



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 04:41 PM UTC

PDB ID : 5A5U / pdb_00005a5u
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)

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:

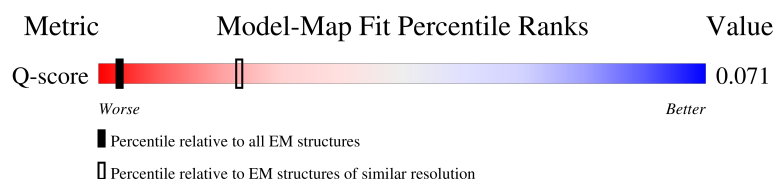
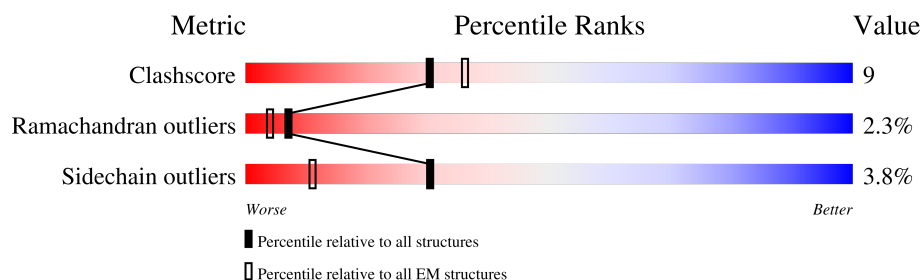
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	257 (8.50 - 9.50)

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	54	
2	B	1121	
3	I	347	

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	C	N	O	0	0
			397	246	74	77		

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

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

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

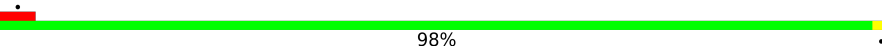
- Molecule 3 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT I.

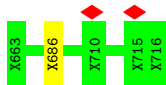
Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	342	Total	C	N	O	S	0	0
			2693	1711	443	530	9		

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.

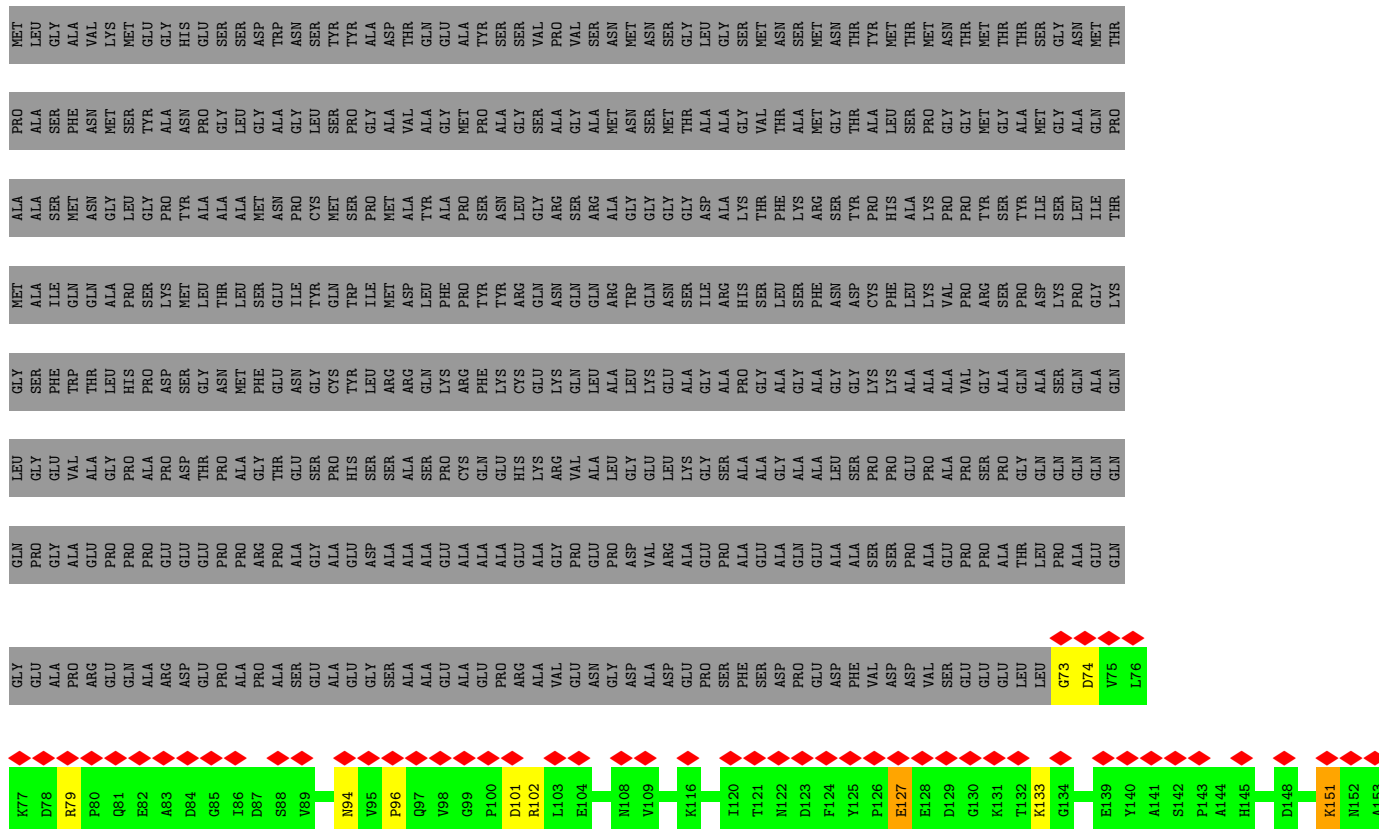
• Molecule 1: EUKARYOTIC INITIATION FACTOR 3

