Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 09:02 pm BST

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	:	6FYX, 5B04

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

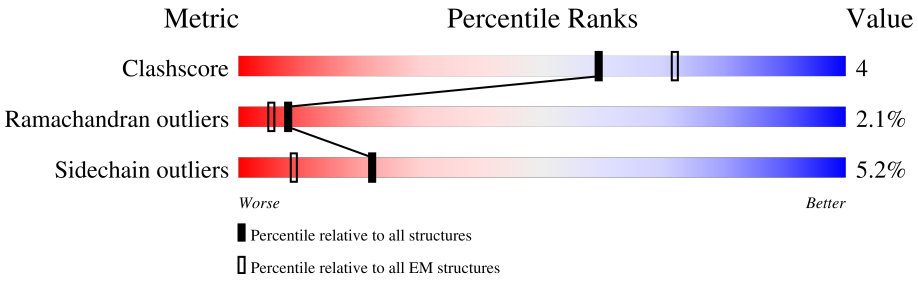
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 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	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 <=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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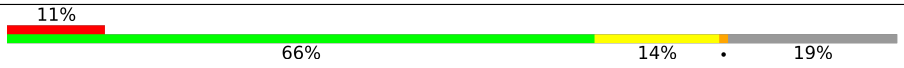
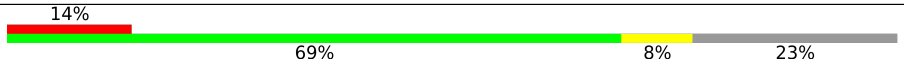
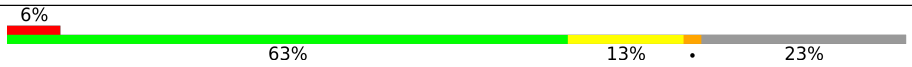
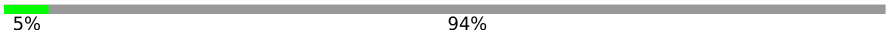
Mol	Chain	Length	Quality of chain
5	I	712	
5	J	712	
6	K	304	
6	L	304	
7	M	527	
7	N	527	
8	O	285	
8	P	285	

2 Entry composition (i)

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	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	C	345	Total	C	N	O	S	0	0
			2665	1694	463	502	6		
2	D	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	K	246	Total	C	N	O	P	S	0	0
			1974	1259	324	382	1	8		
6	L	246	Total	C	N	O	P	S	0	0
			1974	1259	324	382	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.

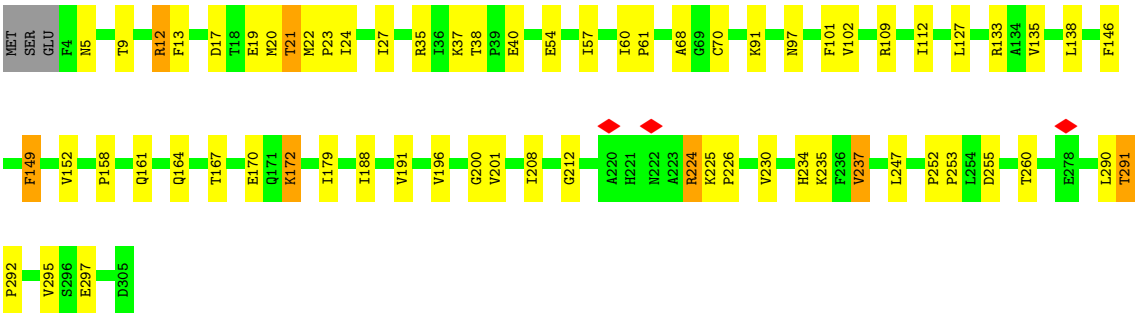
Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	17	Total	C	N	O		0	0
			143	96	24	23			
8	P	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

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.

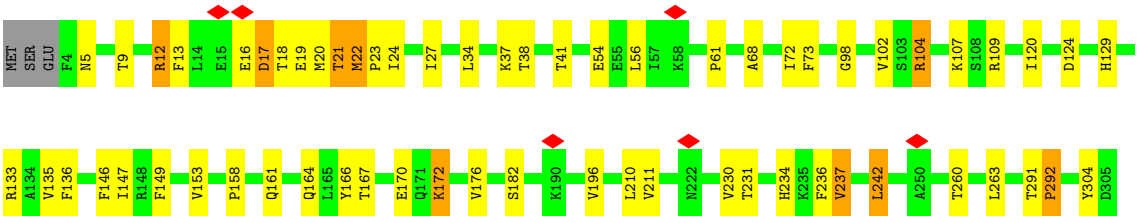
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:



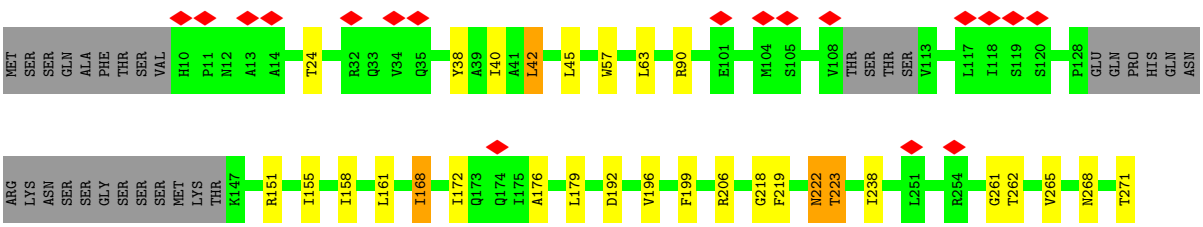
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

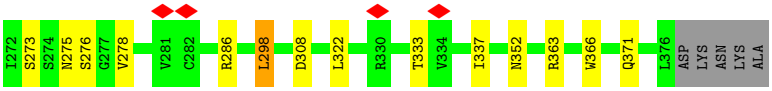
Chain B:



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

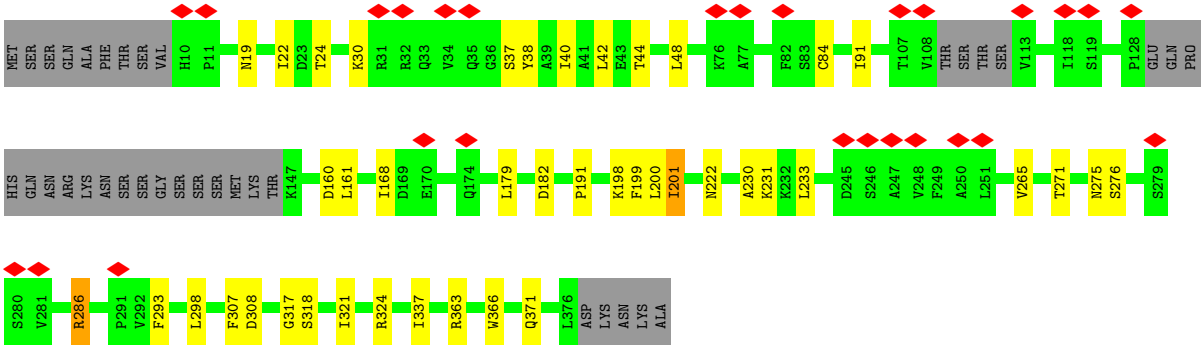
Chain C:





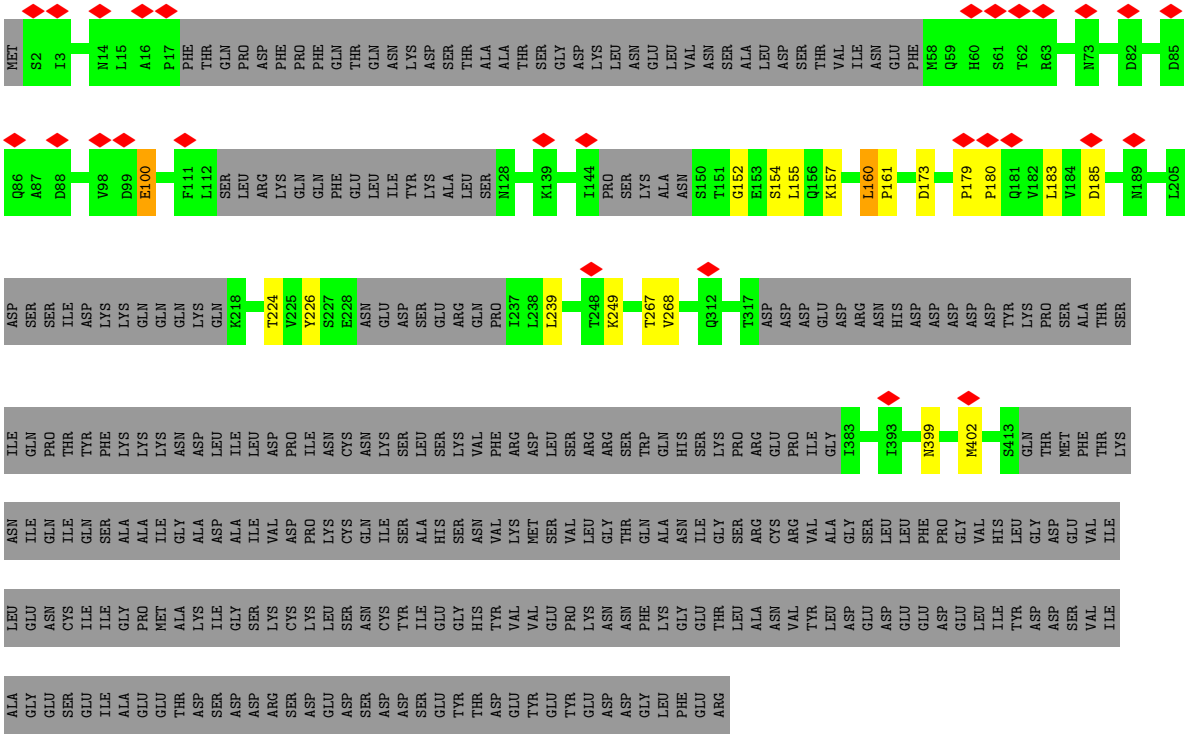
• Molecule 2: Translation initiation factor eIF-2B subunit beta

Chain D:



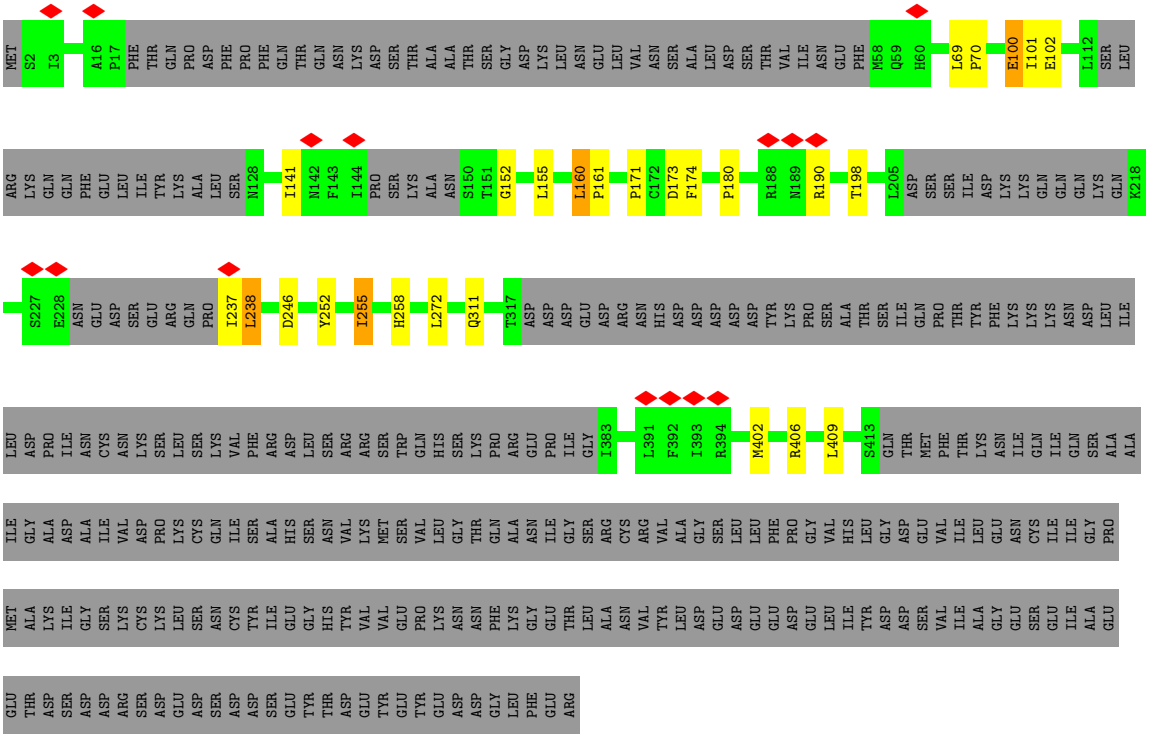
• Molecule 3: Translation initiation factor eIF-2B subunit gamma

Chain E:



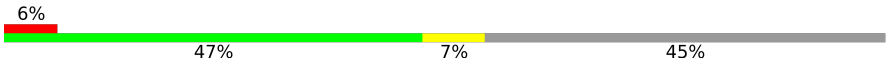
• Molecule 3: Translation initiation factor eIF-2B subunit gamma

