



Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 04:23 PM EDT

PDB ID : 9Y5R / pdb_00009y5r
EMDB ID : EMD-72520
Title : Eukaryotic translation initiation factor 2-B (eIF2B) bound to phosphorylated eIF2alpha (NTD)
Authors : Dalwadi, U.; Croll, T.; Subramanian, A.; Lee, D.J.; Arthur, C.; Walter, P.; Frost, A.
Deposited on : 2025-09-05
Resolution : 3.01 Å (reported)
Based on initial model : 6o9z

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:

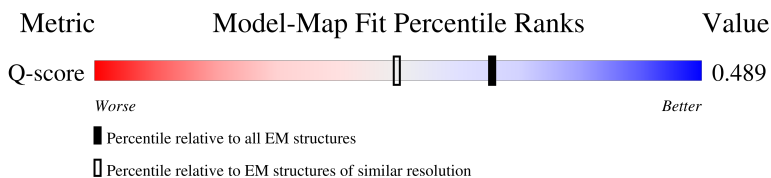
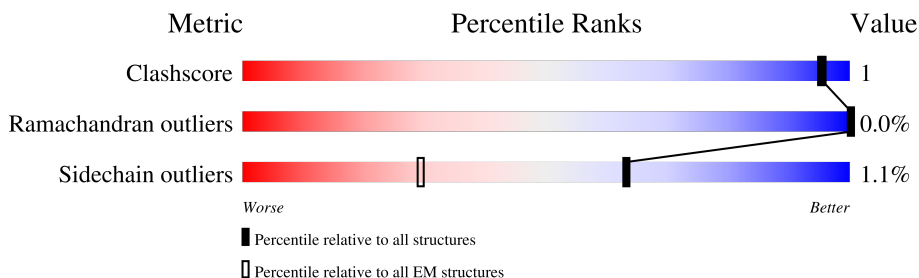
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 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.





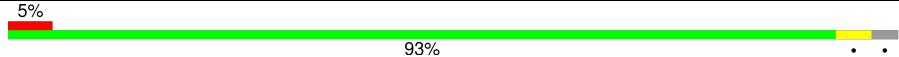
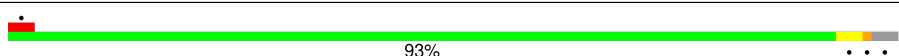
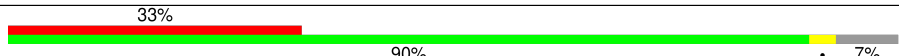
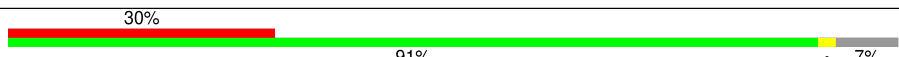
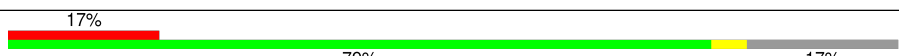

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13882 (2.51 - 3.51)

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	721	 56% 39%
1	B	721	 57% 39%
2	C	368	 79% 9% 12%
2	D	368	 80% 7% 12%

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Mol	Chain	Length	Quality of chain
3	E	523	
3	F	523	
4	G	305	
4	H	305	
5	I	452	
5	J	452	
6	L	222	
6	M	222	

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 31588 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 eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	587	VAL	ILE	conflict	UNP Q13144
B	587	VAL	ILE	conflict	UNP Q13144

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	322	Total	C	N	O	S	0	0
			2523	1596	442	470	15		
2	D	322	Total	C	N	O	S	0	0
			2523	1596	442	470	15		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P49770
C	-15	HIS	-	expression tag	UNP P49770
C	-14	HIS	-	expression tag	UNP P49770
C	-13	HIS	-	expression tag	UNP P49770
C	-12	HIS	-	expression tag	UNP P49770
C	-11	HIS	-	expression tag	UNP P49770
C	-10	HIS	-	expression tag	UNP P49770
C	-9	GLY	-	expression tag	UNP P49770
C	-8	GLY	-	expression tag	UNP P49770
C	-7	GLY	-	expression tag	UNP P49770
C	-6	SER	-	expression tag	UNP P49770

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLU	-	expression tag	UNP P49770
C	-4	ASN	-	expression tag	UNP P49770
C	-3	LEU	-	expression tag	UNP P49770
C	-2	TYR	-	expression tag	UNP P49770
C	-1	PHE	-	expression tag	UNP P49770
C	0	GLN	-	expression tag	UNP P49770
C	1	SER	-	expression tag	UNP P49770
D	-16	MET	-	initiating methionine	UNP P49770
D	-15	HIS	-	expression tag	UNP P49770
D	-14	HIS	-	expression tag	UNP P49770
D	-13	HIS	-	expression tag	UNP P49770
D	-12	HIS	-	expression tag	UNP P49770
D	-11	HIS	-	expression tag	UNP P49770
D	-10	HIS	-	expression tag	UNP P49770
D	-9	GLY	-	expression tag	UNP P49770
D	-8	GLY	-	expression tag	UNP P49770
D	-7	GLY	-	expression tag	UNP P49770
D	-6	SER	-	expression tag	UNP P49770
D	-5	GLU	-	expression tag	UNP P49770
D	-4	ASN	-	expression tag	UNP P49770
D	-3	LEU	-	expression tag	UNP P49770
D	-2	TYR	-	expression tag	UNP P49770
D	-1	PHE	-	expression tag	UNP P49770
D	0	GLN	-	expression tag	UNP P49770
D	1	SER	-	expression tag	UNP P49770

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit delta.

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

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit alpha.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	420	Total	C	N	O	S	0	0
			3260	2062	560	612	26		
5	J	420	Total	C	N	O	S	0	0
			3260	2062	560	612	26		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
6	L	184	Total	C	N	O	P	S	0	0
			1514	953	267	287	1	6		
6	M	184	Total	C	N	O	P	S	0	0
			1514	953	267	287	1	6		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-34	MET	-	initiating methionine	UNP P05198
L	-33	GLY	-	expression tag	UNP P05198
L	-32	SER	-	expression tag	UNP P05198
L	-31	SER	-	expression tag	UNP P05198
L	-30	HIS	-	expression tag	UNP P05198
L	-29	HIS	-	expression tag	UNP P05198
L	-28	HIS	-	expression tag	UNP P05198
L	-27	HIS	-	expression tag	UNP P05198
L	-26	HIS	-	expression tag	UNP P05198
L	-25	HIS	-	expression tag	UNP P05198
L	-24	SER	-	expression tag	UNP P05198
L	-23	SER	-	expression tag	UNP P05198
L	-22	GLY	-	expression tag	UNP P05198
L	-21	LEU	-	expression tag	UNP P05198
L	-20	VAL	-	expression tag	UNP P05198
L	-19	PRO	-	expression tag	UNP P05198
L	-18	ARG	-	expression tag	UNP P05198
L	-17	GLY	-	expression tag	UNP P05198
L	-16	SER	-	expression tag	UNP P05198
L	-15	HIS	-	expression tag	UNP P05198
L	-14	MET	-	expression tag	UNP P05198
L	-13	ALA	-	expression tag	UNP P05198
L	-12	SER	-	expression tag	UNP P05198
L	-11	MET	-	expression tag	UNP P05198
L	-10	THR	-	expression tag	UNP P05198

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-9	GLY	-	expression tag	UNP P05198
L	-8	GLY	-	expression tag	UNP P05198
L	-7	GLN	-	expression tag	UNP P05198
L	-6	GLN	-	expression tag	UNP P05198
L	-5	MET	-	expression tag	UNP P05198
L	-4	GLY	-	expression tag	UNP P05198
L	-3	ARG	-	expression tag	UNP P05198
L	-2	GLY	-	expression tag	UNP P05198
L	-1	SER	-	expression tag	UNP P05198
L	0	GLU	-	expression tag	UNP P05198
L	1	PHE	-	expression tag	UNP P05198
M	-34	MET	-	initiating methionine	UNP P05198
M	-33	GLY	-	expression tag	UNP P05198
M	-32	SER	-	expression tag	UNP P05198
M	-31	SER	-	expression tag	UNP P05198
M	-30	HIS	-	expression tag	UNP P05198
M	-29	HIS	-	expression tag	UNP P05198
M	-28	HIS	-	expression tag	UNP P05198
M	-27	HIS	-	expression tag	UNP P05198
M	-26	HIS	-	expression tag	UNP P05198
M	-25	HIS	-	expression tag	UNP P05198
M	-24	SER	-	expression tag	UNP P05198
M	-23	SER	-	expression tag	UNP P05198
M	-22	GLY	-	expression tag	UNP P05198
M	-21	LEU	-	expression tag	UNP P05198
M	-20	VAL	-	expression tag	UNP P05198
M	-19	PRO	-	expression tag	UNP P05198
M	-18	ARG	-	expression tag	UNP P05198
M	-17	GLY	-	expression tag	UNP P05198
M	-16	SER	-	expression tag	UNP P05198
M	-15	HIS	-	expression tag	UNP P05198
M	-14	MET	-	expression tag	UNP P05198
M	-13	ALA	-	expression tag	UNP P05198
M	-12	SER	-	expression tag	UNP P05198
M	-11	MET	-	expression tag	UNP P05198
M	-10	THR	-	expression tag	UNP P05198
M	-9	GLY	-	expression tag	UNP P05198
M	-8	GLY	-	expression tag	UNP P05198
M	-7	GLN	-	expression tag	UNP P05198
M	-6	GLN	-	expression tag	UNP P05198
M	-5	MET	-	expression tag	UNP P05198
M	-4	GLY	-	expression tag	UNP P05198

