



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 01:23 pm BST

PDB ID : 6QG0
EMDB ID : EMD-4543
Title : Structure of eIF2B-eIF2 (phosphorylated at Ser51) complex (model 1)
Authors : Llacer, J.L.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2019-01-10
Resolution : 4.15 Å(reported)

This is a wwPDB EM Validation Summary 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

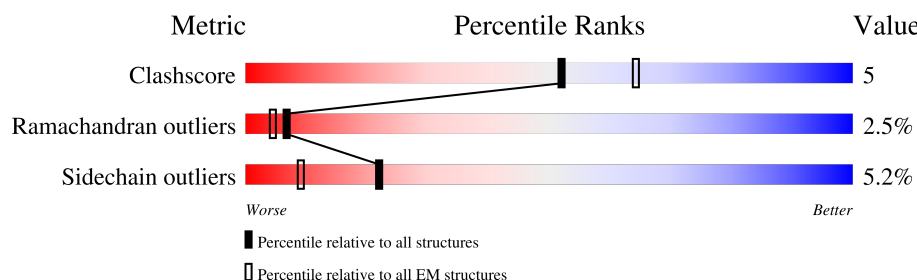
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.15 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	305	<div> <div>37%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
1	B	305	<div> <div>38%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>
2	C	381	<div> <div>19%</div> <div>73%</div> <div>16%</div> <div>• 9%</div> </div>
2	D	381	<div> <div>19%</div> <div>74%</div> <div>15%</div> <div>• 9%</div> </div>
3	E	578	<div> <div>35%</div> <div>41%</div> <div>5%</div> <div>• 54%</div> </div>
3	F	578	<div> <div>35%</div> <div>42%</div> <div>• • 54%</div> </div>
4	G	651	<div> <div>12%</div> <div>43%</div> <div>10%</div> <div>• 45%</div> </div>
4	H	651	<div> <div>12%</div> <div>43%</div> <div>10%</div> <div>• 45%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	712	
5	J	712	
6	K	304	
6	L	304	
7	M	527	
7	N	527	
8	O	285	
8	P	285	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36980 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	302	Total	C	N	O	S	0	0
			2351	1504	394	443	10		
1	B	302	Total	C	N	O	S	0	0
			2351	1504	394	443	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	345	Total	C	N	O	S	0	0
			2665	1694	463	502	6		
2	C	345	Total	C	N	O	S	0	0
			2665	1694	463	502	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	267	Total	C	N	O	S	0	0
			2164	1391	363	400	10		
3	F	267	Total	C	N	O	S	0	0
			2164	1391	363	400	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	355	Total	C	N	O	S	0	0
			2744	1738	474	521	11		
4	H	355	Total	C	N	O	S	0	0
			2744	1738	474	521	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	431	Total	C	N	O	S	0	0
			3406	2147	573	666	20		
5	J	431	Total	C	N	O	S	0	0
			3406	2147	573	666	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	246	Total	C	N	O	P S	0	0
			1973	1259	324	381	1 8		
6	K	246	Total	C	N	O	P S	0	0
			1973	1259	324	381	1 8		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	408	Total	C	N	O	S	0	0
			3044	1934	546	548	16		
7	N	408	Total	C	N	O	S	0	0
			3044	1934	546	548	16		

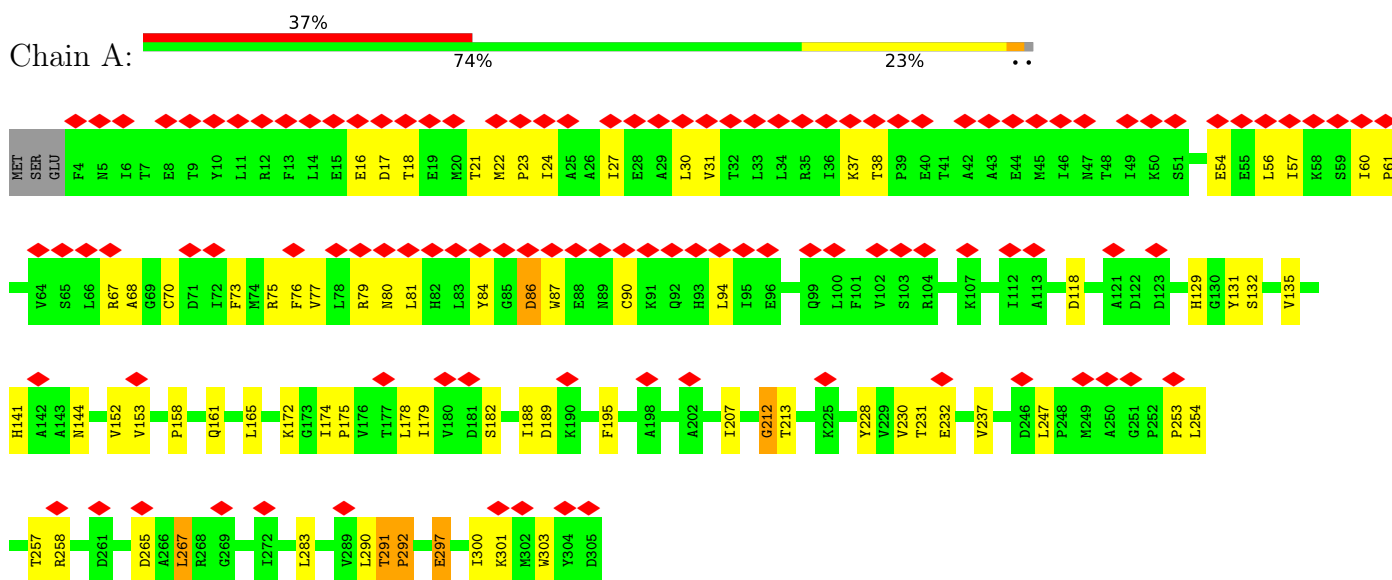
- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	17	Total	C	N	O	0	0
			143	96	24	23		
8	P	17	Total	C	N	O	0	0
			143	96	24	23		

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.

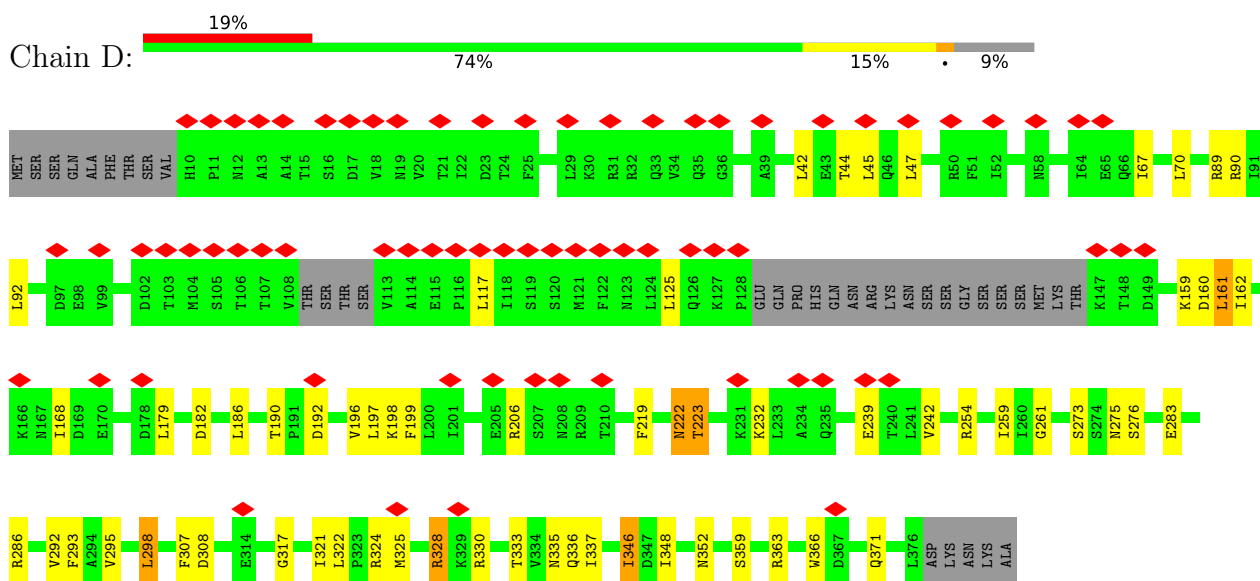
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



