Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 04:17 am GMT

PDB ID	:	6I3M
EMDB ID	:	EMD-4404
Title	:	eIF2B:eIF2 complex, phosphorylated on eIF2 alpha serine 52.
Authors	:	Adomavicius, T.; Roseman, A.M.; Pavitt, G.D.
Deposited on	:	2018-11-06
Resolution	:	3.93 Å(reported)
Based on initial models	:	3JAP, 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:

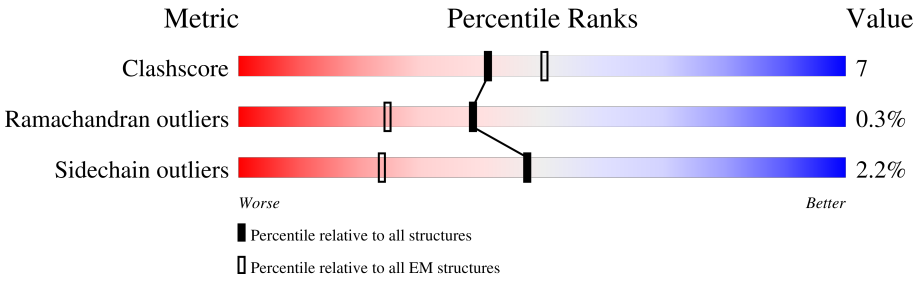
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.93 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	7% 82% 18%
1	B	305	7% 82% 18%
2	C	651	6% 44% 9% 47%
2	D	651	6% 44% 8% 47%
3	E	381	10% 73% 20% 7%
3	F	381	10% 74% 19% 7%
4	G	712	47% 11% 42%
4	H	712	46% 11% 42%

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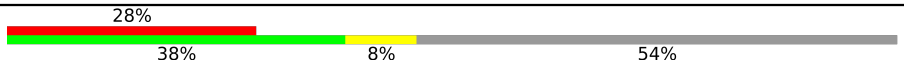
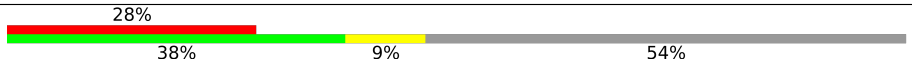
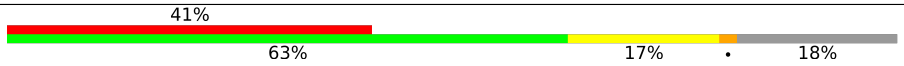
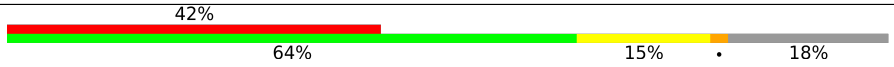
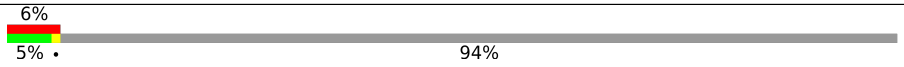
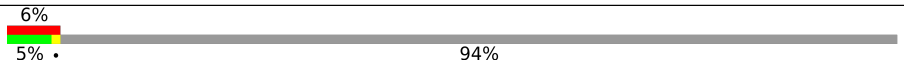
Mol	Chain	Length	Quality of chain
5	I	578	
5	J	578	
6	K	304	
6	L	304	
7	M	285	
7	N	285	
8	O	527	
8	P	527	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 37012 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	305	Total	C	N	O	S	0	0
			2393	1526	400	456	11		
1	B	305	Total	C	N	O	S	0	0
			2393	1526	400	456	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	342	Total	C	N	O	S	0	0
			2677	1715	446	505	11		
2	D	342	Total	C	N	O	S	0	0
			2677	1715	446	505	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	354	Total	C	N	O	S	0	0
			2797	1774	484	530	9		
3	F	354	Total	C	N	O	S	0	0
			2797	1774	484	530	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	410	Total	C	N	O	S	0	0
			3265	2061	549	635	20		
4	H	410	Total	C	N	O	S	0	0
			3265	2061	549	635	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	268	Total	C	N	O	S	0	0
			2187	1398	372	408	9		
5	J	268	Total	C	N	O	S	0	0
			2187	1398	372	408	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	249	Total	C	N	O	P	S	0	0
			2010	1283	333	385	1	8		
6	L	249	Total	C	N	O	P	S	0	0
			2010	1283	333	385	1	8		

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

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

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

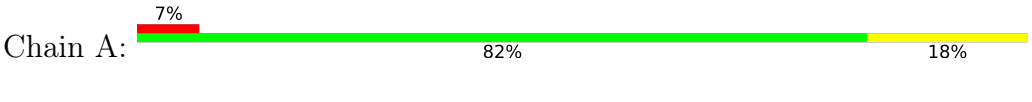
Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		
8	P	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

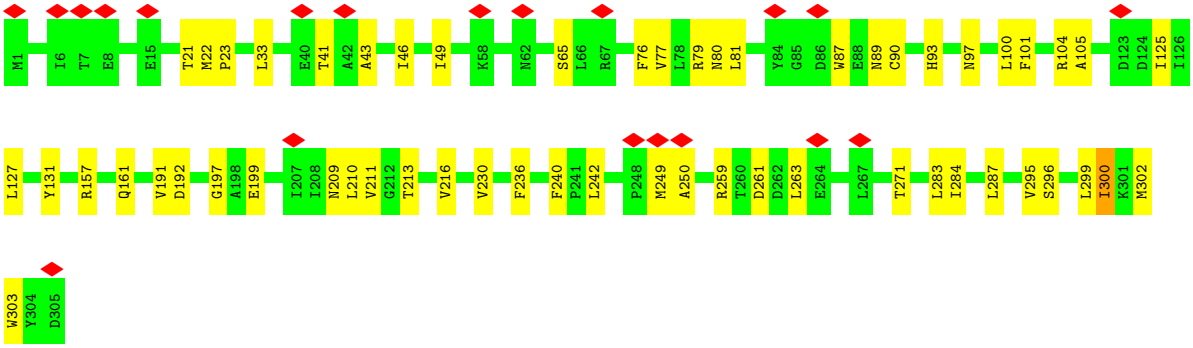
3 Residue-property plots (i)

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

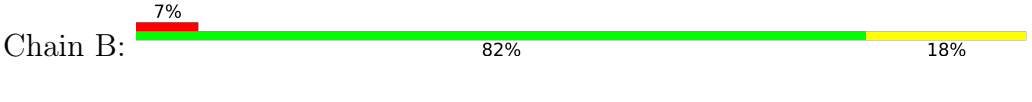
Chain A:

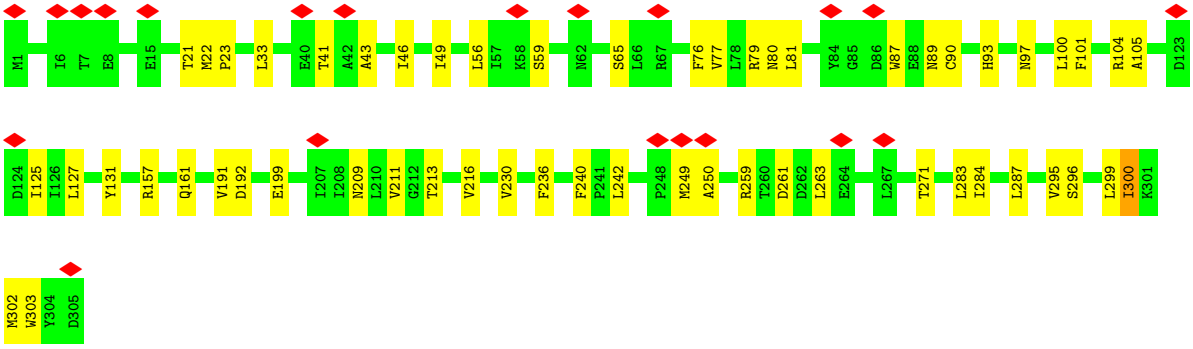




• Molecule 1: Translation initiation factor eIF-2B subunit alpha

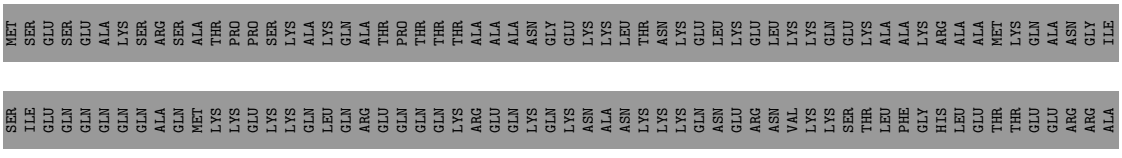
Chain B:

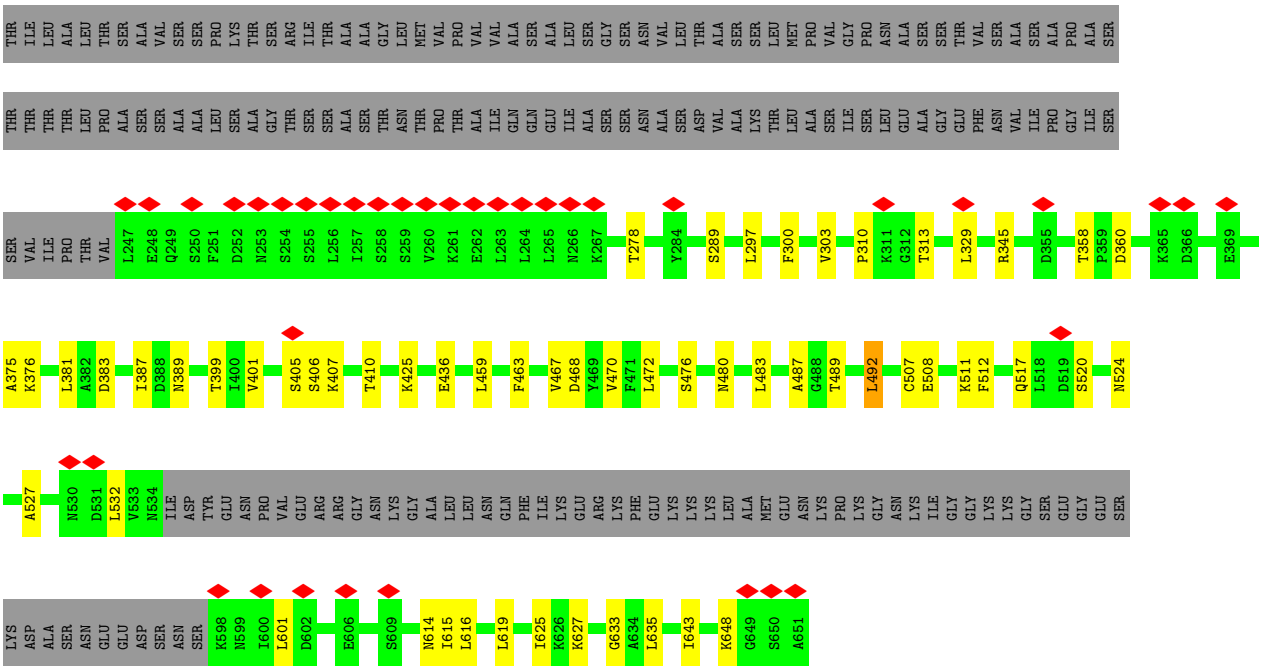




• Molecule 2: Translation initiation factor eIF-2B subunit delta

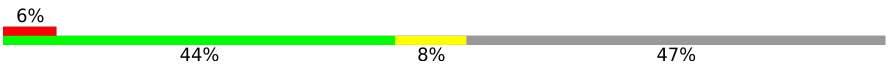
Chain C:

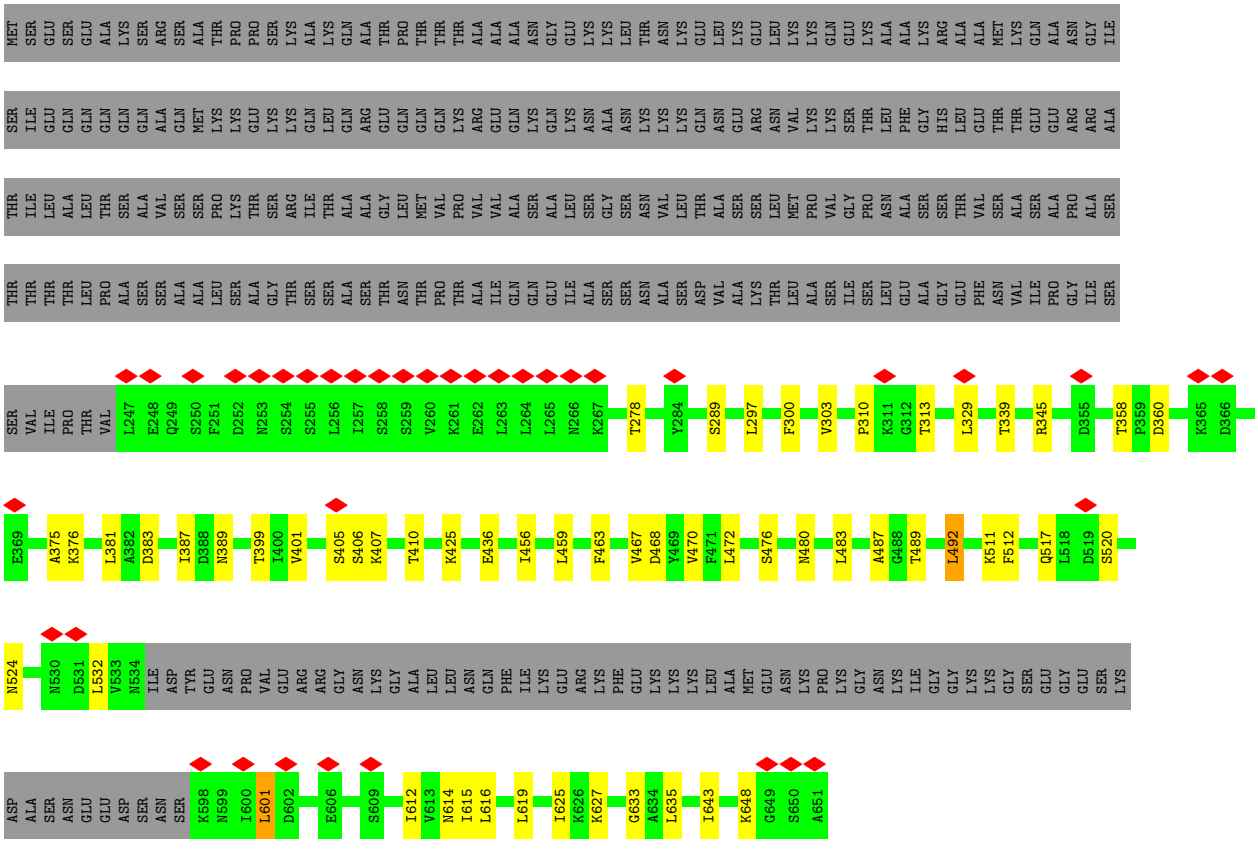




• Molecule 2: Translation initiation factor eIF-2B subunit delta

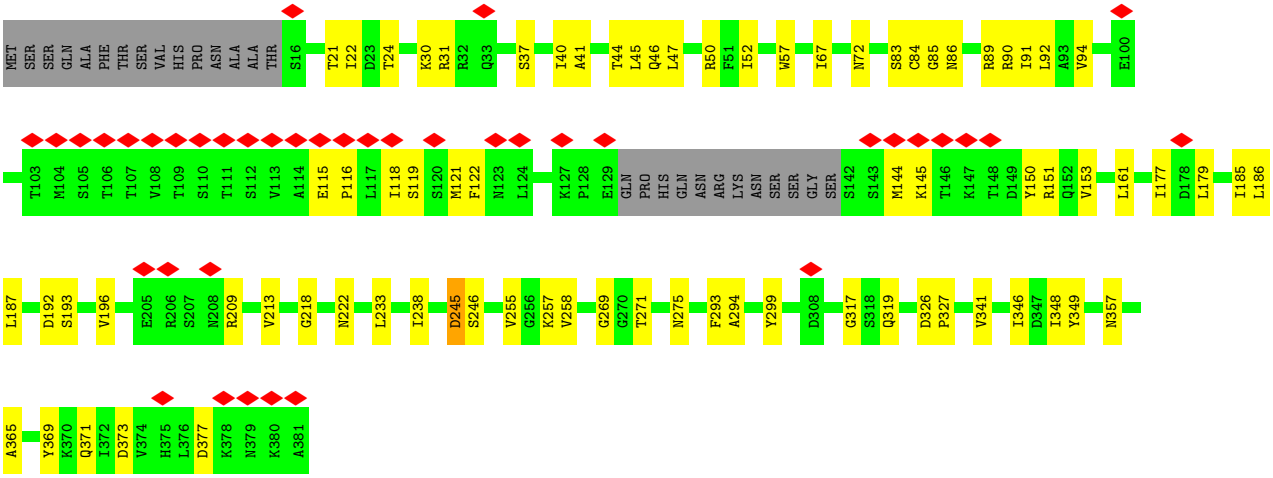
Chain D:





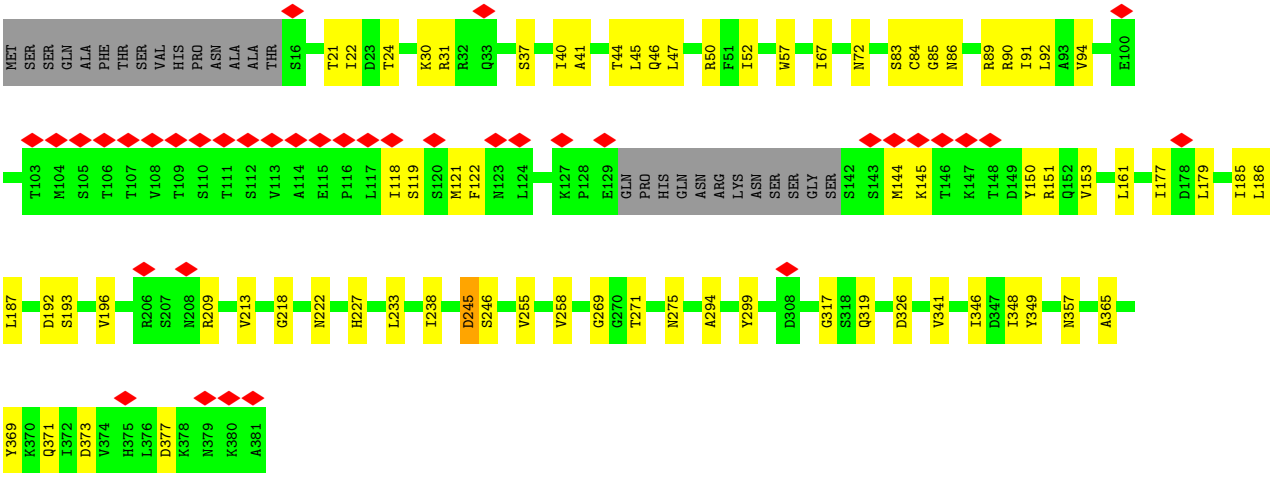
• Molecule 3: Translation initiation factor eIF-2B subunit beta

