WORLDWIDE
wwPDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 11:01 am GMT

PDB ID	:	6QG5
EMDB ID	:	EMD-4547
Title	:	Structure of eIF2B-eIF2 (phosphorylated at Ser51) complex (model C)
Authors	:	Llacer, J.L.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on	:	2019-01-10
Resolution	:	10.10 Å(reported)
Based on initial models	:	5B04, 6FYX

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 10.10 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.
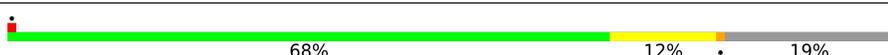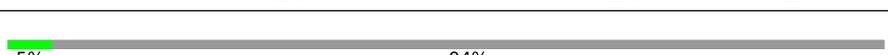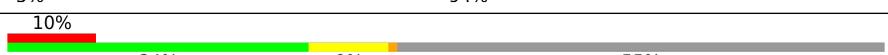
Metric	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		2.1%
Sidechain outliers		5.2%

Worse   *Better*

■ Percentile relative to all structures

▯ Percentile relative to all EM structures
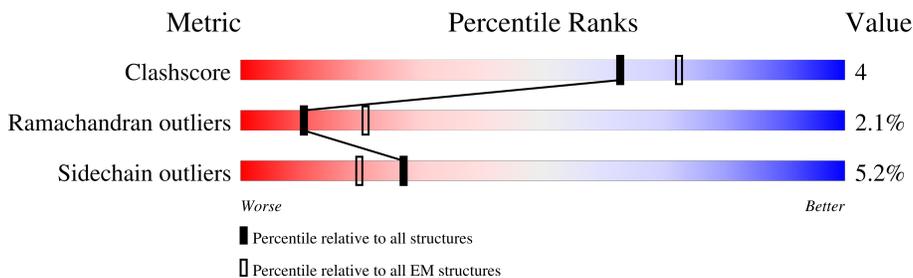
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	77% 19% ••
1	B	305	79% 17% ••
2	C	381	6% 79% 10% • 9%
2	D	381	7% 79% 11% • 9%
3	E	578	5% 43% • 54%
3	F	578	• 42% •• 54%
4	G	651	6% 47% 7% 45%
4	H	651	6% 48% 6% 45%

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Mol	Chain	Length	Quality of chain
5	I	712	53% 7% 39%
5	J	712	51% 9% 39%
6	K	304	11% 66% 14% 19%
6	L	304	68% 12% 19%
7	M	527	14% 69% 8% 23%
7	N	527	6% 63% 13% 23%
8	O	285	5% 94%
8	P	285	10% 34% 9% 55%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 37875 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 2351	C 1504	N 394	O 443	S 10	0	0
1	B	302	Total 2351	C 1504	N 394	O 443	S 10	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	246	Total 1974	C 1259	N 324	O 382	P 1	S 8	0	0
6	L	246	Total 1974	C 1259	N 324	O 382	P 1	S 8	0	0

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

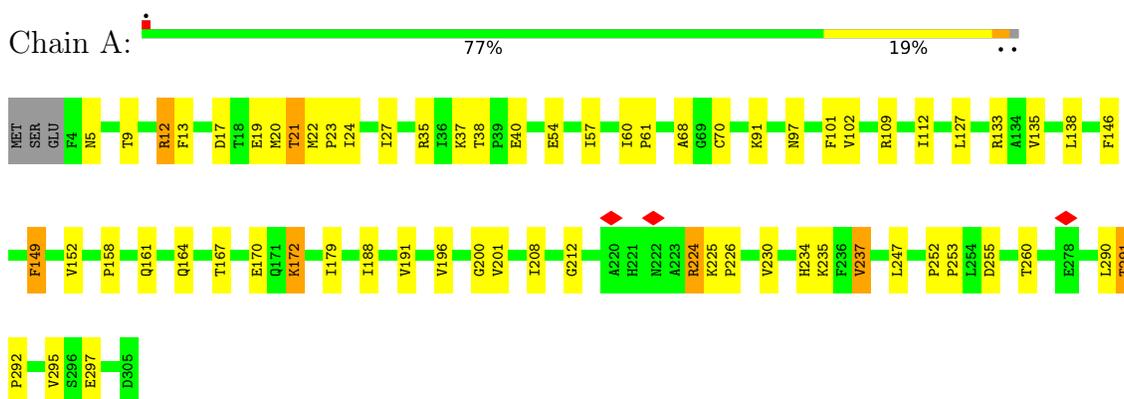| Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	408	Total 3044	C 1934	N 546	O 548	S 16	0	0
7	N	408	Total 3044	C 1934	N 546	O 548	S 16	0	0

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

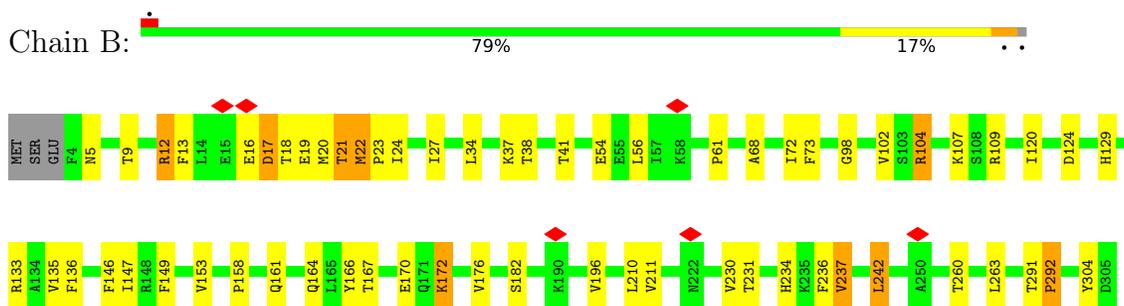| Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	17	Total 143	C 96	N 24	O 23		0	0
8	P	128	Total 1036	C 661	N 186	O 182	S 7	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
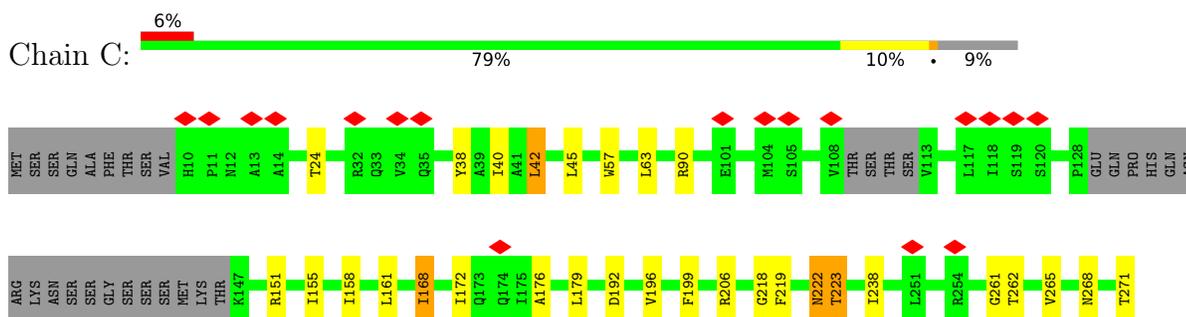
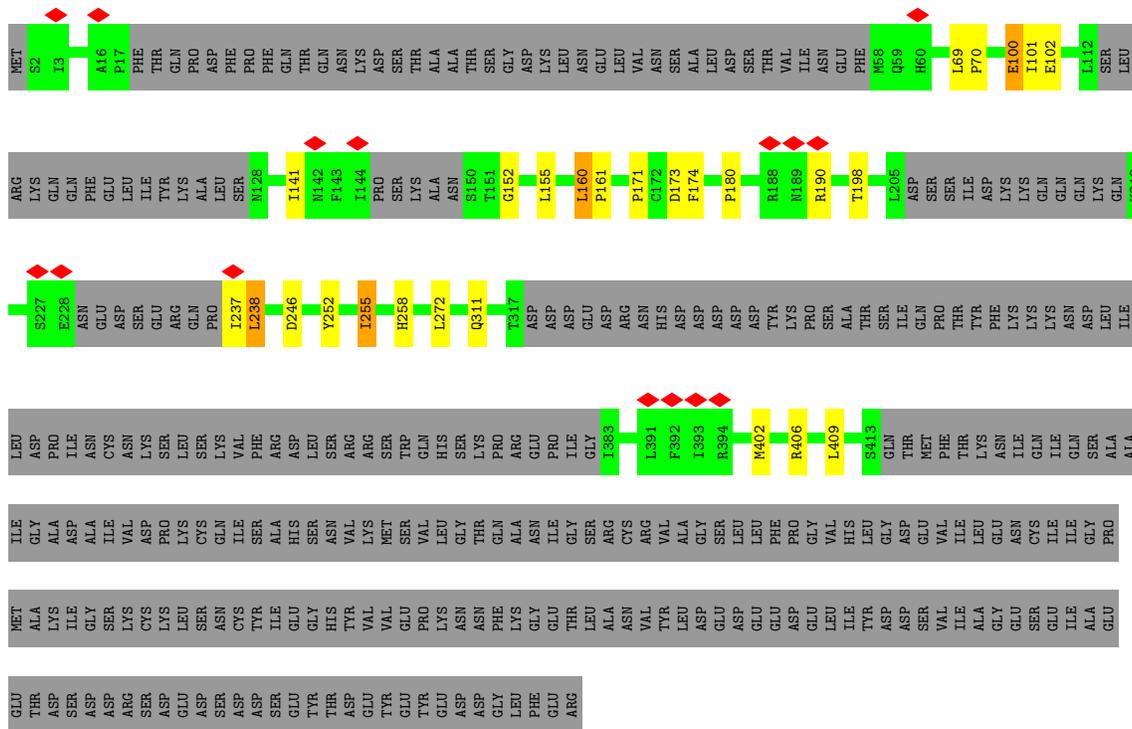- Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:

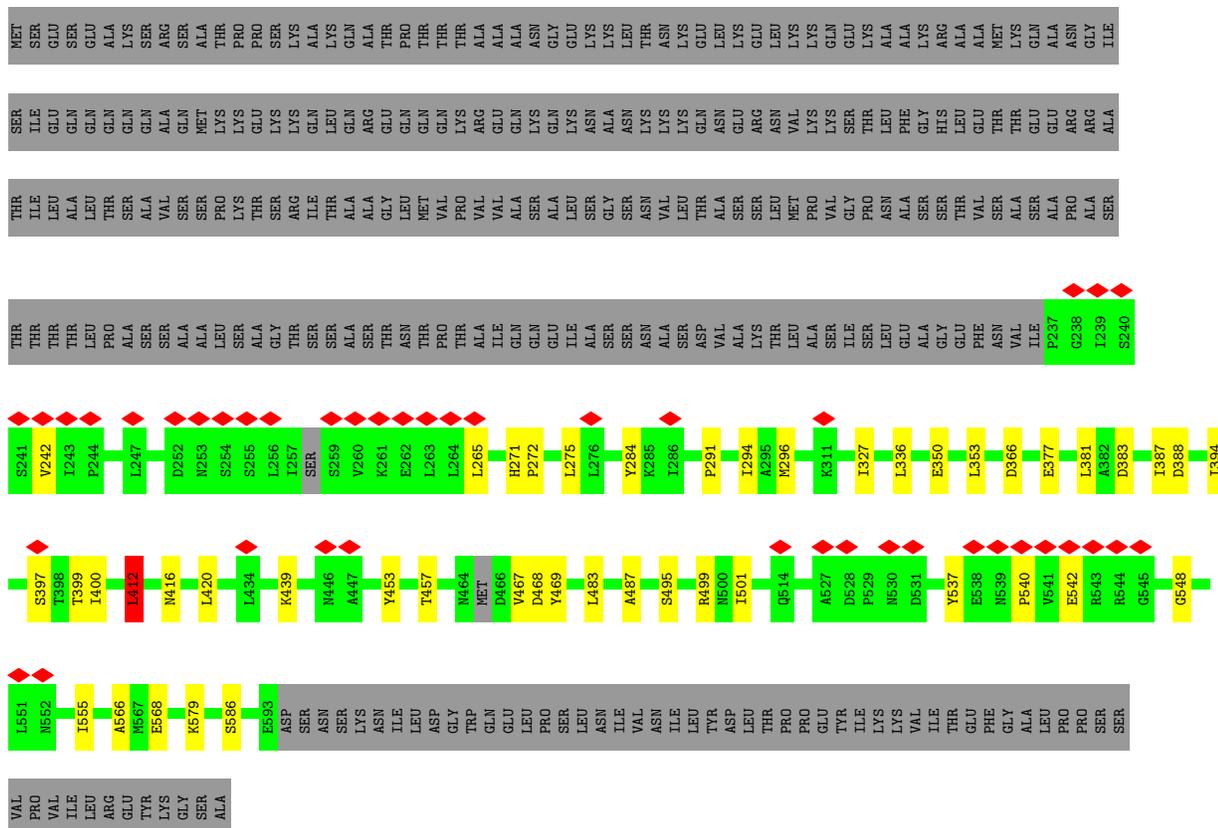- Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain B:

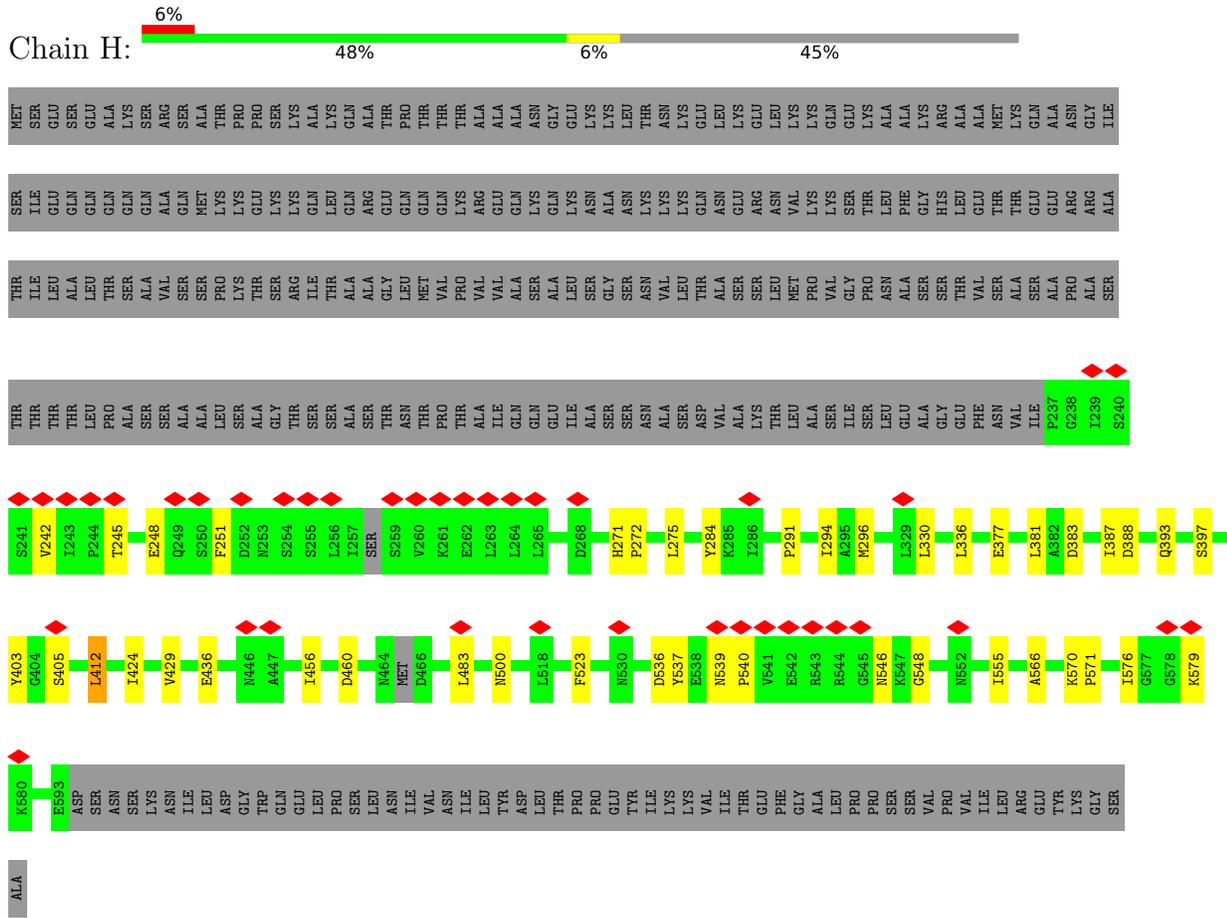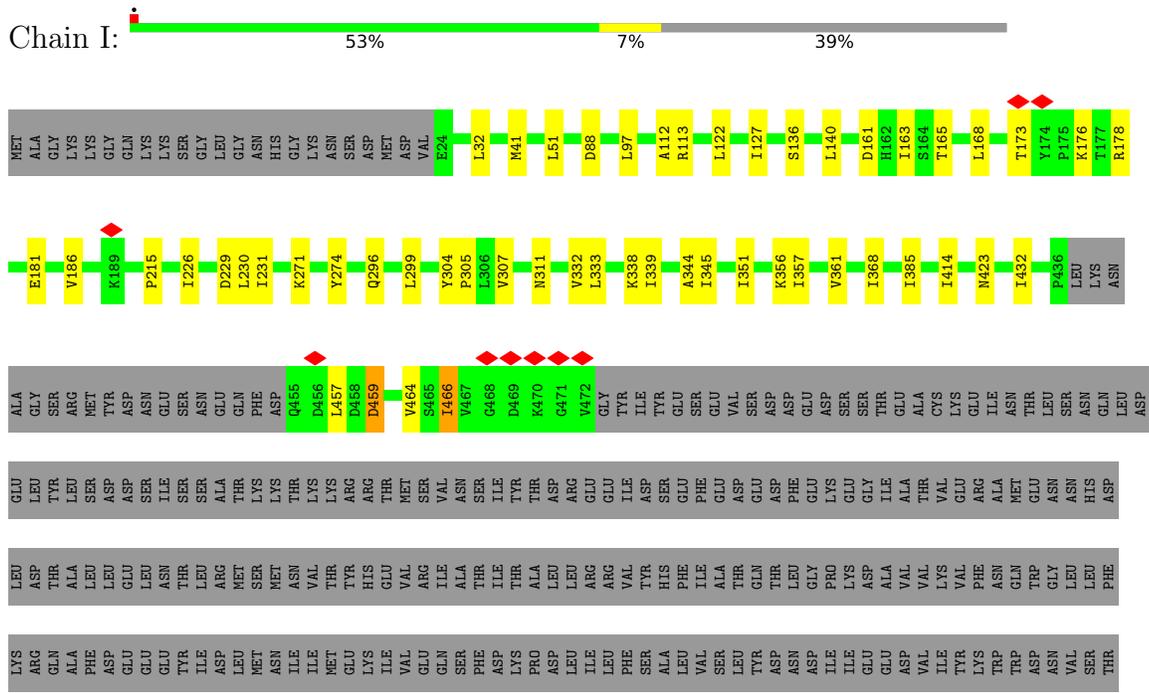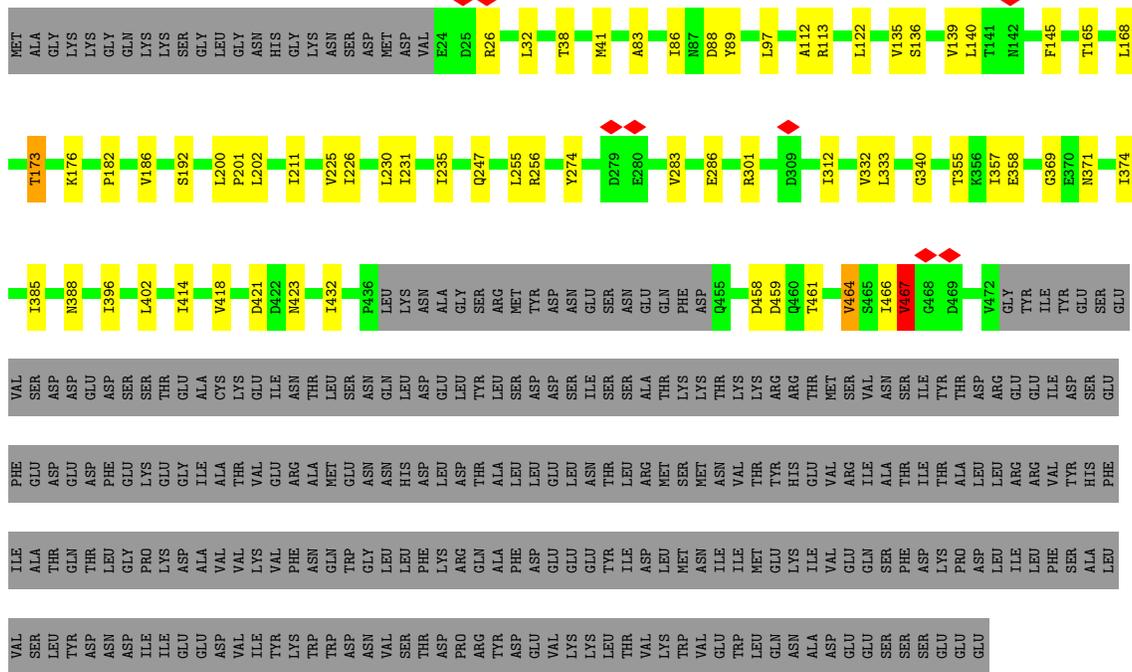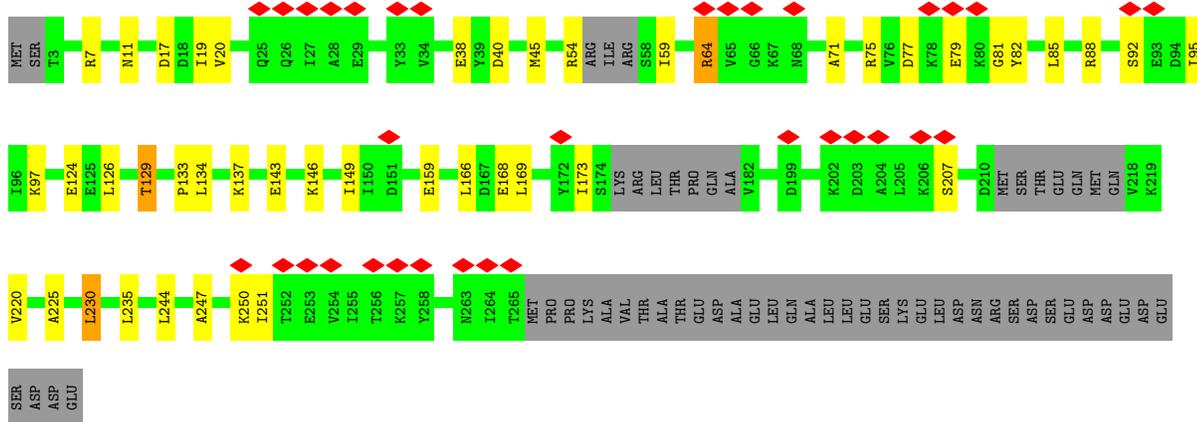- Molecule 2: Translation initiation factor eIF-2B subunit beta

