2:D:297:PHE:CD2	2.53	0.44
5:G:186:ILE:CD1	5:G:189:LYS:HD2	2.46	0.44
5:H:228:VAL:HB	5:H:284:LEU:HD13	2.00	0.44
2:C:188:HIS:CG	2:C:213:GLU:OE2	2.71	0.43
2:C:16:GLU:CD	2:C:67:ARG:HH12	2.26	0.43
5:G:228:VAL:HB	5:G:284:LEU:HD13	2.01	0.43
4:F:388:ILE:N	4:F:389:PRO:CD	2.81	0.43
1:B:379:ILE:HD12	1:B:396:LEU:HD22	2.00	0.42
5:G:89:CYS:SG	5:G:93:MET:HE3	2.59	0.42
2:C:97:HIS:CG	2:C:98:GLY:N	2.87	0.42
6:J:204:LEU:C	6:J:204:LEU:HD23	2.44	0.42
1:B:276:LEU:C	1:B:276:LEU:HD23	2.45	0.42
5:G:229:VAL:HG12	5:G:285:PHE:HB2	2.01	0.42
6:I:78:ILE:HD12	6:I:84:MET:SD	2.60	0.42
2:D:81:MET:HE2	2:D:81:MET:HA	2.02	0.41
3:E:361:VAL:HG22	3:E:386:LEU:CD1	2.49	0.41
6:J:117:VAL:HG21	6:J:131:LEU:HB2	2.01	0.41
6:J:294:SER:O	6:J:297:GLN:NE2	2.54	0.41
1:A:205:VAL:HG11	1:A:289:MET:HE2	2.03	0.41
2:D:14:ARG:NH2	2:D:44:GLN:OE1	2.45	0.41
4:F:345:ILE:CD1	4:F:437:CYS:SG	3.08	0.41
5:H:110:LYS:HD2	5:H:287:ASP:HB2	2.03	0.40
2:D:166:MET:CE	2:D:217:MET:HE1	2.52	0.40
5:H:159:LEU:HD23	5:H:162:LYS:HD2	2.04	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	433/461 (94%)	411 (95%)	22 (5%)	0	100	100
1	B	433/461 (94%)	416 (96%)	17 (4%)	0	100	100
2	C	342/344 (99%)	335 (98%)	7 (2%)	0	100	100
2	D	342/344 (99%)	337 (98%)	5 (2%)	0	100	100
3	E	355/357 (99%)	348 (98%)	7 (2%)	0	100	100
4	F	354/356 (99%)	347 (98%)	7 (2%)	0	100	100
5	G	292/305 (96%)	285 (98%)	7 (2%)	0	100	100
5	H	292/305 (96%)	288 (99%)	4 (1%)	0	100	100
6	I	417/443 (94%)	398 (95%)	18 (4%)	1 (0%)	43	72
6	J	417/443 (94%)	400 (96%)	16 (4%)	1 (0%)	43	72
All	All	3677/3819 (96%)	3565 (97%)	110 (3%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	J	393	MET
6	I	393	MET

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	384/405 (95%)	379 (99%)	5 (1%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	384/405 (95%)	382 (100%)	2 (0%)	81	93
2	C	294/294 (100%)	292 (99%)	2 (1%)	76	92
2	D	294/294 (100%)	292 (99%)	2 (1%)	76	92
3	E	313/313 (100%)	307 (98%)	6 (2%)	50	79
4	F	312/312 (100%)	309 (99%)	3 (1%)	68	89
5	G	253/260 (97%)	252 (100%)	1 (0%)	84	94
5	H	253/260 (97%)	248 (98%)	5 (2%)	48	78
6	I	370/390 (95%)	362 (98%)	8 (2%)	45	77
6	J	370/390 (95%)	363 (98%)	7 (2%)	50	79
All	All	3227/3323 (97%)	3186 (99%)	41 (1%)	59	86

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	PHE
1	A	199	ASP
1	A	250	SER
1	A	394	THR
1	A	408	ILE
1	B	205	VAL
1	B	330	SER
2	C	99	ARG
2	C	205	VAL
2	D	29	ARG
2	D	263	THR
3	E	245	ASN
3	E	291	LYS
3	E	328	SER
3	E	386	LEU
3	E	454	SER
3	E	499	LEU
4	F	190	ASN
4	F	386	LEU
4	F	428	ARG
5	G	266	LEU
5	H	3	ASP
5	H	75	PHE
5	H	133	VAL
5	H	183	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	H	284	LEU
6	I	69	MET
6	I	110	THR
6	I	149	LYS
6	I	177	ASP
6	I	209	LYS
6	I	355	ASP
6	I	362	THR
6	I	366	GLU
6	J	80	ASP
6	J	81	ASP
6	J	128	LEU
6	J	145	GLN
6	J	149	LYS
6	J	307	GLU
6	J	311	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	216	GLN
1	A	388	ASN
1	A	393	GLN
1	A	409	HIS
1	B	337	HIS
2	C	260	HIS
2	C	261	HIS
2	C	349	HIS
2	D	53	ASN
2	D	105	GLN
2	D	128	GLN
2	D	132	ASN
2	D	252	HIS
2	D	277	GLN
3	E	464	GLN
5	H	208	ASN
5	H	244	GLN
6	I	363	GLN
6	I	403	ASN
6	J	115	HIS
6	J	363	GLN

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Mol	Chain	Res	Type
6	J	412	ASN
6	J	440	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 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	IMD	E	603	-	5,5,5	0.99	0	5,5,5	0.50	0
8	IMD	F	602	-	5,5,5	0.93	0	5,5,5	0.48	0

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
8	IMD	E	603	-	-	-	0/1/1/1
8	IMD	F	602	-	-	-	0/1/1/1

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](#)

There are no chain breaks in this entry.

