WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Dec 12, 2022 – 08:23 am GMT

|		
PDB ID	:	5A5U
EMDB ID	:	EMD-3057
Title	:	Structure of mammalian eIF3 in the context of the 43S preinitiation complex
Authors	:	des-Georges, A.; Dhote, V.; Kuhn, L.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.; Hashem, Y.
Deposited on	:	2015-06-21
Resolution	:	9.00 Å(reported)

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 9.00 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.
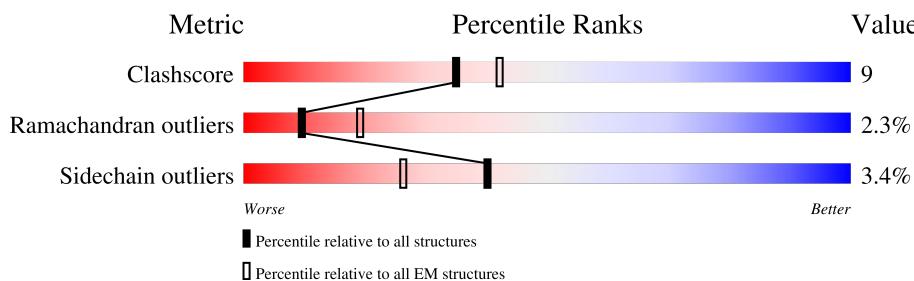
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	54	98%
2	B	1121	12% / 46% / 8% / 45%
3	I	347	65% / 83% / 14%
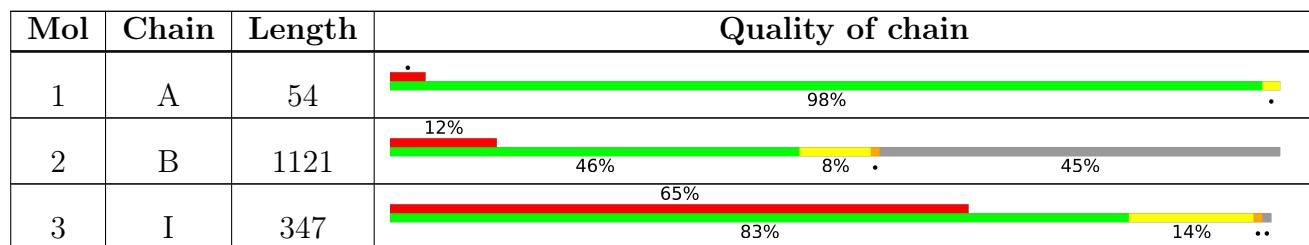
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8124 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 EUKARYOTIC INITIATION FACTOR 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	54	Total 397	C 246	N 74	O 77	0	0

- Molecule 2 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	613	Total 5034	C 3228	N 871	O 915	S 20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	104	GLU	ASP	conflict	UNP G1SZ03
B	124	PHE	TYR	conflict	UNP G1SZ03

- Molecule 3 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	342	Total 2693	C 1711	N 443	O 530	S 9	0	0

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: EUKARYOTIC INITIATION FACTOR 3

Chain A:

• Molecule 2: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT B
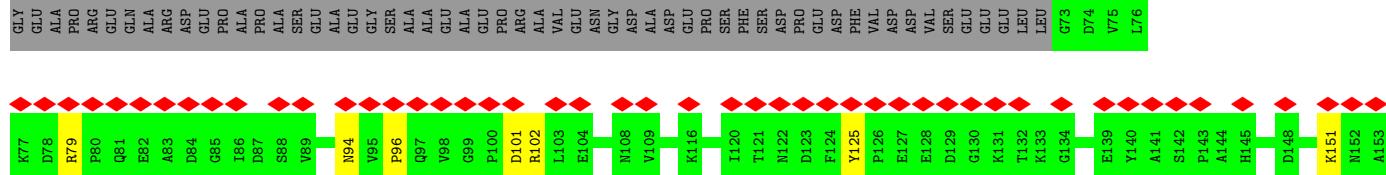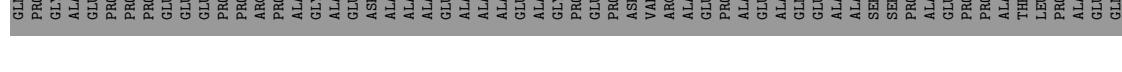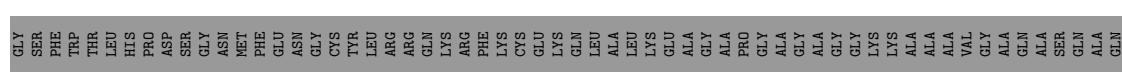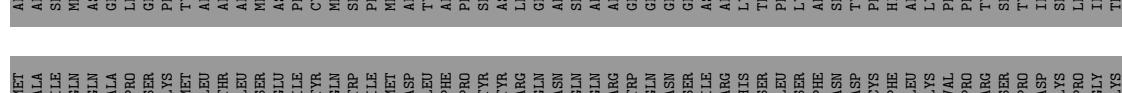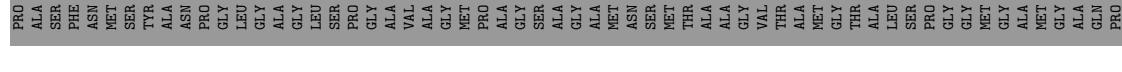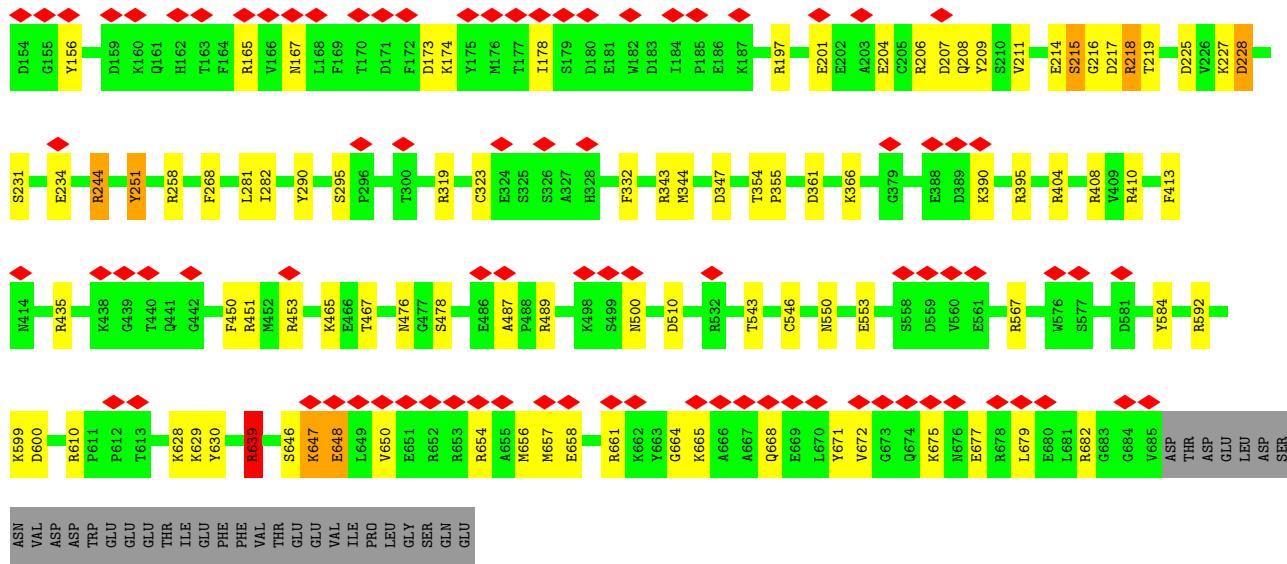
Chain B:

• Molecule 3: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT I

Chain I:
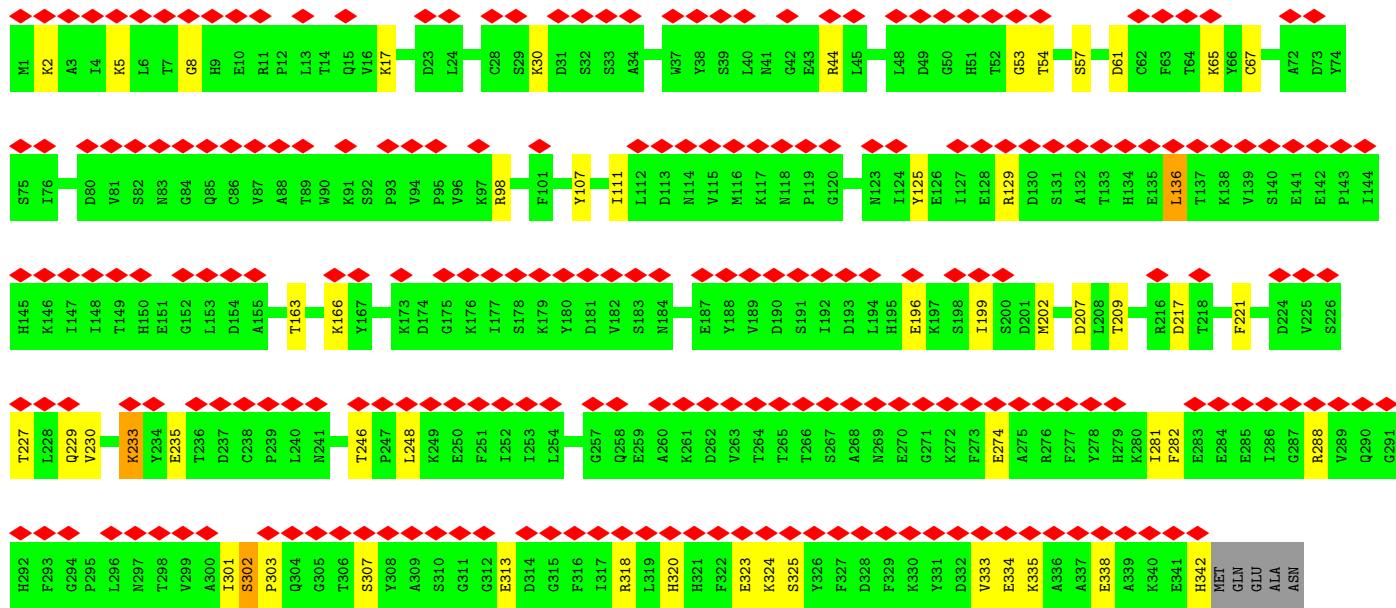
4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54410	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	30120	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.263	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	#$|Z| > 5$
2	B	0.73	1/5168 (0.0%)	1.18	26/6985 (0.4%)
3	I	1.14	3/2757 (0.1%)	0.96	6/3733 (0.2%)
All	All	0.89	4/7925 (0.1%)	1.11	32/10718 (0.3%)

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
2	B	3	22

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	648	GLU	N-CA	-13.23	1.19	1.46
3	I	67	CYS	CB-SG	-8.40	1.68	1.82
3	I	196	GLU	CG-CD	6.87	1.62	1.51
3	I	196	GLU	CB-CG	5.60	1.62	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	LYS	C-N-CA	17.02	164.26	121.70
2	B	215	SER	N-CA-CB	8.95	123.92	110.50
2	B	648	GLU	CA-C-O	-8.70	101.83	120.10
2	B	435	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	B	453	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	B	206	ARG	NE-CZ-NH1	8.07	124.33	120.30
2	B	648	GLU	N-CA-C	7.82	132.12	111.00
2	B	218	ARG	NE-CZ-NH1	7.55	124.08	120.30
3	I	129	ARG	NE-CZ-NH2	-7.22	116.69	120.30
2	B	451	ARG	NE-CZ-NH2	-7.21	116.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	451	ARG	NE-CZ-NH1	7.19	123.89	120.30
2	B	206	ARG	NE-CZ-NH2	-7.15	116.72	120.30
2	B	639	ARG	NE-CZ-NH1	6.87	123.74	120.30
2	B	610	ARG	NE-CZ-NH1	6.85	123.73	120.30
2	B	489	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	B	610	ARG	NE-CZ-NH2	-6.67	116.97	120.30
2	B	218	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	B	197	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	B	258	ARG	NE-CZ-NH1	6.35	123.47	120.30
3	I	202	MET	CG-SD-CE	-6.09	90.45	100.20
2	B	410	ARG	NE-CZ-NH2	-6.03	117.28	120.30
2	B	319	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	B	453	ARG	NE-CZ-NH2	-5.89	117.36	120.30
2	B	251	TYR	CB-CG-CD2	-5.83	117.50	121.00
3	I	318	ARG	NE-CZ-NH2	-5.79	117.41	120.30
3	I	17	LYS	CB-CA-C	-5.57	99.27	110.40
3	I	44	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	B	343	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	B	489	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	125	TYR	CB-CG-CD2	-5.14	117.92	121.00
3	I	61	ASP	CB-CG-OD1	5.04	122.84	118.30
2	B	543	THR	C-N-CA	5.01	134.22	121.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	211	VAL	CA
2	B	213	PHE	CA
2	B	214	GLU	CA