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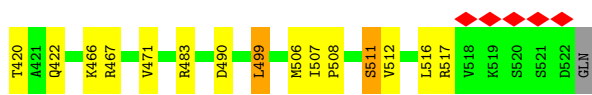
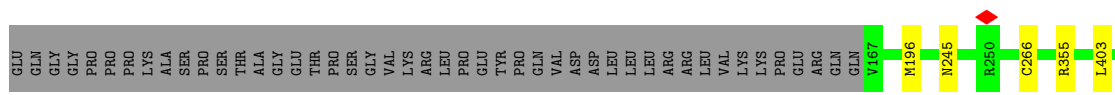
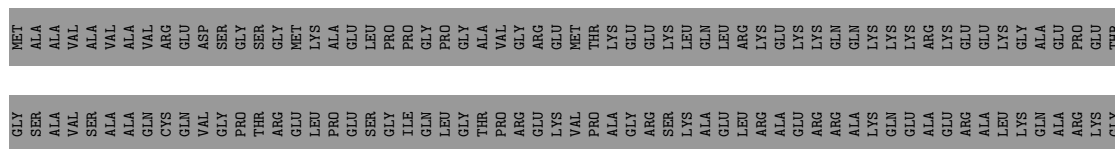
Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	ARG	-	expression tag	UNP P05198
M	-2	GLY	-	expression tag	UNP P05198
M	-1	SER	-	expression tag	UNP P05198
M	0	GLU	-	expression tag	UNP P05198
M	1	PHE	-	expression tag	UNP P05198

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

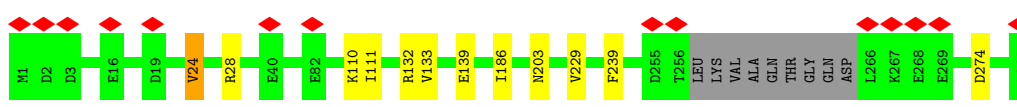
Mol	Chain	Residues	Atoms	AltConf
7	E	1	Total Cl 1 1	0
7	F	1	Total Cl 1 1	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

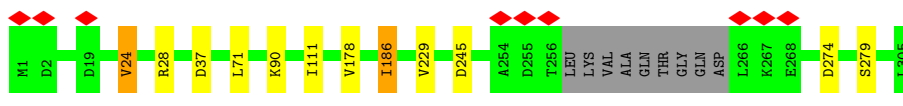
Mol	Chain	Residues	Atoms	AltConf
8	E	1	Total Zn 1 1	0
8	F	1	Total Zn 1 1	0



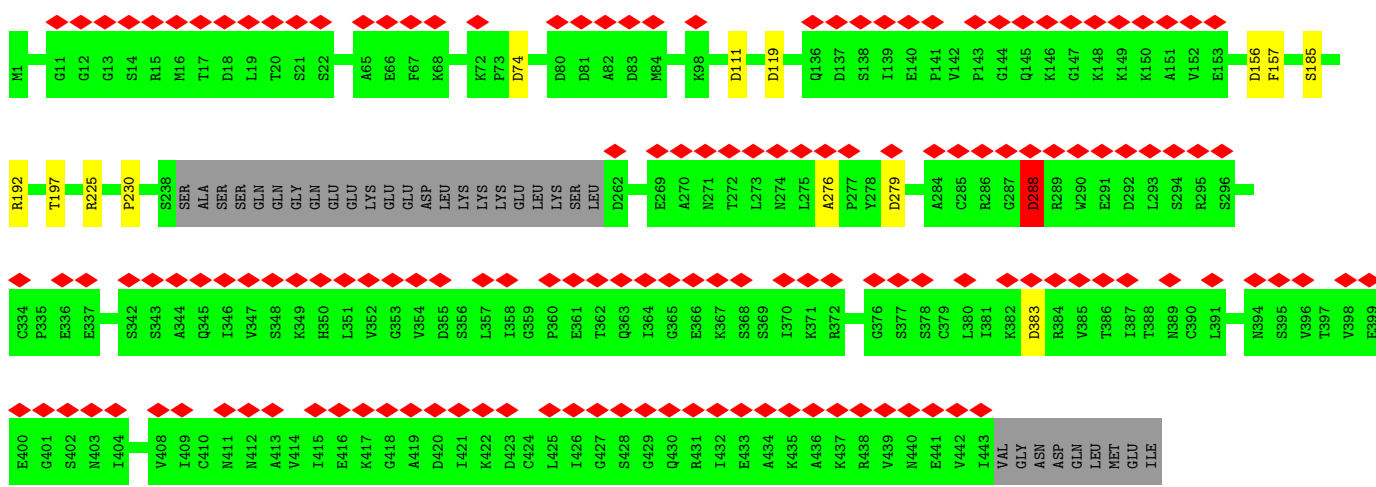
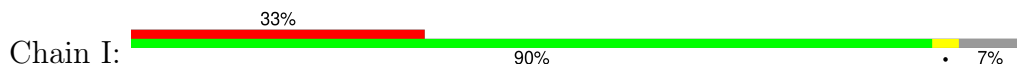
• Molecule 4: Translation initiation factor eIF-2B subunit alpha



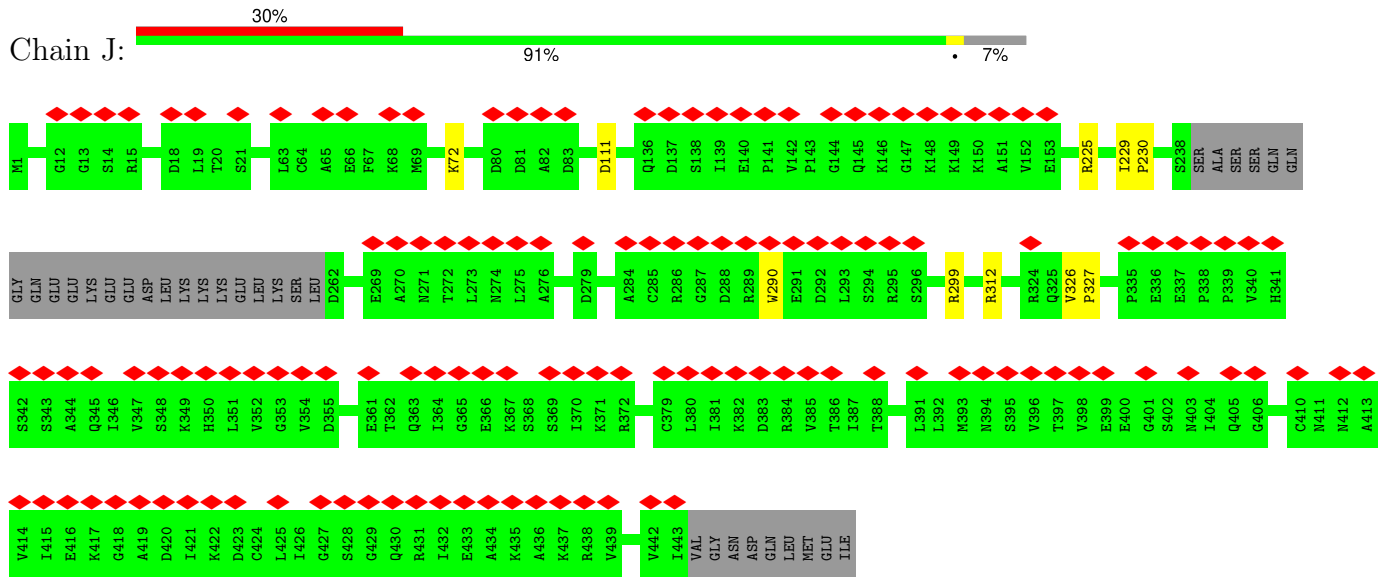
• Molecule 4: Translation initiation factor eIF-2B subunit alpha



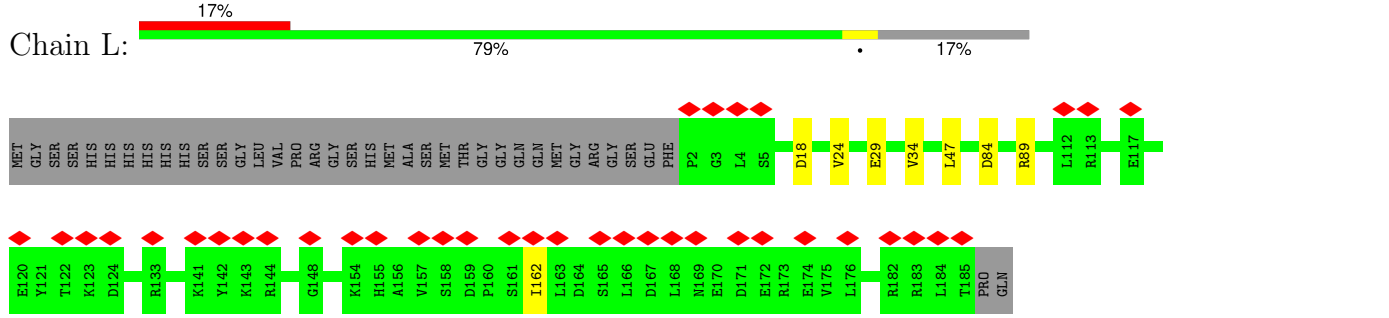
• Molecule 5: Translation initiation factor eIF-2B subunit gamma



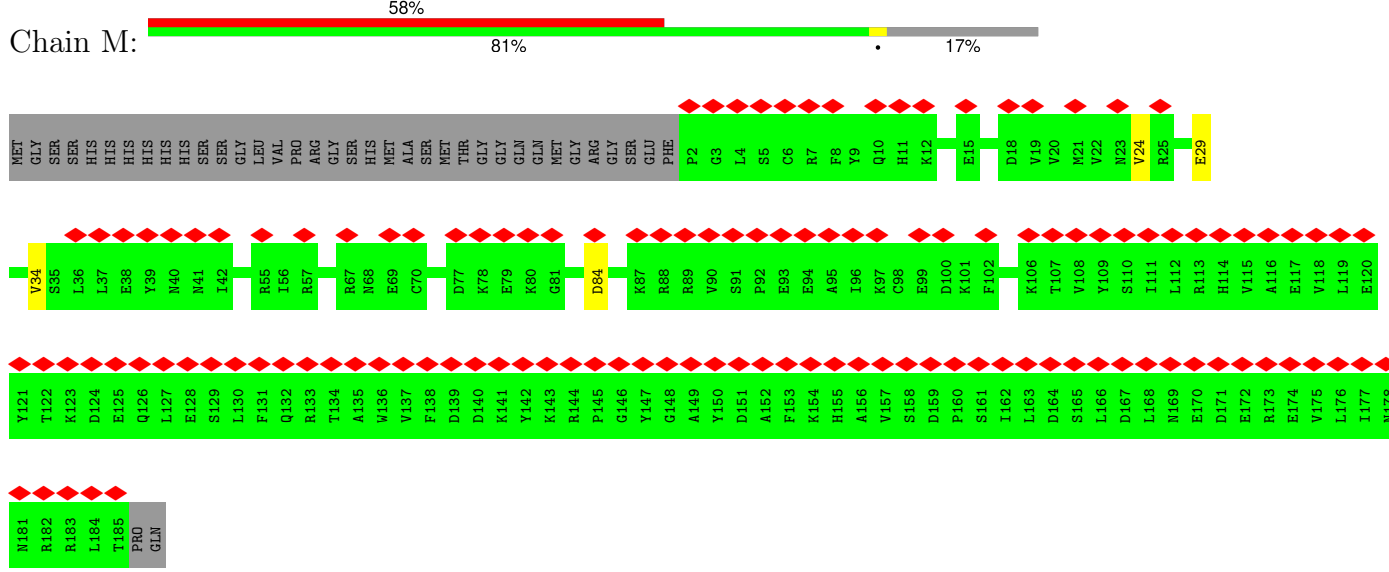
• Molecule 5: Translation initiation factor eIF-2B subunit gamma