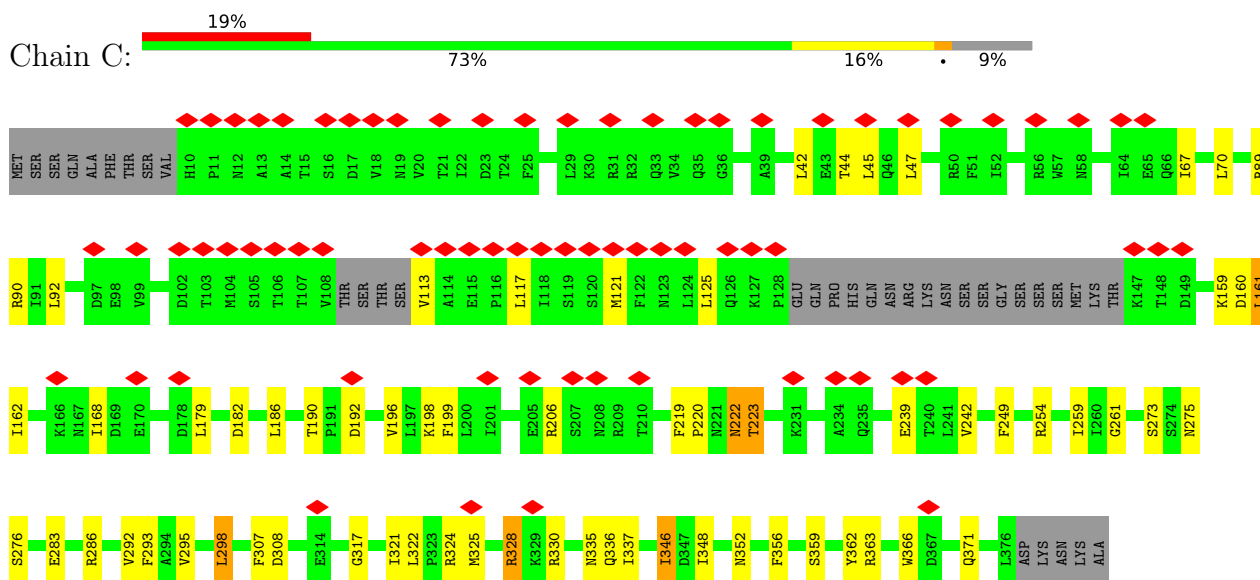
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



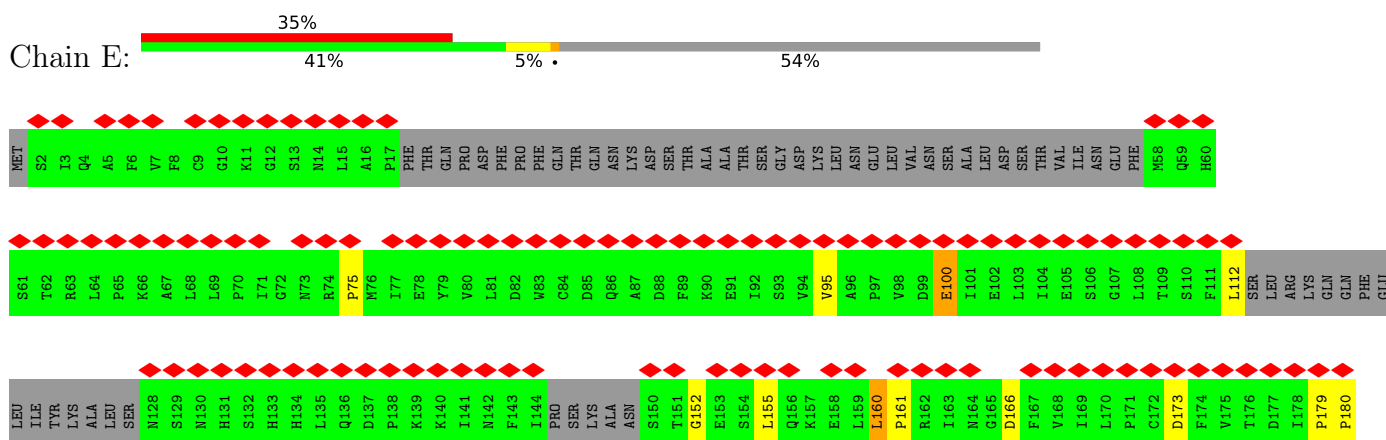
- Molecule 2: Translation initiation factor eIF-2B subunit beta



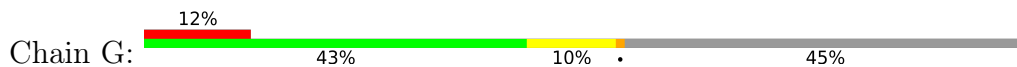
- Molecule 2: Translation initiation factor eIF-2B subunit beta



- Molecule 3: Translation initiation factor eIF-2B subunit gamma



- Molecule 4: Translation initiation factor eIF-2B subunit delta

[illegible]

THR	THR	THR	THR	LEU	PRO	ALA	SER	SER	ALA	LEU	SER	ALA	GLY	THR	SER	SER	ALA	SER	THR	ASN	THR	PRO	THR	ALA	ALA	ILE	GLN	GLN	GLU	ILE	ALA	SER	SER	ASN	ALA	SER	ASP	VAL	ALA	LYS	LEU	THR	ALA	SER	ILE	SER	LEU	GLU	ALA	GLY	GLU	PHE	ASN	VAL	ILE	P237	G238	T239	S240
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S241	V242	P243	P244	T245	V246	L247	E248	Q249	S250	N253	S254	S255	L256	I257	SER	S259	V260	K261	E262	L263	L264	L265	N266	K267	D268	L269	L276	S279	Y284	K285	L286	V287	G288	S289	L290	P291	R292	C293	L294	A295	N296	I302	D306	K311	G312	R317	S324	D328
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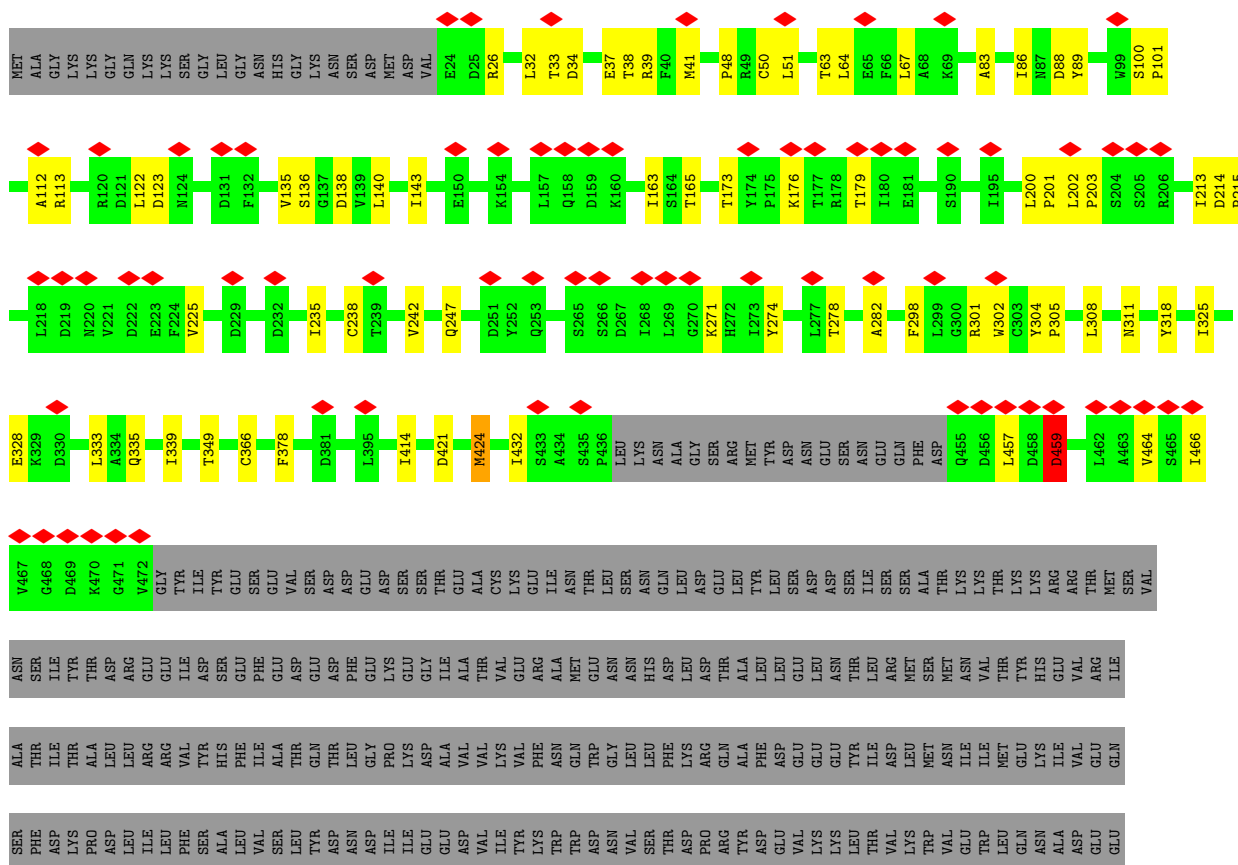
Keyword	Publications
K332	100
A333	95
M340	90
R345	85
W346	80
L347	75
K348	70
I351	65
K361	60
D366	55
Q373	50
E377	45
A382	40
R383	35
Q384	30
L385	25
I386	20
I387	15
D388	10
S397	5
T398	5
V401	5
T410	5
F411	5
L412	5
L413	5
L414	5
H415	5
N416	5
I424	5
I427	5
S431	5
F435	5
M440	5
M452	5
L455	5
I456	5
L459	5
D460	5
T461	5
L462	5