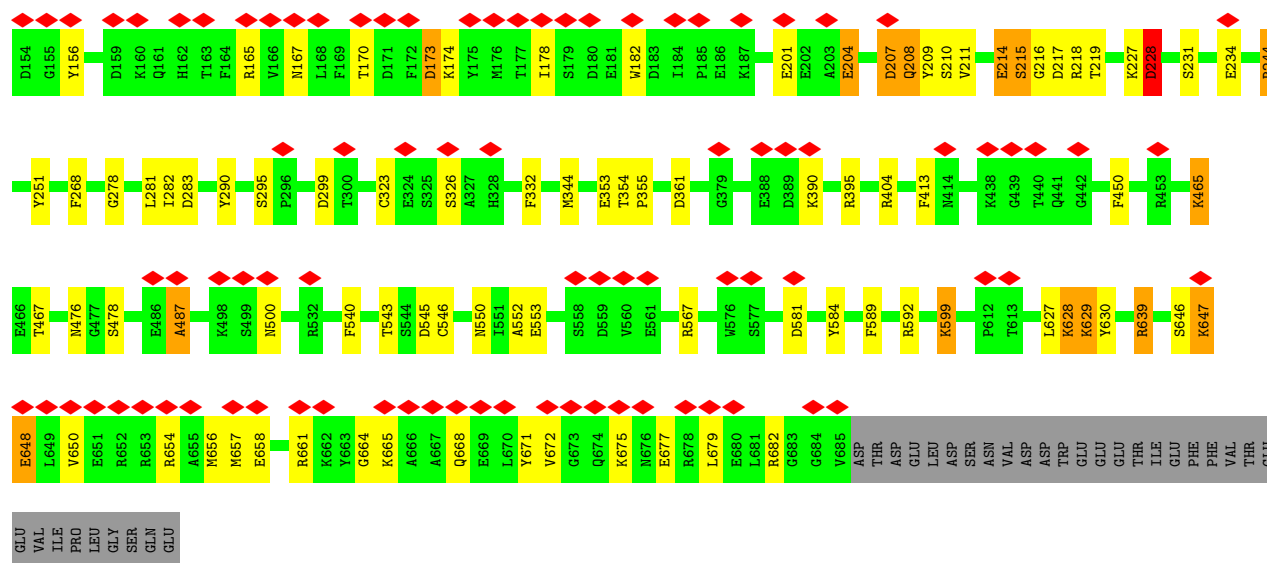
Chain A: 



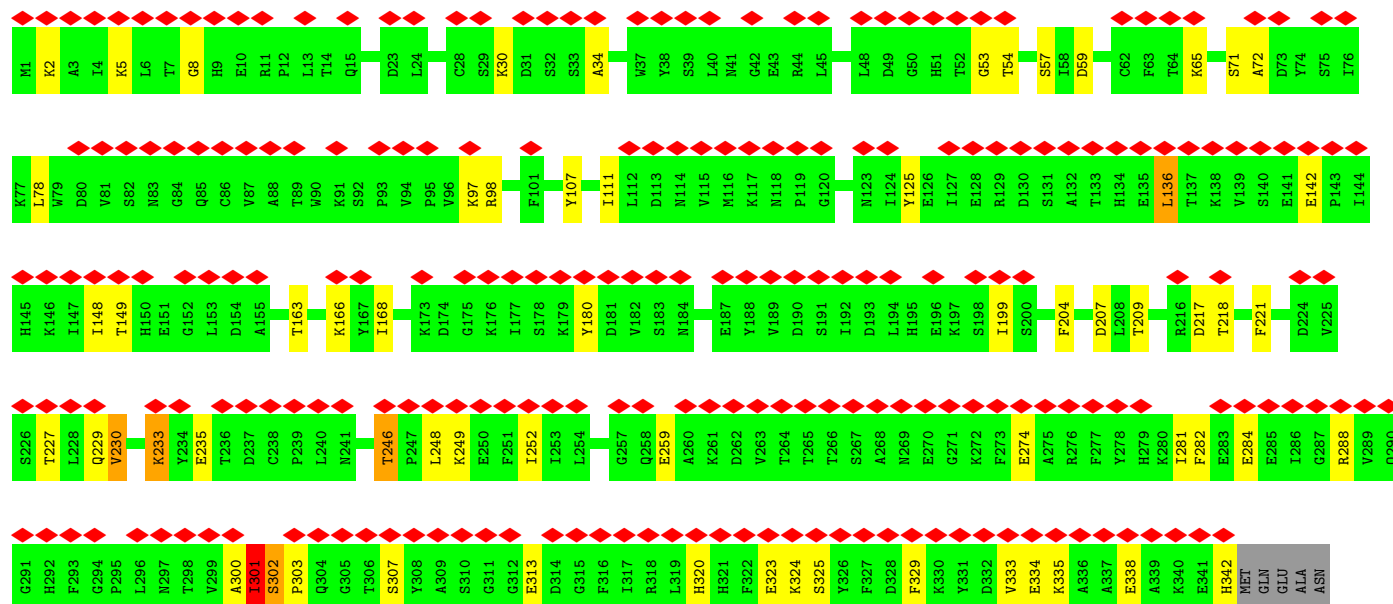
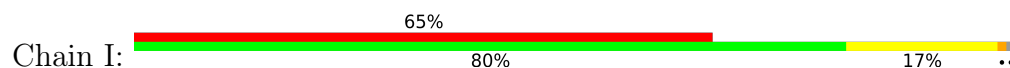
• Molecule 2: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT B

Chain B: 