• Molecule 6: Eukaryotic translation initiation factor 2 subunit 1



• Molecule 6: Eukaryotic translation initiation factor 2 subunit 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130953	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)	6000	Depositor
Maximum defocus (nm)	16000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.564	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	357.44, 357.44, 357.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8936, 0.8936, 0.8936	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.65	0/3497	1.07	3/4758 (0.1%)
1	B	0.65	0/3497	1.10	4/4758 (0.1%)
2	C	0.71	0/2572	1.21	11/3477 (0.3%)
2	D	0.71	0/2572	1.18	10/3477 (0.3%)
3	E	0.70	0/2822	1.13	7/3835 (0.2%)
3	F	0.72	0/2822	1.13	2/3835 (0.1%)
4	G	0.66	0/2338	1.11	4/3155 (0.1%)
4	H	0.67	0/2338	1.12	2/3155 (0.1%)
5	I	0.59	0/3310	1.00	5/4470 (0.1%)
5	J	0.58	0/3310	1.00	2/4470 (0.0%)
6	L	0.54	0/1527	1.10	4/2053 (0.2%)
6	M	0.53	0/1527	1.08	2/2053 (0.1%)
All	All	0.65	0/32132	1.10	56/43496 (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	8
1	B	0	3
2	C	0	4
2	D	0	3
3	E	0	5
3	F	0	5
4	G	0	1
5	I	0	2
5	J	0	4
All	All	0	35

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	317	PRO	CB-CA-C	-8.20	103.68	111.39
4	G	274	ASP	CA-CB-CG	7.02	119.62	112.60
4	G	110	LYS	CB-CA-C	-6.42	100.14	110.79
3	E	490	ASP	CA-CB-CG	6.41	119.01	112.60
3	F	490	ASP	CA-CB-CG	6.37	118.97	112.60
6	L	84	ASP	CA-CB-CG	6.31	118.91	112.60
6	M	84	ASP	CA-CB-CG	6.27	118.87	112.60
5	I	288	ASP	CA-CB-CG	6.21	118.81	112.60
3	E	431	ASN	CB-CA-C	6.17	120.02	111.63
1	A	53	ASP	CA-CB-CG	5.95	118.55	112.60
5	J	72	LYS	CB-CA-C	5.93	118.05	110.34
2	D	48	ASP	CA-CB-CG	5.93	118.53	112.60
6	L	29	GLU	CB-CA-C	-5.87	101.00	110.74
2	D	282	GLU	CB-CG-CD	5.74	122.36	112.60
2	C	160	HIS	CA-CB-CG	-5.64	108.16	113.80
2	D	213	GLU	CB-CA-C	5.62	118.69	110.26
2	D	340	MET	CG-SD-CE	5.58	113.19	100.90
2	C	282	GLU	CB-CA-C	5.58	118.42	109.27
3	E	487	LEU	N-CA-CB	-5.56	102.16	110.17
2	C	259	LYS	CB-CA-C	-5.53	100.40	110.63
1	B	271	ASP	CA-CB-CG	5.51	118.11	112.60
3	E	446	ARG	N-CA-CB	-5.46	101.95	109.97
6	M	29	GLU	CB-CA-C	-5.45	102.09	110.81
2	C	237	LYS	N-CA-C	-5.41	104.80	111.40
2	C	13	GLU	CB-CA-C	-5.41	101.49	110.68
1	B	199	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	392	ASP	CA-CB-CG	5.39	117.99	112.60
2	C	197	PHE	CA-CB-CG	-5.35	108.45	113.80
2	D	84	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	B	392	ASP	CB-CA-C	5.33	118.98	109.65
2	C	48	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	271	ASP	CA-CB-CG	5.32	117.92	112.60
2	D	160	HIS	CA-CB-CG	-5.24	108.56	113.80
3	F	422	GLN	N-CA-CB	-5.24	102.40	110.20
2	D	36	ARG	CB-CA-C	-5.23	102.11	110.79
5	I	383	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	53	ASP	CA-CB-CG	5.19	117.79	112.60
2	D	305	LYS	N-CA-CB	-5.18	103.70	110.59
4	G	110	LYS	N-CA-CB	5.18	117.73	110.12
3	E	172	ASP	CA-CB-CG	5.16	117.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	177	PHE	CA-CB-CG	5.16	118.96	113.80
2	C	338	ARG	CG-CD-NE	-5.16	100.65	112.00
3	E	351	THR	CA-CB-OG1	-5.15	101.87	109.60
4	H	245	ASP	CA-CB-CG	5.15	117.75	112.60
6	L	18	ASP	CA-CB-CG	5.13	117.73	112.60
2	C	202	GLU	CB-CA-C	-5.13	102.82	110.88
5	I	74	ASP	CA-CB-CG	5.11	117.71	112.60
4	H	274	ASP	CA-CB-CG	5.10	117.70	112.60
2	C	314	ASP	CA-CB-CG	5.09	117.69	112.60
5	I	111	ASP	CA-CB-CG	5.08	117.68	112.60
5	I	156	ASP	CA-CB-CG	5.08	117.67	112.60
5	J	111	ASP	CA-CB-CG	5.07	117.67	112.60
4	G	139	GLU	CB-CA-C	-5.02	102.15	110.68
3	E	378	HIS	CB-CA-C	5.01	119.36	110.85
2	C	294	VAL	N-CA-CB	-5.00	103.47	111.82
6	L	89	ARG	N-CA-CB	-5.00	102.94	111.20