Chain C:

I272 S273 S274 N275 S276 G277 V278 V281 C282 R286 L298 D308 L322 R330 T333 V334 I337 N352 R363 W366 Q371 L376 ASP LYS ASN LYS ALA

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

Chain D:

7%

79%   11%   •   9%

MET SER SER GLN PHE THR SER VAL H10 P11 N19 I22 D23 T24 K30 R31 R32 Q33 V34 Q35 G36 S37 Y38 A39 I40 A41 L42 E43 T44 L48 K76 A77 F82 S83 C84 I91 T107 V108 THR SER THR SER V113 I118 S119 P128 GLU GLN PRO

HIS GLN ASN ARG LYS ASN SER SER GLY SER SER MET LYS THR K147 D160 L161 I168 D169 E170 Q174 L179 D182 P191 K198 F199 L200 I201 N222 A230 K231 K232 L233 D245 S246 A247 V248 F249 A250 L251 V265 T271 N275 S276 S279

S280 V281 R286 P291 V292 F293 L298 F307 D308 G317 S318 I321 R324 I337 R363 W366 Q371 L376 ASP LYS ASN LYS ALA

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

Chain E:

5%

43%   •   54%

MET S2 I3 N14 L15 A16 P17 PHE THR GLN PRO ASP PHE PRO PHE GLN THR GLN THR GLN ASN LYS ASP SER THR ALA ALA THR SER GLY ASP LYS LEU ASN GLU LEU VAL ASN SER ALA LEU ASP SER THR VAL ILE ASN GLU PHE M58 Q59 H60 S61 T62 R63 N73 D82 D85

Q86 A87 D88 V98 D99 E100 F111 L112 SER LEU ARG LYS GLN GLN PHE GLU LEU ILE TYR LYS ALA LEU SER N128 K139 I144 PRO SER LYS ALA ASN S150 T151 G152 E153 S154 L155 Q156 K157 L160 P161 D173 P179 P180 Q181 V182 L183 V184 D185 N189 L205

ASP SER SER ILE ASP LYS LYS GLN GLN LYS GLN LYS GLN K218 T224 V225 Y226 S227 E228 ASN GLU ASP SER GLU ARG GLN PRO I237 L238 L239 T248 K249 T267 V268 Q312 T317 ASP ASP ASP GLU ARG ASN HIS ASP ASP ASP TYR LYS PRO SER ALA THR SER

ILE GLN PRO THR TYR PHE LYS LYS LYS ASN ASP LEU ILE LEU ASP ALA ILE VAL ASP PRO ILE ASN CYS ASN SER GLN ILE SER SER ALA HIS SER ASN VAL LYS MET SER VAL LEU GLY THR GLN ALA ASN ILE GLY SER ARG GLU GLU PRO ILE GLY I383 I393 N399 M402 S413 GLN THR MET PHE THR LYS

ASN ILE GLN ILE GLN SER ALA ALA ILE GLY ALA ASP ALA ILE VAL ASP PRO ILE ASN CYS GLN ILE SER SER ALA HIS SER ASN VAL LYS MET SER VAL LEU GLY THR GLN ALA ASN ILE GLY SER ARG GLU GLU PRO ILE GLY

LEU GLU ASN CYS ILE ILE GLY PRO MET ALA LYS ILE GLY SER LYS CYS LYS LEU SER ASN CYS TYR ILE GLU GLY HIS TYR VAL VAL GLU PRO LYS ASN ASN PHE LYS GLY GLU THR LEU ALA ASN VAL TYR LEU ASP GLU GLU GLU GLU ASP GLU LEU ILE TYR ASP ASP SER VAL ILE

ALA GLY GLU SER ILE GLU ALA GLU THR ASP SER ASP ARG SER ASP GLU ASP SER ASP SER GLU THR ASP TYR GLU GLU ASP GLY LEU PHE GLU ARG

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

Chain F:

•

42%   • •   54%

MET S2 I3 A16 P17 PHE THR GLN PRO ASP PHE PRO GLN THR GLN ASN LYS ASP SER THR ALA ALA THR SER GLY ASP LYS LEU ASN GLU LEU VAL ASN SER ALA LEU ASP SER THR VAL ILE ASN GLU PHE M58 Q59 H60 L69 P70 E100 I101 E102 L112 SER LEU

ARG LYS GLN GLN PHE GLU LEU ILE TYR LYS ALA LEU SER N128 I141 N142 F143 I144 PRO SER LYS ALA ASN S150 T151 G152 L155 L160 P161 P171 C172 D173 F174 P180 R188 N189 R190 T198 L205 ASP SER SER ILE ASP LYS LYS GLN GLN LYS GLN LYS K218