• Molecule 3: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT I



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	498.0, 498.0, 498.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.87	2/5168 (0.0%)	1.59	55/6985 (0.8%)
3	I	1.30	9/2757 (0.3%)	1.19	8/3733 (0.2%)
All	All	1.04	11/7925 (0.1%)	1.46	63/10718 (0.6%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	648	GLU	N-CA	-13.87	1.19	1.46
3	I	168	ILE	N-CA	-6.74	1.38	1.46
2	B	647	LYS	C-N	6.19	1.42	1.33
3	I	72	ALA	CA-C	-5.54	1.45	1.52
3	I	34	ALA	CA-CB	5.50	1.62	1.53
3	I	78	LEU	C-O	-5.44	1.17	1.24
3	I	300	ALA	CA-C	-5.35	1.46	1.52
3	I	168	ILE	CA-CB	-5.30	1.48	1.54
3	I	301	ILE	C-O	-5.21	1.18	1.24
3	I	204	PHE	CA-C	-5.14	1.46	1.52
3	I	180	TYR	CA-C	-5.04	1.46	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	LYS	CA-C-N	23.64	164.26	121.70
2	B	647	LYS	C-N-CA	23.64	164.26	121.70
2	B	648	GLU	CA-C-O	-11.16	101.83	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	215	SER	N-CA-CB	7.95	123.92	110.49
2	B	648	GLU	N-CA-C	7.54	132.12	111.00
2	B	589	PHE	CA-C-N	7.33	130.10	120.28
2	B	589	PHE	C-N-CA	7.33	130.10	120.28
2	B	207	ASP	N-CA-C	7.15	118.61	108.74
2	B	151	LYS	CA-C-N	7.14	129.84	120.28
2	B	151	LYS	C-N-CA	7.14	129.84	120.28
2	B	173	ASP	CA-CB-CG	7.05	119.65	112.60
2	B	543	THR	CA-C-N	6.96	134.22	121.70
2	B	543	THR	C-N-CA	6.96	134.22	121.70
2	B	545	ASP	CA-CB-CG	-6.88	105.72	112.60
2	B	543	THR	O-C-N	-6.81	115.64	123.33
2	B	326	SER	O-C-N	-6.68	115.21	123.36
2	B	599	LYS	CA-C-N	6.66	129.20	120.28
2	B	599	LYS	C-N-CA	6.66	129.20	120.28
3	I	246	THR	CA-C-N	6.61	126.58	120.03
3	I	246	THR	C-N-CA	6.61	126.58	120.03
2	B	173	ASP	CB-CA-C	6.47	119.37	109.34
2	B	228	ASP	N-CA-C	-6.20	102.64	108.22
2	B	545	ASP	CA-C-N	6.13	133.25	121.54
2	B	545	ASP	C-N-CA	6.13	133.25	121.54
2	B	204	GLU	O-C-N	-6.10	115.81	123.01
2	B	73	GLY	CA-C-N	6.09	129.06	120.28
2	B	73	GLY	C-N-CA	6.09	129.06	120.28
2	B	74	ASP	N-CA-C	6.05	118.67	111.71
2	B	182	TRP	N-CA-C	5.96	117.98	107.61
2	B	214	GLU	CA-C-N	5.94	132.89	121.54
2	B	214	GLU	C-N-CA	5.94	132.89	121.54
2	B	208	GLN	N-CA-C	5.93	123.44	110.80
2	B	207	ASP	CA-C-N	5.82	132.66	121.54
2	B	207	ASP	C-N-CA	5.82	132.66	121.54
3	I	71	SER	N-CA-C	5.77	118.46	109.52
2	B	487	ALA	O-C-N	-5.65	114.82	121.32
2	B	299	ASP	CA-CB-CG	5.63	118.23	112.60
2	B	581	ASP	N-CA-C	-5.61	100.82	109.52
3	I	59	ASP	CA-C-N	-5.61	115.14	122.94
3	I	59	ASP	C-N-CA	-5.61	115.14	122.94
2	B	278	GLY	CA-C-N	5.60	128.00	120.50
2	B	278	GLY	C-N-CA	5.60	128.00	120.50
3	I	142	GLU	CA-C-N	-5.52	114.56	120.03
3	I	142	GLU	C-N-CA	-5.52	114.56	120.03
2	B	627	LEU	CA-C-N	5.37	131.80	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	627	LEU	C-N-CA	5.37	131.80	121.54
2	B	283	ASP	CA-CB-CG	-5.33	107.27	112.60
2	B	204	GLU	CA-C-N	5.27	131.19	121.70
2	B	204	GLU	C-N-CA	5.27	131.19	121.70
2	B	540	PHE	CA-CB-CG	-5.24	108.56	113.80
2	B	465	LYS	CA-C-N	5.23	128.13	120.71
2	B	465	LYS	C-N-CA	5.23	128.13	120.71
2	B	210	SER	CA-C-N	5.21	131.07	121.70
2	B	210	SER	C-N-CA	5.21	131.07	121.70
2	B	628	LYS	N-CA-CB	5.15	119.19	110.49
2	B	326	SER	CA-C-N	5.11	130.90	121.70
2	B	326	SER	C-N-CA	5.11	130.90	121.70
2	B	552	ALA	CA-C-N	5.07	127.90	120.71
2	B	552	ALA	C-N-CA	5.07	127.90	120.71
2	B	629	LYS	CA-C-N	5.06	131.20	121.54
2	B	629	LYS	C-N-CA	5.06	131.20	121.54
2	B	353	GLU	N-CA-C	5.02	116.57	108.34
3	I	230	VAL	N-CA-CB	5.01	116.56	110.95

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
2	B	281	LEU	Peptide
2	B	290	TYR	Sidechain
2	B	344	MET	Peptide
2	B	354	THR	Peptide

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Mol	Chain	Res	Type	Group
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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	397	0	156	1	0
2	B	5034	0	4953	120	0
3	I	2693	0	2609	115	0
All	All	8124	0	7718	141	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 (141) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.17	1.05
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	1.37	0.88
2:B:682:ARG:HD3	3:I:248:LEU:CD1	2.02	0.88
2:B:218:ARG:CG	3:I:2:LYS:HZ1	1.87	0.87
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:592:ARG:NH2	3:I:342:HIS:CG	2.44	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:MET:HE1	3:I:282:PHE:HA	1.61	0.81
2:B:656:MET:HE2	3:I:281:ILE:O	1.81	0.81
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:671:TYR:CD2	2:B:677:GLU:C	2.59	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: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: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
2:B:218:ARG:CD	3:I:2:LYS:HZ3	1.98	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:675:LYS:HD3	3:I:166:LYS:HZ2	1.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:218:ARG:CD	3:I:2:LYS:HZ1	2.14	0.51
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: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:646:SER:C	2:B:650:VAL:HG11	2.36	0.50
3:I:217:ASP:OD1	3:I:217:ASP:C	2.56	0.48
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:53:GLY:O	3:I:54:THR:C	2.57	0.46
3:I:233:LYS:HE2	3:I:235:GLU:HG3	1.98	0.46
3:I:136:LEU:C	3:I:136:LEU:HD12	2.41	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
3:I:302:SER:HA	3:I:303:PRO:HD3	1.78	0.44
3:I:313:GLU:O	3:I:313:GLU:HG3	2.16	0.44
2:B:218:ARG:HG3	3:I:2:LYS:HE2	1.99	0.44
2:B:218:ARG:HH11	3:I:2:LYS:HZ3	1.66	0.44
2:B:646:SER:C	2:B:654:ARG:NH1	2.75	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:148:ILE:O	3:I:149:THR:C	2.60	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
2:B:664:GLY:O	2:B:668:GLN:CG	2.53	0.42
2:B:127:GLU:CD	2:B:133:LYS:HZ1	2.27	0.42
2:B:231:SER:HG	3:I:325:SER:CB	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:249:LYS:NZ	3:I:329:PHE:O	2.44	0.41
3:I:217:ASP:O	3:I:218:THR:OG1	2.33	0.41
2:B:679:LEU:HD22	3:I:209:THR:HG21	1.96	0.41
3:I:329:PHE:CD1	3:I:329:PHE:C	2.99	0.40
1:A:686:UNK:CD	2:B:567:ARG:HH12	2.34	0.40
2:B:657:MET:HE3	3:I:334:GLU:HG2	2.02	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	611/1121 (54%)	534 (87%)	56 (9%)	21 (3%)	3	21
3	I	340/347 (98%)	323 (95%)	16 (5%)	1 (0%)	36	72
All	All	951/1468 (65%)	857 (90%)	72 (8%)	22 (2%)	7	28