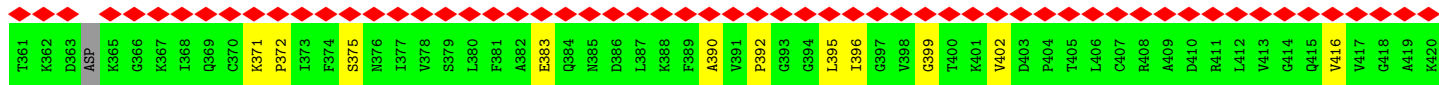
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N464
MET
D466
L472
L478
F482
L483
A487
M494
R498
IS01
PS02
VS05
ES08
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V516
Q517
V521
T522
F523
N524
ES25
L526
A527
D528
PS29
N530
D531
L532
V533
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E542
R543
R544
G545
N546
K547
G548
L551
N552

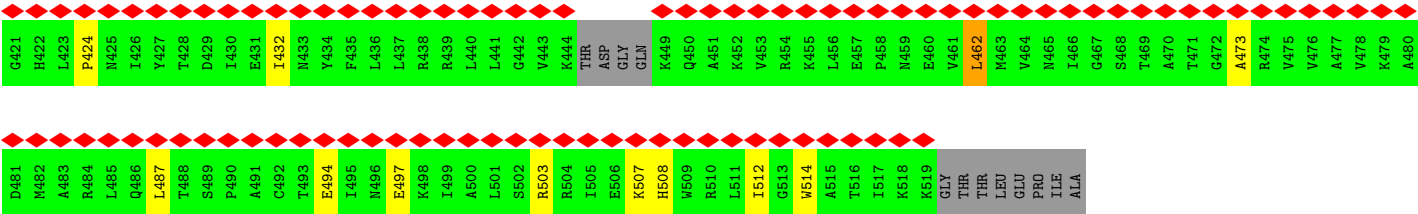
VAL	ILE	THR	GLU	PHE	GLY	ALA	LEU	PRO	PRO	SER	SER	VAL	PRO	VAL	ILE	LEU	ARG	GLU	TYR	LYS	GLY	SER	ALA
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- Molecule 4: Translation initiation factor eIF-2B subunit delta

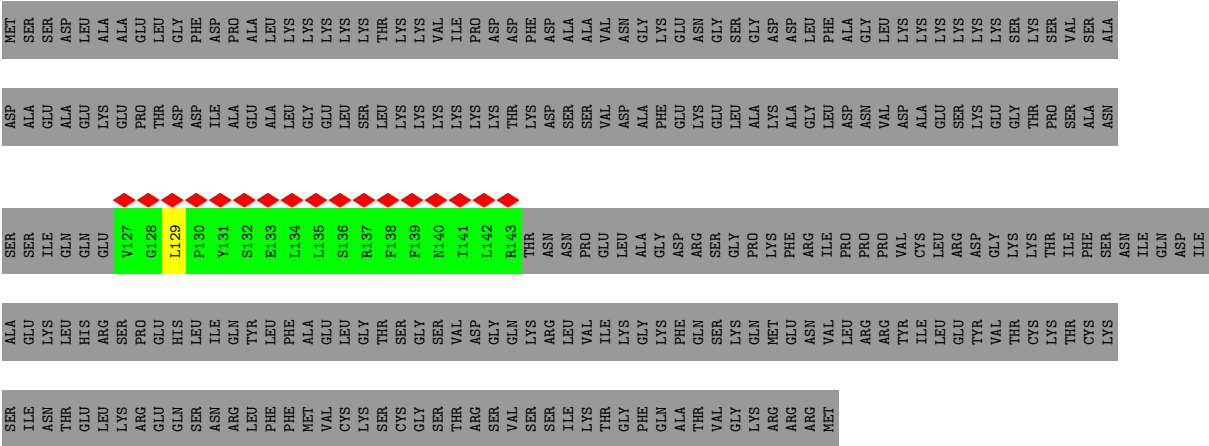
[illegible]



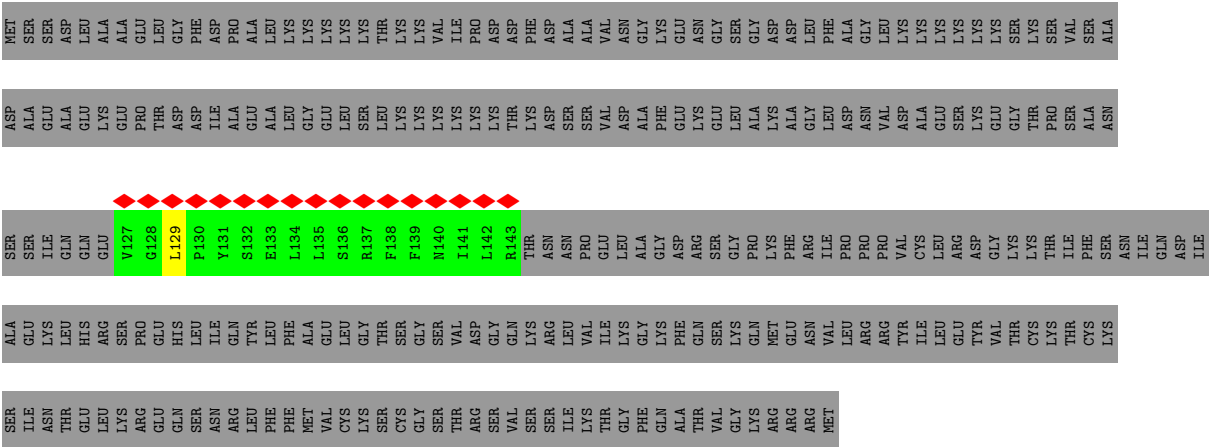




• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta



• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	131663	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.579	Depositor
Minimum map value	-0.341	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.47	0/2395	0.66	0/3251
1	B	0.48	0/2395	0.65	0/3251
2	C	0.41	0/2714	0.64	0/3693
2	D	0.41	0/2714	0.64	0/3693
3	E	0.45	0/2209	0.59	0/2989
3	F	0.45	0/2209	0.59	0/2989
4	G	0.43	0/2781	0.66	1/3747 (0.0%)
4	H	0.43	0/2781	0.66	0/3747
5	I	0.41	0/3468	0.63	0/4704
5	J	0.41	0/3468	0.63	0/4704
6	K	0.46	0/1988	0.64	0/2674
6	L	0.47	0/1988	0.62	0/2674
7	M	0.42	0/3087	0.58	0/4173
7	N	0.42	0/3087	0.58	0/4173
8	O	0.51	0/146	0.62	0/196
8	P	0.51	0/146	0.63	0/196
All	All	0.43	0/37576	0.63	1/50854 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	412	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2351	0	2365	46	0
1	B	2351	0	2365	55	0
2	C	2665	0	2626	38	0
2	D	2665	0	2626	32	0
3	E	2164	0	2154	12	0
3	F	2164	0	2154	10	0
4	G	2744	0	2819	34	0
4	H	2744	0	2819	35	0
5	I	3406	0	3359	31	0
5	J	3406	0	3359	26	0
6	K	1973	0	2016	40	0
6	L	1973	0	2014	49	0
7	M	3044	0	3126	18	0
7	N	3044	0	3126	16	0
8	O	143	0	148	0	0
8	P	143	0	148	0	0
All	All	36980	0	37224	388	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 5.