S227 E228 ASN GLU ASP SER GLU ARG GLN PRO I237 L238 D246 Y252 I255 H258 L272 Q311 T317 ASP ASP ASP GLU ASP ARG ASN HIS ASP ASP ASP ASP ASP TYR LYS PRO SER ALA THR SER ILE GLN PRO THR TYR PHE LYS LYS GLN GLN LYS ASN ASP LEU ILE

LEU ASP PRO ILE ASN CYS ASN LYS SER SER LYS VAL PHE ARG LEU SER ARG ARG SER TRP GLN HIS SER LYS PRO ARG GLU PRO ILE GLY I383 L391 F392 I393 R394 M402 R406 L409 S413 GLN THR MET PHE THR LYS ASN ILE GLN ILE GLN SER ALA ALA

ILE GLY ALA ASP ALA ILE ASP ASP PRO LYS CYS GLN ILE ILE SER ALA HIS SER ASN VAL LYS MET SER VAL LEU GLY THR GLN ASN ILE GLY SER ARG CYS ARG VAL ALA GLY SER LEU LEU PHE PRO GLY VAL HIS LEU ASP GLU GLU VAL ILE LEU GLU ASN CYS ILE ILE GLY PRO

MET ALA LYS ILE GLY SER LYS CYS LYS LEU SER ASN CYS TYR ILE GLU GLY GLY HIS TYR VAL VAL GLU PRO LYS ASN ASN PHE LYS GLY GLU THR LEU ALA ASN VAL TYR LEU ASP GLU GLU ASP GLU ILE ILE TYR ASP SER SER VAL ILE ALA GLY GLU SER ILE ALA GLU

GLU THR ASP SER ASP ASP ARG SER ASP GLU SER ASP ASP SER GLU TYR THR ASP GLU TYR GLU ASP GLY GLY LEU PHE GLU ARG

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

Chain G:

6% 47% 7% 45%

MET SER GLU GLU GLU ALA LYS SER ARG SER ALA THR PRO PRO SER LYS ALA LYS GLN ALA THR PRO THR THR ALA ALA ASN GLY LYS LYS GLU THR ASN LYS GLU LEU LYS GLU LYS LYS GLN LEU GLU LYS LYS ALA ALA LYS ARG ALA ALA MET LYS GLN ALA ASN GLY ILE

SER ILE GLU GLN GLN GLN GLN GLN ALA GLN MET LYS LYS GLU LYS GLN GLN LEU GLN LEU ARG GLU GLU GLN GLN GLN LYS ARG GLU GLU ASN VAL LYS LYS LYS GLN SER GLU LYS GLN ARG ASN VAL LYS SER THR LEU PHE GLY HIS LEU GLU GLN THR GLU GLU ARG ARG ALA

THR ILE LEU ALA LEU THR SER SER ALA VAL SER SER PRO LYS THR SER ARG ILE THR ALA ALA GLY LEU MET VAL PRO VAL VAL ALA SER ALA LEU SER GLY ASN VAL LEU THR ALA SER SER ASN ALA SER ASP VAL LYS SER GLY LEU LEU ALA ILE SER SER THR VAL SER ALA PRO ALA SER

THR THR THR LEU PRO ALA SER SER ALA ALA LEU SER ALA GLY THR SER SER ALA SER THR ASN THR PRO THR ALA ILE GLN GLN GLN ILE ALA SER SER ASN ALA SER ASP VAL ALA LYS THR ALA LEU ALA ILE SER LEU GLU ALA GLY GLU PHE ASN VAL P237 G238 I239 S240

S241 V242 I243 P244 L247 D252 N253 S254 S255 L256 I257 SER S259 V260 K261 E262 L263 L264 L265 H271 P272 L275 L276 Y284 K285 I286 P291 I294 A295 M296 K311 I327 L336 E350 L353 D366 E377 L381 A382 D383 I387 D388 I394

S397 T398 T399 I400 L412 M416 L420 L434 K439 N446 A447 Y453 T457 N464 MET D466 V467 D468 Y469 L483 A487 S495 R499 N500 I501 Q514 A527 D528 P529 N530 D531 Y537 E538 N539 P540 V541 E542 R643 R544 G545 G548

L551 N552 I555 A566 M567 E568 K579 S586 E593 ASP SER ASN SER LYS ASN ILE LEU ASP GLY TRP GLN LEU GLU LEU PRO SER GLU ASN ILE VAL ASN ILE LEU TYR ASP LEU THR PRO PRO GLU TYR ILE LYS LYS VAL ILE THR GLU PHE GLY ALA LEU GLU PRO SER SER

VAL PRO VAL ILE LEU ARG GLU TYR LYS GLY SER ALA

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

Chain H:

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

Chain I:

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

Chain J:

• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain K:

• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain L:

• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

Chain M:

14%

69%　　　8%　　23%

• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

Chain N:

6%

63%　　13%　　•　　23%

• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta

Chain O:

• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta

Chain P:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23909	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 $(e^-/\text{Å}^2)$	45	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	0.126	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.39	0/2395	0.61	0/3251
1	B	0.38	0/2395	0.59	0/3251
2	C	0.40	0/2714	0.62	0/3693
2	D	0.39	0/2714	0.62	0/3693
3	E	0.42	0/2209	0.59	0/2989
3	F	0.42	0/2209	0.59	0/2989
4	G	0.39	0/2781	0.62	1/3747 (0.0%)
4	H	0.39	0/2781	0.62	0/3747
5	I	0.40	0/3468	0.61	0/4704
5	J	0.41	0/3468	0.60	0/4704
6	K	0.39	0/1989	0.63	0/2675
6	L	0.39	0/1989	0.63	0/2675
7	M	0.38	0/3087	0.57	0/4173
7	N	0.36	0/3087	0.55	0/4173
8	O	0.46	0/146	0.63	0/196
8	P	0.38	0/1051	0.59	1/1402 (0.1%)
All	All	0.39	0/38483	0.60	2/52062 (0.0%)

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
7	N	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	166	LEU	CA-CB-CG	6.07	129.27	115.30
4	G	412	LEU	CA-CB-CG	5.47	127.87	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	N	423	LEU	Peptide

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	2351	0	2367	43	0
1	B	2351	0	2367	57	0
2	C	2665	0	2626	14	0
2	D	2665	0	2626	12	0
3	E	2164	0	2154	8	0
3	F	2164	0	2154	10	0
4	G	2744	0	2819	17	0
4	H	2744	0	2819	15	0
5	I	3406	0	3359	19	0
5	J	3406	0	3359	26	0
6	K	1974	0	2020	13	0
6	L	1974	0	2020	24	0
7	M	3044	0	3126	23	0
7	N	3044	0	3126	71	0
8	O	143	0	148	1	0
8	P	1036	0	1080	18	0
All	All	37875	0	38170	331	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 4.

The worst 5 of 331 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)
1:B:20:MET:SD	1:B:102:VAL:HG13	1.27	1.70
7:N:312:SER:HB2	7:N:422:HIS:CE1	1.47	1.49
1:B:20:MET:SD	1:B:102:VAL:CG1	2.22	1.27
7:N:314:ARG:HH21	7:N:423:LEU:C	1.47	1.18
1:A:20:MET:SD	1:A:102:VAL:CG1	2.34	1.16

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%)	254 (85%)	39 (13%)	7 (2%)	6	34
1	B	300/305 (98%)	256 (85%)	35 (12%)	9 (3%)	4	28
2	C	339/381 (89%)	308 (91%)	28 (8%)	3 (1%)	17	57
2	D	339/381 (89%)	309 (91%)	25 (7%)	5 (2%)	10	46
3	E	253/578 (44%)	217 (86%)	34 (13%)	2 (1%)	19	60
3	F	253/578 (44%)	211 (83%)	37 (15%)	5 (2%)	7	38
4	G	349/651 (54%)	303 (87%)	35 (10%)	11 (3%)	4	26
4	H	349/651 (54%)	302 (86%)	36 (10%)	11 (3%)	4	26
5	I	427/712 (60%)	379 (89%)	41 (10%)	7 (2%)	9	44
5	J	427/712 (60%)	365 (86%)	45 (10%)	17 (4%)	3	23
6	K	237/304 (78%)	208 (88%)	27 (11%)	2 (1%)	19	60
6	L	237/304 (78%)	211 (89%)	25 (10%)	1 (0%)	34	72
7	M	398/527 (76%)	345 (87%)	48 (12%)	5 (1%)	12	48
7	N	398/527 (76%)	330 (83%)	55 (14%)	13 (3%)	4	26
8	O	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	15
8	P	120/285 (42%)	100 (83%)	18 (15%)	2 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4741/7486 (63%)	4111 (87%)	529 (11%)	101 (2%)	10	36

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	PRO
3	E	100	GLU
3	F	100	GLU
4	G	487	ALA
4	H	536	ASP