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	102	ARG	Sidechain
2	B	156	TYR	Peptide
2	B	165	ARG	Sidechain
2	B	204	GLU	Peptide
2	B	209	TYR	Sidechain
2	B	219	THR	Peptide
2	B	228	ASP	Peptide
2	B	244	ARG	Sidechain
2	B	251	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	281	LEU	Peptide
2	B	290	TYR	Sidechain
2	B	344	MET	Peptide
2	B	354	THR	Peptide
2	B	395	ARG	Sidechain
2	B	404	ARG	Sidechain
2	B	450	PHE	Sidechain
2	B	553	GLU	Peptide
2	B	599	LYS	Peptide
2	B	639	ARG	Sidechain
2	B	647	LYS	Peptide
2	B	648	GLU	Mainchain
2	B	79	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	397	0	156	1	0
2	B	5034	0	4952	120	0
3	I	2693	0	2609	112	0
All	All	8124	0	7717	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (137) 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:B:646:SER:CB	2:B:654:ARG:HH12	1.05	1.61
2:B:675:LYS:HZ3	3:I:166:LYS:CG	1.30	1.44
2:B:218:ARG:NH1	3:I:2:LYS:HD2	1.12	1.43
2:B:682:ARG:NH1	3:I:248:LEU:HD12	1.26	1.41
2:B:218:ARG:NH1	3:I:2:LYS:CD	1.87	1.34
2:B:646:SER:HB2	2:B:654:ARG:CZ	1.55	1.34
2:B:675:LYS:NZ	3:I:166:LYS:CG	1.92	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:584:TYR:OH	3:I:324:LYS:HE3	1.33	1.28
2:B:675:LYS:NZ	3:I:166:LYS:HG3	1.43	1.28
2:B:646:SER:HB2	2:B:654:ARG:NH1	0.92	1.24
2:B:218:ARG:HH11	3:I:2:LYS:CD	1.49	1.21
2:B:592:ARG:HH22	3:I:342:HIS:CG	1.60	1.19
2:B:682:ARG:NH1	3:I:248:LEU:CD1	2.05	1.19
2:B:584:TYR:OH	3:I:324:LYS:CE	1.95	1.15
2:B:682:ARG:CD	3:I:248:LEU:HD13	1.77	1.13
2:B:682:ARG:CZ	3:I:248:LEU:CD1	2.25	1.13
2:B:216:GLY:N	3:I:323:GLU:OE1	1.85	1.10
2:B:227:LYS:CE	3:I:335:LYS:HD2	1.82	1.10
2:B:227:LYS:HD2	3:I:335:LYS:HB3	1.21	1.09
2:B:218:ARG:HH11	3:I:2:LYS:CE	1.65	1.06
2:B:218:ARG:HD3	3:I:2:LYS:HZ3	1.16	1.06
2:B:682:ARG:NE	3:I:248:LEU:HD13	1.72	1.05
2:B:675:LYS:HZ1	3:I:166:LYS:HD2	1.22	1.05
2:B:671:TYR:HD2	2:B:677:GLU:O	1.40	1.03
2:B:584:TYR:HH	3:I:324:LYS:HE3	0.96	1.01
2:B:646:SER:CB	2:B:654:ARG:NH1	1.81	1.00
2:B:218:ARG:HD3	3:I:2:LYS:NZ	1.75	1.00
2:B:675:LYS:NZ	3:I:166:LYS:CD	2.25	0.99
2:B:682:ARG:HD3	3:I:248:LEU:HD13	1.40	0.98
2:B:679:LEU:HD21	3:I:209:THR:HG21	1.45	0.98
2:B:227:LYS:HD2	3:I:335:LYS:CB	1.94	0.97
2:B:682:ARG:HH11	3:I:248:LEU:HA	1.28	0.97
2:B:682:ARG:HH11	3:I:248:LEU:HD12	1.19	0.94
2:B:675:LYS:HZ1	3:I:166:LYS:CD	1.80	0.94
2:B:664:GLY:O	2:B:668:GLN:HG3	1.67	0.93
2:B:592:ARG:NH2	3:I:342:HIS:CB	2.32	0.93
2:B:646:SER:HB3	2:B:654:ARG:HH22	1.34	0.93
2:B:671:TYR:CD2	2:B:677:GLU:O	2.23	0.92
2:B:227:LYS:HE2	3:I:335:LYS:HD2	1.52	0.92
2:B:592:ARG:HH22	3:I:342:HIS:CB	1.83	0.91
2:B:227:LYS:HE3	3:I:335:LYS:HD2	1.48	0.90
2:B:218:ARG:HG2	3:I:2:LYS:HZ1	1.38	0.88
2:B:682:ARG:HD3	3:I:248:LEU:CD1	2.02	0.88
2:B:679:LEU:CD2	3:I:209:THR:HG21	2.04	0.87
2:B:675:LYS:NZ	3:I:166:LYS:HD2	1.85	0.87
2:B:218:ARG:CG	3:I:2:LYS:HZ1	1.88	0.86
2:B:656:MET:HE2	3:I:281:ILE:O	1.74	0.86
2:B:592:ARG:NH2	3:I:342:HIS:CG	2.44	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:682:ARG:CZ	3:I:248:LEU:HD13	2.00	0.84
2:B:592:ARG:NH2	3:I:342:HIS:HB3	1.93	0.82
2:B:682:ARG:CZ	3:I:248:LEU:HD12	1.99	0.82
2:B:646:SER:CB	2:B:654:ARG:NH2	2.43	0.82
2:B:646:SER:HB2	2:B:654:ARG:NH2	1.94	0.82
2:B:218:ARG:CD	3:I:2:LYS:NZ	2.43	0.81
2:B:646:SER:CB	2:B:654:ARG:HH22	1.93	0.81
2:B:650:VAL:HG13	3:I:333:VAL:CG1	2.10	0.80
2:B:646:SER:CB	2:B:654:ARG:CZ	2.44	0.80
2:B:227:LYS:HE2	3:I:335:LYS:CD	2.12	0.79
2:B:592:ARG:CZ	3:I:342:HIS:HB3	2.13	0.79
2:B:675:LYS:HZ1	3:I:166:LYS:CG	1.93	0.78
2:B:227:LYS:CD	3:I:335:LYS:HB3	2.10	0.77
2:B:646:SER:CA	2:B:654:ARG:HH12	1.97	0.77
2:B:675:LYS:NZ	3:I:166:LYS:CB	2.48	0.74
2:B:671:TYR:CD2	2:B:677:GLU:C	2.59	0.74
2:B:654:ARG:O	2:B:658:GLU:HG3	1.87	0.74
2:B:656:MET:CE	3:I:282:PHE:HA	2.19	0.71
2:B:675:LYS:HZ3	3:I:166:LYS:HG3	0.57	0.71
2:B:218:ARG:CD	3:I:2:LYS:HZ3	1.97	0.71
2:B:218:ARG:CG	3:I:2:LYS:NZ	2.54	0.71
2:B:584:TYR:OH	3:I:324:LYS:HE2	1.88	0.71
2:B:218:ARG:HH12	3:I:2:LYS:HD2	0.87	0.70
3:I:307:SER:HB2	3:I:320:HIS:O	1.93	0.69
2:B:234:GLU:OE1	3:I:323:GLU:HB3	1.93	0.68
2:B:646:SER:CA	2:B:654:ARG:NH1	2.55	0.67
2:B:656:MET:CE	3:I:281:ILE:O	2.41	0.67
2:B:682:ARG:HD3	3:I:248:LEU:CB	2.25	0.66
3:I:221:PHE:CE1	3:I:233:LYS:HG3	2.31	0.66
2:B:592:ARG:NH1	3:I:342:HIS:HB3	2.11	0.65
2:B:218:ARG:NH1	3:I:2:LYS:CG	2.58	0.64
2:B:646:SER:O	2:B:654:ARG:NH1	2.29	0.64
2:B:218:ARG:HH12	3:I:2:LYS:CD	1.76	0.62
2:B:218:ARG:HH11	3:I:2:LYS:NZ	1.98	0.62
2:B:656:MET:HE2	3:I:282:PHE:HA	1.82	0.61
2:B:668:GLN:HA	2:B:679:LEU:HD12	1.81	0.60
2:B:216:GLY:CA	3:I:323:GLU:OE1	2.50	0.60
3:I:30:LYS:HA	3:I:54:THR:HG23	1.82	0.60
2:B:679:LEU:HD21	3:I:209:THR:CG2	2.28	0.59
2:B:227:LYS:CE	3:I:335:LYS:CD	2.67	0.58
2:B:682:ARG:HD3	3:I:248:LEU:CA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:274:GLU:OE2	3:I:288:ARG:HD3	2.04	0.57
2:B:231:SER:OG	3:I:325:SER:HA	2.05	0.57
2:B:218:ARG:NH1	3:I:2:LYS:CE	2.47	0.54
2:B:661:ARG:O	2:B:665:LYS:HG3	2.09	0.53
3:I:57:SER:CB	3:I:98:ARG:HA	2.40	0.52
3:I:57:SER:HB2	3:I:98:ARG:HA	1.91	0.52
2:B:650:VAL:HG13	3:I:333:VAL:HG11	1.87	0.52
2:B:677:GLU:OE1	3:I:163:THR:HG21	2.10	0.52
2:B:679:LEU:CD2	3:I:209:THR:CG2	2.82	0.52
2:B:677:GLU:OE1	3:I:163:THR:CG2	2.58	0.51
2:B:650:VAL:HG13	3:I:333:VAL:HG12	1.92	0.51
3:I:246:THR:HG22	3:I:301:ILE:HD13	1.91	0.51
2:B:656:MET:HE1	3:I:282:PHE:HA	1.92	0.51
2:B:682:ARG:HH11	3:I:248:LEU:CD1	1.97	0.50
3:I:227:THR:OG1	3:I:229:GLN:HB2	2.11	0.50
2:B:218:ARG:CD	3:I:2:LYS:HZ1	2.15	0.50
2:B:675:LYS:HD3	3:I:166:LYS:HZ2	1.77	0.50
2:B:347:ASP:CG	2:B:366:LYS:HZ1	2.16	0.49
2:B:682:ARG:HD3	3:I:248:LEU:HA	1.95	0.48
2:B:234:GLU:OE1	3:I:323:GLU:CB	2.60	0.48
2:B:675:LYS:CE	3:I:166:LYS:HD2	2.43	0.47
2:B:668:GLN:CA	2:B:679:LEU:HD12	2.44	0.47
3:I:98:ARG:HB3	3:I:111:ILE:HD12	1.97	0.47
2:B:668:GLN:O	2:B:672:VAL:HG23	2.14	0.47
2:B:682:ARG:HD3	3:I:248:LEU:HB2	1.96	0.47
3:I:233:LYS:HE2	3:I:235:GLU:HG3	1.98	0.46
2:B:227:LYS:HE2	3:I:335:LYS:HD3	1.93	0.46
2:B:671:TYR:CE1	3:I:163:THR:HG21	2.50	0.45
2:B:646:SER:C	2:B:650:VAL:HG11	2.36	0.45
3:I:313:GLU:O	3:I:313:GLU:HG3	2.16	0.45
3:I:302:SER:HA	3:I:303:PRO:HD3	1.78	0.44
2:B:218:ARG:HH11	3:I:2:LYS:HZ3	1.65	0.44
2:B:657:MET:HE1	3:I:334:GLU:HA	2.00	0.44
2:B:218:ARG:HG3	3:I:2:LYS:HE2	1.99	0.44
3:I:217:ASP:OD1	3:I:217:ASP:C	2.56	0.44
2:B:234:GLU:OE2	3:I:324:LYS:HB3	2.18	0.43
2:B:657:MET:SD	3:I:333:VAL:HG23	2.58	0.43
3:I:307:SER:CB	3:I:320:HIS:O	2.65	0.43
2:B:679:LEU:HD22	3:I:207:ASP:OD2	2.18	0.43
2:B:675:LYS:HD3	3:I:166:LYS:NZ	2.34	0.42
2:B:218:ARG:NH1	3:I:323:GLU:OE2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:664:GLY:O	2:B:668:GLN:CG	2.53	0.42
2:B:231:SER:HG	3:I:325:SER:CB	2.31	0.42
3:I:53:GLY:O	3:I:54:THR:C	2.57	0.41
3:I:136:LEU:C	3:I:136:LEU:HD12	2.41	0.41
2:B:679:LEU:HD22	3:I:209:THR:HG21	1.96	0.41
1:A:686:UNK:CD	2:B:567:ARG:HH12	2.34	0.40
3:I:107:TYR:HA	3:I:125:TYR:O	2.21	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	
2	B	611/1121 (54%)	534 (87%)	56 (9%)	21 (3%)	3	26
3	I	340/347 (98%)	323 (95%)	16 (5%)	1 (0%)	41	77
All	All	951/1468 (65%)	857 (90%)	72 (8%)	22 (2%)	9	34