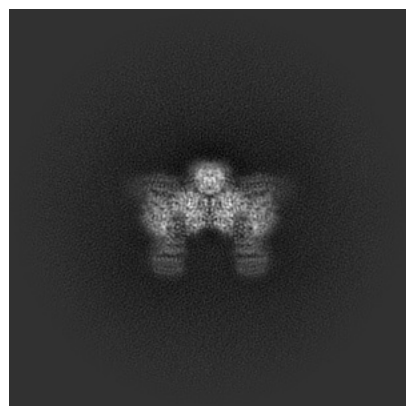
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72462. These allow visual inspection of the internal detail of the map and identification of artifacts.

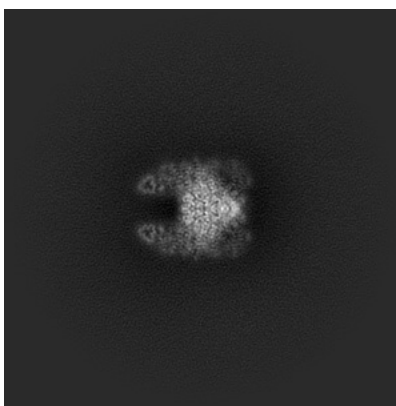
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

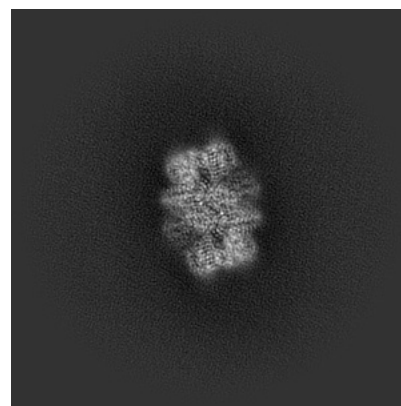
6.1.1 Primary map



X

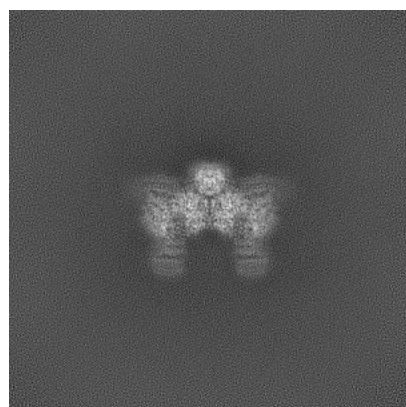


Y

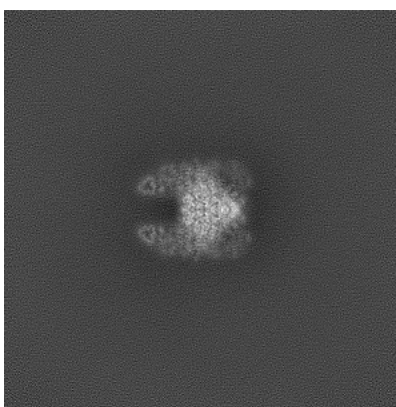


Z

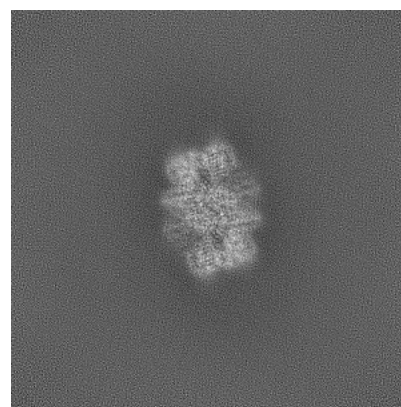
6.1.2 Raw map



X



Y

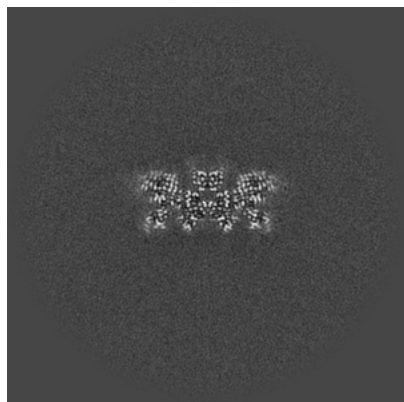


Z

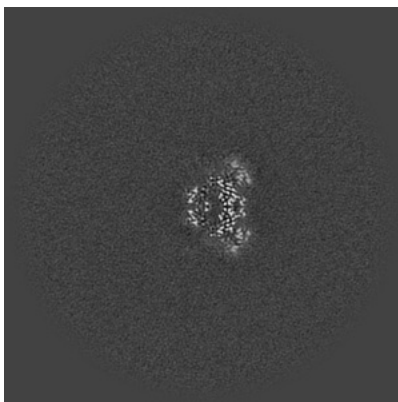
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

