Full wwPDB EM Validation Report

Mar 30, 2024 – 12:25 PM EDT

PDB ID	:	8TQZ
EMDB ID	:	EMD-41566
Title	:	Eukaryotic translation initiation factor 2B with a mutation (L516A) in the delta subunit
Authors	:	Wang, L.; Lawrence, R.; Sangwan, S.; Anand, A.; Shoemaker, S.; Deal, A.; Marqusee, S.; Watler, P.
Deposited on	:	2023-08-08
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

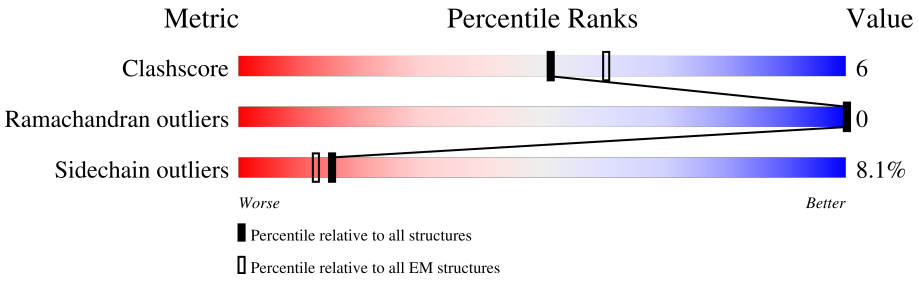
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	G	322	66% 15% • 17%
1	H	322	62% 17% • 19%
2	A	721	47% 9% • 43%
2	B	721	46% 10% • 43%
3	C	368	74% 12% 14%
3	D	368	69% 16% • 14%
4	E	523	37% 11% • 51%
4	F	523	55% 10% • 34%

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Mol	Chain	Length	Quality of chain
5	I	452	
5	J	452	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22334 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	G	266	Total 2039	C 1312	N 346	O 370	S 11	0	0
1	H	260	Total 2002	C 1293	N 336	O 364	S 9	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	MET	-	initiating methionine	UNP Q14232
G	-15	HIS	-	expression tag	UNP Q14232
G	-14	HIS	-	expression tag	UNP Q14232
G	-13	HIS	-	expression tag	UNP Q14232
G	-12	HIS	-	expression tag	UNP Q14232
G	-11	HIS	-	expression tag	UNP Q14232
G	-10	HIS	-	expression tag	UNP Q14232
G	-9	GLY	-	expression tag	UNP Q14232
G	-8	GLY	-	expression tag	UNP Q14232
G	-7	GLY	-	expression tag	UNP Q14232
G	-6	SER	-	expression tag	UNP Q14232
G	-5	GLU	-	expression tag	UNP Q14232
G	-4	ASN	-	expression tag	UNP Q14232
G	-3	LEU	-	expression tag	UNP Q14232
G	-2	TYR	-	expression tag	UNP Q14232
G	-1	PHE	-	expression tag	UNP Q14232
G	0	GLN	-	expression tag	UNP Q14232
G	1	SER	-	expression tag	UNP Q14232
H	-16	MET	-	initiating methionine	UNP Q14232
H	-15	HIS	-	expression tag	UNP Q14232
H	-14	HIS	-	expression tag	UNP Q14232
H	-13	HIS	-	expression tag	UNP Q14232
H	-12	HIS	-	expression tag	UNP Q14232
H	-11	HIS	-	expression tag	UNP Q14232
H	-10	HIS	-	expression tag	UNP Q14232
H	-9	GLY	-	expression tag	UNP Q14232

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-8	GLY	-	expression tag	UNP Q14232
H	-7	GLY	-	expression tag	UNP Q14232
H	-6	SER	-	expression tag	UNP Q14232
H	-5	GLU	-	expression tag	UNP Q14232
H	-4	ASN	-	expression tag	UNP Q14232
H	-3	LEU	-	expression tag	UNP Q14232
H	-2	TYR	-	expression tag	UNP Q14232
H	-1	PHE	-	expression tag	UNP Q14232
H	0	GLN	-	expression tag	UNP Q14232
H	1	SER	-	expression tag	UNP Q14232

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	414	Total	C	N	O	S	0	0
			3244	2048	576	605	15		
2	B	413	Total	C	N	O	S	0	0
			3239	2046	576	602	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 3 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	318	Total	C	N	O	S	0	0
			2483	1570	437	461	15		
3	C	318	Total	C	N	O	S	0	0
			2486	1571	438	462	15		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	256	Total	C	N	O	S	0	0
			1983	1254	356	363	10		
4	F	346	Total	C	N	O	S	0	0
			2690	1701	478	497	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	516	ALA	LEU	engineered mutation	UNP Q9UI10
F	516	ALA	LEU	engineered mutation	UNP Q9UI10

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

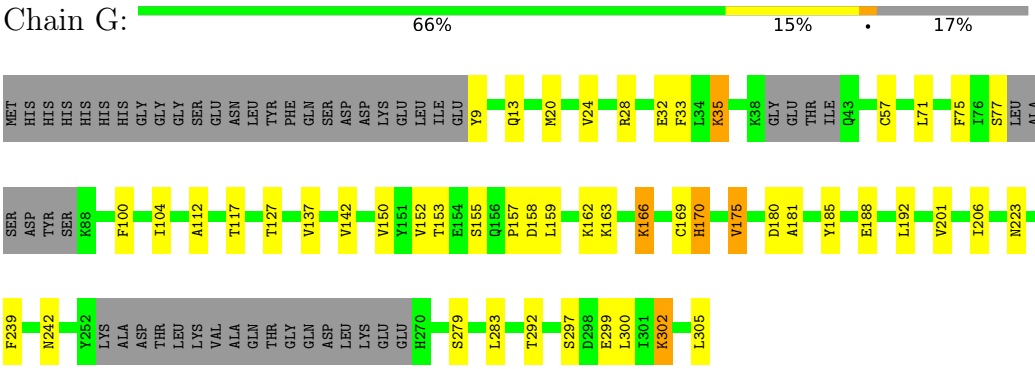
Mol	Chain	Residues	Atoms	AltConf	Trace
5	I	46	Total C N O S 380 252 69 57 2	0	0
5	J	226	Total C N O S 1788 1159 300 314 15	0	0

3 Residue-property plots (i)

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.

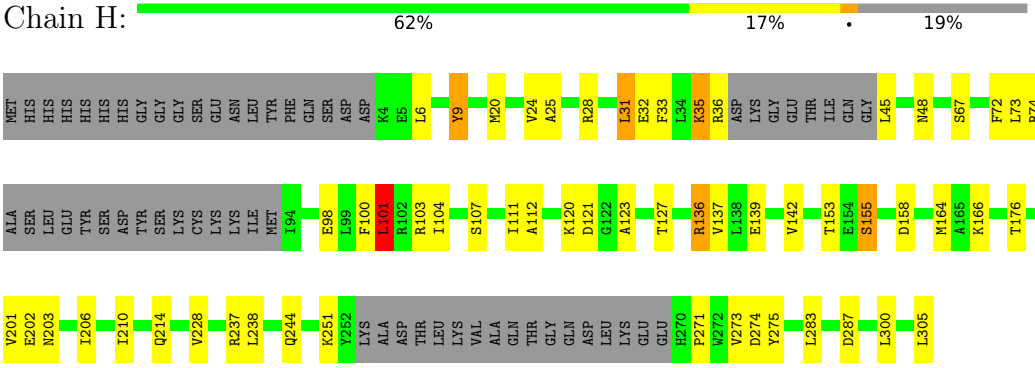
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain G:



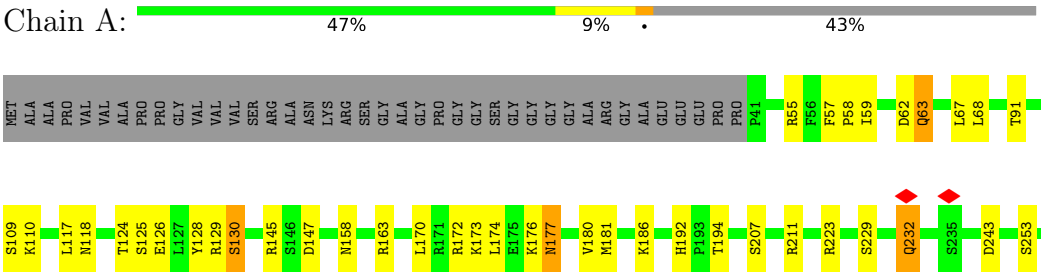
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

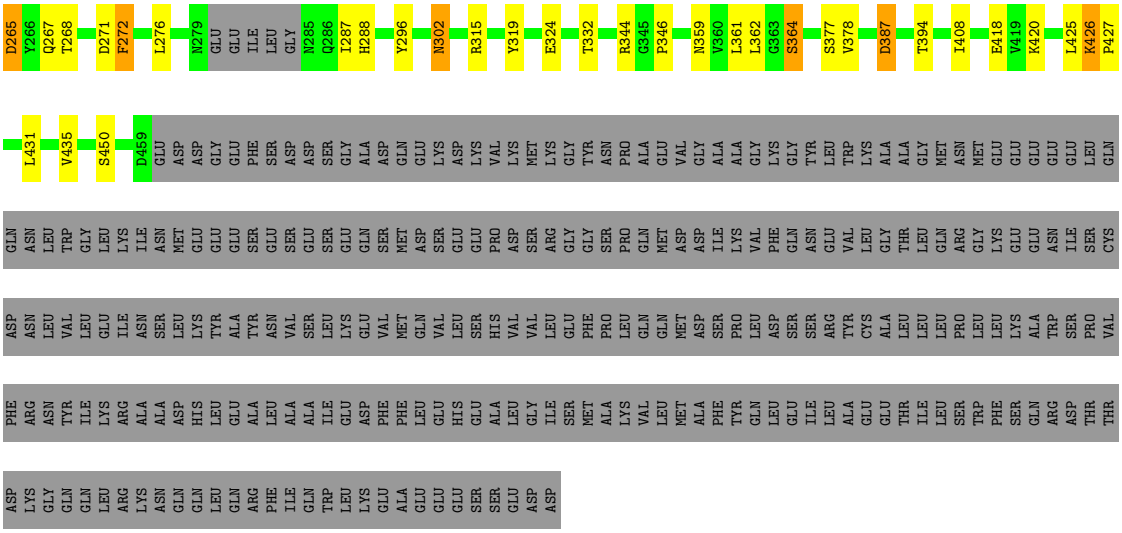
Chain H:



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

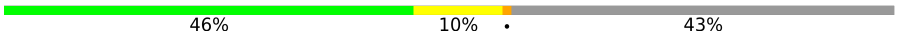
Chain A:

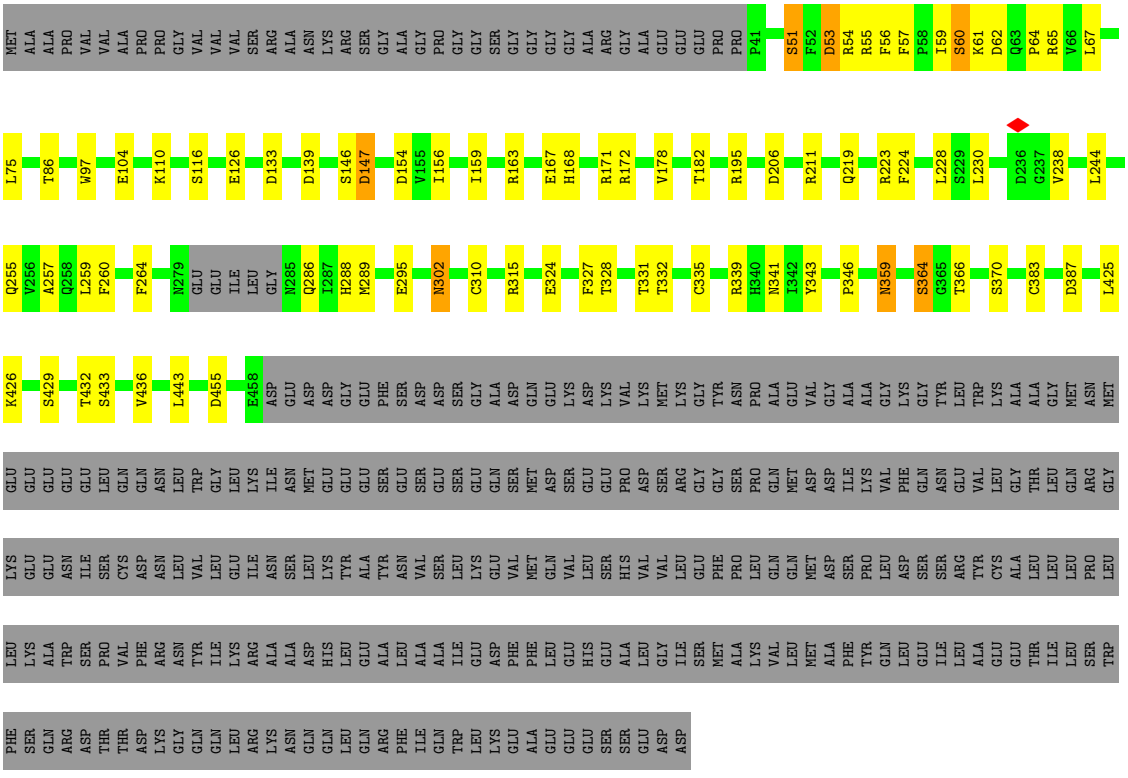




• Molecule 2: Translation initiation factor eIF-2B subunit epsilon

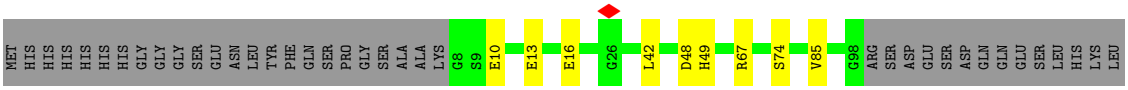
Chain B:

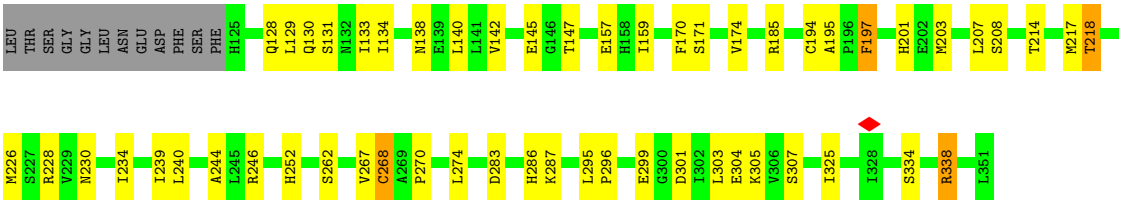




• Molecule 3: Translation initiation factor eIF-2B subunit beta

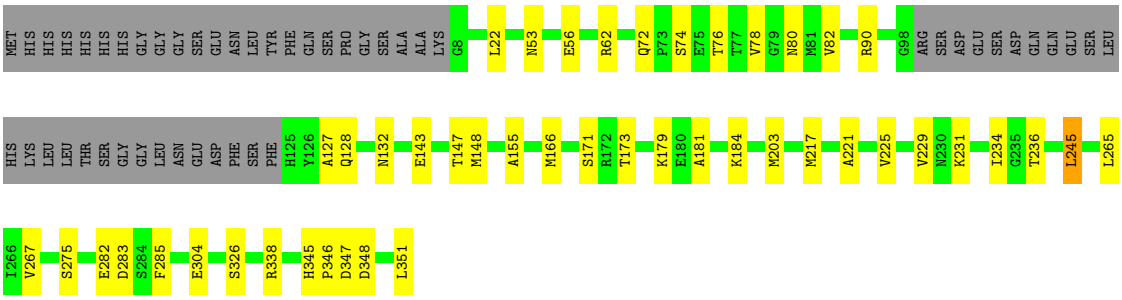
Chain D:





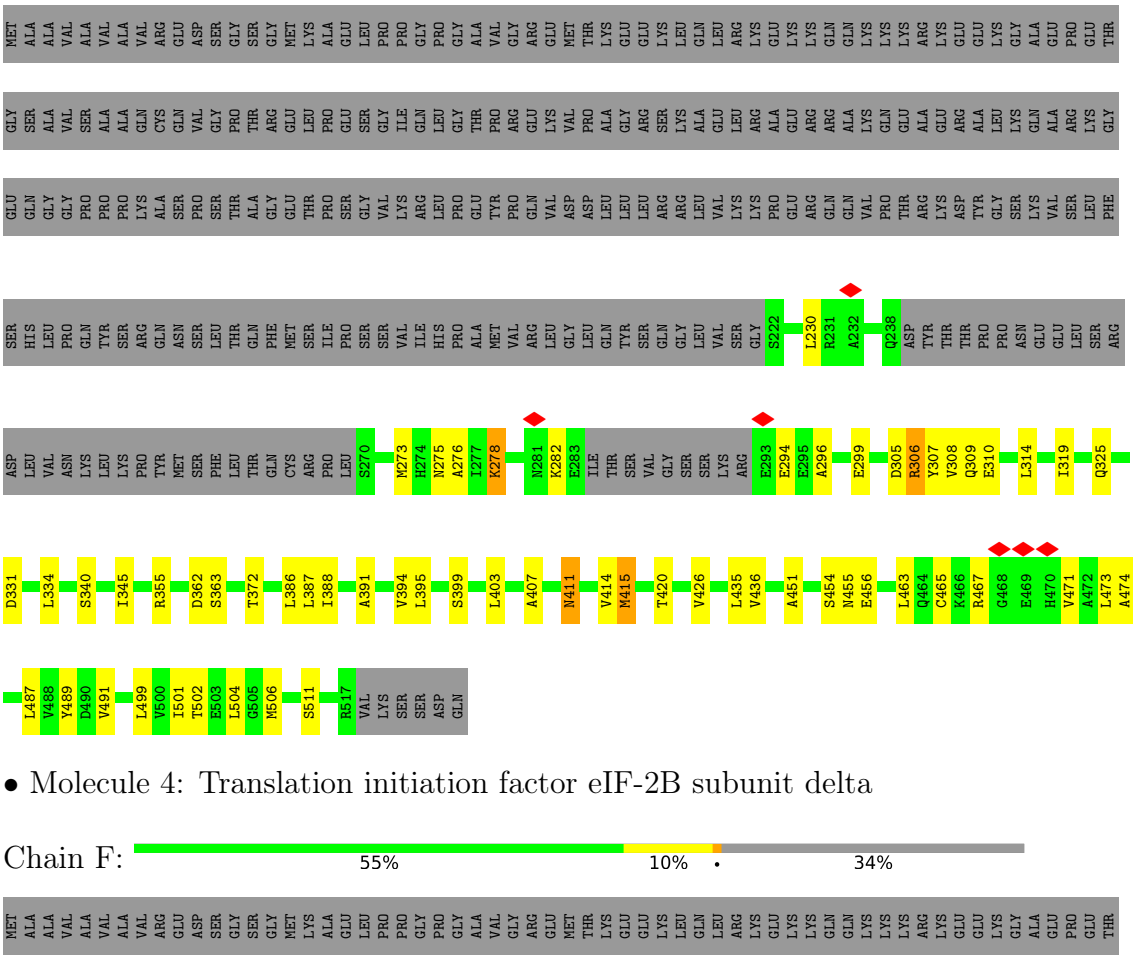
• Molecule 3: Translation initiation factor eIF-2B subunit beta

Chain C:



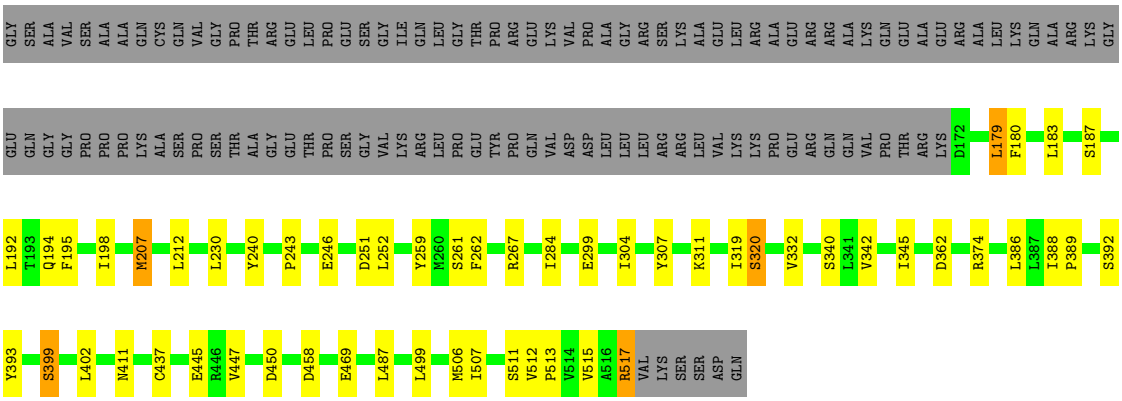
• Molecule 4: Translation initiation factor eIF-2B subunit delta

Chain E:



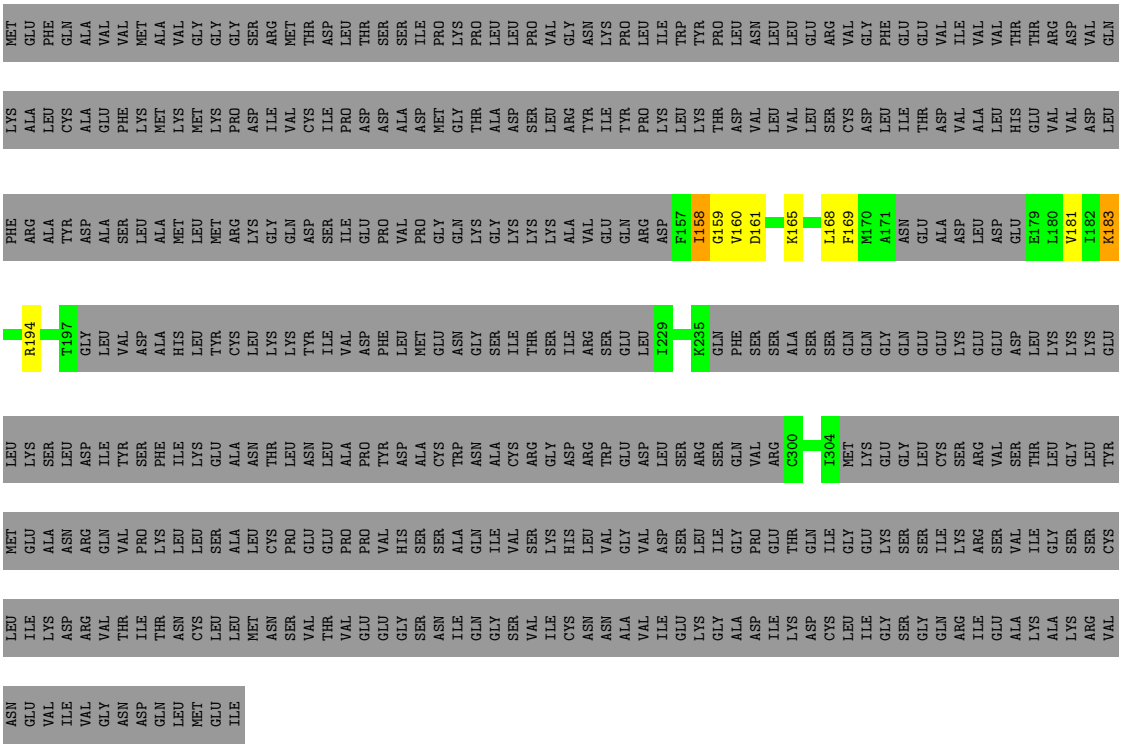
• Molecule 4: Translation initiation factor eIF-2B subunit delta

Chain F:



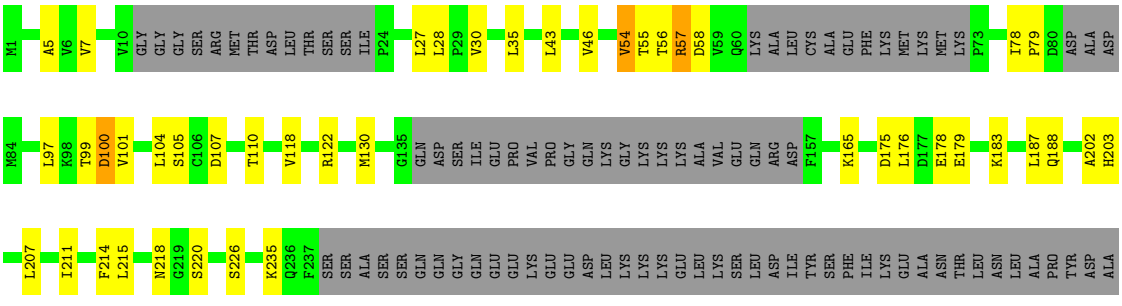
• Molecule 5: Translation initiation factor eIF-2B subunit gamma

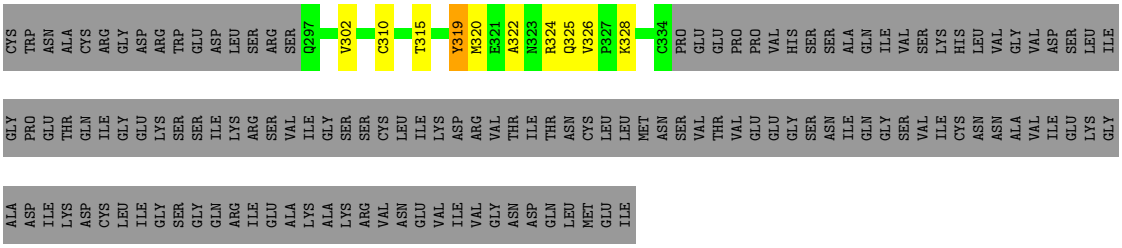
Chain I:



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

Chain J:




CYS TRP ASN ALA CYS ARG GLY ASP ARG TRP GLU ASP LEU SER ARG SER Q297 V302 C310 T315 Y319 M320 E321 A322 N323 R324 Q325 V326 P327 K328 C334 PRO GLU GLU PRO PRO VAL HIS SER SER ALA GLN ILE VAL SER LYS HIS LEU VAL GLY VAL ASP SER LEU ILE
GLY PRO GLU THR GLN ILE GLY GLU LYS SER SER ILE LYS ARG SER VAL ILE GLY SER SER CYS LEU ILE LYS ASP ARG VAL THR ILE THR ASN CYS LEU LEU MET ASN SER VAL THR VAL GLU GLU GLY SER ASN ILE GLN GLY SER VAL ILE CYS ASN ASN ALA VAL ILE GLU LYS GLY
ALA ASP ILE LYS ASP CYS LEU ILE GLY SER GLY GLN ARG ILE GLU ALA LYS ALA LYS ARG VAL ASN GLU VAL ILE VAL GLY ASN ASP GLN LEU MET GLU ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	327000	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 ($e^-/Å^2$)	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.823	Depositor
Minimum map value	-1.005	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	334.0, 334.0, 334.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	G	0.24	0/2071	0.47	0/2797
1	H	0.25	0/2034	0.49	1/2752 (0.0%)
2	A	0.24	0/3311	0.50	0/4507
2	B	0.24	0/3306	0.49	0/4500
3	C	0.25	0/2533	0.49	0/3426
3	D	0.25	0/2530	0.48	0/3422
4	E	0.24	0/2015	0.49	0/2738
4	F	0.25	0/2741	0.48	0/3726
5	I	0.24	0/386	0.52	0/513
5	J	0.25	0/1816	0.53	1/2449 (0.0%)
All	All	0.24	0/22743	0.49	2/30830 (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
2	B	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})
5	J	79	PRO	CA-N-CD	-5.54	103.74	111.50
1	H	101	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	57	PHE	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	G	2039	0	2094	21	0
1	H	2002	0	2060	29	0
2	A	3244	0	3222	42	0
2	B	3239	0	3221	38	0
3	C	2486	0	2500	22	0
3	D	2483	0	2496	29	0
4	E	1983	0	2025	27	0
4	F	2690	0	2739	29	0
5	I	380	0	407	11	0
5	J	1788	0	1863	31	0
All	All	22334	0	22627	261	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 6.