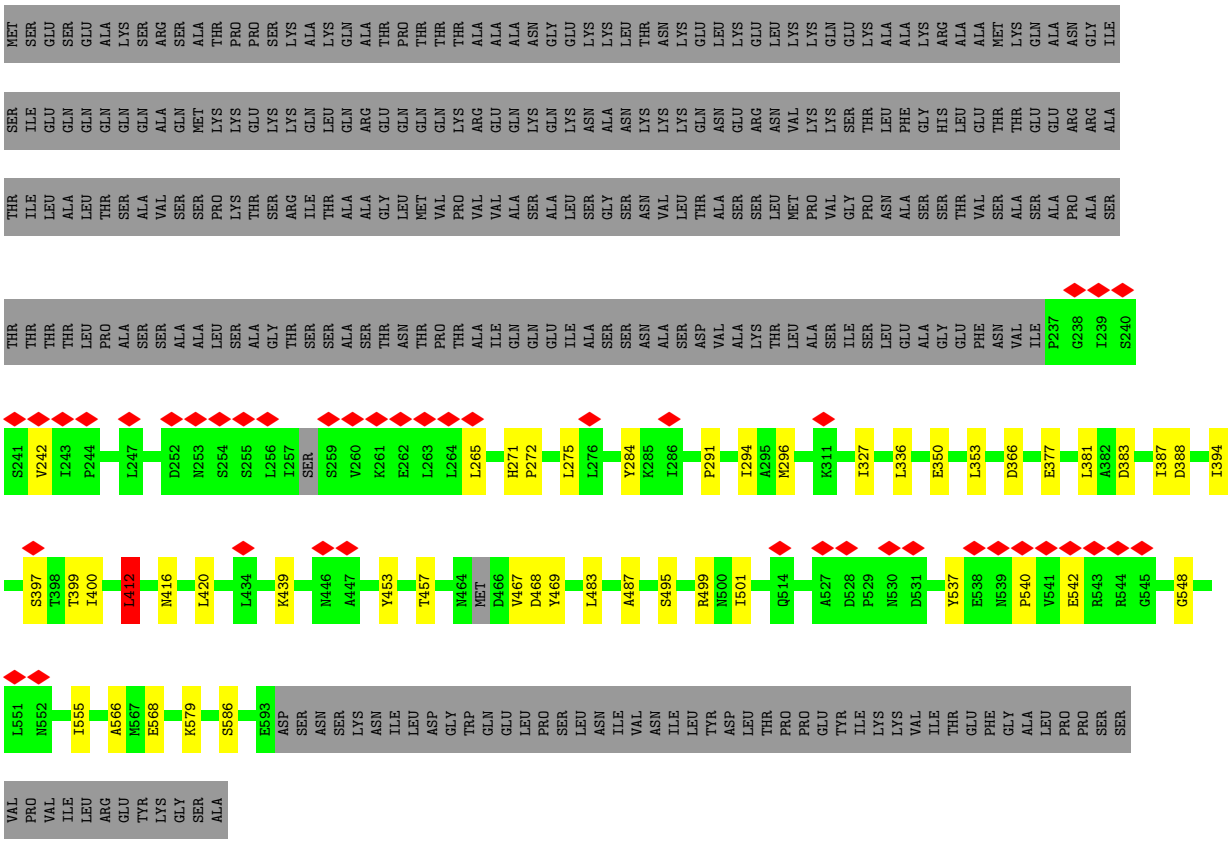
Chain F:



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

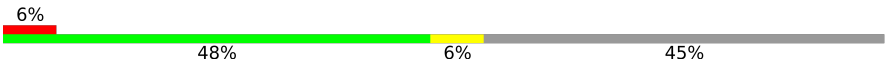
Chain G:

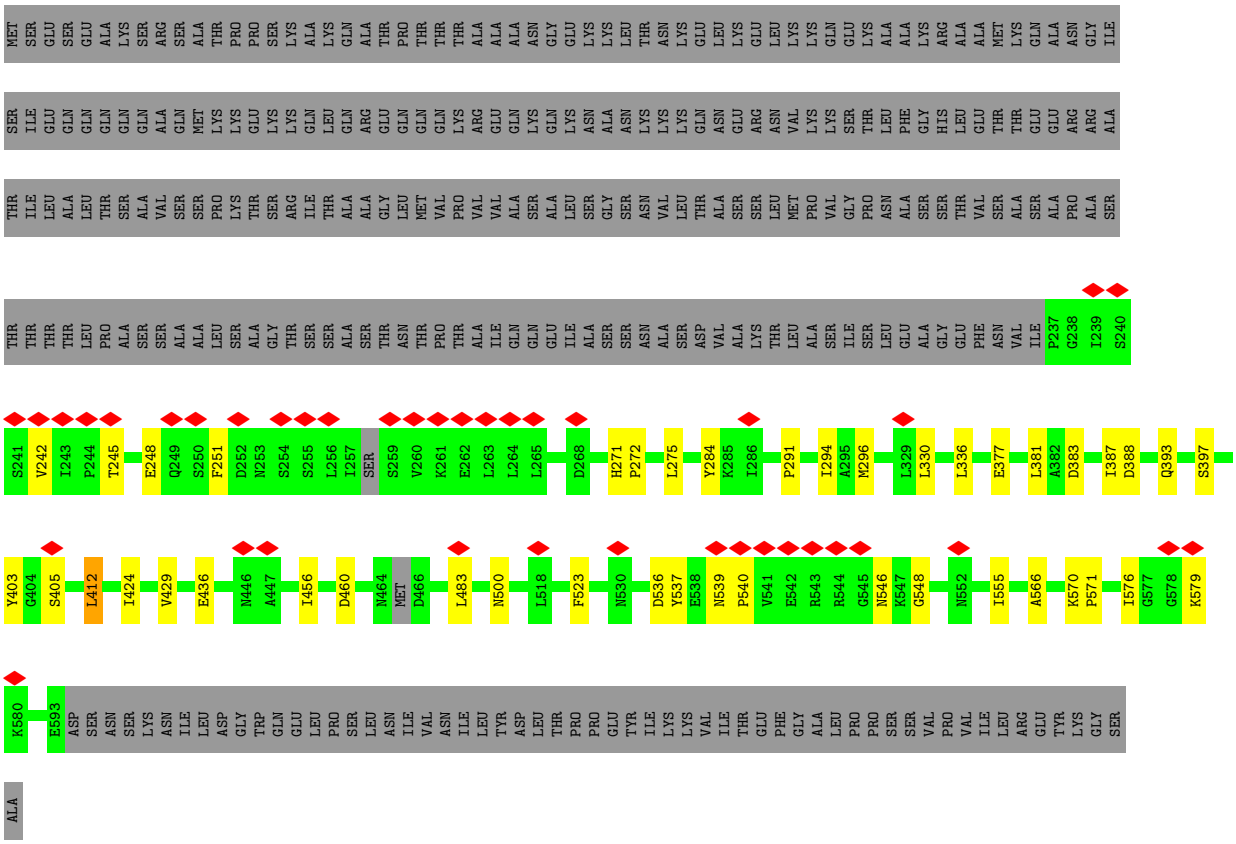




• Molecule 4: Translation initiation factor eIF-2B subunit delta

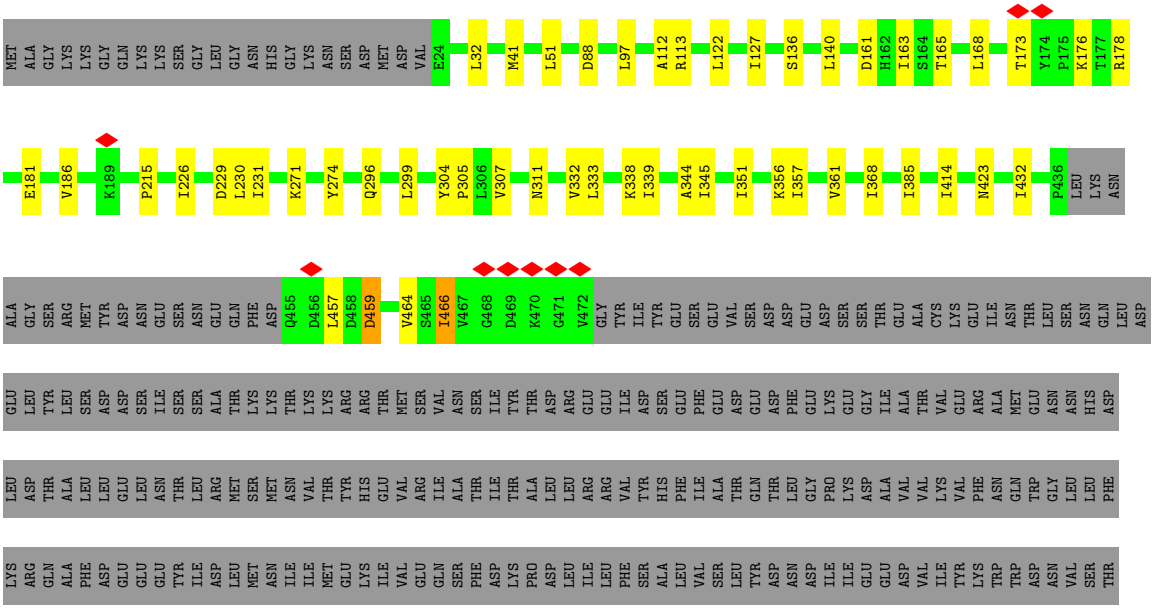
Chain H:





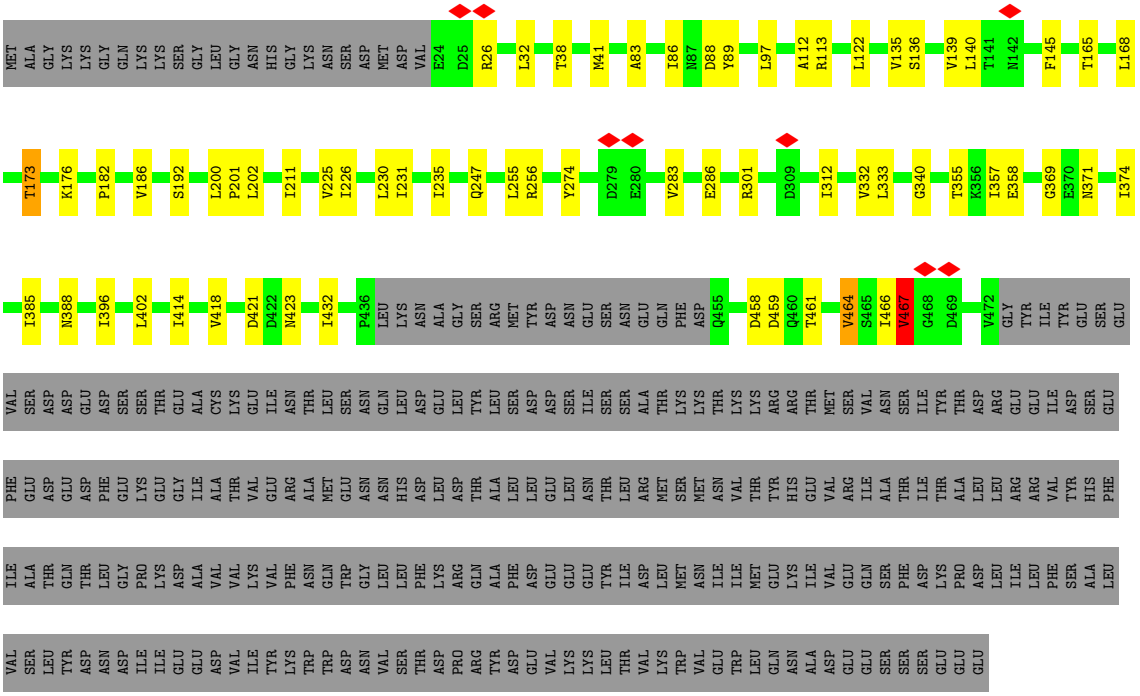
• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

Chain I:



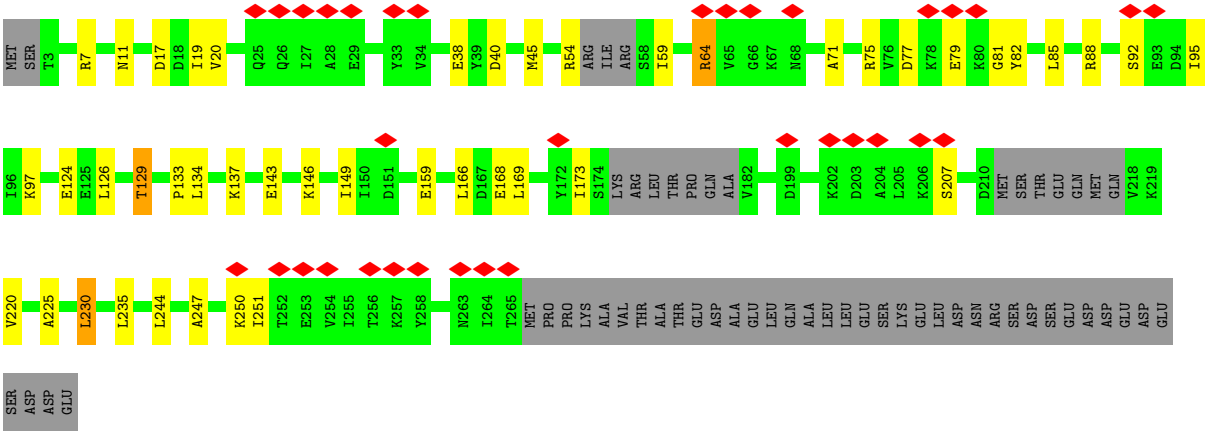
• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

Chain J:



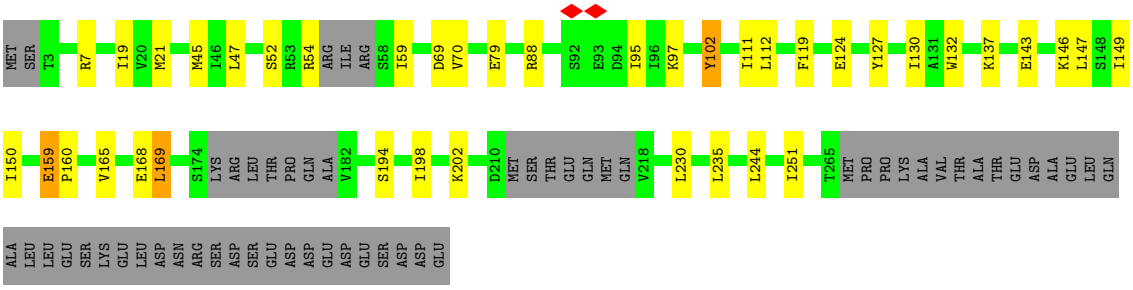
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain K:

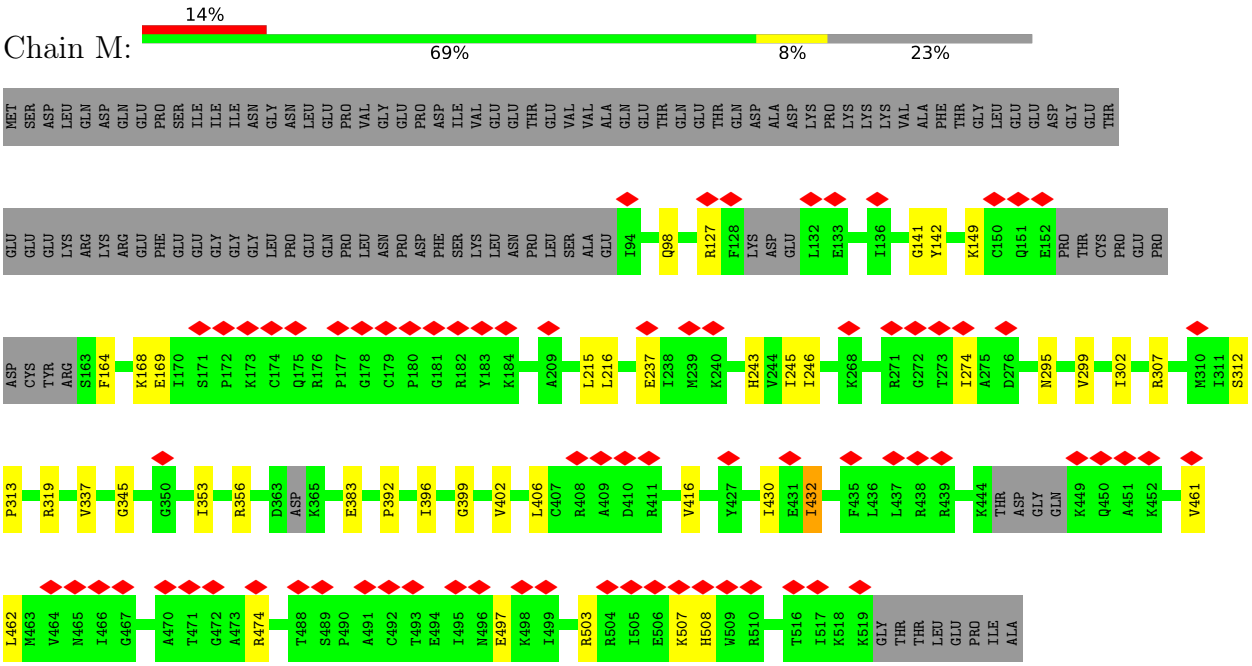


• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

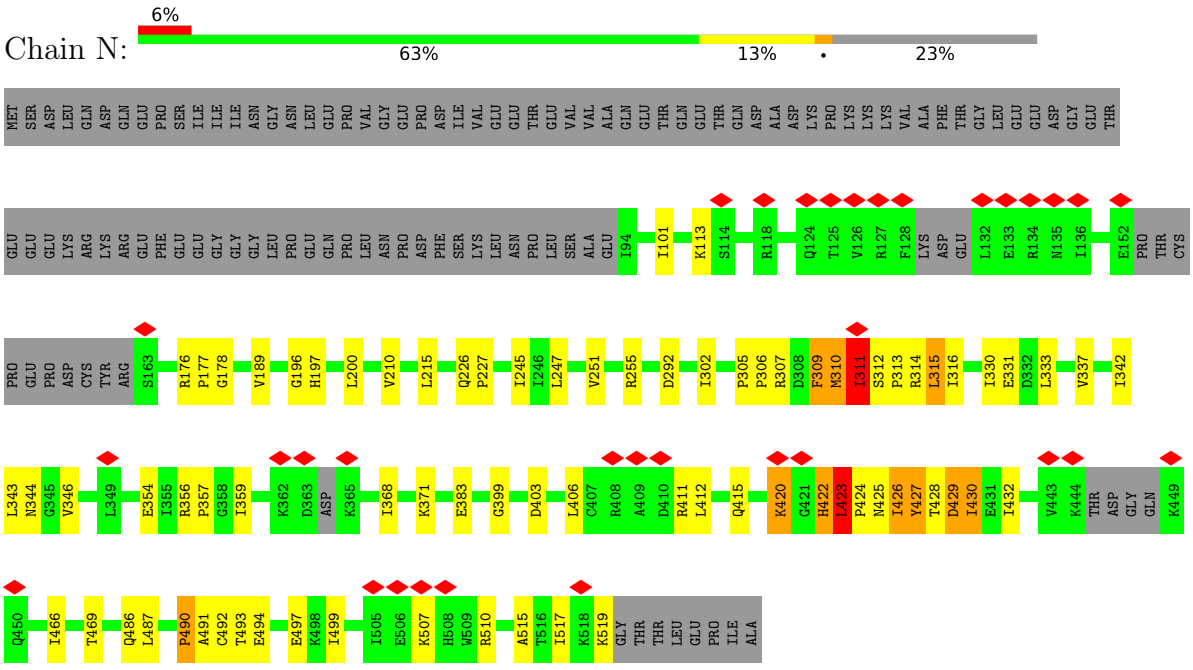
Chain L:



• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

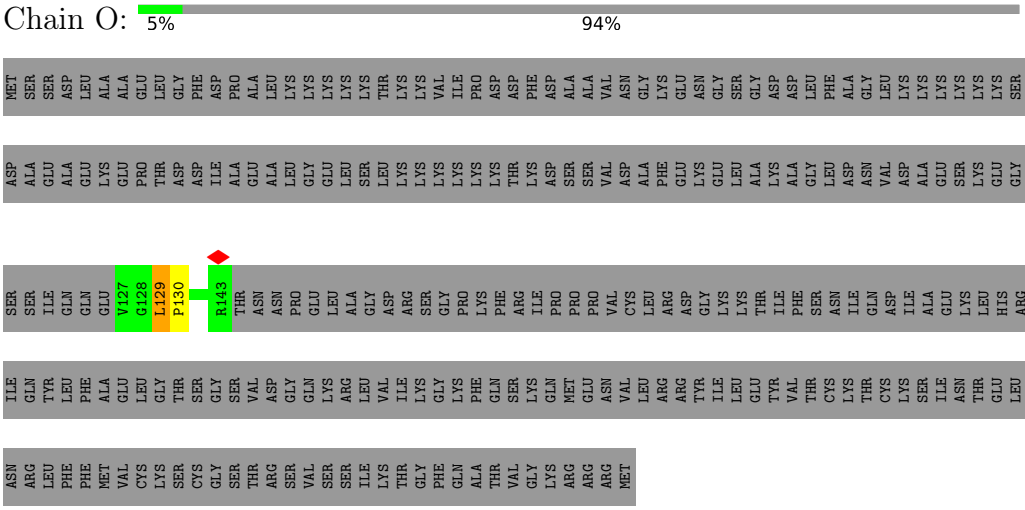


• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma



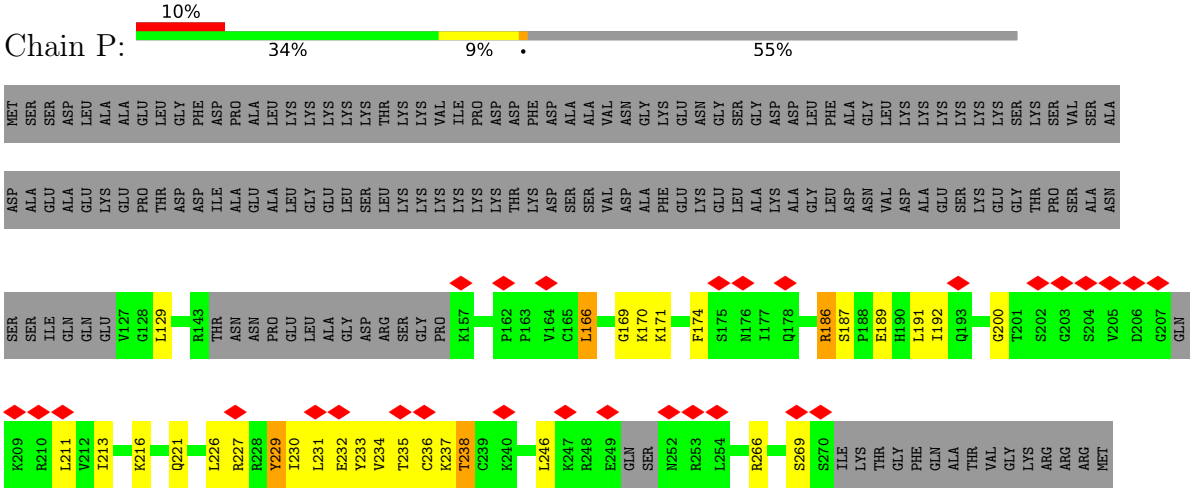
• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta

Chain O:



• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta

Chain P:



4 Experimental information (i)

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 ($e^-/Å^2$)	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.