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	175	GLU	Peptide
1	A	211	ARG	Sidechain
1	A	315	ARG	Sidechain
1	A	401	ARG	Sidechain
1	A	422	ARG	Sidechain
1	A	65	ARG	Sidechain
1	B	211	ARG	Sidechain
1	B	422	ARG	Sidechain
1	B	65	ARG	Sidechain
2	C	172	ARG	Sidechain
2	C	228	ARG	Sidechain
2	C	284	SER	Peptide
2	C	338	ARG	Sidechain
2	D	183	ARG	Sidechain
2	D	185	ARG	Sidechain
2	D	228	ARG	Sidechain
3	E	188	ARG	Sidechain
3	E	209	ARG	Sidechain
3	E	417	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	E	467	ARG	Sidechain
3	E	499	LEU	Peptide
3	F	266	CYS	Peptide
3	F	355	ARG	Sidechain
3	F	467	ARG	Sidechain
3	F	483	ARG	Sidechain
3	F	517	ARG	Sidechain
4	G	132	ARG	Sidechain
5	I	192	ARG	Sidechain
5	I	225	ARG	Sidechain
5	J	225	ARG	Sidechain
5	J	290	TRP	Peptide
5	J	299	ARG	Sidechain
5	J	312	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	3423	0	3419	11	0
1	B	3423	0	3419	11	0
2	C	2523	0	2527	9	0
2	D	2523	0	2527	9	0
3	E	2770	0	2829	12	0
3	F	2770	0	2830	5	0
4	G	2302	0	2378	5	0
4	H	2302	0	2378	4	0
5	I	3260	0	3357	4	0
5	J	3260	0	3357	2	0
6	L	1514	0	1526	1	0
6	M	1514	0	1526	1	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
All	All	31588	0	32073	66	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 (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:LEU:HB3	2:C:340:MET:HE1	1.68	0.74
1:A:66:VAL:HG13	1:A:76:ILE:HB	1.71	0.71
2:D:236:THR:HG21	2:D:245:LEU:HD22	1.71	0.71
1:B:66:VAL:HG13	1:B:76:ILE:HB	1.73	0.70
2:C:236:THR:HG21	2:C:245:LEU:HD22	1.77	0.67
2:C:303:LEU:O	1:B:315:ARG:NH1	2.34	0.60
3:E:499:LEU:HD23	4:G:239:PHE:CZ	2.40	0.57
3:E:402:LEU:HD11	3:E:437:CYS:SG	2.45	0.57
4:G:111:ILE:HG21	4:G:229:VAL:HG13	1.88	0.55
3:F:499:LEU:HD21	3:F:506:MET:HB3	1.87	0.55
1:A:47:LEU:C	1:A:47:LEU:HD23	2.34	0.53
1:B:47:LEU:C	1:B:47:LEU:HD23	2.35	0.52
3:E:467:ARG:NH1	2:D:293:GLU:OE1	2.43	0.52
4:H:37:ASP:O	4:H:90:LYS:NZ	2.41	0.51
1:B:66:VAL:CG1	1:B:76:ILE:HB	2.38	0.51
4:G:133:VAL:HG22	4:G:229:VAL:CG1	2.41	0.50
2:D:271:MET:HA	2:D:271:MET:HE2	1.93	0.50
2:C:297:PHE:CD2	1:B:186:LYS:HE3	2.47	0.49
2:C:274:LEU:HB3	2:C:340:MET:CE	2.39	0.49
1:B:394:THR:HG22	1:B:396:LEU:CD1	2.42	0.49
2:C:239:ILE:HD11	2:C:269:ALA:HB1	1.95	0.49
3:E:371:HIS:CD2	5:I:288:ASP:HB3	2.49	0.48
5:I:276:ALA:HB1	5:I:279:ASP:OD2	2.13	0.48
1:B:156:ILE:HG13	1:B:309:VAL:HG11	1.95	0.47
4:H:178:VAL:HG11	4:H:186:ILE:HG13	1.97	0.47
3:E:269:LEU:HD22	3:E:273:MET:HE2	1.96	0.47
4:H:111:ILE:HG21	4:H:229:VAL:HG13	1.97	0.47
5:J:229:ILE:HB	5:J:230:PRO:HD3	1.96	0.46
2:C:271:MET:HE2	2:C:271:MET:HA	1.97	0.46
3:E:395:LEU:N	3:E:396:PRO:HD2	2.31	0.45
3:E:388:ILE:N	3:E:389:PRO:CD	2.79	0.45
1:A:432:THR:HG22	1:A:433:SER:H	1.81	0.45
3:F:512:VAL:HG13	3:F:516:LEU:HD22	1.98	0.45
1:A:186:LYS:HE3	2:D:297:PHE:CD2	2.53	0.44
3:E:449:THR:O	3:E:450:ASP:HB3	2.17	0.44
1:A:338:SER:HA	2:D:283:ASP:HB3	1.99	0.44
3:F:403:LEU:HD13	3:F:420:THR:HG23	1.99	0.44
1:B:161:ILE:HD13	1:B:161:ILE:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:CG	1:A:193:PRO:HD2	2.53	0.43
2:C:175:GLU:HG2	2:C:179:LYS:HD3	2.00	0.43
3:F:466:LYS:HA	3:F:471:VAL:HG22	2.02	0.42
4:H:24:VAL:O	4:H:28:ARG:HB2	2.19	0.42
3:E:257:LYS:HB2	3:E:258:PRO:HD3	2.02	0.42
1:B:56:PHE:CE1	1:B:65:ARG:HD2	2.54	0.42
1:A:161:ILE:HD13	1:A:161:ILE:HA	1.83	0.42
6:M:24:VAL:HA	6:M:34:VAL:HG12	2.02	0.42
2:C:62:ARG:NH2	2:C:351:LEU:O	2.52	0.42
1:A:396:LEU:HG	1:A:400:VAL:HG11	2.01	0.41
2:D:326:SER:C	2:D:328:ILE:H	2.28	0.41
5:J:326:VAL:N	5:J:327:PRO:CD	2.82	0.41
2:D:197:PHE:HZ	2:D:289:VAL:HG21	1.86	0.41
3:E:335:VAL:HG11	3:E:346:LEU:HD11	2.02	0.41
6:L:24:VAL:HA	6:L:34:VAL:HG12	2.02	0.41
1:A:178:VAL:HG13	1:A:284:GLY:O	2.21	0.41
1:B:276:LEU:C	1:B:276:LEU:HD23	2.46	0.41
2:D:236:THR:CG2	2:D:245:LEU:HD13	2.51	0.41
1:A:409:HIS:O	1:A:410:GLN:C	2.63	0.41
1:B:432:THR:HG22	1:B:433:SER:H	1.85	0.41
1:A:362:LEU:CD2	1:A:379:ILE:HD12	2.51	0.41
3:F:508:PRO:HG2	3:F:511:SER:HB3	2.03	0.41
4:G:24:VAL:O	4:G:28:ARG:HB2	2.20	0.40
3:E:193:THR:HG21	5:I:119:ASP:OD2	2.21	0.40
3:E:435:LEU:HD12	3:E:435:LEU:N	2.36	0.40
5:I:157:PHE:CD1	5:I:197:THR:HG22	2.56	0.40
2:D:173:THR:HG22	2:D:268:CYS:HB3	2.04	0.40
4:G:203:ASN:HB3	4:G:239:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/721 (60%)	418 (96%)	15 (4%)	0	100	100
1	B	433/721 (60%)	417 (96%)	16 (4%)	0	100	100
2	C	318/368 (86%)	310 (98%)	7 (2%)	1 (0%)	36	68
2	D	318/368 (86%)	312 (98%)	6 (2%)	0	100	100
3	E	354/523 (68%)	347 (98%)	7 (2%)	0	100	100
3	F	354/523 (68%)	350 (99%)	4 (1%)	0	100	100
4	G	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
4	H	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
5	I	416/452 (92%)	386 (93%)	30 (7%)	0	100	100
5	J	416/452 (92%)	394 (95%)	22 (5%)	0	100	100
6	L	181/222 (82%)	175 (97%)	6 (3%)	0	100	100
6	M	181/222 (82%)	175 (97%)	6 (3%)	0	100	100
All	All	3988/5182 (77%)	3856 (97%)	131 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	194	CYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/626 (61%)	378 (98%)	6 (2%)	55	78
1	B	384/626 (61%)	379 (99%)	5 (1%)	61	80
2	C	274/312 (88%)	269 (98%)	5 (2%)	51	76
2	D	274/312 (88%)	273 (100%)	1 (0%)	84	89
3	E	312/444 (70%)	305 (98%)	7 (2%)	45	73
3	F	312/444 (70%)	307 (98%)	5 (2%)	55	78
4	G	253/260 (97%)	251 (99%)	2 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	253/260 (97%)	249 (98%)	4 (2%)	55	78
5	I	369/398 (93%)	366 (99%)	3 (1%)	73	85
5	J	369/398 (93%)	369 (100%)	0	100	100
6	L	168/198 (85%)	166 (99%)	2 (1%)	63	81
6	M	168/198 (85%)	168 (100%)	0	100	100
All	All	3520/4476 (79%)	3480 (99%)	40 (1%)	63	82

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	161	ILE
1	A	180	VAL
1	A	294	LYS
1	A	318	VAL
1	A	401	ARG
2	C	139	GLU
2	C	142	VAL
2	C	161	SER
2	C	277	GLN
2	C	281	GLU
3	E	178	SER
3	E	188	ARG
3	E	209	ARG
3	E	258	PRO
3	E	386	LEU
3	E	462	ASP
3	E	512	VAL
4	G	24	VAL
4	G	186	ILE
5	I	185	SER
5	I	230	PRO
5	I	288	ASP
1	B	151	VAL
1	B	161	ILE
1	B	180	VAL
1	B	189	SER
1	B	258	GLN
2	D	29	ARG
3	F	196	MET

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Mol	Chain	Res	Type
3	F	245	ASN
3	F	499	LEU
3	F	507	ILE
3	F	511	SER
4	H	24	VAL
4	H	71	LEU
4	H	186	ILE
4	H	279	SER
6	L	47	LEU
6	L	162	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	GLN
1	A	352	HIS
1	A	398	GLN
2	C	160	HIS
3	E	235	GLN
3	E	347	GLN
3	E	470	HIS
3	E	477	GLN
5	I	363	GLN
1	B	160	ASN
1	B	216	GLN
1	B	393	GLN
1	B	398	GLN
2	D	160	HIS
4	H	208	ASN
5	J	271	ASN
5	J	297	GLN
5	J	363	GLN
6	L	23	ASN
6	L	41	ASN
6	M	23	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SEP	M	52	6	8,9,10	0.61	0	7,12,14	0.80	0
6	SEP	L	52	6	8,9,10	0.58	0	7,12,14	0.84	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
6	SEP	M	52	6	-	1/6/8/10	-
6	SEP	L	52	6	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	52	SEP	CB-OG-P-O1P
6	M	52	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

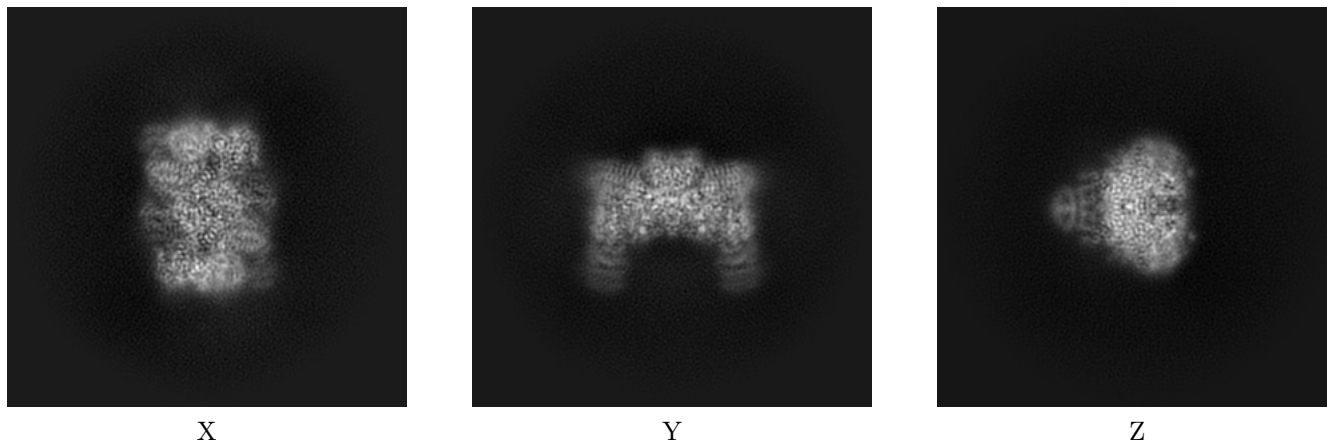
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72520. These allow visual inspection of the internal detail of the map and identification of artifacts.

