Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 11:02 am GMT

PDB ID	:	6QG2
EMDB ID	:	EMD-4545
Title	:	Structure of eIF2B-eIF2 (phosphorylated at Ser51) complex (model A)
Authors	:	Llacer, J.L.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on	:	2019-01-10
Resolution	:	4.60 Å(reported)
Based on initial models	:	5B04, 6FYX

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:

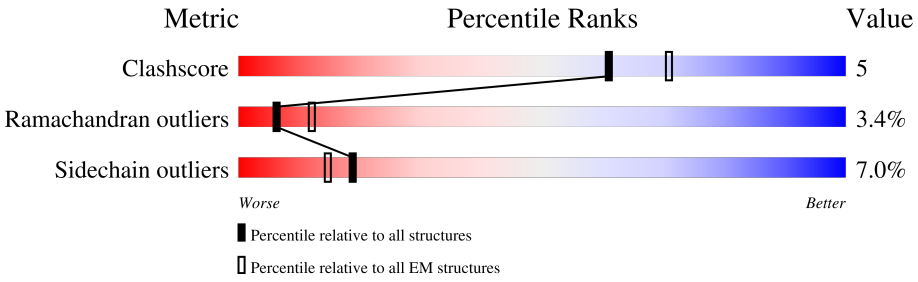
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	305	12% 72% 23%
1	B	305	21% 74% 22%
2	C	381	20% 71% 19% 9%
2	D	381	18% 73% 16% 9%
3	E	578	18% 39% 7% 54%
3	F	578	39% 56% 8% 35%
4	G	651	10% 46% 8% 45%
4	H	651	14% 44% 10% 45%

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Mol	Chain	Length	Quality of chain
5	I	712	8% 48% 11% 39%
5	J	712	47% 12% 39%
6	K	304	42% 64% 15% 19%
6	L	304	8% 64% 14% 19%
7	M	527	56% 68% 9% 23%
7	N	527	47% 67% 9% 23%
8	O	285	6% 5% 94%
8	P	285	36% 38% 6% 55%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 38664 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	375	Total	C	N	O	S	0	0
			2967	1895	504	550	18		

- 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
			1967	1256	321	381	1	8		
6	L	246	Total	C	N	O	P	S	0	0
			1967	1256	321	381	1	8		

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

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

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

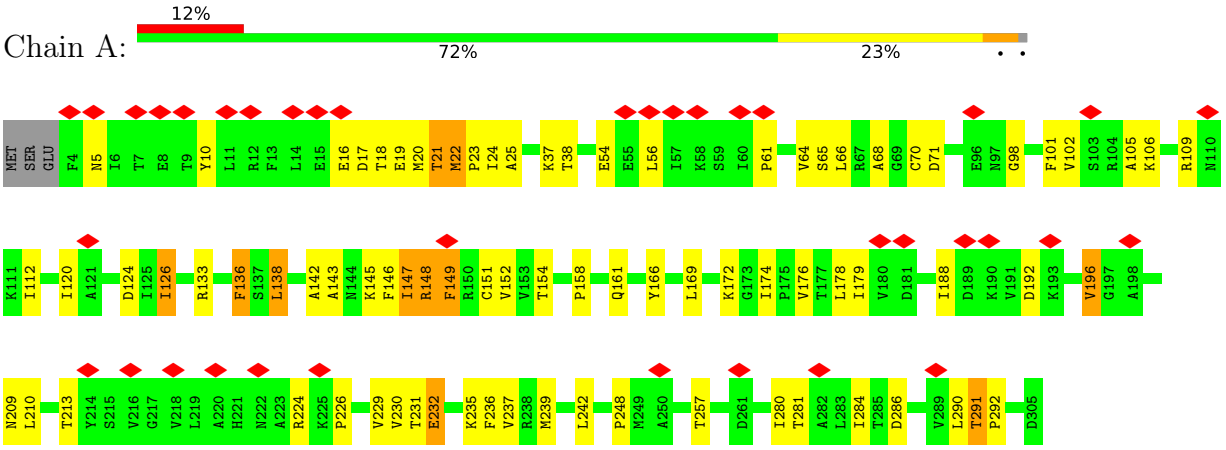
Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	17	Total	C	N	O		0	0
			143	96	24	23			
8	P	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

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.

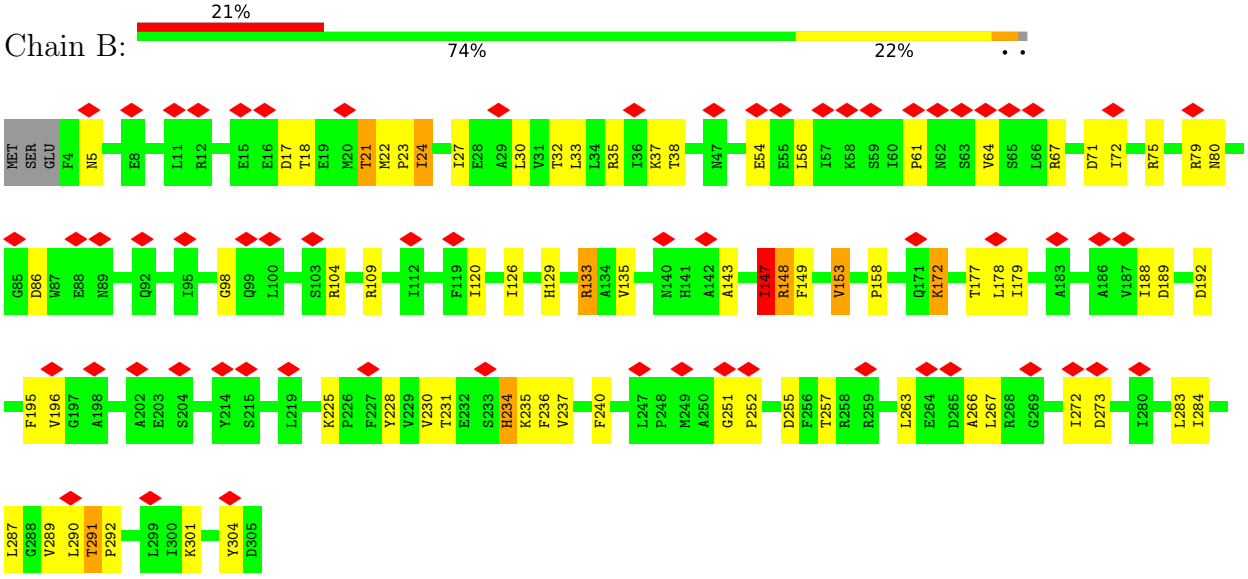
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:



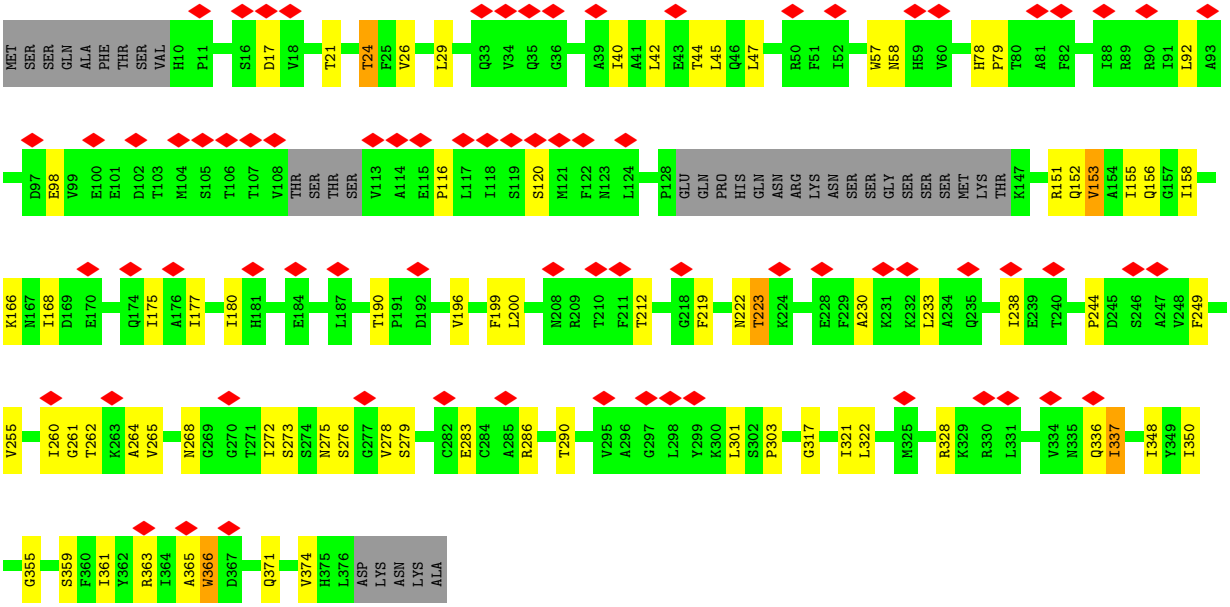
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain B:



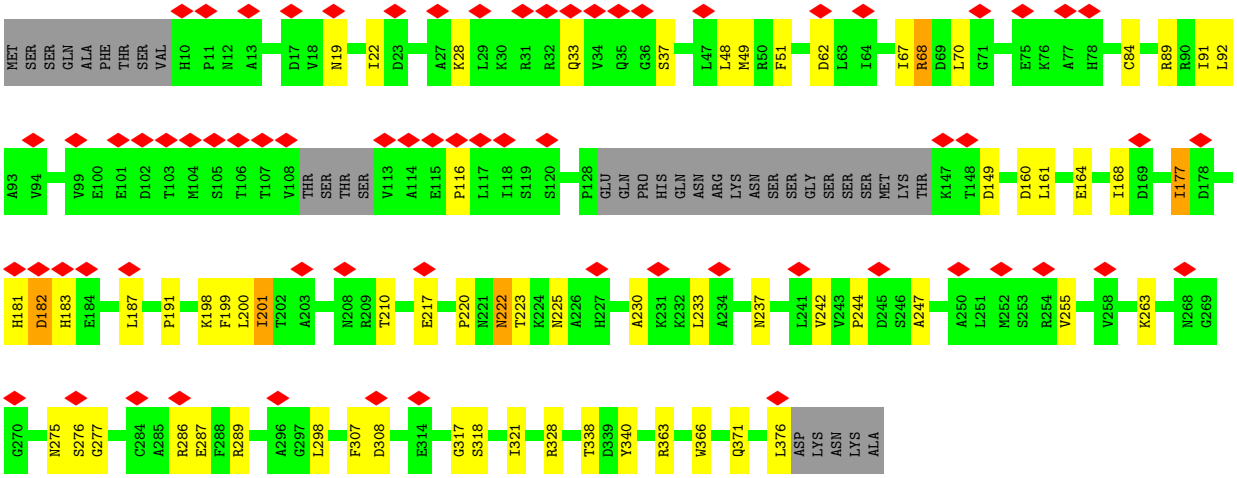
• Molecule 2: Translation initiation factor eIF-2B subunit beta

Chain C:



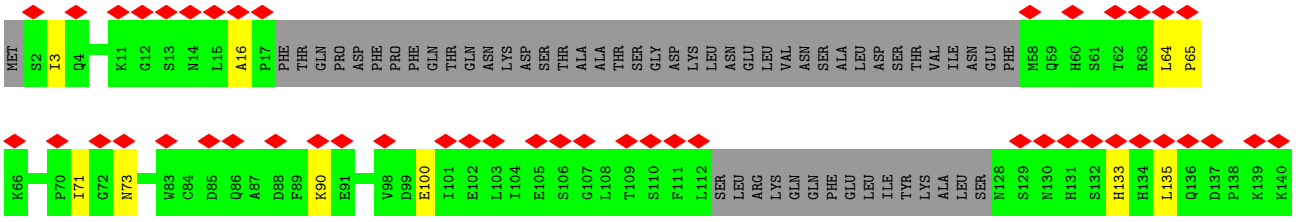
• Molecule 2: Translation initiation factor eIF-2B subunit beta