The worst 5 of 388 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)
6:L:25:GLN:OE1	6:L:35:LYS:HE2	1.34	1.21
6:L:25:GLN:OE1	6:L:35:LYS:CE	1.98	1.11
6:L:26:GLN:HG2	6:L:33:TYR:N	1.34	1.10
6:L:26:GLN:CG	6:L:33:TYR:N	2.18	1.06
1:A:31:VAL:HG22	1:A:73:PHE:CE2	1.89	1.06

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/305 (98%)	260 (87%)	28 (9%)	12 (4%)	2	21
1	B	300/305 (98%)	261 (87%)	26 (9%)	13 (4%)	2	21
2	C	339/381 (89%)	302 (89%)	31 (9%)	6 (2%)	7	36
2	D	339/381 (89%)	302 (89%)	31 (9%)	6 (2%)	7	36
3	E	253/578 (44%)	218 (86%)	30 (12%)	5 (2%)	6	34
3	F	253/578 (44%)	222 (88%)	26 (10%)	5 (2%)	6	34
4	G	349/651 (54%)	298 (85%)	41 (12%)	10 (3%)	3	27
4	H	349/651 (54%)	300 (86%)	35 (10%)	14 (4%)	2	21
5	I	427/712 (60%)	388 (91%)	31 (7%)	8 (2%)	6	35
5	J	427/712 (60%)	387 (91%)	32 (8%)	8 (2%)	6	35
6	K	237/304 (78%)	199 (84%)	30 (13%)	8 (3%)	3	24
6	L	237/304 (78%)	199 (84%)	29 (12%)	9 (4%)	2	22
7	M	398/527 (76%)	347 (87%)	47 (12%)	4 (1%)	13	48
7	N	398/527 (76%)	351 (88%)	43 (11%)	4 (1%)	13	48
8	O	15/285 (5%)	12 (80%)	2 (13%)	1 (7%)	1	15
8	P	15/285 (5%)	12 (80%)	2 (13%)	1 (7%)	1	15
All	All	4636/7486 (62%)	4058 (88%)	464 (10%)	114 (2%)	7	29

5 of 114 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	PRO
1	B	158	PRO
1	B	292	PRO
4	H	487	ALA
5	I	202	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/265 (97%)	239 (93%)	18 (7%)	12	35
1	B	257/265 (97%)	238 (93%)	19 (7%)	11	33
2	C	286/338 (85%)	267 (93%)	19 (7%)	14	37
2	D	286/338 (85%)	267 (93%)	19 (7%)	14	37
3	E	249/529 (47%)	241 (97%)	8 (3%)	34	55
3	F	249/529 (47%)	242 (97%)	7 (3%)	38	59
4	G	305/561 (54%)	295 (97%)	10 (3%)	33	55
4	H	305/561 (54%)	292 (96%)	13 (4%)	25	48
5	I	389/649 (60%)	373 (96%)	16 (4%)	26	49
5	J	389/649 (60%)	373 (96%)	16 (4%)	26	49
6	K	218/273 (80%)	191 (88%)	27 (12%)	4	18
6	L	218/273 (80%)	190 (87%)	28 (13%)	3	17
7	M	319/449 (71%)	312 (98%)	7 (2%)	47	65
7	N	319/449 (71%)	313 (98%)	6 (2%)	52	69
8	O	16/246 (6%)	16 (100%)	0	100	100
8	P	16/246 (6%)	16 (100%)	0	100	100
All	All	4078/6620 (62%)	3865 (95%)	213 (5%)	22	43

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	113	ARG
6	L	137	LYS
2	C	206	ARG
5	J	176	LYS
6	L	45	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
6	L	60	GLN
6	K	60	GLN
7	M	98	GLN
7	N	197	HIS
2	C	61	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	K	52	6	8,9,10	0.86	0	8,12,14	1.28	0
6	SEP	L	52	6	8,9,10	0.78	0	8,12,14	1.13	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	K	52	6	-	5/5/8/10	-
6	SEP	L	52	6	-	5/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	52	SEP	CA-CB-OG-P
6	L	52	SEP	CB-OG-P-O2P
6	L	52	SEP	CB-OG-P-O3P
6	K	52	SEP	CB-OG-P-O2P
6	K	52	SEP	CB-OG-P-O3P

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 [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.

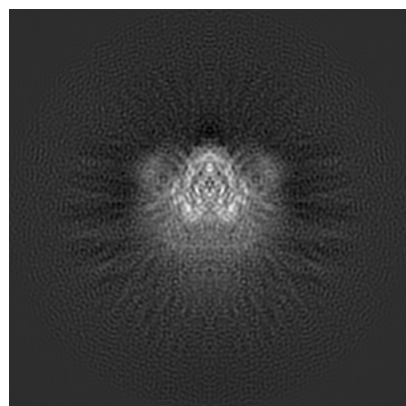
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4543. These allow visual inspection of the internal detail of the map and identification of artifacts.

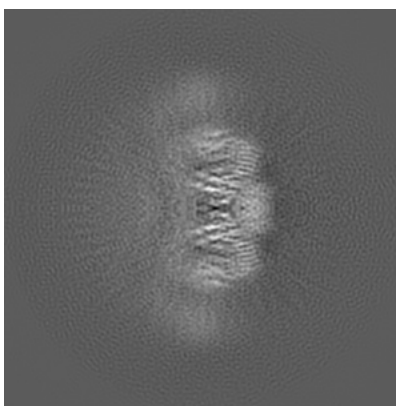
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

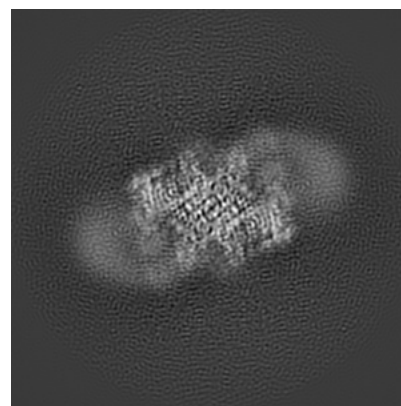
6.1.1 Primary map



X

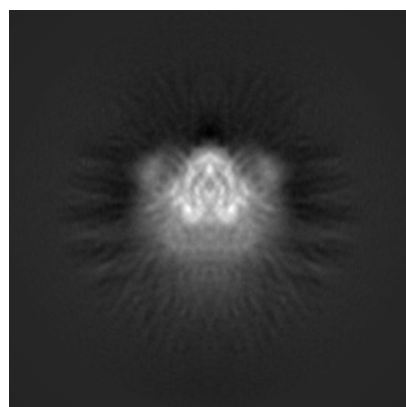


Y

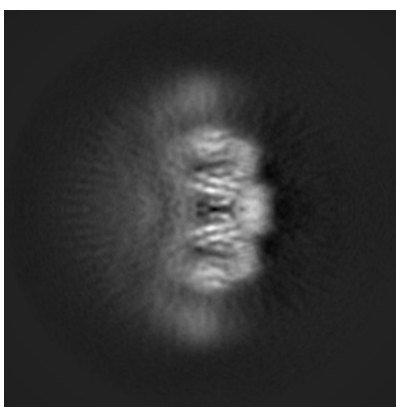


Z

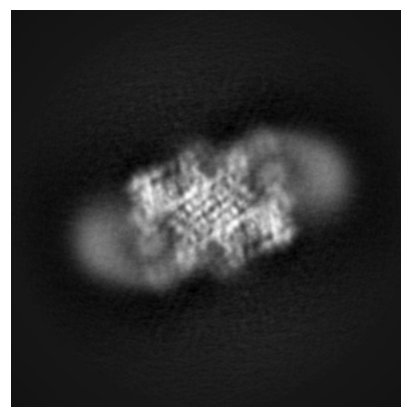
6.1.2 Raw map



X



Y

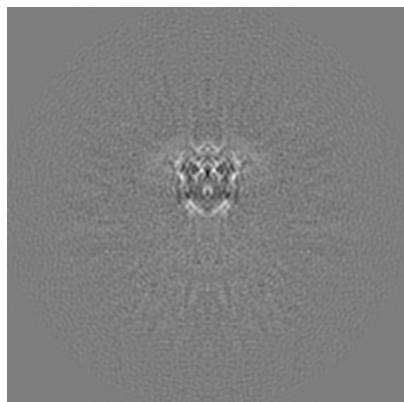


Z

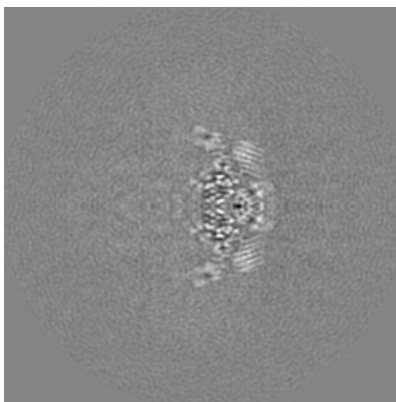
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