All (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
1:B:21:THR:HB	1:B:24:ILE:CD1	1.74	1.15
1:A:20:MET:SD	1:A:102:VAL:HG13	1.87	1.14
7:N:314:ARG:NH2	7:N:423:LEU:O	1.78	1.14
7:N:429:ASP:O	7:N:430:ILE:HG13	1.44	1.13
7:N:429:ASP:O	7:N:430:ILE:CG1	1.98	1.11
7:M:142:TYR:HB2	7:M:319:ARG:HH22	1.03	1.08
7:N:314:ARG:HH22	7:N:423:LEU:HG	1.12	1.08
1:B:20:MET:SD	1:B:24:ILE:HG21	1.95	1.06
7:M:142:TYR:HB2	7:M:319:ARG:NH2	1.71	1.05
7:N:368:ILE:HD13	7:N:428:THR:HG21	1.39	1.04
1:B:21:THR:HB	1:B:24:ILE:HD12	1.41	1.03
7:N:312:SER:CB	7:N:422:HIS:CE1	2.43	1.01
8:P:226:LEU:O	8:P:230:ILE:HG13	1.59	1.00
1:A:146:PHE:HB3	5:J:332:VAL:HG13	1.42	0.98
7:M:142:TYR:CB	7:M:319:ARG:HH22	1.76	0.97
1:B:21:THR:CB	1:B:24:ILE:HD13	1.94	0.97
1:B:21:THR:HB	1:B:24:ILE:HD13	1.48	0.96
1:B:120:ILE:HG21	1:B:147:ILE:HG21	1.51	0.93
1:B:9:THR:HA	1:B:12:ARG:HD2	1.52	0.92
1:B:20:MET:SD	1:B:24:ILE:CG2	2.58	0.91
7:N:312:SER:CB	7:N:422:HIS:HE1	1.78	0.91
1:A:146:PHE:CB	5:J:332:VAL:HG13	2.01	0.91
7:N:426:ILE:HD12	7:N:426:ILE:H	1.32	0.91
1:B:146:PHE:HB3	5:I:332:VAL:HG13	1.51	0.91
1:B:120:ILE:HG21	1:B:147:ILE:CG2	2.00	0.90
1:B:21:THR:CB	1:B:24:ILE:CD1	2.50	0.90
7:N:314:ARG:NH2	7:N:423:LEU:HG	1.85	0.90
7:N:314:ARG:NH2	7:N:423:LEU:C	2.22	0.88
1:A:9:THR:O	1:A:12:ARG:HB2	1.73	0.88
1:B:9:THR:O	1:B:12:ARG:HB2	1.75	0.86
1:B:120:ILE:CG2	1:B:147:ILE:HG21	2.04	0.86
1:B:20:MET:CE	1:B:102:VAL:CG1	2.52	0.86
8:P:238:THR:HG22	8:P:266:ARG:HH21	1.41	0.84
1:B:20:MET:CE	1:B:102:VAL:HG13	2.07	0.84
1:A:21:THR:HG22	1:A:23:PRO:HD2	1.60	0.83
7:N:428:THR:O	7:N:487:LEU:HD12	1.79	0.83
1:A:20:MET:SD	1:A:102:VAL:HG11	2.19	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:368:ILE:HD13	7:N:428:THR:CG2	2.12	0.79
7:N:429:ASP:O	7:N:430:ILE:HG12	1.82	0.79
1:B:146:PHE:CB	5:I:332:VAL:HG13	2.14	0.78
6:L:198:ILE:HG12	7:N:333:LEU:HB2	1.63	0.78
1:A:9:THR:HA	1:A:12:ARG:HD2	1.63	0.78
6:L:202:LYS:CE	7:N:331:GLU:HA	2.14	0.78
7:N:422:HIS:HB3	7:N:424:PRO:HD2	1.68	0.75
6:L:198:ILE:HG23	7:N:333:LEU:HD12	1.69	0.75
7:N:312:SER:HB2	7:N:422:HIS:HE1	0.99	0.74
1:B:120:ILE:CG2	1:B:147:ILE:CG2	2.65	0.74
1:B:21:THR:HG22	1:B:23:PRO:HD2	1.69	0.74
1:A:112:ILE:HG22	1:A:138:LEU:HD21	1.70	0.73
7:N:368:ILE:CD1	7:N:428:THR:HG21	2.18	0.72
8:P:169:GLY:HA3	8:P:216:LYS:HG3	1.72	0.72
7:N:314:ARG:HH22	7:N:423:LEU:CG	1.99	0.71
7:N:429:ASP:C	7:N:430:ILE:HG12	2.10	0.71
1:B:20:MET:CE	1:B:102:VAL:HG11	2.21	0.71
3:E:160:LEU:H	3:E:161:PRO:HD2	1.55	0.70
6:L:198:ILE:CG2	7:N:330:ILE:O	2.40	0.69
7:M:142:TYR:HB2	7:M:319:ARG:CZ	2.21	0.69
7:N:429:ASP:C	7:N:430:ILE:CG1	2.57	0.68
3:F:160:LEU:H	3:F:161:PRO:HD2	1.58	0.68
1:B:21:THR:OG1	1:B:24:ILE:HD13	1.94	0.68
1:B:20:MET:HE1	1:B:102:VAL:HG11	1.73	0.68
1:A:164:GLN:O	1:A:167:THR:OG1	2.09	0.67
1:B:164:GLN:O	1:B:167:THR:OG1	2.12	0.67
5:J:414:ILE:HG12	5:J:432:ILE:HD12	1.77	0.66
4:H:387:ILE:HD13	4:H:412:LEU:HD22	1.76	0.66
7:M:142:TYR:HB2	7:M:319:ARG:HH12	1.62	0.64
6:L:198:ILE:HG23	7:N:330:ILE:O	1.98	0.64
7:M:142:TYR:HB2	7:M:319:ARG:NH1	2.12	0.64
4:H:383:ASP:O	4:H:387:ILE:HG12	1.98	0.63
1:A:260:THR:OG1	1:B:170:GLU:OE2	2.07	0.63
1:B:23:PRO:O	1:B:27:ILE:HD12	1.98	0.63
6:L:146:LYS:O	6:L:149:ILE:HG13	1.99	0.62
2:C:333:THR:HG22	4:G:453:TYR:HB3	1.81	0.62
7:N:210:VAL:HG22	7:N:343:LEU:HA	1.81	0.62
1:B:9:THR:HA	1:B:12:ARG:CD	2.28	0.61
6:L:194:SER:N	7:N:403:ASP:OD2	2.33	0.61
1:A:260:THR:O	1:B:170:GLU:HG2	2.01	0.61
6:K:149:ILE:HG21	6:K:173:ILE:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:427:TYR:OH	7:N:519:LYS:HG3	2.02	0.60
5:J:464:VAL:HB	5:J:467:VAL:HG23	1.84	0.60
1:B:20:MET:SD	1:B:24:ILE:HG22	2.42	0.60
6:L:198:ILE:HG12	7:N:333:LEU:CD1	2.32	0.59
5:I:459:ASP:H	5:I:466:ILE:HD12	1.68	0.59
1:B:120:ILE:HG21	1:B:147:ILE:HG22	1.80	0.58
2:C:196:VAL:HG21	2:C:261:GLY:HA2	1.85	0.58
6:K:146:LYS:O	6:K:149:ILE:HG13	2.03	0.58
3:F:255:ILE:H	8:P:216:LYS:HD3	1.69	0.58
1:A:208:ILE:HD12	1:A:247:LEU:HD21	1.85	0.57
1:B:109:ARG:HH22	1:B:133:ARG:HB3	1.69	0.57
7:N:101:ILE:HD12	7:N:305:PRO:HG3	1.87	0.56
1:B:135:VAL:HG22	1:B:230:VAL:HB	1.87	0.56
1:A:149:PHE:HD1	1:A:149:PHE:O	1.88	0.56
6:L:198:ILE:CG1	7:N:333:LEU:CD1	2.84	0.56
6:L:198:ILE:HG13	7:N:333:LEU:HD13	1.87	0.56
6:L:202:LYS:HE2	7:N:331:GLU:HA	1.86	0.56
8:P:233:TYR:OH	8:P:269:SER:C	2.43	0.56
4:G:468:ASP:HA	4:G:501:ILE:HD13	1.87	0.56
6:L:198:ILE:CG2	7:N:333:LEU:HD12	2.35	0.56
2:D:317:GLY:HA2	5:J:301:ARG:HB3	1.88	0.55
6:K:92:SER:HA	6:K:95:ILE:HD12	1.88	0.55
4:G:394:ILE:HD13	4:G:416:ASN:HD21	1.71	0.55
8:P:186:ARG:NH2	8:P:234:VAL:HG22	2.22	0.55
1:A:21:THR:HG21	1:A:234:HIS:CE1	2.42	0.55
1:A:23:PRO:O	1:A:27:ILE:HD12	2.07	0.54
5:I:351:ILE:HG12	5:I:368:ILE:HD12	1.88	0.54
3:F:190:ARG:HH22	3:F:238:LEU:HD12	1.73	0.54
1:A:291:THR:H	1:A:292:PRO:HD3	1.73	0.54
5:J:165:THR:HA	5:J:274:TYR:HB2	1.90	0.53
1:B:153:VAL:HG11	1:B:166:TYR:HB2	1.90	0.53
1:A:22:MET:HB2	1:A:23:PRO:HD3	1.89	0.53
2:D:231:LYS:HD2	4:H:546:ASN:HD21	1.74	0.53
2:D:318:SER:HA	2:D:321:ILE:HD12	1.91	0.53
4:G:483:LEU:HB3	4:G:566:ALA:HB3	1.91	0.52
6:L:111:ILE:HG23	6:L:169:LEU:HD21	1.92	0.52
1:B:22:MET:CB	1:B:23:PRO:HD3	2.40	0.52
7:N:499:ILE:HB	7:N:515:ALA:HB3	1.91	0.52
8:P:186:ARG:HH21	8:P:234:VAL:HG22	1.75	0.52
8:P:189:GLU:HA	8:P:192:ILE:HD12	1.92	0.52
1:A:57:ILE:HA	1:A:60:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:466:ILE:HG12	7:N:499:ILE:HG12	1.92	0.52
7:N:313:PRO:HA	7:N:344:ASN:O	2.10	0.52
6:L:70:VAL:HG21	6:L:95:ILE:HA	1.90	0.51
7:N:469:THR:HG21	7:N:491:ALA:HA	1.93	0.51
6:L:198:ILE:CG1	7:N:333:LEU:HD13	2.41	0.51
1:A:146:PHE:HB3	5:J:332:VAL:CG1	2.30	0.51
4:H:377:GLU:HA	4:H:381:LEU:HD12	1.92	0.51
1:B:19:GLU:HA	1:B:19:GLU:OE1	2.11	0.51
1:B:129:HIS:HB3	1:B:196:VAL:HG22	1.92	0.51
4:H:330:LEU:HB3	4:H:336:LEU:HD21	1.93	0.51
3:E:226:TYR:HB3	3:E:239:LEU:H	1.75	0.50
8:P:237:LYS:HB2	8:P:266:ARG:CZ	2.41	0.50
6:L:198:ILE:HG12	7:N:333:LEU:HD12	1.92	0.50
7:M:142:TYR:CB	7:M:319:ARG:HH12	2.24	0.50
7:M:237:GLU:HB3	7:M:274:ILE:HD12	1.93	0.50
1:A:68:ALA:HB2	1:A:237:VAL:HG22	1.93	0.50
1:A:224:ARG:HH22	2:D:286:ARG:HE	1.60	0.49
5:J:414:ILE:HA	5:J:432:ILE:HB	1.93	0.49
6:L:198:ILE:HG12	7:N:333:LEU:CB	2.38	0.49
1:A:22:MET:CB	1:A:23:PRO:HD3	2.42	0.49
5:I:414:ILE:HG12	5:I:432:ILE:HD12	1.93	0.49
1:B:21:THR:HG21	1:B:234:HIS:CE1	2.48	0.49
4:H:291:PRO:HA	4:H:294:ILE:HD12	1.93	0.49
2:C:168:ILE:HG23	2:C:352:ASN:HD22	1.77	0.49
5:J:340:GLY:HA3	5:J:358:GLU:HG3	1.95	0.49
8:P:233:TYR:OH	8:P:269:SER:O	2.29	0.49
2:C:90:ARG:HH22	2:C:298:LEU:HD13	1.77	0.48
5:I:178:ARG:HH22	5:I:229:ASP:HA	1.78	0.48
5:J:396:ILE:HG13	5:J:414:ILE:HD12	1.93	0.48
7:N:426:ILE:HD12	7:N:426:ILE:N	2.13	0.48
1:A:152:VAL:HG13	1:A:179:ILE:HD13	1.94	0.48
1:A:135:VAL:HG22	1:A:230:VAL:HB	1.95	0.48
1:A:146:PHE:HB2	5:J:332:VAL:HG13	1.90	0.48
1:B:21:THR:O	1:B:24:ILE:HB	2.14	0.48
7:N:113:LYS:HE3	7:N:196:GLY:H	1.78	0.48
7:N:426:ILE:H	7:N:426:ILE:CD1	2.01	0.48
5:I:168:LEU:HB3	5:I:230:LEU:HD22	1.96	0.48
8:P:236:CYS:SG	8:P:237:LYS:N	2.86	0.48
4:G:291:PRO:HA	4:G:294:ILE:HD12	1.95	0.47
5:I:163:ILE:HD11	5:I:271:LYS:HB3	1.96	0.47
5:I:304:TYR:HB3	5:I:305:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:307:ARG:HD3	7:N:307:ARG:HA	1.75	0.47
1:B:242:LEU:HB3	4:H:393:GLN:HG2	1.96	0.47
3:F:101:ILE:HG23	3:F:102:GLU:HG3	1.97	0.47
5:J:458:ASP:HB3	5:J:466:ILE:HD11	1.96	0.47
6:K:133:PRO:HG2	6:K:134:LEU:HD12	1.97	0.47
7:N:428:THR:O	7:N:487:LEU:CD1	2.59	0.47
1:A:127:LEU:HB2	1:A:191:VAL:HG11	1.95	0.47
7:N:310:MET:HB3	7:N:311:ILE:H	1.57	0.47
1:B:20:MET:HE1	1:B:102:VAL:CG1	2.33	0.47
7:N:356:ARG:O	7:N:426:ILE:HG23	2.14	0.47
3:E:267:THR:HG23	5:J:225:VAL:HA	1.96	0.47
3:F:171:PRO:HD2	3:F:174:PHE:HE1	1.80	0.47
5:J:139:VAL:HG11	5:J:235:ILE:HD11	1.97	0.47
8:P:238:THR:HG22	8:P:266:ARG:NH2	2.21	0.47
4:H:483:LEU:HB3	4:H:566:ALA:HB3	1.97	0.47
5:I:32:LEU:HB2	5:I:136:SER:HA	1.97	0.47
7:N:315:LEU:CD1	7:N:342:ILE:HG12	2.45	0.47
8:P:187:SER:H	8:P:246:LEU:HD13	1.80	0.47
7:N:197:HIS:HB3	7:N:200:LEU:H	1.78	0.47
5:J:200:LEU:HD11	5:J:211:ILE:HD11	1.96	0.46
3:F:152:GLY:HA2	3:F:155:LEU:HD12	1.97	0.46
1:B:13:PHE:CD1	1:B:13:PHE:N	2.81	0.46
7:N:429:ASP:HA	7:N:486:GLN:HA	1.97	0.46
8:P:227:ARG:O	8:P:231:LEU:HD12	2.15	0.46
8:O:129:LEU:H	8:O:130:PRO:HD2	1.80	0.46
1:B:292:PRO:HG3	2:C:268:ASN:HA	1.98	0.46
5:I:165:THR:HA	5:I:274:TYR:HB2	1.97	0.46
4:H:272:PRO:HA	4:H:275:LEU:HD12	1.98	0.46
5:I:296:GLN:HA	5:I:299:LEU:HD12	1.97	0.46
4:H:403:TYR:HD1	4:H:429:VAL:HB	1.80	0.46
5:J:385:ILE:HG12	5:J:402:LEU:HD12	1.96	0.46
6:L:198:ILE:CG1	7:N:333:LEU:HD12	2.46	0.46
4:G:495:SER:HB2	4:G:499:ARG:HH21	1.81	0.45
1:B:17:ASP:HB3	1:B:18:THR:H	1.50	0.45
7:N:226:GLN:HA	7:N:227:PRO:HD3	1.83	0.45
1:B:22:MET:HB3	1:B:23:PRO:HD3	1.99	0.45
3:F:406:ARG:HA	3:F:409:LEU:HD12	1.99	0.45
8:P:237:LYS:HB2	8:P:266:ARG:NH2	2.31	0.45
4:G:377:GLU:HA	4:G:381:LEU:HD12	1.99	0.45
6:K:20:VAL:HG12	6:K:38:GLU:HB3	1.98	0.45
6:L:147:LEU:O	6:L:150:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:313:PRO:HA	7:M:345:GLY:HA3	1.98	0.45
2:C:42:LEU:HA	2:C:45:LEU:HD12	1.99	0.45
2:C:192:ASP:HB2	2:C:222:ASN:HD21	1.82	0.45
5:J:357:ILE:HA	5:J:374:ILE:HB	1.99	0.45
6:K:220:VAL:HG13	6:K:230:LEU:HB3	1.98	0.45
6:L:202:LYS:HG3	7:N:330:ILE:HG22	1.98	0.45
7:N:245:ILE:HD11	7:N:302:ILE:HD11	1.98	0.45
2:C:262:THR:HA	2:C:273:SER:HA	1.98	0.45
3:E:179:PRO:HA	3:E:180:PRO:HD3	1.78	0.45
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.17	0.44
2:D:30:LYS:HD3	5:J:312:ILE:HA	1.98	0.44
4:G:350:GLU:HA	4:G:353:LEU:HD12	1.99	0.44
4:H:381:LEU:HD22	6:K:64:ARG:HD3	1.99	0.44
5:I:339:ILE:HG22	5:I:357:ILE:HB	2.00	0.44
2:C:218:GLY:HA2	4:G:457:THR:HG21	1.98	0.44
1:A:21:THR:HG21	1:A:234:HIS:NE2	2.33	0.44
1:A:23:PRO:HG2	1:A:234:HIS:CD2	2.53	0.44
1:B:9:THR:CA	1:B:12:ARG:HD2	2.37	0.44
7:M:462:LEU:HD22	7:M:503:ARG:HG2	1.99	0.44
5:J:83:ALA:HA	5:J:86:ILE:HD12	1.99	0.44
7:M:216:LEU:HD23	7:M:246:ILE:HG12	2.00	0.44
7:M:337:VAL:HA	7:M:399:GLY:HA2	1.99	0.44
7:N:427:TYR:OH	7:N:519:LYS:CG	2.66	0.44
1:B:72:ILE:HD11	1:B:236:PHE:HB2	1.99	0.44
4:G:399:THR:HB	4:G:467:VAL:HA	1.99	0.44
7:M:168:LYS:CB	7:M:295:ASN:HB3	2.48	0.44
7:M:243:HIS:HB3	7:M:302:ILE:HG12	2.00	0.44
8:P:232:GLU:HG3	8:P:233:TYR:HD1	1.83	0.44
1:A:170:GLU:HG2	1:B:260:THR:O	2.18	0.43
1:A:225:LYS:HA	1:A:226:PRO:HD3	1.88	0.43
2:D:230:ALA:HA	2:D:233:LEU:HD12	2.00	0.43
2:D:37:SER:HA	2:D:40:ILE:HD12	2.00	0.43
4:G:387:ILE:HD13	4:G:412:LEU:HD22	2.00	0.43
7:N:337:VAL:HA	7:N:399:GLY:HA2	1.99	0.43
2:C:219:PHE:HA	2:C:223:THR:HG23	2.00	0.43
3:E:154:SER:HA	3:E:157:LYS:HE3	1.98	0.43
4:H:405:SER:HB3	4:H:436:GLU:HB3	2.01	0.43
5:J:168:LEU:HD22	5:J:230:LEU:HD13	2.01	0.43
5:J:255:LEU:HD12	5:J:256:ARG:HG2	2.01	0.43
7:N:314:ARG:NE	7:N:424:PRO:HD3	2.33	0.43
7:M:141:GLY:O	7:M:319:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:HG3	1:A:91:LYS:HE3	2.01	0.43
7:N:316:ILE:HD11	7:N:343:LEU:HD12	2.00	0.43
7:N:357:PRO:O	7:N:426:ILE:CG2	2.67	0.43
2:C:155:ILE:HA	2:C:158:ILE:HD12	2.00	0.43
1:A:149:PHE:C	1:A:149:PHE:CD1	2.92	0.43
2:D:179:LEU:HD13	2:D:293:PHE:HE2	1.84	0.43
6:L:112:LEU:HD21	6:L:130:ILE:HG13	2.01	0.43
1:A:109:ARG:HH22	1:A:133:ARG:HB3	1.84	0.43
1:A:149:PHE:HD1	1:A:149:PHE:C	2.22	0.43
1:A:200:GLY:HA2	1:A:235:LYS:HB3	2.01	0.43
6:K:77:ASP:HB3	6:K:82:TYR:HB2	1.99	0.43
1:B:41:THR:HG22	6:K:75:ARG:HB3	2.00	0.43
6:L:159:GLU:HA	6:L:160:PRO:HD3	1.88	0.43
6:L:202:LYS:HE2	7:N:331:GLU:HG2	2.00	0.43
6:L:21:MET:HG2	6:L:102:TYR:HB2	2.01	0.42
7:M:312:SER:HA	7:M:313:PRO:HD3	1.93	0.42
2:C:265:VAL:HA	2:C:271:THR:HG22	1.99	0.42
3:E:173:ASP:HB2	3:E:399:ASN:HD21	1.84	0.42
7:N:309:PHE:HB3	7:N:346:VAL:HG23	2.02	0.42
3:F:252:TYR:HE1	5:I:215:PRO:HG3	1.85	0.42
4:G:271:HIS:HA	4:G:272:PRO:HD3	1.89	0.42
6:K:71:ALA:HB3	6:K:85:LEU:HD23	2.02	0.42
8:P:229:TYR:O	8:P:229:TYR:CG	2.71	0.42
1:B:16:GLU:HB3	1:B:17:ASP:H	1.69	0.42
4:G:272:PRO:HA	4:G:275:LEU:HD12	2.00	0.42
4:G:327:ILE:HG23	4:G:336:LEU:HD11	2.00	0.42
5:I:186:VAL:HG22	5:I:226:ILE:HG23	2.00	0.42
1:B:68:ALA:HB2	1:B:237:VAL:HG22	2.02	0.42
4:G:416:ASN:HA	4:G:420:LEU:HD12	2.02	0.42
1:A:212:GLY:HA3	1:B:182:SER:HB2	2.01	0.42
1:B:210:LEU:HB3	1:B:211:VAL:H	1.63	0.42
3:E:224:THR:HG22	3:E:268:VAL:HG22	2.01	0.42
1:B:21:THR:OG1	1:B:24:ILE:CD1	2.63	0.42
7:M:215:LEU:HD23	7:M:245:ILE:HB	2.02	0.42
2:D:265:VAL:HA	2:D:271:THR:HG22	2.01	0.42
3:F:198:THR:HB	3:F:272:LEU:HB3	2.02	0.42
5:I:344:ALA:HB3	5:I:361:VAL:HG13	2.02	0.42
5:J:135:VAL:HG22	5:J:235:ILE:HG23	2.02	0.42
7:M:149:LYS:HE3	7:M:299:VAL:HG21	2.01	0.42
1:B:34:LEU:HD22	1:B:73:PHE:HZ	1.84	0.42
1:A:201:VAL:HG11	1:A:295:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:LEU:HD13	2:D:91:ILE:HD13	2.02	0.42
5:J:231:ILE:HG21	5:J:283:VAL:HG22	2.02	0.42
7:N:432:ILE:HG12	7:N:499:ILE:HD13	2.02	0.41
1:B:104:ARG:HA	1:B:107:LYS:HE3	2.02	0.41
3:E:152:GLY:HA2	3:E:155:LEU:HD12	2.02	0.41
5:I:338:LYS:HE3	5:I:356:LYS:HE2	2.01	0.41
5:J:418:VAL:HG22	5:J:461:THR:HG22	2.03	0.41
7:N:357:PRO:HB2	7:N:490:PRO:HB3	2.02	0.41
1:A:252:PRO:HA	1:A:253:PRO:HD3	1.94	0.41
5:I:368:ILE:HG12	5:I:385:ILE:HD12	2.02	0.41
7:N:423:LEU:N	7:N:424:PRO:HD2	2.35	0.41
1:B:172:LYS:HE2	1:B:172:LYS:HA	2.01	0.41
7:N:309:PHE:CD1	7:N:309:PHE:N	2.88	0.41
7:N:359:ILE:HD11	7:N:411:ARG:HH11	1.86	0.41
6:K:207:SER:HB2	6:K:250:LYS:HD2	2.01	0.41
7:M:98:GLN:HE22	7:M:396:ILE:HD11	1.85	0.41
7:M:307:ARG:HD3	7:M:392:PRO:HB2	2.02	0.41
2:C:172:ILE:HG22	2:C:176:ALA:HB2	2.02	0.41
7:M:430:ILE:HD12	7:M:432:ILE:HD12	2.03	0.41
2:D:19:ASN:HB2	2:D:22:ILE:HD11	2.03	0.41
8:P:211:LEU:HD13	8:P:213:ILE:HD11	2.02	0.41
1:A:109:ARG:HH12	1:A:133:ARG:HB3	1.85	0.41
1:B:166:TYR:HE1	1:B:176:VAL:HG23	1.86	0.41
5:I:161:ASP:HB3	5:I:271:LYS:HG2	2.03	0.41
5:J:186:VAL:HG22	5:J:226:ILE:HG12	2.02	0.41
6:K:247:ALA:HA	6:K:250:LYS:HE3	2.03	0.41
4:G:400:ILE:HG12	4:G:469:TYR:HB2	2.03	0.41
4:H:271:HIS:HA	4:H:272:PRO:HD3	1.86	0.41
4:H:570:LYS:HB2	4:H:571:PRO:HD3	2.03	0.41
4:G:383:ASP:O	4:G:387:ILE:HG12	2.20	0.40
7:M:461:VAL:HG22	7:M:474:ARG:HE	1.86	0.40
7:N:412:LEU:HA	7:N:415:GLN:HE21	1.86	0.40
2:D:198:LYS:O	2:D:201:ILE:HG22	2.20	0.40
7:N:215:LEU:HD22	7:N:247:LEU:HD11	2.03	0.40
1:A:291:THR:H	1:A:292:PRO:CD	2.34	0.40
5:J:32:LEU:HB2	5:J:136:SER:HA	2.02	0.40
6:K:126:LEU:O	6:K:129:THR:HG22	2.21	0.40
7:M:356:ARG:HB2	7:M:416:VAL:HG23	2.03	0.40
1:A:172:LYS:HD3	1:A:172:LYS:HA	1.75	0.40
2:C:57:TRP:HB3	2:C:63:LEU:HD13	2.04	0.40
3:F:69:LEU:HA	3:F:70:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:539:ASN:HB2	4:H:540:PRO:HD3	2.03	0.40
7:N:499:ILE:HD11	7:N:517:ILE:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/305 (98%)	254 (85%)	39 (13%)	7 (2%)	5	28
1	B	300/305 (98%)	256 (85%)	35 (12%)	9 (3%)	3	23
2	C	339/381 (89%)	308 (91%)	28 (8%)	3 (1%)	14	52
2	D	339/381 (89%)	309 (91%)	25 (7%)	5 (2%)	8	40
3	E	253/578 (44%)	217 (86%)	34 (13%)	2 (1%)	16	55
3	F	253/578 (44%)	211 (83%)	37 (15%)	5 (2%)	6	32
4	G	349/651 (54%)	303 (87%)	35 (10%)	11 (3%)	3	21
4	H	349/651 (54%)	302 (86%)	36 (10%)	11 (3%)	3	21
5	I	427/712 (60%)	379 (89%)	41 (10%)	7 (2%)	8	38
5	J	427/712 (60%)	365 (86%)	45 (10%)	17 (4%)	2	18
6	K	237/304 (78%)	208 (88%)	27 (11%)	2 (1%)	16	55
6	L	237/304 (78%)	211 (89%)	25 (10%)	1 (0%)	30	68
7	M	398/527 (76%)	345 (87%)	48 (12%)	5 (1%)	10	43
7	N	398/527 (76%)	330 (83%)	55 (14%)	13 (3%)	3	21
8	O	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	12
8	P	120/285 (42%)	100 (83%)	18 (15%)	2 (2%)	7	37
All	All	4741/7486 (63%)	4111 (87%)	529 (11%)	101 (2%)	8	30