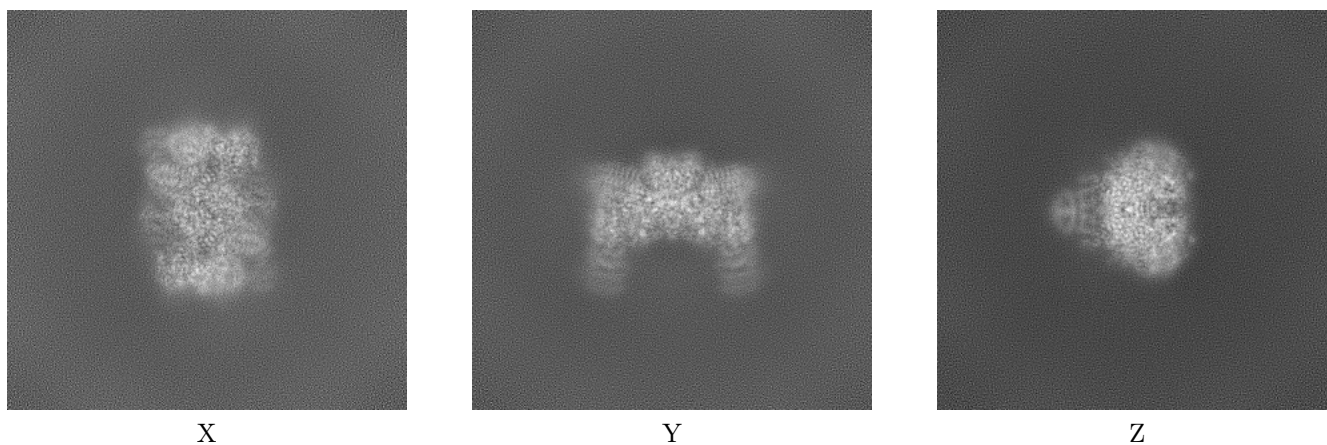
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



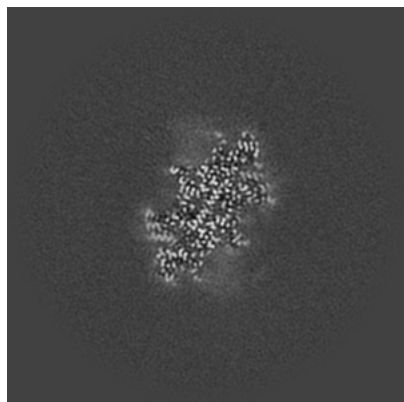
6.1.2 Raw map



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

6.2 Central slices [i](#)

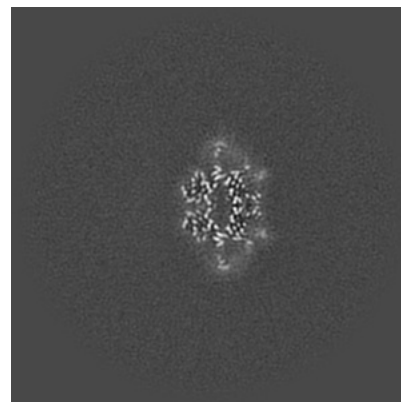
6.2.1 Primary map



X Index: 200

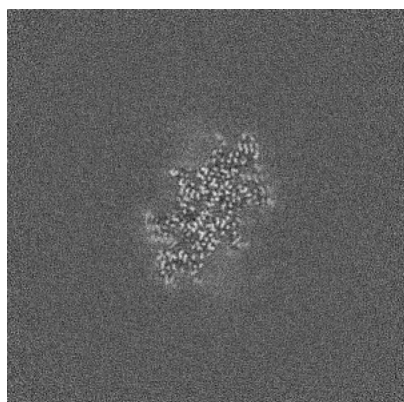


Y Index: 200

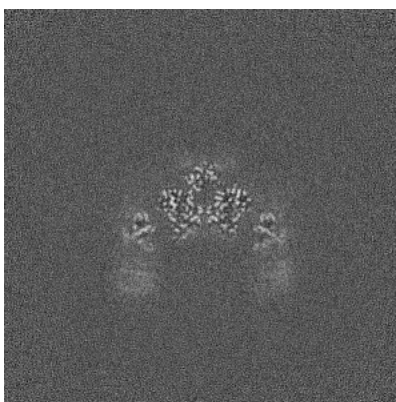


Z Index: 200

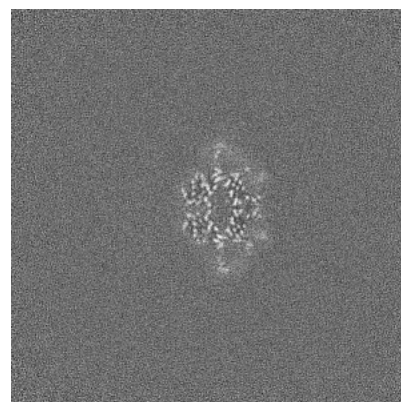
6.2.2 Raw map



X Index: 200



Y Index: 200

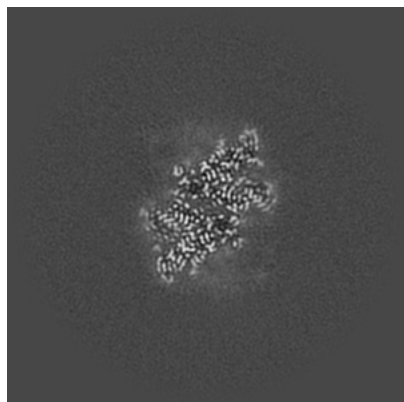


Z Index: 200

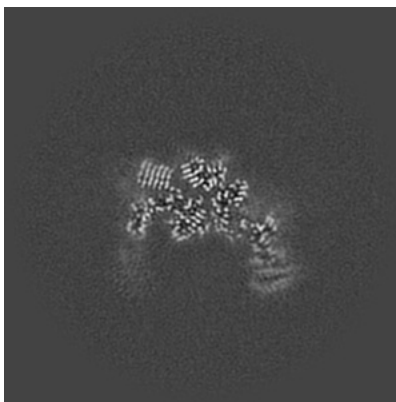
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

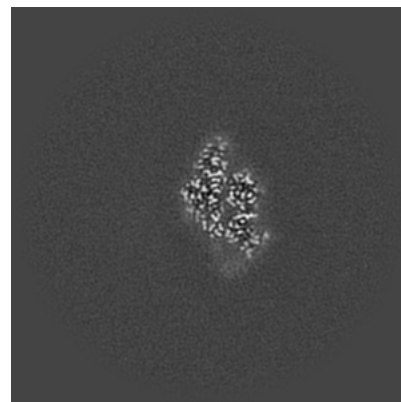
6.3.1 Primary map



X Index: 204

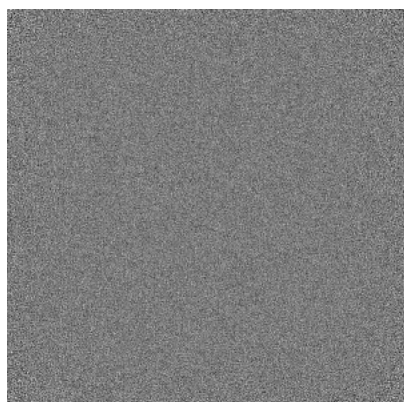


Y Index: 189

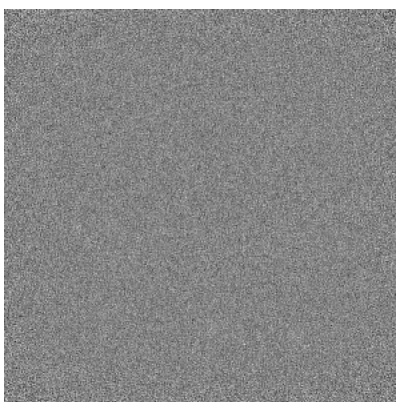


Z Index: 210

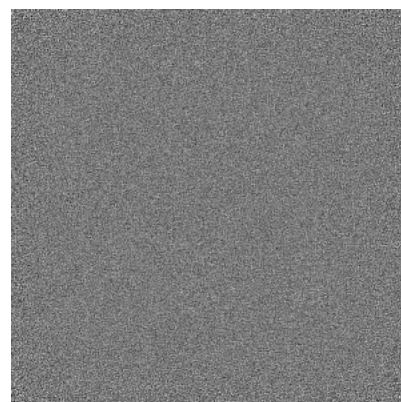
6.3.2 Raw map



X Index: 0



Y Index: 0

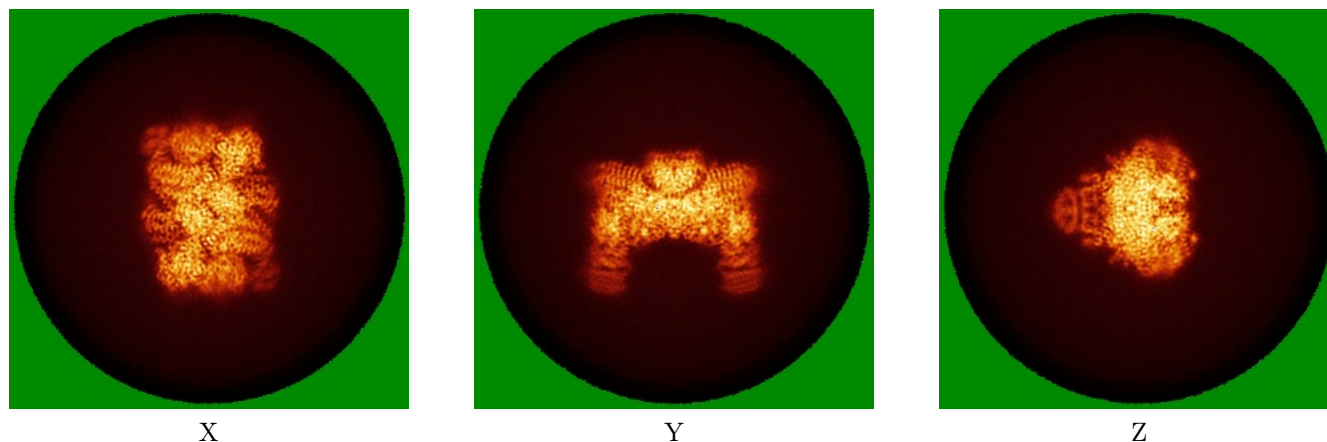


Z Index: 0

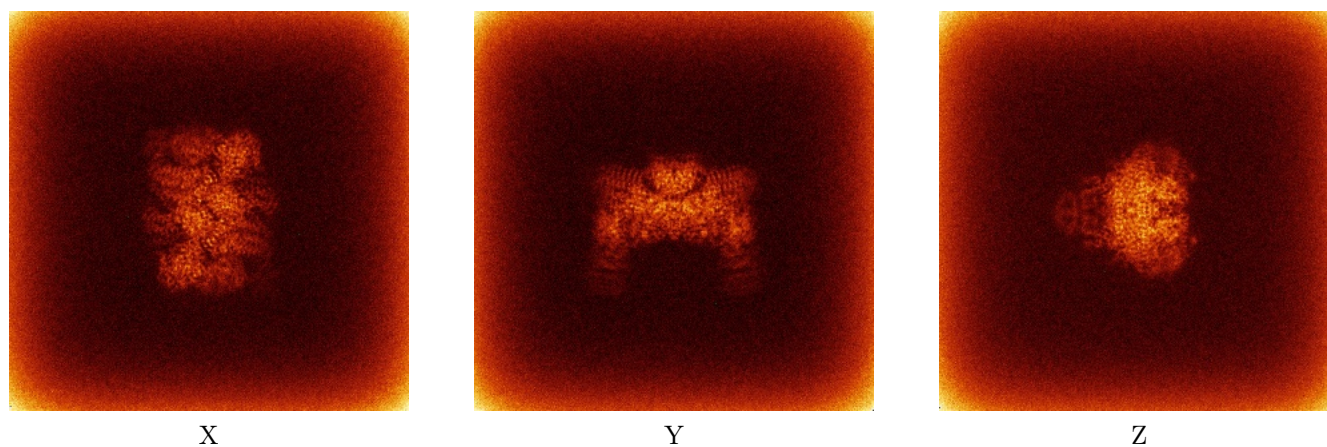
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