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	208	GLN
2	B	211	VAL
2	B	214	GLU
2	B	215	SER
2	B	323	CYS
2	B	178	ILE
2	B	217	ASP
2	B	282	ILE
2	B	467	THR
2	B	546	CYS
2	B	628	LYS

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Mol	Chain	Res	Type
2	B	629	LYS
2	B	630	TYR
2	B	390	LYS
3	I	8	GLY
2	B	101	ASP
2	B	268	PHE
2	B	413	PHE
2	B	478	SER
2	B	355	PRO
2	B	96	PRO
2	B	487	ALA

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	
2	B	547/928 (59%)	526 (96%)	21 (4%)	33	57
3	I	297/301 (99%)	289 (97%)	8 (3%)	44	65
All	All	844/1229 (69%)	815 (97%)	29 (3%)	40	60

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	94	ASN
2	B	151	LYS
2	B	167	ASN
2	B	173	ASP
2	B	174	LYS
2	B	201	GLU
2	B	207	ASP
2	B	225	ASP
2	B	228	ASP
2	B	244	ARG
2	B	295	SER
2	B	332	PHE

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Mol	Chain	Res	Type
2	B	361	ASP
2	B	408	ARG
2	B	465	LYS
2	B	476	ASN
2	B	500	ASN
2	B	510	ASP
2	B	550	ASN
2	B	600	ASP
2	B	639	ARG
3	I	5	LYS
3	I	65	LYS
3	I	136	LEU
3	I	199	ILE
3	I	230	VAL
3	I	233	LYS
3	I	302	SER
3	I	338	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	414	ASN
3	I	269	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