All (261) 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)
5:I:159:GLY:N	5:I:169:PHE:O	2.05	0.89
2:B:168:HIS:HA	2:B:171:ARG:HE	1.51	0.75
3:D:201:HIS:ND1	4:E:465:CYS:SG	2.61	0.74
1:H:101:LEU:HA	1:H:104:ILE:HG12	1.70	0.72
3:D:128:GLN:N	3:D:128:GLN:OE1	2.24	0.70
2:A:265:ASP:OD1	2:A:265:ASP:N	2.24	0.69
2:B:315:ARG:HH22	3:C:304:GLU:HA	1.59	0.68
3:C:338:ARG:O	3:C:338:ARG:NH1	2.27	0.68
3:C:128:GLN:OE1	3:C:128:GLN:N	2.25	0.68
2:A:302:ASN:OD1	2:A:302:ASN:N	2.27	0.66
2:A:223:ARG:HH12	5:I:183:LYS:HA	1.61	0.65
2:B:168:HIS:HD1	2:B:182:THR:HG1	1.44	0.65
4:E:455:ASN:ND2	4:E:489:TYR:O	2.31	0.64
2:B:139:ASP:HB2	2:B:257:ALA:HB1	1.80	0.64
5:J:322:ALA:O	5:J:326:VAL:HG23	1.98	0.62
3:D:195:ALA:HB1	4:E:387:LEU:HD13	1.81	0.62
4:F:207:MET:HG2	4:F:259:TYR:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:240:TYR:OH	4:F:251:ASP:OD2	2.17	0.62
1:H:206:ILE:HG21	1:H:228:VAL:HG11	1.81	0.61
3:C:128:GLN:O	3:C:132:ASN:ND2	2.32	0.61
3:D:171:SER:HB3	3:D:174:VAL:HB	1.82	0.61
1:G:180:ASP:OD1	1:G:180:ASP:N	2.34	0.61
1:G:150:VAL:HB	1:G:175:VAL:HG23	1.81	0.61
5:J:178:GLU:HG3	5:J:179:GLU:HG2	1.82	0.61
2:A:57:PHE:CD1	2:A:58:PRO:HD3	2.35	0.61
3:C:53:ASN:ND2	3:C:56:GLU:OE1	2.34	0.61
1:H:25:ALA:HA	1:H:28:ARG:HD2	1.83	0.60
2:A:55:ARG:HH21	2:A:302:ASN:HB3	1.67	0.60
2:B:56:PHE:O	2:B:60:SER:OG	2.14	0.59
4:E:471:VAL:HB	4:E:474:ALA:HB2	1.85	0.58
2:B:302:ASN:OD1	2:B:302:ASN:N	2.36	0.58
4:F:512:VAL:HG23	4:F:513:PRO:HD3	1.85	0.58
2:B:126:GLU:OE1	2:B:126:GLU:N	2.34	0.58
5:J:99:THR:HG22	5:J:100:ASP:H	1.67	0.58
1:G:188:GLU:OE2	1:H:244:GLN:NE2	2.37	0.57
1:H:202:GLU:OE2	1:H:237:ARG:NH1	2.37	0.57
2:A:315:ARG:NH1	3:D:303:LEU:O	2.35	0.57
5:J:130:MET:HB3	5:J:302:VAL:HG23	1.86	0.57
1:G:201:VAL:HG12	1:G:238:LEU:HB2	1.87	0.57
2:A:186:LYS:HE2	2:A:296:TYR:HA	1.87	0.57
1:H:287:ASP:N	1:H:287:ASP:OD1	2.33	0.57
2:A:163:ARG:HB2	2:A:163:ARG:NH1	2.18	0.57
4:E:395:LEU:HD11	4:E:426:VAL:HG13	1.87	0.57
2:B:366:THR:HG23	2:B:383:CYS:HB2	1.87	0.57
1:H:45:LEU:HA	1:H:48:ASN:HD21	1.68	0.56
2:B:339:ARG:NH2	4:F:393:TYR:O	2.38	0.56
1:G:71:LEU:HD13	1:G:305:LEU:HD12	1.86	0.56
1:G:112:ALA:HA	1:G:137:VAL:HG22	1.87	0.56
1:G:206:ILE:HG21	1:G:228:VAL:HG11	1.87	0.56
2:B:432:THR:HG22	2:B:433:SER:H	1.70	0.56
1:G:299:GLU:HA	1:G:302:LYS:HG2	1.88	0.56
2:B:65:ARG:NH2	2:B:154:ASP:OD2	2.40	0.55
2:A:170:LEU:O	2:A:174:LEU:HD22	2.06	0.55
3:D:130:GLN:O	3:D:134:ILE:HG12	2.06	0.55
4:F:499:LEU:HD11	4:F:506:MET:HG2	1.89	0.55
1:G:100:PHE:O	1:G:104:ILE:HD12	2.07	0.54
2:B:53:ASP:OD1	2:B:65:ARG:NH1	2.40	0.54
4:F:469:GLU:N	4:F:469:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:306:ARG:HB2	4:E:306:ARG:NH1	2.23	0.54
4:E:435:LEU:HD23	4:E:501:ILE:HD11	1.88	0.54
5:J:7:VAL:HG12	5:J:7:VAL:O	2.07	0.54
2:A:181:MET:HB3	2:A:287:ILE:HD13	1.90	0.54
2:A:361:LEU:HB3	2:A:378:VAL:HG22	1.90	0.54
2:A:426:LYS:HG3	2:A:427:PRO:HD2	1.90	0.54
2:B:223:ARG:HH12	5:J:183:LYS:HG2	1.72	0.54
5:J:56:THR:OG1	5:J:57:ARG:N	2.41	0.54
1:H:203:ASN:ND2	1:H:275:TYR:OH	2.41	0.54
2:A:180:VAL:HG22	2:A:256:VAL:HG23	1.88	0.54
4:E:411:ASN:O	4:E:411:ASN:ND2	2.38	0.53
4:F:198:ILE:O	5:J:122:ARG:NH2	2.41	0.53
3:C:62:ARG:NH1	3:C:351:LEU:O	2.41	0.53
5:J:105:SER:HB2	5:J:203:HIS:HB3	1.90	0.53
2:A:346:PRO:HD2	2:A:364:SER:HB2	1.90	0.53
2:B:59:ILE:HG23	2:B:432:THR:HG23	1.91	0.53
1:H:120:LYS:HG3	1:H:123:ALA:HB2	1.91	0.52
3:C:78:VAL:O	3:C:82:VAL:HG23	2.09	0.52
2:A:176:LYS:O	2:A:177:ASN:ND2	2.42	0.52
3:D:74:SER:O	3:D:246:ARG:NH1	2.42	0.52
2:A:268:THR:OG1	2:A:271:ASP:OD2	2.23	0.52
5:J:100:ASP:OD1	5:J:100:ASP:N	2.43	0.51
2:A:272:PHE:HE1	2:A:276:LEU:HD22	1.76	0.51
2:A:211:ARG:HA	2:A:288:HIS:HA	1.92	0.51
4:E:319:ILE:HG22	4:E:345:ILE:HD11	1.93	0.51
2:B:195:ARG:NH2	2:B:244:LEU:O	2.44	0.51
5:I:159:GLY:HA3	5:I:169:PHE:H	1.75	0.50
2:B:61:LYS:NZ	2:B:455:ASP:OD2	2.44	0.50
4:F:445:GLU:OE1	4:F:517:ARG:NH2	2.42	0.50
5:J:325:GLN:HA	5:J:328:LYS:HZ1	1.77	0.50
2:A:229:SER:HA	2:A:232:GLN:HB2	1.93	0.50
2:A:243:ASP:OD1	2:A:243:ASP:N	2.43	0.50
1:H:210:ILE:HD12	1:H:274:ASP:HB3	1.93	0.50
2:A:130:SER:OG	2:A:267:GLN:O	2.29	0.50
4:E:403:LEU:HD13	4:E:420:THR:HG23	1.93	0.49
1:G:153:THR:HG22	1:G:155:SER:H	1.78	0.49
3:D:239:ILE:HB	3:D:274:LEU:HD12	1.94	0.49
4:F:320:SER:HA	4:F:345:ILE:HG12	1.94	0.49
3:C:282:GLU:HB3	3:C:285:PHE:HB2	1.94	0.49
4:F:299:GLU:OE1	4:F:299:GLU:N	2.45	0.49
1:H:9:TYR:HD2	1:H:9:TYR:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:304:GLU:HG3	3:D:305:LYS:HG3	1.94	0.49
2:B:56:PHE:HB2	2:B:65:ARG:HD2	1.95	0.49
3:C:90:ARG:NH1	3:C:348:ASP:OD1	2.46	0.49
4:F:230:LEU:HD22	4:F:304:ILE:HG23	1.95	0.49
4:F:319:ILE:HG22	4:F:345:ILE:HD11	1.93	0.49
4:F:243:PRO:HG2	4:F:246:GLU:HB3	1.95	0.48
5:J:55:THR:OG1	5:J:56:THR:N	2.46	0.48
2:A:106:LEU:O	2:A:109:SER:OG	2.27	0.48
3:D:129:LEU:O	3:D:133:ILE:HG12	2.13	0.48
5:I:158:ILE:HG22	5:I:160:VAL:HG23	1.95	0.48
5:J:214:PHE:O	5:J:218:ASN:ND2	2.46	0.48
4:F:342:VAL:HG13	4:F:402:LEU:HD23	1.96	0.48
2:A:67:LEU:HD21	2:A:102:ILE:HG23	1.96	0.48
2:A:431:LEU:HB3	2:A:435:VAL:HG21	1.95	0.48
3:D:218:THR:HG23	4:E:463:LEU:HD21	1.95	0.48
5:J:97:LEU:HD22	5:J:101:VAL:HG11	1.96	0.48
5:I:159:GLY:HA3	5:I:169:PHE:N	2.28	0.48
3:D:147:THR:HG21	3:D:270:PRO:HB3	1.96	0.47
2:A:418:GLU:OE2	2:A:420:LYS:NZ	2.47	0.47
4:E:502:THR:HG22	4:E:504:LEU:H	1.79	0.47
4:F:332:VAL:H	4:F:399:SER:HB3	1.79	0.47
3:C:76:THR:O	3:C:80:ASN:ND2	2.46	0.47
4:F:388:ILE:HG22	4:F:389:PRO:HD3	1.96	0.47
4:E:305:ASP:O	4:E:309:GLN:HG2	2.14	0.47
5:I:158:ILE:HD12	5:I:158:ILE:HA	1.74	0.47
1:H:136:ARG:HA	1:H:139:GLU:HG2	1.97	0.47
5:I:161:ASP:HB3	5:I:168:LEU:HD13	1.97	0.47
4:F:511:SER:O	4:F:511:SER:OG	2.33	0.47
4:E:363:SER:HB2	4:E:388:ILE:HG13	1.97	0.46
2:B:64:PRO:HD2	2:B:67:LEU:HD12	1.96	0.46
2:A:207:SER:OG	5:I:194:ARG:NH2	2.48	0.46
3:D:138:ASN:O	3:D:142:VAL:HG12	2.16	0.46
5:J:320:MET:HB3	5:J:324:ARG:HH22	1.80	0.46
4:E:275:ASN:HA	4:E:278:LYS:HD3	1.97	0.46
2:A:387:ASP:N	2:A:387:ASP:OD1	2.48	0.46
4:F:192:LEU:HD11	4:F:262:PHE:HE1	1.80	0.46
4:F:252:LEU:HD23	4:F:284:ILE:HG12	1.98	0.46
4:F:507:ILE:HD13	4:F:515:VAL:HG11	1.98	0.46
3:D:128:GLN:O	3:D:131:SER:OG	2.34	0.46
1:G:32:GLU:HA	1:G:35:LYS:HE2	1.98	0.46
2:A:145:ARG:HB3	2:A:145:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:268:CYS:HA	3:D:325:ILE:HB	1.96	0.46
5:J:110:THR:HG22	5:J:310:CYS:HA	1.98	0.46
2:B:51:SER:OG	2:B:53:ASP:OD1	2.34	0.45
2:A:192:HIS:HE2	3:D:303:LEU:HD12	1.81	0.45
2:B:346:PRO:HG2	2:B:364:SER:HB2	1.97	0.45
4:F:411:ASN:HD22	4:F:447:VAL:HG13	1.81	0.45
2:B:255:GLN:O	2:B:259:LEU:HD13	2.15	0.45
5:J:5:ALA:HB1	5:J:43:LEU:HD13	1.98	0.45
2:B:211:ARG:HA	2:B:288:HIS:HA	1.98	0.45
5:J:235:LYS:HD2	5:J:235:LYS:HA	1.64	0.45
2:A:129:ARG:HA	2:A:129:ARG:HD3	1.79	0.45
3:D:338:ARG:HA	3:D:338:ARG:HD3	1.66	0.45
4:E:499:LEU:HD11	4:E:506:MET:HB3	1.99	0.45
2:B:425:LEU:HG	2:B:443:LEU:HD12	1.98	0.45
1:H:158:ASP:OD1	1:H:158:ASP:N	2.50	0.45
5:J:27:LEU:HD11	5:J:58:ASP:HB2	1.99	0.45
4:E:391:ALA:HA	4:E:394:VAL:HG12	1.98	0.45
4:F:450:ASP:OD1	4:F:450:ASP:N	2.50	0.45
1:H:201:VAL:HG12	1:H:238:LEU:HB2	1.99	0.44
2:A:276:LEU:HD23	2:A:287:ILE:HD11	1.99	0.44
2:B:178:VAL:HG12	2:B:286:GLN:HG3	1.99	0.44
3:C:155:ALA:HB1	3:C:181:ALA:HB2	1.98	0.44
1:H:107:SER:O	1:H:111:ILE:HG13	2.18	0.44
2:B:324:GLU:H	2:B:324:GLU:HG3	1.66	0.44
1:H:98:GLU:O	1:H:101:LEU:HD23	2.17	0.44
2:B:228:LEU:HD11	5:J:176:LEU:HD11	1.98	0.44
3:C:231:LYS:HE3	3:C:231:LYS:HB2	1.61	0.44
3:D:295:LEU:HG	3:D:299:GLU:HG3	1.99	0.44
2:B:238:VAL:HG22	2:B:238:VAL:O	2.17	0.44
2:B:341:ASN:HB2	2:B:359:ASN:HB3	2.00	0.44
2:A:63:GLN:HG2	2:A:68:LEU:HD23	2.00	0.43
3:D:10:GLU:O	3:D:13:GLU:HG2	2.18	0.43
1:H:32:GLU:HA	1:H:35:LYS:HE2	2.00	0.43
2:A:276:LEU:HD12	2:A:276:LEU:HA	1.80	0.43
4:E:487:LEU:HA	4:E:487:LEU:HD23	1.81	0.43
5:I:165:LYS:HD3	5:I:165:LYS:N	2.33	0.43
4:F:179:LEU:H	4:F:179:LEU:HD12	1.83	0.43
3:D:159:ILE:O	3:D:185:ARG:NH1	2.51	0.43
4:E:414:VAL:HG11	4:E:436:VAL:HG11	1.99	0.43
1:H:35:LYS:H	1:H:35:LYS:HD2	1.83	0.43
1:H:112:ALA:HA	1:H:137:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:344:ARG:HG2	2:A:362:LEU:HD12	2.00	0.43
1:G:242:ASN:N	1:G:242:ASN:OD1	2.51	0.43
3:C:143:GLU:O	3:C:147:THR:HG23	2.19	0.43
1:H:283:LEU:HD12	1:H:283:LEU:HA	1.91	0.43
5:I:159:GLY:CA	5:I:169:PHE:O	2.67	0.43
2:B:370:SER:OG	2:B:387:ASP:OD2	2.35	0.43
3:C:221:ALA:HB1	4:F:487:LEU:HD13	2.00	0.43
4:F:198:ILE:HD12	5:J:118:VAL:HG11	2.01	0.43
1:H:24:VAL:HG12	1:H:28:ARG:HE	1.84	0.43
4:F:307:TYR:O	4:F:311:LYS:HB2	2.19	0.43
2:A:272:PHE:CE1	2:A:276:LEU:HD22	2.54	0.42
1:G:181:ALA:HA	1:H:214:GLN:HE22	1.83	0.42
1:G:13:GLN:OE1	1:G:13:GLN:N	2.50	0.42
1:G:158:ASP:N	1:G:158:ASP:OD1	2.52	0.42
2:A:173:LYS:HB2	2:A:173:LYS:HE2	1.75	0.42
2:A:260:PHE:HD1	2:A:260:PHE:HA	1.67	0.42
3:D:194:CYS:HB2	3:D:197:PHE:O	2.19	0.42
5:J:101:VAL:HG23	5:J:207:LEU:HB2	2.00	0.42
3:D:301:ASP:OD1	3:D:301:ASP:N	2.43	0.42
4:E:310:GLU:HA	4:E:314:LEU:HD12	2.01	0.42
3:D:240:LEU:HD12	3:D:244:ALA:HB3	2.01	0.42
2:B:163:ARG:O	2:B:167:GLU:HG2	2.18	0.42
5:J:30:VAL:HG21	5:J:35:LEU:HD13	2.01	0.42
3:D:42:LEU:HD13	3:D:85:VAL:HG21	2.01	0.42
1:G:166:LYS:HB2	1:G:166:LYS:HE2	1.90	0.42
2:A:59:ILE:N	2:A:59:ILE:HD12	2.34	0.42
3:D:234:ILE:HG13	3:D:267:VAL:HG22	2.00	0.42
4:E:296:ALA:O	4:E:299:GLU:HG3	2.20	0.42
2:B:54:ARG:HD3	2:B:54:ARG:HA	1.80	0.42
2:B:335:CYS:SG	2:B:343:TYR:HB3	2.60	0.42
3:C:234:ILE:HD11	3:C:265:LEU:HD21	2.00	0.42
5:J:28:LEU:HD13	5:J:319:TYR:CE1	2.54	0.42
3:D:67:ARG:HE	3:D:67:ARG:HB3	1.62	0.42
5:J:57:ARG:HA	5:J:57:ARG:HD2	1.87	0.42
4:E:407:ALA:HB3	4:E:415:MET:HE2	2.01	0.42
5:J:207:LEU:HD22	5:J:211:ILE:HG21	2.02	0.42
1:H:203:ASN:OD1	1:H:203:ASN:N	2.49	0.41
2:A:125:SER:OG	2:A:126:GLU:N	2.53	0.41
1:G:24:VAL:O	1:G:28:ARG:HG2	2.20	0.41
1:H:251:LYS:HA	1:H:273:VAL:HG22	2.02	0.41
2:A:408:ILE:HG23	2:A:425:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ASP:OD1	2:B:154:ASP:N	2.51	0.41
5:J:54:VAL:HG13	5:J:78:ILE:HG23	2.02	0.41
1:G:185:TYR:CE2	1:H:271:PRO:HG3	2.56	0.41
4:E:305:ASP:HA	4:E:308:VAL:HG22	2.03	0.41
5:J:187:LEU:HD23	5:J:187:LEU:HA	1.90	0.41
1:G:170:HIS:ND1	1:G:170:HIS:C	2.73	0.41
1:H:153:THR:HG22	1:H:155:SER:H	1.85	0.41
3:D:129:LEU:CD2	3:D:133:ILE:HD11	2.51	0.41
5:J:325:GLN:HA	5:J:328:LYS:NZ	2.34	0.41
3:C:127:ALA:HB3	3:C:128:GLN:OE1	2.20	0.41
1:H:100:PHE:O	1:H:104:ILE:HG23	2.21	0.41
3:D:207:LEU:HB3	3:D:214:THR:HG21	2.03	0.41
1:G:283:LEU:HD23	1:G:283:LEU:HA	1.89	0.41
2:B:230:LEU:H	2:B:230:LEU:HD12	1.86	0.41
4:E:511:SER:O	4:E:511:SER:OG	2.38	0.41
2:B:146:SER:OG	2:B:147:ASP:N	2.53	0.41
3:C:245:LEU:HD21	3:C:267:VAL:HG21	2.03	0.41
3:C:345:HIS:ND1	3:C:346:PRO:HD2	2.36	0.41
4:F:194:GLN:H	4:F:194:GLN:HG2	1.59	0.41
4:F:212:LEU:HD12	4:F:212:LEU:HA	1.96	0.41
4:E:230:LEU:HD21	4:E:276:ALA:HB1	2.03	0.41
4:E:451:ALA:HA	4:E:491:VAL:HG22	2.02	0.41
2:B:75:LEU:HD22	2:B:156:ILE:HD11	2.02	0.41
2:B:110:LYS:NZ	2:B:327:PHE:O	2.44	0.41
3:C:22:LEU:HG	3:C:72:GLN:HB2	2.02	0.41
3:D:296:PRO:HG2	3:D:299:GLU:HG2	2.02	0.40
2:B:159:ILE:HG12	2:B:295:GLU:HB2	2.02	0.40
3:C:234:ILE:HG13	3:C:267:VAL:HG22	2.03	0.40
1:H:28:ARG:HA	1:H:31:LEU:CD2	2.51	0.40
2:A:158:ASN:ND2	2:A:319:TYR:O	2.50	0.40
4:E:387:LEU:HA	4:E:387:LEU:HD23	1.86	0.40
5:I:158:ILE:CG2	5:I:160:VAL:HG23	2.50	0.40
3:C:166:MET:HE2	3:C:229:VAL:HG21	2.02	0.40
3:C:236:THR:HB	3:C:245:LEU:HD22	2.04	0.40
5:J:202:ALA:HB2	5:J:310:CYS:SG	2.61	0.40
4:F:180:PHE:HD1	4:F:183:LEU:HD12	1.87	0.40
5:J:215:LEU:HD23	5:J:215:LEU:HA	1.91	0.40
1:G:157:PRO:HG3	1:H:179:LEU:HD13	2.04	0.40
2:A:426:LYS:HB2	2:A:426:LYS:HE2	1.96	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	G	258/322 (80%)	251 (97%)	7 (3%)	0	100	100
1	H	252/322 (78%)	243 (96%)	9 (4%)	0	100	100
2	A	410/721 (57%)	389 (95%)	21 (5%)	0	100	100
2	B	409/721 (57%)	393 (96%)	16 (4%)	0	100	100
3	C	314/368 (85%)	303 (96%)	11 (4%)	0	100	100
3	D	314/368 (85%)	303 (96%)	11 (4%)	0	100	100
4	E	250/523 (48%)	245 (98%)	5 (2%)	0	100	100
4	F	344/523 (66%)	338 (98%)	6 (2%)	0	100	100
5	I	38/452 (8%)	38 (100%)	0	0	100	100
5	J	214/452 (47%)	202 (94%)	12 (6%)	0	100	100
All	All	2803/4772 (59%)	2705 (96%)	98 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	G	219/274 (80%)	192 (88%)	27 (12%)	4	14
1	H	216/274 (79%)	192 (89%)	24 (11%)	6	19
2	A	366/626 (58%)	337 (92%)	29 (8%)	12	34
2	B	365/626 (58%)	337 (92%)	28 (8%)	13	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	270/312 (86%)	256 (95%)	14 (5%)	23 55
3	D	269/312 (86%)	245 (91%)	24 (9%)	9 29
4	E	217/443 (49%)	196 (90%)	21 (10%)	8 25
4	F	301/443 (68%)	285 (95%)	16 (5%)	22 54
5	I	42/398 (11%)	39 (93%)	3 (7%)	14 40
5	J	200/398 (50%)	187 (94%)	13 (6%)	17 45
All	All	2465/4106 (60%)	2266 (92%)	199 (8%)	15 33