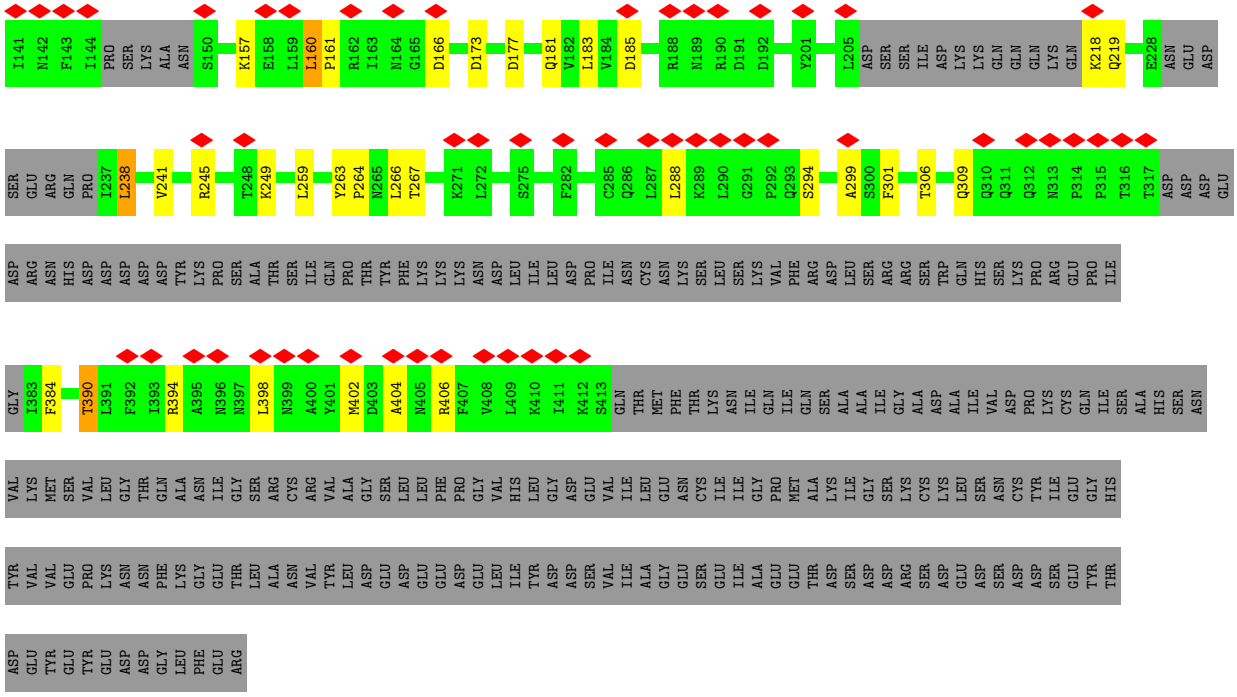
Chain D:



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

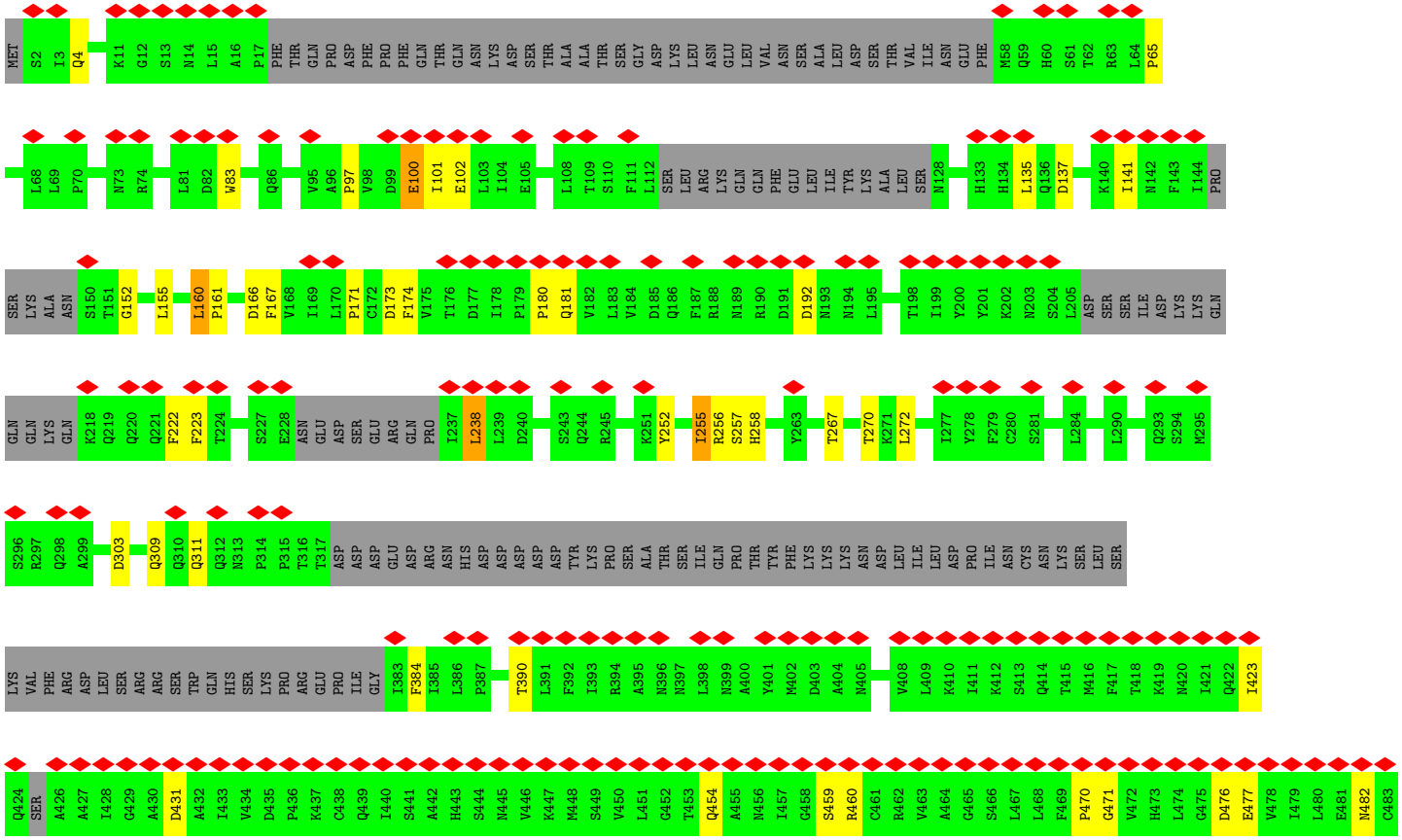
Chain E:

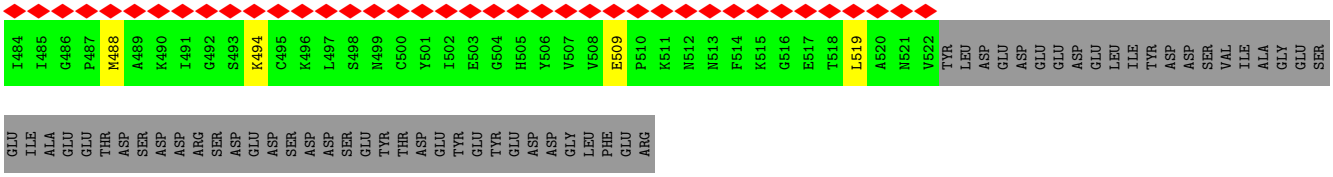




• Molecule 3: Translation initiation factor eIF-2B subunit gamma

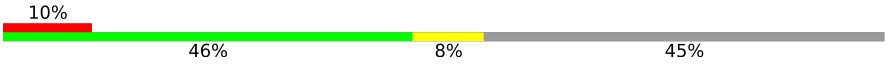
Chain F:

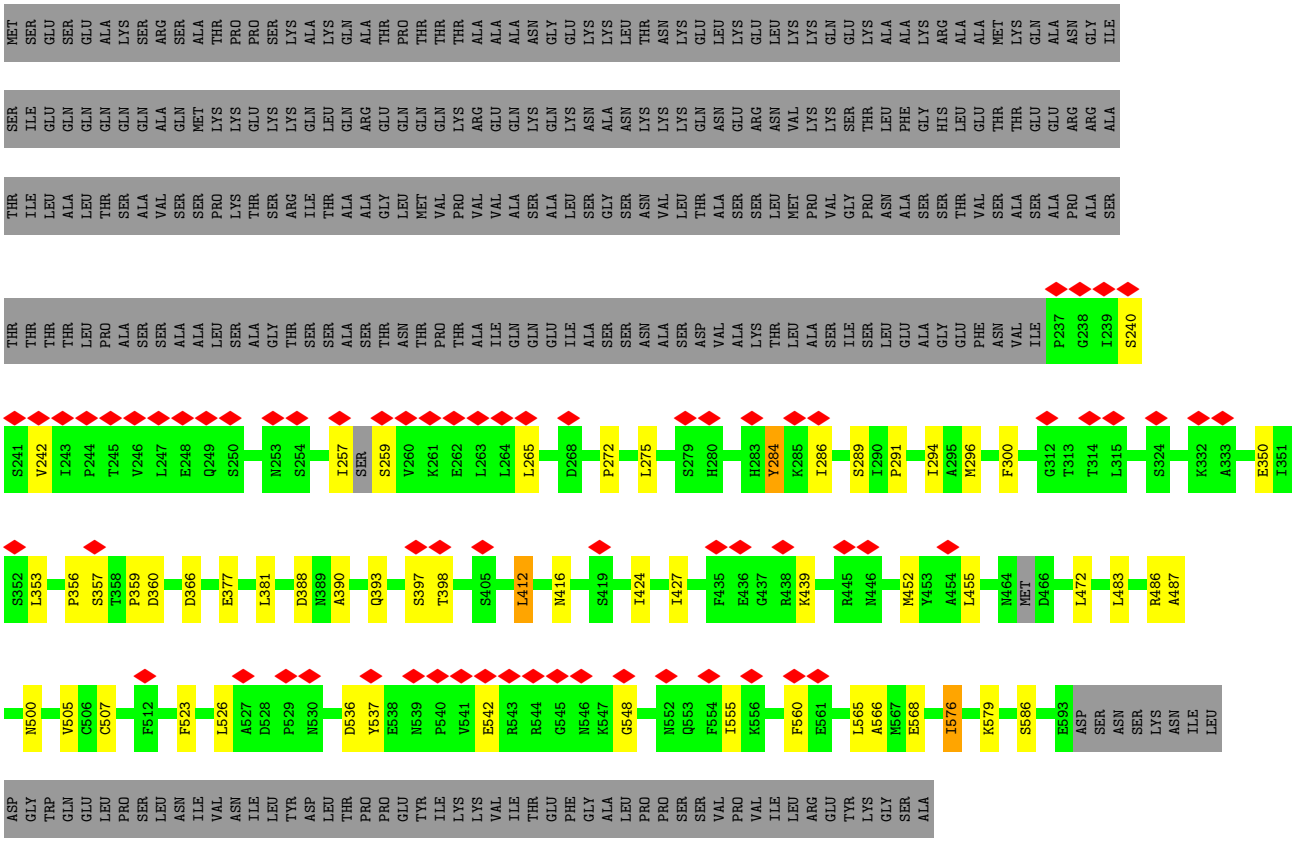




• Molecule 4: Translation initiation factor eIF-2B subunit delta

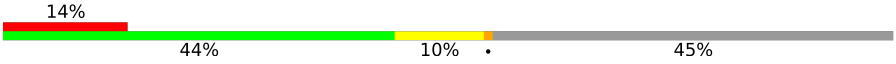
Chain G:

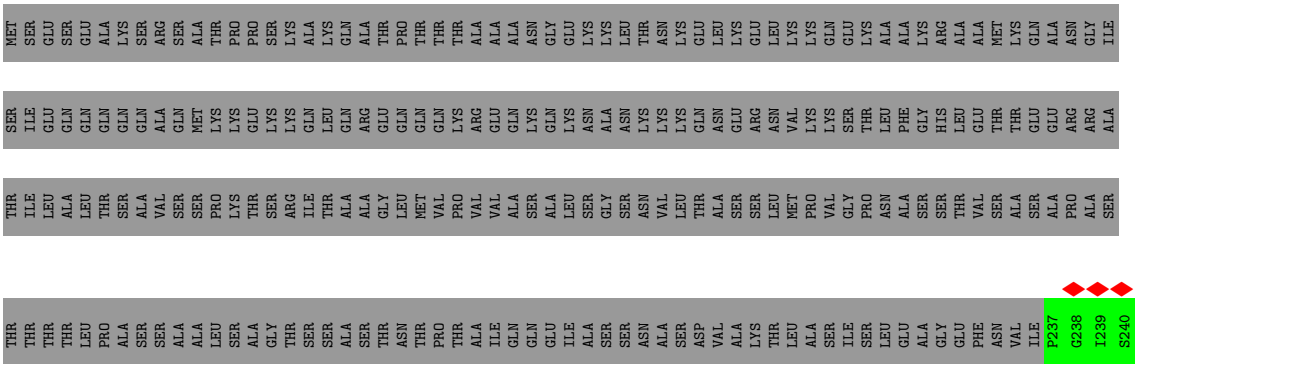


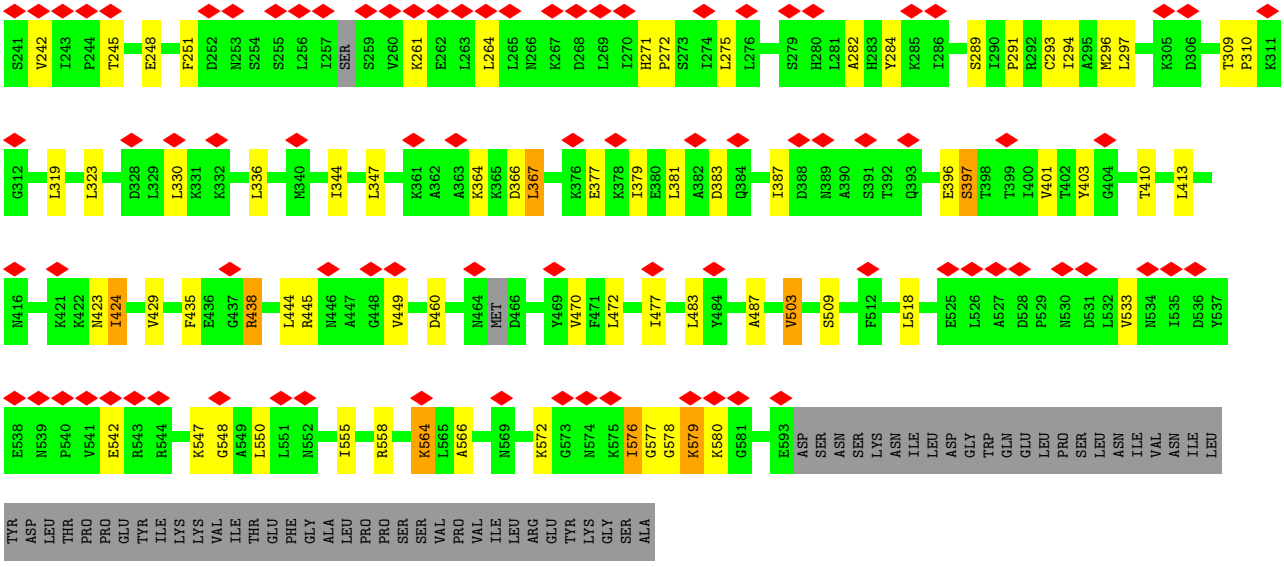


• Molecule 4: Translation initiation factor eIF-2B subunit delta

Chain H:

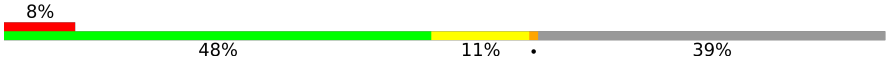


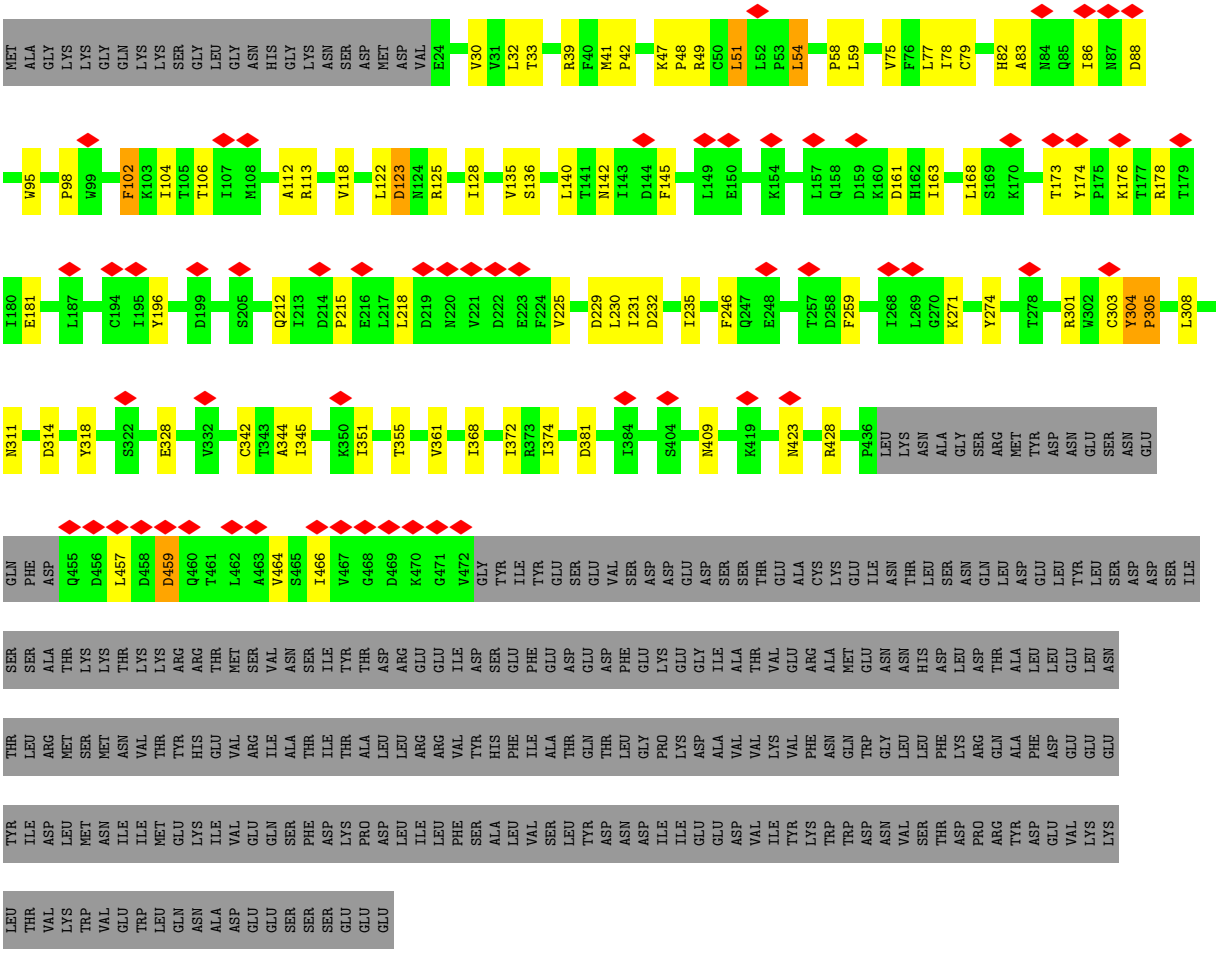




• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

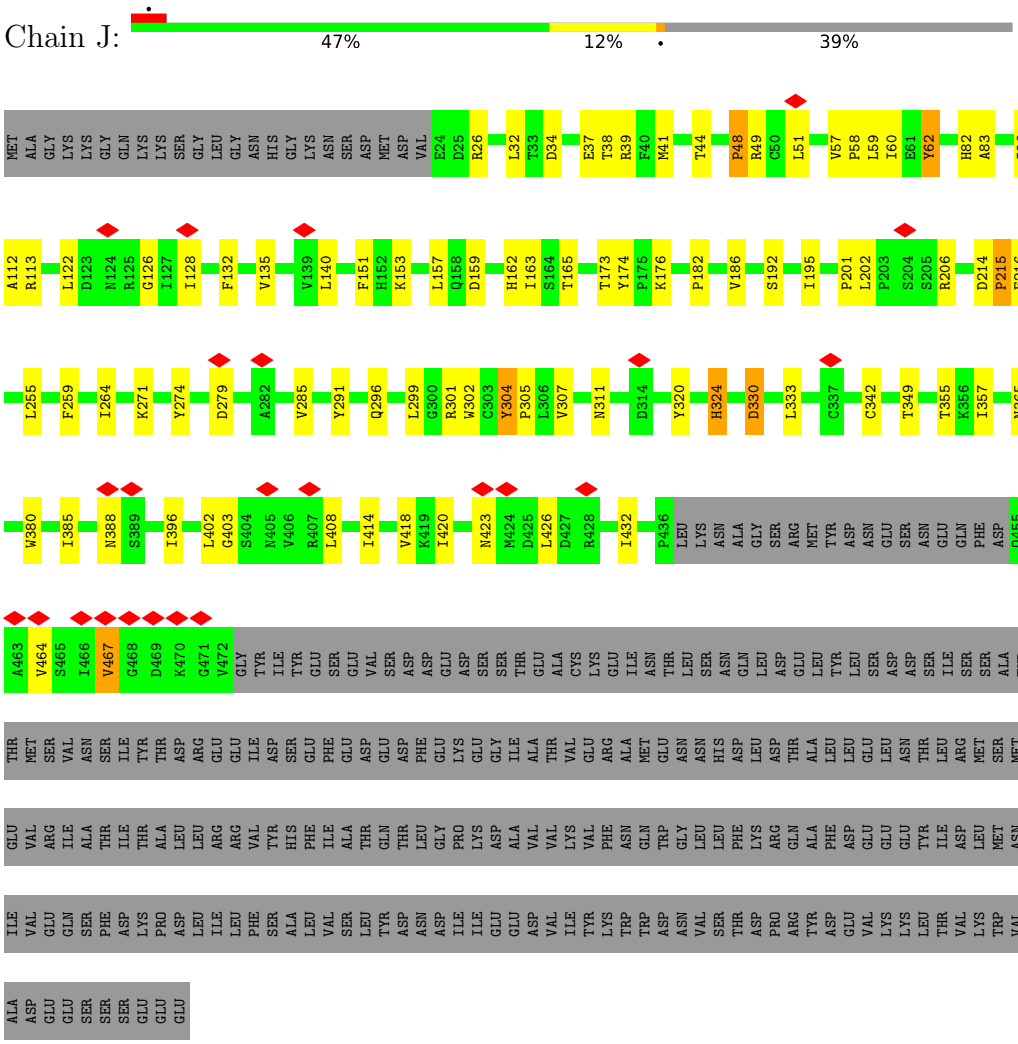
Chain I:





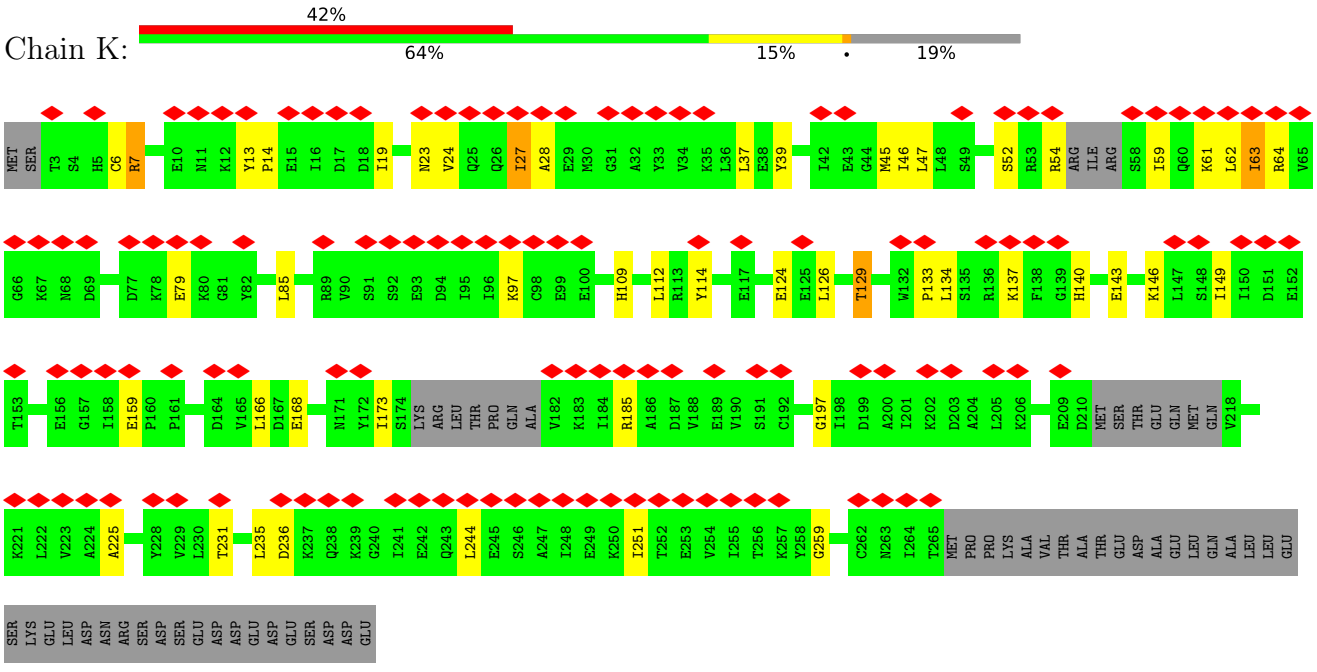
• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