All (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	J	202	LEU
1	B	158	PRO
1	B	304	TYR
2	C	275	ASN
2	C	276	SER
2	C	337	ILE
2	D	275	ASN
2	D	276	SER
2	D	337	ILE
4	G	579	LYS
4	H	537	TYR
4	H	579	LYS
5	I	173	THR
5	I	464	VAL
5	J	201	PRO
5	J	459	ASP
5	J	464	VAL
7	M	507	LYS
7	N	311	ILE
7	N	430	ILE
1	A	97	ASN
1	A	158	PRO
1	A	291	THR
1	B	38	THR
1	B	98	GLY
1	B	291	THR
3	E	160	LEU
4	G	265	LEU
4	G	397	SER
4	G	537	TYR
4	G	586	SER
4	H	397	SER
5	I	112	ALA
5	I	423	ASN
5	J	112	ALA
5	J	173	THR
5	J	182	PRO

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Mol	Chain	Res	Type
5	J	355	THR
5	J	371	ASN
5	J	388	ASN
5	J	423	ASN
6	K	225	ALA
6	L	132	TRP
7	M	127	ARG
7	M	164	PHE
7	M	383	GLU
7	N	178	GLY
7	N	255	ARG
7	N	497	GLU
7	N	507	LYS
1	A	5	ASN
1	A	38	THR
1	B	5	ASN
1	B	263	LEU
3	F	160	LEU
3	F	311	GLN
4	H	251	PHE
5	I	311	ASN
5	I	459	ASP
5	J	26	ARG
5	J	192	SER
5	J	421	ASP
8	O	129	LEU
7	N	176	ARG
7	N	306	PRO
8	P	129	LEU
1	A	61	PRO
2	D	324	ARG
3	F	238	LEU
4	G	242	VAL
4	G	542	GLU
4	G	548	GLY
4	H	242	VAL
4	H	248	GLU
4	H	500	ASN
4	H	548	GLY
4	H	555	ILE
5	J	369	GLY
6	K	81	GLY

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Mol	Chain	Res	Type
7	M	497	GLU
7	N	383	GLU
7	N	420	LYS
8	P	200	GLY
1	A	35	ARG
2	D	191	PRO
3	F	180	PRO
4	H	245	THR
5	J	38	THR
7	N	494	GLU
4	G	555	ILE
5	I	466	ILE
5	J	467	VAL
7	N	490	PRO
4	G	540	PRO
7	N	177	PRO
1	B	292	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/265 (97%)	238 (93%)	19 (7%)	11	31
1	B	257/265 (97%)	241 (94%)	16 (6%)	15	36
2	C	286/338 (85%)	265 (93%)	21 (7%)	11	31
2	D	286/338 (85%)	266 (93%)	20 (7%)	12	32
3	E	249/529 (47%)	244 (98%)	5 (2%)	50	68
3	F	249/529 (47%)	241 (97%)	8 (3%)	34	53
4	G	305/561 (54%)	298 (98%)	7 (2%)	45	64
4	H	305/561 (54%)	296 (97%)	9 (3%)	36	55
5	I	389/649 (60%)	374 (96%)	15 (4%)	27	48
5	J	389/649 (60%)	375 (96%)	14 (4%)	30	50
6	K	219/273 (80%)	195 (89%)	24 (11%)	5	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	L	219/273 (80%)	195 (89%)	24 (11%)	5 18
7	M	319/449 (71%)	313 (98%)	6 (2%)	52 69
7	N	319/449 (71%)	299 (94%)	20 (6%)	15 36
8	O	16/246 (6%)	16 (100%)	0	100 100
8	P	119/246 (48%)	109 (92%)	10 (8%)	9 27
All	All	4183/6620 (63%)	3965 (95%)	218 (5%)	22 40

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	PHE
1	A	17	ASP
1	A	21	THR
1	A	24	ILE
1	A	37	LYS
1	A	54	GLU
1	A	70	CYS
1	A	101	PHE
1	A	149	PHE
1	A	161	GLN
1	A	172	LYS
1	A	188	ILE
1	A	196	VAL
1	A	224	ARG
1	A	237	VAL
1	A	255	ASP
1	A	290	LEU
1	A	297	GLU
1	B	12	ARG
1	B	17	ASP
1	B	21	THR
1	B	22	MET
1	B	37	LYS
1	B	54	GLU
1	B	56	LEU
1	B	104	ARG
1	B	124	ASP
1	B	136	PHE
1	B	149	PHE

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Mol	Chain	Res	Type
1	B	161	GLN
1	B	172	LYS
1	B	231	THR
1	B	237	VAL
1	B	242	LEU
2	C	24	THR
2	C	38	TYR
2	C	40	ILE
2	C	42	LEU
2	C	151	ARG
2	C	161	LEU
2	C	168	ILE
2	C	179	LEU
2	C	199	PHE
2	C	206	ARG
2	C	222	ASN
2	C	223	THR
2	C	238	ILE
2	C	278	VAL
2	C	286	ARG
2	C	298	LEU
2	C	308	ASP
2	C	322	LEU
2	C	363	ARG
2	C	366	TRP
2	C	371	GLN
2	D	24	THR
2	D	38	TYR
2	D	42	LEU
2	D	44	THR
2	D	84	CYS
2	D	160	ASP
2	D	161	LEU
2	D	168	ILE
2	D	182	ASP
2	D	199	PHE
2	D	200	LEU
2	D	201	ILE
2	D	222	ASN
2	D	286	ARG
2	D	298	LEU
2	D	307	PHE

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Mol	Chain	Res	Type
2	D	308	ASP
2	D	363	ARG
2	D	366	TRP
2	D	371	GLN
3	E	100	GLU
3	E	183	LEU
3	E	185	ASP
3	E	249	LYS
3	E	402	MET
3	F	100	GLU
3	F	141	ILE
3	F	173	ASP
3	F	237	ILE
3	F	246	ASP
3	F	255	ILE
3	F	258	HIS
3	F	402	MET
4	G	284	TYR
4	G	296	MET
4	G	366	ASP
4	G	388	ASP
4	G	412	LEU
4	G	439	LYS
4	G	568	GLU
4	H	284	TYR
4	H	296	MET
4	H	388	ASP
4	H	412	LEU
4	H	424	ILE
4	H	456	ILE
4	H	460	ASP
4	H	523	PHE
4	H	576	ILE
5	I	41	MET
5	I	51	LEU
5	I	88	ASP
5	I	97	LEU
5	I	113	ARG
5	I	122	LEU
5	I	127	ILE
5	I	140	LEU
5	I	176	LYS

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Mol	Chain	Res	Type
5	I	181	GLU
5	I	231	ILE
5	I	307	VAL
5	I	333	LEU
5	I	345	ILE
5	I	457	LEU
5	J	41	MET
5	J	88	ASP
5	J	89	TYR
5	J	97	LEU
5	J	113	ARG
5	J	122	LEU
5	J	140	LEU
5	J	145	PHE
5	J	173	THR
5	J	176	LYS
5	J	247	GLN
5	J	286	GLU
5	J	333	LEU
5	J	467	VAL
6	K	7	ARG
6	K	11	ASN
6	K	17	ASP
6	K	19	ILE
6	K	40	ASP
6	K	45	MET
6	K	54	ARG
6	K	59	ILE
6	K	64	ARG
6	K	79	GLU
6	K	88	ARG
6	K	97	LYS
6	K	124	GLU
6	K	129	THR
6	K	137	LYS
6	K	143	GLU
6	K	159	GLU
6	K	166	LEU
6	K	168	GLU
6	K	169	LEU
6	K	230	LEU
6	K	235	LEU