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%)	528 (96%)	19 (4%)	32	53
3	I	297/301 (99%)	284 (96%)	13 (4%)	25	47
All	All	844/1229 (69%)	812 (96%)	32 (4%)	30	50

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	94	ASN
2	B	127	GLU
2	B	151	LYS
2	B	167	ASN
2	B	170	THR
2	B	173	ASP
2	B	174	LYS
2	B	201	GLU
2	B	207	ASP
2	B	228	ASP
2	B	244	ARG
2	B	295	SER

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Mol	Chain	Res	Type
2	B	332	PHE
2	B	361	ASP
2	B	465	LYS
2	B	476	ASN
2	B	500	ASN
2	B	550	ASN
2	B	639	ARG
3	I	5	LYS
3	I	65	LYS
3	I	97	LYS
3	I	136	LEU
3	I	199	ILE
3	I	230	VAL
3	I	233	LYS
3	I	252	ILE
3	I	259	GLU
3	I	284	GLU
3	I	301	ILE
3	I	302	SER
3	I	338	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	316	HIS
2	B	322	HIS
2	B	400	GLN
2	B	421	HIS
2	B	441	GLN
2	B	512	GLN
2	B	597	ASN
2	B	619	GLN
2	B	636	GLN
3	I	85	GLN
3	I	150	HIS
3	I	219	ASN
3	I	269	ASN
3	I	321	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](#)

There are no ligands in this entry.

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.

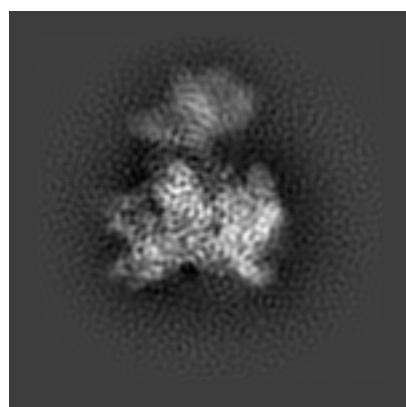
6 Map visualisation [i](#)

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

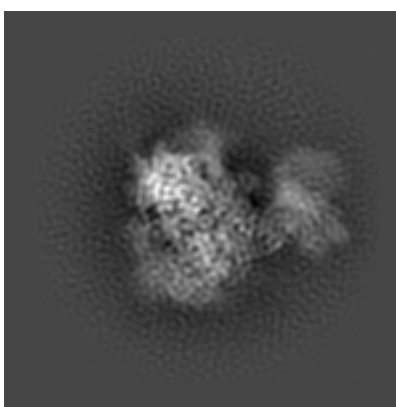
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

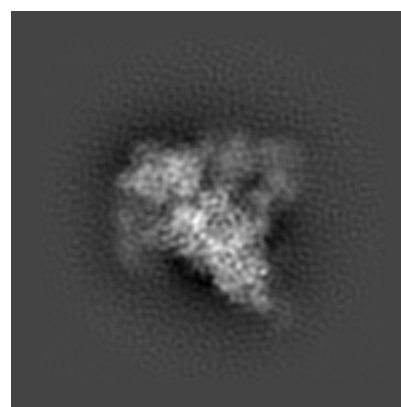
6.1.1 Primary map



X



Y

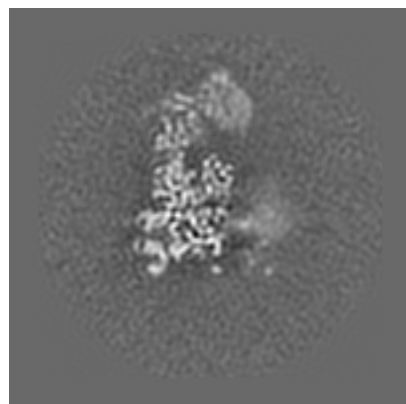


Z

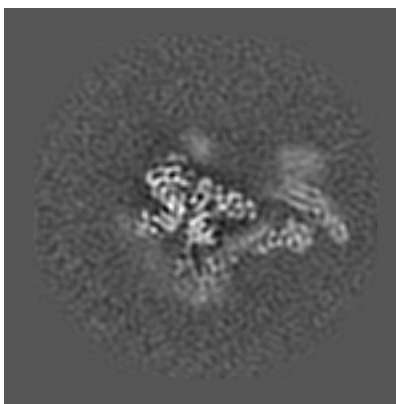
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