Chain E:



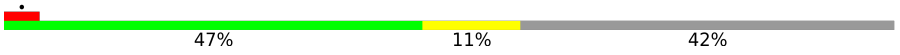
• Molecule 3: Translation initiation factor eIF-2B subunit beta

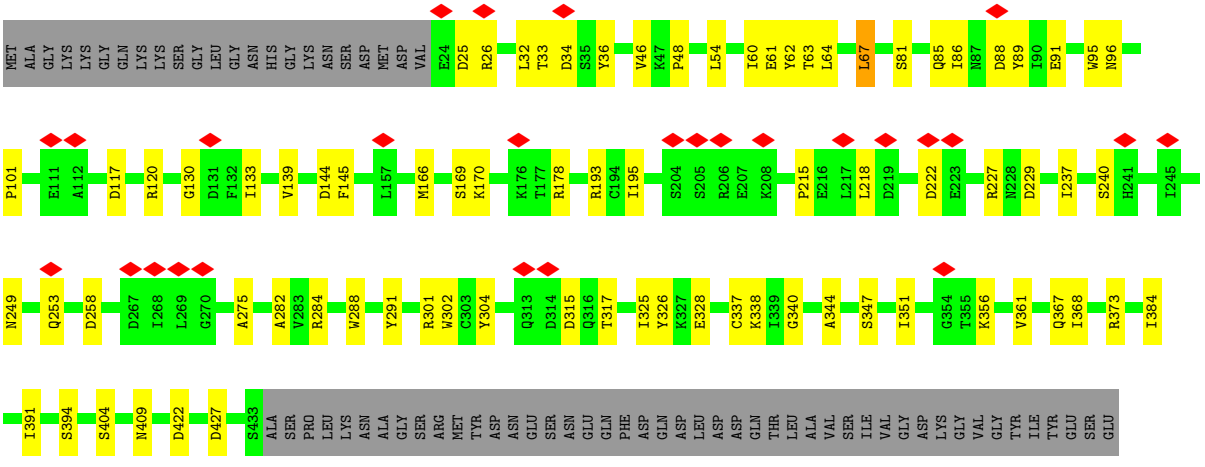
Chain F:

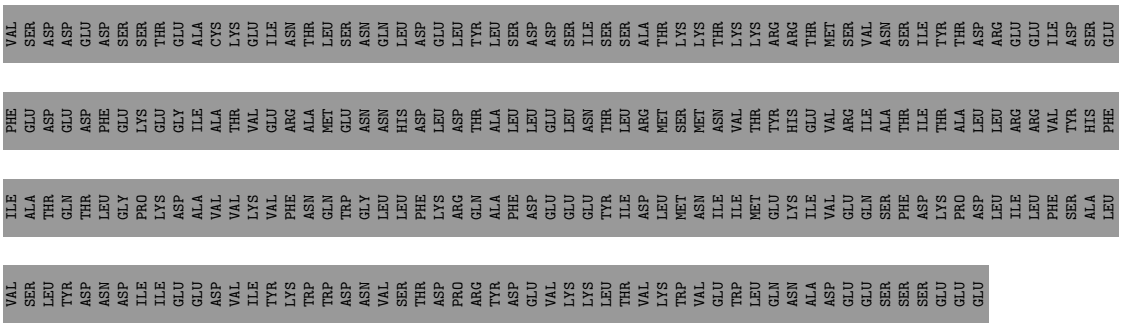


• Molecule 4: Translation initiation factor eIF-2B subunit epsilon

Chain G:

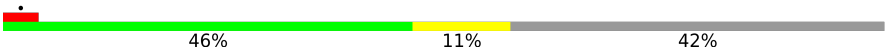


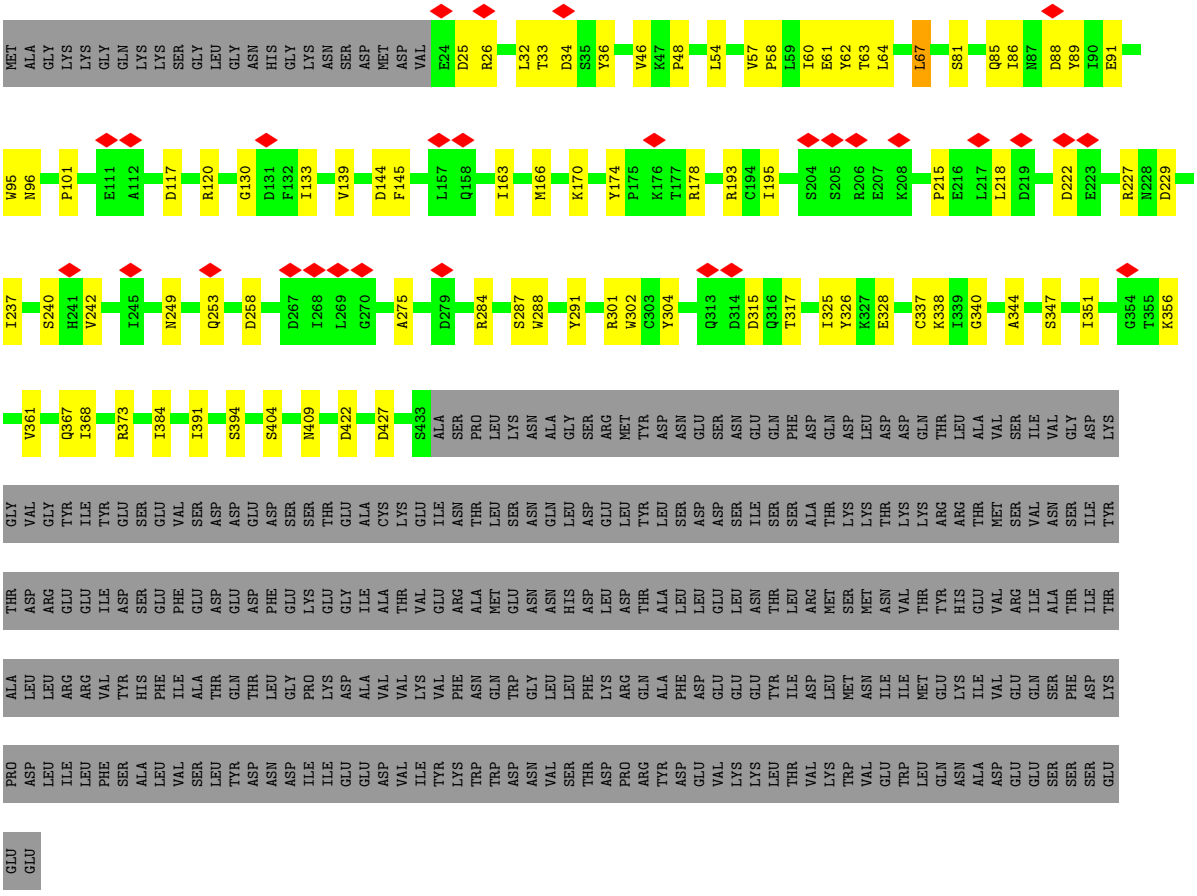




• Molecule 4: Translation initiation factor eIF-2B subunit epsilon

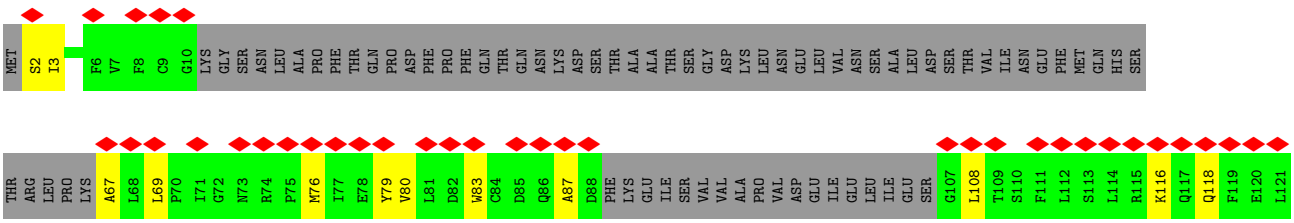
Chain H:

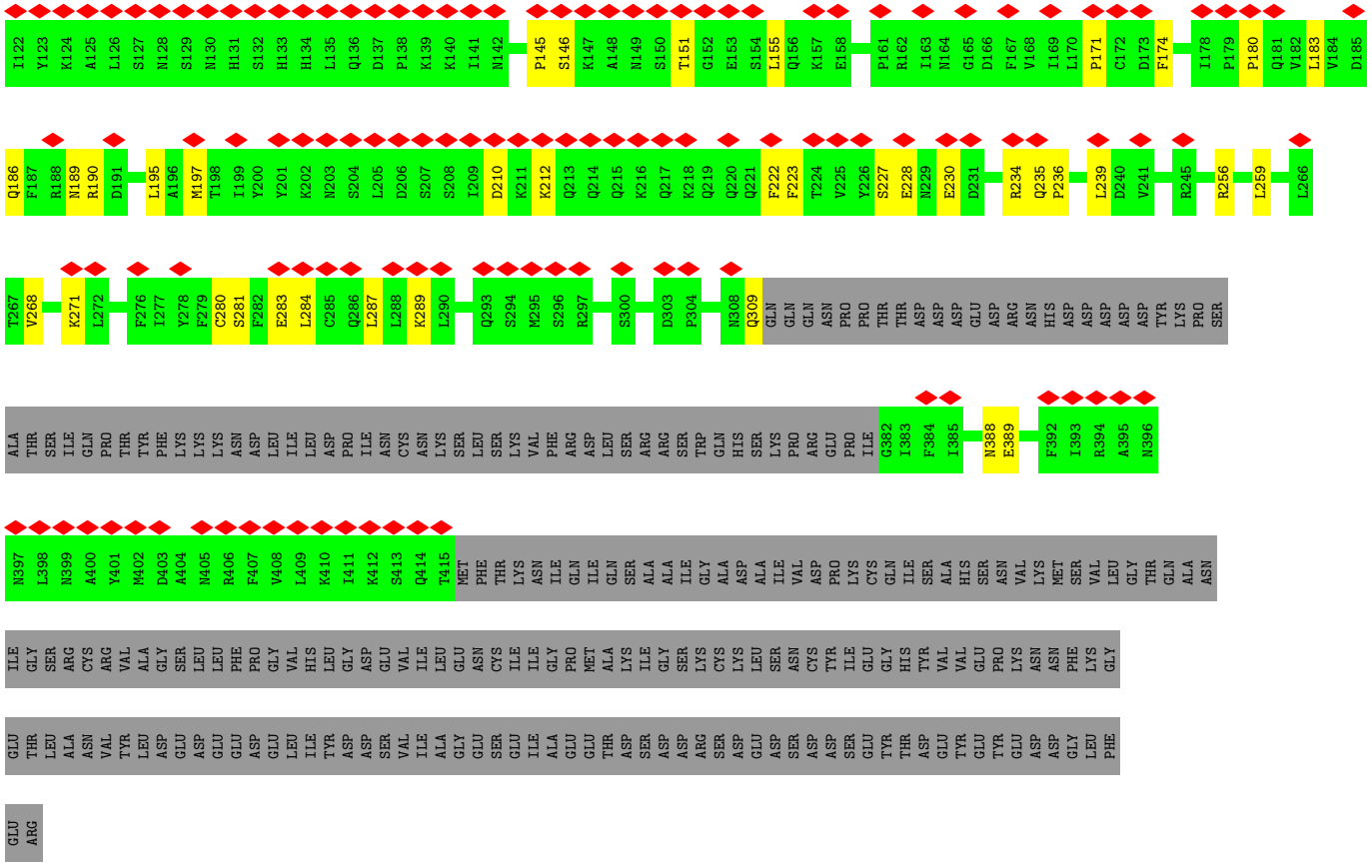




• Molecule 5: Translation initiation factor eIF-2B subunit gamma

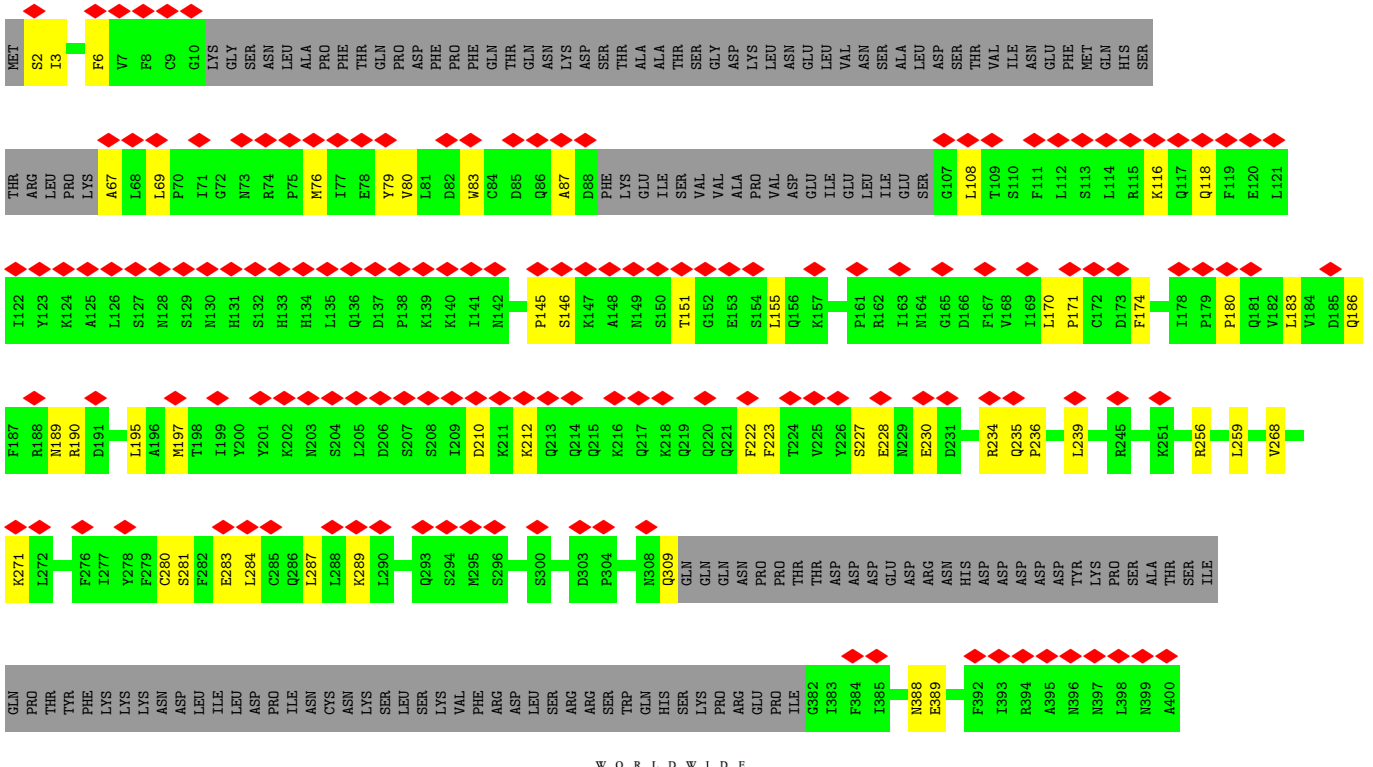
Chain I:

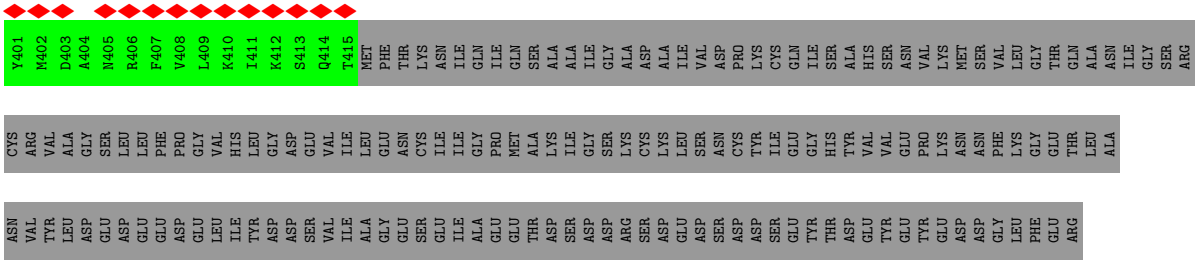




• Molecule 5: Translation initiation factor eIF-2B subunit gamma

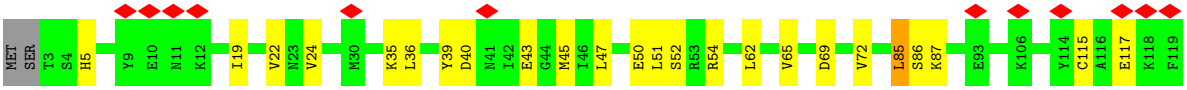
Chain J:

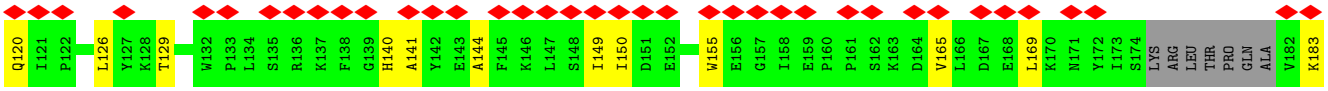


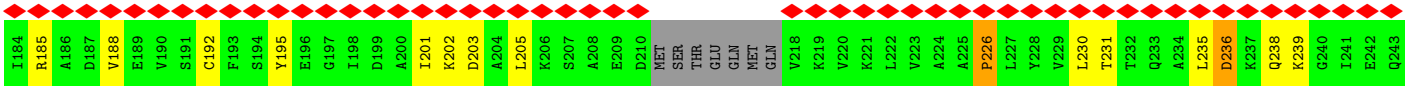


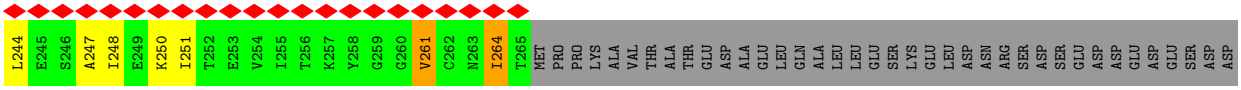
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain K:



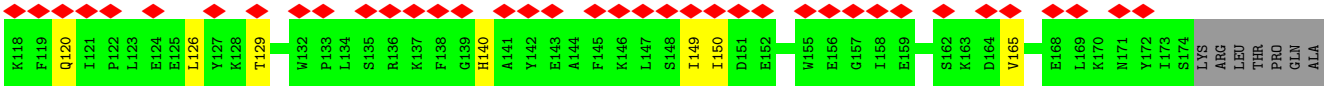


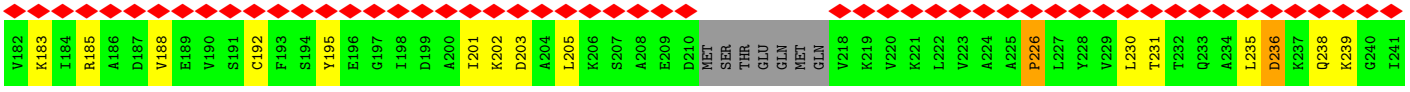


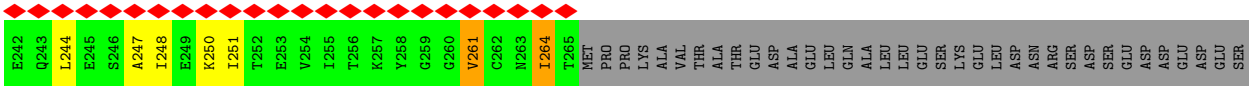


• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain L:

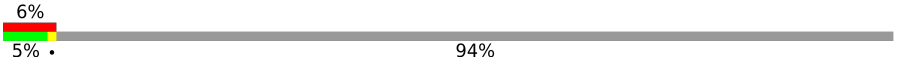


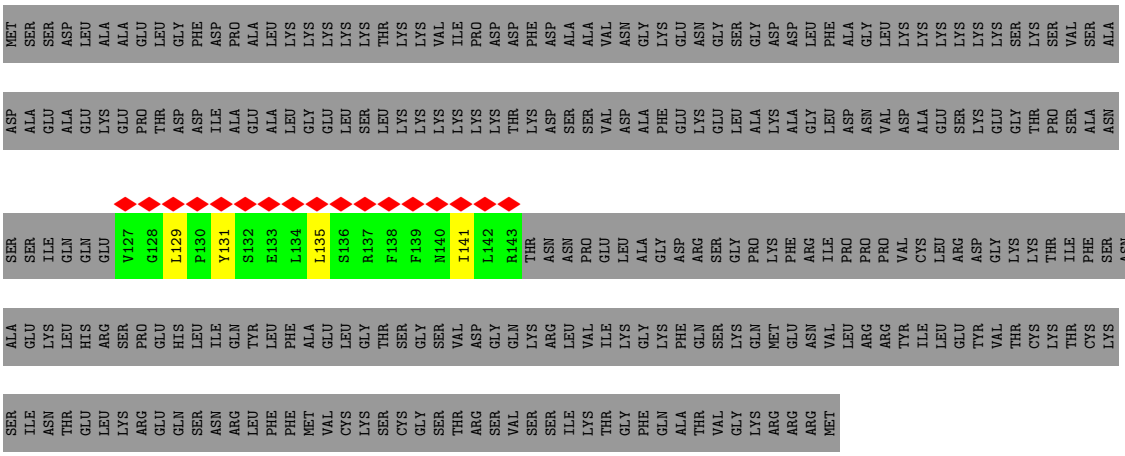




• Molecule 7: Eukaryotic translation initiation factor 2 subunit beta

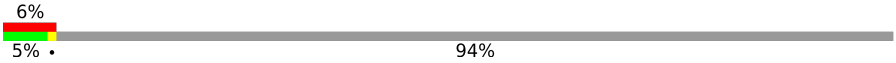
Chain M:

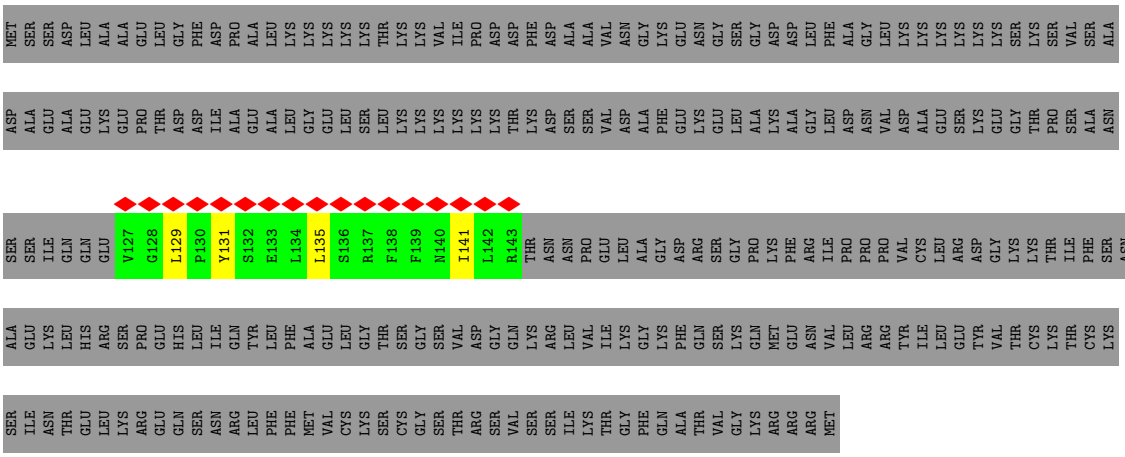




• Molecule 7: Eukaryotic translation initiation factor 2 subunit beta

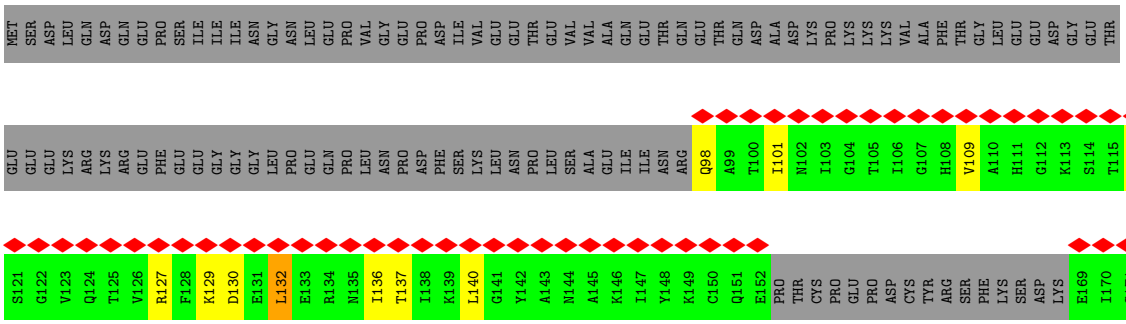
Chain N:

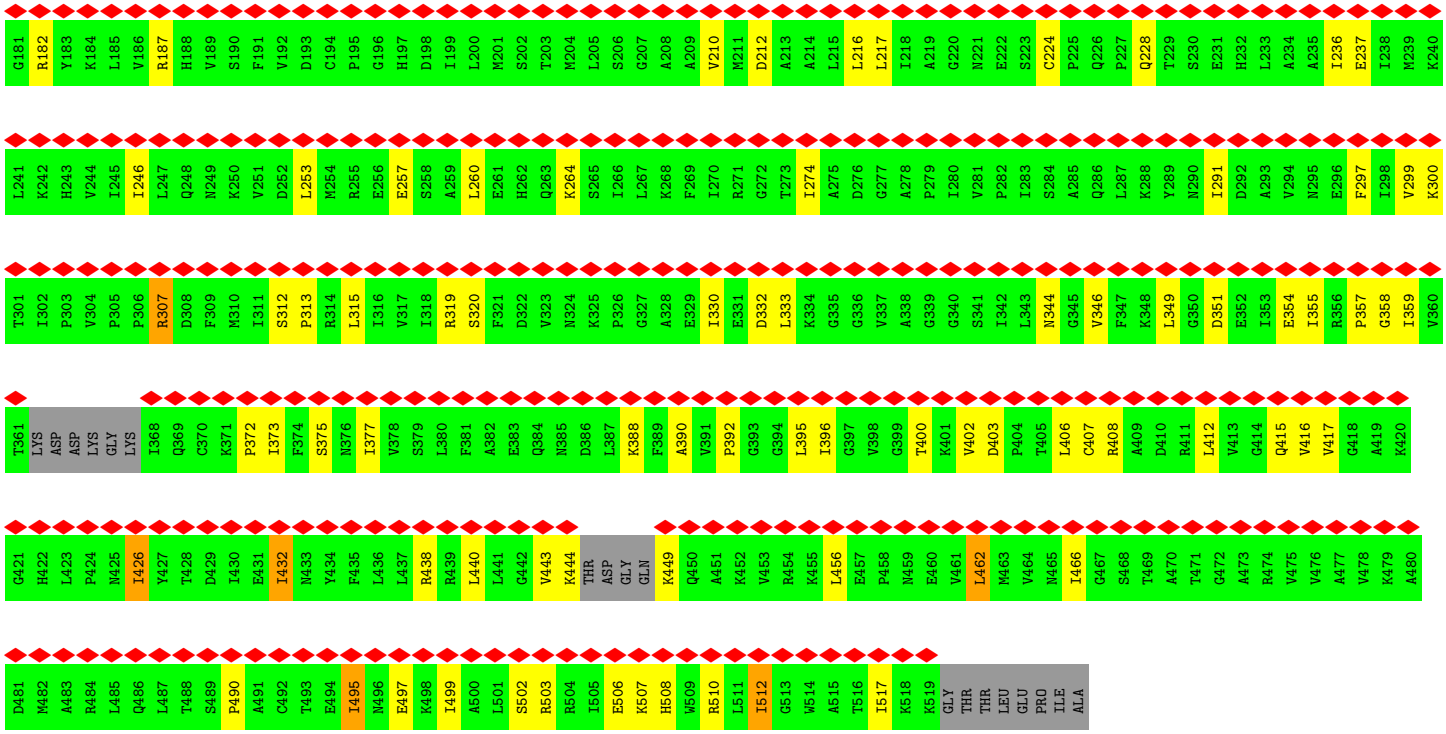




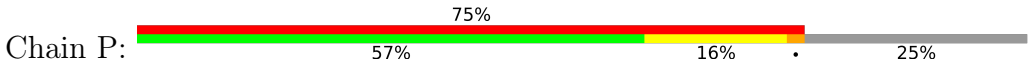
• Molecule 8: Eukaryotic translation initiation factor 2 subunit gamma

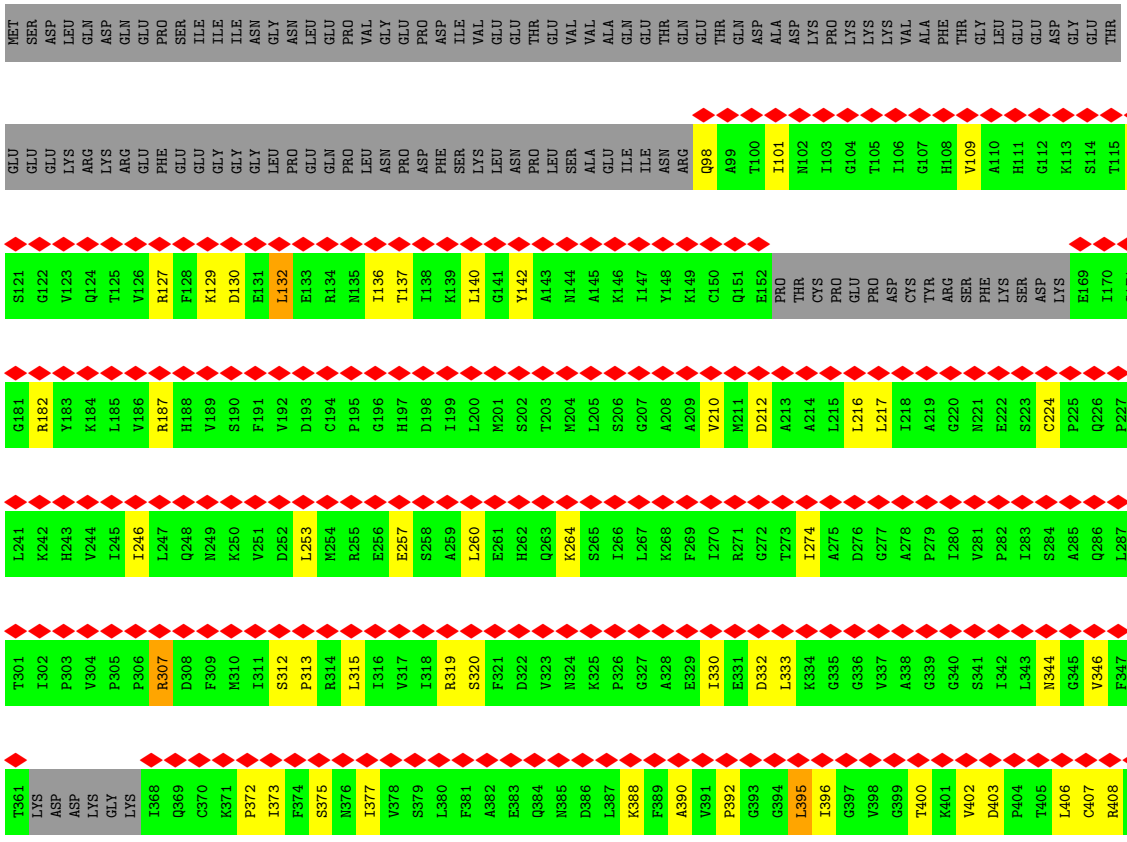
Chain O:

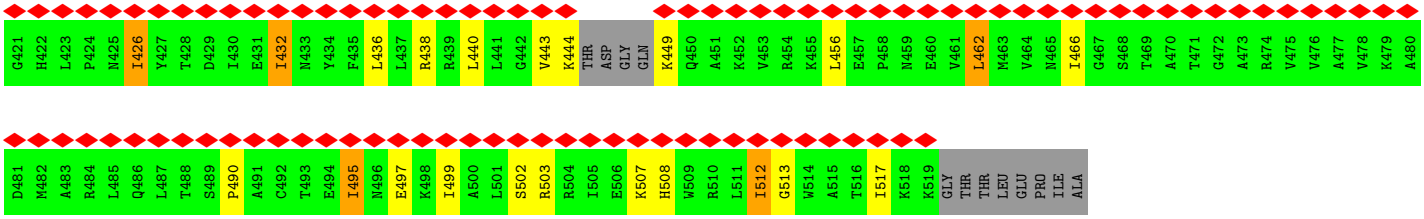




• Molecule 8: Eukaryotic translation initiation factor 2 subunit gamma






G421 H422 L423 P424 N425 I426 Y427 T428 D429 I430 E431 I432 N433 Y434 F435 L436 L437 R438 R439 L440 L441 G442 V443 K444 THR ASP GLY GLN K449 Q450 A451 K452 V453 R454 K455 L456 E457 P458 N459 E460 V461 L462 M463 V464 N465 I466 G467 S468 T469 A470 T471 G472 A473 R474 V475 V476 A477 V478 K479 A480

D481 M482 A483 R484 L485 Q486 L487 T488 S489 P490 A491 C492 T493 E494 I495 N496 E497 K498 I499 A500 L501 S502 R503 R504 I505 E506 K507 H508 W509 R510 L511 I512 G513 W514 A515 T516 I517 K518 K519 GLY THR THR LEU GLU PRO ILE ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64541	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF determination was performed per micrograph initially. After particle picking and initial reconstruction, per particle CTF determination was performed.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	37313	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.304	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	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	0.34	0/2437	0.62	0/3304
1	B	0.34	0/2437	0.62	0/3304
2	C	0.33	0/2720	0.65	2/3685 (0.1%)
2	D	0.33	0/2720	0.65	2/3685 (0.1%)
3	E	0.35	0/2846	0.65	1/3857 (0.0%)
3	F	0.36	0/2846	0.65	1/3857 (0.0%)
4	G	0.35	0/3327	0.66	3/4512 (0.1%)
4	H	0.35	0/3327	0.66	3/4512 (0.1%)
5	I	0.32	0/2232	0.66	0/3015
5	J	0.32	0/2232	0.66	0/3015
6	K	0.37	0/2027	0.67	2/2726 (0.1%)
6	L	0.37	0/2027	0.67	2/2726 (0.1%)
7	M	0.53	0/146	0.71	0/196
7	N	0.53	0/146	0.71	0/196
8	O	0.47	0/3079	0.70	1/4157 (0.0%)
8	P	0.47	0/3079	0.70	1/4157 (0.0%)
All	All	0.37	0/37628	0.66	18/50904 (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
4	G	0	1
4	H	0	1
6	K	0	2
6	L	0	2
All	All	0	6

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	245	ASP	CB-CG-OD1	6.49	124.14	118.30
3	E	245	ASP	CB-CG-OD1	6.44	124.09	118.30
4	G	32	LEU	CA-CB-CG	6.05	129.21	115.30
4	H	32	LEU	CA-CB-CG	6.04	129.19	115.30
6	L	85	LEU	CA-CB-CG	5.99	129.07	115.30
6	K	85	LEU	CA-CB-CG	5.99	129.07	115.30
2	D	601	LEU	CA-CB-CG	5.50	127.95	115.30
2	C	601	LEU	CA-CB-CG	5.50	127.94	115.30
4	G	315	ASP	CB-CG-OD1	5.46	123.21	118.30
4	H	315	ASP	CB-CG-OD1	5.46	123.21	118.30
2	D	492	LEU	CA-CB-CG	5.23	127.32	115.30
2	C	492	LEU	CA-CB-CG	5.22	127.31	115.30
4	G	67	LEU	CA-CB-CG	5.15	127.14	115.30
4	H	67	LEU	CA-CB-CG	5.13	127.11	115.30
6	K	85	LEU	CB-CG-CD2	5.12	119.71	111.00
6	L	85	LEU	CB-CG-CD2	5.12	119.70	111.00
8	P	462	LEU	CA-CB-CG	5.04	126.90	115.30
8	O	462	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	178	ARG	Peptide
4	H	178	ARG	Peptide
6	K	140	HIS	Peptide
6	K	39	TYR	Peptide
6	L	140	HIS	Peptide
6	L	39	TYR	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	2393	0	2416	39	0
1	B	2393	0	2416	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2677	0	2787	34	0
2	D	2677	0	2787	36	0
3	E	2797	0	2835	51	0
3	F	2797	0	2835	46	0
4	G	3265	0	3229	45	0
4	H	3265	0	3229	49	0
5	I	2187	0	2173	31	0
5	J	2187	0	2173	32	0
6	K	2010	0	2064	29	0
6	L	2010	0	2064	27	0
7	M	143	0	148	0	0
7	N	143	0	148	0	0
8	O	3034	0	3195	44	0
8	P	3034	0	3195	44	0
All	All	37012	0	37694	498	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 7.