Chain J:



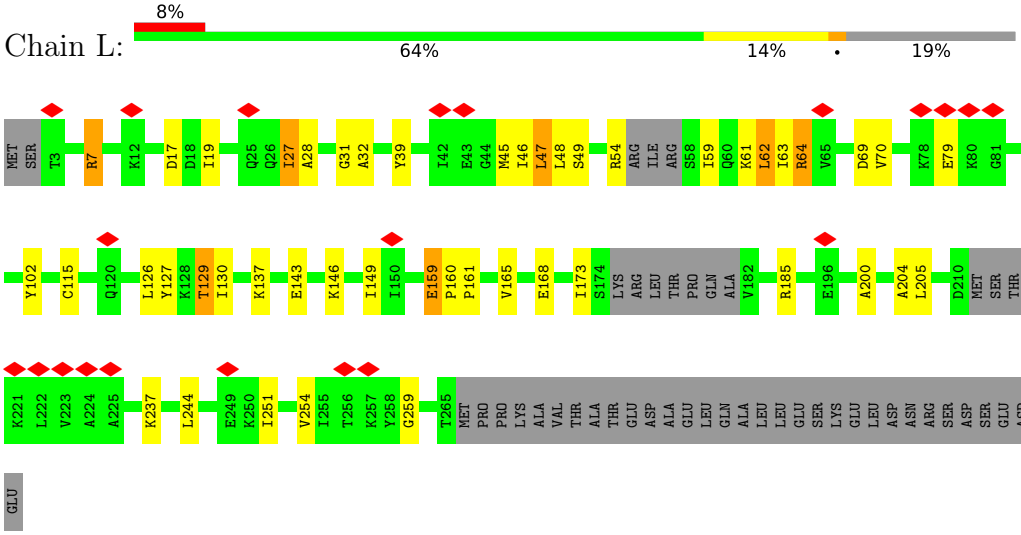
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain K:



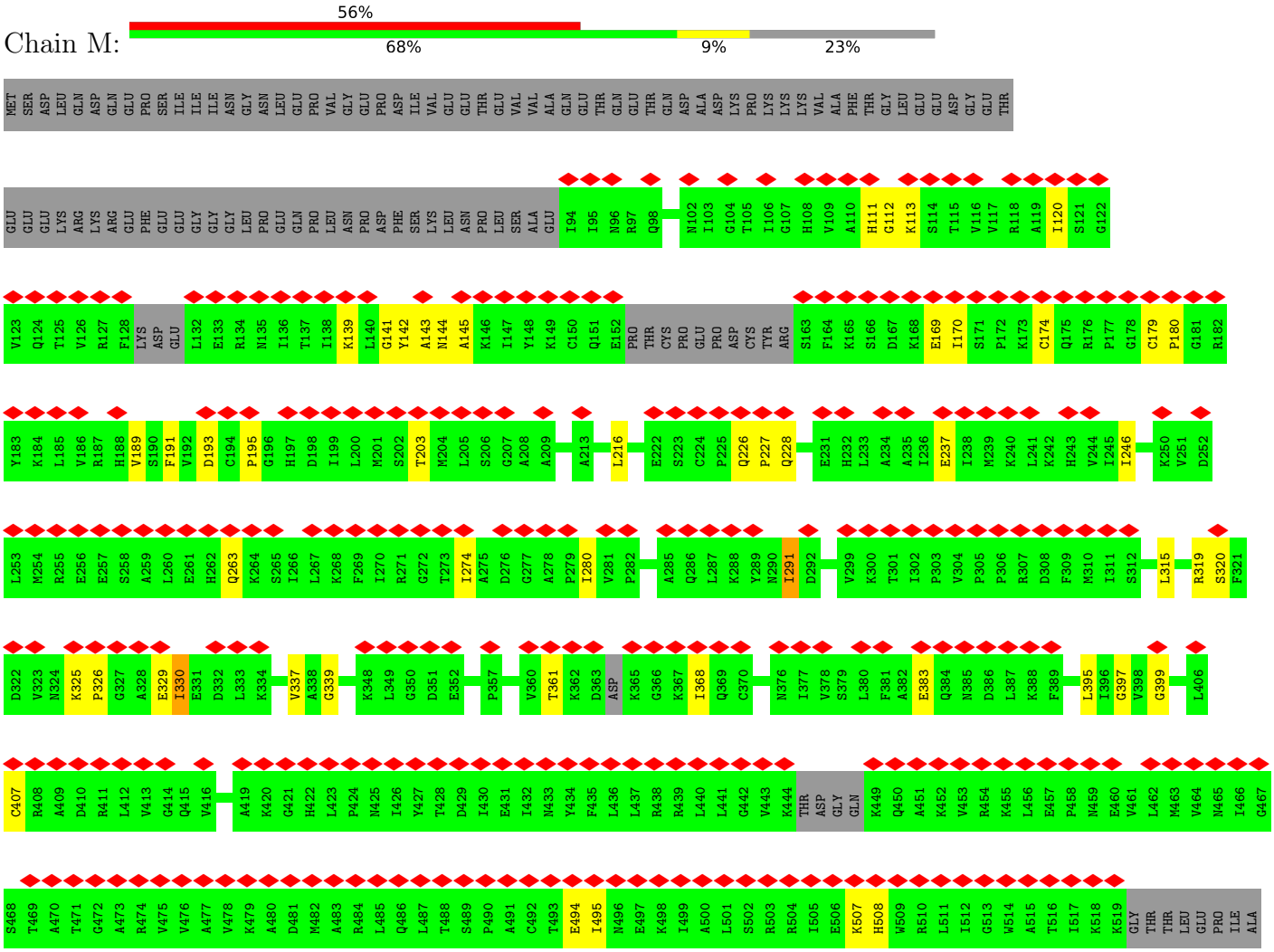
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain L:

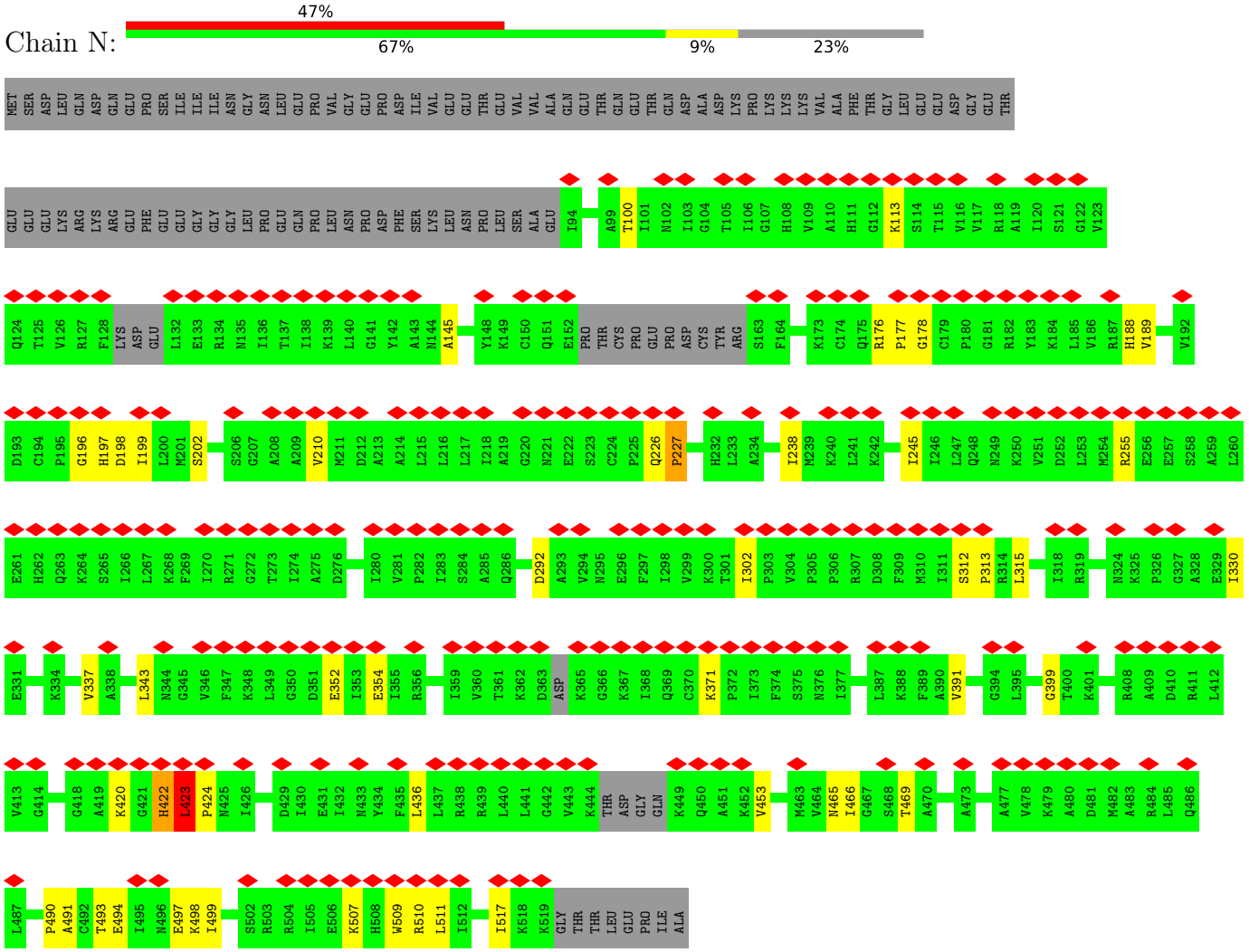


• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

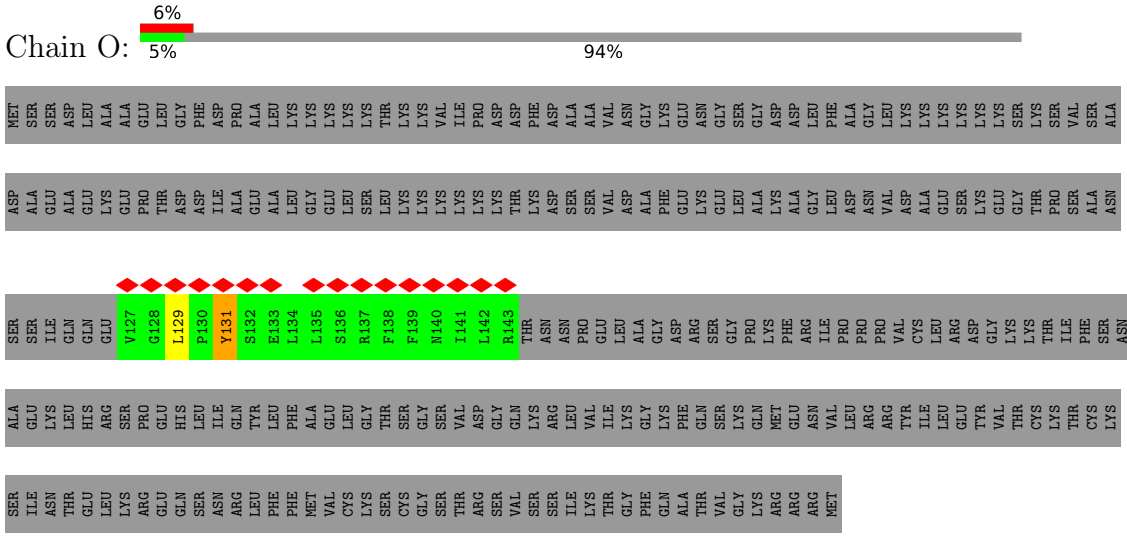
Chain M:



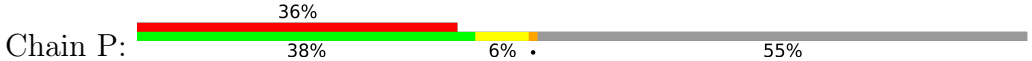
• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

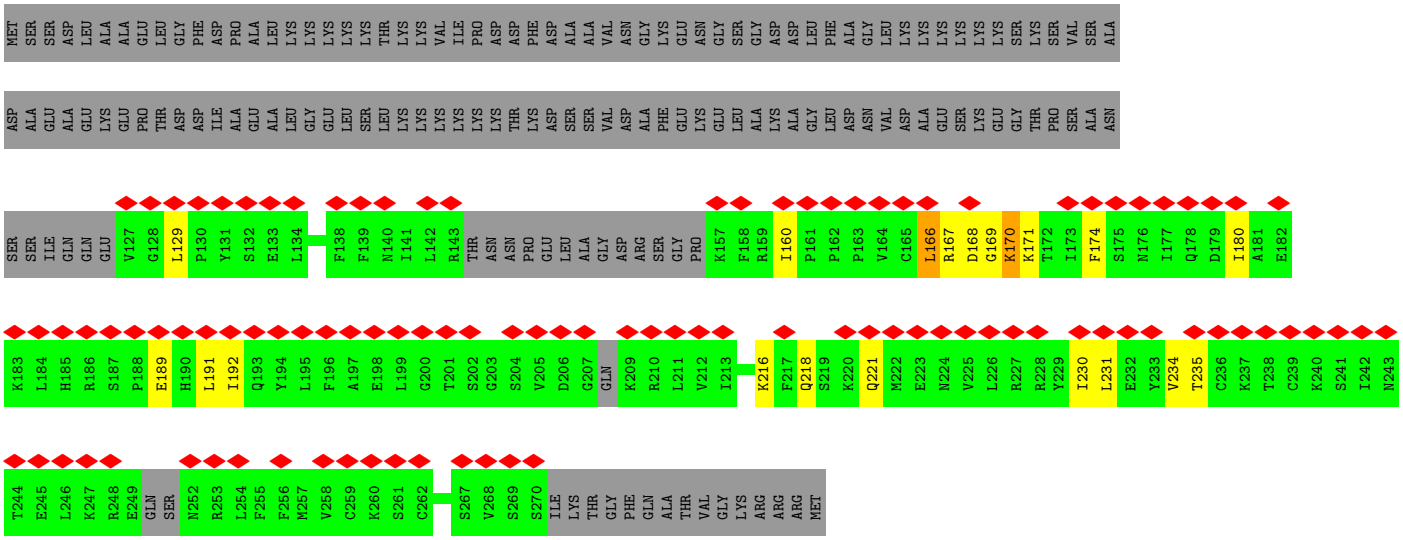


• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta



• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta




MET SER SER ASP LEU ALA ALA GLU LEU GLY PHE ASP PRO ALA LEU LYS LYS LYS LYS LYS LYS THR LYS LYS VAL ILE PRO ASP ASP PHE ASP ALA ALA VAL ASN GLY LYS GLU ASN GLY SER GLY ASP ASP LEU PHE ALA GLY LEU LYS LYS LYS LYS LYS LYS SER LYS SER VAL SER ALA
ASP ALA GLU ALA GLU LYS GLU PRO THR ASP ASP ILE ALA GLU ALA GLU LEU GLY GLU GLU LEU SER LEU LYS LYS LYS LYS LYS LYS THR LYS ASP SER SER VAL ASP ALA PHE GLU LYS GLU LEU ALA LYS ALA GLY LEU ASP ASN VAL ASP ALA GLU SER LYS GLU GLY THR PRO SER ALA ASN
SER SER ILE GLN GLN GLU V127 G128 L129 P130 Y131 S132 E133 L134 F138 F139 N140 I141 L142 R143 THR ASN ASN PRO GLU LEU ALA GLY ASP ARG SER GLY PRO K157 F158 R159 I160 P161 P162 P163 V164 C165 L166 R167 D168 G169 K170 K171 T172 I173 F174 S175 N176 I177 Q178 D179 I180 A181 E182
K183 L184 H185 R186 S187 P188 E189 H190 L191 I192 Q193 Y194 L195 F196 A197 E198 L199 G200 T201 S202 G203 S204 V205 D206 G207 GLN K209 R210 L211 V212 I213 K216 F217 Q218 S219 K220 Q221 M222 E223 N224 V225 L226 R227 R228 Y229 I230 L231 E232 Y233 V234 T235 C236 K237 T238 C239 K240 S241 I242 N243
T244 E245 L246 K247 R248 E249 GLN SER N252 R253 L254 F255 F256 M257 V258 C259 K260 S261 C262 S267 V268 S269 S270 ILE LYS THR GLY PHE GLN ALA THR VAL GLY LYS ARG ARG ARG MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	119037	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	0.256	Depositor
Minimum map value	-0.118	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.045	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	0.40	0/2395	0.65	0/3251
1	B	0.41	0/2395	0.66	0/3251
2	C	0.40	0/2714	0.66	0/3693
2	D	0.40	0/2714	0.65	0/3693
3	E	0.44	0/2209	0.62	1/2989 (0.0%)
3	F	0.45	0/3022	0.63	1/4084 (0.0%)
4	G	0.39	0/2781	0.65	0/3747
4	H	0.39	0/2781	0.64	0/3747
5	I	0.41	0/3468	0.64	0/4704
5	J	0.42	0/3468	0.63	0/4704
6	K	0.42	0/1982	0.65	0/2667
6	L	0.42	0/1982	0.66	0/2667
7	M	0.40	0/3087	0.59	0/4173
7	N	0.40	0/3087	0.58	0/4173
8	O	0.48	0/146	0.69	0/196
8	P	0.42	0/1051	0.63	1/1402 (0.1%)
All	All	0.41	0/39282	0.63	3/53141 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	166	LEU	CA-CB-CG	6.31	129.81	115.30
3	F	135	LEU	CA-CB-CG	5.61	128.20	115.30
3	E	135	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