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Mol	Chain	Res	Type
6	K	244	LEU
6	K	251	ILE
6	L	7	ARG
6	L	19	ILE
6	L	45	MET
6	L	47	LEU
6	L	54	ARG
6	L	59	ILE
6	L	69	ASP
6	L	79	GLU
6	L	88	ARG
6	L	97	LYS
6	L	102	TYR
6	L	119	PHE
6	L	124	GLU
6	L	127	TYR
6	L	137	LYS
6	L	143	GLU
6	L	159	GLU
6	L	165	VAL
6	L	168	GLU
6	L	169	LEU
6	L	230	LEU
6	L	235	LEU
6	L	244	LEU
6	L	251	ILE
7	M	169	GLU
7	M	353	ILE
7	M	402	VAL
7	M	406	LEU
7	M	432	ILE
7	M	508	HIS
7	N	189	VAL
7	N	251	VAL
7	N	292	ASP
7	N	309	PHE
7	N	310	MET
7	N	311	ILE
7	N	315	LEU
7	N	354	GLU
7	N	371	LYS
7	N	406	LEU

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Mol	Chain	Res	Type
7	N	420	LYS
7	N	422	HIS
7	N	423	LEU
7	N	425	ASN
7	N	426	ILE
7	N	427	TYR
7	N	429	ASP
7	N	492	CYS
7	N	493	THR
7	N	510	ARG
8	P	166	LEU
8	P	170	LYS
8	P	171	LYS
8	P	174	PHE
8	P	186	ARG
8	P	191	LEU
8	P	221	GLN
8	P	229	TYR
8	P	235	THR
8	P	238	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	163	ASN
2	C	152	GLN
2	C	156	GLN
2	C	222	ASN
2	C	236	HIS
2	C	237	ASN
2	C	275	ASN
2	C	352	ASN
2	D	78	HIS
2	D	221	ASN
3	E	156	GLN
3	E	258	HIS
3	E	399	ASN
3	F	219	GLN
3	F	221	GLN
4	G	271	HIS
4	G	416	ASN

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Mol	Chain	Res	Type
4	G	475	HIS
4	H	271	HIS
4	H	480	ASN
4	H	500	ASN
5	I	73	HIS
5	I	124	ASN
5	I	296	GLN
5	I	376	ASN
6	K	41	ASN
6	L	23	ASN
6	L	103	GLN
7	M	98	GLN
7	M	108	HIS
7	M	151	GLN
7	M	197	HIS
7	M	248	GLN
7	N	243	HIS
7	N	422	HIS
7	N	425	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	L	52	6	8,9,10	0.65	0	8,12,14	1.25	1 (12%)
6	SEP	K	52	6	8,9,10	0.65	0	8,12,14	1.21	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	L	52	6	-	1/5/8/10	-
6	SEP	K	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 (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.

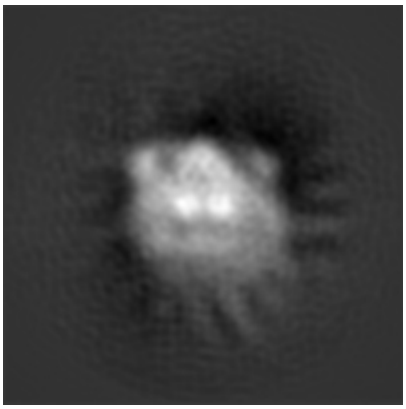
6 Map visualisation

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.

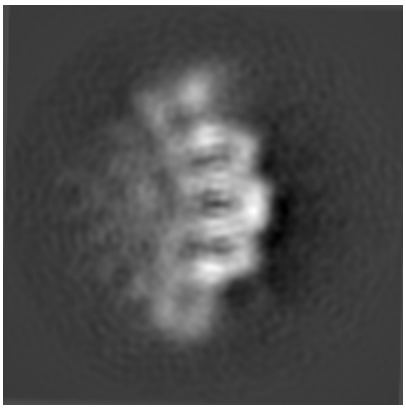
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

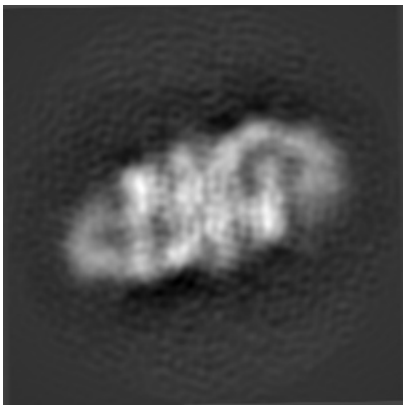
6.1.1 Primary map



X

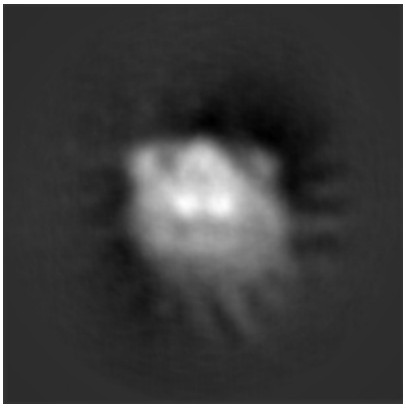


Y

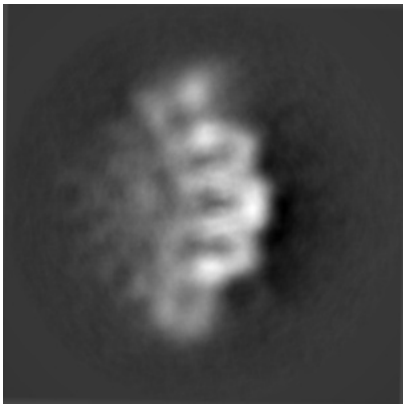


Z

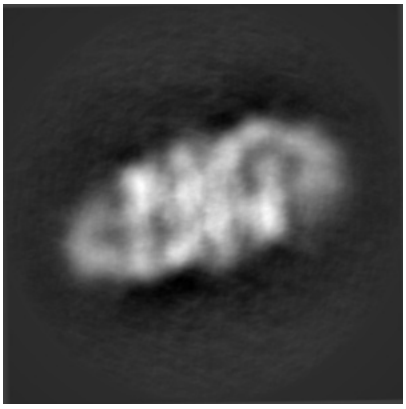
6.1.2 Raw map



X



Y

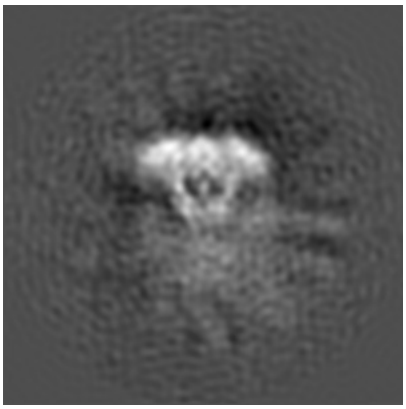


Z

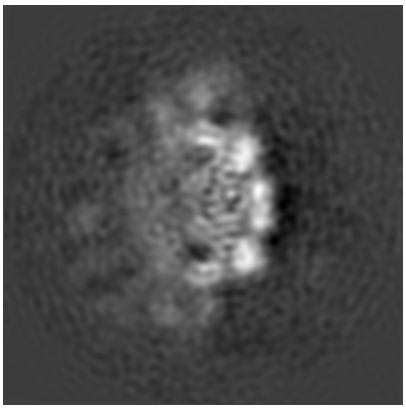
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

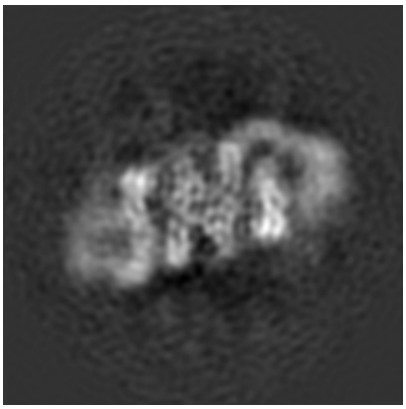
6.2.1 Primary map



X Index: 140

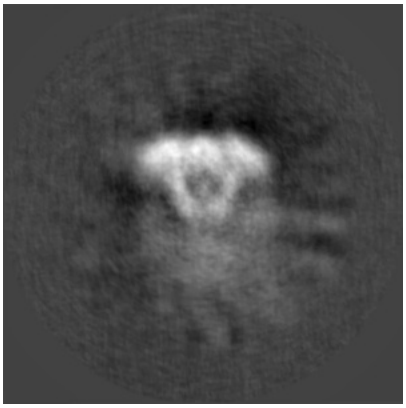


Y Index: 140

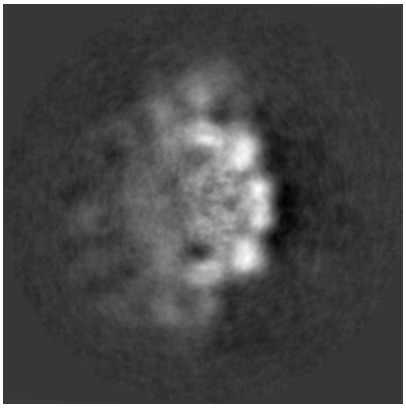


Z Index: 140

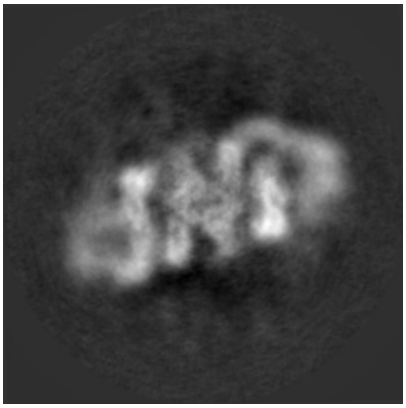
6.2.2 Raw map



X Index: 140



Y Index: 140

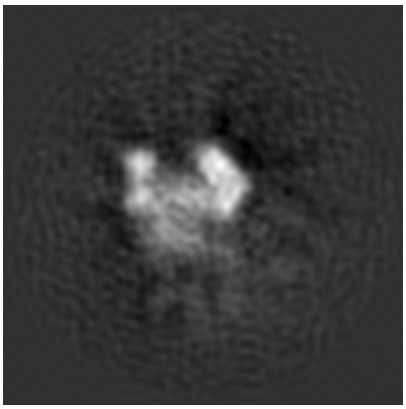


Z Index: 140

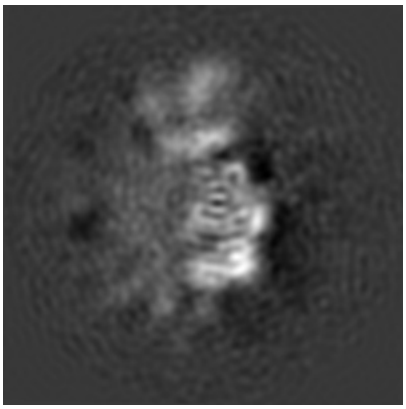
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

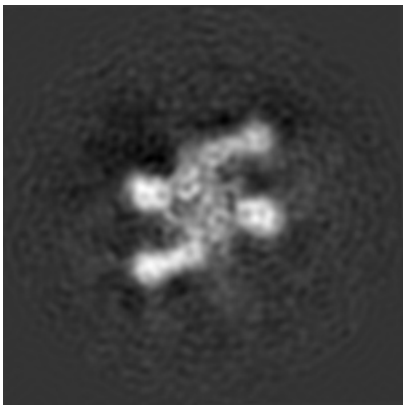
6.3.1 Primary map



X Index: 96

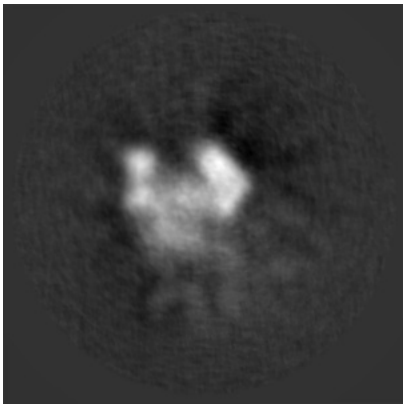


Y Index: 152

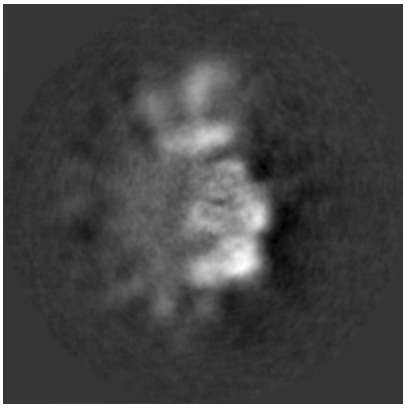


Z Index: 169

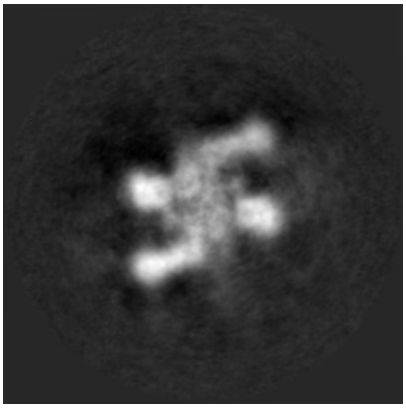
6.3.2 Raw map



X Index: 96



Y Index: 150

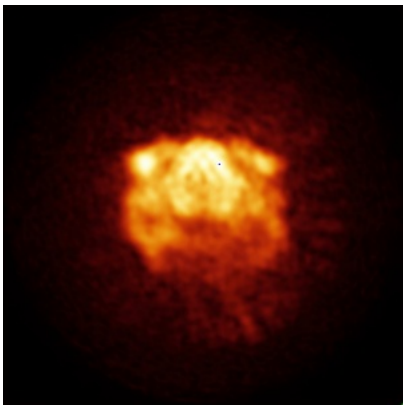


Z Index: 168

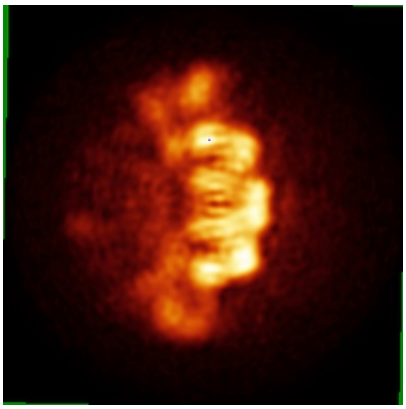
The images above show the largest variance slices of the map in three orthogonal directions.