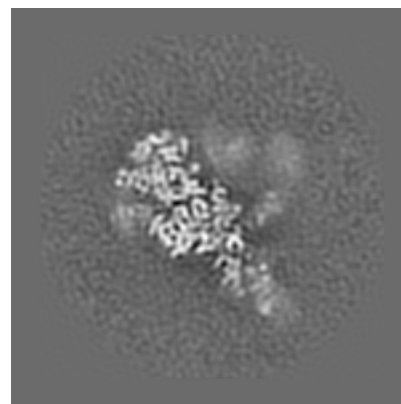
6.2.1 Primary map



X Index: 150



Y Index: 150

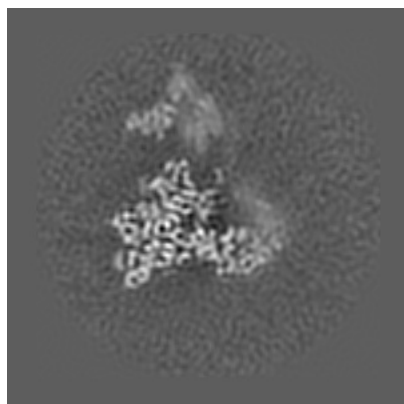


Z Index: 150

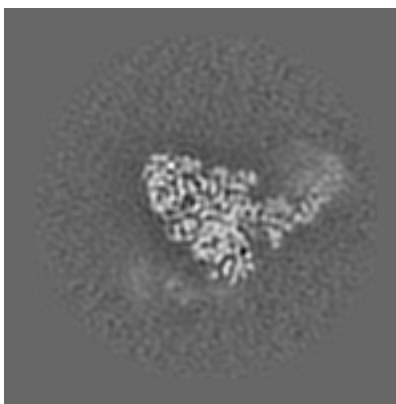
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

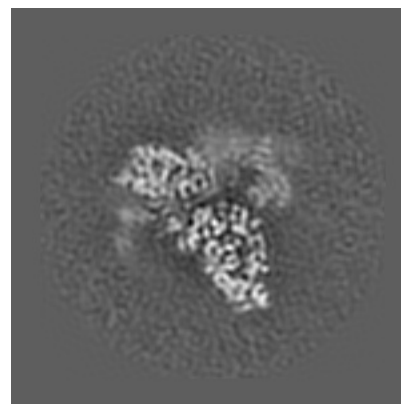
6.3.1 Primary map



X Index: 164



Y Index: 127

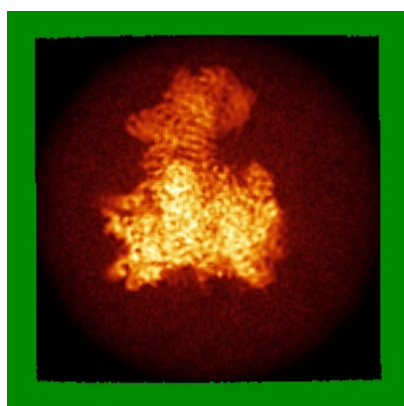


Z Index: 136

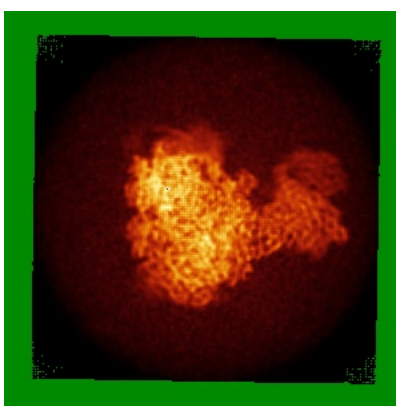
The images above show the largest variance slices of the map in three orthogonal directions.