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	53	0
1	B	2351	0	2367	56	0
2	C	2665	0	2626	26	0
2	D	2665	0	2626	20	0
3	E	2164	0	2154	11	0
3	F	2967	0	2974	10	0
4	G	2744	0	2819	15	0
4	H	2744	0	2819	29	0
5	I	3406	0	3359	33	0
5	J	3406	0	3359	33	0
6	K	1967	0	2005	12	0
6	L	1967	0	2006	17	0
7	M	3044	0	3126	31	0
7	N	3044	0	3126	20	0
8	O	143	0	148	0	0
8	P	1036	0	1080	6	0
All	All	38664	0	38961	351	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (351) 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:A:22:MET:CB	1:A:23:PRO:HD3	1.52	1.39
1:A:22:MET:HB3	1:A:23:PRO:CD	1.39	1.36
1:B:17:ASP:OD2	1:B:133:ARG:NH1	1.70	1.23
1:A:22:MET:CG	1:A:235:LYS:HE3	1.68	1.22
7:M:144:ASN:ND2	7:M:383:GLU:OE1	1.78	1.17
1:A:21:THR:HG21	1:A:232:GLU:HG2	1.36	1.07
1:B:120:ILE:HB	1:B:147:ILE:HD12	1.39	1.05
1:A:22:MET:HG3	1:A:235:LYS:HE3	1.01	1.00
1:A:22:MET:CB	1:A:23:PRO:CD	2.16	0.99
7:M:142:TYR:CE2	7:M:395:LEU:HB3	1.97	0.99
7:M:169:GLU:HB3	7:M:174:CYS:SG	2.09	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:MET:HG3	1:A:235:LYS:CE	1.98	0.91
1:A:22:MET:CG	1:A:235:LYS:CE	2.50	0.90
1:A:17:ASP:O	1:A:19:GLU:N	2.07	0.87
1:B:17:ASP:OD2	1:B:133:ARG:CZ	2.24	0.86
1:B:21:THR:HG22	1:B:23:PRO:HD2	1.64	0.80
7:M:142:TYR:CE2	7:M:395:LEU:CB	2.66	0.79
1:B:172:LYS:HA	1:B:172:LYS:CE	2.12	0.78
1:A:22:MET:SD	1:A:65:SER:OG	2.42	0.77
1:A:112:ILE:HG22	1:A:138:LEU:HD21	1.64	0.77
1:A:21:THR:HG21	1:A:232:GLU:CG	2.12	0.76
1:B:143:ALA:HA	1:B:149:PHE:CZ	2.21	0.76
1:A:22:MET:HG2	1:A:235:LYS:HE3	1.70	0.72
1:B:143:ALA:HA	1:B:149:PHE:HZ	1.55	0.72
1:A:17:ASP:C	1:A:19:GLU:H	1.92	0.72
1:B:22:MET:HB3	1:B:23:PRO:HD3	1.71	0.72
1:A:22:MET:HG2	1:A:235:LYS:CE	2.20	0.71
1:B:172:LYS:HA	1:B:172:LYS:NZ	2.06	0.70
7:M:141:GLY:O	7:M:193:ASP:N	2.21	0.68
1:B:120:ILE:HD13	1:B:147:ILE:CD1	2.25	0.67
5:J:414:ILE:HG12	5:J:432:ILE:HD12	1.76	0.67
1:B:21:THR:HB	1:B:24:ILE:HD13	1.78	0.66
3:E:160:LEU:H	3:E:161:PRO:HD2	1.61	0.65
1:B:126:ILE:HD12	1:B:149:PHE:HB2	1.78	0.65
1:B:126:ILE:CD1	1:B:149:PHE:HB2	2.26	0.64
1:B:23:PRO:HG2	1:B:235:LYS:HZ3	1.62	0.64
2:C:262:THR:HA	2:C:273:SER:HA	1.78	0.64
4:H:383:ASP:O	4:H:387:ILE:HG12	1.98	0.63
1:A:24:ILE:HG13	1:A:102:VAL:HA	1.81	0.63
6:L:200:ALA:HB1	6:L:254:VAL:HG13	1.81	0.61
1:A:145:LYS:O	1:A:146:PHE:HB2	1.98	0.61
6:K:149:ILE:HG21	6:K:173:ILE:HG21	1.81	0.61
4:H:435:PHE:HB3	4:H:438:ARG:HD2	1.82	0.61
7:M:143:ALA:O	7:M:191:PHE:N	2.28	0.61
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.00	0.61
7:M:141:GLY:HA3	7:M:193:ASP:HB3	1.83	0.61
2:D:183:HIS:H	2:D:210:THR:HB	1.66	0.61
5:J:324:HIS:HB3	5:J:342:CYS:H	1.66	0.60
5:J:414:ILE:HA	5:J:432:ILE:HB	1.83	0.60
1:B:72:ILE:HD11	1:B:236:PHE:H	1.67	0.60
7:M:142:TYR:CD2	7:M:395:LEU:HB3	2.37	0.60
1:A:209:ASN:HB3	1:A:213:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:HG21	1:B:234:HIS:CE1	2.38	0.59
5:I:79:CYS:HB2	5:I:86:ILE:HD13	1.85	0.59
1:B:135:VAL:HG22	1:B:230:VAL:HB	1.83	0.59
7:M:141:GLY:N	7:M:193:ASP:O	2.27	0.59
2:D:37:SER:HB3	2:D:263:LYS:HE3	1.85	0.59
4:H:487:ALA:HA	4:H:564:LYS:HE3	1.85	0.59
1:A:22:MET:CB	1:A:23:PRO:HD2	2.29	0.59
7:M:120:ILE:O	7:M:170:ILE:HD13	2.03	0.58
8:P:167:ARG:HG3	8:P:218:GLN:HA	1.85	0.58
1:A:120:ILE:HG12	1:A:126:ILE:HG12	1.84	0.58
6:L:70:VAL:HG21	6:L:95:ILE:HG23	1.86	0.58
1:B:23:PRO:CG	1:B:235:LYS:HZ3	2.15	0.58
6:L:146:LYS:O	6:L:149:ILE:HG13	2.04	0.58
5:I:304:TYR:HB3	5:I:305:PRO:HD3	1.87	0.57
1:A:24:ILE:CG1	1:A:102:VAL:HA	2.35	0.56
7:M:237:GLU:HB3	7:M:274:ILE:HD12	1.87	0.56
4:H:403:TYR:HD1	4:H:429:VAL:HB	1.72	0.55
5:I:178:ARG:HH22	5:I:229:ASP:HA	1.71	0.55
1:A:24:ILE:CG2	1:A:25:ALA:N	2.68	0.55
5:J:385:ILE:HG12	5:J:402:LEU:HD12	1.88	0.55
4:H:424:ILE:HD13	4:H:449:VAL:HG13	1.89	0.55
5:J:349:THR:HA	5:J:366:CYS:H	1.71	0.55
2:C:219:PHE:HA	2:C:223:THR:HG23	1.88	0.55
2:C:29:LEU:HD13	2:C:78:HIS:HB2	1.89	0.55
3:E:294:SER:HA	3:E:299:ALA:HB3	1.88	0.54
1:A:257:THR:H	1:B:177:THR:HB	1.73	0.54
5:J:195:ILE:HG12	5:J:264:ILE:HG21	1.89	0.54
7:M:142:TYR:HB3	7:M:319:ARG:NH2	2.22	0.54
5:I:77:LEU:HB2	5:I:106:THR:HG22	1.90	0.53
1:A:22:MET:HB3	1:A:23:PRO:HD3	0.59	0.53
4:H:364:LYS:HA	4:H:367:LEU:HB2	1.89	0.53
1:A:142:ALA:C	1:A:149:PHE:HE2	2.12	0.53
8:P:189:GLU:HA	8:P:192:ILE:HD12	1.91	0.53
2:C:98:GLU:HG3	2:C:153:VAL:HG11	1.91	0.53
1:B:64:VAL:HA	1:B:67:ARG:HD2	1.91	0.53
7:N:113:LYS:HE3	7:N:196:GLY:H	1.74	0.53
4:G:377:GLU:HA	4:G:381:LEU:HD12	1.91	0.52
1:B:240:PHE:HZ	4:H:572:LYS:HB3	1.73	0.52
5:I:32:LEU:HB2	5:I:136:SER:HA	1.92	0.52
3:E:157:LYS:HG2	3:E:288:LEU:HB3	1.91	0.52
1:A:178:LEU:HD22	1:B:267:LEU:HA	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:GLY:HA2	5:J:301:ARG:HB3	1.91	0.52
1:B:120:ILE:HD13	1:B:147:ILE:HD11	1.91	0.52
7:N:423:LEU:N	7:N:424:PRO:HD2	2.25	0.52
1:B:301:LYS:HB3	2:C:120:SER:HA	1.91	0.52
5:J:403:GLY:H	5:J:420:ILE:HG22	1.75	0.52
7:N:199:ILE:HG12	7:N:509:TRP:HB2	1.92	0.51
1:B:24:ILE:N	1:B:24:ILE:CD1	2.74	0.51
2:D:67:ILE:HA	2:D:70:LEU:HD12	1.92	0.51
2:C:26:VAL:HA	2:C:29:LEU:HD12	1.93	0.51
7:M:337:VAL:HA	7:M:399:GLY:HA2	1.93	0.51
3:F:238:LEU:HD13	3:F:390:THR:HG23	1.93	0.51
5:J:128:ILE:HG21	5:J:132:PHE:HB3	1.93	0.51
1:B:129:HIS:HD2	1:B:196:VAL:HG13	1.77	0.50
2:D:198:LYS:O	2:D:201:ILE:HG22	2.11	0.50
5:J:83:ALA:HA	5:J:86:ILE:HD12	1.94	0.50
4:G:272:PRO:HA	4:G:275:LEU:HD12	1.93	0.50
4:H:261:LYS:HE2	4:H:282:ALA:HB1	1.94	0.50
5:I:142:ASN:HD22	5:I:304:TYR:HB2	1.77	0.50
7:M:120:ILE:O	7:M:170:ILE:HG21	2.12	0.50
7:M:143:ALA:O	7:M:191:PHE:HB2	2.11	0.50
3:E:177:ASP:HB3	3:E:394:ARG:HH11	1.74	0.50
4:G:483:LEU:HB3	4:G:566:ALA:HB3	1.94	0.50
7:M:339:GLY:HA2	7:M:397:GLY:HA2	1.93	0.49
1:A:239:MET:HG2	1:A:248:PRO:HG2	1.94	0.49
7:M:113:LYS:HE3	7:M:195:PRO:HA	1.94	0.49
1:B:252:PRO:HB2	1:B:255:ASP:HB2	1.94	0.49
2:D:19:ASN:HD22	2:D:22:ILE:HD11	1.77	0.49
7:M:320:SER:HB2	7:M:407:CYS:HB3	1.93	0.49
1:A:291:THR:H	1:A:292:PRO:HD3	1.77	0.49
6:K:146:LYS:O	6:K:149:ILE:HG13	2.13	0.49
6:K:133:PRO:HG2	6:K:134:LEU:HD12	1.93	0.49
7:N:422:HIS:HB3	7:N:424:PRO:HD2	1.94	0.49
1:A:143:ALA:HB2	1:A:149:PHE:HZ	1.77	0.49
2:D:68:ARG:HH21	2:D:376:LEU:HB3	1.77	0.49
3:F:4:GLN:HG3	3:F:167:PHE:HB3	1.95	0.49
1:B:120:ILE:CB	1:B:147:ILE:HD12	2.27	0.49
1:B:189:ASP:HA	1:B:225:LYS:HE3	1.94	0.49
7:N:245:ILE:HD11	7:N:302:ILE:HD11	1.95	0.49
4:G:390:ALA:HB1	4:G:412:LEU:HD13	1.95	0.48
5:I:75:VAL:HG23	5:I:102:PHE:HB2	1.95	0.48
7:N:469:THR:HG21	7:N:491:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:330:LEU:HB3	4:H:336:LEU:HD21	1.95	0.48
5:J:418:VAL:HG22	5:J:461:THR:HG22	1.95	0.48
5:I:33:THR:HA	5:I:49:ARG:HH21	1.79	0.48
5:J:163:ILE:HD11	5:J:271:LYS:HB3	1.96	0.48
1:B:120:ILE:HD13	1:B:147:ILE:HD12	1.95	0.48
4:H:397:SER:HB2	4:H:423:ASN:HB2	1.94	0.48
1:A:68:ALA:HB2	1:A:237:VAL:HA	1.94	0.48
3:F:160:LEU:H	3:F:161:PRO:HD2	1.79	0.48
1:A:145:LYS:HB3	1:A:147:ILE:HG13	1.96	0.48
2:C:42:LEU:HA	2:C:45:LEU:HD12	1.96	0.48
1:A:17:ASP:OD1	1:A:20:MET:HB2	2.13	0.48
4:H:319:LEU:O	4:H:323:LEU:HG	2.13	0.48
5:I:123:ASP:HA	5:I:128:ILE:HD11	1.96	0.48
5:J:159:ASP:HB3	5:J:162:HIS:CD2	2.49	0.48
4:G:507:CYS:HB3	4:G:576:ILE:HG12	1.94	0.47
4:H:550:LEU:HG	4:H:558:ARG:HH11	1.79	0.47
6:L:27:ILE:HG13	6:L:28:ALA:H	1.79	0.47
7:N:499:ILE:HD11	7:N:517:ILE:HB	1.96	0.47
1:B:292:PRO:HB3	2:C:359:SER:HA	1.95	0.47
4:G:381:LEU:HD13	6:L:62:LEU:HA	1.97	0.47
4:H:509:SER:HB3	4:H:577:GLY:H	1.79	0.47
5:I:163:ILE:HD11	5:I:271:LYS:HB3	1.96	0.47
5:J:357:ILE:HA	5:J:374:ILE:HB	1.96	0.47
1:B:257:THR:HG21	1:B:266:ALA:HA	1.95	0.47
5:I:351:ILE:HG12	5:I:368:ILE:HD12	1.96	0.47
1:A:17:ASP:C	1:A:19:GLU:N	2.58	0.47
1:B:23:PRO:HG2	1:B:234:HIS:NE2	2.29	0.47
1:B:23:PRO:CG	1:B:235:LYS:NZ	2.77	0.47
6:L:27:ILE:HG22	6:L:64:ARG:HH11	1.79	0.47
1:B:143:ALA:CA	1:B:149:PHE:HZ	2.23	0.47
2:C:350:ILE:HA	2:C:355:GLY:HA2	1.97	0.47
4:H:291:PRO:HA	4:H:294:ILE:HD12	1.97	0.47
4:H:579:LYS:HG2	4:H:580:LYS:HG3	1.97	0.47
7:N:226:GLN:HA	7:N:227:PRO:HD3	1.78	0.47
1:A:146:PHE:O	1:A:148:ARG:N	2.48	0.46
1:A:291:THR:H	1:A:292:PRO:CD	2.28	0.46
3:E:267:THR:HG23	5:J:226:ILE:H	1.80	0.46
2:C:255:VAL:HG12	2:C:290:THR:HG21	1.97	0.46
5:I:168:LEU:HB3	5:I:230:LEU:HD22	1.97	0.46
7:N:100:THR:HG22	7:N:391:VAL:HG11	1.97	0.46
7:N:466:ILE:HG12	7:N:499:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:CD1	1:B:147:ILE:HD12	2.45	0.46
5:I:161:ASP:HB3	5:I:271:LYS:HA	1.97	0.46
6:K:46:ILE:HG13	6:K:85:LEU:HB2	1.97	0.46
6:L:149:ILE:HG21	6:L:173:ILE:HD12	1.97	0.46
2:D:275:ASN:HA	2:D:338:THR:HA	1.96	0.46
1:A:22:MET:HB2	1:A:23:PRO:CD	2.34	0.46