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	9	TYR
1	G	20	MET
1	G	33	PHE
1	G	35	LYS
1	G	57	CYS
1	G	75	PHE
1	G	77	SER
1	G	117	THR
1	G	127	THR
1	G	142	VAL
1	G	152	VAL
1	G	159	LEU
1	G	162	LYS
1	G	163	LYS
1	G	166	LYS
1	G	169	CYS
1	G	170	HIS
1	G	175	VAL
1	G	192	LEU
1	G	223	ASN
1	G	229	VAL
1	G	239	PHE
1	G	279	SER
1	G	292	THR
1	G	297	SER
1	G	300	LEU
1	G	302	LYS
1	H	6	LEU
1	H	9	TYR

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Mol	Chain	Res	Type
1	H	20	MET
1	H	31	LEU
1	H	33	PHE
1	H	35	LYS
1	H	36	ARG
1	H	67	SER
1	H	72	PHE
1	H	73	LEU
1	H	74	ARG
1	H	101	LEU
1	H	103	ARG
1	H	121	ASP
1	H	127	THR
1	H	136	ARG
1	H	142	VAL
1	H	155	SER
1	H	164	MET
1	H	166	LYS
1	H	176	THR
1	H	192	LEU
1	H	300	LEU
1	H	305	LEU
2	A	62	ASP
2	A	63	GLN
2	A	91	THR
2	A	110	LYS
2	A	117	LEU
2	A	118	ASN
2	A	124	THR
2	A	128	TYR
2	A	130	SER
2	A	147	ASP
2	A	172	ARG
2	A	177	ASN
2	A	194	THR
2	A	232	GLN
2	A	253	SER
2	A	256	VAL
2	A	260	PHE
2	A	265	ASP
2	A	272	PHE
2	A	302	ASN

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Mol	Chain	Res	Type
2	A	324	GLU
2	A	332	THR
2	A	359	ASN
2	A	364	SER
2	A	377	SER
2	A	387	ASP
2	A	394	THR
2	A	426	LYS
2	A	450	SER
3	D	16	GLU
3	D	48	ASP
3	D	49	HIS
3	D	140	LEU
3	D	145	GLU
3	D	157	GLU
3	D	170	PHE
3	D	197	PHE
3	D	203	MET
3	D	208	SER
3	D	217	MET
3	D	218	THR
3	D	226	MET
3	D	228	ARG
3	D	230	ASN
3	D	252	HIS
3	D	262	SER
3	D	268	CYS
3	D	283	ASP
3	D	286	HIS
3	D	287	LYS
3	D	307	SER
3	D	334	SER
3	D	338	ARG
4	E	273	MET
4	E	278	LYS
4	E	282	LYS
4	E	294	GLU
4	E	306	ARG
4	E	307	TYR
4	E	325	GLN
4	E	331	ASP
4	E	334	LEU

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Mol	Chain	Res	Type
4	E	340	SER
4	E	355	ARG
4	E	362	ASP
4	E	372	THR
4	E	386	LEU
4	E	399	SER
4	E	411	ASN
4	E	415	MET
4	E	454	SER
4	E	456	GLU
4	E	467	ARG
4	E	473	LEU
5	I	158	ILE
5	I	181	VAL
5	I	183	LYS
2	B	51	SER
2	B	53	ASP
2	B	55	ARG
2	B	60	SER
2	B	62	ASP
2	B	86	THR
2	B	97	TRP
2	B	104	GLU
2	B	116	SER
2	B	133	ASP
2	B	147	ASP
2	B	172	ARG
2	B	206	ASP
2	B	219	GLN
2	B	224	PHE
2	B	260	PHE
2	B	264	PHE
2	B	289	MET
2	B	302	ASN
2	B	310	CYS
2	B	328	THR
2	B	331	THR
2	B	332	THR
2	B	359	ASN
2	B	364	SER
2	B	426	LYS
2	B	429	SER

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Mol	Chain	Res	Type
2	B	436	VAL
3	C	74	SER
3	C	148	MET
3	C	171	SER
3	C	173	THR
3	C	179	LYS
3	C	184	LYS
3	C	203	MET
3	C	217	MET
3	C	225	VAL
3	C	245	LEU
3	C	275	SER
3	C	283	ASP
3	C	326	SER
3	C	347	ASP
4	F	179	LEU
4	F	187	SER
4	F	195	PHE
4	F	207	MET
4	F	261	SER
4	F	267	ARG
4	F	320	SER
4	F	340	SER
4	F	362	ASP
4	F	374	ARG
4	F	386	LEU
4	F	392	SER
4	F	399	SER
4	F	437	CYS
4	F	458	ASP
4	F	517	ARG
5	J	46	VAL
5	J	54	VAL
5	J	57	ARG
5	J	100	ASP
5	J	104	LEU
5	J	107	ASP
5	J	165	LYS
5	J	175	ASP
5	J	188	GLN
5	J	220	SER
5	J	226	SER

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Mol	Chain	Res	Type
5	J	315	THR
5	J	319	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	214	GLN
2	A	118	ASN
4	E	411	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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.

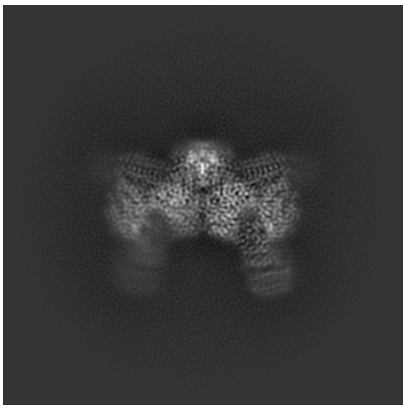
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41566. These allow visual inspection of the internal detail of the map and identification of artifacts.

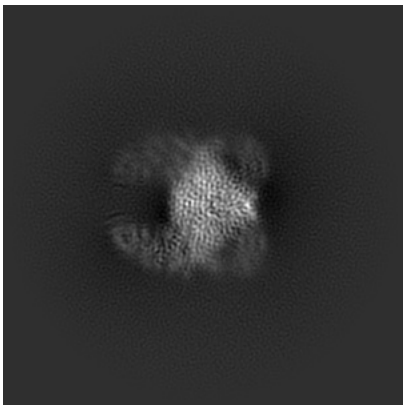
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

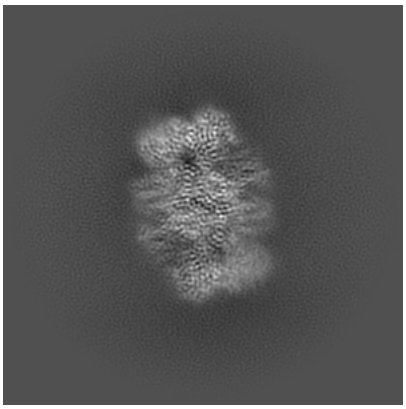
6.1.1 Primary map



X

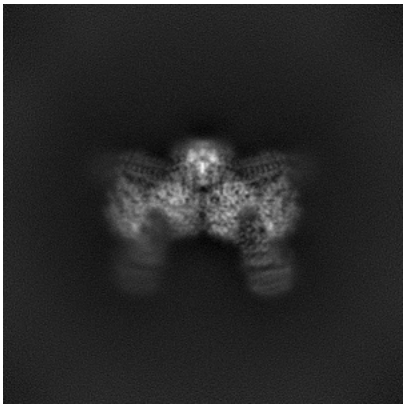


Y

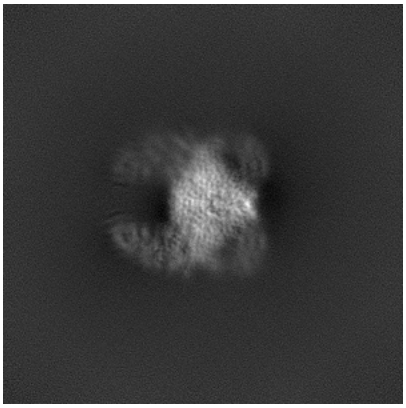


Z

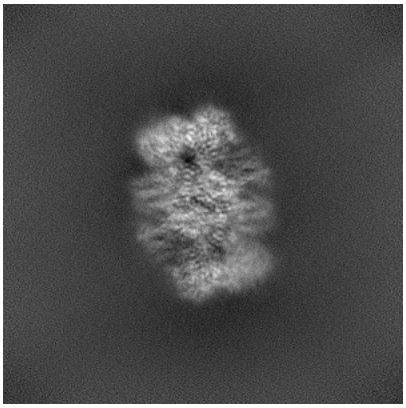
6.1.2 Raw map



X



Y

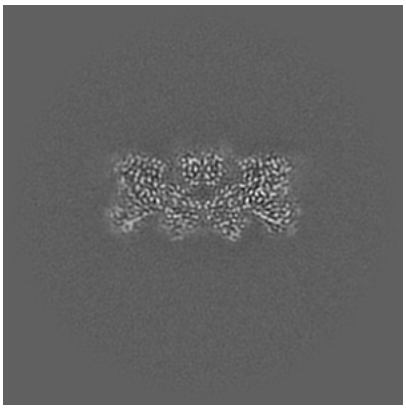


Z

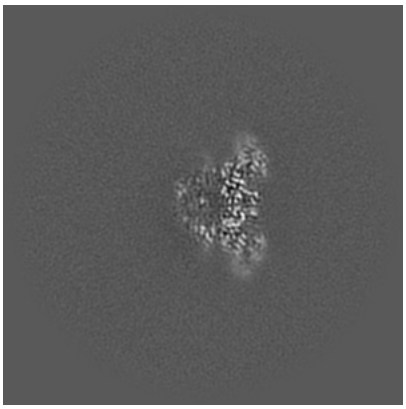
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