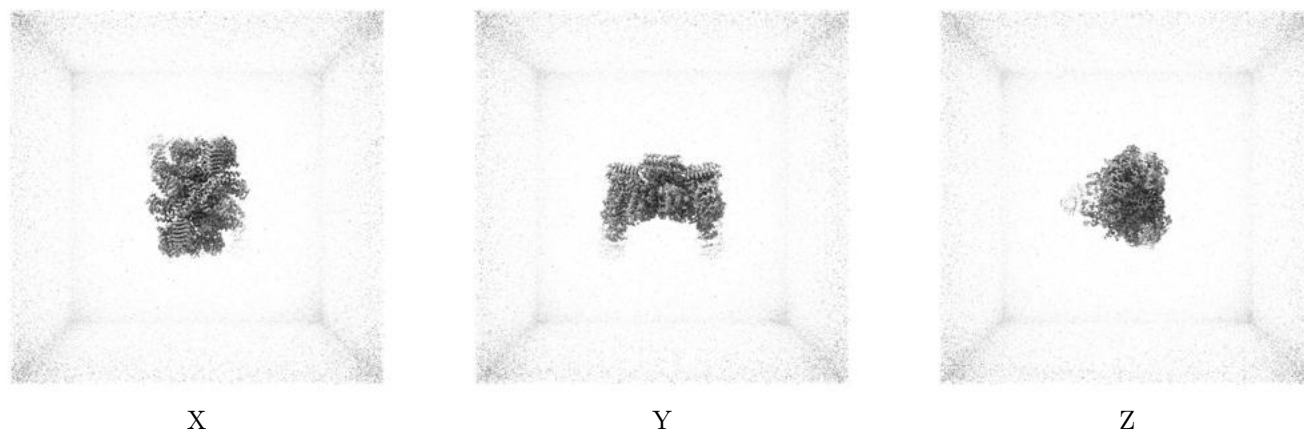
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

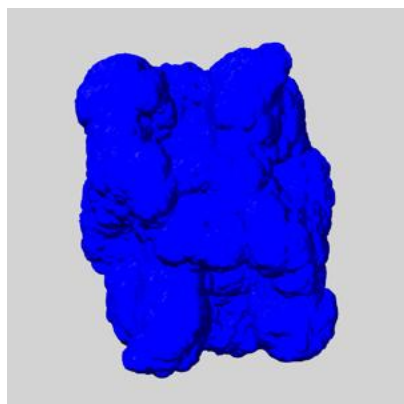
6.6 Mask visualisation [i](#)

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

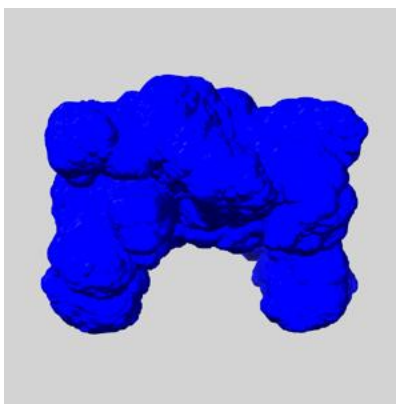
A mask typically either:

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

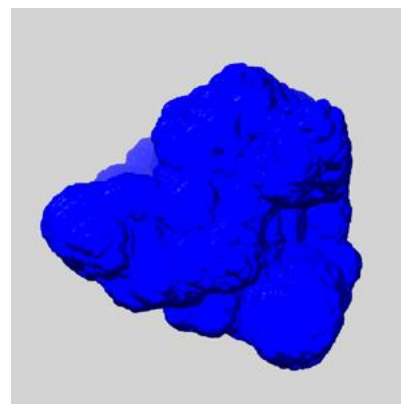
6.6.1 emd_72520_msk_1.map [i](#)