All (498) 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)
8:P:499:ILE:HD11	8:P:517:ILE:HG13	1.63	0.81
8:O:499:ILE:HD11	8:O:517:ILE:HG13	1.63	0.79
5:J:79:TYR:O	5:J:83:TRP:HB2	1.89	0.72
5:I:79:TYR:O	5:I:83:TRP:HB2	1.89	0.71
6:L:201:ILE:HG22	8:P:330:ILE:HG21	1.73	0.69
4:G:301:ARG:HB3	3:F:317:GLY:HA2	1.73	0.69
6:K:201:ILE:HG22	8:O:330:ILE:HG21	1.73	0.69
8:O:116:VAL:HG21	8:O:217:LEU:HD21	1.75	0.69
5:I:171:PRO:HG2	5:I:174:PHE:HB2	1.75	0.68
6:K:248:ILE:HG12	6:K:264:ILE:HG21	1.74	0.68
8:P:116:VAL:HG21	8:P:217:LEU:HD21	1.75	0.68
5:J:171:PRO:HG2	5:J:174:PHE:HB2	1.75	0.68
6:L:248:ILE:HG12	6:L:264:ILE:HG21	1.74	0.68
4:H:61:GLU:HA	4:H:64:LEU:HB2	1.77	0.67
4:G:61:GLU:HA	4:G:64:LEU:HB2	1.77	0.66
1:B:259:ARG:HG3	1:B:263:LEU:HG	1.78	0.66
3:F:218:GLY:H	3:F:222:ASN:HB2	1.60	0.66
3:E:218:GLY:H	3:E:222:ASN:HB2	1.59	0.66
3:E:317:GLY:HA2	4:H:301:ARG:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:222:PHE:H	5:J:268:VAL:HG12	1.61	0.66
5:I:222:PHE:H	5:I:268:VAL:HG12	1.61	0.65
1:A:259:ARG:HG3	1:A:263:LEU:HG	1.78	0.64
1:A:157:ARG:HH11	1:B:157:ARG:HH11	1.44	0.64
5:J:256:ARG:HH21	5:J:309:GLN:HE22	1.47	0.62
4:G:222:ASP:HB3	5:J:271:LYS:HZ2	1.64	0.61
2:C:532:LEU:HD11	2:C:614:ASN:HB3	1.83	0.61
1:B:79:ARG:HB3	3:F:122:PHE:CE2	2.36	0.61
8:P:426:ILE:HG22	8:P:490:PRO:HB2	1.82	0.61
5:I:256:ARG:HH21	5:I:309:GLN:HE22	1.47	0.61
2:D:532:LEU:HD11	2:D:614:ASN:HB3	1.83	0.61
8:O:426:ILE:HG22	8:O:490:PRO:HB2	1.82	0.61
2:C:459:LEU:HD11	2:C:492:LEU:HB3	1.83	0.60
3:E:269:GLY:O	3:E:349:TYR:OH	2.20	0.60
6:L:205:LEU:HG	8:P:330:ILE:HB	1.84	0.60
5:I:151:THR:O	5:I:155:LEU:HB2	2.02	0.59
8:O:320:SER:HB3	8:O:412:LEU:H	1.68	0.59
3:F:269:GLY:O	3:F:349:TYR:OH	2.20	0.59
1:A:79:ARG:HB3	3:E:122:PHE:CE2	2.38	0.59
4:H:91:GLU:HA	4:H:96:ASN:HD22	1.67	0.59
6:K:226:PRO:HG3	8:O:408:ARG:HD2	1.85	0.59
1:B:287:LEU:HD11	3:F:121:MET:HG2	1.84	0.59
6:K:24:VAL:HG23	6:K:65:VAL:HA	1.85	0.59
2:D:459:LEU:HD11	2:D:492:LEU:HB3	1.83	0.59
5:J:151:THR:O	5:J:155:LEU:HB2	2.03	0.59
8:O:358:GLY:HA2	8:O:372:PRO:HA	1.84	0.59
8:P:358:GLY:HA2	8:P:372:PRO:HA	1.84	0.59
5:I:271:LYS:HZ2	4:H:222:ASP:HB3	1.67	0.58
4:G:91:GLU:HA	4:G:96:ASN:HD22	1.67	0.58
6:K:205:LEU:HG	8:O:330:ILE:HB	1.84	0.58
6:L:226:PRO:HG3	8:P:408:ARG:HD2	1.85	0.58
8:O:346:VAL:HG22	8:O:392:PRO:HD3	1.84	0.58
8:O:313:PRO:HA	8:O:344:ASN:O	2.03	0.58
8:P:320:SER:HB3	8:P:412:LEU:H	1.68	0.58
8:P:313:PRO:HA	8:P:344:ASN:O	2.03	0.58
6:K:51:LEU:HG	6:K:87:LYS:HE2	1.85	0.58
8:P:346:VAL:HG22	8:P:392:PRO:HD3	1.84	0.58
3:F:233:LEU:HD22	3:F:238:ILE:HD11	1.85	0.58
6:L:24:VAL:HG23	6:L:65:VAL:HA	1.85	0.58
6:L:51:LEU:HG	6:L:87:LYS:HE2	1.85	0.58
5:J:186:GLN:O	5:J:190:ARG:NH2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:233:LEU:HD22	3:E:238:ILE:HD11	1.85	0.57
4:G:170:LYS:HD2	5:J:228:GLU:OE2	2.04	0.57
8:P:307:ARG:HG2	8:P:392:PRO:HB2	1.87	0.57
5:J:230:GLU:HG3	5:J:234:ARG:HH21	1.70	0.57
5:J:197:MET:HA	5:J:388:ASN:HB2	1.87	0.57
3:F:41:ALA:HB2	3:F:83:SER:HB3	1.86	0.57
1:A:287:LEU:HD11	3:E:121:MET:HG2	1.86	0.56
1:A:127:LEU:HB2	1:A:191:VAL:HG11	1.87	0.56
2:D:381:LEU:HB2	6:K:62:LEU:HD23	1.87	0.56
8:P:140:LEU:HD12	8:P:319:ARG:HH21	1.70	0.56
4:G:391:ILE:HG23	4:G:394:SER:HB2	1.87	0.56
1:B:127:LEU:HB2	1:B:191:VAL:HG11	1.87	0.56
3:F:85:GLY:O	3:F:89:ARG:NH1	2.39	0.56
8:O:140:LEU:HD12	8:O:319:ARG:HH21	1.70	0.56
3:E:85:GLY:O	3:E:89:ARG:NH1	2.39	0.56
5:I:230:GLU:HG3	5:I:234:ARG:HH21	1.70	0.56
5:I:228:GLU:OE2	4:H:170:LYS:HD2	2.05	0.56
1:B:76:PHE:HA	3:F:122:PHE:CZ	2.41	0.56
3:E:37:SER:HG	3:E:83:SER:HG	1.52	0.56
4:H:351:ILE:HA	4:H:368:ILE:HB	1.87	0.56
3:E:41:ALA:HB2	3:E:83:SER:HB3	1.86	0.56
3:E:192:ASP:OD2	3:E:275:ASN:ND2	2.39	0.56
3:F:192:ASP:OD2	3:F:275:ASN:ND2	2.39	0.56
5:I:197:MET:HA	5:I:388:ASN:HB2	1.87	0.56
1:A:230:VAL:HG22	1:A:284:ILE:HD12	1.88	0.56
5:J:118:GLN:NE2	5:J:146:SER:OG	2.39	0.56
1:B:101:PHE:O	1:B:105:ALA:N	2.38	0.56
2:C:512:PHE:O	2:C:648:LYS:NZ	2.39	0.55
4:G:351:ILE:HA	4:G:368:ILE:HB	1.87	0.55
1:A:259:ARG:NH1	1:A:261:ASP:O	2.40	0.55
2:D:517:GLN:HG3	2:D:619:LEU:HD21	1.88	0.55
4:H:391:ILE:HG23	4:H:394:SER:HB2	1.87	0.55
8:O:307:ARG:HG2	8:O:392:PRO:HB2	1.87	0.55
8:P:503:ARG:HD3	8:P:512:ILE:HG21	1.89	0.55
3:F:44:THR:HG21	3:F:84:CYS:HA	1.89	0.55
3:F:37:SER:HG	3:F:83:SER:HG	1.53	0.55
8:O:503:ARG:HD3	8:O:512:ILE:HG21	1.88	0.55
3:E:326:ASP:OD1	3:E:326:ASP:N	2.40	0.55
2:C:517:GLN:HG3	2:C:619:LEU:HD21	1.88	0.55
4:H:120:ARG:NH2	4:H:249:ASN:O	2.40	0.55
4:G:120:ARG:NH2	4:G:249:ASN:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:118:GLN:NE2	5:I:146:SER:OG	2.39	0.54
1:B:259:ARG:NH1	1:B:261:ASP:O	2.40	0.54
1:B:81:LEU:HD21	6:L:47:LEU:HD12	1.89	0.54
3:E:52:ILE:O	3:E:151:ARG:NH1	2.41	0.54
5:I:186:GLN:O	5:I:190:ARG:NH2	2.31	0.54
5:I:180:PRO:HA	5:I:183:LEU:HD13	1.90	0.54
3:F:90:ARG:HD3	3:F:161:LEU:HD11	1.90	0.54
6:L:149:ILE:HD12	6:L:150:ILE:HG23	1.90	0.54
1:A:90:CYS:HA	1:A:93:HIS:HB3	1.90	0.54
1:B:230:VAL:HG22	1:B:284:ILE:HD12	1.88	0.54
3:E:44:THR:HG21	3:E:84:CYS:HA	1.89	0.53
1:A:101:PHE:O	1:A:105:ALA:N	2.38	0.53
5:I:271:LYS:NZ	4:H:222:ASP:O	2.40	0.53
4:H:344:ALA:HB3	4:H:361:VAL:HG23	1.89	0.53
5:J:87:ALA:H	5:J:108:LEU:HD22	1.74	0.53
1:B:90:CYS:HA	1:B:93:HIS:HB3	1.90	0.53
2:C:463:PHE:HA	2:C:467:VAL:HG11	1.91	0.53
3:F:86:ASN:ND2	3:F:299:TYR:O	2.41	0.53
4:H:25:ASP:OD2	4:H:26:ARG:NH2	2.42	0.53
1:A:76:PHE:HA	3:E:122:PHE:CZ	2.43	0.53
3:E:86:ASN:ND2	3:E:299:TYR:O	2.41	0.53
3:F:52:ILE:O	3:F:151:ARG:NH1	2.41	0.53
1:A:213:THR:HA	1:A:216:VAL:HG12	1.91	0.53
3:F:326:ASP:N	3:F:326:ASP:OD1	2.40	0.53
1:A:296:SER:O	1:A:300:ILE:HB	2.09	0.53
5:J:180:PRO:HA	5:J:183:LEU:HD13	1.90	0.53
1:B:296:SER:O	1:B:300:ILE:HB	2.09	0.53
6:K:149:ILE:HD12	6:K:150:ILE:HG23	1.90	0.53
2:D:512:PHE:O	2:D:648:LYS:NZ	2.39	0.52
1:A:131:TYR:H	1:A:161:GLN:HB3	1.74	0.52
2:D:463:PHE:HA	2:D:467:VAL:HG11	1.91	0.52
5:I:87:ALA:H	5:I:108:LEU:HD22	1.74	0.52
1:B:213:THR:HA	1:B:216:VAL:HG12	1.90	0.52
4:H:64:LEU:HA	4:H:67:LEU:HD23	1.91	0.52
8:O:109:VAL:HG23	8:O:136:ILE:HG21	1.92	0.52
1:A:100:LEU:O	1:A:104:ARG:CB	2.58	0.52
4:G:344:ALA:HB3	4:G:361:VAL:HG23	1.89	0.52
1:B:100:LEU:O	1:B:104:ARG:CB	2.58	0.52
6:L:117:GLU:O	6:L:120:GLN:NE2	2.43	0.52
3:E:90:ARG:HD3	3:E:161:LEU:HD11	1.90	0.52
3:E:40:ILE:HG12	3:E:84:CYS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:98:GLN:HE22	8:O:396:ILE:HD11	1.75	0.52
8:P:109:VAL:HG23	8:P:136:ILE:HG21	1.92	0.52
8:P:456:LEU:HD23	8:P:503:ARG:HD2	1.92	0.52
2:D:300:PHE:HA	2:D:303:VAL:HG12	1.92	0.52
4:G:64:LEU:HA	4:G:67:LEU:HD23	1.91	0.52
4:H:60:ILE:HG22	4:H:64:LEU:HD13	1.91	0.52
3:F:40:ILE:HG12	3:F:84:CYS:HB3	1.91	0.52
6:K:117:GLU:O	6:K:120:GLN:NE2	2.43	0.52
2:D:376:LYS:HG2	2:D:381:LEU:HD23	1.92	0.51
4:G:48:PRO:HG2	4:G:86:ILE:HD11	1.92	0.51
1:A:242:LEU:HB3	2:D:627:LYS:HZ1	1.74	0.51
1:B:131:TYR:H	1:B:161:GLN:HB3	1.74	0.51
6:K:35:LYS:HA	6:K:43:GLU:HA	1.93	0.51
2:C:520:SER:HA	2:C:619:LEU:HD13	1.91	0.51
3:F:91:ILE:HA	3:F:94:VAL:HG12	1.92	0.51
8:O:349:LEU:HD12	8:O:388:LYS:HA	1.93	0.51
2:C:627:LYS:HZ1	1:B:242:LEU:HB3	1.75	0.51
5:I:271:LYS:NZ	4:H:222:ASP:HB3	2.25	0.51
6:K:183:LYS:HB3	6:K:231:THR:HB	1.92	0.51
4:G:25:ASP:OD2	4:G:26:ARG:NH2	2.42	0.51
6:L:35:LYS:HA	6:L:43:GLU:HA	1.92	0.51
3:E:91:ILE:HA	3:E:94:VAL:HG12	1.92	0.51
6:L:183:LYS:HB3	6:L:231:THR:HB	1.92	0.51
8:P:98:GLN:HE22	8:P:396:ILE:HD11	1.75	0.51
1:A:209:ASN:HD21	1:A:213:THR:HG21	1.75	0.51
2:C:300:PHE:HA	2:C:303:VAL:HG12	1.92	0.51
2:D:520:SER:HA	2:D:619:LEU:HD13	1.91	0.51
4:G:36:TYR:OH	4:G:284:ARG:NH1	2.44	0.51
4:H:326:TYR:HB2	4:H:344:ALA:HA	1.93	0.51
8:P:349:LEU:HD12	8:P:388:LYS:HA	1.93	0.51
2:C:376:LYS:HG2	2:C:381:LEU:HD23	1.92	0.51
4:G:60:ILE:HG22	4:G:64:LEU:HD13	1.91	0.51
1:B:80:ASN:HD21	1:B:97:ASN:HD22	1.59	0.51
4:H:36:TYR:OH	4:H:284:ARG:NH1	2.44	0.51
1:A:80:ASN:HD21	1:A:97:ASN:HD22	1.59	0.50
4:G:222:ASP:O	5:J:271:LYS:NZ	2.44	0.50
1:A:81:LEU:HD21	6:K:47:LEU:HD12	1.94	0.50
8:P:216:LEU:HD23	8:P:246:ILE:HG12	1.92	0.50
5:I:210:ASP:HB2	5:I:212:LYS:HE2	1.94	0.50
4:H:48:PRO:HG2	4:H:86:ILE:HD11	1.92	0.50
4:H:166:MET:H	4:H:275:ALA:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:SER:HB3	2:D:410:THR:HG23	1.94	0.50
8:O:237:GLU:HB3	8:O:274:ILE:HD12	1.94	0.50
8:P:320:SER:HB2	8:P:407:CYS:HA	1.94	0.50
2:C:406:SER:HB3	2:C:410:THR:HG23	1.94	0.50
4:G:326:TYR:HB2	4:G:344:ALA:HA	1.93	0.50
1:B:209:ASN:HD21	1:B:213:THR:HG21	1.75	0.50
8:P:237:GLU:HB3	8:P:274:ILE:HD12	1.94	0.50
8:O:216:LEU:HD23	8:O:246:ILE:HG12	1.92	0.50
4:H:404:SER:N	4:H:422:ASP:OD1	2.44	0.50
4:H:34:ASP:OD2	4:H:81:SER:N	2.45	0.50
8:O:320:SER:HB2	8:O:407:CYS:HA	1.94	0.50
4:G:288:TRP:HA	4:G:291:TYR:HB3	1.92	0.50
8:O:456:LEU:HD23	8:O:503:ARG:HD2	1.92	0.50
4:G:95:TRP:HZ3	4:G:101:PRO:HD2	1.77	0.49
5:J:189:ASN:OD1	5:J:190:ARG:NH2	2.45	0.49
1:A:125:ILE:HG23	1:A:192:ASP:H	1.77	0.49
5:J:284:LEU:HA	5:J:287:LEU:HD22	1.93	0.49
4:H:54:LEU:HB3	4:H:62:TYR:HE2	1.77	0.49
4:H:288:TRP:HA	4:H:291:TYR:HB3	1.92	0.49
1:A:77:VAL:O	1:A:81:LEU:HB2	2.13	0.49
5:I:284:LEU:HA	5:I:287:LEU:HD22	1.93	0.49
5:I:189:ASN:OD1	5:I:190:ARG:NH2	2.45	0.49
5:J:210:ASP:HB2	5:J:212:LYS:HE2	1.94	0.49
4:H:193:ARG:HE	4:H:195:ILE:HD13	1.78	0.49
4:H:409:ASN:HD21	4:H:427:ASP:HA	1.77	0.49
2:C:399:THR:HG22	2:C:425:LYS:HB2	1.94	0.49
3:E:45:LEU:HD11	3:E:161:LEU:HB3	1.95	0.49
4:G:54:LEU:HB3	4:G:62:TYR:HE2	1.77	0.49
4:G:166:MET:H	4:G:275:ALA:HA	1.76	0.49
3:F:118:ILE:HG22	3:F:119:SER:O	2.13	0.49
3:F:271:THR:HG22	3:F:341:VAL:HG22	1.95	0.49
8:P:187:ARG:HH21	8:P:299:VAL:HG13	1.78	0.49
3:E:317:GLY:HA3	4:H:304:TYR:HB2	1.95	0.49
1:B:125:ILE:HG23	1:B:192:ASP:H	1.77	0.49
4:H:95:TRP:HZ3	4:H:101:PRO:HD2	1.77	0.49
3:F:45:LEU:HD11	3:F:161:LEU:HB3	1.95	0.49
3:E:118:ILE:HG22	3:E:119:SER:O	2.13	0.49
5:J:223:PHE:HZ	5:J:227:SER:HB3	1.78	0.49
3:F:177:ILE:O	3:F:209:ARG:NH1	2.35	0.49
6:L:115:CYS:HB3	6:L:165:VAL:HG13	1.95	0.49
8:P:390:ALA:HB1	8:P:396:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:HD1	1:A:299:LEU:HD12	1.78	0.49
2:D:399:THR:HG22	2:D:425:LYS:HB2	1.94	0.49
4:G:409:ASN:HD21	4:G:427:ASP:HA	1.77	0.49
8:O:355:ILE:HG12	8:O:417:VAL:HG22	1.95	0.49
4:H:337:CYS:SG	4:H:338:LYS:N	2.86	0.48
8:O:444:LYS:HB2	8:O:449:LYS:HB2	1.95	0.48
1:A:23:PRO:HG3	1:A:65:SER:HB2	1.95	0.48
4:G:337:CYS:SG	4:G:338:LYS:N	2.86	0.48
5:I:223:PHE:HZ	5:I:227:SER:HB3	1.78	0.48
4:G:193:ARG:HE	4:G:195:ILE:HD13	1.78	0.48
4:H:130:GLY:N	4:H:240:SER:OG	2.46	0.48
8:O:320:SER:HB3	8:O:412:LEU:HB2	1.94	0.48
4:G:34:ASP:OD2	4:G:81:SER:N	2.45	0.48
5:J:76:MET:HA	5:J:79:TYR:HD2	1.78	0.48
1:B:46:ILE:HD12	6:L:45:MET:HE1	1.94	0.48
1:B:236:PHE:HD1	1:B:299:LEU:HD12	1.79	0.48
8:O:357:PRO:HD3	8:O:416:VAL:HG22	1.95	0.48
8:P:355:ILE:HG12	8:P:417:VAL:HG22	1.95	0.48
5:I:2:SER:OG	5:I:3:ILE:N	2.43	0.48
1:B:79:ARG:HB3	3:F:122:PHE:HE2	1.77	0.48
2:D:524:ASN:HD21	2:D:615:ILE:HG23	1.79	0.48
5:I:76:MET:HA	5:I:79:TYR:HD2	1.78	0.48
8:P:444:LYS:HB2	8:P:449:LYS:HB2	1.95	0.48
4:G:404:SER:N	4:G:422:ASP:OD1	2.44	0.48
1:B:23:PRO:HG3	1:B:65:SER:HB2	1.95	0.48
1:B:77:VAL:O	1:B:81:LEU:HB2	2.12	0.48
8:O:187:ARG:HH21	8:O:299:VAL:HG13	1.78	0.48
1:A:100:LEU:O	1:A:104:ARG:HB3	2.14	0.48
3:E:179:LEU:HD21	3:E:348:ILE:HG21	1.96	0.48
4:G:130:GLY:N	4:G:240:SER:OG	2.46	0.48
3:E:245:ASP:OD1	3:E:246:SER:N	2.47	0.48
1:B:100:LEU:O	1:B:104:ARG:HB3	2.14	0.47
3:F:179:LEU:HD21	3:F:348:ILE:HG21	1.96	0.47
6:K:236:ASP:C	6:K:238:GLN:H	2.17	0.47
8:P:320:SER:HB3	8:P:412:LEU:HB2	1.94	0.47