This section contains visualisations of the EMDB entry EMD-3057. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

| X | Y | Z |
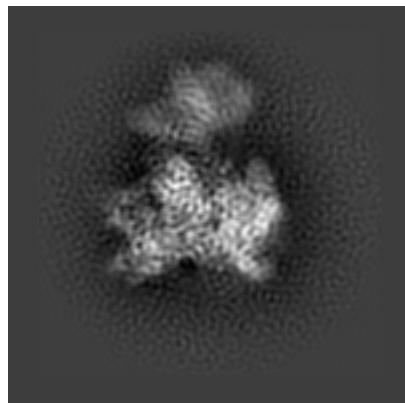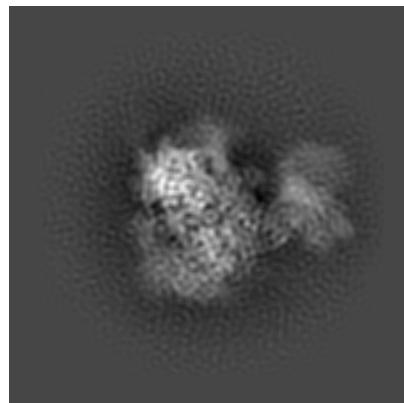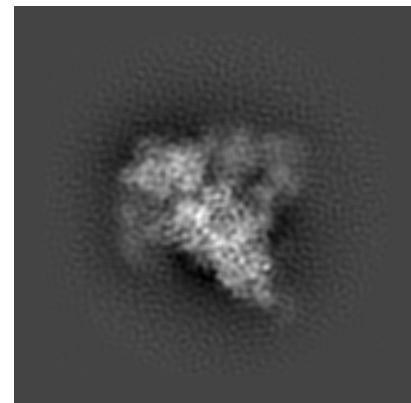
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
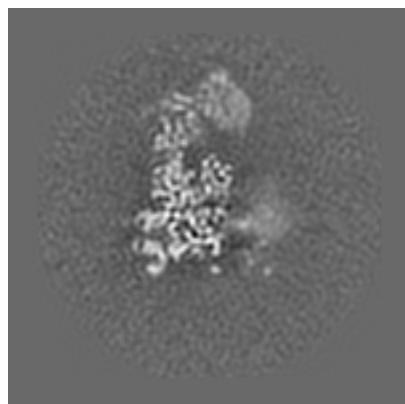
6.2.1 Primary map
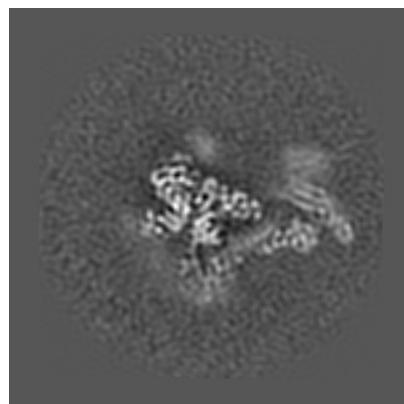
| X Index: 150 | Y Index: 150 | Z Index: 150 |
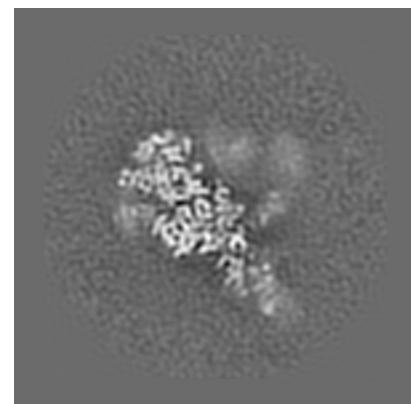
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
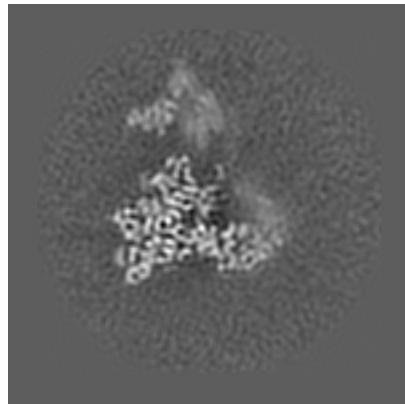