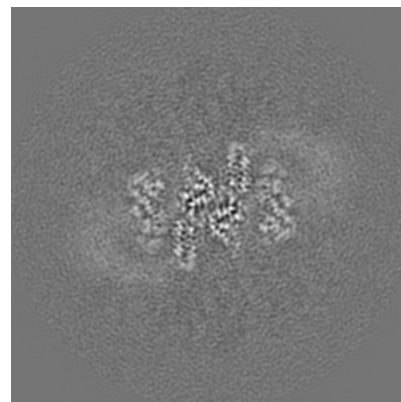
6.2.1 Primary map



X Index: 140

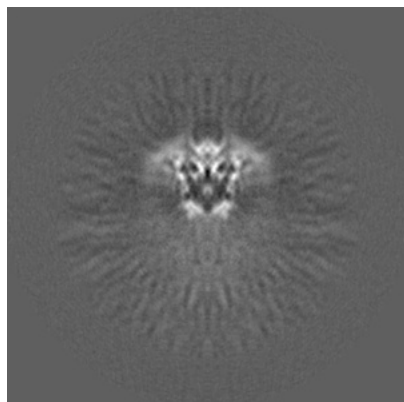


Y Index: 140

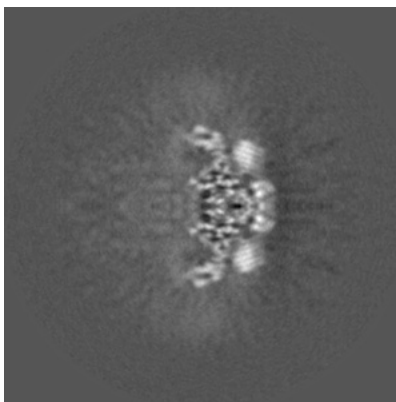


Z Index: 140

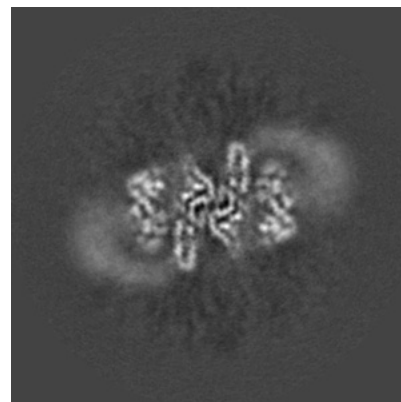
6.2.2 Raw map



X Index: 140



Y Index: 140

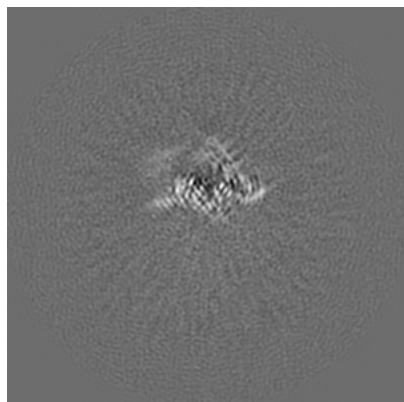


Z Index: 140

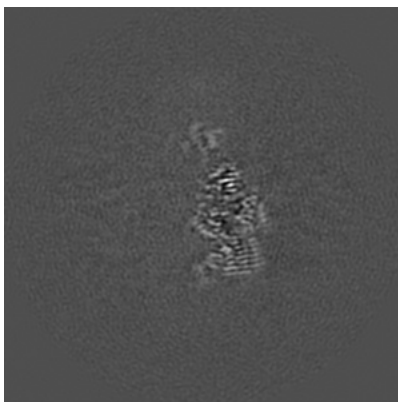
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

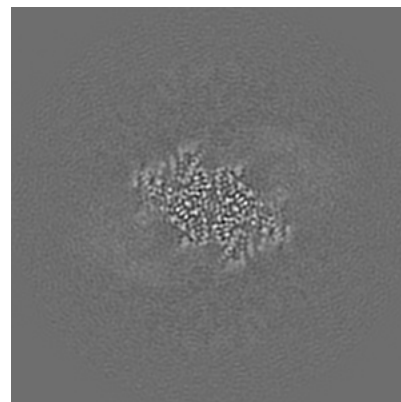
6.3.1 Primary map



X Index: 127

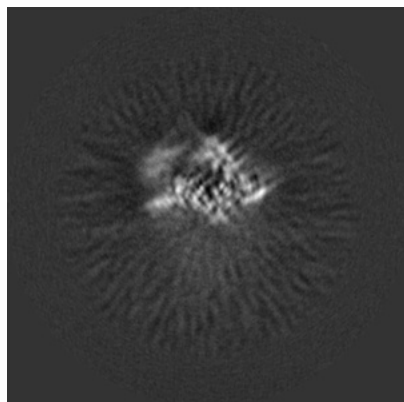


Y Index: 147

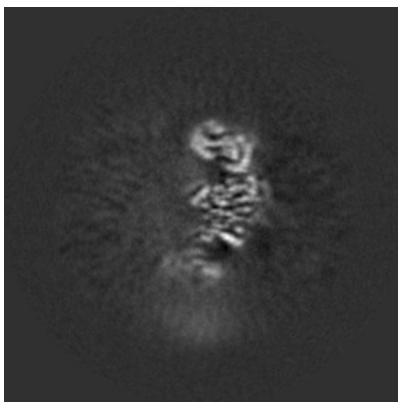


Z Index: 153

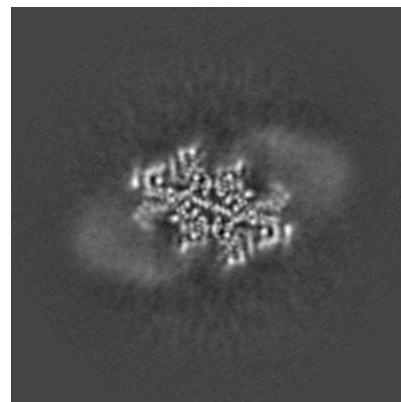
6.3.2 Raw map



X Index: 127



Y Index: 126

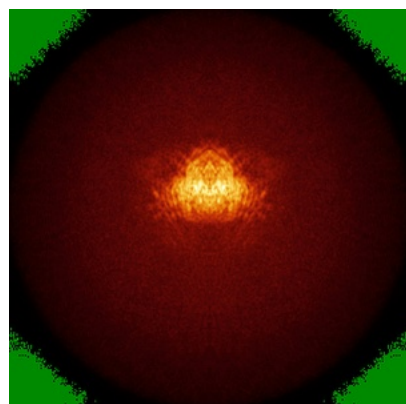


Z Index: 151

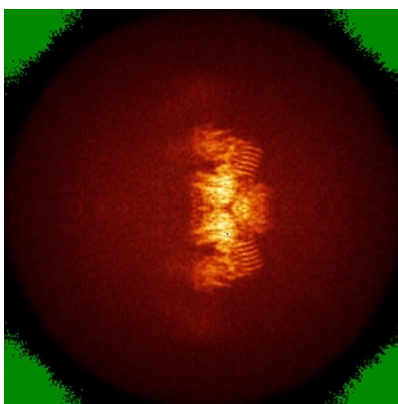
The images above show the largest variance slices of the map in three orthogonal directions.

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

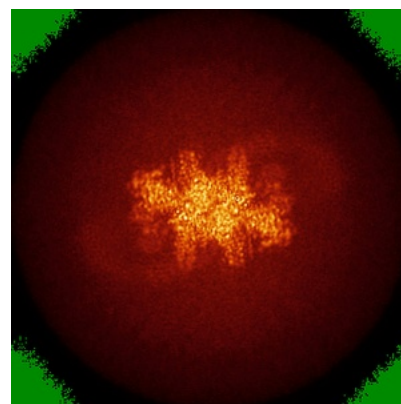
6.4.1 Primary map



X

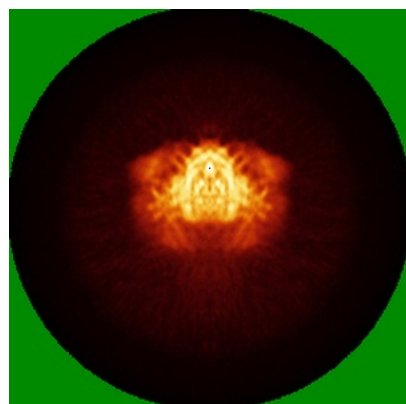


Y

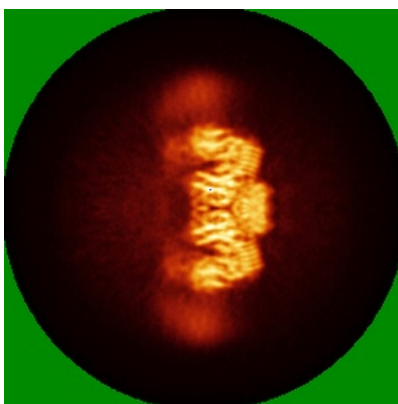


Z

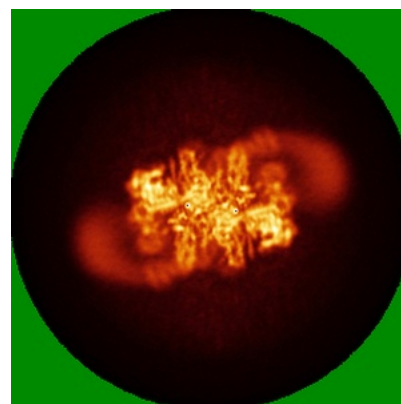
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