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%)	238 (93%)	19 (7%)	13	38
1	B	257/265 (97%)	241 (94%)	16 (6%)	18	43
2	C	286/338 (85%)	265 (93%)	21 (7%)	14	39
2	D	286/338 (85%)	266 (93%)	20 (7%)	15	40
3	E	249/529 (47%)	244 (98%)	5 (2%)	55	74
3	F	249/529 (47%)	241 (97%)	8 (3%)	39	61
4	G	305/561 (54%)	298 (98%)	7 (2%)	50	70
4	H	305/561 (54%)	296 (97%)	9 (3%)	41	63
5	I	389/649 (60%)	374 (96%)	15 (4%)	32	56
5	J	389/649 (60%)	375 (96%)	14 (4%)	35	59
6	K	219/273 (80%)	195 (89%)	24 (11%)	6	22
6	L	219/273 (80%)	195 (89%)	24 (11%)	6	22
7	M	319/449 (71%)	313 (98%)	6 (2%)	57	75
7	N	319/449 (71%)	299 (94%)	20 (6%)	18	43
8	O	16/246 (6%)	16 (100%)	0	100	100
8	P	119/246 (48%)	109 (92%)	10 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4183/6620 (63%)	3965 (95%)	218 (5%)	27	48

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	231	ILE
6	K	79	GLU
7	N	422	HIS
5	I	457	LEU
5	J	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
6	L	103	GLN
7	N	422	HIS
7	M	98	GLN
7	M	197	HIS
3	E	258	HIS

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	0.65	0	8,12,14	1.21	0
6	SEP	L	52	6	8,9,10	0.65	0	8,12,14	1.25	1 (12%)

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	-	1/5/8/10	-
6	SEP	L	52	6	-	1/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	52	SEP	OG-CB-CA	2.01	110.11	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	52	SEP	N-CA-CB-OG
6	L	52	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-4547. 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 ⓘ
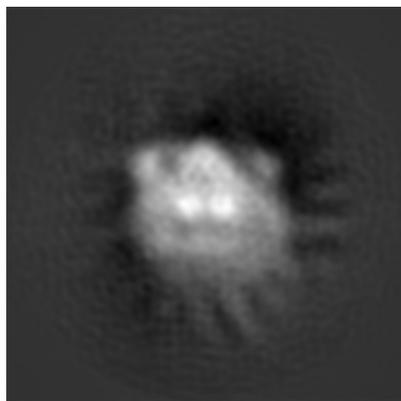
6.1.1 Primary map

X
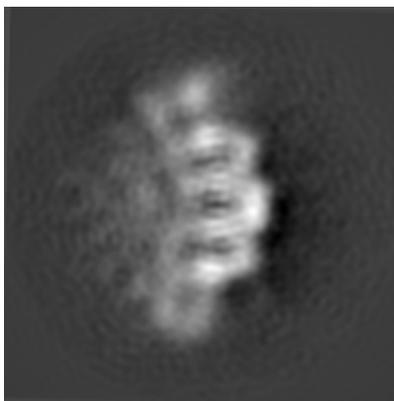
Y
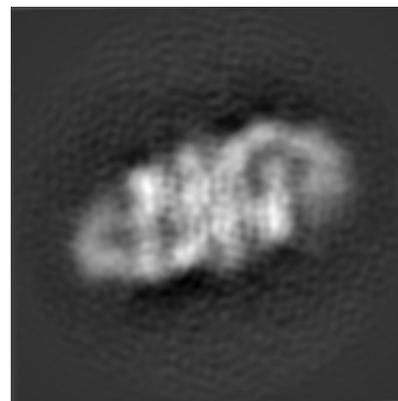
Z

6.1.2 Raw map

X

Y

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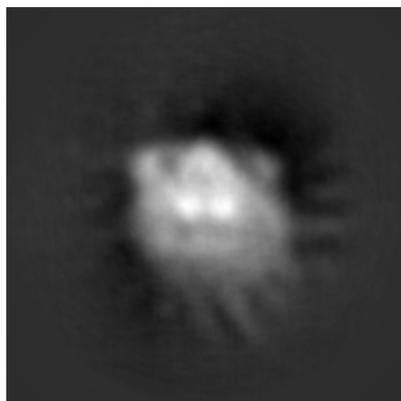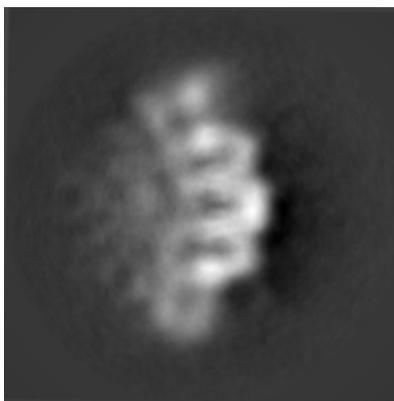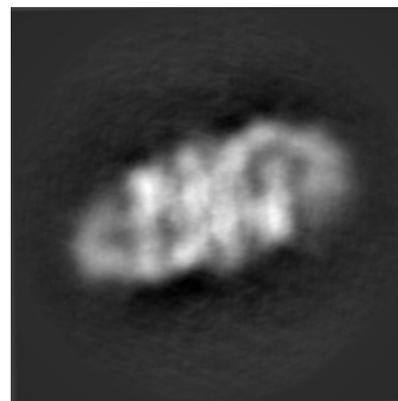
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map
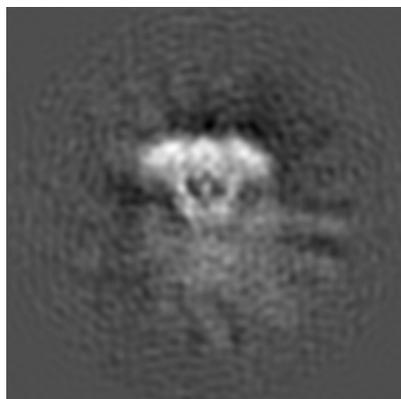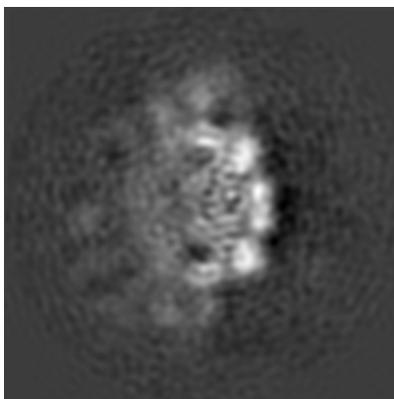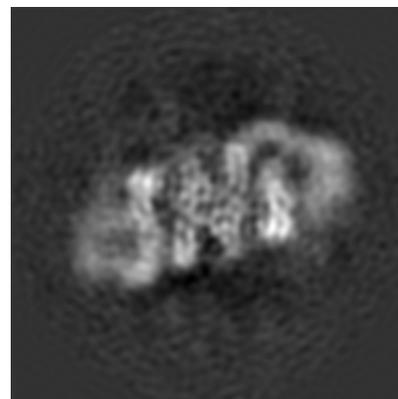
X Index: 140   Y Index: 140   Z Index: 140

6.2.2 Raw map
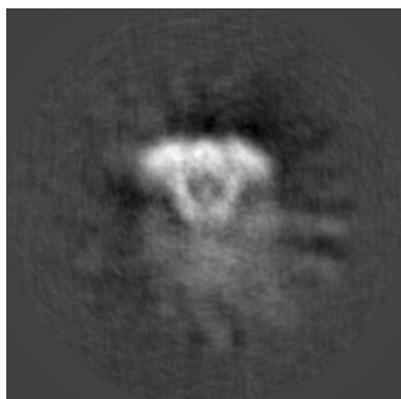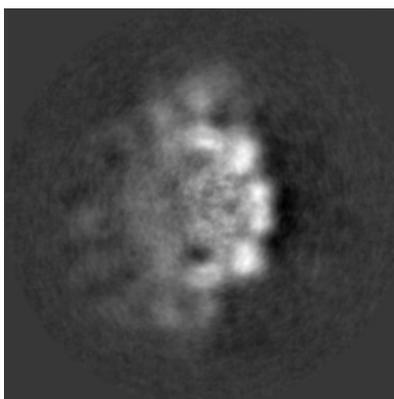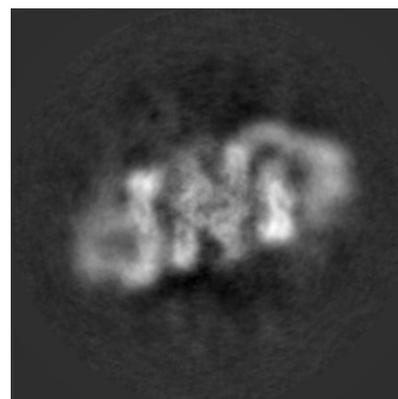
X Index: 140   Y Index: 140   Z Index: 140