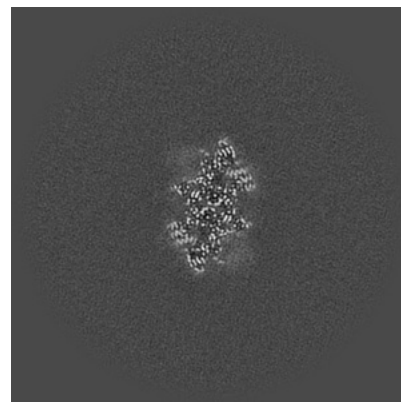
6.2.1 Primary map



X Index: 200

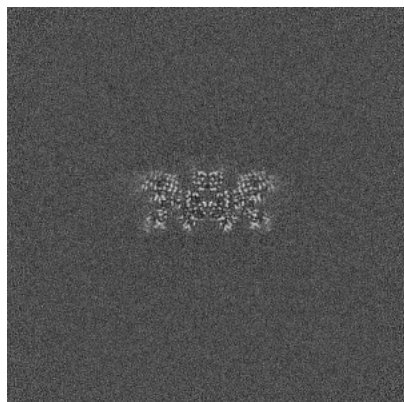


Y Index: 200

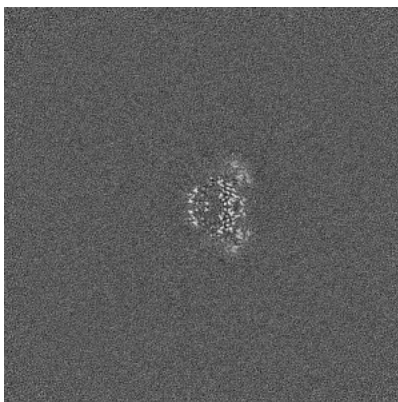


Z Index: 200

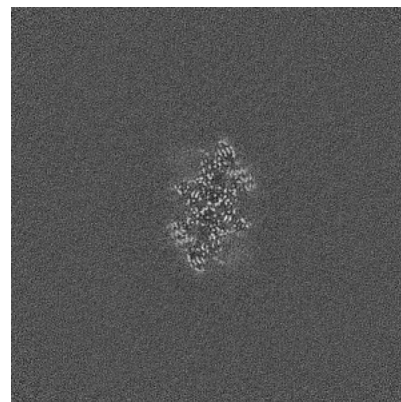
6.2.2 Raw map



X Index: 200



Y Index: 200

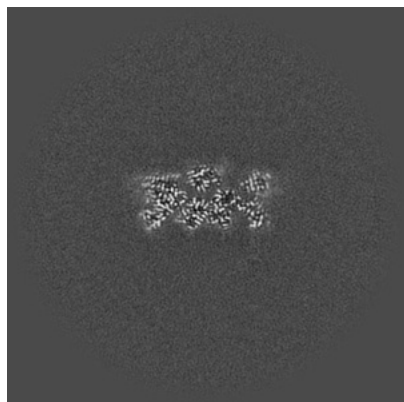


Z Index: 200

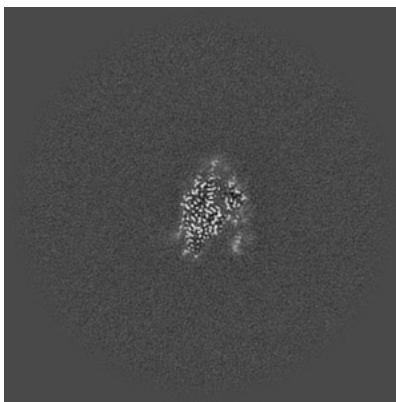
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

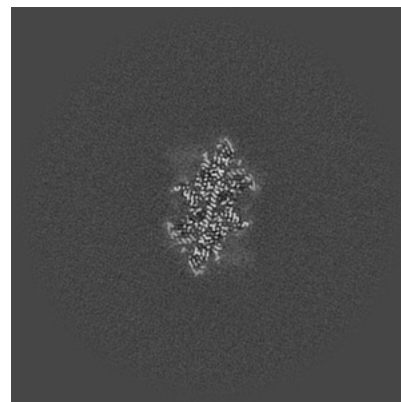
6.3.1 Primary map



X Index: 196

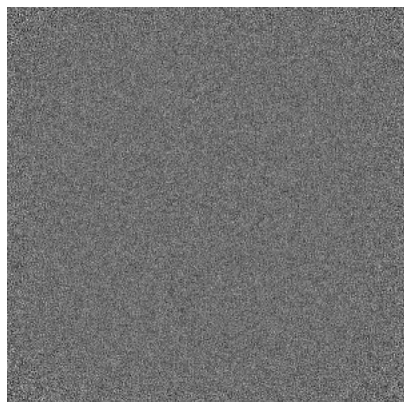


Y Index: 213

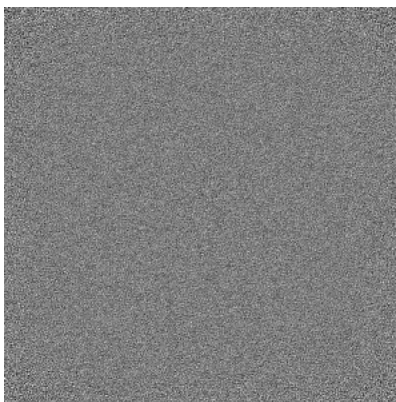


Z Index: 202

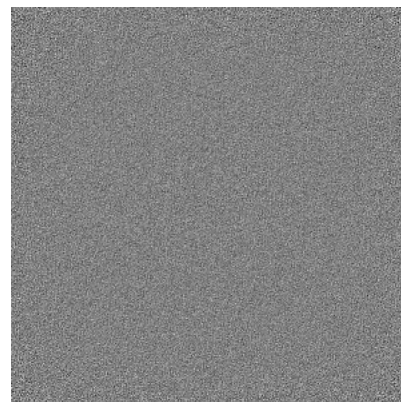
6.3.2 Raw map



X Index: 0



Y Index: 0

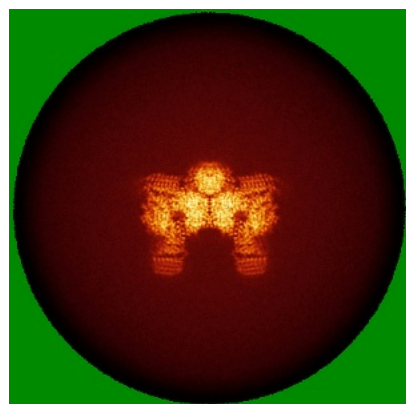


Z Index: 0

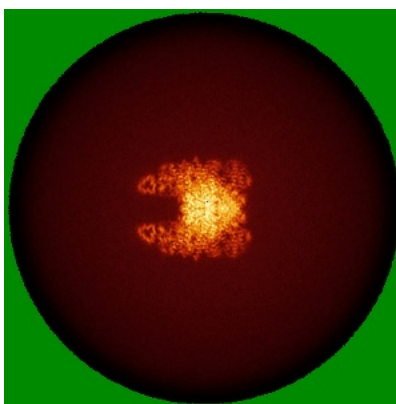
The images above show the largest variance slices of the map in three orthogonal directions.