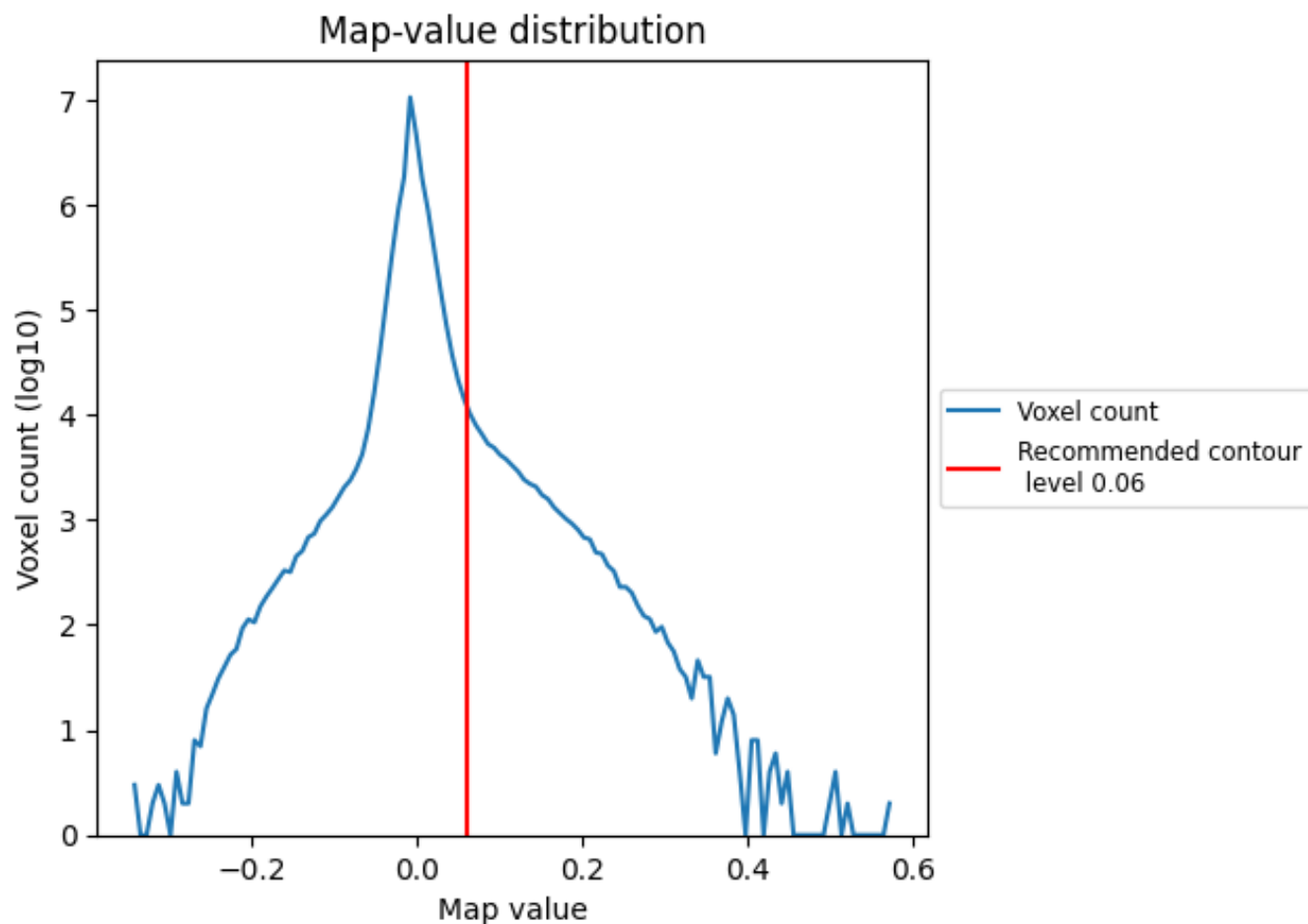
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

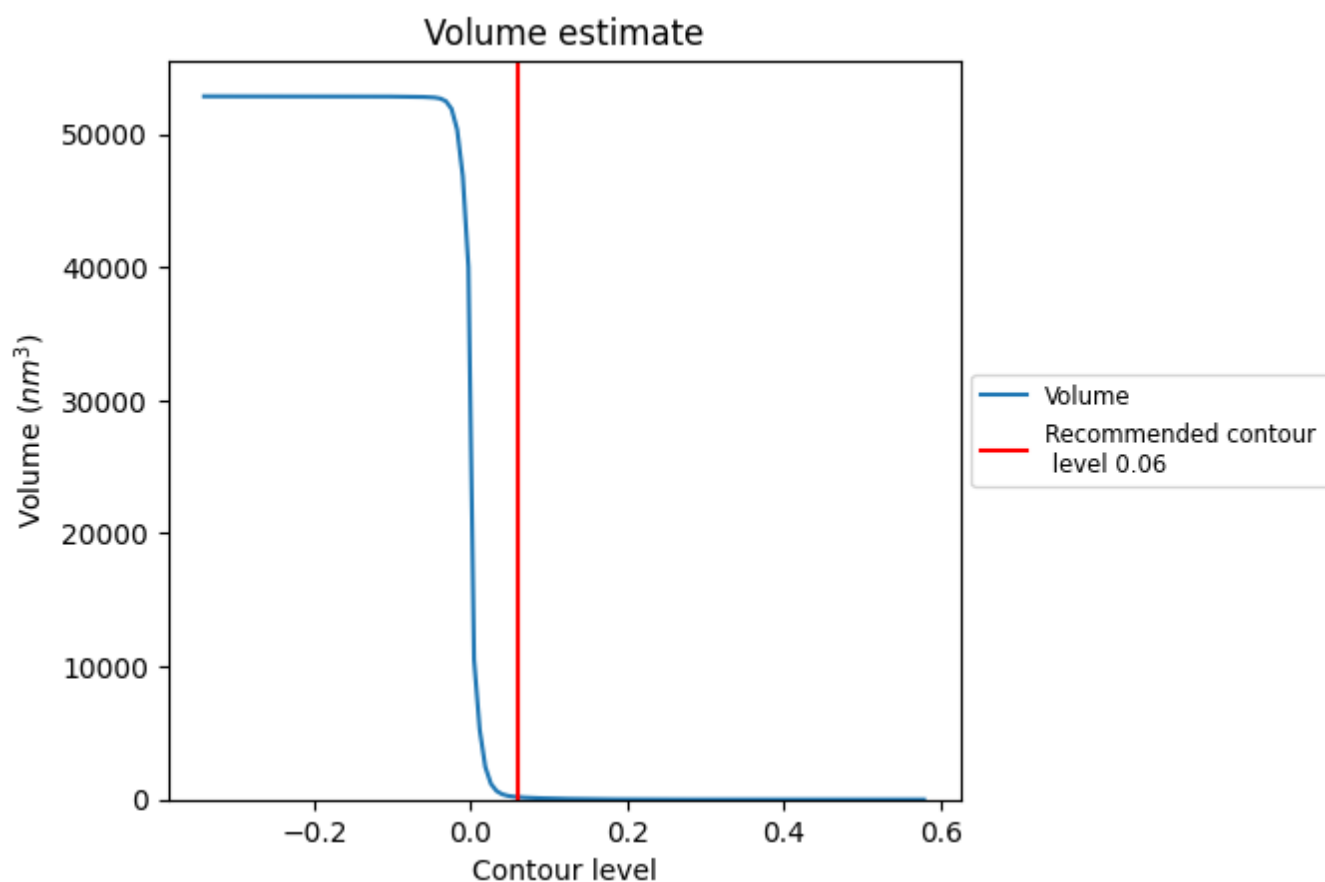
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