2:C:468:ASP:OD1	2:C:468:ASP:N	2.47	0.47
8:O:390:ALA:HB1	8:O:396:ILE:HD13	1.95	0.47
1:A:41:THR:HG22	1:A:43:ALA:H	1.79	0.47
1:A:240:PHE:HE2	2:D:627:LYS:HG3	1.79	0.47
3:F:245:ASP:OD1	3:F:246:SER:N	2.47	0.47
6:L:236:ASP:C	6:L:238:GLN:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:389:ASN:HD21	2:C:633:GLY:HA2	1.80	0.47
5:I:116:LYS:HD2	5:I:145:PRO:HG2	1.96	0.47
5:J:280:CYS:SG	5:J:281:SER:N	2.87	0.47
2:C:524:ASN:HD21	2:C:615:ILE:HG23	1.79	0.47
2:D:289:SER:OG	2:D:511:LYS:NZ	2.48	0.47
3:E:271:THR:HG22	3:E:341:VAL:HG22	1.95	0.47
6:K:115:CYS:HB3	6:K:165:VAL:HG13	1.95	0.47
3:E:294:ALA:HB2	3:E:346:ILE:HD11	1.97	0.47
6:L:236:ASP:HB2	6:L:239:LYS:HG3	1.96	0.47
5:I:239:LEU:HB3	5:I:259:LEU:HD21	1.96	0.47
8:P:297:PHE:HA	8:P:300:LYS:HB2	1.96	0.47
8:P:357:PRO:HD3	8:P:416:VAL:HG22	1.95	0.47
1:A:199:GLU:HB2	1:A:209:ASN:HA	1.96	0.47
2:C:289:SER:OG	2:C:511:LYS:NZ	2.48	0.47
5:J:239:LEU:HB3	5:J:259:LEU:HD21	1.96	0.47
1:B:33:LEU:HD23	1:B:49:ILE:HG22	1.97	0.47
3:F:150:TYR:HA	3:F:153:VAL:HG12	1.97	0.47
6:K:236:ASP:HB2	6:K:239:LYS:HG3	1.96	0.47
5:J:2:SER:OG	5:J:3:ILE:N	2.43	0.47
4:G:46:VAL:O	4:G:85:GLN:NE2	2.42	0.47
4:H:133:ILE:HA	4:H:237:ILE:HG22	1.97	0.47
3:F:294:ALA:HB2	3:F:346:ILE:HD11	1.97	0.46
6:K:69:ASP:OD2	6:K:87:LYS:NZ	2.37	0.46
2:D:389:ASN:HD21	2:D:633:GLY:HA2	1.80	0.46
5:I:280:CYS:SG	5:I:281:SER:N	2.87	0.46
4:H:328:GLU:OE1	4:H:347:SER:N	2.47	0.46
8:O:357:PRO:HB2	8:O:415:GLN:HE21	1.79	0.46
8:O:375:SER:HB2	8:O:400:THR:HB	1.98	0.46
3:E:177:ILE:O	3:E:209:ARG:NH1	2.35	0.46
4:G:215:PRO:HA	4:G:218:LEU:HD23	1.97	0.46
4:H:215:PRO:HA	4:H:218:LEU:HD23	1.97	0.46
3:F:92:LEU:HD22	3:F:373:ASP:HB3	1.98	0.46
3:E:72:ASN:ND2	3:E:377:ASP:OD1	2.43	0.46
1:B:199:GLU:HB2	1:B:209:ASN:HA	1.96	0.46
8:O:297:PHE:HA	8:O:300:LYS:HB2	1.96	0.46
2:D:480:ASN:O	3:E:357:ASN:ND2	2.45	0.46
4:G:328:GLU:OE1	4:G:347:SER:N	2.47	0.46
2:D:483:LEU:HB2	2:D:625:ILE:HD11	1.97	0.46
3:E:92:LEU:HD22	3:E:373:ASP:HB3	1.97	0.46
5:J:116:LYS:HD2	5:J:145:PRO:HG2	1.96	0.46
3:F:57:TRP:HH2	3:F:151:ARG:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:357:PRO:HB2	8:P:415:GLN:HE21	1.79	0.46
3:E:57:TRP:HH2	3:E:151:ARG:HB2	1.81	0.46
3:E:150:TYR:HA	3:E:153:VAL:HG12	1.97	0.46
4:G:133:ILE:HA	4:G:237:ILE:HG22	1.97	0.46
1:B:41:THR:HG22	1:B:43:ALA:H	1.79	0.46
6:K:201:ILE:HG22	8:O:330:ILE:CG2	2.43	0.46
2:C:472:LEU:HD22	2:C:489:THR:HG23	1.98	0.46
3:F:365:ALA:O	3:F:369:TYR:N	2.49	0.46
2:C:358:THR:HG22	2:C:360:ASP:H	1.81	0.46
2:D:358:THR:HG22	2:D:360:ASP:H	1.81	0.46
2:D:468:ASP:N	2:D:468:ASP:OD1	2.47	0.46
3:E:118:ILE:HG22	3:E:119:SER:N	2.31	0.46
8:O:174:CYS:HB2	8:O:182:ARG:HA	1.98	0.46
5:I:151:THR:O	5:I:155:LEU:CB	2.64	0.45
5:J:151:THR:O	5:J:155:LEU:CB	2.64	0.45
1:A:33:LEU:HD23	1:A:49:ILE:HG22	1.97	0.45
2:D:472:LEU:HD22	2:D:489:THR:HG23	1.98	0.45
8:O:351:ASP:HB2	8:O:377:ILE:HD12	1.98	0.45
3:E:187:LEU:HB3	3:E:258:VAL:HG12	1.97	0.45
3:E:365:ALA:O	3:E:369:TYR:N	2.49	0.45
4:G:302:TRP:O	3:F:319:GLN:NE2	2.50	0.45
3:F:187:LEU:HB3	3:F:258:VAL:HG12	1.97	0.45
8:P:351:ASP:HB2	8:P:377:ILE:HD12	1.98	0.45
1:A:249:MET:HG3	1:A:250:ALA:H	1.81	0.45
2:C:381:LEU:HB2	6:L:62:LEU:HD23	1.97	0.45
1:B:249:MET:HG3	1:B:250:ALA:H	1.81	0.45
2:C:310:PRO:HG2	2:C:313:THR:HB	1.98	0.45
2:C:483:LEU:HB2	2:C:625:ILE:HD11	1.97	0.45
2:D:310:PRO:HG2	2:D:313:THR:HB	1.98	0.45
4:H:46:VAL:O	4:H:85:GLN:NE2	2.42	0.45
1:A:197:GLY:O	1:A:209:ASN:ND2	2.39	0.45
2:C:406:SER:OG	2:C:407:LYS:N	2.49	0.45
8:P:375:SER:HB2	8:P:400:THR:HB	1.98	0.45
5:J:87:ALA:HB3	5:J:108:LEU:HD13	1.98	0.45
2:D:406:SER:OG	2:D:407:LYS:N	2.49	0.45
6:K:126:LEU:HA	6:K:129:THR:HG22	1.99	0.45
4:H:144:ASP:OD1	4:H:144:ASP:N	2.50	0.45
1:A:79:ARG:HB3	3:E:122:PHE:HE2	1.82	0.44
4:H:367:GLN:HB2	4:H:384:ILE:HG12	1.99	0.44
5:I:87:ALA:HB3	5:I:108:LEU:HD13	1.98	0.44
5:J:195:LEU:HD12	5:J:283:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:192:CYS:HA	6:K:261:VAL:H	1.82	0.44
4:G:304:TYR:HB2	3:F:317:GLY:HA3	1.99	0.44
5:J:80:VAL:HG11	5:J:174:PHE:HB3	1.99	0.44
4:H:88:ASP:OD1	4:H:89:TYR:N	2.50	0.44
2:C:278:THR:HG21	2:C:329:LEU:HG	2.00	0.44
2:C:480:ASN:O	3:F:357:ASN:ND2	2.46	0.44
3:F:118:ILE:HG22	3:F:119:SER:N	2.31	0.44
8:P:174:CYS:HB2	8:P:182:ARG:HA	1.99	0.44
4:G:117:ASP:OD1	4:G:120:ARG:NH1	2.50	0.44
4:G:367:GLN:HB2	4:G:384:ILE:HG12	1.99	0.44
5:I:195:LEU:HD12	5:I:283:GLU:HB3	2.00	0.44
6:L:192:CYS:HA	6:L:261:VAL:H	1.83	0.44
4:G:144:ASP:OD1	4:G:144:ASP:N	2.50	0.44
5:I:80:VAL:HG11	5:I:174:PHE:HB3	1.99	0.44
8:P:315:LEU:HB3	8:P:417:VAL:HB	1.99	0.44
4:G:63:THR:HG22	4:G:139:VAL:H	1.83	0.44
4:G:88:ASP:OD1	4:G:89:TYR:N	2.50	0.44
4:H:253:GLN:N	4:H:258:ASP:OD2	2.48	0.44
8:O:315:LEU:HB3	8:O:417:VAL:HB	1.99	0.44
4:H:117:ASP:OD1	4:H:120:ARG:NH1	2.50	0.44
6:L:126:LEU:HA	6:L:129:THR:HG22	1.99	0.44
3:F:193:SER:HB3	3:F:196:VAL:HG22	2.00	0.43
6:L:201:ILE:HG22	8:P:330:ILE:CG2	2.43	0.43
3:E:319:GLN:NE2	4:H:302:TRP:O	2.50	0.43
8:P:466:ILE:HG12	8:P:499:ILE:HG12	2.01	0.43
3:E:22:ILE:HG22	3:E:47:LEU:HD11	2.00	0.43
6:K:188:VAL:HG22	6:K:264:ILE:HG23	2.01	0.43
8:O:176:ARG:HB2	8:O:177:PRO:HD3	2.00	0.43
8:O:466:ILE:HG12	8:O:499:ILE:HG12	2.01	0.43
6:L:19:ILE:HG13	6:L:72:VAL:HG23	2.00	0.43
8:P:176:ARG:HB2	8:P:177:PRO:HD3	2.00	0.43
1:A:87:TRP:HA	1:A:90:CYS:HB2	2.00	0.43
3:F:22:ILE:HG22	3:F:47:LEU:HD11	2.00	0.43
6:K:19:ILE:HG13	6:K:72:VAL:HG23	2.00	0.43
3:E:30:LYS:HB2	3:E:31:ARG:HD2	2.01	0.43
3:F:30:LYS:HB2	3:F:31:ARG:HD2	2.01	0.43
2:C:627:LYS:HG3	1:B:240:PHE:HE2	1.83	0.43
5:I:190:ARG:NH1	5:I:235:GLN:OE1	2.52	0.43
5:J:190:ARG:NH1	5:J:235:GLN:OE1	2.52	0.43
8:P:432:ILE:HD11	8:P:499:ILE:HD13	2.01	0.43
6:K:247:ALA:HA	6:K:250:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:432:ILE:HD11	8:O:499:ILE:HD13	2.01	0.43
2:C:383:ASP:O	2:C:387:ILE:HG12	2.19	0.42
2:D:278:THR:HG21	2:D:329:LEU:HG	2.00	0.42
2:D:383:ASP:O	2:D:387:ILE:HG12	2.19	0.42
3:E:185:ILE:HG13	3:E:255:VAL:HA	2.01	0.42
3:E:115:GLU:HA	3:E:116:PRO:HD3	1.80	0.42
3:E:144:MET:HG2	3:E:145:LYS:HD2	2.01	0.42
3:F:52:ILE:HD11	3:F:67:ILE:HD12	2.01	0.42
6:L:188:VAL:HG22	6:L:264:ILE:HG23	2.01	0.42
4:G:33:THR:OG1	4:G:34:ASP:N	2.52	0.42
4:H:33:THR:OG1	4:H:34:ASP:N	2.52	0.42
3:F:144:MET:HG2	3:F:145:LYS:HD2	2.01	0.42
8:O:312:SER:HA	8:O:313:PRO:HD3	1.84	0.42
6:L:52:SEP:HB2	6:L:53:ARG:H	1.68	0.42
1:B:56:LEU:O	1:B:59:SER:OG	2.31	0.42
1:B:87:TRP:HA	1:B:90:CYS:HB2	2.00	0.42
4:H:287:SER:O	4:H:291:TYR:N	2.48	0.42
3:F:72:ASN:ND2	3:F:377:ASP:OD1	2.43	0.42
6:K:5:HIS:HD1	6:K:40:ASP:HB2	1.85	0.42
1:B:283:LEU:HD21	1:B:295:VAL:HG11	2.02	0.42
8:O:132:LEU:HD13	8:O:137:THR:HA	2.02	0.42
6:L:5:HIS:HD1	6:L:40:ASP:HB2	1.85	0.42
1:A:21:THR:OG1	1:A:22:MET:N	2.52	0.42
3:E:327:PRO:HG3	4:H:174:TYR:HB3	2.01	0.42
6:L:202:LYS:HG3	8:P:333:LEU:HD12	2.01	0.42
1:A:89:ASN:O	1:A:93:HIS:N	2.40	0.42
2:C:401:VAL:HB	2:C:470:VAL:HG22	2.02	0.42
3:E:193:SER:HB3	3:E:196:VAL:HG22	2.00	0.42
4:H:356:LYS:HD2	4:H:373:ARG:HG2	2.01	0.42
1:A:283:LEU:HD21	1:A:295:VAL:HG11	2.02	0.42
1:A:76:PHE:HD1	3:E:122:PHE:HZ	1.67	0.42
4:G:227:ARG:NH2	4:G:229:ASP:OD2	2.52	0.42
3:F:21:THR:HA	3:F:24:THR:HG22	2.02	0.42
8:P:260:LEU:O	8:P:264:LYS:HG2	2.20	0.42
2:D:401:VAL:HB	2:D:470:VAL:HG22	2.02	0.42
3:E:21:THR:HA	3:E:24:THR:HG22	2.02	0.42
4:G:145:PHE:HZ	4:G:237:ILE:HG21	1.84	0.42
4:G:317:THR:O	4:G:328:GLU:HA	2.20	0.42
5:I:67:ALA:HB3	5:I:69:LEU:HG	2.02	0.42
4:H:57:VAL:HA	4:H:58:PRO:HD3	1.90	0.42
4:H:145:PHE:HZ	4:H:237:ILE:HG21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:50:GLU:OE2	6:K:86:SER:OG	2.32	0.42
2:C:405:SER:HB2	2:C:436:GLU:HB2	2.02	0.41
1:B:21:THR:OG1	1:B:22:MET:N	2.52	0.41
8:P:132:LEU:HD13	8:P:137:THR:HA	2.02	0.41
1:A:46:ILE:HD12	6:K:45:MET:HE1	2.01	0.41
3:E:186:LEU:HB2	3:E:213:VAL:HG12	2.02	0.41
4:H:63:THR:HG22	4:H:139:VAL:H	1.83	0.41
4:H:227:ARG:NH2	4:H:229:ASP:OD2	2.52	0.41
6:L:247:ALA:HA	6:L:250:LYS:HE3	2.01	0.41
4:G:169:SER:OG	4:G:282:ALA:O	2.30	0.41
6:K:22:VAL:HG12	6:K:36:LEU:HA	2.02	0.41
3:E:52:ILE:HD11	3:E:67:ILE:HD12	2.01	0.41
3:F:46:GLN:OE1	3:F:50:ARG:NH1	2.54	0.41
2:D:476:SER:HA	2:D:511:LYS:HG2	2.02	0.41
2:D:601:LEU:HD23	3:F:227:HIS:HB3	2.01	0.41
1:B:302:MET:HG3	1:B:303:TRP:CD1	2.56	0.41
4:H:163:ILE:HG23	4:H:242:VAL:HG11	2.03	0.41
6:K:202:LYS:HG3	8:O:333:LEU:HD12	2.02	0.41
8:P:101:ILE:HG13	8:P:212:ASP:HB2	2.02	0.41
8:P:312:SER:HA	8:P:313:PRO:HD3	1.84	0.41
2:C:487:ALA:N	2:C:616:LEU:O	2.54	0.41
2:D:456:ILE:HG13	2:D:459:LEU:HD12	2.02	0.41
3:E:192:ASP:OD1	3:E:192:ASP:N	2.50	0.41
4:H:317:THR:O	4:H:328:GLU:HA	2.20	0.41
4:H:325:ILE:HD11	4:H:340:GLY:O	2.21	0.41
3:F:185:ILE:HG13	3:F:255:VAL:HA	2.01	0.41
2:C:476:SER:HA	2:C:511:LYS:HG2	2.02	0.41
2:D:635:LEU:HD22	2:D:643:ILE:HD12	2.03	0.41
4:G:356:LYS:HD2	4:G:373:ARG:HG2	2.01	0.41
5:J:234:ARG:HD3	5:J:234:ARG:HA	1.85	0.41
1:B:211:VAL:HG22	1:B:271:THR:HA	2.03	0.41
8:O:260:LEU:O	8:O:264:LYS:HG2	2.20	0.41
6:L:22:VAL:HG12	6:L:36:LEU:HA	2.02	0.41
6:L:69:ASP:OD2	6:L:87:LYS:NZ	2.37	0.41
8:P:355:ILE:HD12	8:P:373:ILE:HB	2.02	0.41
1:A:211:VAL:HG22	1:A:271:THR:HA	2.03	0.41
2:C:297:LEU:HD23	2:C:375:ALA:HB2	2.03	0.41
2:C:527:ALA:O	2:C:614:ASN:ND2	2.41	0.41
2:D:487:ALA:N	2:D:616:LEU:O	2.54	0.41
5:I:236:PRO:O	5:I:389:GLU:N	2.54	0.41
3:F:186:LEU:HB2	3:F:213:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:472:LEU:HD21	2:C:492:LEU:HD11	2.03	0.41
2:D:405:SER:HB2	2:D:436:GLU:HB2	2.02	0.41
5:J:67:ALA:HB3	5:J:69:LEU:HG	2.02	0.41
2:C:507:CYS:SG	2:C:508:GLU:N	2.94	0.40
3:E:46:GLN:OE1	3:E:50:ARG:NH1	2.54	0.40
3:E:257:LYS:HD3	3:E:293:PHE:CE2	2.56	0.40
5:J:6:PHE:O	5:J:170:LEU:N	2.54	0.40
1:A:302:MET:HG3	1:A:303:TRP:CD1	2.56	0.40
2:D:339:THR:HG21	2:D:511:LYS:HZ3	1.85	0.40
2:D:472:LEU:HD21	2:D:492:LEU:HD11	2.03	0.40
3:E:373:ASP:OD1	3:E:373:ASP:N	2.53	0.40
4:G:325:ILE:HD11	4:G:340:GLY:O	2.21	0.40
5:J:236:PRO:O	5:J:389:GLU:N	2.54	0.40
8:O:116:VAL:HG21	8:O:217:LEU:CD2	2.47	0.40
1:A:210:LEU:HG	1:A:211:VAL:H	1.87	0.40
2:D:601:LEU:HD11	2:D:612:ILE:HD11	2.04	0.40
1:B:21:THR:HG23	1:B:23:PRO:HD2	2.04	0.40
8:P:142:TYR:CE1	8:P:395:LEU:HB3	2.56	0.40
2:D:297:LEU:HD23	2:D:375:ALA:HB2	2.03	0.40
4:G:253:GLN:N	4:G:258:ASP:OD2	2.48	0.40
6:K:141:ALA:HA	6:K:144:ALA:HB3	2.03	0.40
6:K:155:TRP:HH2	6:K:169:LEU:HB3	1.87	0.40
8:O:355:ILE:HD12	8:O:373:ILE:HB	2.02	0.40
8:P:436:LEU:HD23	8:P:513:GLY:HA3	2.04	0.40
2:C:635:LEU:HD22	2:C:643:ILE:HD12	2.03	0.40
1:B:89:ASN:O	1:B:93:HIS:N	2.40	0.40
8:O:101:ILE:HG13	8:O:212:ASP:HB2	2.02	0.40
8:O:506:GLU:HB2	8:O:510:ARG:NE	2.37	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	303/305 (99%)	264 (87%)	39 (13%)	0	100	100
1	B	303/305 (99%)	265 (88%)	38 (12%)	0	100	100
2	C	338/651 (52%)	303 (90%)	35 (10%)	0	100	100
2	D	338/651 (52%)	303 (90%)	35 (10%)	0	100	100
3	E	350/381 (92%)	327 (93%)	23 (7%)	0	100	100
3	F	350/381 (92%)	327 (93%)	23 (7%)	0	100	100
4	G	408/712 (57%)	364 (89%)	44 (11%)	0	100	100
4	H	408/712 (57%)	364 (89%)	44 (11%)	0	100	100
5	I	260/578 (45%)	214 (82%)	46 (18%)	0	100	100
5	J	260/578 (45%)	215 (83%)	45 (17%)	0	100	100
6	K	242/304 (80%)	212 (88%)	29 (12%)	1 (0%)	30	65
6	L	242/304 (80%)	212 (88%)	29 (12%)	1 (0%)	30	65
7	M	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	15
7	N	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	15
8	O	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	8	38
8	P	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	8	38
All	All	4608/7486 (62%)	4074 (88%)	518 (11%)	16 (0%)	38	70