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

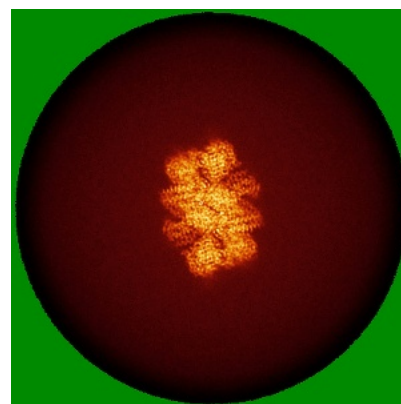
6.4.1 Primary map



X

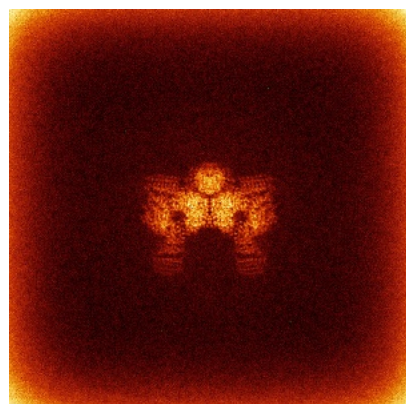


Y

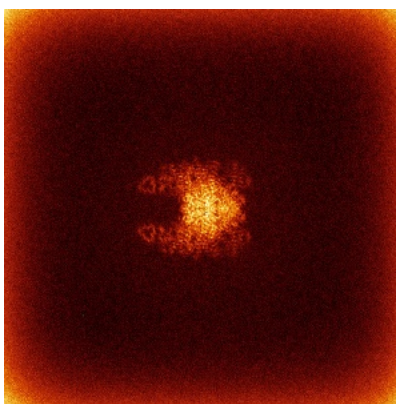


Z

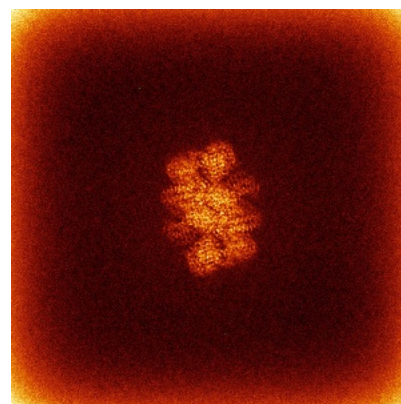
6.4.2 Raw map



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.

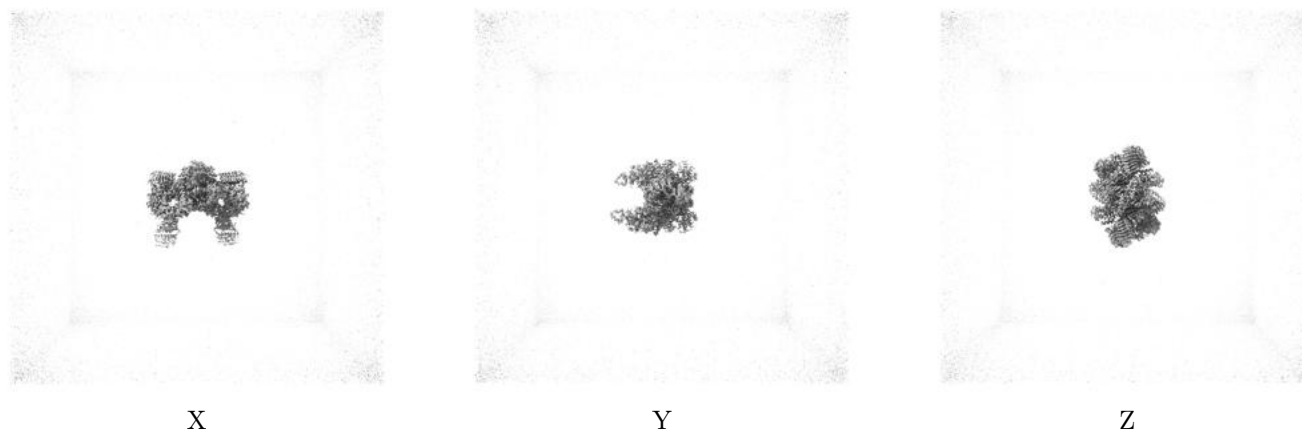
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