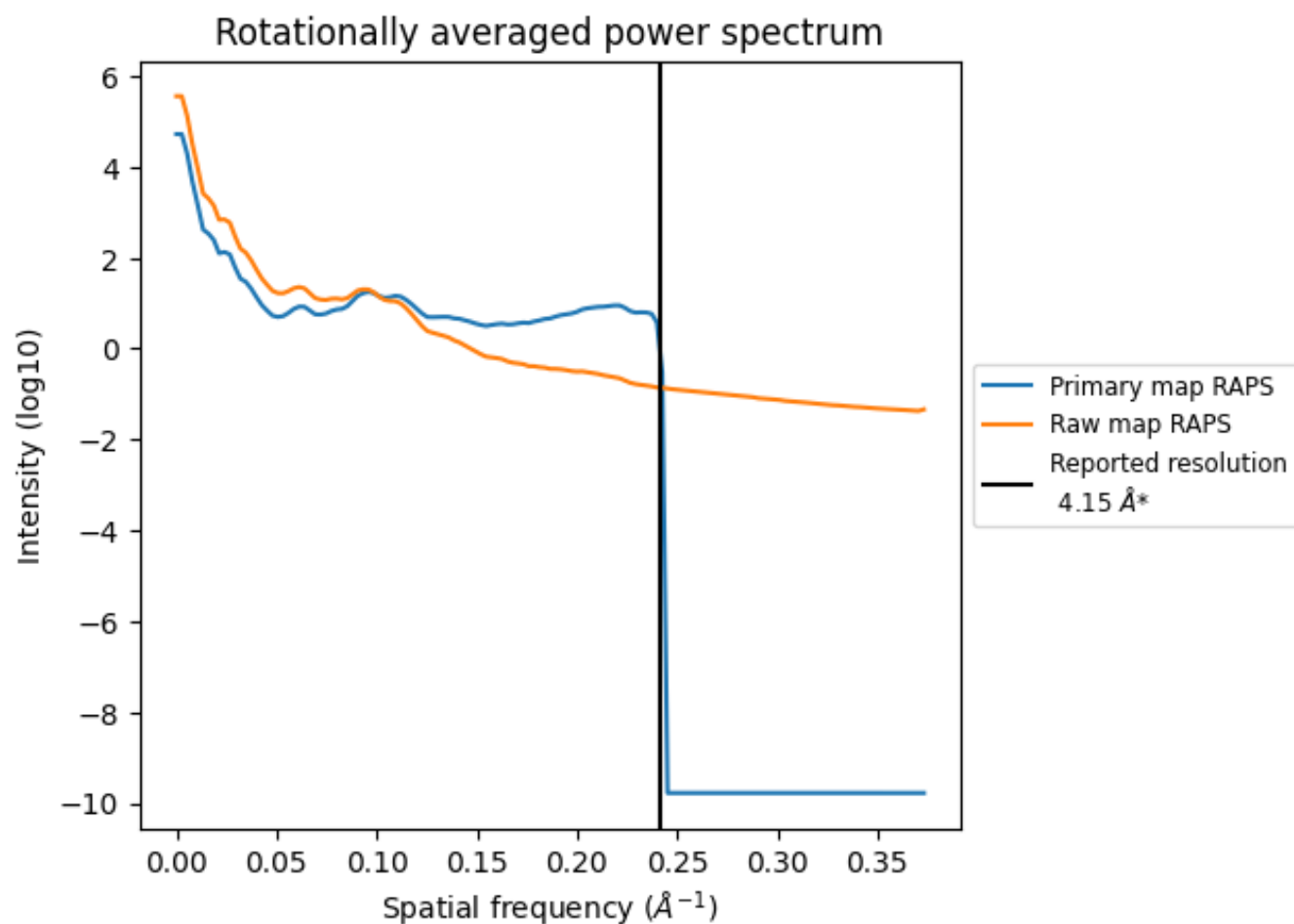
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm³; this corresponds to an approximate mass of 170 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 ⓘ

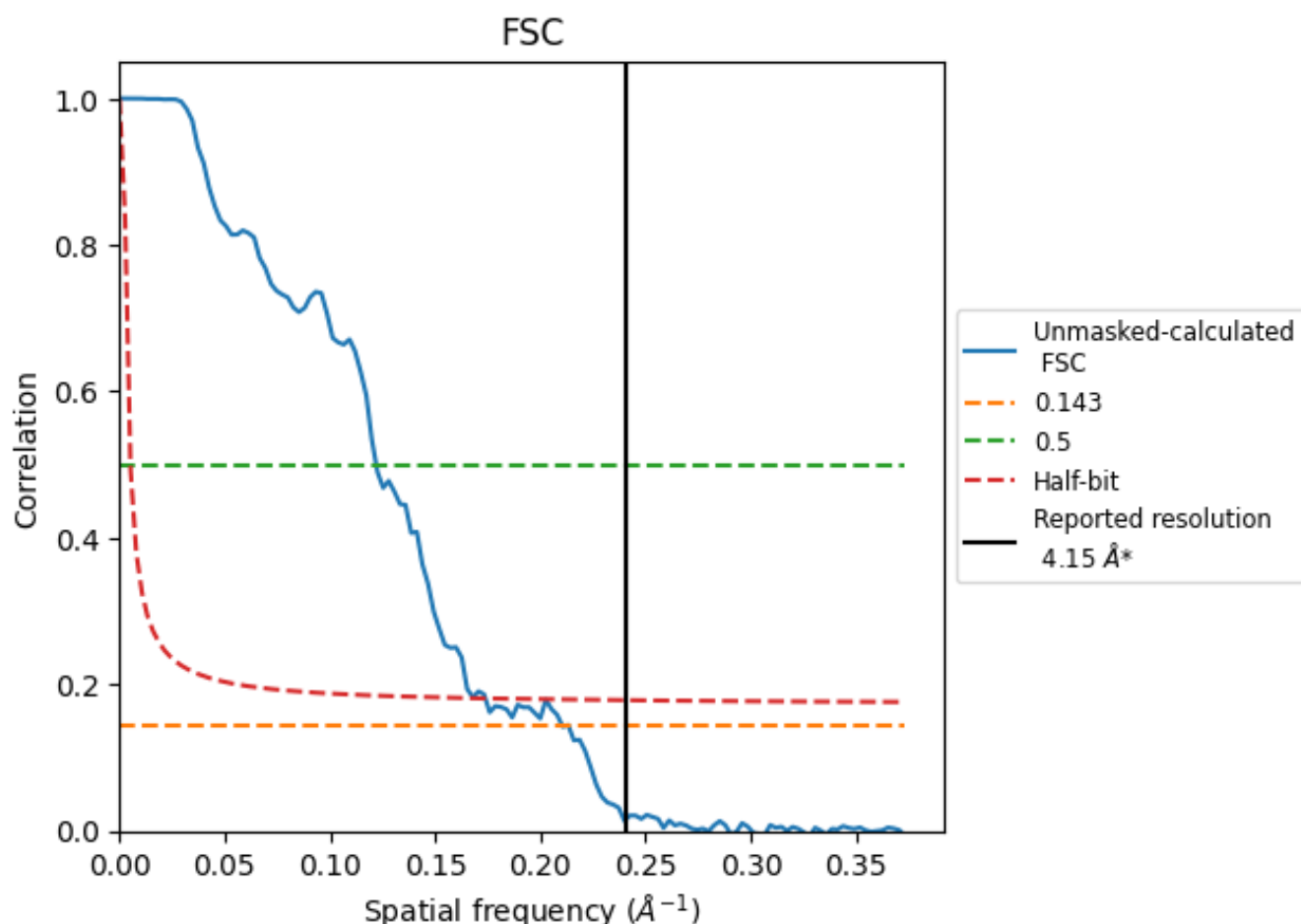


*Reported resolution corresponds to spatial frequency of 0.241 Å⁻¹

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 0.241 Å⁻¹

8.2 Resolution estimates [i](#)

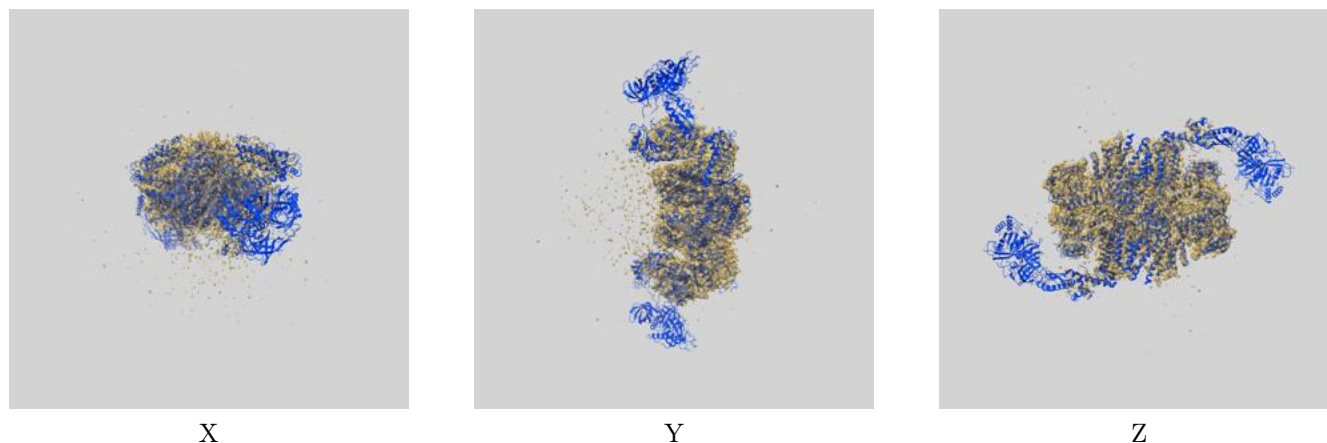
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.75	8.20	5.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.75 differs from the reported value 4.15 by more than 10 %