6.3.1 Primary map
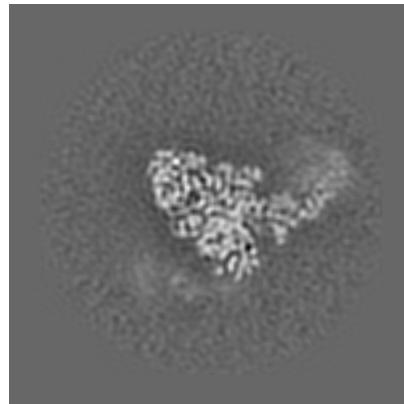
| X Index: 164 | Y Index: 127 | Z Index: 136 |
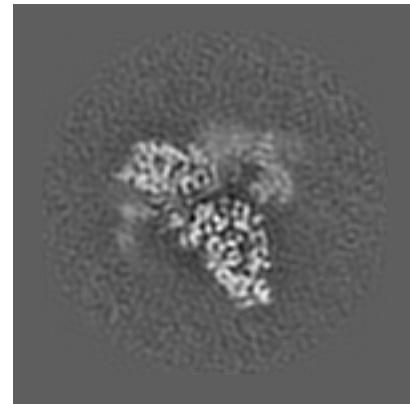
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ
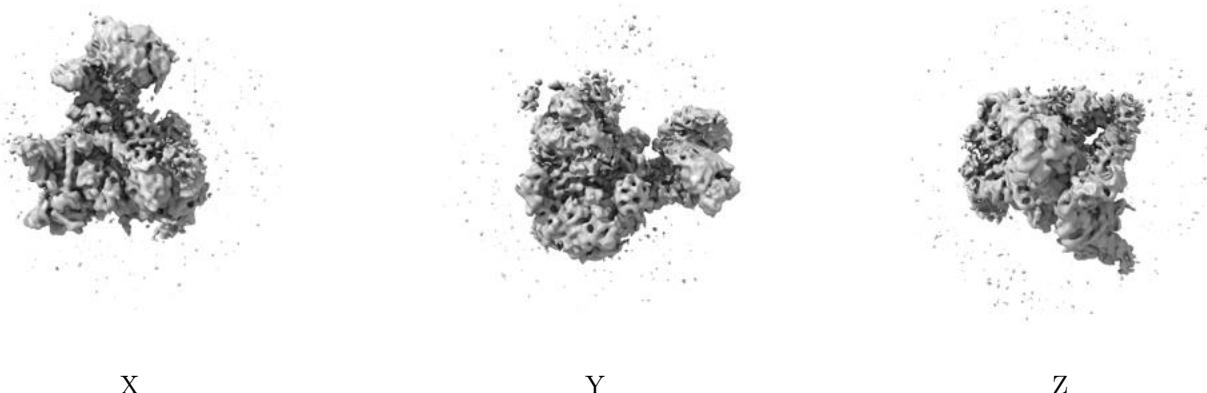
6.4.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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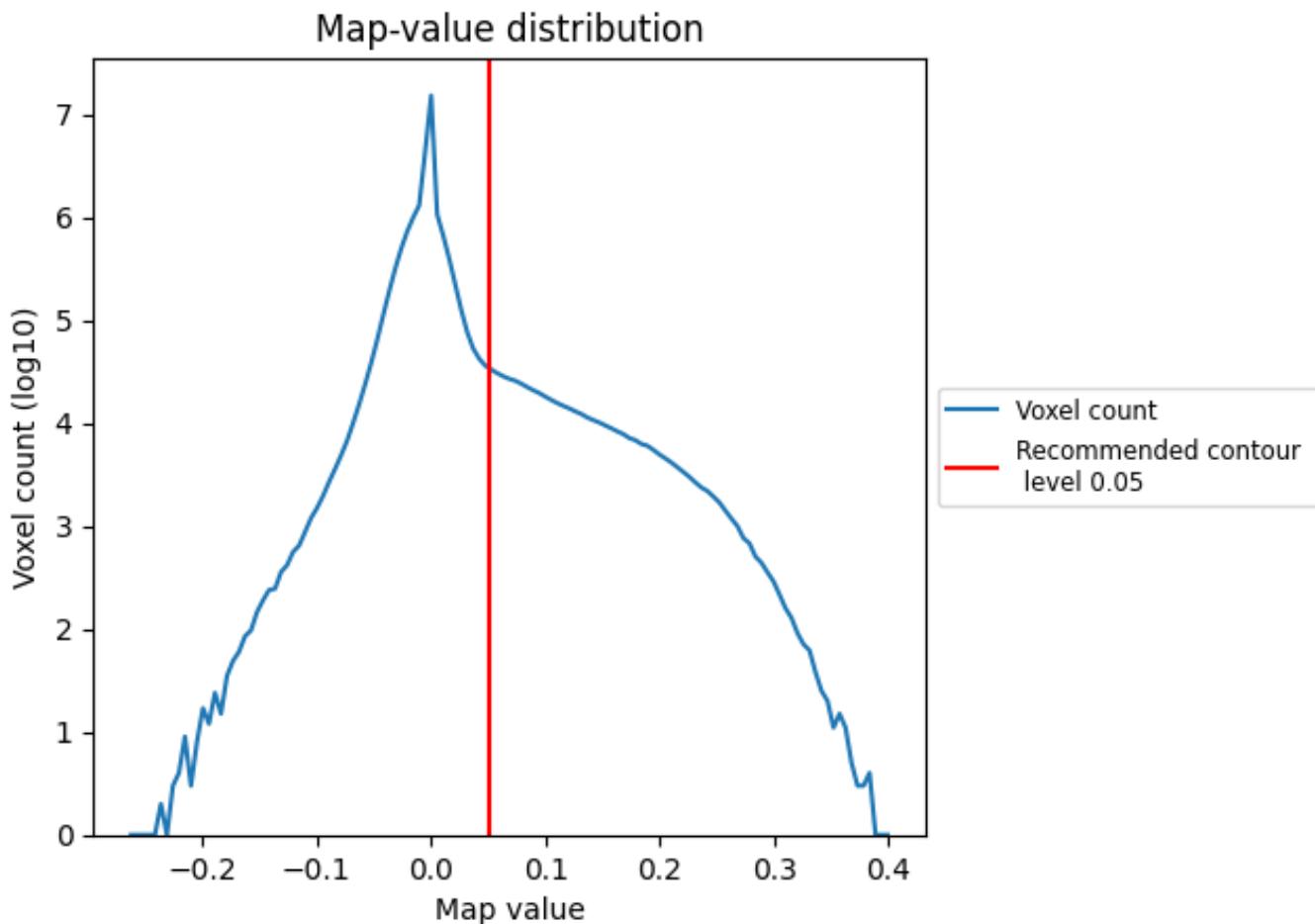
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
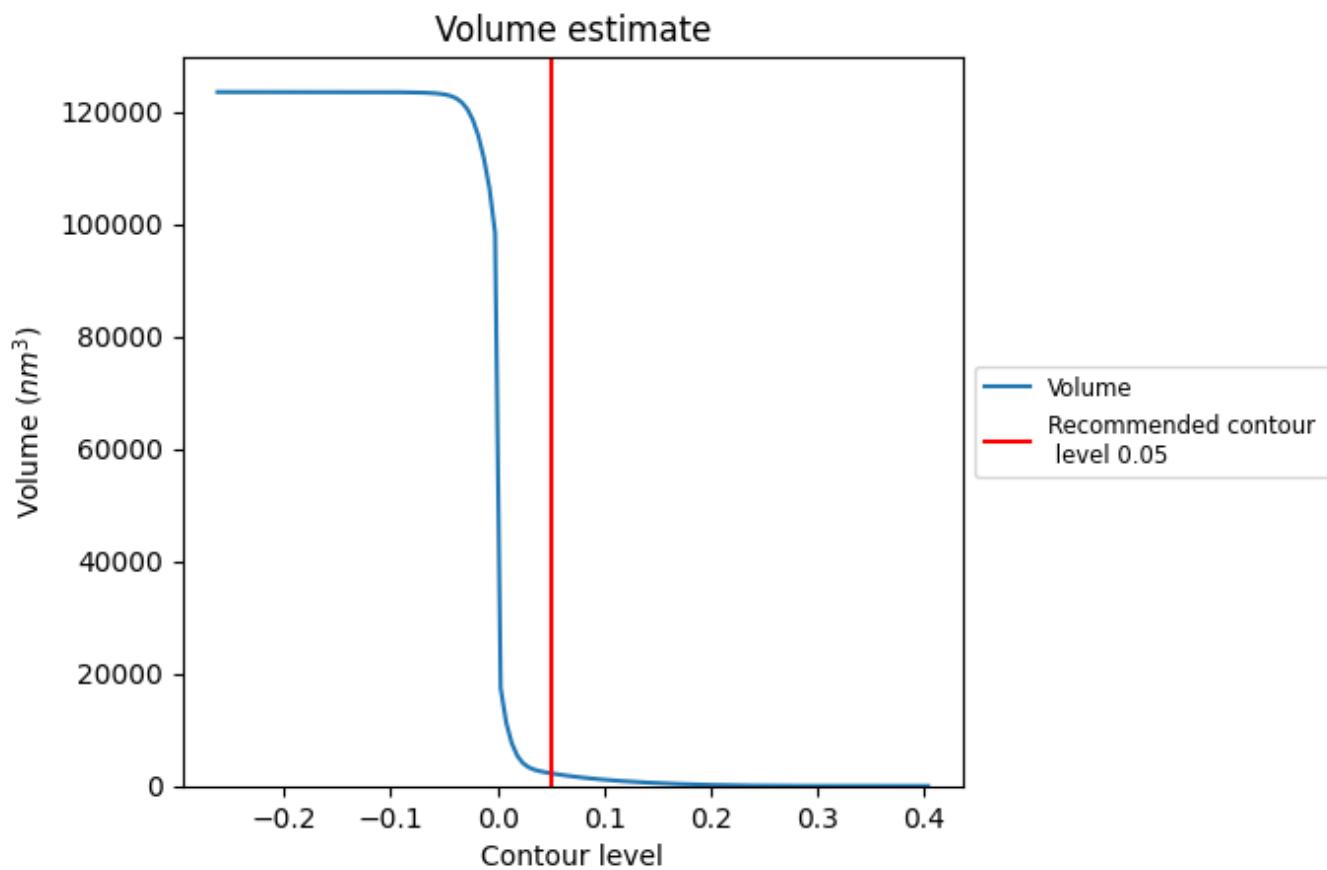
The volume at the recommended contour level is 2255 nm^3; this corresponds to an approximate mass of 2037 kDa.