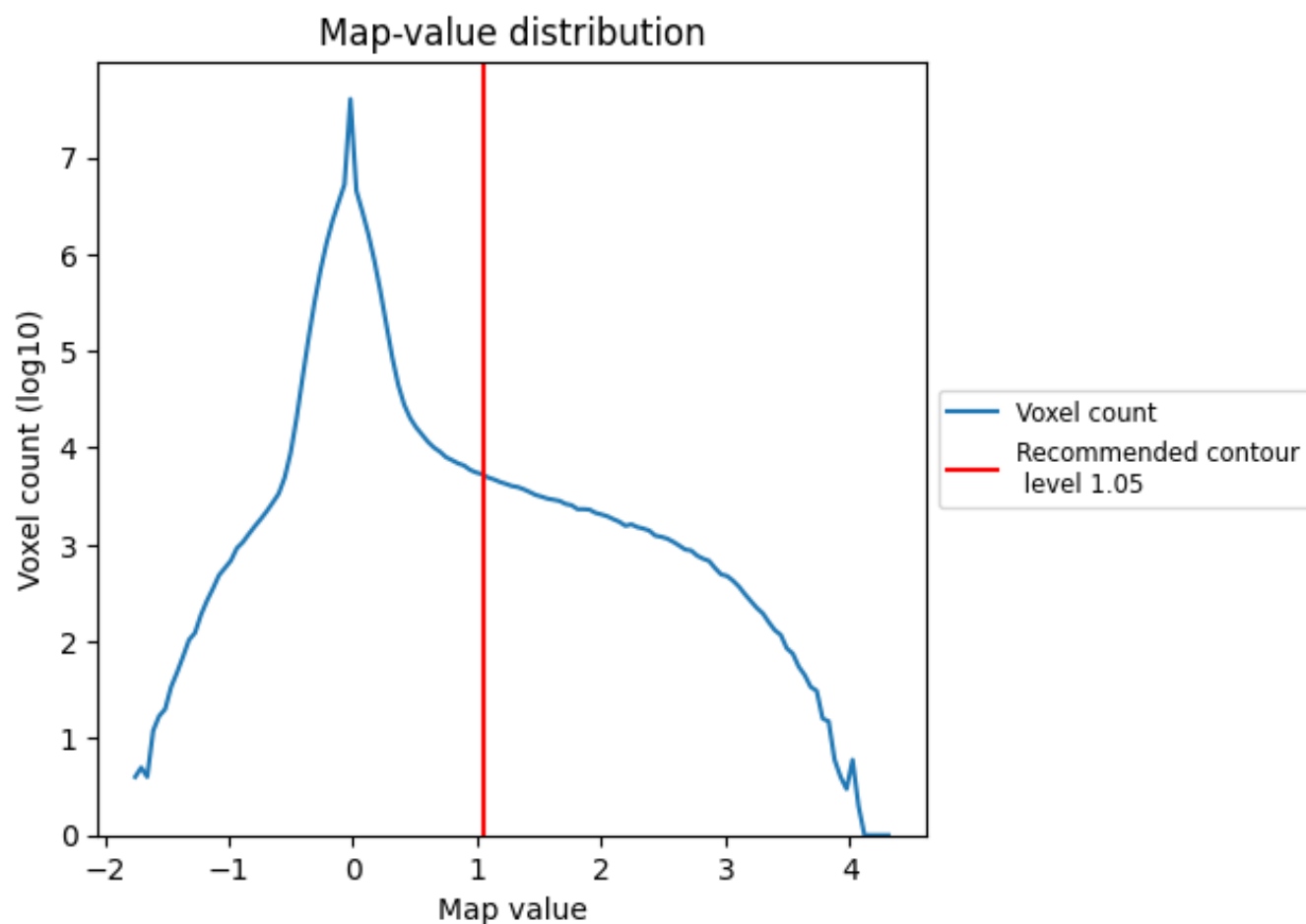
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

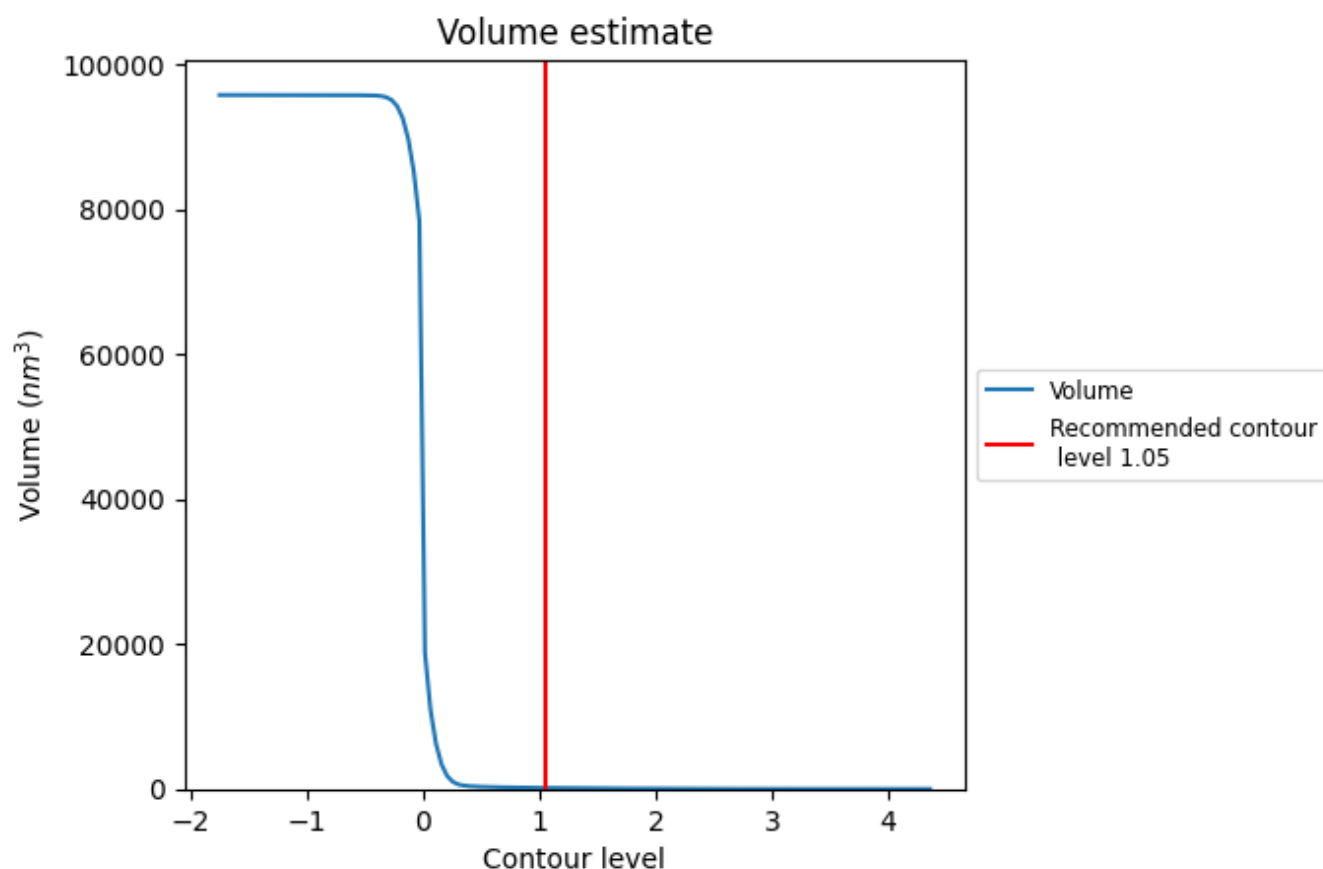
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