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

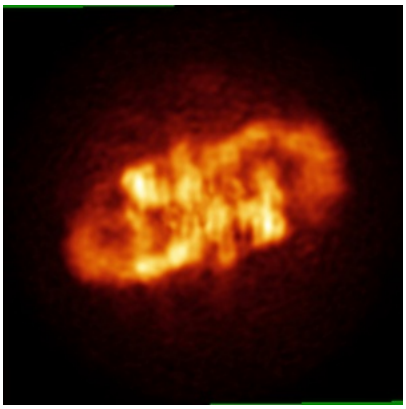
6.4.1 Primary map



X

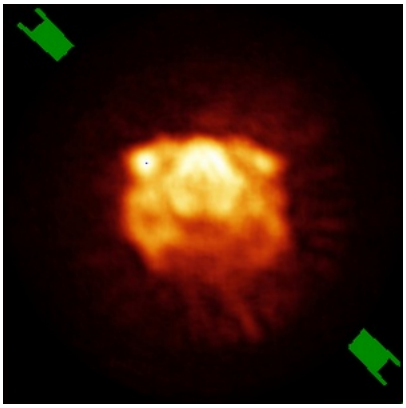


Y

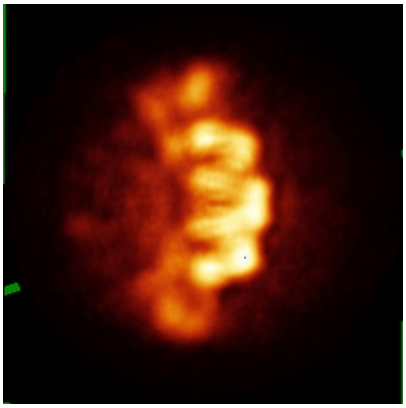


Z

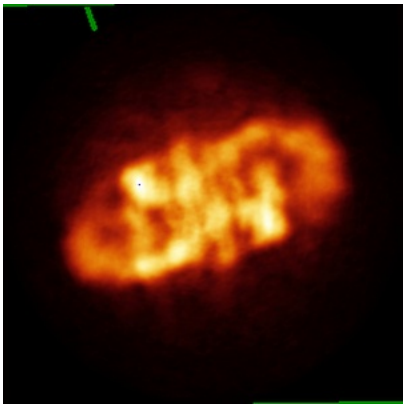
6.4.2 Raw map



X



Y

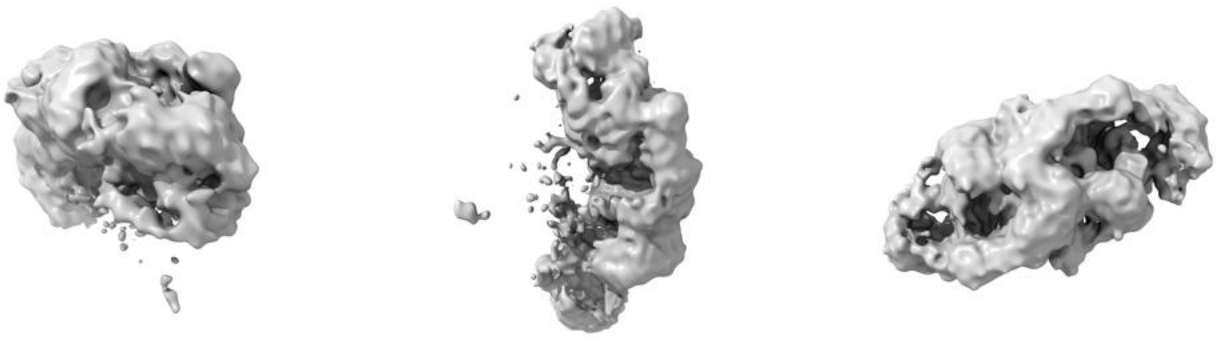


Z

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)

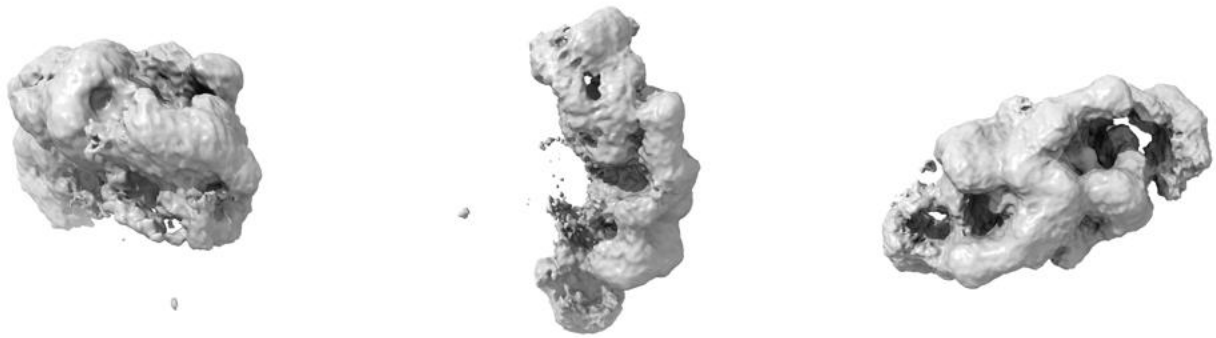
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

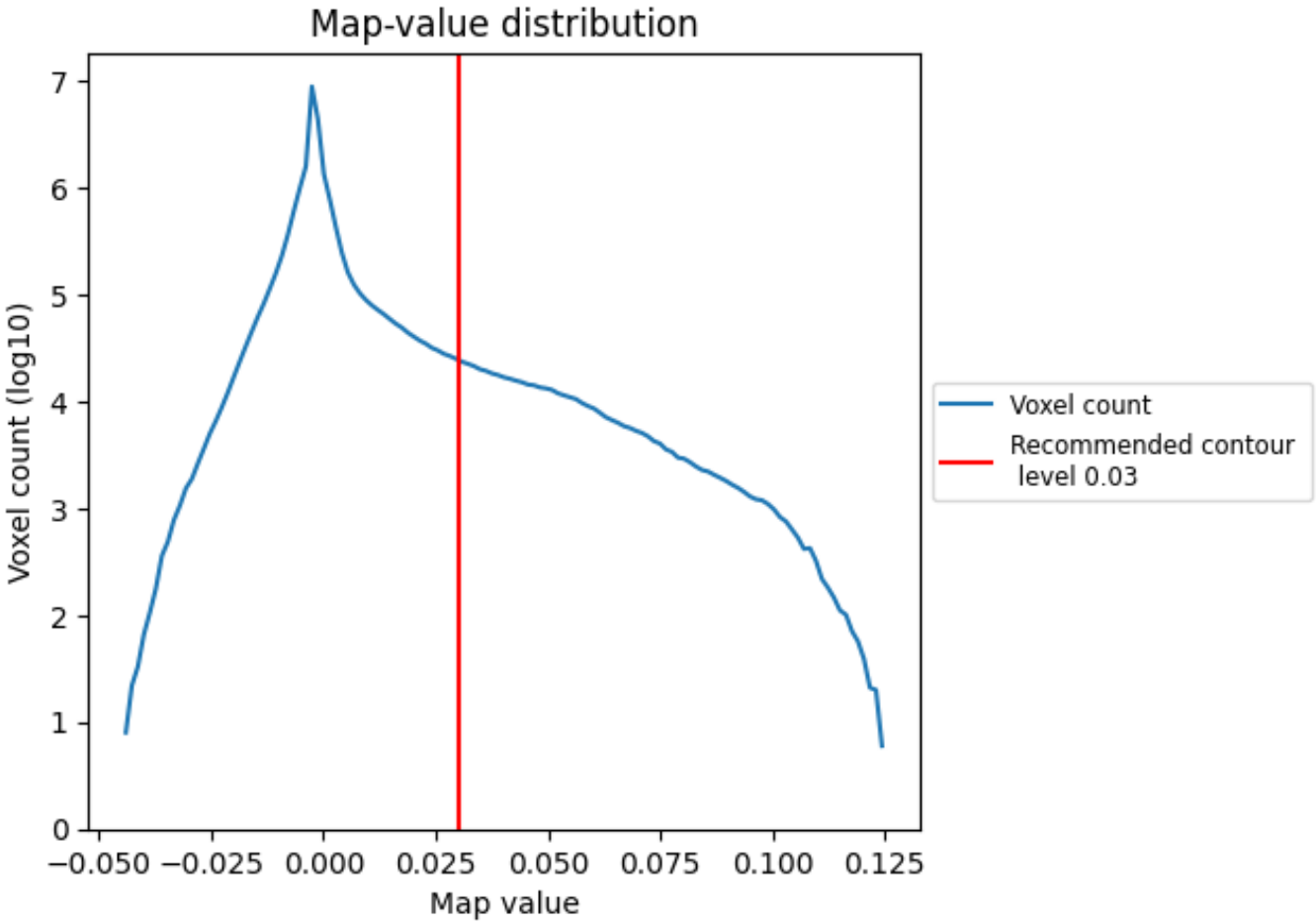
6.6 Mask visualisation (i)

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

7 Map analysis

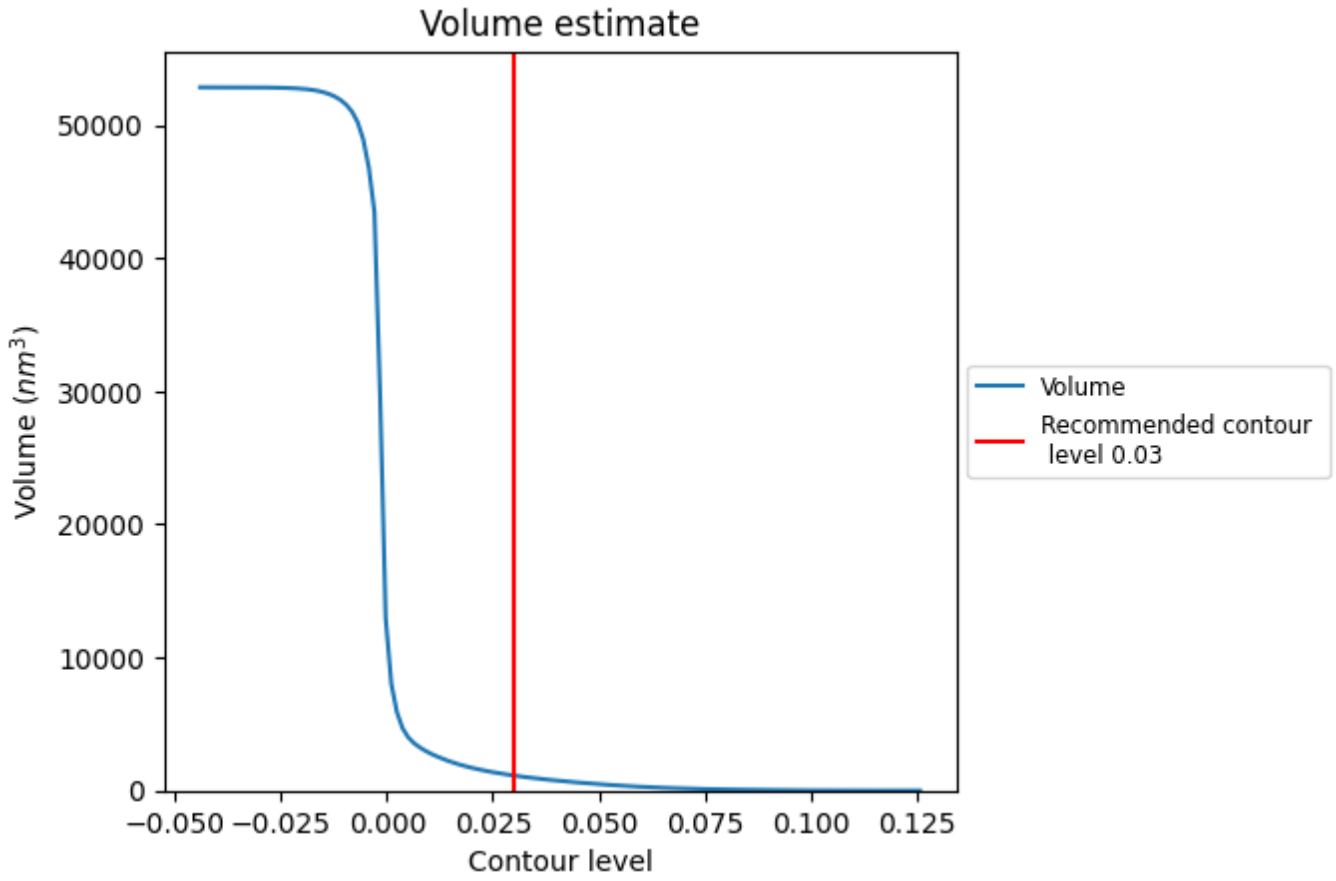
This section contains the results of statistical analysis of the map.

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.