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

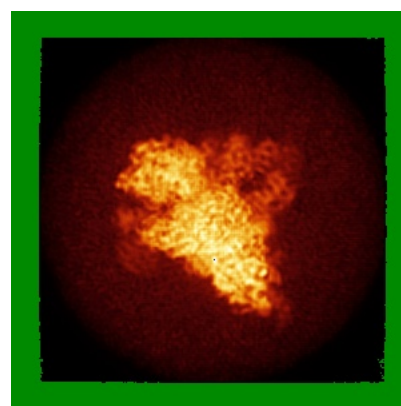
6.4.1 Primary map



X



Y

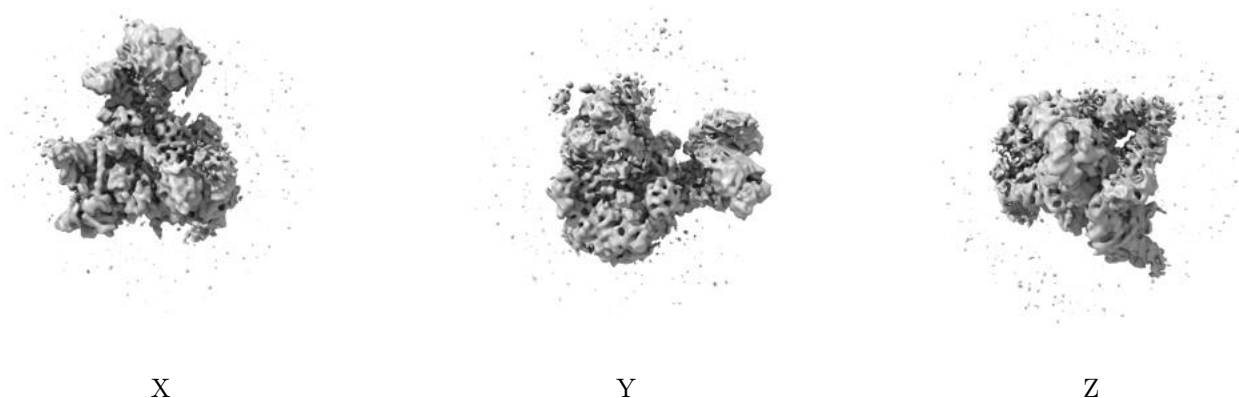


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

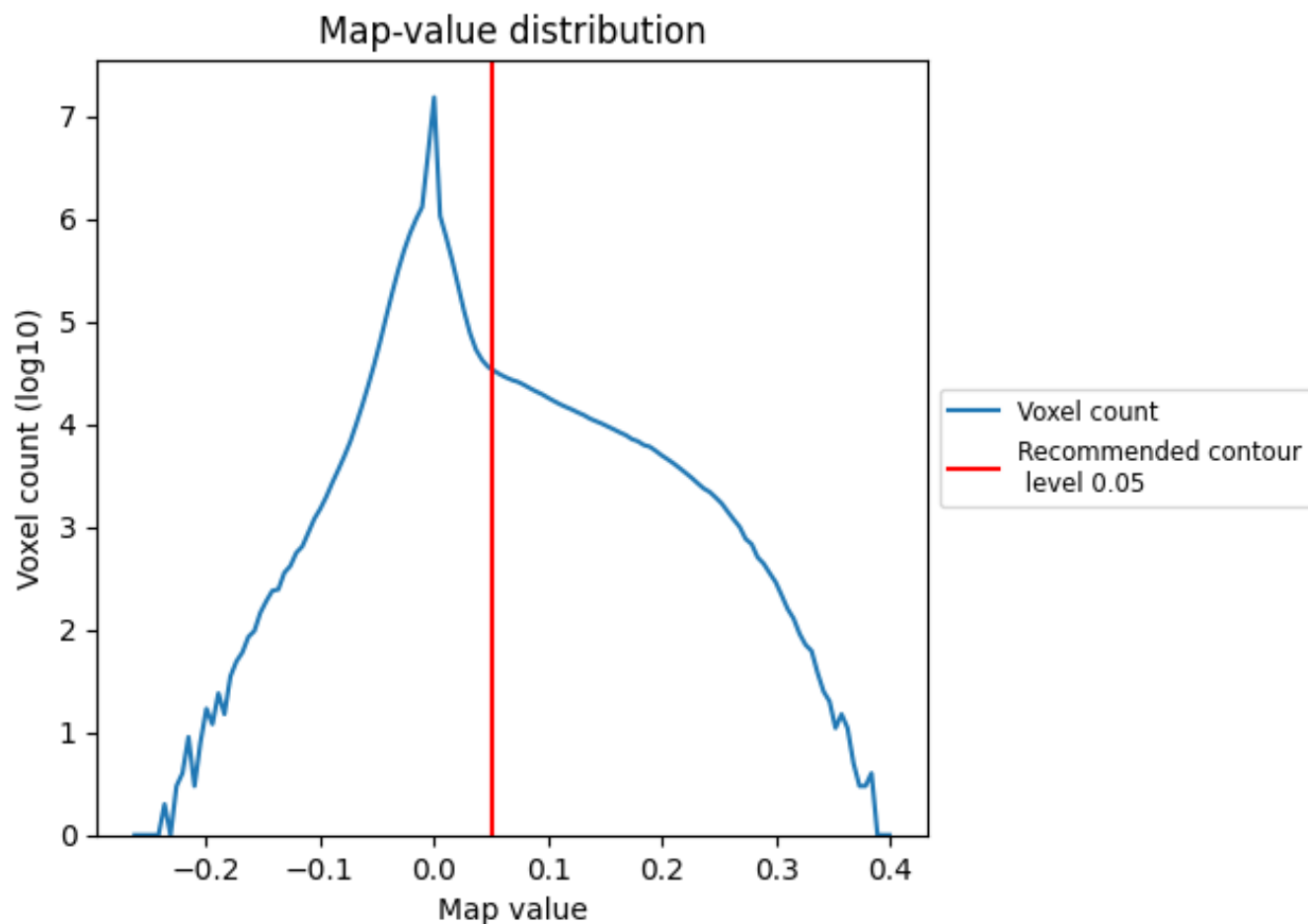
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

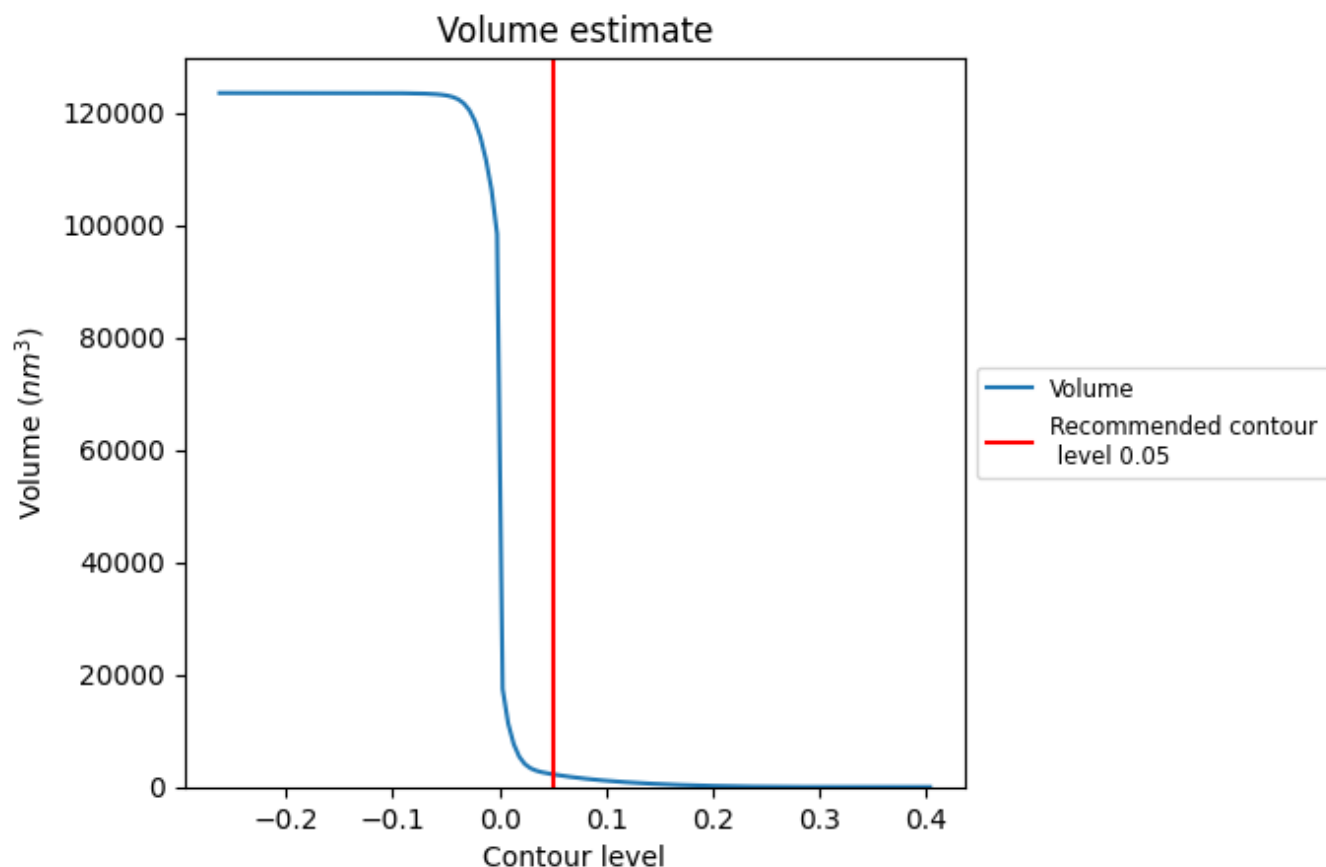
This section contains the results of statistical analysis of the map.