9 Map-model fit [i](#)

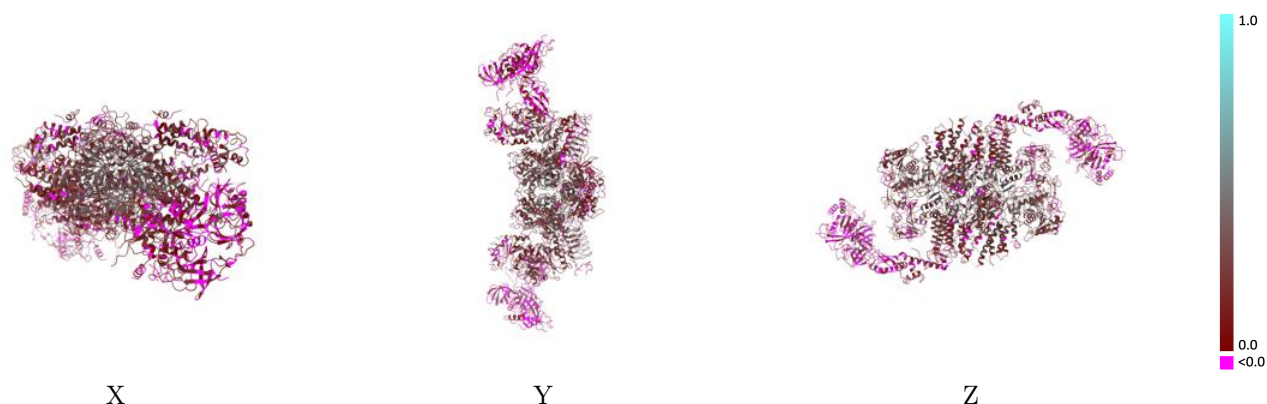
This section contains information regarding the fit between EMDB map EMD-4543 and PDB model 6QG0. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



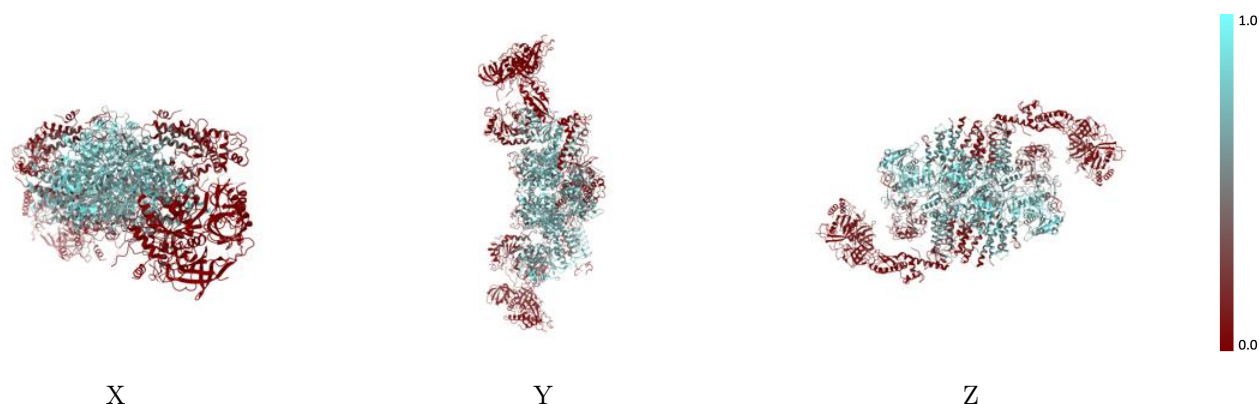
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



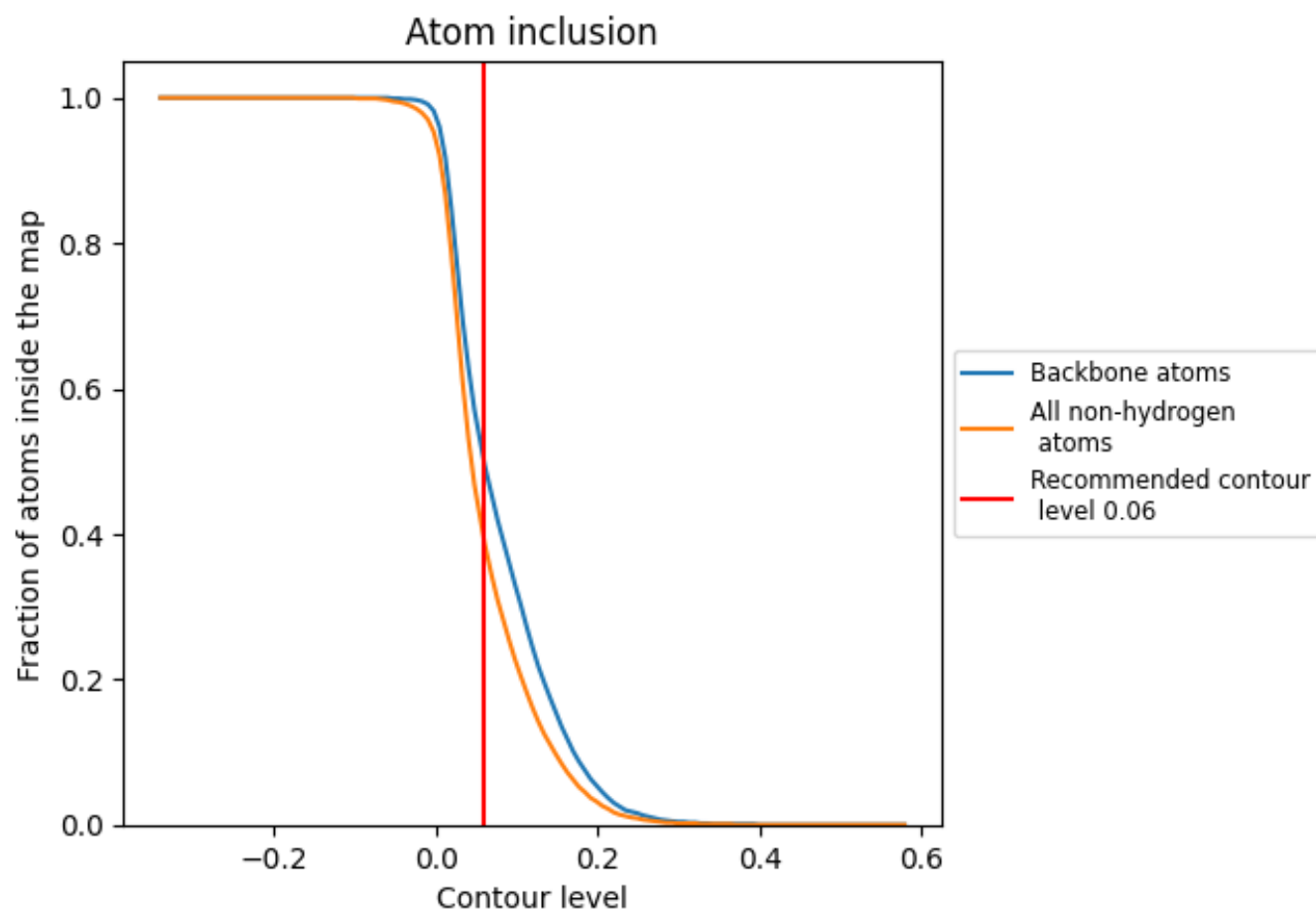
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 39% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3870	 0.1950
A	 0.4840	 0.2220
B	 0.4870	 0.2170
C	 0.6190	 0.2960
D	 0.6180	 0.2930
E	 0.2190	 0.1470
F	 0.2220	 0.1510
G	 0.5890	 0.2820
H	 0.5900	 0.2900
I	 0.6360	 0.2680
J	 0.6360	 0.2700
K	 0.0560	 0.1120
L	 0.0580	 0.1090
M	 0.0000	 0.0240
N	 0.0010	 0.0230
O	 0.0000	 0.0020
P	 0.0000	 -0.0320