X



Y

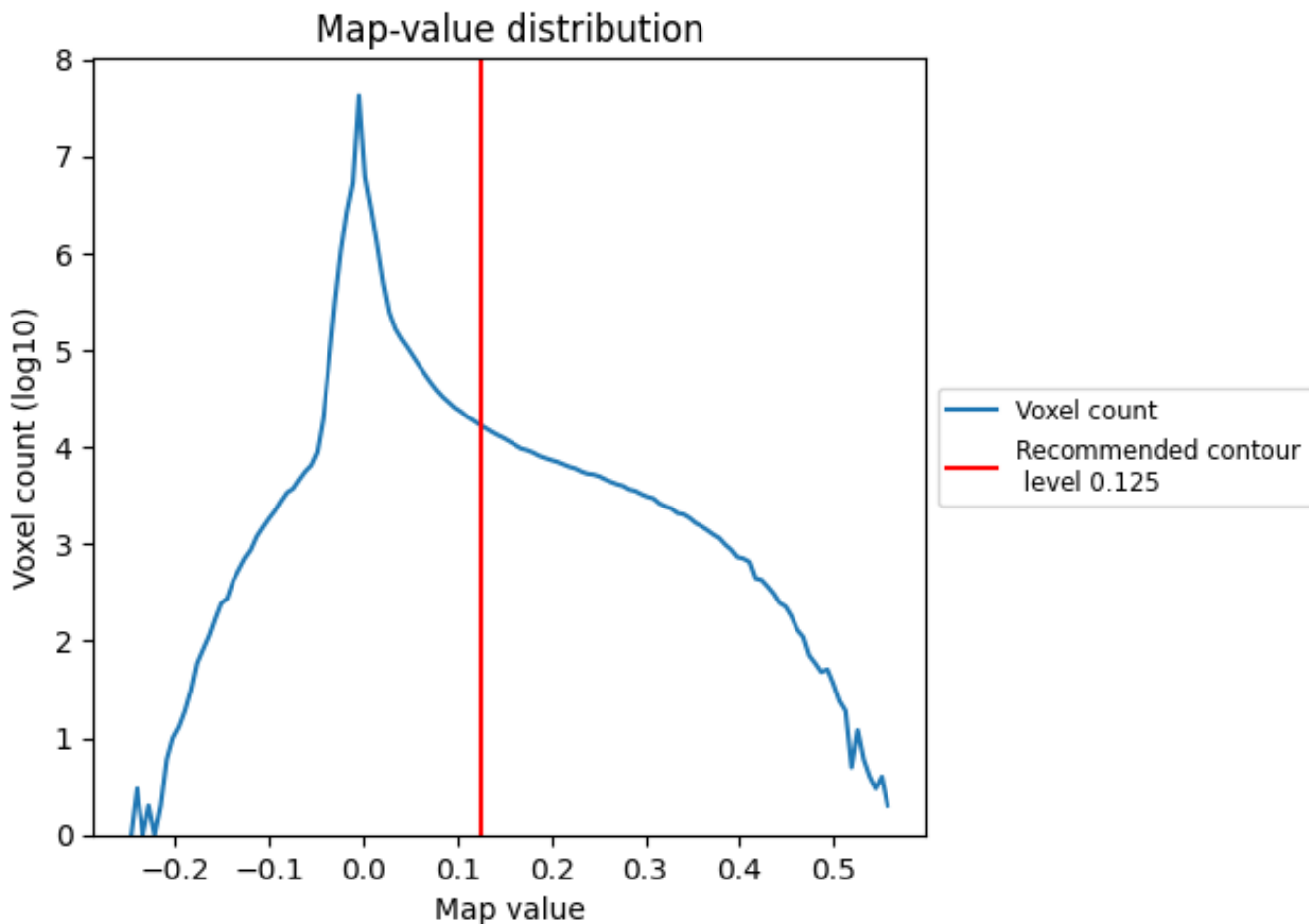


Z

7 Map analysis [i](#)

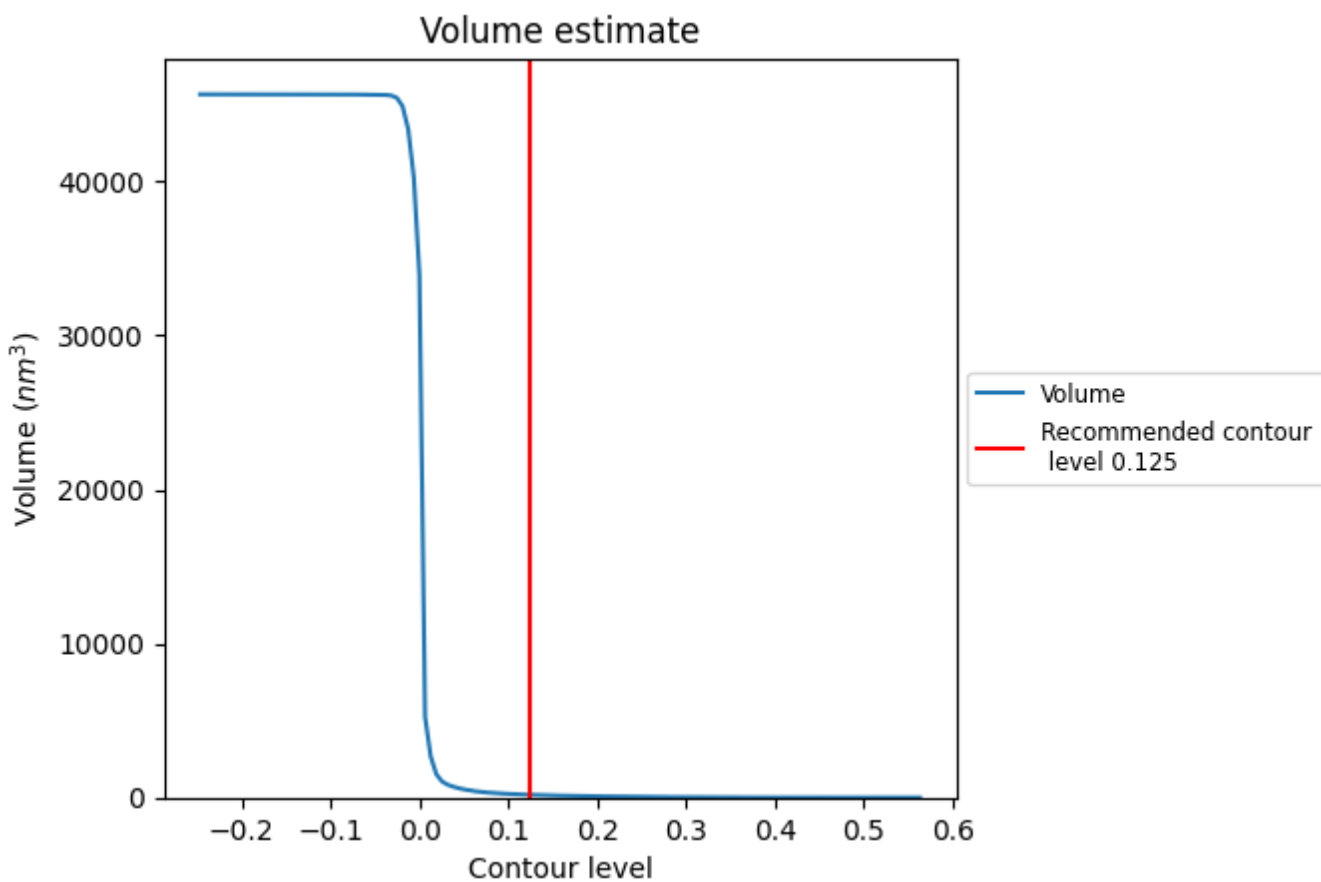
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

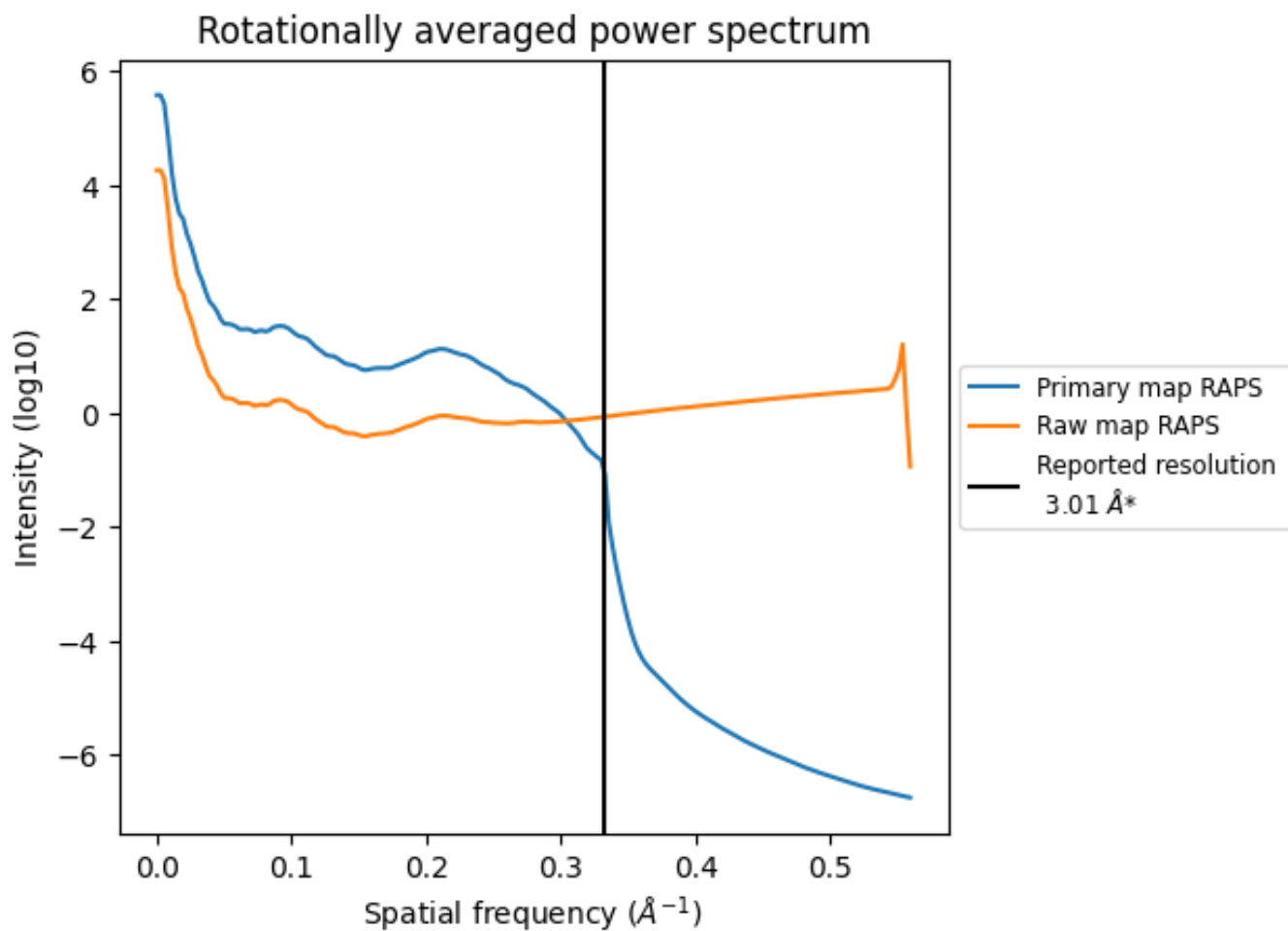
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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](#)