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	O	129	LYS
8	P	129	LYS
8	O	495	ILE
8	O	507	LYS
8	P	495	ILE
8	P	507	LYS
8	O	127	ARG
8	O	497	GLU
8	P	127	ARG
8	P	497	GLU
7	M	129	LEU
7	N	129	LEU
6	K	226	PRO
6	L	226	PRO
8	O	210	VAL
8	P	210	VAL

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	265/265 (100%)	264 (100%)	1 (0%)	89 91
1	B	265/265 (100%)	264 (100%)	1 (0%)	89 91
2	C	308/561 (55%)	307 (100%)	1 (0%)	91 91
2	D	308/561 (55%)	307 (100%)	1 (0%)	91 91
3	E	315/338 (93%)	314 (100%)	1 (0%)	91 91
3	F	315/338 (93%)	314 (100%)	1 (0%)	91 91
4	G	375/649 (58%)	375 (100%)	0	100 100
4	H	375/649 (58%)	375 (100%)	0	100 100
5	I	250/529 (47%)	249 (100%)	1 (0%)	89 91
5	J	250/529 (47%)	249 (100%)	1 (0%)	89 91
6	K	223/273 (82%)	211 (95%)	12 (5%)	18 42
6	L	223/273 (82%)	211 (95%)	12 (5%)	18 42
7	M	16/246 (6%)	13 (81%)	3 (19%)	1 8
7	N	16/246 (6%)	13 (81%)	3 (19%)	1 8
8	O	332/449 (74%)	306 (92%)	26 (8%)	10 33
8	P	332/449 (74%)	306 (92%)	26 (8%)	10 33
All	All	4168/6620 (63%)	4078 (98%)	90 (2%)	47 65

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	ILE
2	C	345	ARG
2	D	345	ARG
3	E	371	GLN
5	I	289	LYS
5	J	289	LYS
1	B	300	ILE
3	F	371	GLN

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Mol	Chain	Res	Type
6	K	54	ARG
6	K	85	LEU
6	K	185	ARG
6	K	195	TYR
6	K	203	ASP
6	K	230	LEU
6	K	235	LEU
6	K	236	ASP
6	K	244	LEU
6	K	251	ILE
6	K	261	VAL
6	K	264	ILE
7	M	131	TYR
7	M	135	LEU
7	M	141	ILE
8	O	130	ASP
8	O	132	LEU
8	O	224	CYS
8	O	228	GLN
8	O	236	ILE
8	O	253	LEU
8	O	257	GLU
8	O	291	ILE
8	O	307	ARG
8	O	332	ASP
8	O	354	GLU
8	O	359	ILE
8	O	395	LEU
8	O	402	VAL
8	O	403	ASP
8	O	406	LEU
8	O	426	ILE
8	O	432	ILE
8	O	438	ARG
8	O	440	LEU
8	O	443	VAL
8	O	462	LEU
8	O	495	ILE
8	O	502	SER
8	O	508	HIS
8	O	512	ILE
6	L	54	ARG

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Mol	Chain	Res	Type
6	L	85	LEU
6	L	185	ARG
6	L	195	TYR
6	L	203	ASP
6	L	230	LEU
6	L	235	LEU
6	L	236	ASP
6	L	244	LEU
6	L	251	ILE
6	L	261	VAL
6	L	264	ILE
7	N	131	TYR
7	N	135	LEU
7	N	141	ILE
8	P	130	ASP
8	P	132	LEU
8	P	224	CYS
8	P	228	GLN
8	P	236	ILE
8	P	253	LEU
8	P	257	GLU
8	P	291	ILE
8	P	307	ARG
8	P	332	ASP
8	P	354	GLU
8	P	359	ILE
8	P	395	LEU
8	P	402	VAL
8	P	403	ASP
8	P	406	LEU
8	P	426	ILE
8	P	432	ILE
8	P	438	ARG
8	P	440	LEU
8	P	443	VAL
8	P	462	LEU
8	P	495	ILE
8	P	502	SER
8	P	508	HIS
8	P	512	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
2	C	271	HIS
2	C	325	HIS
2	C	342	ASN
2	C	389	ASN
2	C	416	ASN
2	D	271	HIS
2	D	325	HIS
2	D	342	ASN
2	D	389	ASN
2	D	416	ASN
3	E	227	HIS
4	G	87	ASN
4	G	96	ASN
4	G	371	ASN
5	I	118	GLN
5	I	309	GLN
5	I	388	ASN
5	J	118	GLN
5	J	309	GLN
5	J	388	ASN
1	B	80	ASN
4	H	87	ASN
4	H	96	ASN
4	H	371	ASN
3	F	227	HIS
3	F	368	ASN
6	K	120	GLN
8	O	98	GLN
8	O	248	GLN
8	O	415	GLN
8	O	508	HIS
6	L	109	HIS
6	L	120	GLN
8	P	98	GLN
8	P	248	GLN
8	P	415	GLN
8	P	508	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SEP	L	52	6	8,9,10	1.53	1 (12%)	8,12,14	1.62	2 (25%)
6	SEP	K	52	6	8,9,10	1.53	1 (12%)	8,12,14	1.62	2 (25%)

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	-	5/5/8/10	-
6	SEP	K	52	6	-	5/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	52	SEP	P-O1P	3.33	1.61	1.50
6	K	52	SEP	P-O1P	3.32	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	52	SEP	P-OG-CB	-3.19	109.50	118.30
6	L	52	SEP	P-OG-CB	-3.18	109.53	118.30
6	L	52	SEP	OG-CB-CA	2.80	110.87	108.14
6	K	52	SEP	OG-CB-CA	2.79	110.86	108.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	52	SEP	N-CA-CB-OG
6	K	52	SEP	CB-OG-P-O2P
6	L	52	SEP	N-CA-CB-OG
6	L	52	SEP	CB-OG-P-O2P
6	K	52	SEP	CB-OG-P-O1P
6	L	52	SEP	CB-OG-P-O1P
6	K	52	SEP	CB-OG-P-O3P
6	L	52	SEP	CB-OG-P-O3P
6	K	52	SEP	CA-CB-OG-P
6	L	52	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	52	SEP	1	0

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.

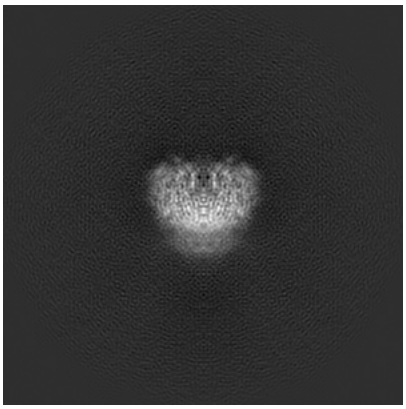
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4404. These allow visual inspection of the internal detail of the map and identification of artifacts.

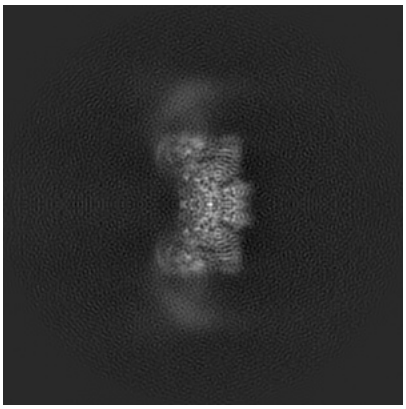
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

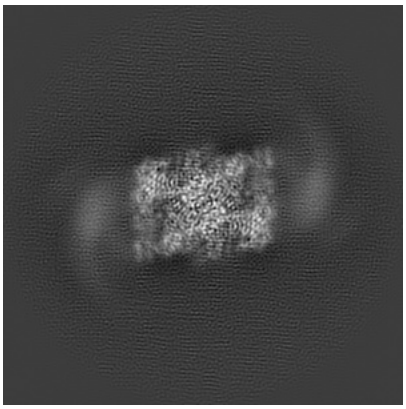
6.1.1 Primary map



X

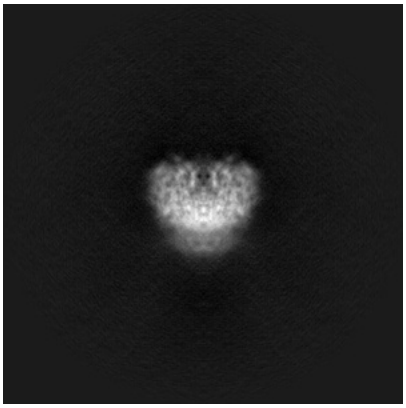


Y

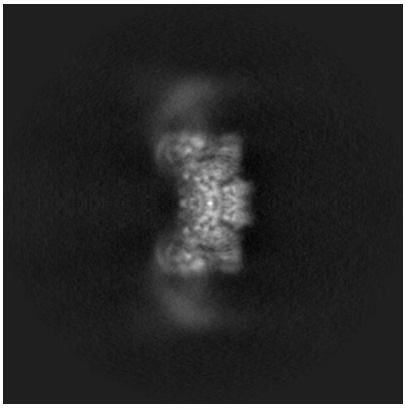


Z

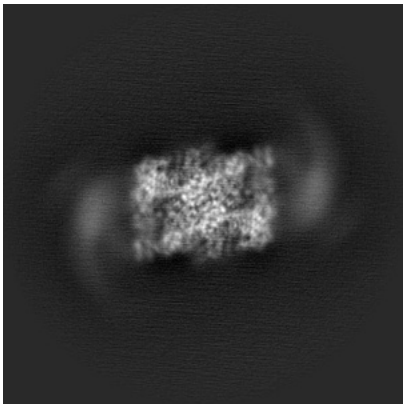
6.1.2 Raw map



X



Y



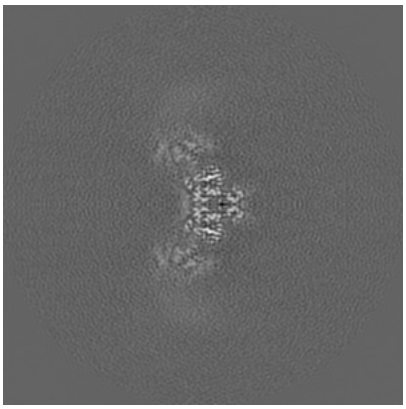
Z

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

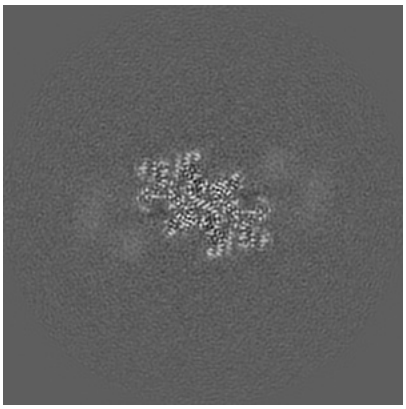
6.2 Central slices (i)