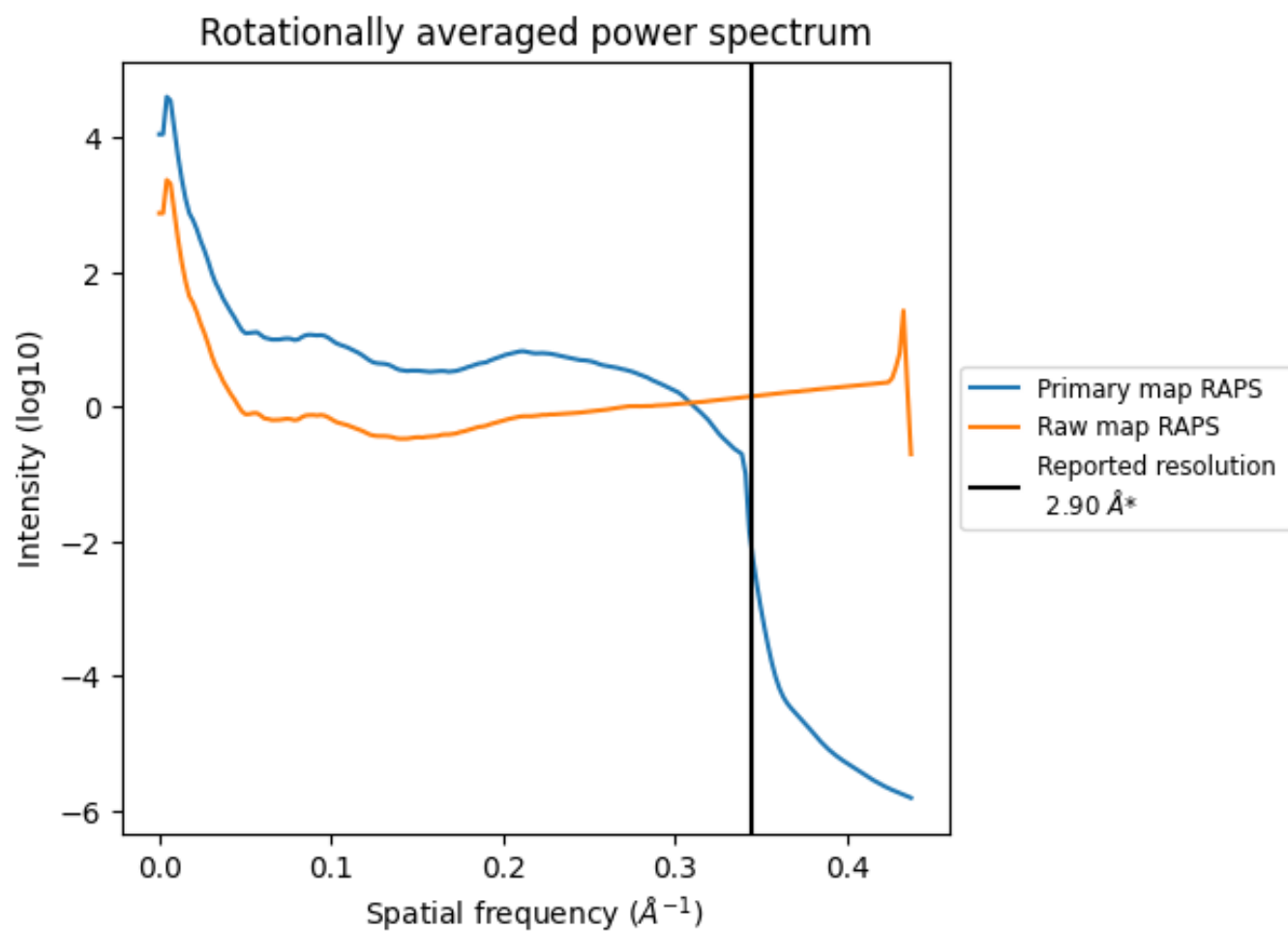
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 143 nm³; this corresponds to an approximate mass of 130 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](#)