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

6.3 Largest variance slices ⓘ
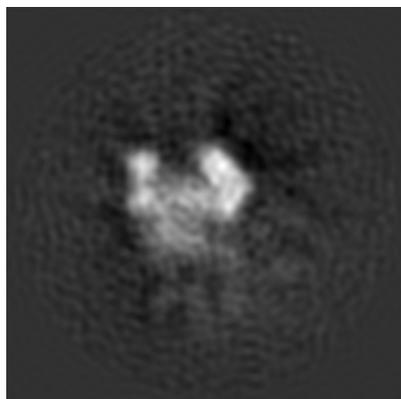
6.3.1 Primary map
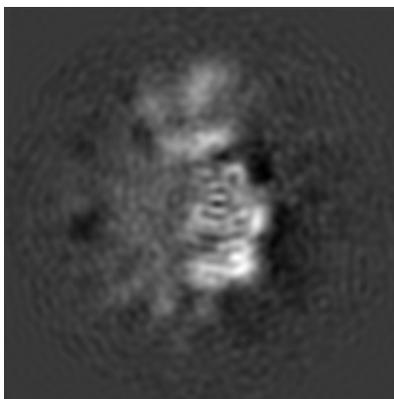
| X Index: 96 | Y Index: 152 | Z Index: 169 |
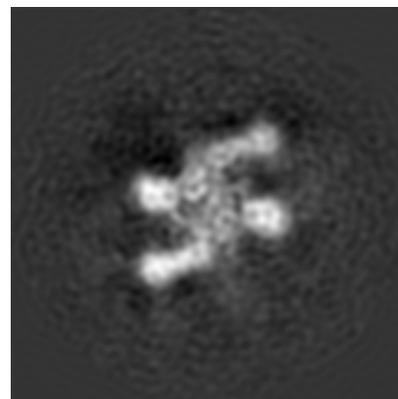
6.3.2 Raw map
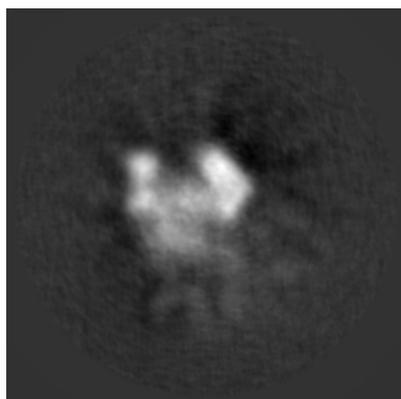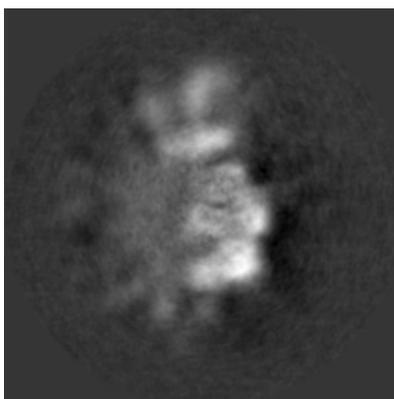
| X Index: 96 | Y Index: 150 | Z Index: 168 |
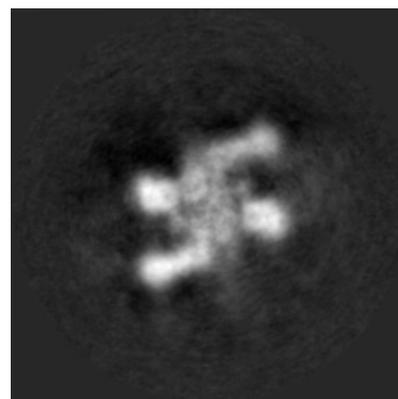
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X   Y   Z

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.

6.5 Mask visualisation (i)

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

7   Map analysis ⓘ

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

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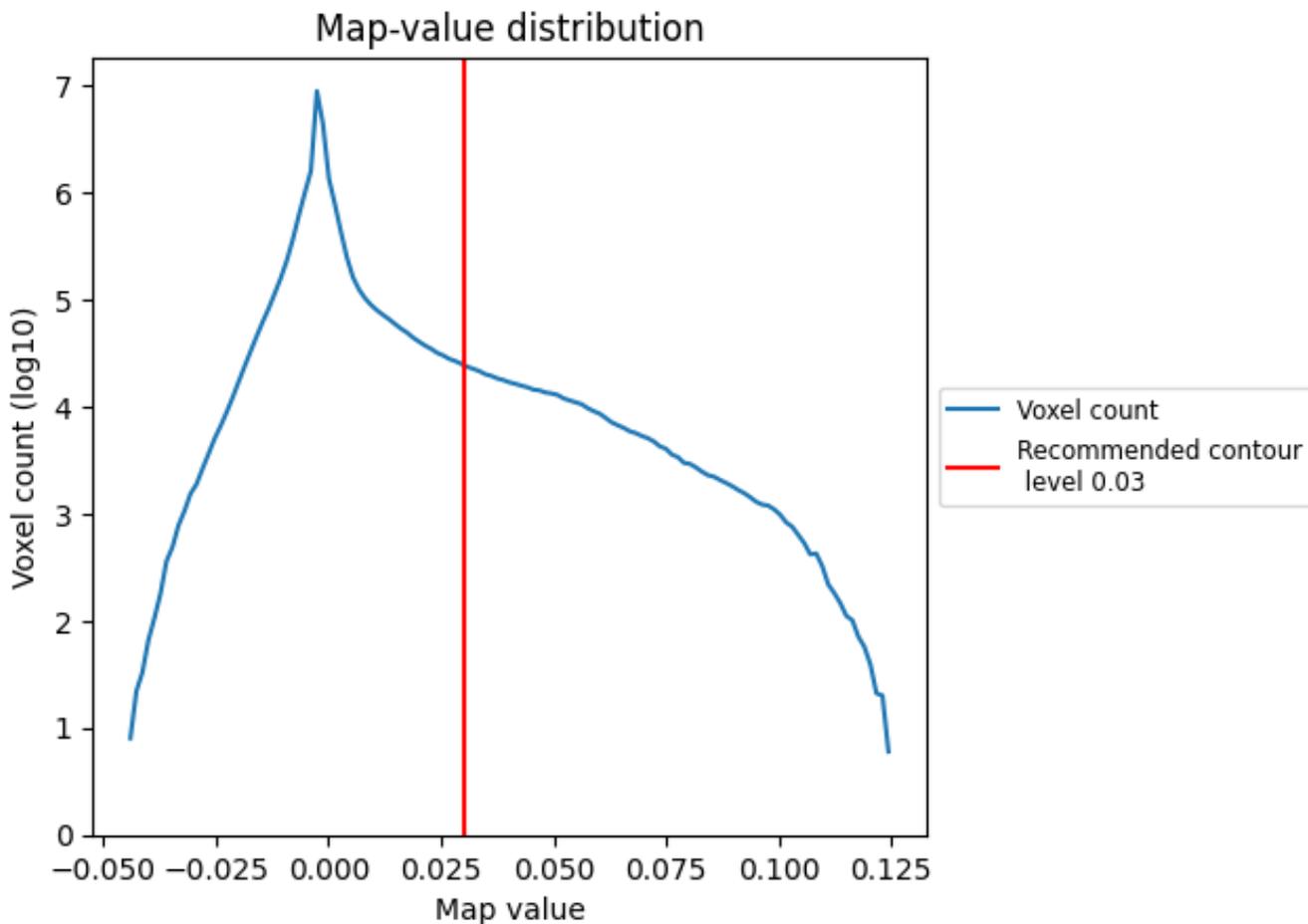
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate (i)
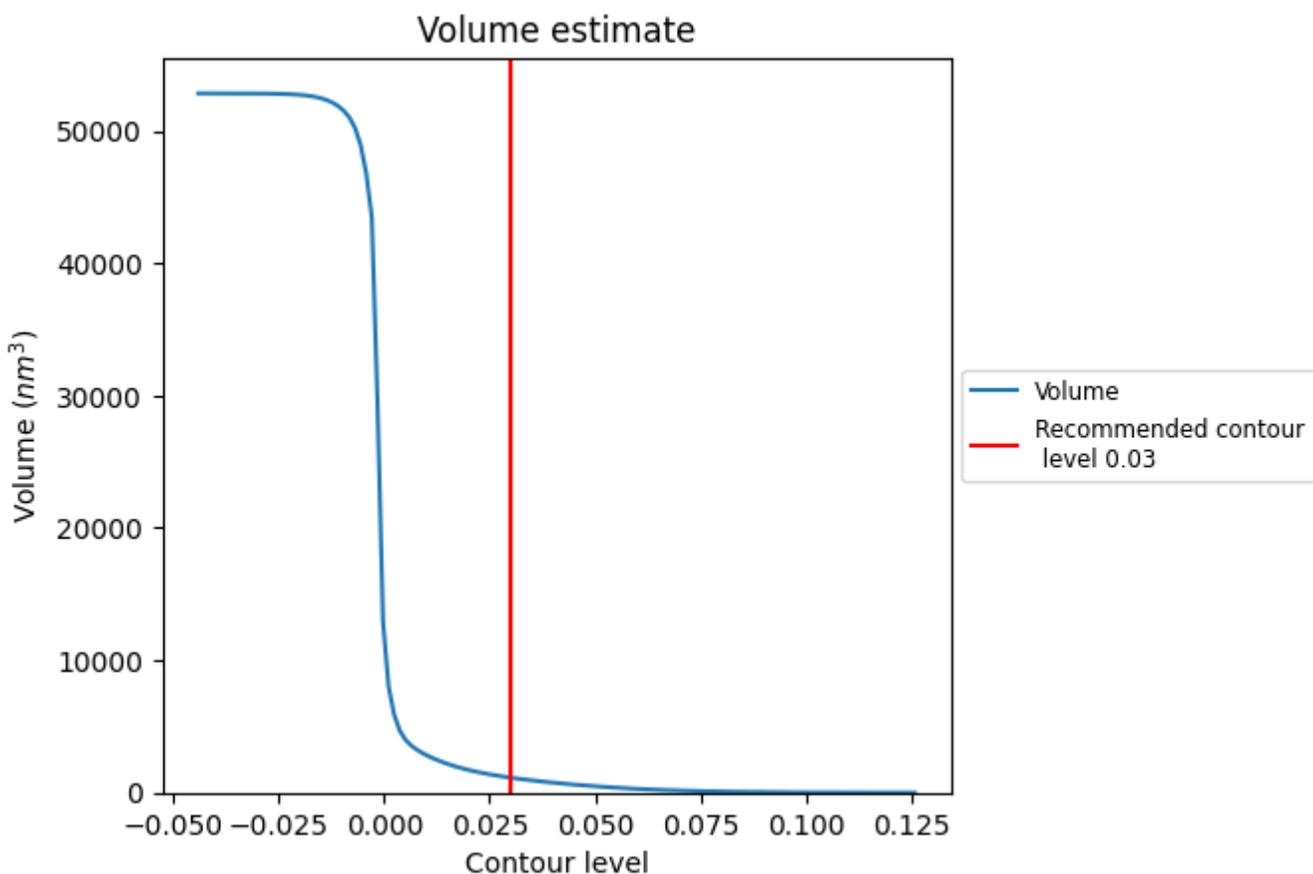
The volume at the recommended contour level is 1127 nm^3; this corresponds to an approximate mass of 1018 kDa.