6.2.1 Primary map

X Index: 160

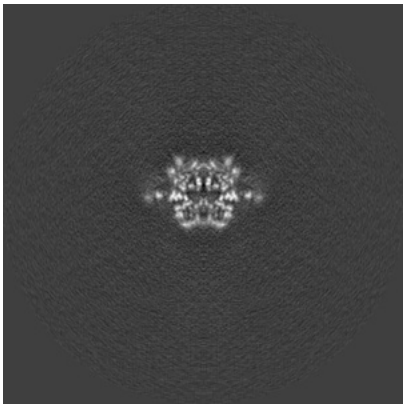


Y Index: 160

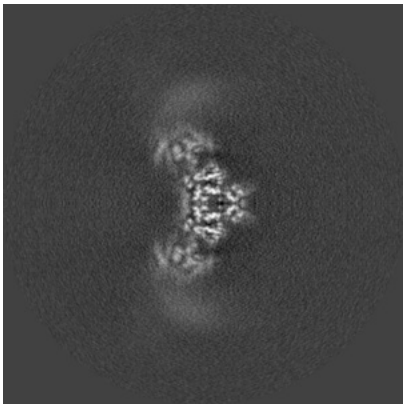


Z Index: 160

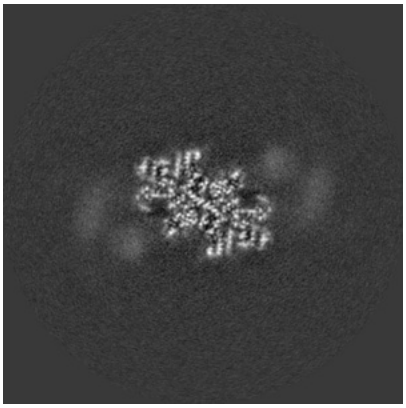
6.2.2 Raw map



X Index: 160



Y Index: 160

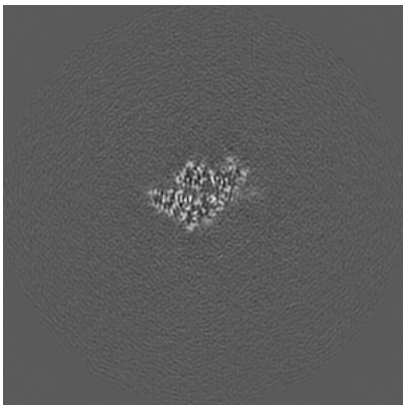


Z Index: 160

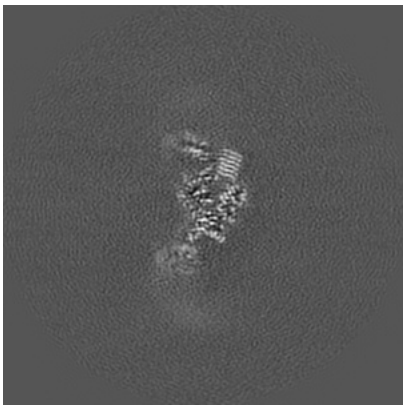
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

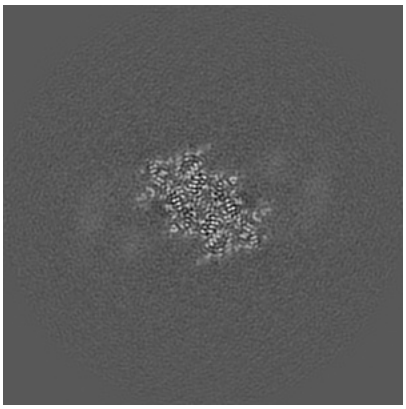
6.3.1 Primary map



X Index: 167

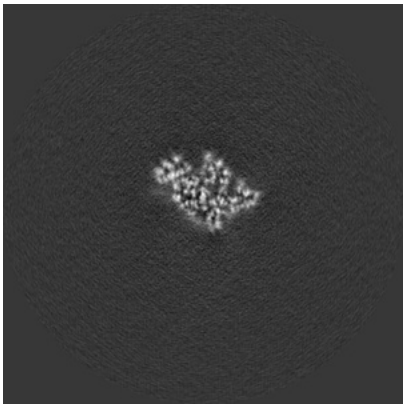


Y Index: 151

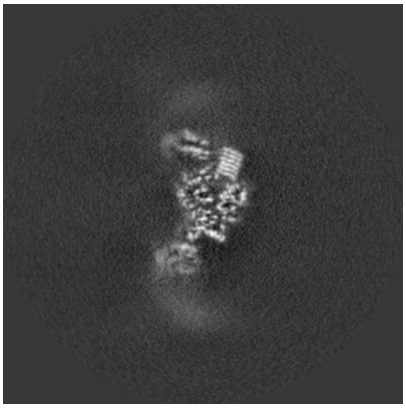


Z Index: 163

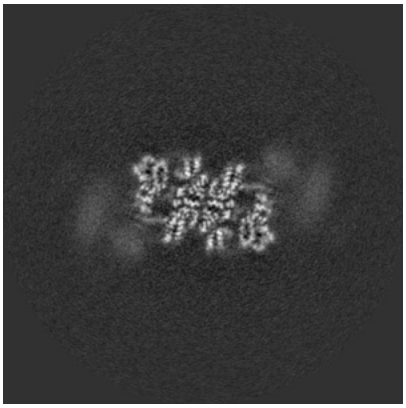
6.3.2 Raw map



X Index: 149



Y Index: 151

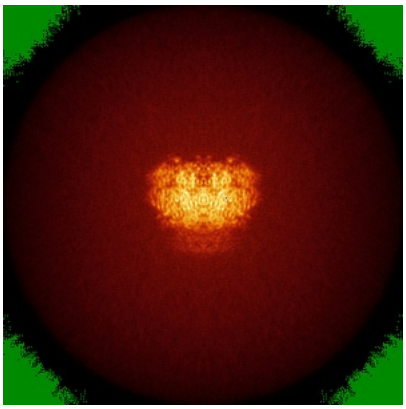


Z Index: 156

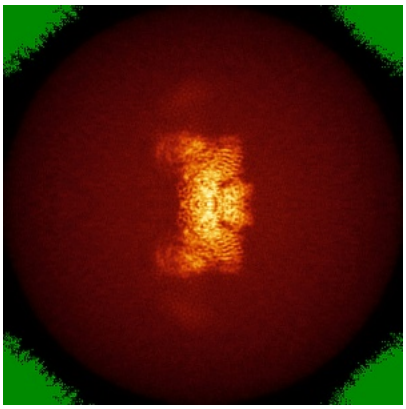
The images above show the largest variance slices of the map in three orthogonal directions.

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

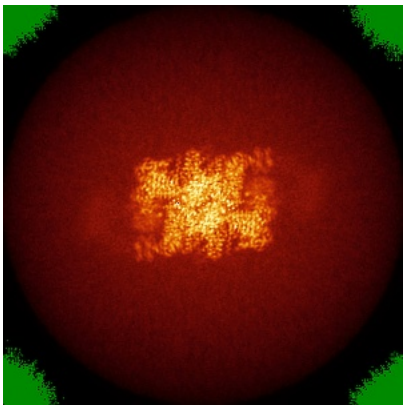
6.4.1 Primary map



X

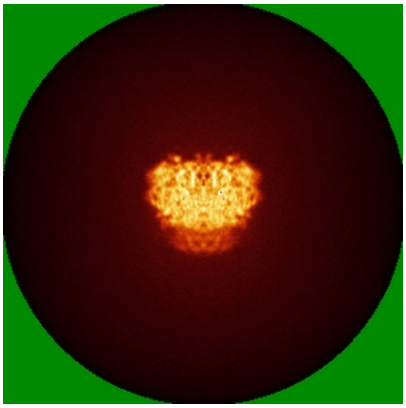


Y

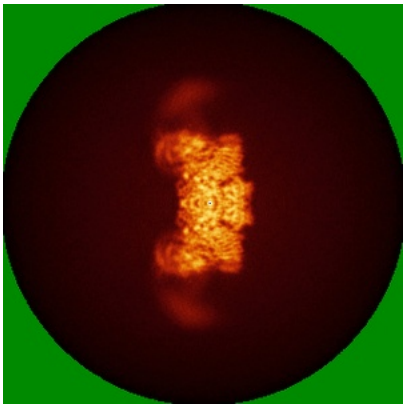


Z

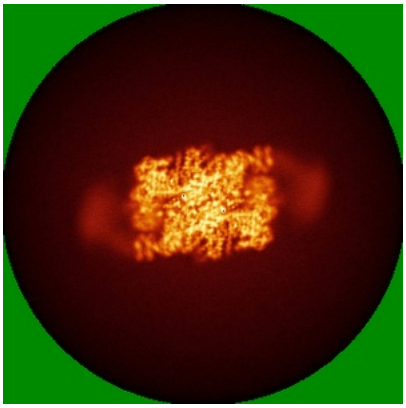
6.4.2 Raw map



X



Y



Z

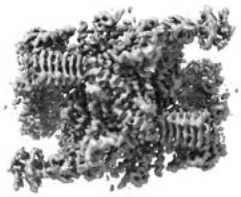
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

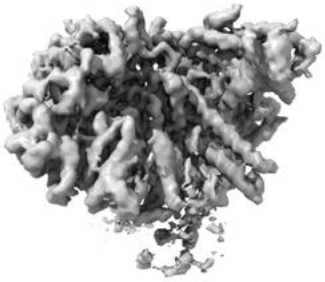
Y



Z

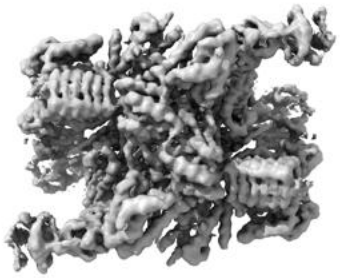
The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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.

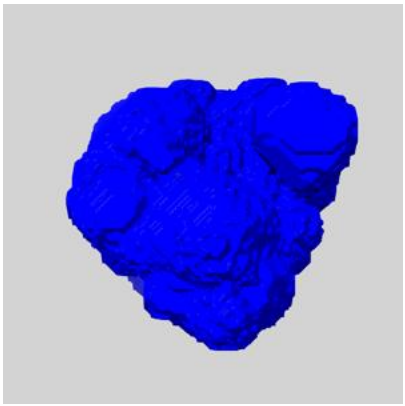
6.6 Mask visualisation

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

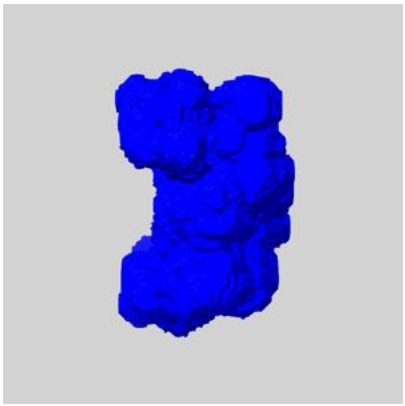
A mask typically either:

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

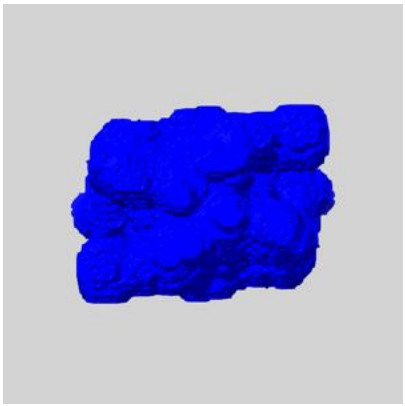
6.6.1 emd_4404_msk_1.map



X



Y

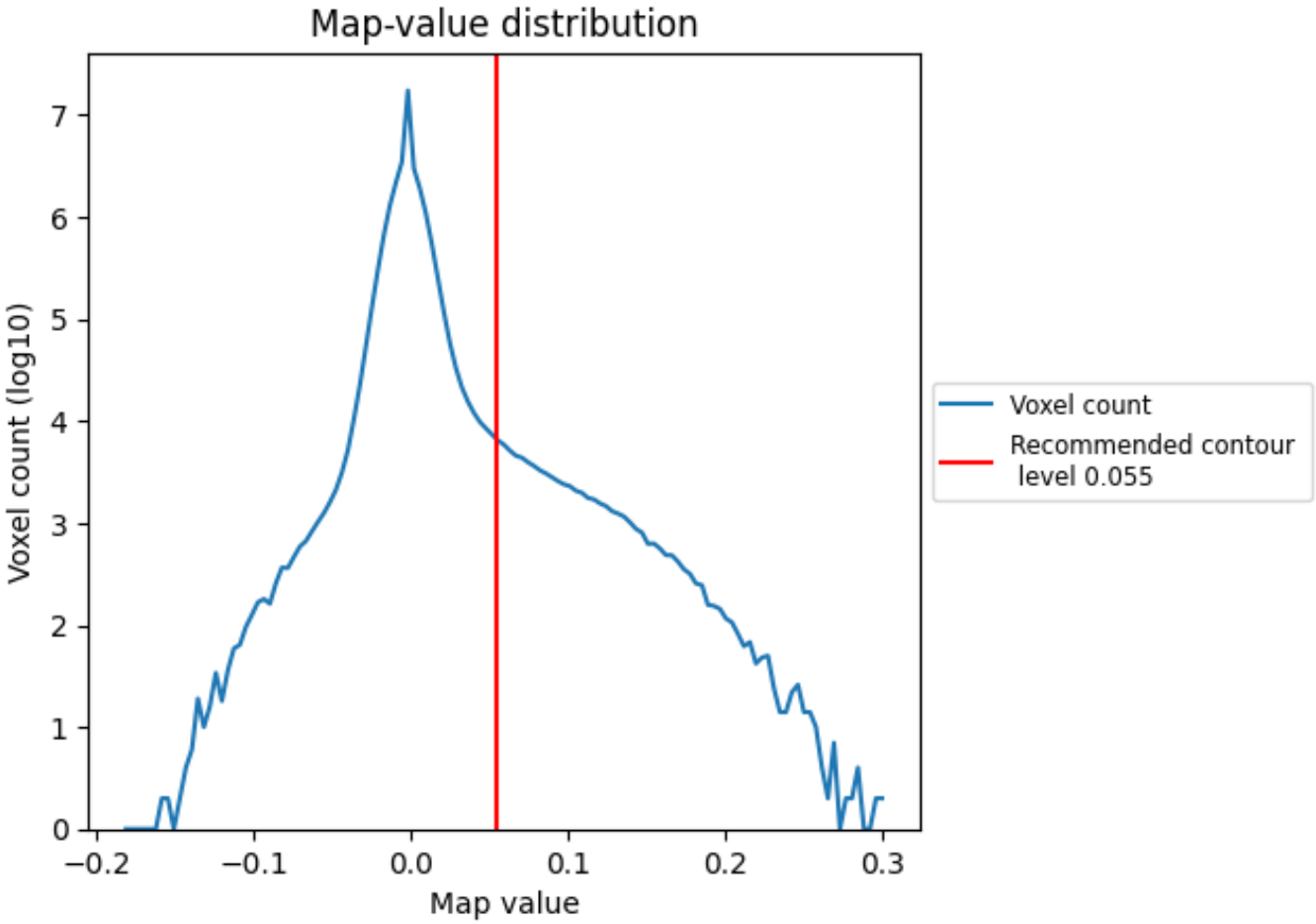


Z

7 Map analysis

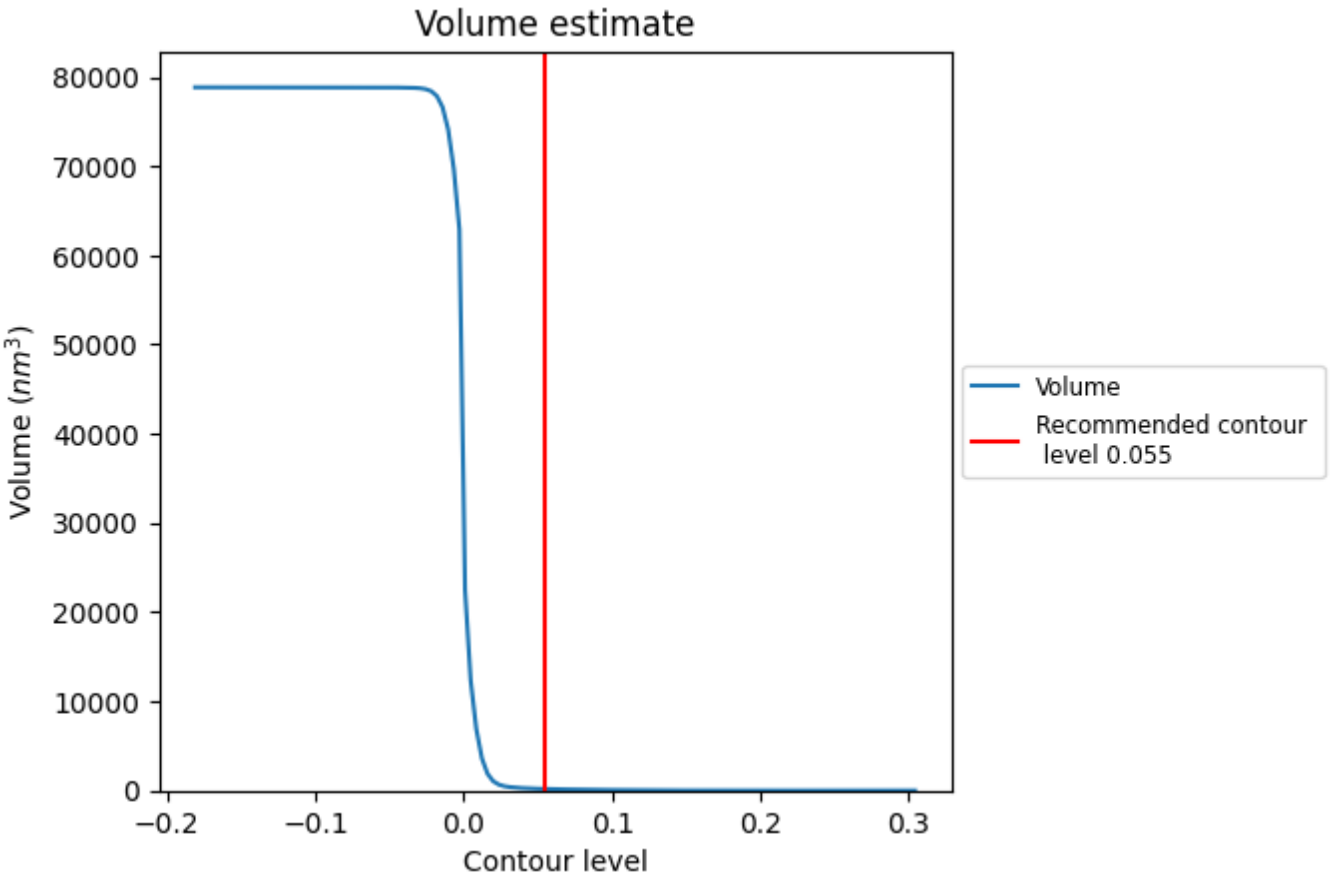
This section contains the results of statistical analysis of the map.