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.

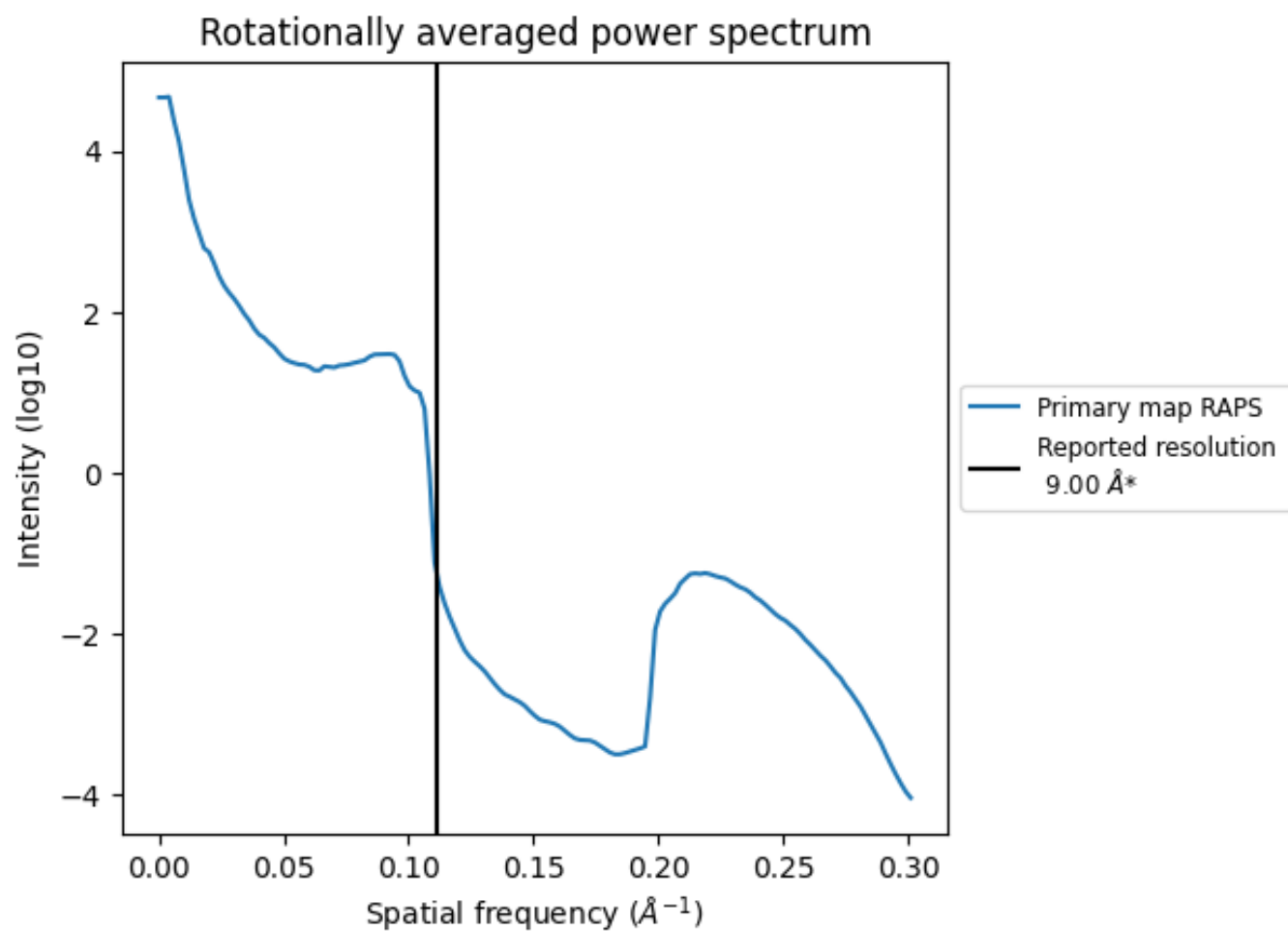
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2255 nm³; 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

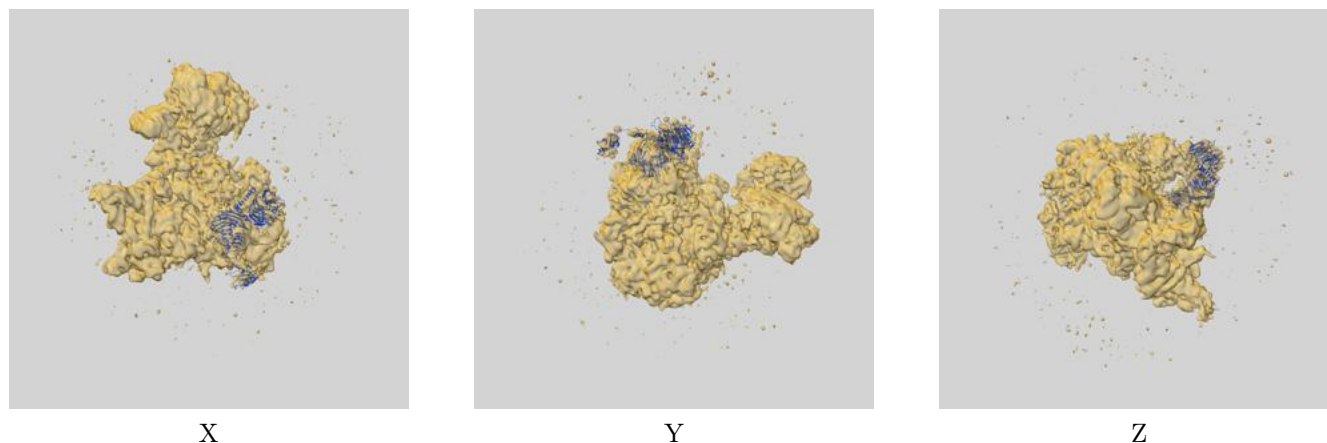
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