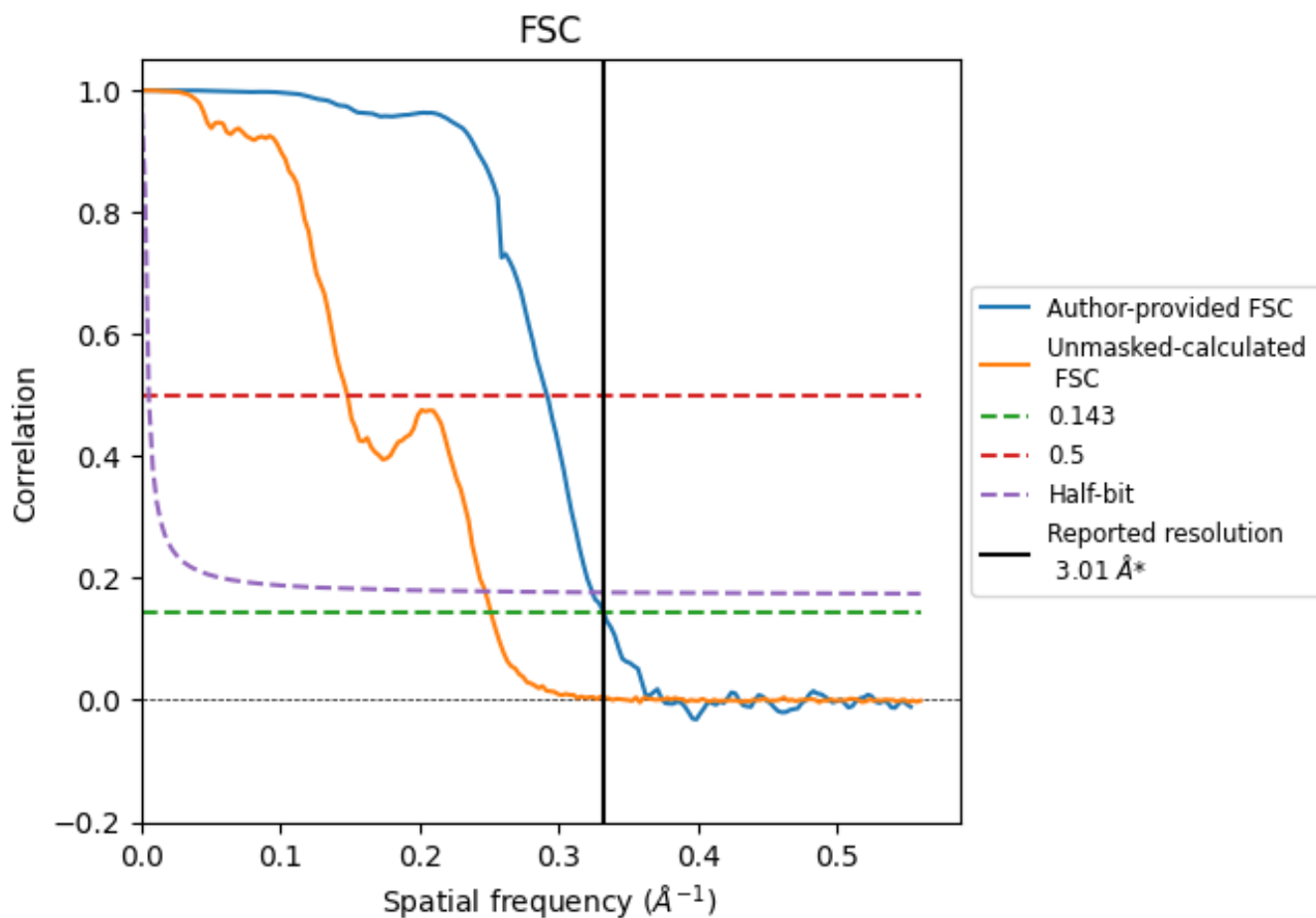


*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

8.2 Resolution estimates [i](#)

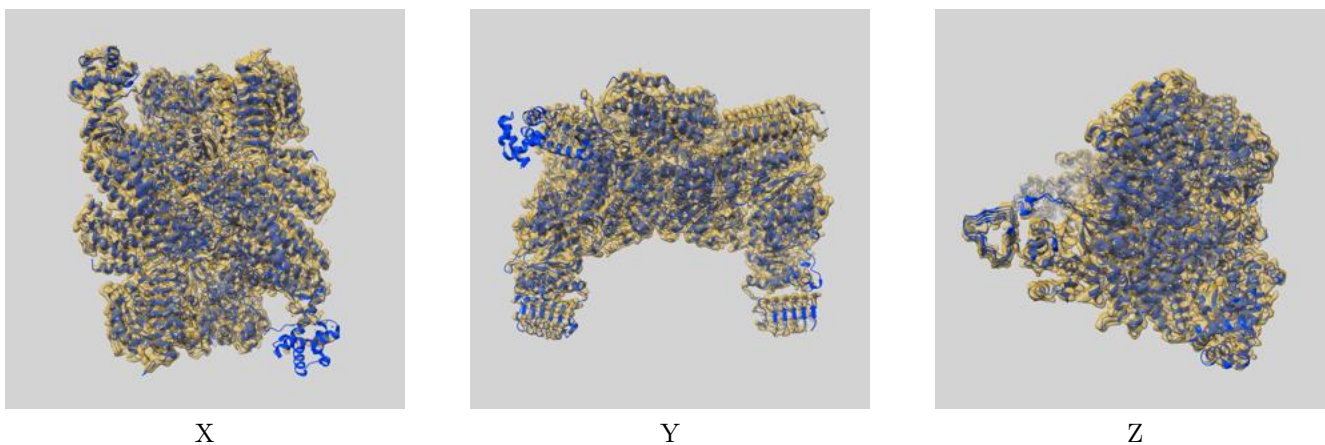
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.43	3.09
Unmasked-calculated*	3.98	6.76	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.01 by more than 10 %

9 Map-model fit [i](#)

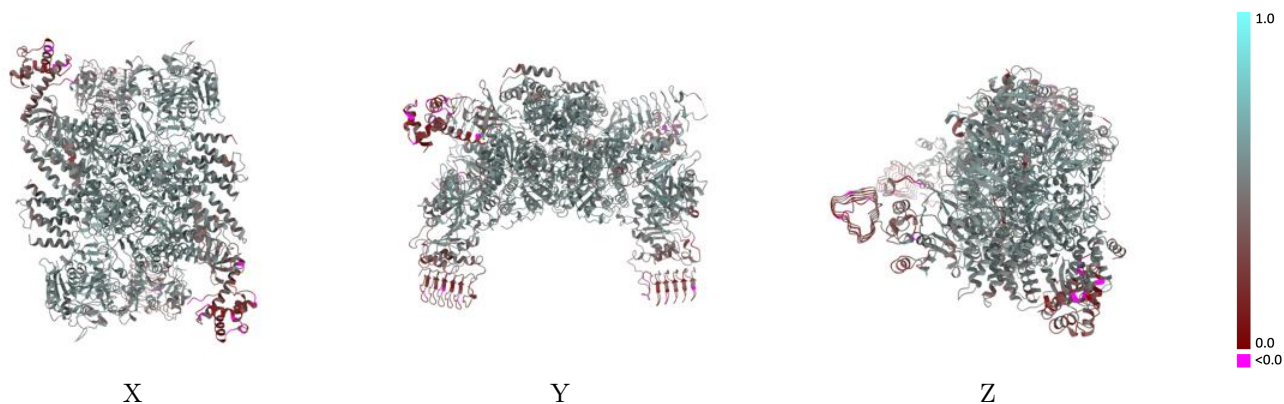
This section contains information regarding the fit between EMDB map EMD-72520 and PDB model 9Y5R. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



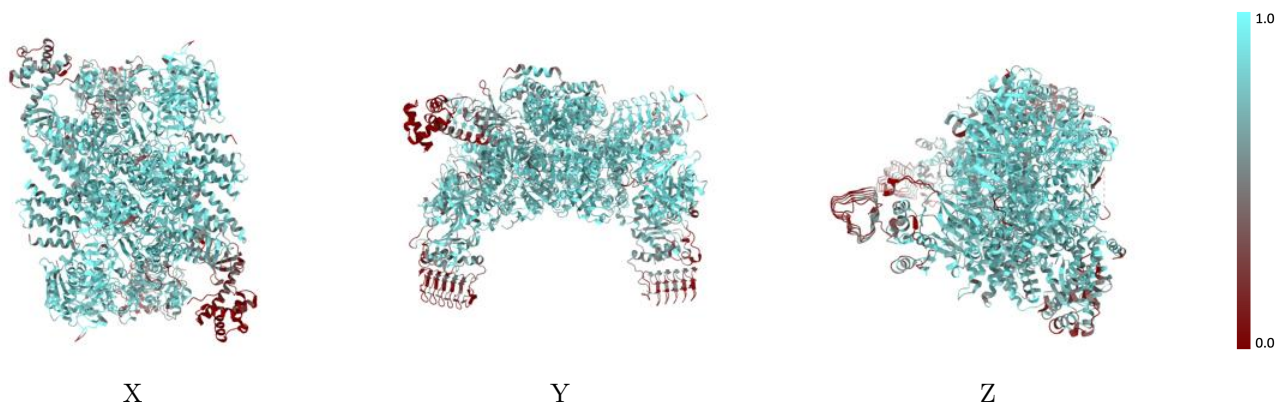
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



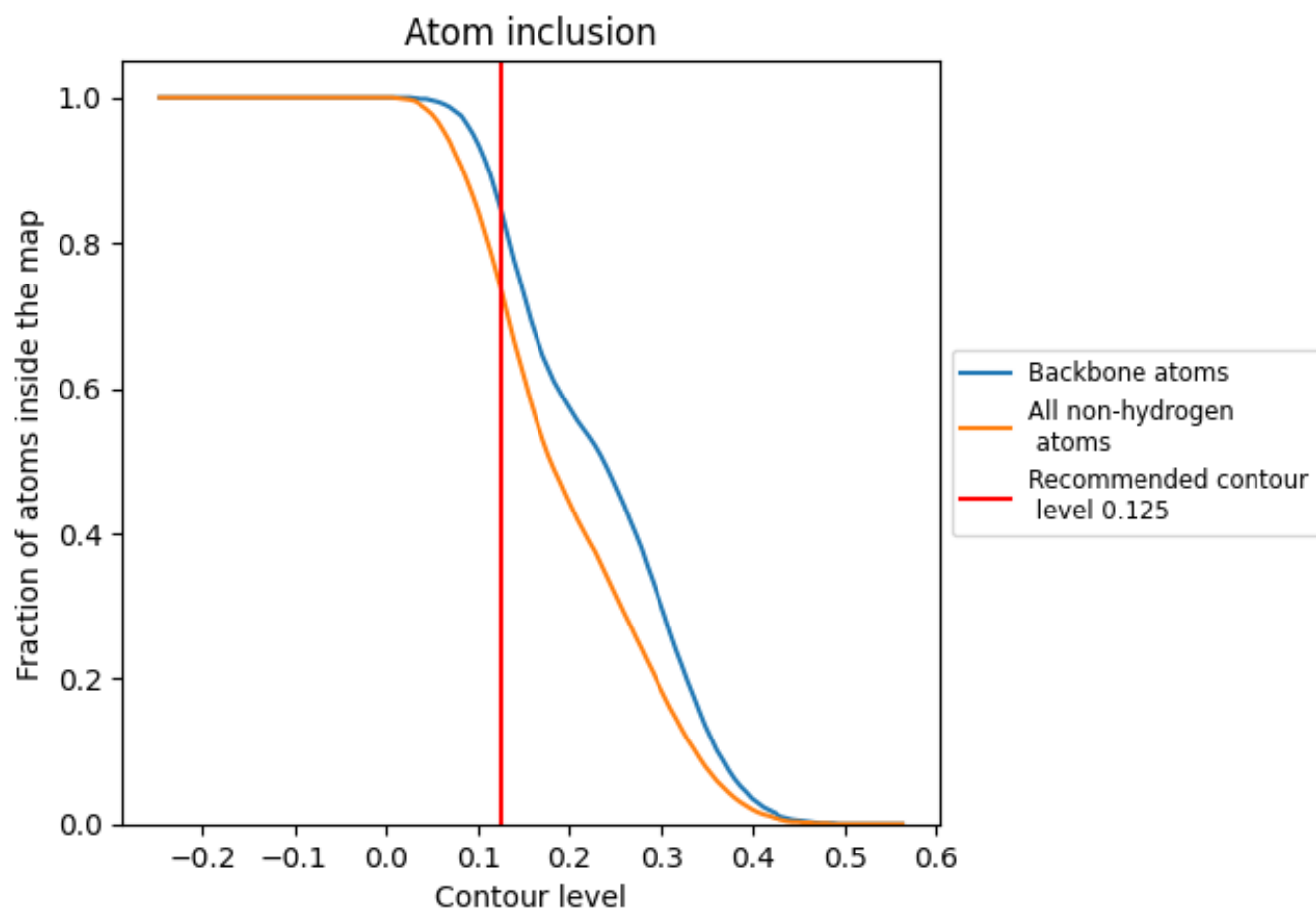
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.125).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.4890
A	 0.8330	 0.5340
B	 0.8430	 0.5330
C	 0.8490	 0.5310
D	 0.8420	 0.5290
E	 0.8450	 0.5450
F	 0.8440	 0.5440
G	 0.8050	 0.5240
H	 0.8260	 0.5280
I	 0.5340	 0.4030
J	 0.5580	 0.4080
L	 0.5950	 0.3700
M	 0.2460	 0.3060