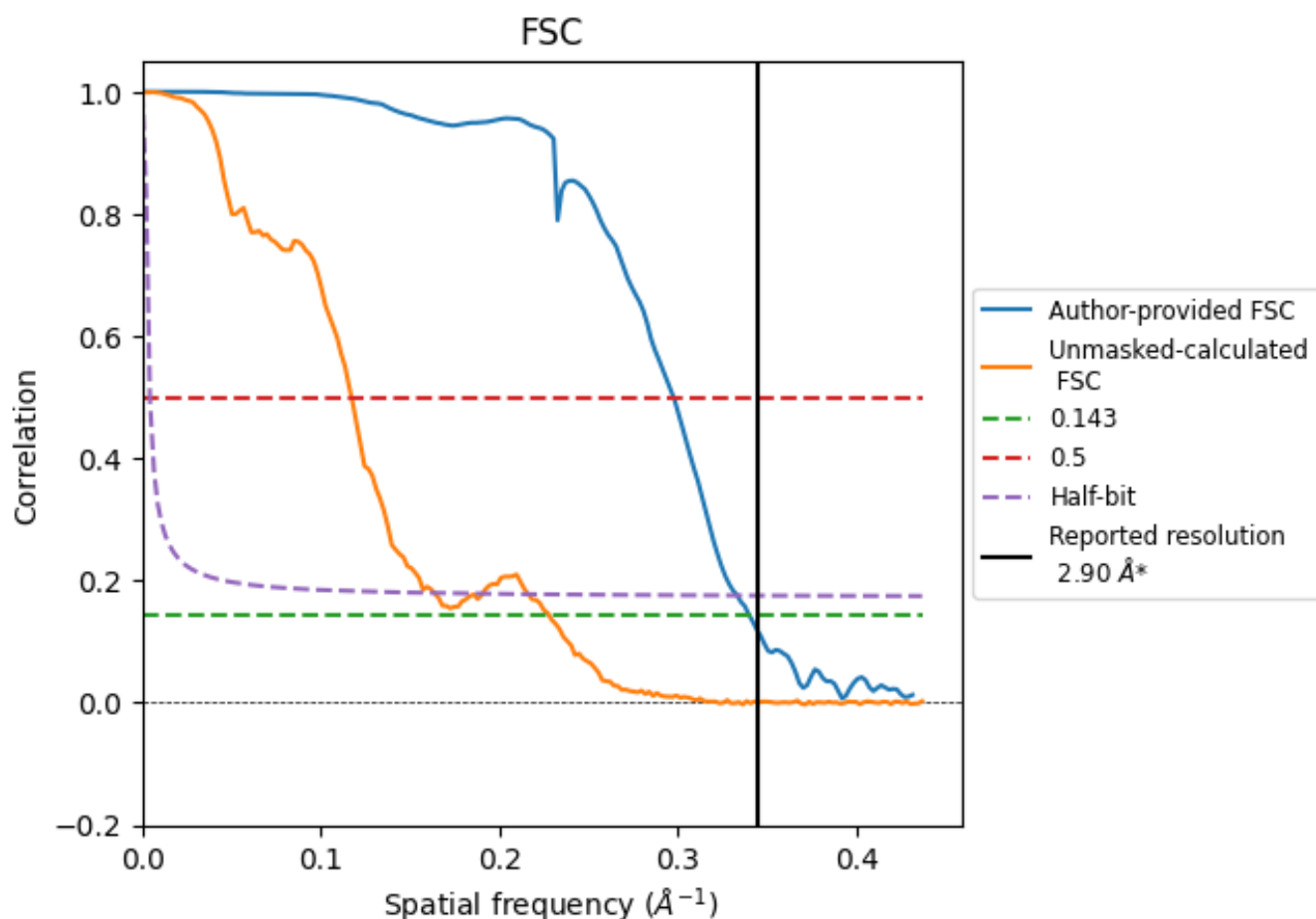


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

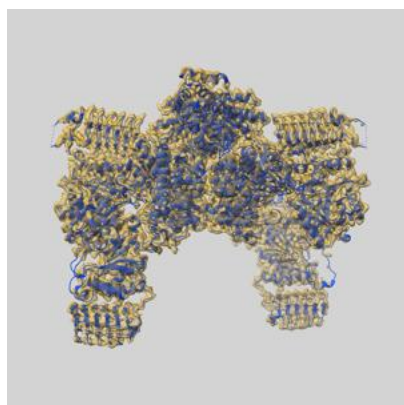
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.36	3.00
Unmasked-calculated*	4.39	8.53	6.11

*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 4.39 differs from the reported value 2.9 by more than 10 %

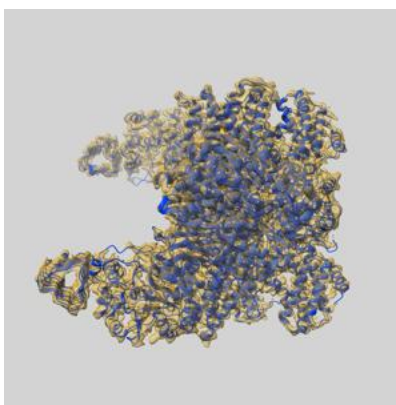
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72462 and PDB model 9Y3P. Per-residue inclusion information can be found in section [3](#) on page [7](#).

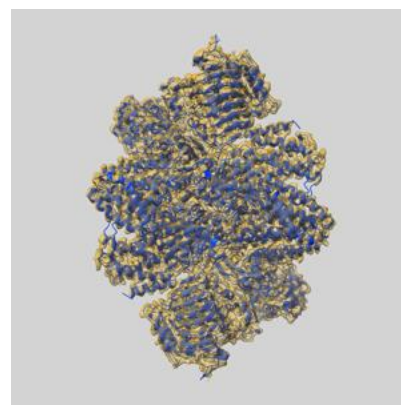
9.1 Map-model overlay [i](#)