2:D:187:LEU:HB2	2:D:255:VAL:HG11	1.97	0.46
2:D:217:GLU:HB3	2:D:223:THR:HG22	1.97	0.46
1:A:24:ILE:HG22	1:A:25:ALA:N	2.31	0.46
1:B:120:ILE:HG21	1:B:147:ILE:HB	1.97	0.46
1:A:19:GLU:HG3	1:A:106:LYS:HE2	1.98	0.46
1:B:189:ASP:HB3	4:G:500:ASN:HD22	1.81	0.46
2:D:230:ALA:HA	2:D:233:LEU:HD12	1.97	0.46
5:I:142:ASN:HB3	5:I:303:CYS:HB3	1.98	0.46
1:B:153:VAL:HB	1:B:178:LEU:HD12	1.97	0.46
6:L:7:ARG:HD3	6:L:7:ARG:H	1.80	0.46
5:I:48:PRO:HG2	5:I:51:LEU:HB2	1.98	0.45
7:N:436:LEU:HD22	7:N:453:VAL:HG11	1.98	0.45
2:C:244:PRO:HG3	4:G:560:PHE:HB2	1.98	0.45
5:J:255:LEU:HA	5:J:259:PHE:HB3	1.98	0.45
2:C:230:ALA:HA	2:C:233:LEU:HD12	1.97	0.45
2:D:244:PRO:HG2	2:D:247:ALA:HB3	1.97	0.45
3:F:101:ILE:HG23	3:F:102:GLU:HG3	1.97	0.45
4:G:350:GLU:HA	4:G:353:LEU:HD12	1.99	0.45
2:D:28:LYS:HG2	2:D:33:GLN:HB3	1.99	0.45
5:J:135:VAL:HG22	5:J:235:ILE:HG23	1.99	0.45
6:L:47:LEU:HD13	6:L:49:SER:HB2	1.99	0.45
7:N:238:ILE:HG21	7:N:498:LYS:HE3	1.98	0.45
2:C:260:ILE:HG23	2:C:278:VAL:HG11	1.98	0.45
5:I:212:GLN:HG3	8:P:167:ARG:HB3	1.98	0.45
5:J:34:ASP:HA	5:J:49:ARG:HE	1.81	0.45
6:L:31:GLY:HA2	6:L:48:LEU:HG	1.99	0.45
3:F:267:THR:HG23	5:I:225:VAL:HG22	1.99	0.45
4:H:377:GLU:HB3	6:K:61:LYS:HG2	1.98	0.45
7:M:226:GLN:HA	7:M:227:PRO:HD3	1.82	0.45
7:N:337:VAL:HA	7:N:399:GLY:HA2	1.98	0.45
5:I:409:ASN:HB3	5:I:428:ARG:HG3	1.99	0.45
6:L:204:ALA:HB2	6:L:254:VAL:HG21	1.99	0.45
1:B:32:THR:HA	1:B:35:ARG:HG2	1.99	0.44
2:D:48:LEU:HD13	2:D:91:ILE:HD13	1.99	0.44
1:B:120:ILE:CG2	1:B:147:ILE:HB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:576:ILE:HG12	4:H:578:GLY:H	1.81	0.44
1:B:126:ILE:HD11	1:B:149:PHE:HB2	1.99	0.44
5:I:78:ILE:HG21	5:I:118:VAL:HG13	1.99	0.44
7:M:361:THR:HG22	7:M:368:ILE:HG22	1.99	0.44
1:A:136:PHE:HZ	1:A:169:LEU:HG	1.82	0.44
1:A:151:CYS:HB2	1:A:176:VAL:HG12	1.98	0.44
4:H:472:LEU:HG	4:H:503:VAL:HG11	1.99	0.44
2:C:279:SER:O	2:C:283:GLU:HG2	2.18	0.44
2:C:303:PRO:HB2	2:C:374:VAL:HG22	2.00	0.44
5:J:432:ILE:HA	5:J:459:ASP:HB2	1.99	0.44
2:C:264:ALA:HB3	2:C:272:ILE:HB	2.00	0.44
7:M:291:ILE:H	7:M:291:ILE:HG13	1.70	0.44
1:A:112:ILE:HD11	1:A:286:ASP:HB3	2.00	0.44
1:B:195:PHE:HA	1:B:228:TYR:HB2	2.00	0.44
4:H:294:ILE:HG12	4:H:379:ILE:HD13	2.00	0.44
5:I:215:PRO:HA	5:I:218:LEU:HB2	2.00	0.44
8:P:169:GLY:HA2	8:P:216:LYS:HG3	2.00	0.44
2:C:196:VAL:HG21	2:C:261:GLY:HA2	2.00	0.43
4:G:284:TYR:HD1	4:G:286:ILE:H	1.66	0.43
1:B:283:LEU:HB3	1:B:291:THR:HA	2.00	0.43
1:A:64:VAL:HG12	1:A:237:VAL:HG11	2.01	0.43
3:E:71:ILE:HG21	3:E:404:ALA:HB1	2.00	0.43
7:M:179:CYS:HA	7:M:180:PRO:HD3	1.91	0.43
4:G:291:PRO:HA	4:G:294:ILE:HD12	1.99	0.43
2:C:152:GLN:HG2	2:C:156:GLN:HE21	1.83	0.43
4:H:271:HIS:HA	4:H:272:PRO:HD3	1.86	0.43
1:B:27:ILE:HA	1:B:30:LEU:HD12	1.99	0.43
1:B:22:MET:CB	1:B:23:PRO:HD3	2.42	0.43
4:H:401:VAL:HB	4:H:470:VAL:HG13	2.00	0.43
1:B:290:LEU:HB3	2:C:366:TRP:HH2	1.83	0.43
5:J:48:PRO:HB3	5:J:82:HIS:HB2	2.00	0.43
1:A:56:LEU:HD11	1:A:66:LEU:HD22	2.00	0.43
1:A:152:VAL:HG13	1:A:179:ILE:HD13	2.01	0.43
3:E:259:LEU:HD13	3:E:306:THR:HG22	2.01	0.43
4:G:427:ILE:HG12	4:G:452:MET:HB2	2.00	0.43
5:I:30:VAL:HG11	5:I:122:LEU:HD11	2.01	0.43
5:I:47:LYS:HD3	5:I:51:LEU:HD22	2.00	0.43
6:K:126:LEU:O	6:K:129:THR:HG22	2.18	0.43
6:L:159:GLU:HA	6:L:160:PRO:HD3	1.91	0.43
1:A:109:ARG:HH22	1:A:133:ARG:HB3	1.83	0.43
1:A:226:PRO:HB3	1:A:281:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:54:LEU:HD13	5:I:59:LEU:HD13	2.00	0.43
5:J:59:LEU:HA	5:J:62:TYR:CE2	2.53	0.43
5:J:396:ILE:HG13	5:J:414:ILE:HD12	2.01	0.43
1:A:154:THR:HA	1:A:179:ILE:HB	2.00	0.42
1:A:230:VAL:HG22	1:A:284:ILE:HD12	1.99	0.42
3:F:171:PRO:HD2	3:F:174:PHE:HE2	1.84	0.42
5:I:355:THR:HG22	5:I:372:ILE:H	1.84	0.42
1:B:109:ARG:HH22	1:B:133:ARG:HB3	1.83	0.42
1:B:230:VAL:HG22	1:B:284:ILE:HD12	2.01	0.42
4:H:533:VAL:HA	4:H:547:LYS:HD3	2.00	0.42
3:F:223:PHE:HB3	3:F:272:LEU:HD12	2.01	0.42
5:I:135:VAL:HG22	5:I:235:ILE:HG23	2.01	0.42
5:J:37:GLU:C	5:J:39:ARG:H	2.22	0.42
1:A:149:PHE:HE1	1:A:174:ILE:HD13	1.85	0.42
2:D:222:ASN:HA	2:D:225:ASN:HD22	1.85	0.42
2:D:242:VAL:HB	4:H:558:ARG:HA	2.00	0.42
2:D:318:SER:HA	2:D:321:ILE:HD12	2.01	0.42
1:A:196:VAL:HG12	1:A:229:VAL:HG13	2.01	0.42
2:D:89:ARG:HA	2:D:92:LEU:HD12	2.02	0.42
5:I:168:LEU:HD22	5:I:230:LEU:HB3	2.00	0.42
7:M:169:GLU:OE1	7:M:169:GLU:HA	2.19	0.42
5:J:296:GLN:HA	5:J:299:LEU:HD12	2.02	0.42
6:L:205:LEU:HG	7:N:330:ILE:HG21	2.02	0.42
7:N:198:ASP:HB2	7:N:511:LEU:HB2	2.00	0.42
1:B:188:ILE:HD12	4:G:500:ASN:HB3	2.02	0.42
4:H:444:LEU:HB3	4:H:449:VAL:HB	2.01	0.42
7:N:493:THR:HG21	7:N:517:ILE:HD13	2.01	0.42
1:A:143:ALA:N	1:A:149:PHE:HE2	2.18	0.42
4:H:309:THR:HA	4:H:310:PRO:HD3	1.90	0.42
5:I:196:TYR:CZ	5:I:212:GLN:HB3	2.55	0.42
1:B:22:MET:HB3	1:B:23:PRO:CD	2.46	0.42
1:B:251:GLY:HA2	1:B:252:PRO:HD3	1.90	0.42
3:E:241:VAL:HG21	3:E:266:LEU:HD22	2.02	0.42
5:J:408:LEU:HD23	5:J:426:LEU:HB2	2.01	0.42
6:K:13:TYR:HA	6:K:14:PRO:HD3	1.91	0.42
4:H:410:THR:HA	4:H:413:LEU:HD12	2.01	0.41
5:I:83:ALA:HA	5:I:86:ILE:HD12	2.02	0.41
5:J:285:VAL:HG11	5:J:291:TYR:HD1	1.85	0.41
6:K:185:ARG:HG3	6:K:231:THR:HG22	2.02	0.41
7:M:139:LYS:H	7:M:203:THR:HG21	1.85	0.41
7:N:312:SER:HA	7:N:313:PRO:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:472:LEU:HB2	4:G:505:VAL:HG22	2.01	0.41
7:M:325:LYS:HA	7:M:326:PRO:HD3	1.95	0.41
1:B:147:ILE:HB	1:B:148:ARG:H	1.59	0.41
3:F:255:ILE:HB	3:F:256:ARG:H	1.72	0.41
5:I:95:TRP:HD1	5:I:104:ILE:HD11	1.85	0.41
6:L:126:LEU:O	6:L:129:THR:HG22	2.20	0.41
1:B:22:MET:N	1:B:23:PRO:CD	2.82	0.41
2:C:21:THR:O	2:C:24:THR:HG22	2.21	0.41
3:F:152:GLY:HA2	3:F:155:LEU:HD12	2.01	0.41
4:H:272:PRO:HA	4:H:275:LEU:HD12	2.02	0.41
5:J:214:ASP:HA	5:J:215:PRO:HD3	1.86	0.41
2:C:155:ILE:HA	2:C:158:ILE:HD12	2.01	0.41
2:C:265:VAL:HB	2:C:301:LEU:HA	2.01	0.41
5:I:318:TYR:HA	5:I:328:GLU:HA	2.01	0.41
2:D:328:ARG:HG3	5:J:302:TRP:HE1	1.86	0.41
1:A:24:ILE:CD1	1:A:105:ALA:HB2	2.51	0.41
6:K:23:ASN:HB2	6:K:37:LEU:HD12	2.03	0.41
7:M:142:TYR:CE2	7:M:395:LEU:HB2	2.52	0.41
3:E:64:LEU:HA	3:E:65:PRO:HD3	1.86	0.41
7:M:145:ALA:HB3	7:M:189:VAL:HG23	2.02	0.41
7:N:145:ALA:HB3	7:N:189:VAL:HG23	2.02	0.41
2:C:301:LEU:HD21	2:C:365:ALA:HA	2.02	0.41
2:C:317:GLY:HA2	5:I:301:ARG:HB3	2.03	0.41
5:I:459:ASP:H	5:I:466:ILE:HD12	1.85	0.41
5:J:186:VAL:HG13	5:J:226:ILE:HG12	2.03	0.41
7:M:330:ILE:H	7:M:330:ILE:HG13	1.75	0.41
7:N:202:SER:HB3	7:N:465:ASN:HB3	2.02	0.41
7:N:210:VAL:HG22	7:N:343:LEU:HA	2.03	0.41
3:E:218:LYS:HB3	3:E:219:GLN:H	1.72	0.41
4:H:483:LEU:HB3	4:H:566:ALA:HB3	2.03	0.41
5:J:57:VAL:HA	5:J:58:PRO:HD3	1.95	0.41
8:P:160:ILE:HG12	8:P:230:ILE:HD13	2.03	0.41
1:B:126:ILE:HD11	1:B:149:PHE:CB	2.51	0.40
5:J:60:ILE:H	5:J:60:ILE:HG13	1.75	0.40
6:L:115:CYS:HB3	6:L:165:VAL:HG13	2.03	0.40
6:K:24:VAL:HG11	6:K:63:ILE:HG22	2.04	0.40
6:L:46:ILE:HG13	6:L:85:LEU:HB2	2.03	0.40
7:M:216:LEU:HD23	7:M:246:ILE:HG23	2.04	0.40
7:M:263:GLN:HE22	7:M:280:ILE:HB	1.87	0.40
2:D:181:HIS:HB3	2:D:182:ASP:H	1.66	0.40
3:F:252:TYR:HB2	8:P:218:GLN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:153:LYS:HE2	5:J:157:LEU:HD11	2.02	0.40
5:J:304:TYR:HB3	5:J:305:PRO:HD3	2.04	0.40
6:K:7:ARG:HD3	6:K:7:ARG:H	1.86	0.40
2:C:44:THR:HA	2:C:47:LEU:HD12	2.02	0.40
6:K:27:ILE:HG13	6:K:28:ALA:H	1.87	0.40
7:M:142:TYR:CD2	7:M:395:LEU:CB	3.01	0.40
1:B:292:PRO:HG3	2:C:268:ASN:HA	2.03	0.40
3:E:238:LEU:HD13	3:E:390:THR:HG23	2.03	0.40
4:G:257:ILE:HG22	4:G:259:SER:HB3	2.02	0.40
4:H:344:ILE:HA	4:H:347:LEU:HD12	2.03	0.40
5:I:344:ALA:HB3	5:I:361:VAL:HG13	2.03	0.40
6:L:27:ILE:HD12	6:L:32:ALA:HB2	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%)	246 (82%)	41 (14%)	13 (4%)	2	25
1	B	300/305 (98%)	249 (83%)	40 (13%)	11 (4%)	3	27
2	C	339/381 (89%)	287 (85%)	44 (13%)	8 (2%)	6	36
2	D	339/381 (89%)	296 (87%)	35 (10%)	8 (2%)	6	36
3	E	253/578 (44%)	205 (81%)	38 (15%)	10 (4%)	3	26
3	F	357/578 (62%)	285 (80%)	52 (15%)	20 (6%)	2	21
4	G	349/651 (54%)	286 (82%)	45 (13%)	18 (5%)	2	22
4	H	349/651 (54%)	294 (84%)	44 (13%)	11 (3%)	4	30
5	I	427/712 (60%)	357 (84%)	56 (13%)	14 (3%)	4	30
5	J	427/712 (60%)	358 (84%)	46 (11%)	23 (5%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	K	237/304 (78%)	196 (83%)	36 (15%)	5 (2%)	7 38
6	L	237/304 (78%)	200 (84%)	33 (14%)	4 (2%)	9 43
7	M	398/527 (76%)	333 (84%)	62 (16%)	3 (1%)	19 60
7	N	398/527 (76%)	332 (83%)	56 (14%)	10 (2%)	5 35
8	O	15/285 (5%)	11 (73%)	2 (13%)	2 (13%)	0 4
8	P	120/285 (42%)	103 (86%)	12 (10%)	5 (4%)	3 25
All	All	4845/7486 (65%)	4038 (83%)	642 (13%)	165 (3%)	6 29