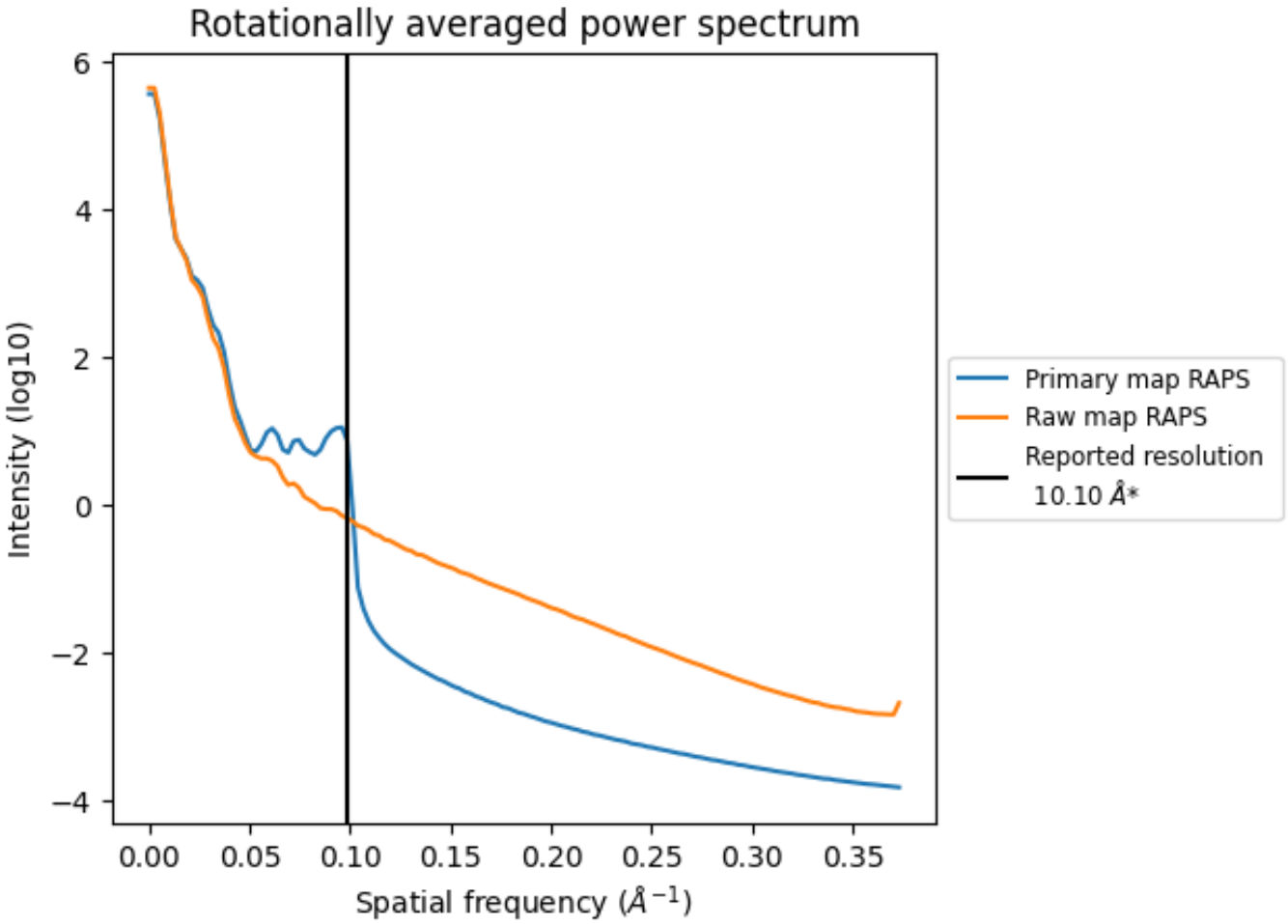
7.2 Volume estimate (i)



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 (i)

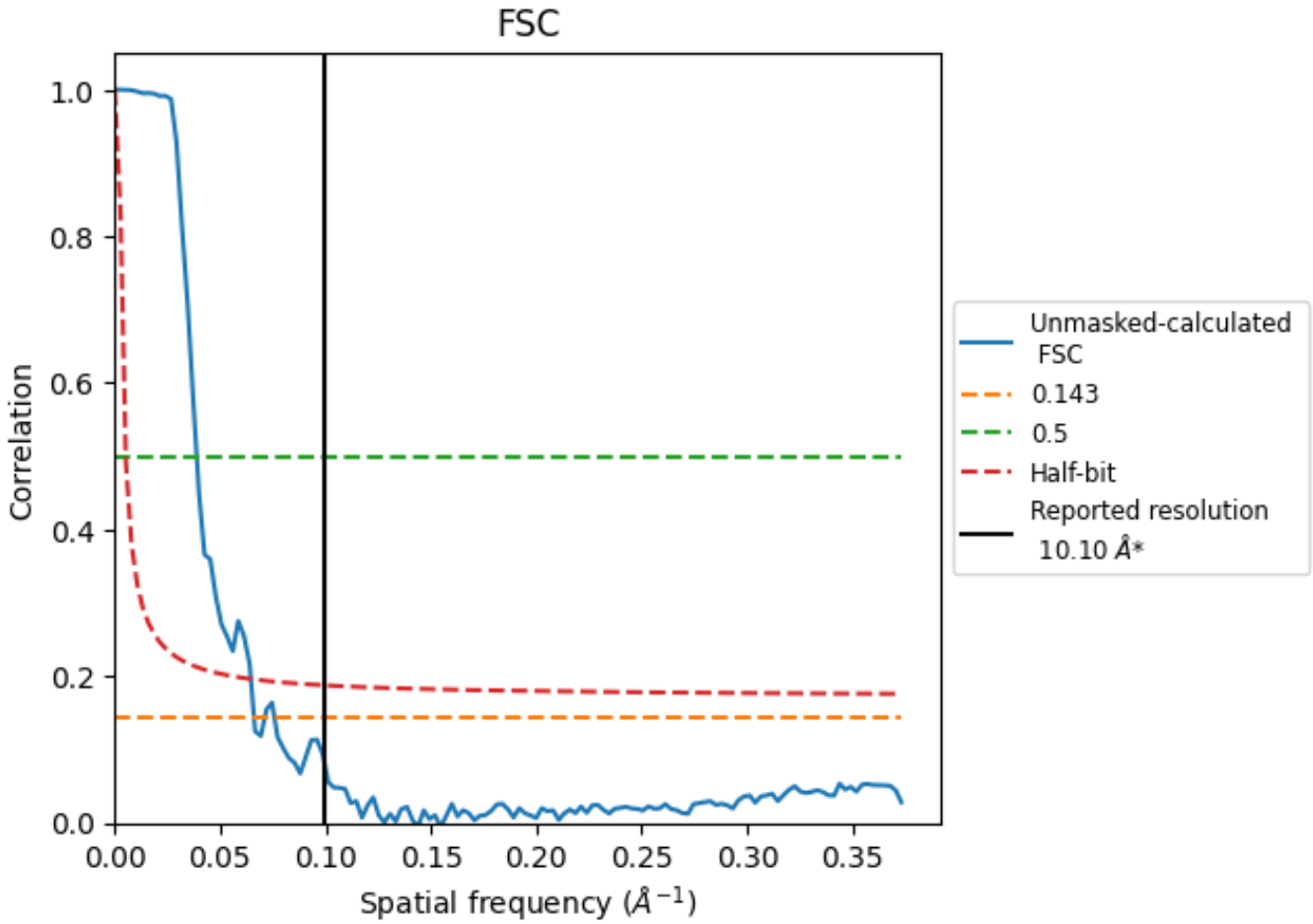


*Reported resolution corresponds to spatial frequency of 0.099 Å^{-1}

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)

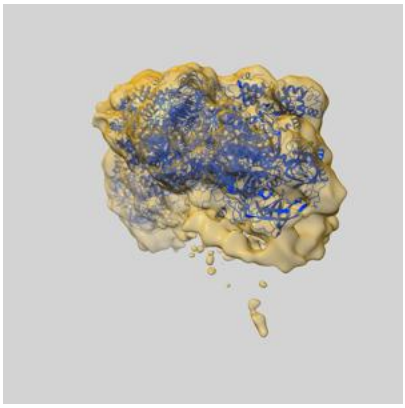
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	15.13	25.71	15.48

*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 %

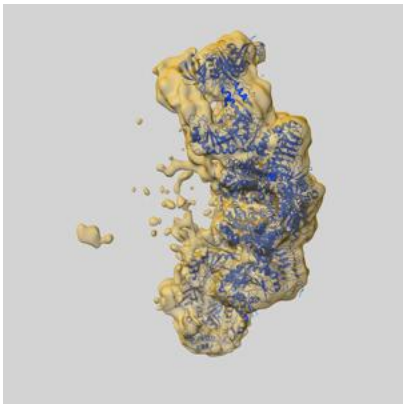
9 Map-model fit

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.

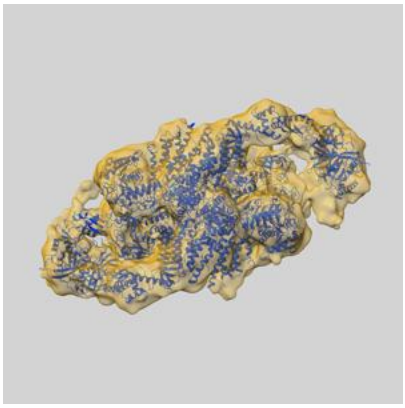
9.1 Map-model overlay



X



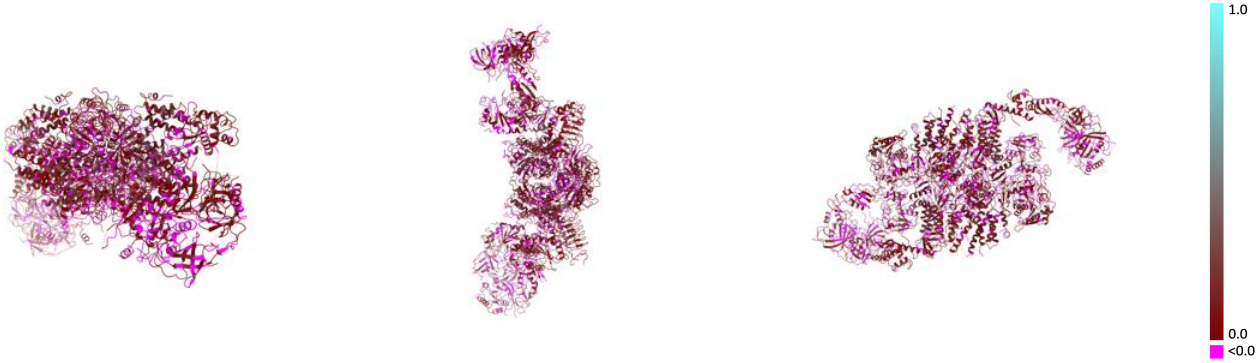
Y



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.

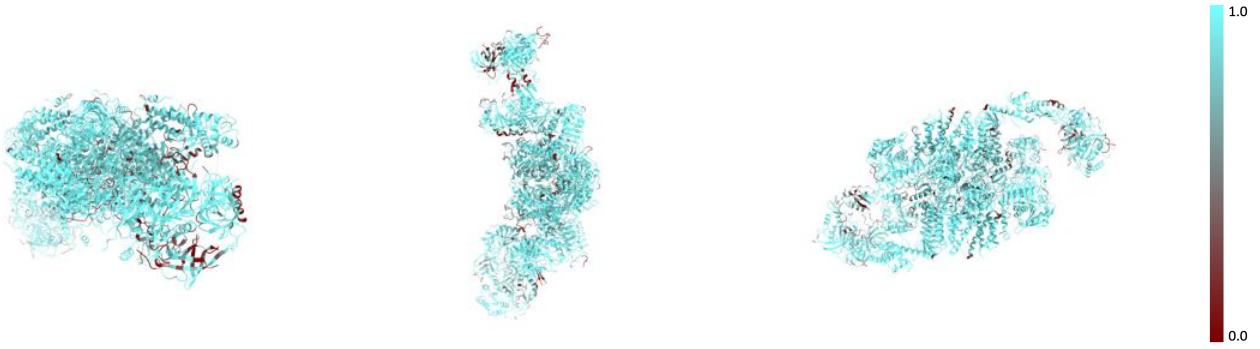
9.2 Q-score mapped to coordinate model



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.

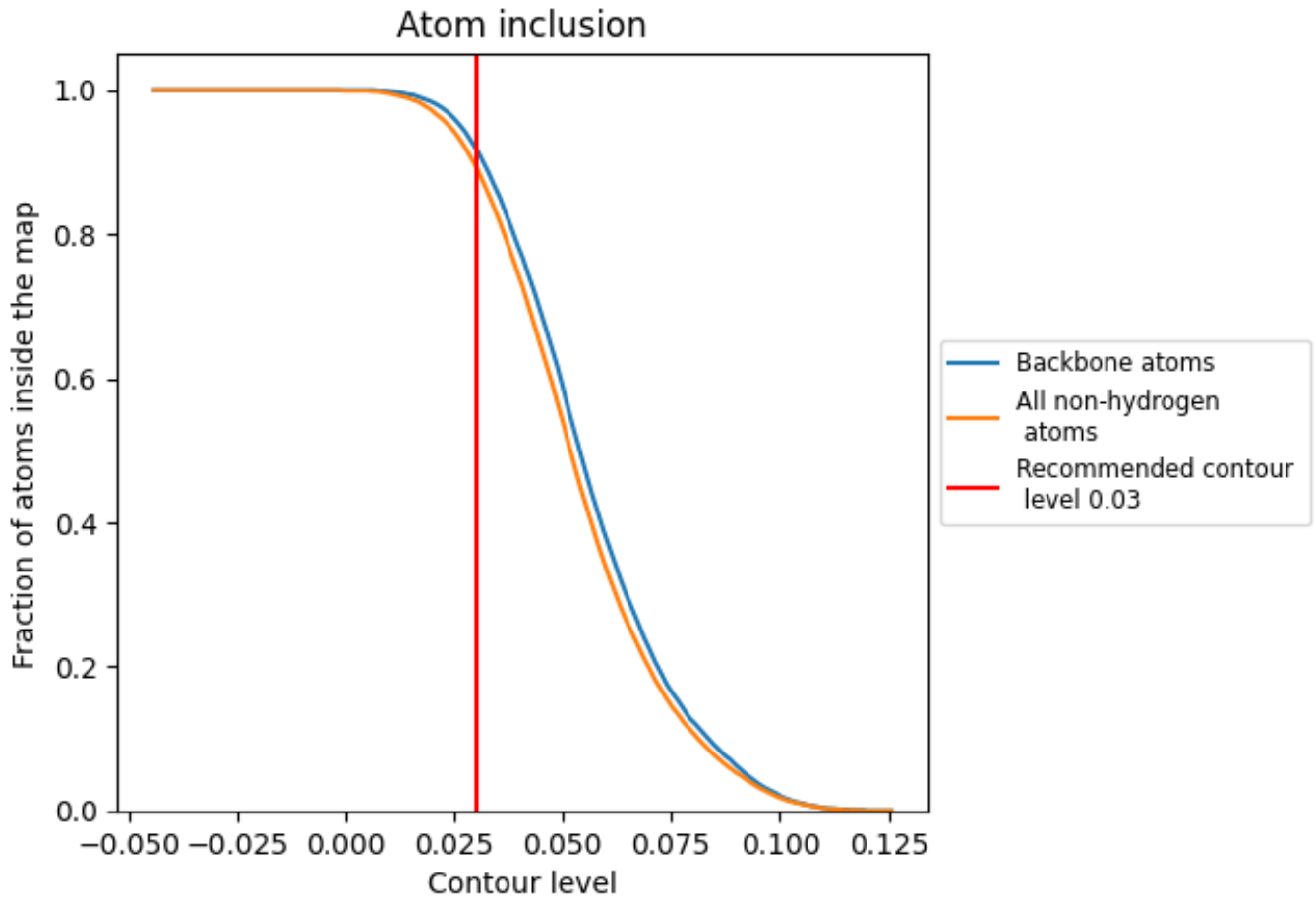
9.3 Atom inclusion mapped to coordinate model



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 (i)



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	0.8940	0.0690
A	0.9750	0.0770
B	0.9600	0.0810
C	0.9020	0.0750
D	0.8880	0.0740
E	0.8670	0.0430
F	0.9120	0.0500
G	0.8500	0.0880
H	0.8390	0.0890
I	0.9590	0.0820
J	0.9620	0.0820
K	0.8280	0.0670
L	0.9840	0.0760
M	0.7870	0.0350
N	0.8860	0.0430
O	0.9130	0.0540
P	0.6850	0.0590