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 ⓘ
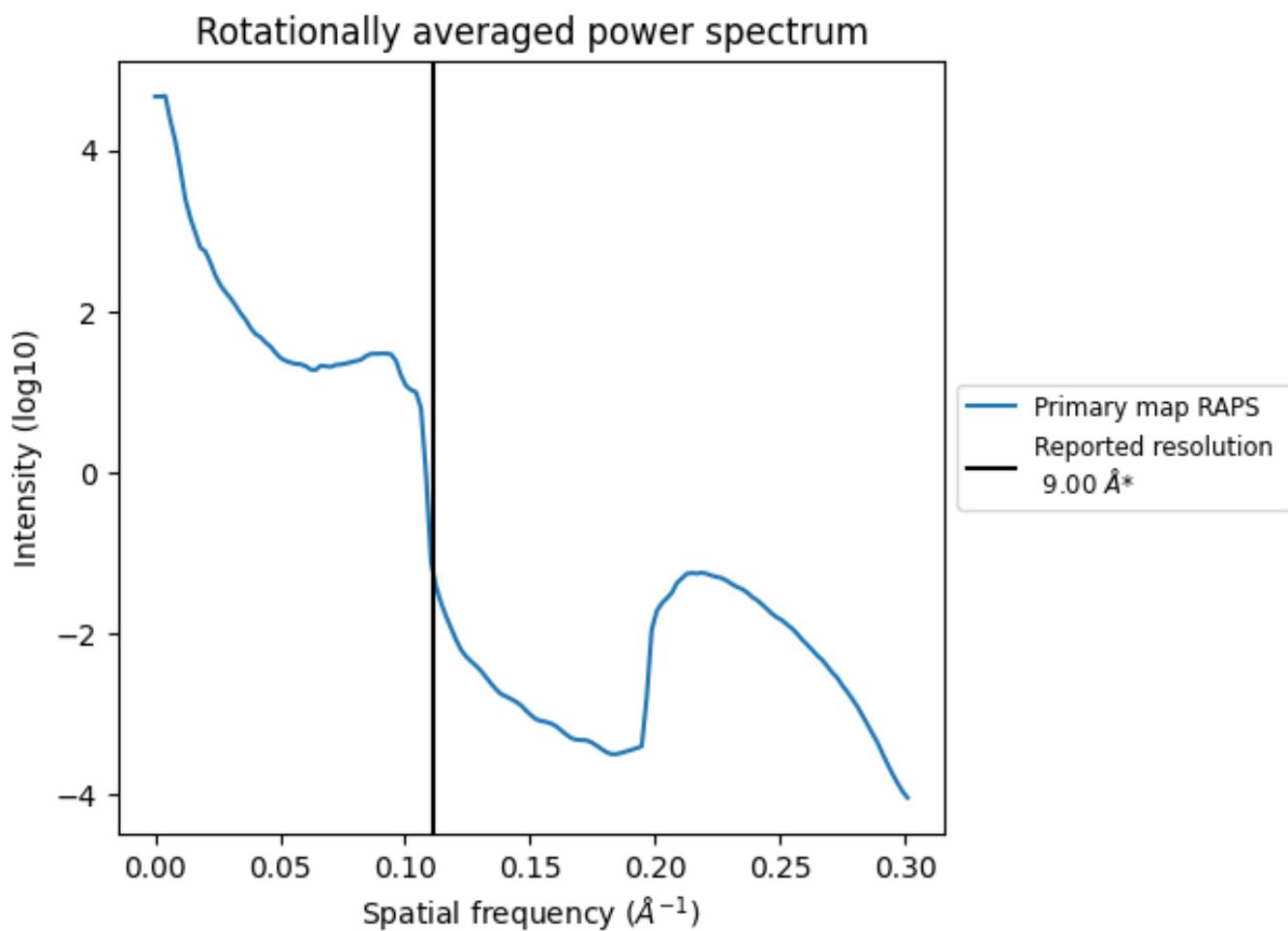
*Reported resolution corresponds to spatial frequency of 0.111 Å^{-1}

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-3057 and PDB model 5A5U. Per-residue inclusion information can be found in section 3 on page 4.