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 ⓘ
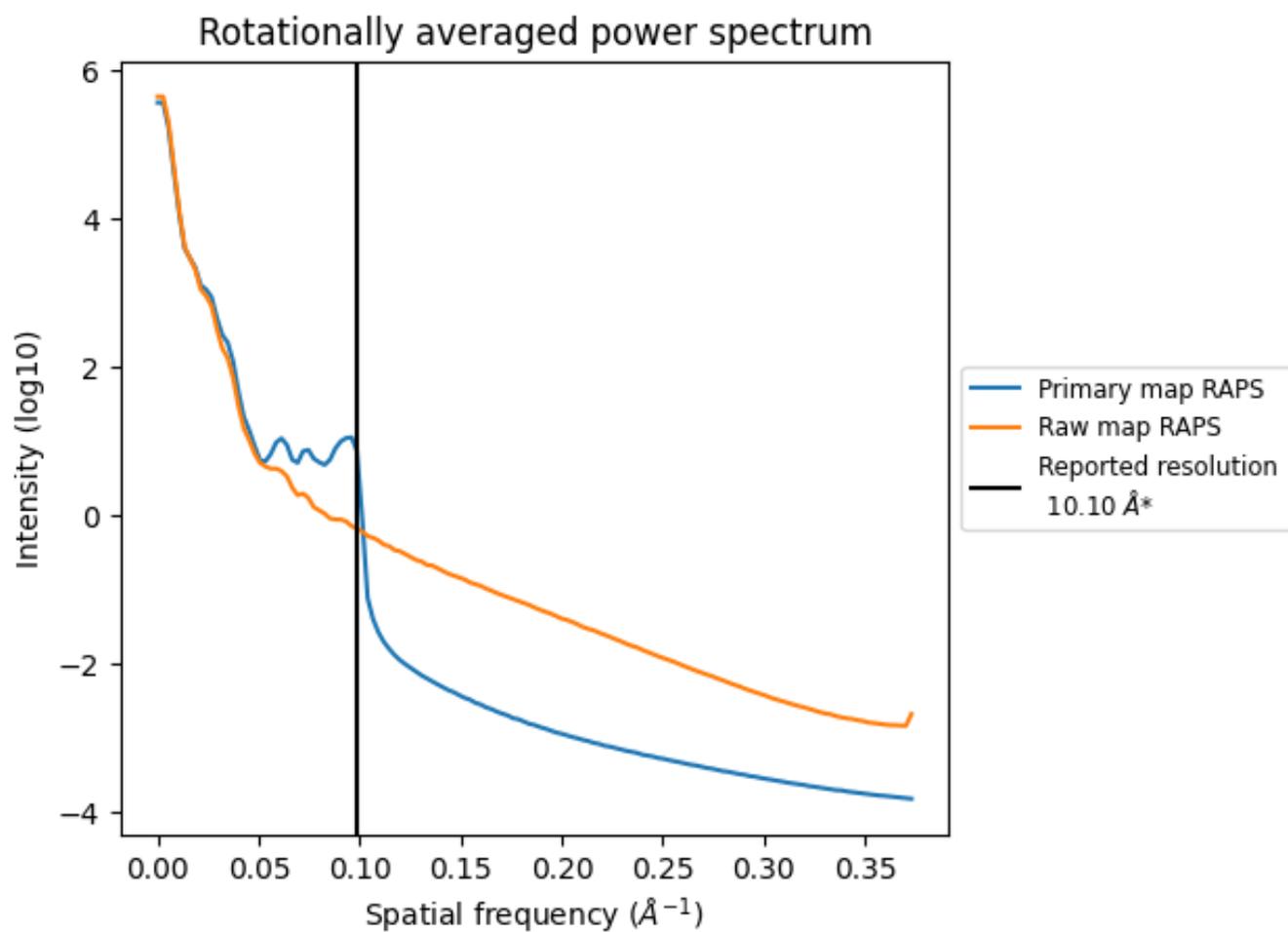
*Reported resolution corresponds to spatial frequency of 0.099 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
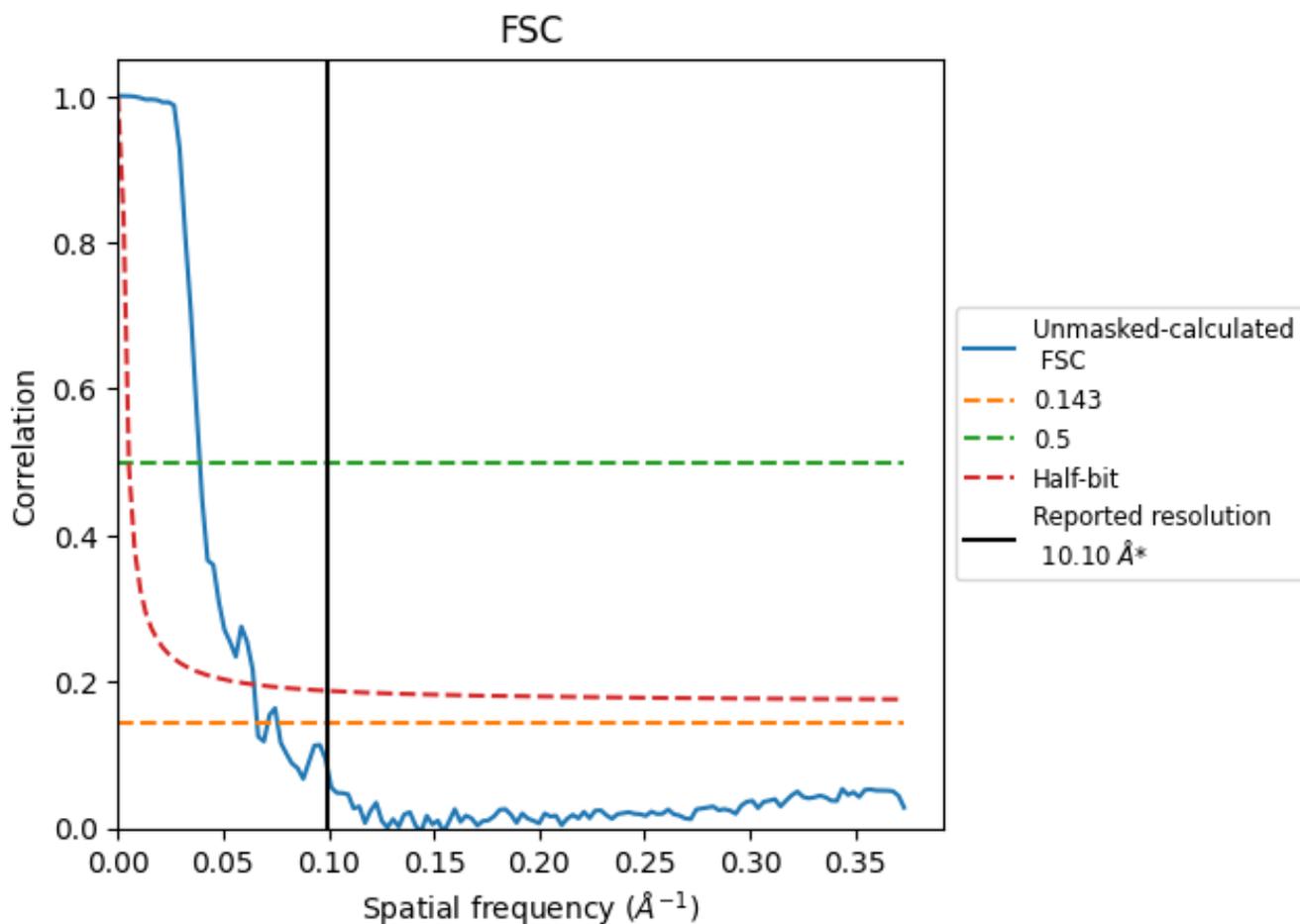
*Reported resolution corresponds to spatial frequency of 0.099 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	15.13	25.71	15.48

*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 15.13 differs from the reported value 10.1 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-4547 and PDB model 6QG5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ


X   Y   Z
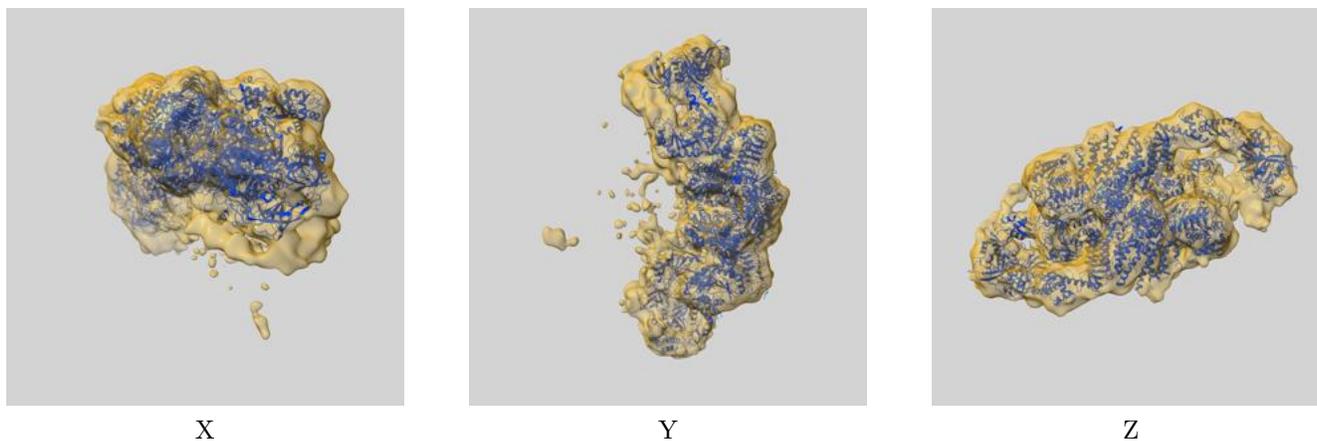
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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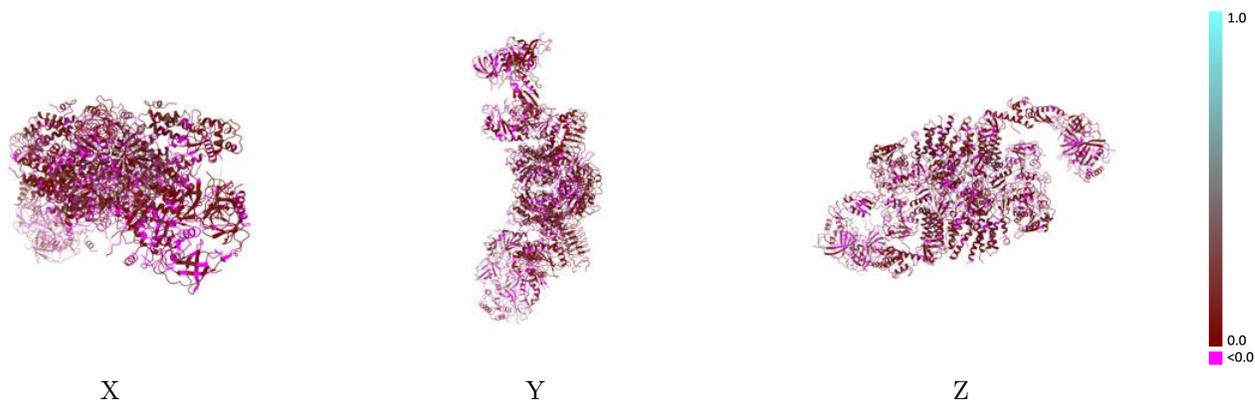
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
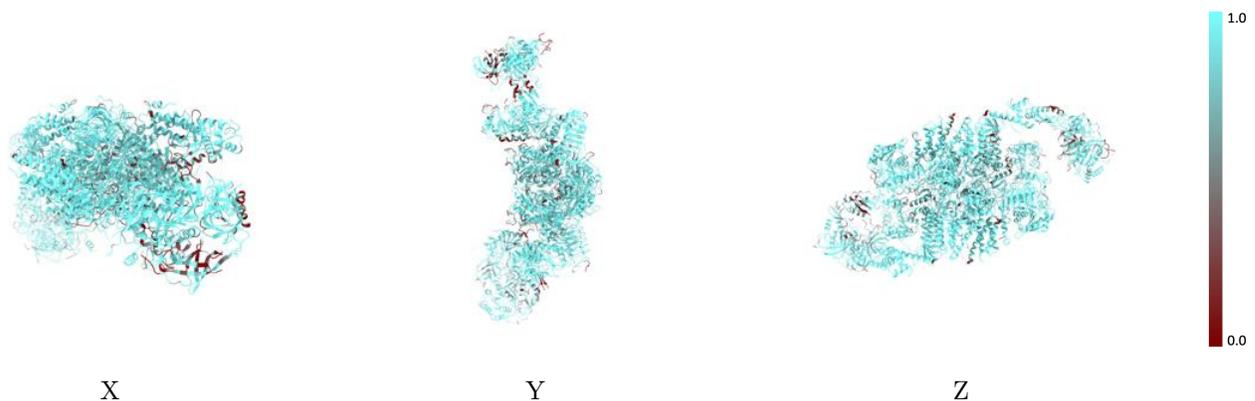
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4   Atom inclusion ⓘ
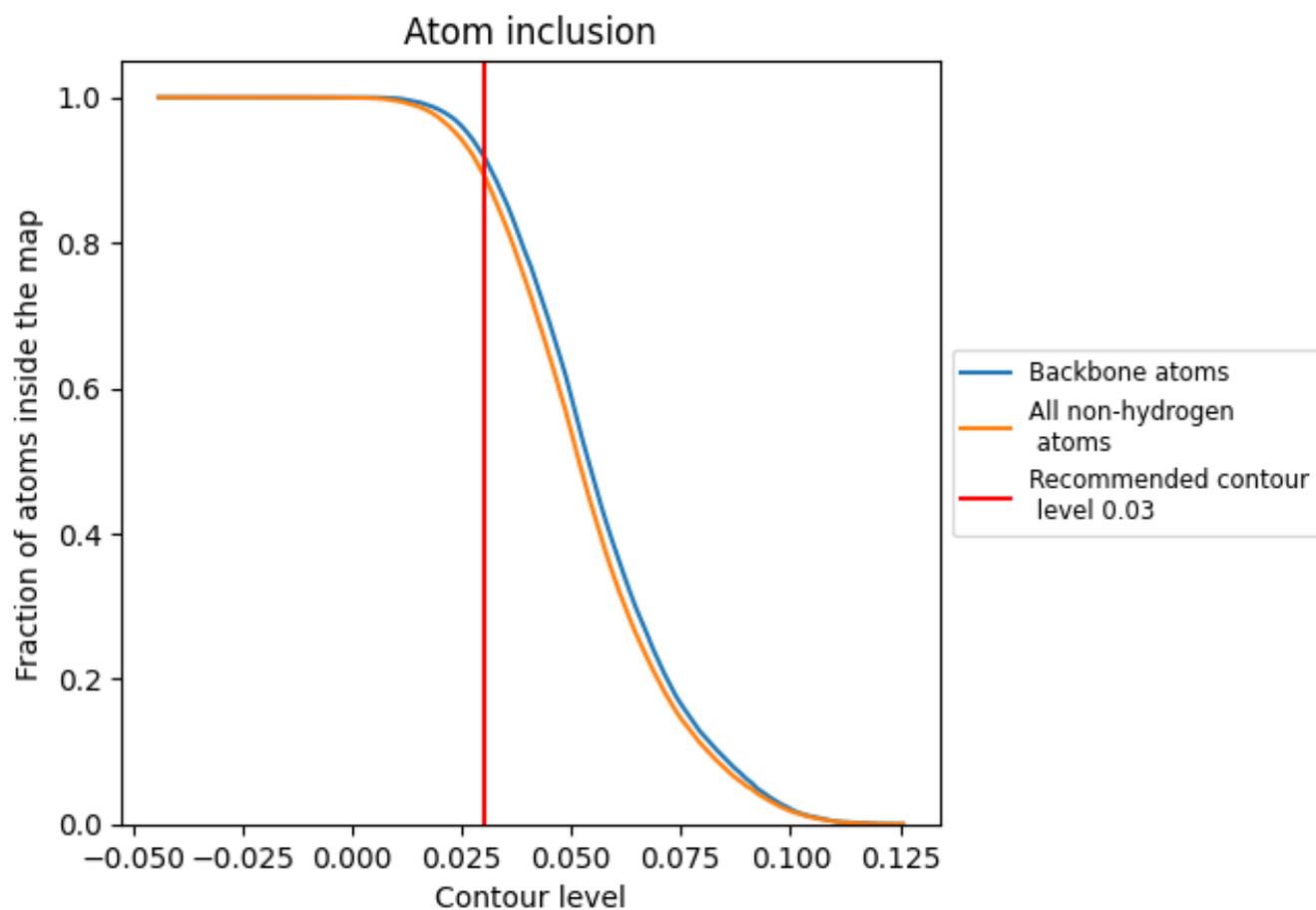
At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8939	0.0690
A	0.9745	0.0770
B	0.9597	0.0810
C	0.9019	0.0750
D	0.8881	0.0740
E	0.8669	0.0430
F	0.9119	0.0500
G	0.8504	0.0880
H	0.8393	0.0890
I	0.9588	0.0820
J	0.9618	0.0820
K	0.8277	0.0670
L	0.9835	0.0760
M	0.7875	0.0350
N	0.8862	0.0430
O	0.9130	0.0540
P	0.6851	0.0590

1.0

0.0
<0.0