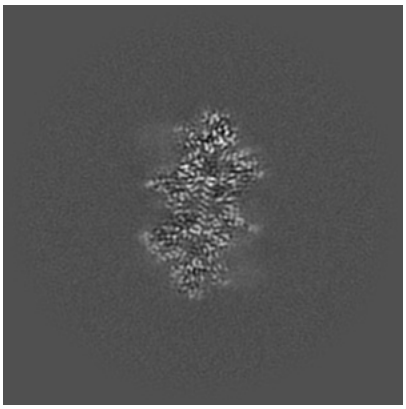
6.2.1 Primary map



X Index: 200

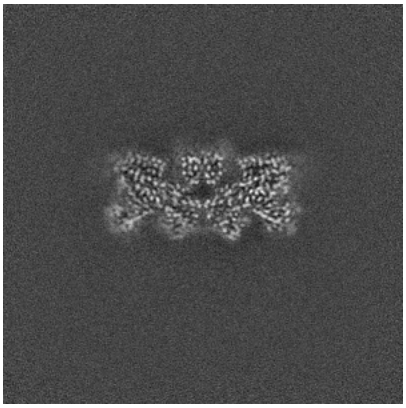


Y Index: 200

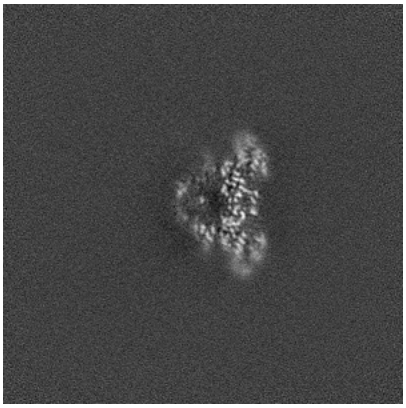


Z Index: 200

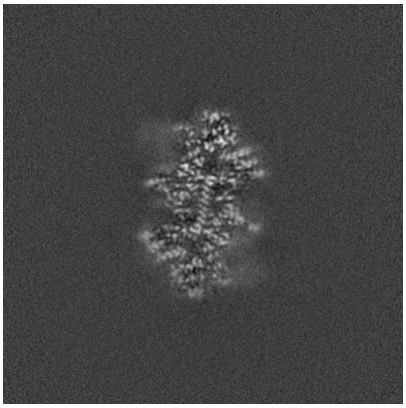
6.2.2 Raw map



X Index: 200



Y Index: 200

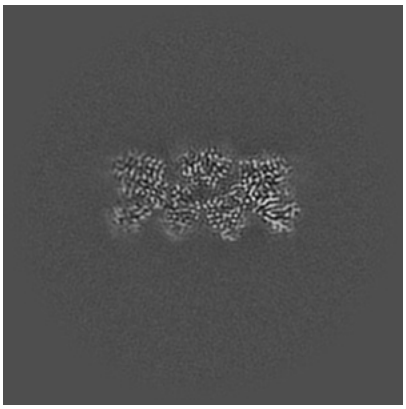


Z Index: 200

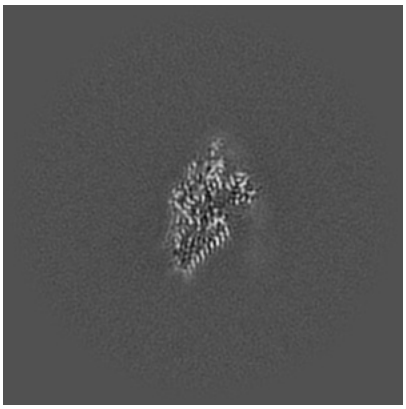
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

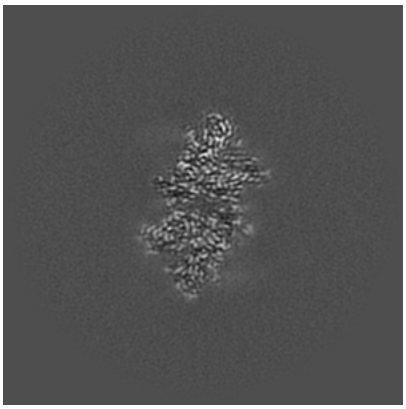
6.3.1 Primary map



X Index: 202

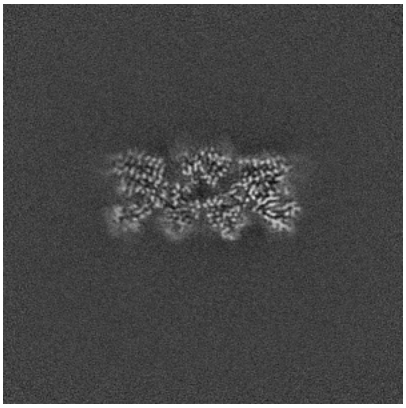


Y Index: 221

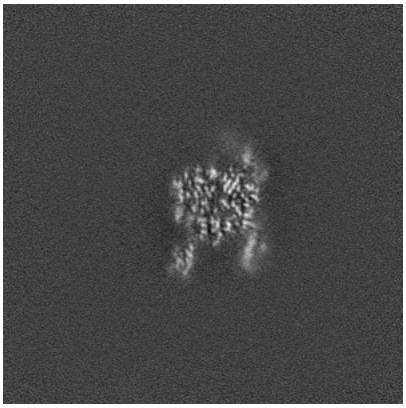


Z Index: 206

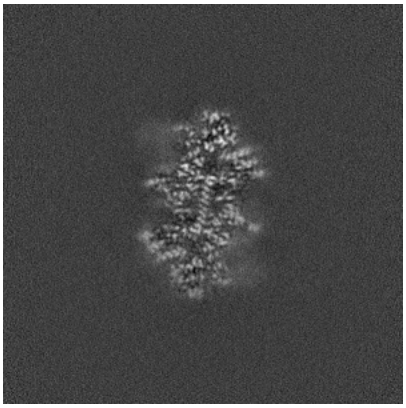
6.3.2 Raw map



X Index: 202



Y Index: 210

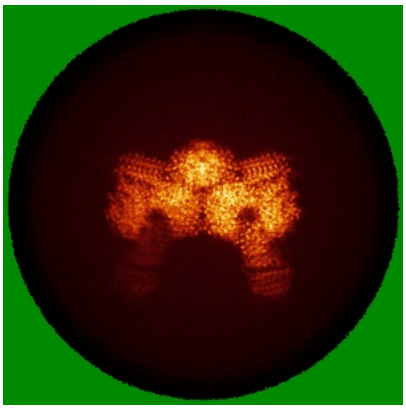


Z Index: 200

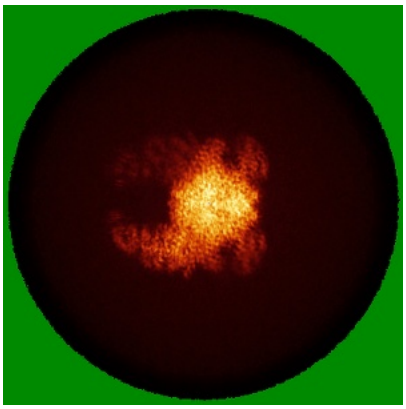
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

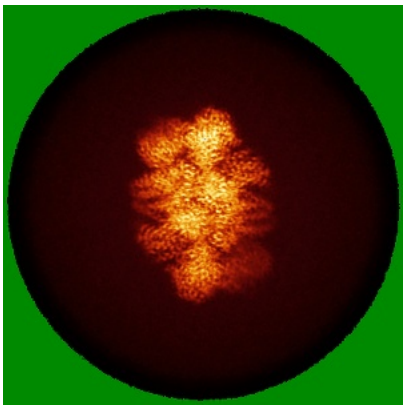
6.4.1 Primary map



X

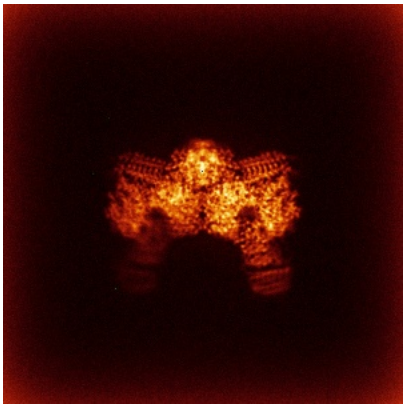


Y

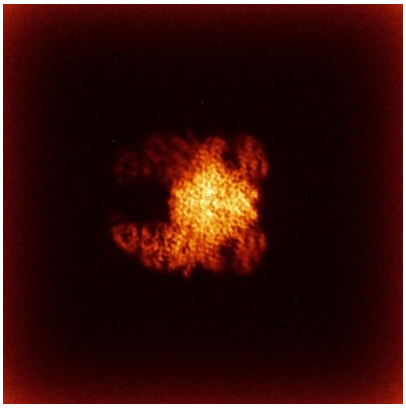


Z

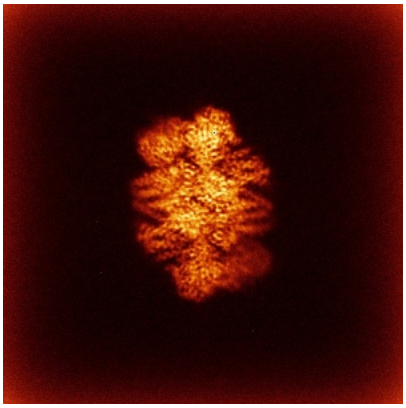
6.4.2 Raw map



X



Y

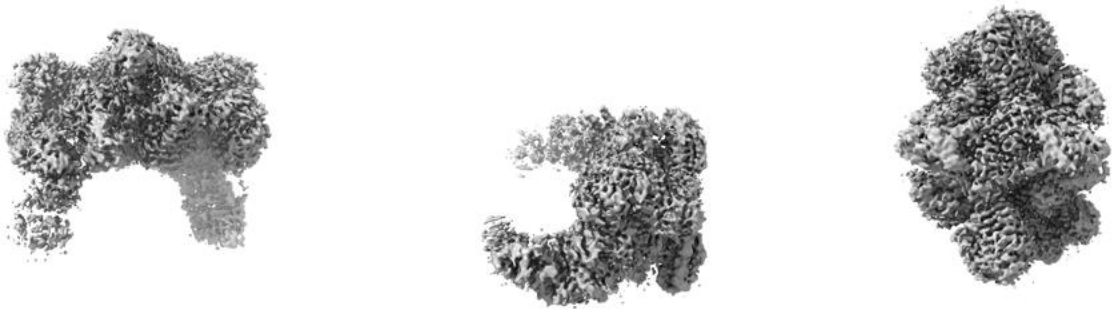


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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

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.