9.1　Map-model overlay ⓘ

X　　　　　　　　　　　　Y　　　　　　　　　　　　Z
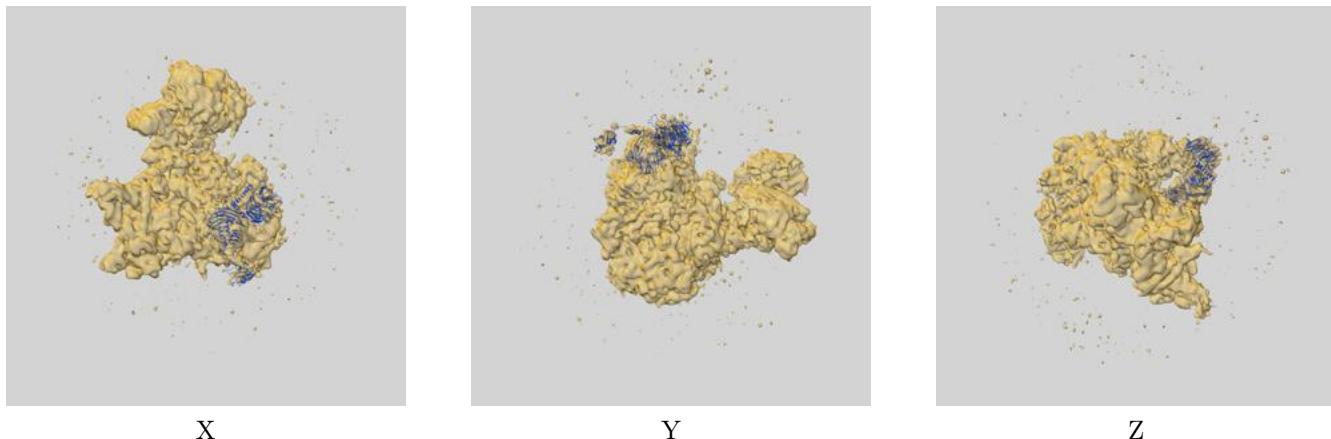
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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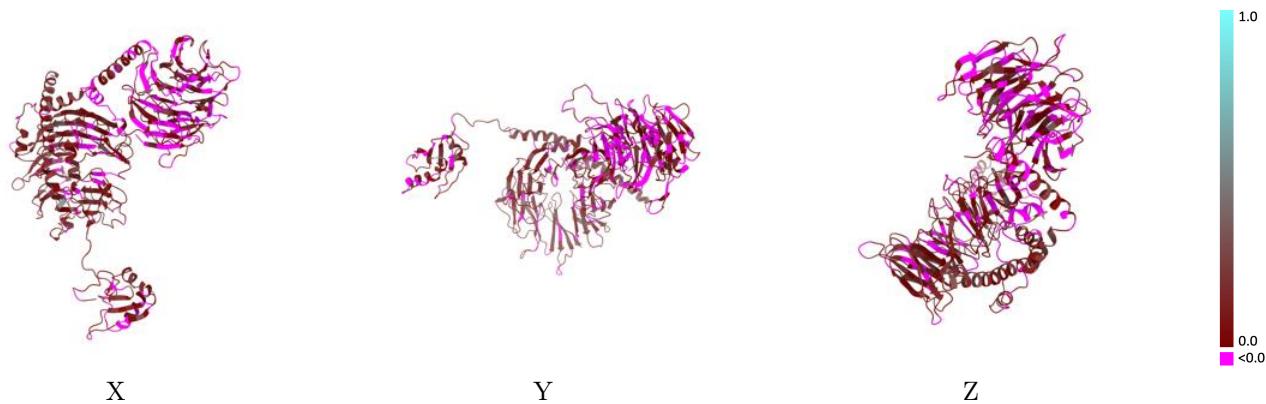
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
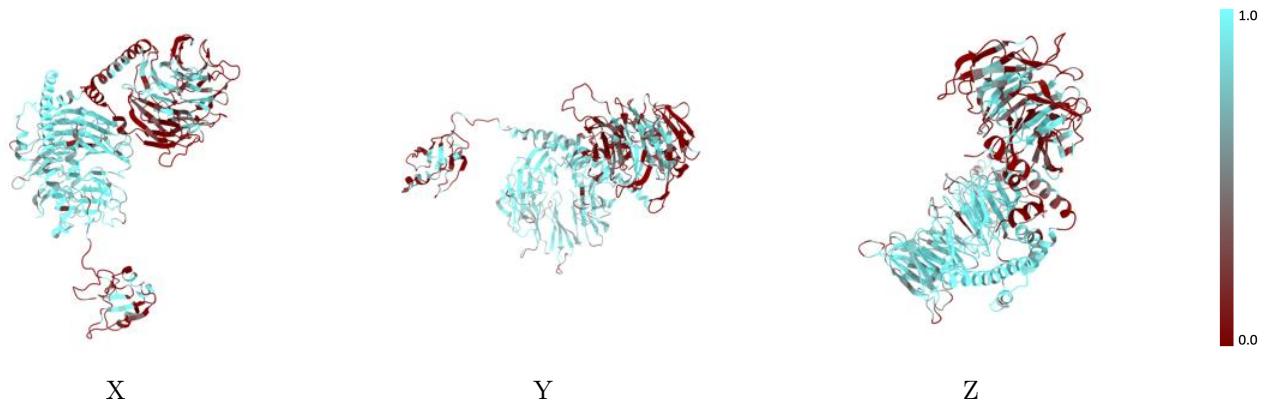
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ
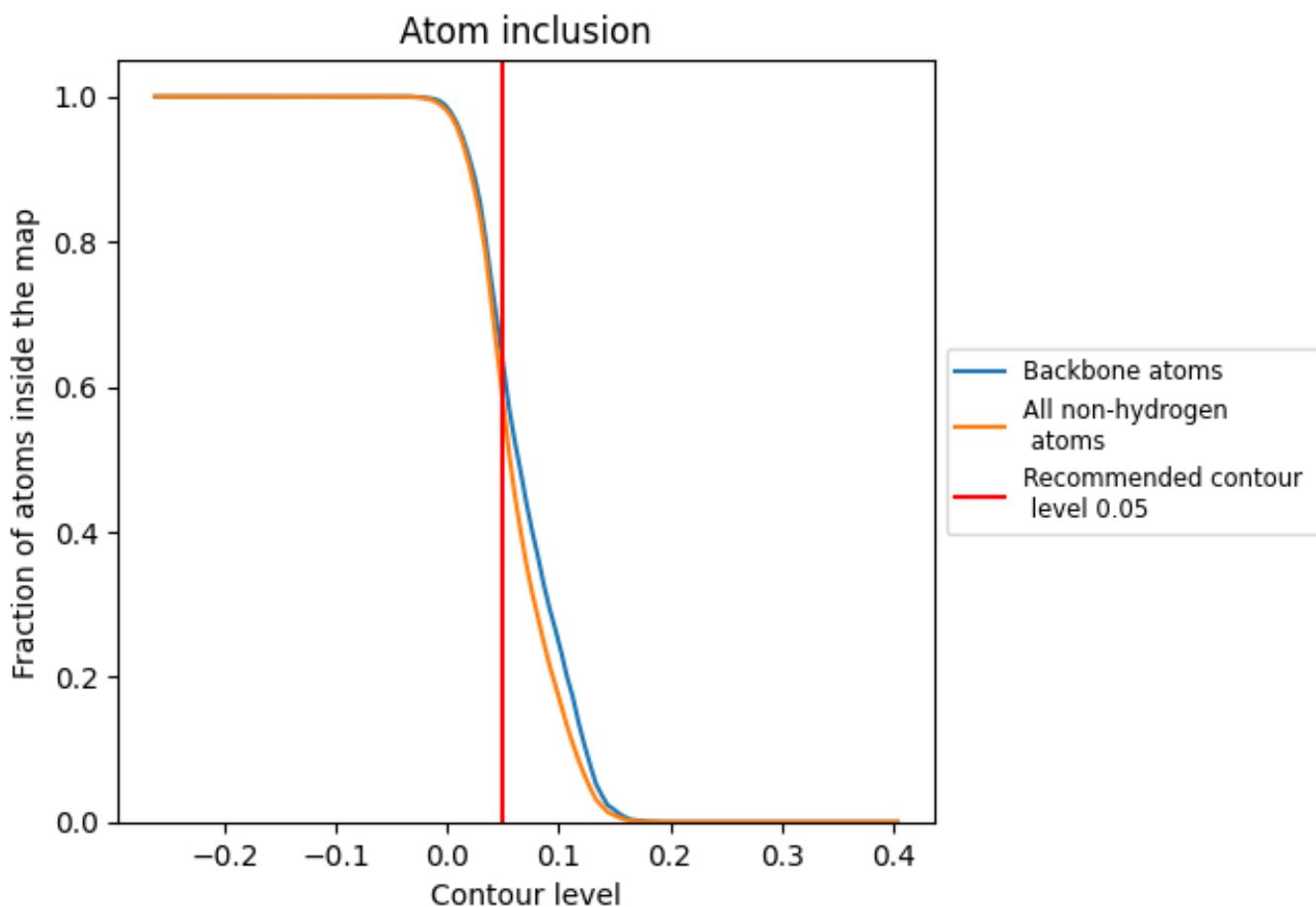
At the recommended contour level, 63% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5775	0.0710
A	0.9154	0.1640
B	0.6918	0.0970
I	0.3159	0.0080

1.0

0.0
<0.0