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 [i](#)



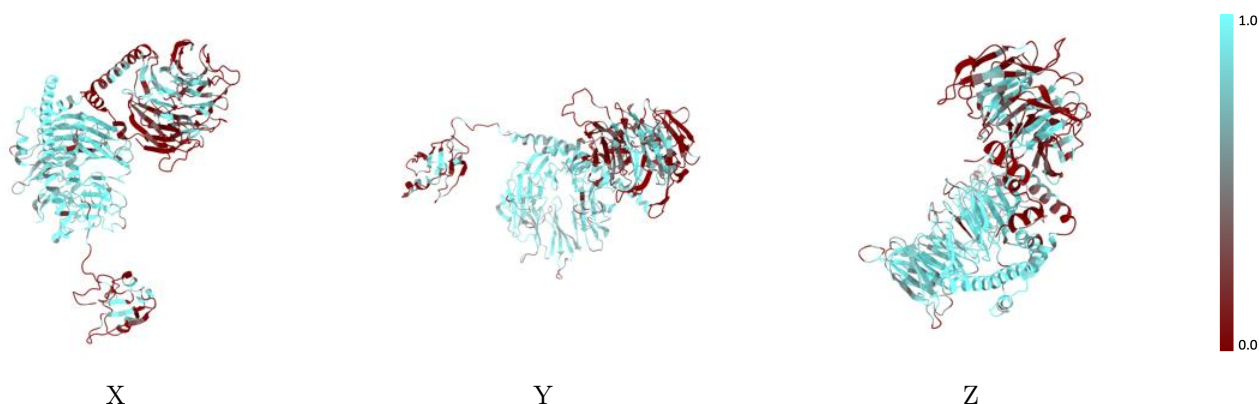
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



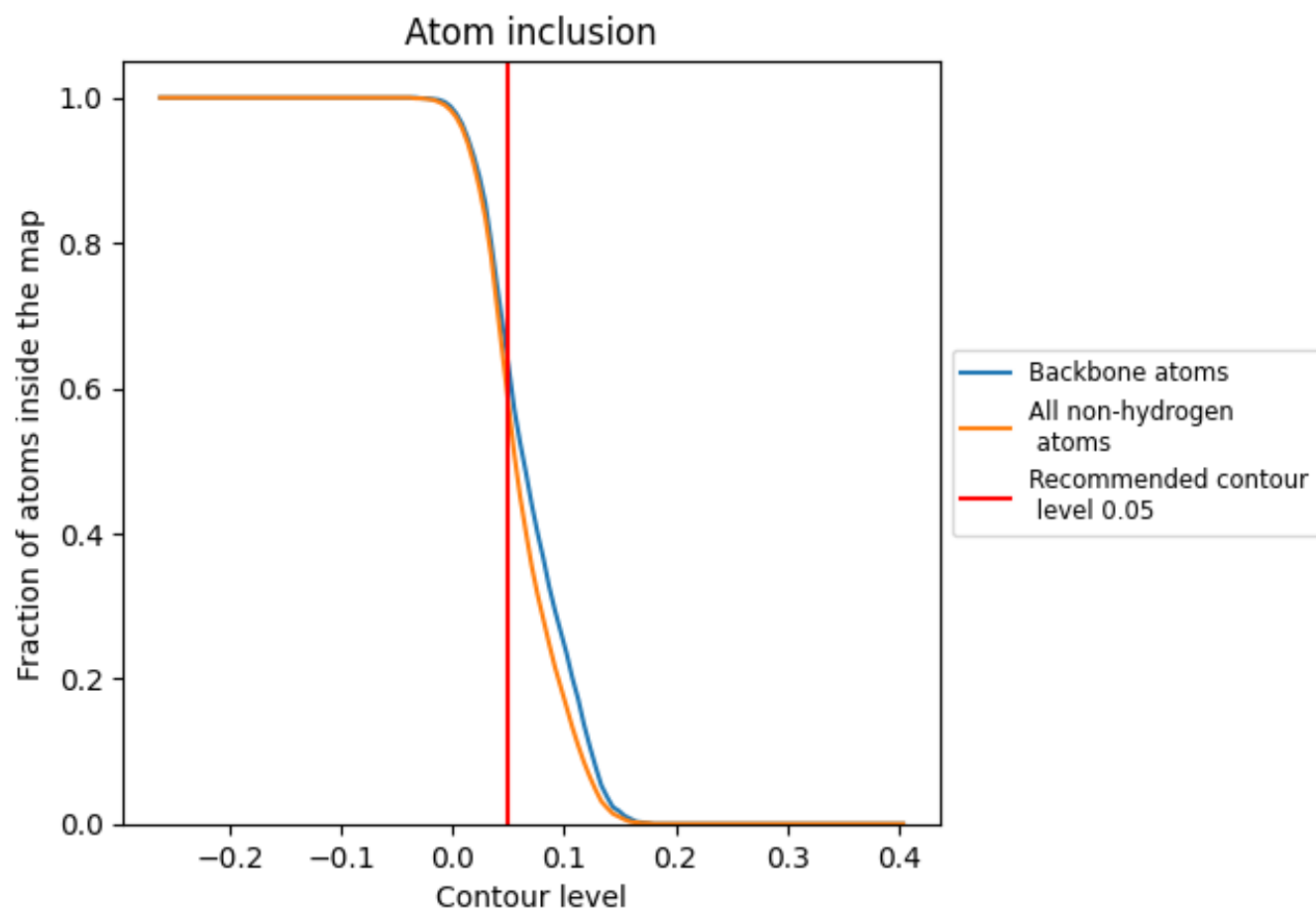
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



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	0.5770	0.0710
A	0.9150	0.1640
B	0.6920	0.0970
I	0.3160	0.0080