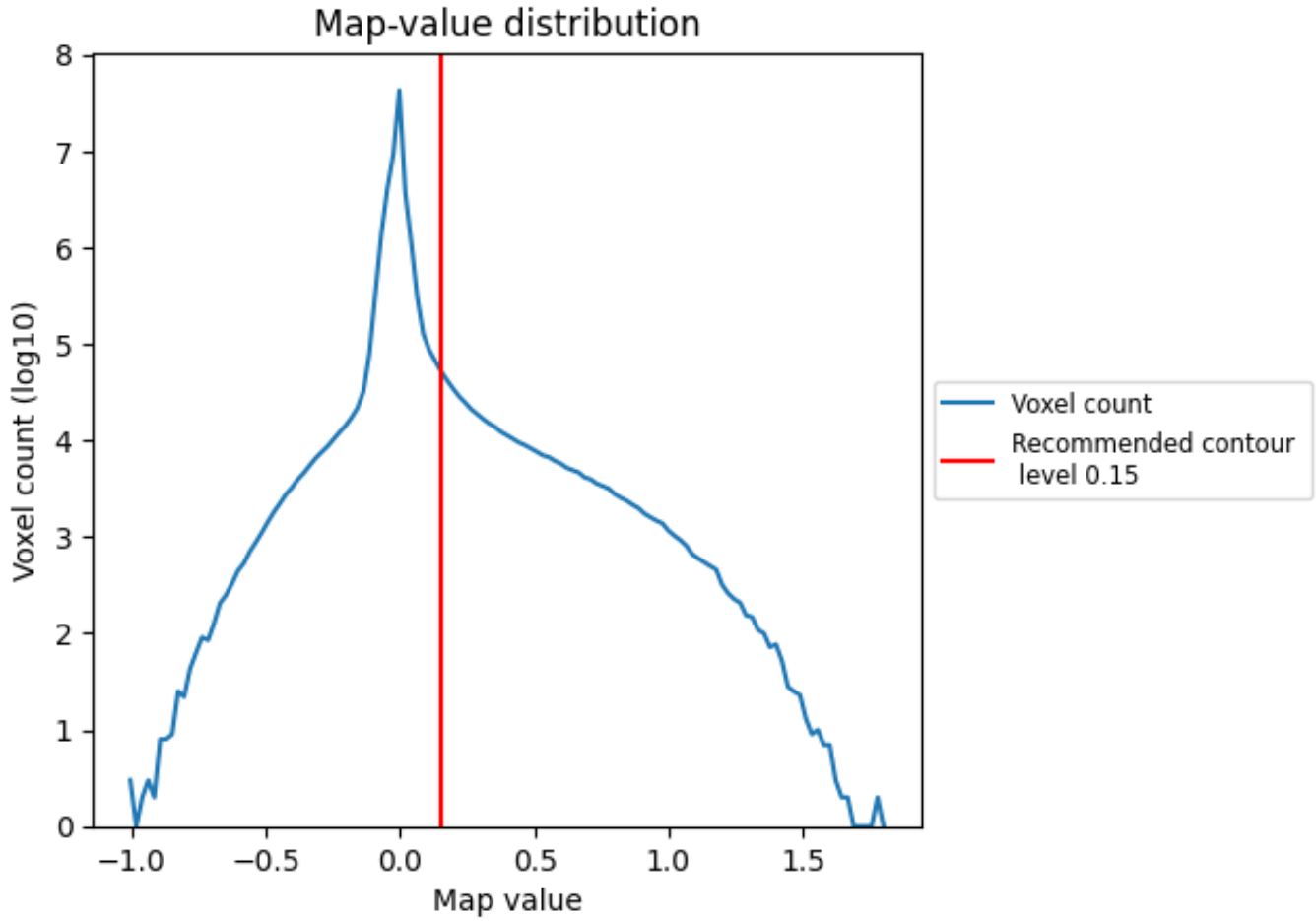
6.6 Mask visualisation (i)

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

7 Map analysis

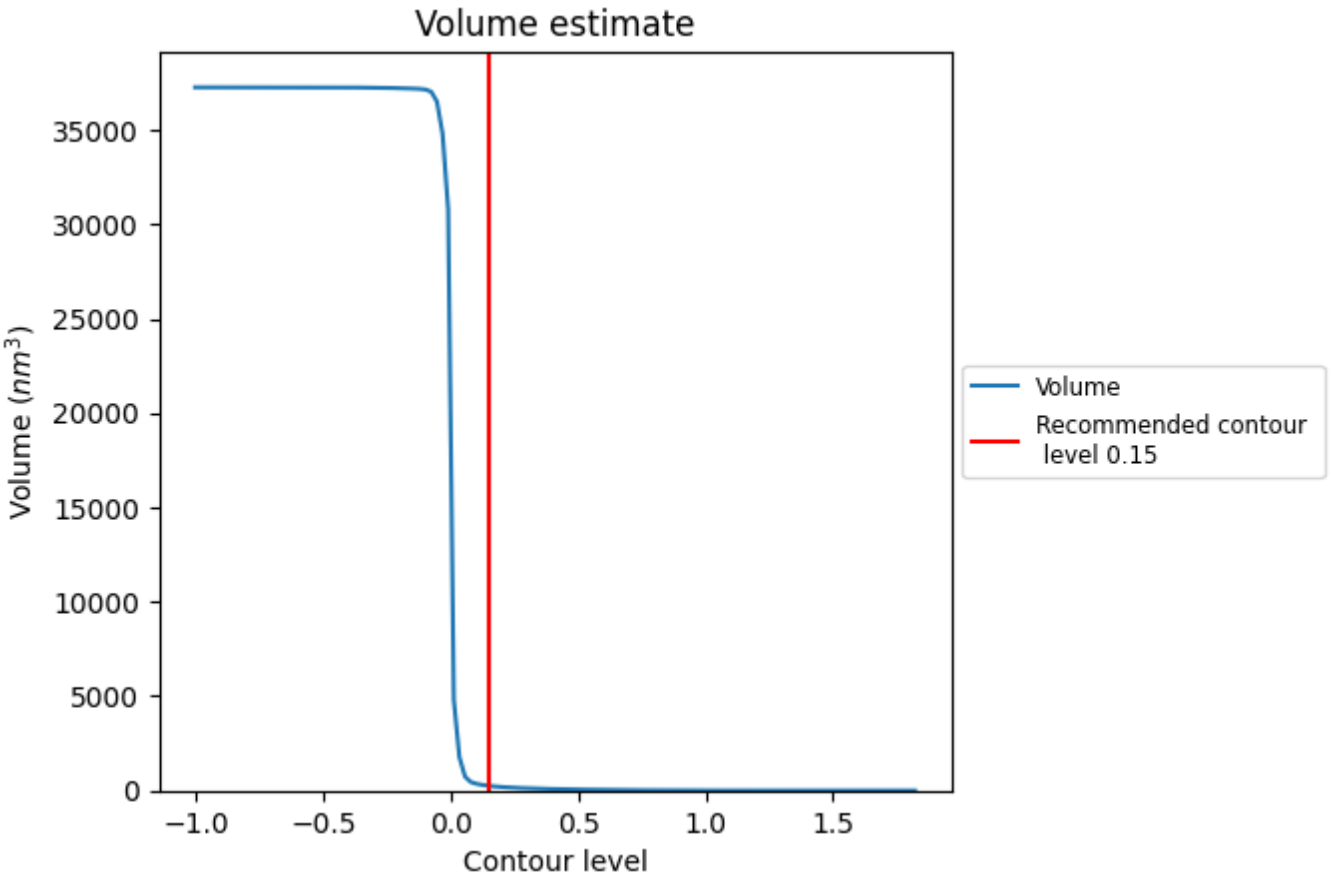
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

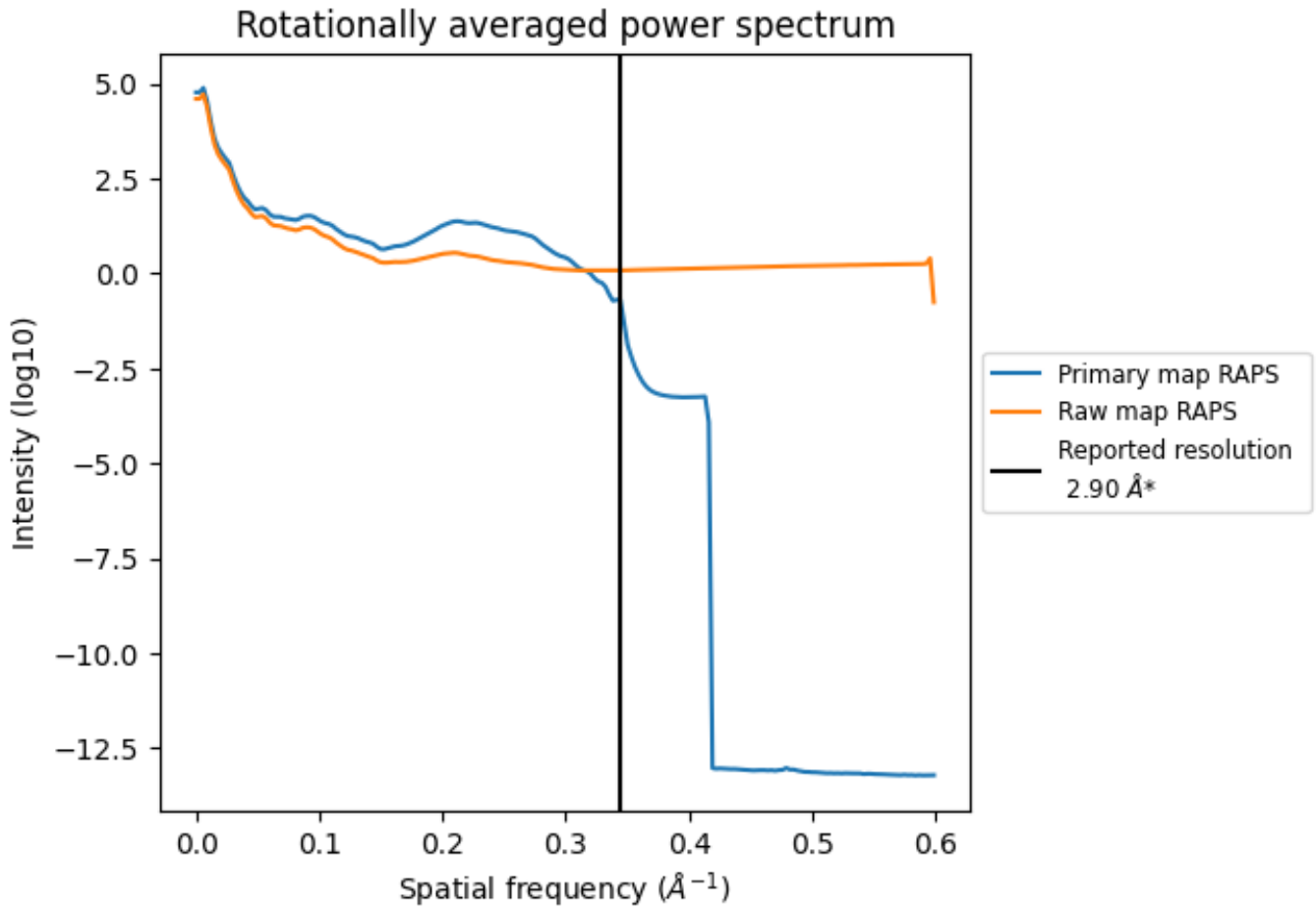
7.2 Volume estimate



The volume at the recommended contour level is 251 nm^3; this corresponds to an approximate mass of 227 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)