X



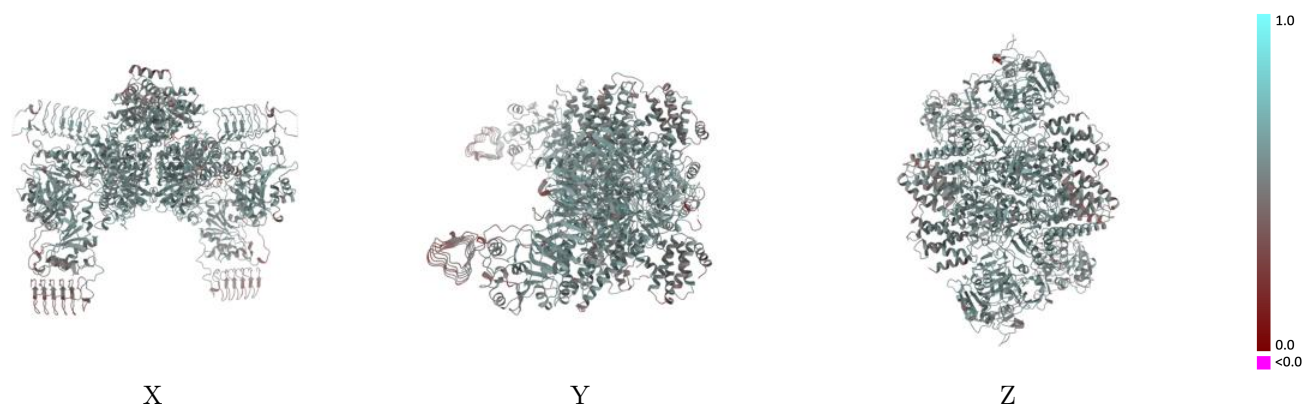
Y



Z

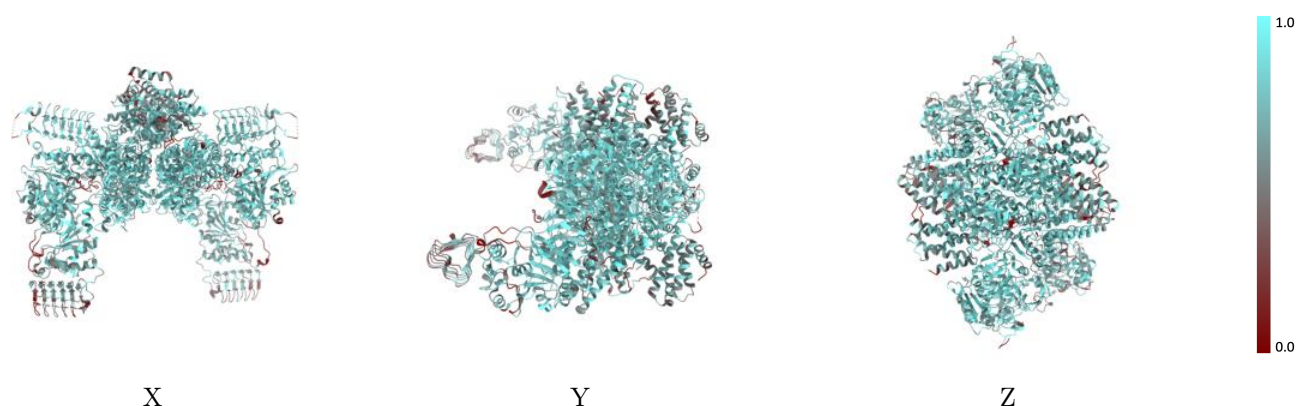
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



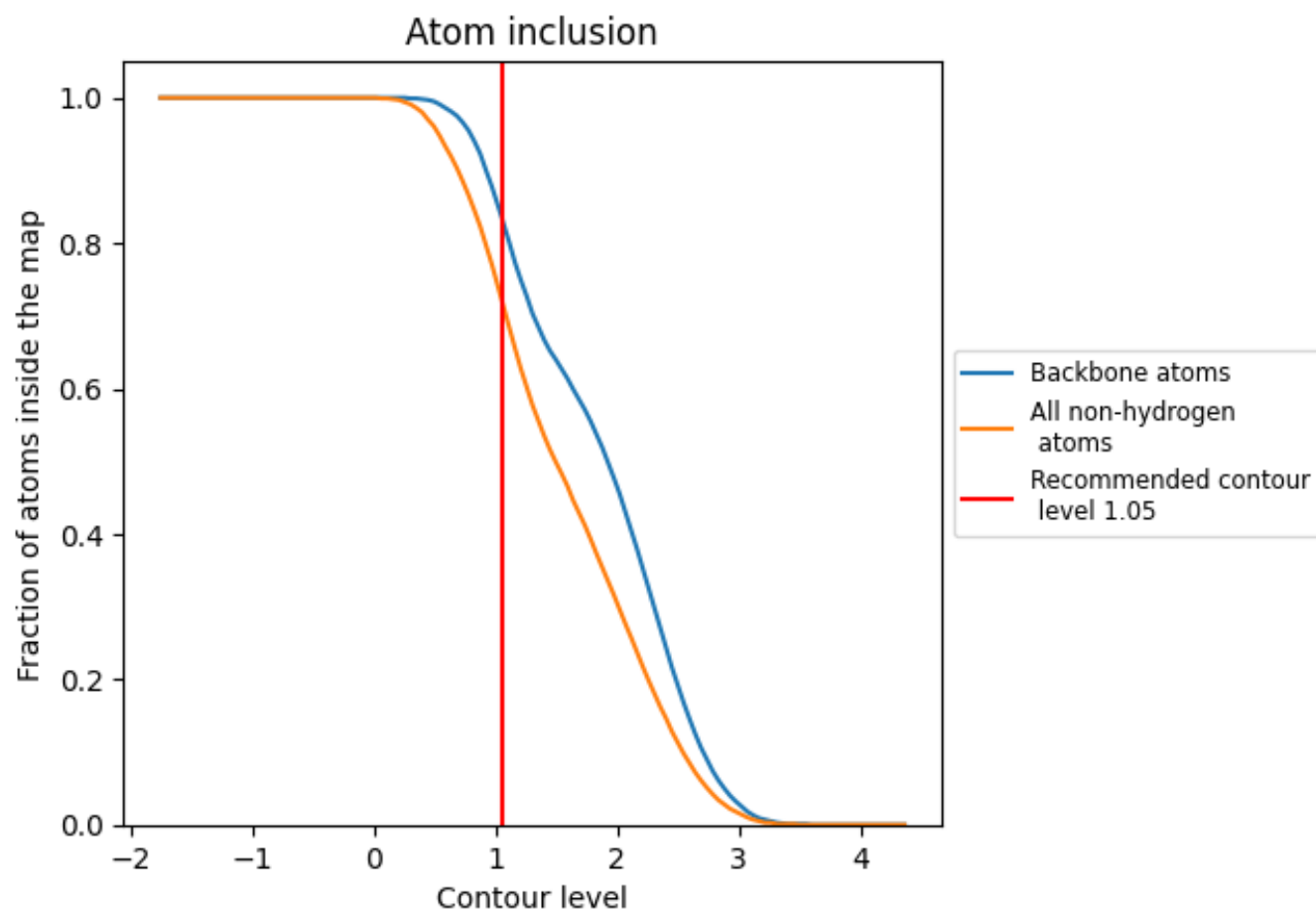
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (1.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7220	<div></div> 0.5370
A	<div></div> 0.7660	<div></div> 0.5510
B	<div></div> 0.7610	<div></div> 0.5510
C	<div></div> 0.7320	<div></div> 0.5460
D	<div></div> 0.7380	<div></div> 0.5440
E	<div></div> 0.7960	<div></div> 0.5680
F	<div></div> 0.8090	<div></div> 0.5720
G	<div></div> 0.6930	<div></div> 0.5300
H	<div></div> 0.7060	<div></div> 0.5350
I	<div></div> 0.6020	<div></div> 0.4920
J	<div></div> 0.6250	<div></div> 0.4870