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.

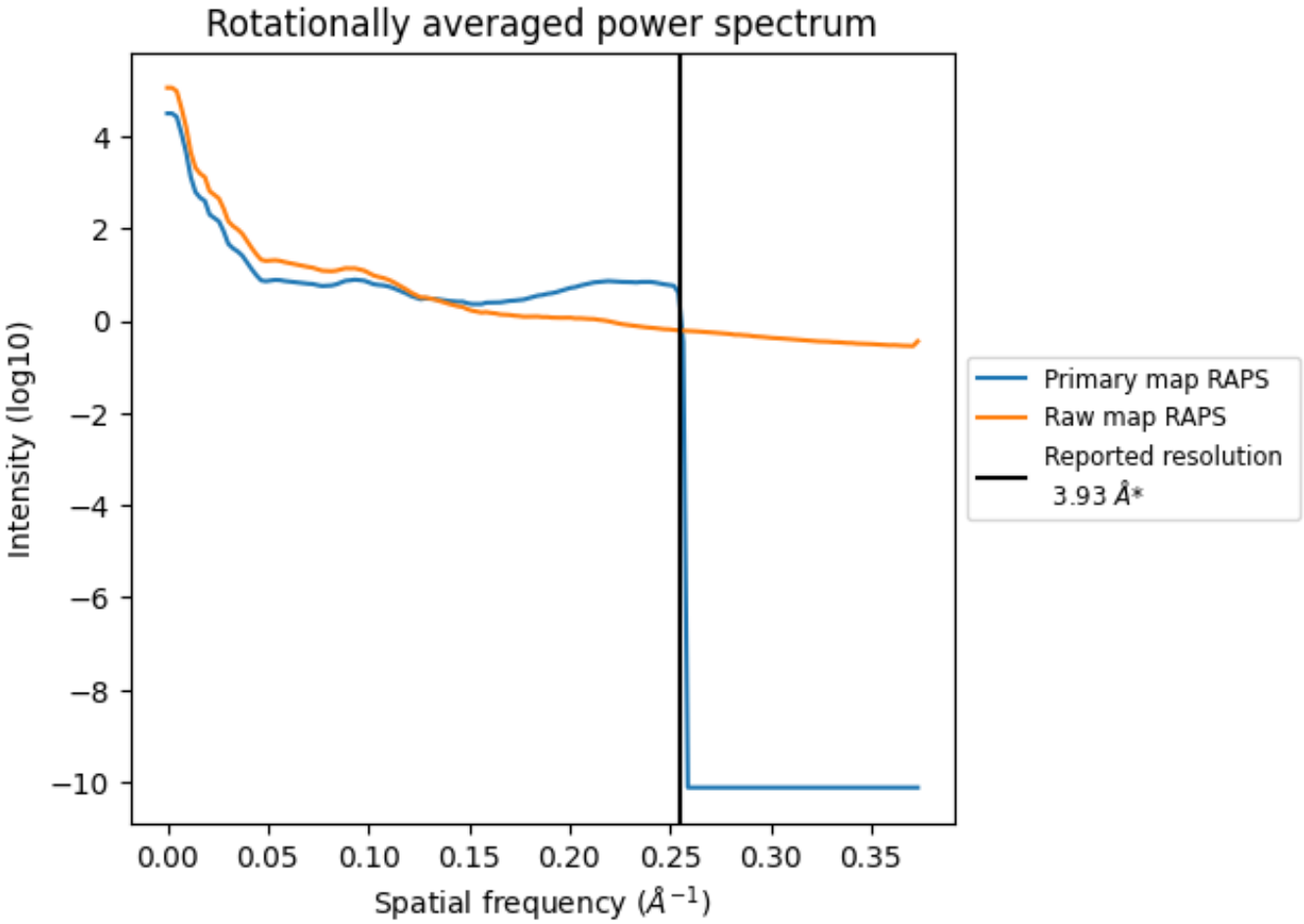
7.2 Volume estimate



The volume at the recommended contour level is 180 nm^3; this corresponds to an approximate mass of 162 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)

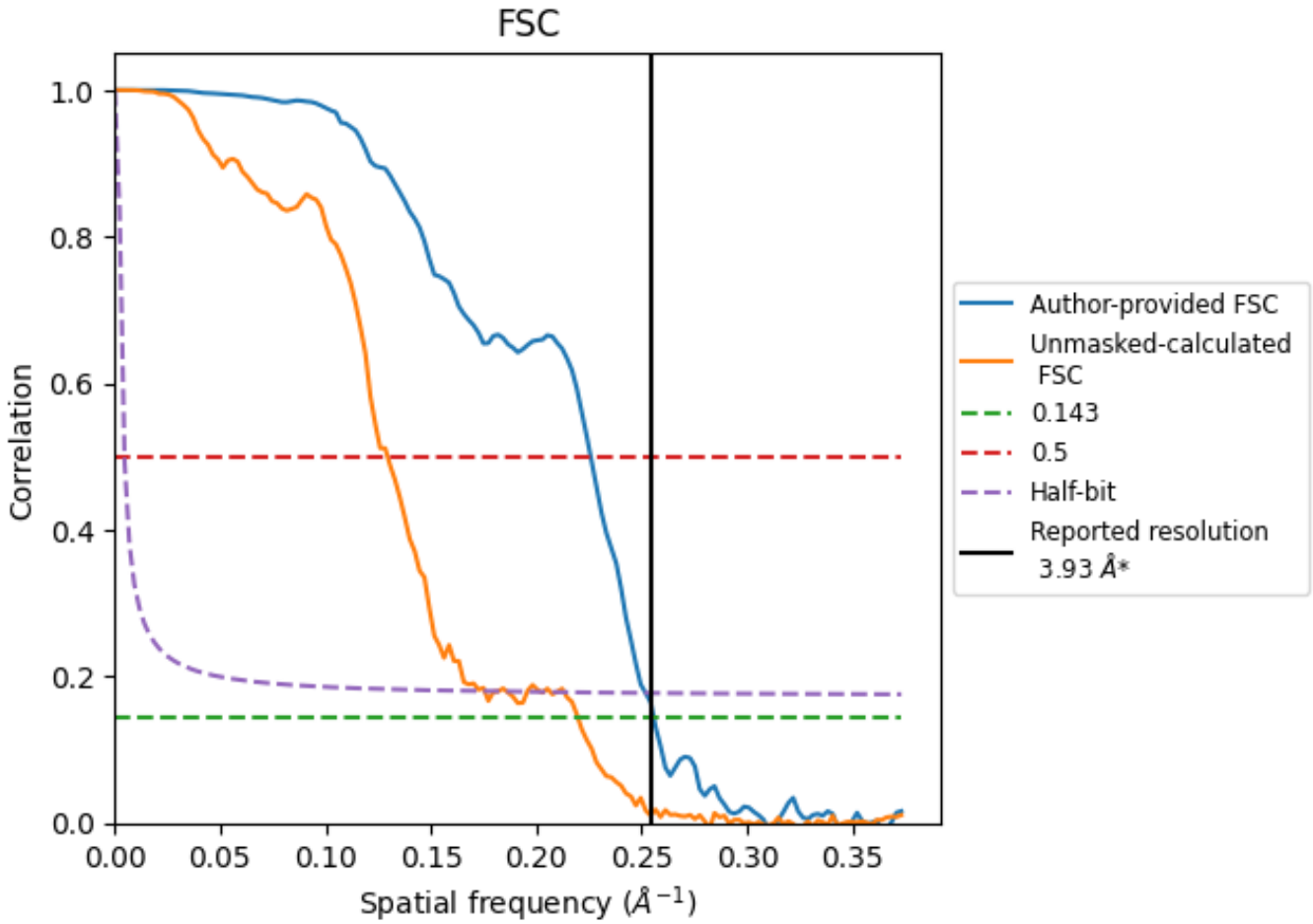


*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

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 0.254 Å^{-1}

8.2 Resolution estimates (i)

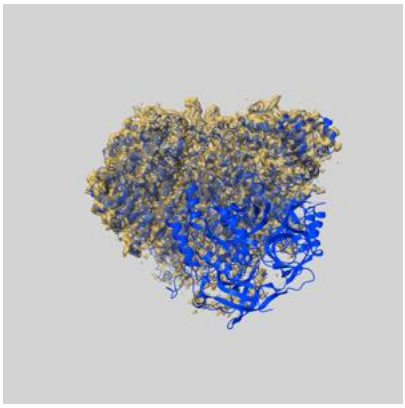
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.91	4.43	3.97
Unmasked-calculated*	4.55	7.73	5.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.93 by more than 10 %

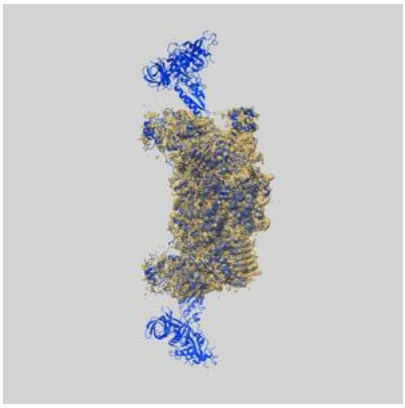
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4404 and PDB model 6I3M. Per-residue inclusion information can be found in section 3 on page 6.

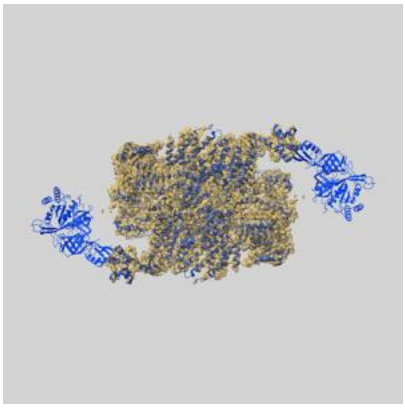
9.1 Map-model overlay



X



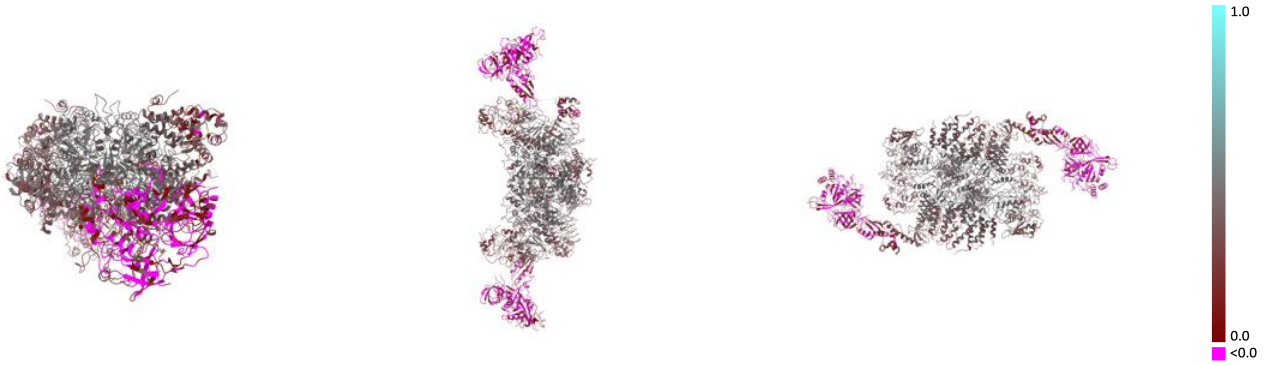
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

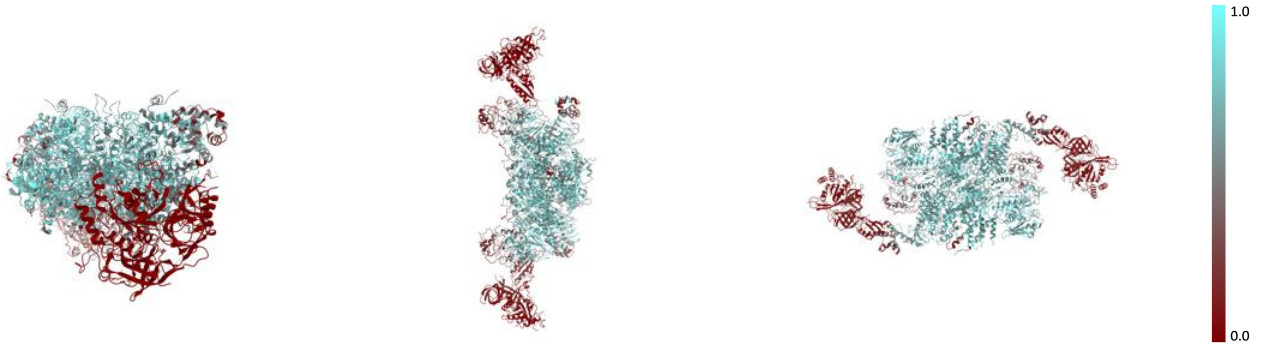
9.2 Q-score mapped to coordinate model (i)



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.

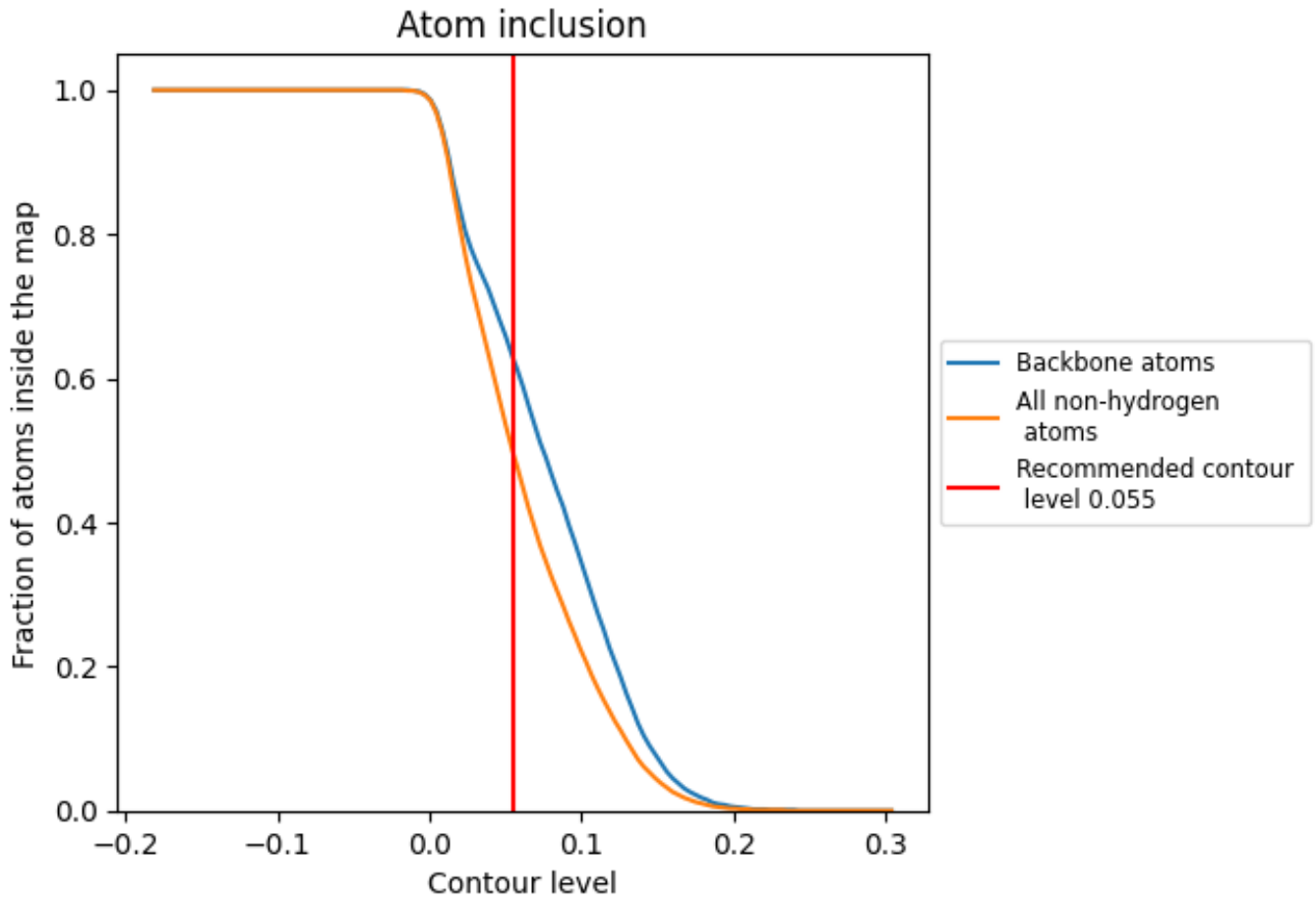
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 50% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4970	0.3070
A	0.7140	0.4080
B	0.7110	0.4080
C	0.6680	0.4200
D	0.6680	0.4210
E	0.6850	0.4110
F	0.6870	0.4120
G	0.6970	0.4000
H	0.6990	0.3990
I	0.3560	0.2950
J	0.3590	0.2960
K	0.3650	0.2370
L	0.3610	0.2380
M	0.0000	0.0040
N	0.0000	0.0410
O	0.0000	-0.0010
P	0.0000	-0.0040