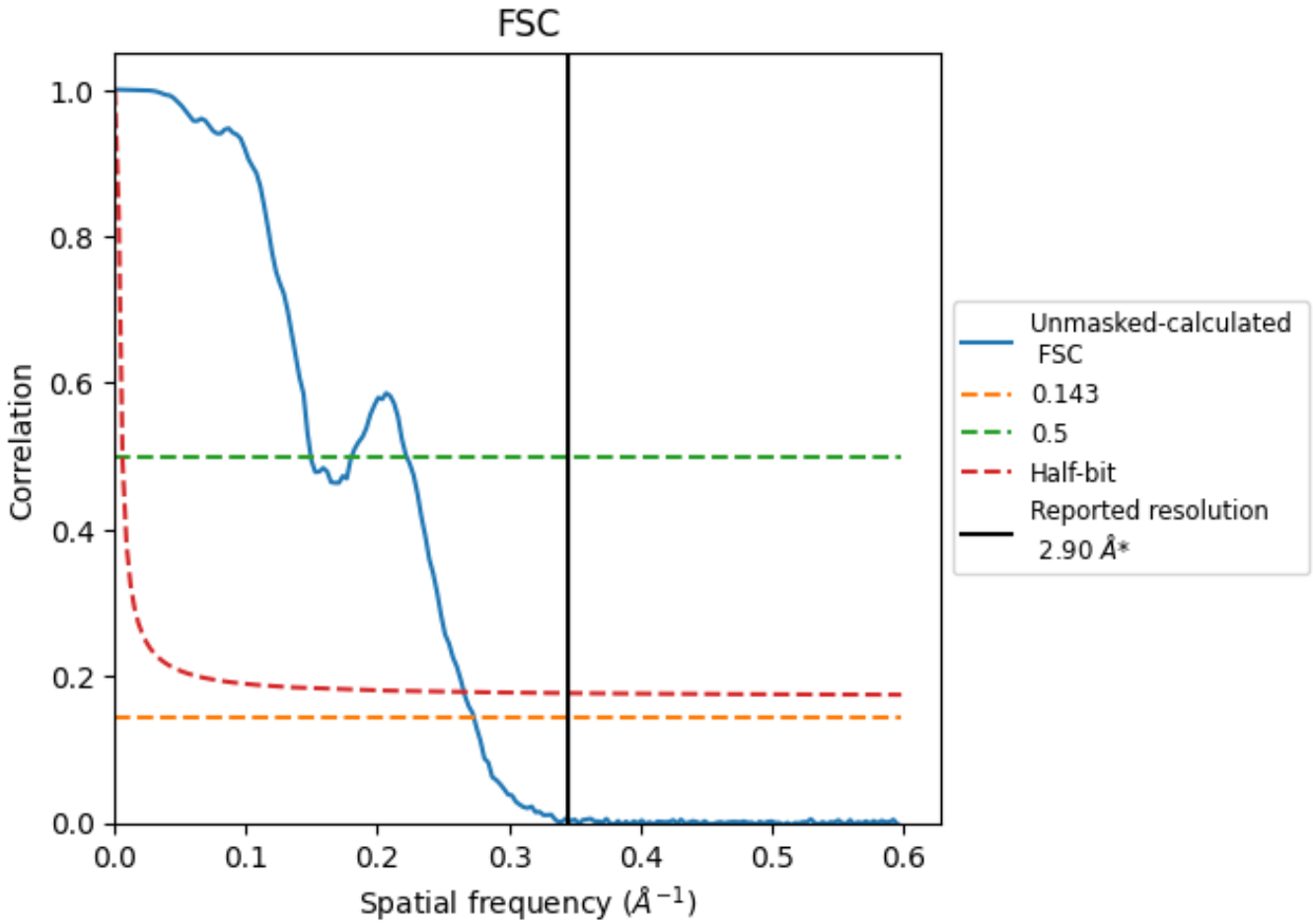


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

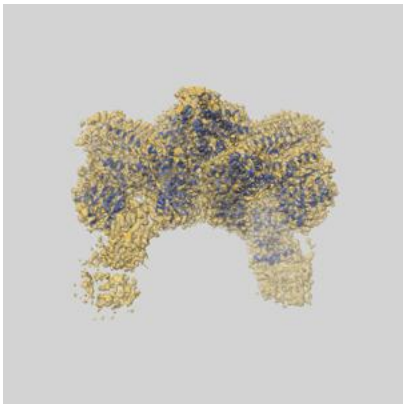
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	6.70	3.76

*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 3.66 differs from the reported value 2.9 by more than 10 %

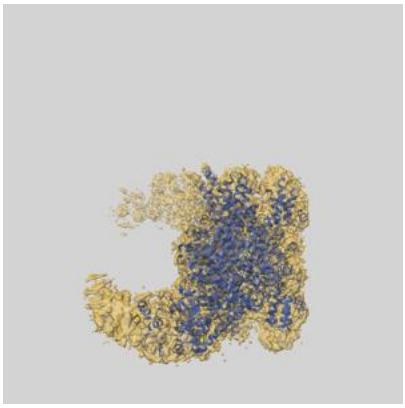
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41566 and PDB model 8TQZ. Per-residue inclusion information can be found in section 3 on page 8.

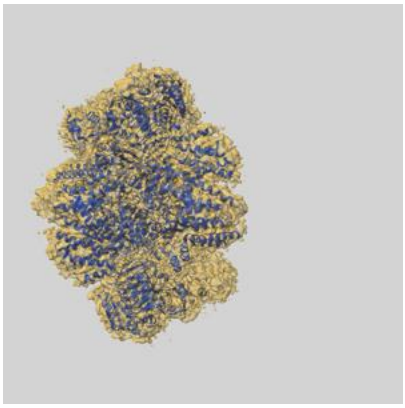
9.1 Map-model overlay



X



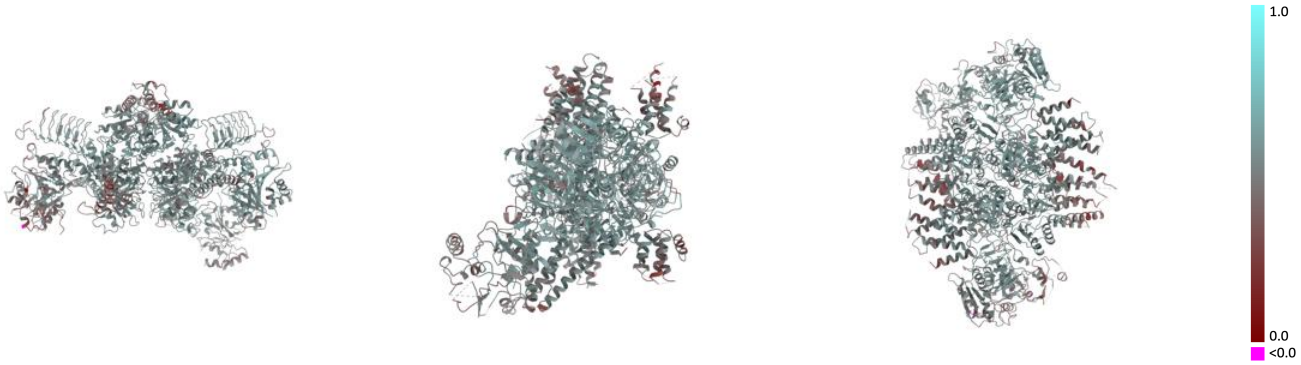
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

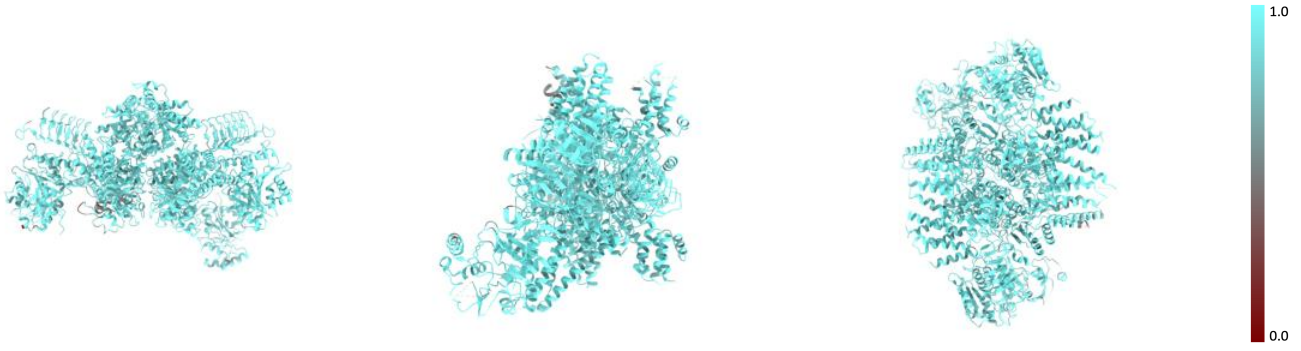
9.2 Q-score mapped to coordinate model (i)



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.

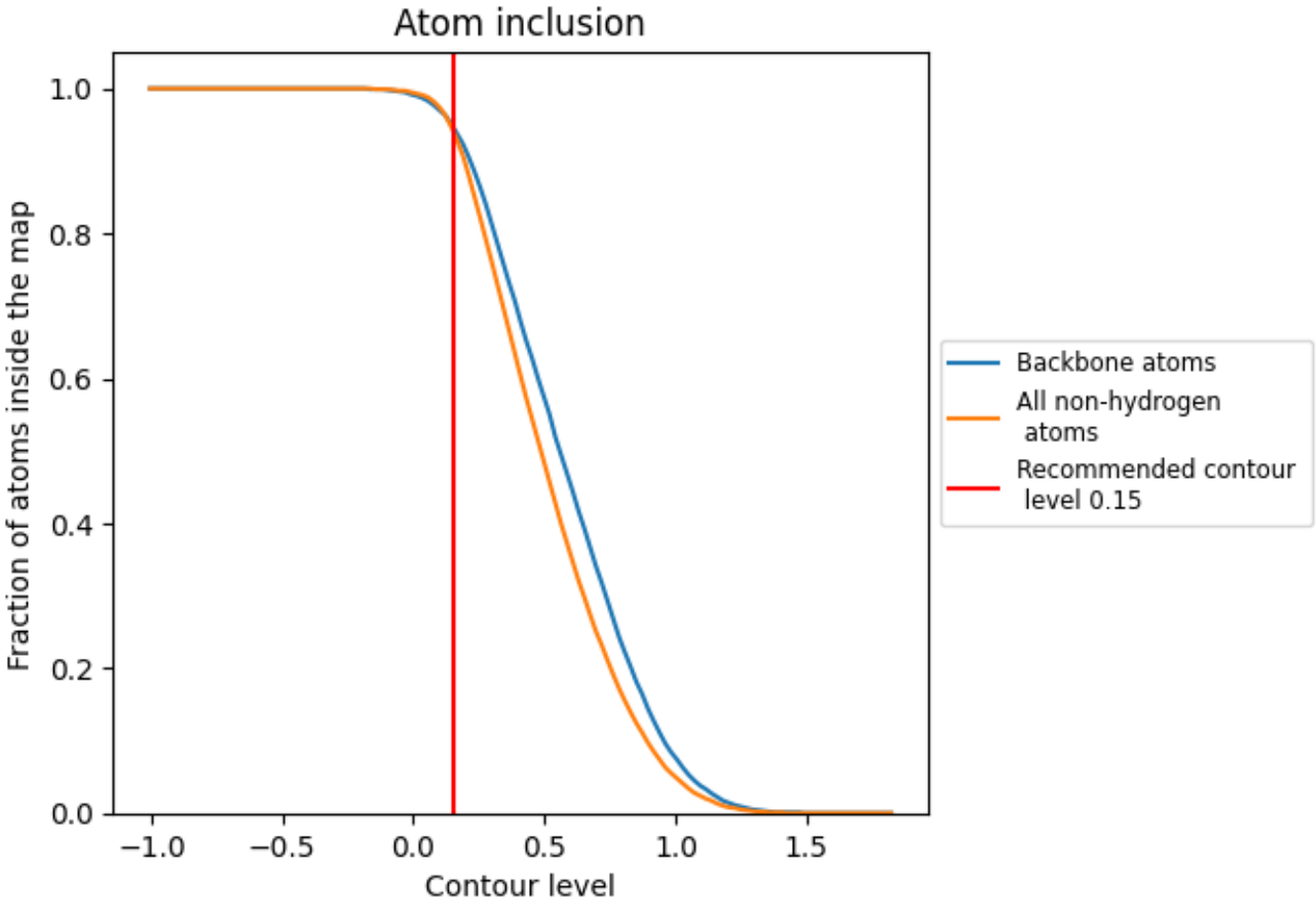
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9430	0.5190
A	0.9190	0.4980
B	0.9640	0.5480
C	0.9580	0.5270
D	0.9440	0.5180
E	0.8990	0.5060
F	0.9550	0.5430
G	0.9560	0.5190
H	0.9590	0.5160
I	0.9080	0.4150
J	0.9370	0.5010