All (165) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	147	ILE
1	B	61	PRO
1	B	147	ILE
1	B	158	PRO
2	D	220	PRO
3	E	100	GLU
3	F	65	PRO
3	F	100	GLU
3	F	180	PRO
4	G	356	PRO
4	G	487	ALA
5	I	314	ASP
5	J	202	LEU
5	J	464	VAL
1	A	18	THR
1	A	98	GLY
1	B	18	THR
1	B	98	GLY
1	B	304	TYR
2	C	166	LYS
2	C	275	ASN
2	C	276	SER
2	D	237	ASN
2	D	277	GLY
3	E	73	ASN
3	E	160	LEU
3	F	454	GLN
3	F	460	ARG

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Mol	Chain	Res	Type
3	F	470	PRO
4	G	265	LEU
4	G	537	TYR
4	G	579	LYS
4	G	586	SER
4	H	397	SER
5	I	173	THR
5	I	305	PRO
5	I	464	VAL
5	J	201	PRO
5	J	216	GLU
5	J	355	THR
5	J	371	ASN
6	L	259	GLY
7	M	507	LYS
7	N	178	GLY
7	N	507	LYS
1	A	5	ASN
1	A	16	GLU
1	A	61	PRO
1	A	148	ARG
1	A	291	THR
1	B	5	ASN
1	B	38	THR
1	B	234	HIS
1	B	263	LEU
1	B	291	THR
2	C	58	ASN
2	C	79	PRO
3	E	90	LYS
3	F	311	GLN
3	F	477	GLU
3	F	488	MET
4	G	240	SER
4	G	397	SER
4	G	542	GLU
4	H	579	LYS
5	I	42	PRO
5	I	54	LEU
5	I	58	PRO
5	I	98	PRO
5	I	112	ALA

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Mol	Chain	Res	Type
5	I	423	ASN
5	J	26	ARG
5	J	126	GLY
5	J	311	ASN
5	J	330	ASP
5	J	388	ASN
5	J	423	ASN
6	K	225	ALA
7	N	255	ARG
7	N	490	PRO
8	P	170	LYS
8	P	231	LEU
8	P	235	THR
1	A	158	PRO
2	C	116	PRO
2	D	276	SER
2	D	289	ARG
3	E	238	LEU
3	E	264	PRO
3	F	160	LEU
3	F	309	GLN
3	F	431	ASP
3	F	476	ASP
3	F	482	ASN
4	G	357	SER
4	G	486	ARG
4	H	248	GLU
4	H	251	PHE
4	H	542	GLU
5	I	82	HIS
5	I	311	ASN
5	I	342	CYS
5	I	459	ASP
5	J	182	PRO
5	J	192	SER
5	J	365	ASN
5	J	459	ASP
6	K	197	GLY
6	K	259	GLY
6	L	237	LYS
8	O	129	LEU
7	N	176	ARG

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Mol	Chain	Res	Type
7	N	494	GLU
7	N	497	GLU
8	P	129	LEU
1	A	38	THR
1	A	210	LEU
2	D	177	ILE
3	E	309	GLN
3	F	238	LEU
3	F	459	SER
4	G	242	VAL
4	G	289	SER
4	G	360	ASP
4	G	536	ASP
4	H	245	THR
4	H	289	SER
4	H	396	GLU
4	H	555	ILE
5	J	44	THR
5	J	467	VAL
6	K	6	CYS
7	M	112	GLY
7	M	329	GLU
8	O	131	TYR
7	N	177	PRO
7	N	227	PRO
1	A	192	ASP
3	E	245	ARG
3	F	255	ILE
3	F	471	GLY
3	F	494	LYS
4	G	359	PRO
4	G	548	GLY
5	J	38	THR
5	J	112	ALA
5	J	215	PRO
6	L	63	ILE
8	P	234	VAL
3	E	16	ALA
3	E	263	TYR
6	K	63	ILE
6	L	161	PRO
2	C	177	ILE

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Mol	Chain	Res	Type
2	D	116	PRO
4	H	548	GLY
5	J	48	PRO
2	D	191	PRO
5	J	304	TYR
2	C	337	ILE
4	G	555	ILE
4	H	242	VAL
7	N	423	LEU
3	F	97	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%)	233 (91%)	24 (9%)	9 30
1	B	257/265 (97%)	232 (90%)	25 (10%)	8 29
2	C	286/338 (85%)	257 (90%)	29 (10%)	7 27
2	D	286/338 (85%)	261 (91%)	25 (9%)	10 33
3	E	249/529 (47%)	235 (94%)	14 (6%)	21 48
3	F	338/529 (64%)	321 (95%)	17 (5%)	24 51
4	G	305/561 (54%)	288 (94%)	17 (6%)	21 48
4	H	305/561 (54%)	288 (94%)	17 (6%)	21 48
5	I	389/649 (60%)	365 (94%)	24 (6%)	18 45
5	J	389/649 (60%)	364 (94%)	25 (6%)	17 44
6	K	217/273 (80%)	190 (88%)	27 (12%)	4 21
6	L	217/273 (80%)	191 (88%)	26 (12%)	5 22
7	M	319/449 (71%)	311 (98%)	8 (2%)	47 68
7	N	319/449 (71%)	308 (97%)	11 (3%)	37 60
8	O	16/246 (6%)	15 (94%)	1 (6%)	18 44
8	P	119/246 (48%)	111 (93%)	8 (7%)	16 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4268/6620 (64%)	3970 (93%)	298 (7%)	19 41

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	21	THR
1	A	37	LYS
1	A	54	GLU
1	A	70	CYS
1	A	71	ASP
1	A	101	PHE
1	A	124	ASP
1	A	126	ILE
1	A	136	PHE
1	A	138	LEU
1	A	149	PHE
1	A	161	GLN
1	A	166	TYR
1	A	172	LYS
1	A	188	ILE
1	A	196	VAL
1	A	224	ARG
1	A	231	THR
1	A	232	GLU
1	A	236	PHE
1	A	242	LEU
1	A	280	ILE
1	A	290	LEU
1	B	21	THR
1	B	24	ILE
1	B	33	LEU
1	B	37	LYS
1	B	54	GLU
1	B	56	LEU
1	B	71	ASP
1	B	75	ARG
1	B	79	ARG
1	B	80	ASN
1	B	86	ASP
1	B	104	ARG
1	B	133	ARG

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Mol	Chain	Res	Type
1	B	147	ILE
1	B	148	ARG
1	B	153	VAL
1	B	172	LYS
1	B	179	ILE
1	B	192	ASP
1	B	231	THR
1	B	237	VAL
1	B	272	ILE
1	B	273	ASP
1	B	287	LEU
1	B	289	VAL
2	C	17	ASP
2	C	24	THR
2	C	40	ILE
2	C	57	TRP
2	C	92	LEU
2	C	151	ARG
2	C	153	VAL
2	C	168	ILE
2	C	175	ILE
2	C	180	ILE
2	C	190	THR
2	C	199	PHE
2	C	200	LEU
2	C	212	THR
2	C	222	ASN
2	C	223	THR
2	C	238	ILE
2	C	249	PHE
2	C	286	ARG
2	C	321	ILE
2	C	322	LEU
2	C	328	ARG
2	C	336	GLN
2	C	337	ILE
2	C	348	ILE
2	C	361	ILE
2	C	363	ARG
2	C	366	TRP
2	C	371	GLN
2	D	49	MET

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Mol	Chain	Res	Type
2	D	51	PHE
2	D	62	ASP
2	D	68	ARG
2	D	84	CYS
2	D	149	ASP
2	D	160	ASP
2	D	161	LEU
2	D	164	GLU
2	D	168	ILE
2	D	177	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	287	GLU
2	D	298	LEU
2	D	307	PHE
2	D	308	ASP
2	D	340	TYR
2	D	363	ARG
2	D	366	TRP
2	D	371	GLN
3	E	3	ILE
3	E	133	HIS
3	E	166	ASP
3	E	173	ASP
3	E	181	GLN
3	E	183	LEU
3	E	185	ASP
3	E	249	LYS
3	E	301	PHE
3	E	384	PHE
3	E	390	THR
3	E	398	LEU
3	E	402	MET
3	E	406	ARG
3	F	83	TRP
3	F	100	GLU
3	F	137	ASP
3	F	141	ILE

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Mol	Chain	Res	Type
3	F	166	ASP
3	F	173	ASP
3	F	181	GLN
3	F	192	ASP
3	F	222	PHE
3	F	257	SER
3	F	258	HIS
3	F	270	THR
3	F	303	ASP
3	F	384	PHE
3	F	423	ILE
3	F	509	GLU
3	F	519	LEU
4	G	284	TYR
4	G	296	MET
4	G	300	PHE
4	G	366	ASP
4	G	388	ASP
4	G	393	GLN
4	G	398	THR
4	G	412	LEU
4	G	416	ASN
4	G	424	ILE
4	G	439	LYS
4	G	455	LEU
4	G	523	PHE
4	G	526	LEU
4	G	565	LEU
4	G	568	GLU
4	G	576	ILE
4	H	264	LEU
4	H	284	TYR
4	H	293	CYS
4	H	296	MET
4	H	297	LEU
4	H	366	ASP
4	H	367	LEU
4	H	381	LEU
4	H	424	ILE
4	H	438	ARG
4	H	445	ARG
4	H	460	ASP

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Mol	Chain	Res	Type
4	H	477	ILE
4	H	503	VAL
4	H	518	LEU
4	H	564	LYS
4	H	576	ILE
5	I	39	ARG
5	I	41	MET
5	I	51	LEU
5	I	88	ASP
5	I	102	PHE
5	I	113	ARG
5	I	123	ASP
5	I	125	ARG
5	I	140	LEU
5	I	145	PHE
5	I	174	TYR
5	I	176	LYS
5	I	181	GLU
5	I	231	ILE
5	I	232	ASP
5	I	246	PHE
5	I	259	PHE
5	I	274	TYR
5	I	304	TYR
5	I	308	LEU
5	I	345	ILE
5	I	374	ILE
5	I	381	ASP
5	I	457	LEU
5	J	32	LEU
5	J	41	MET
5	J	51	LEU
5	J	62	TYR
5	J	88	ASP
5	J	99	TRP
5	J	113	ARG
5	J	122	LEU
5	J	140	LEU
5	J	151	PHE
5	J	165	THR
5	J	173	THR
5	J	174	TYR

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Mol	Chain	Res	Type
5	J	176	LYS
5	J	206	ARG
5	J	274	TYR
5	J	279	ASP
5	J	307	VAL
5	J	320	TYR
5	J	324	HIS
5	J	330	ASP
5	J	333	LEU
5	J	372	ILE
5	J	380	TRP
5	J	467	VAL
6	K	7	ARG
6	K	19	ILE
6	K	27	ILE
6	K	39	TYR
6	K	45	MET
6	K	47	LEU
6	K	54	ARG
6	K	59	ILE
6	K	62	LEU
6	K	64	ARG
6	K	79	GLU
6	K	97	LYS
6	K	109	HIS
6	K	112	LEU
6	K	114	TYR
6	K	124	GLU
6	K	129	THR
6	K	137	LYS
6	K	140	HIS
6	K	143	GLU
6	K	159	GLU
6	K	166	LEU
6	K	168	GLU
6	K	235	LEU
6	K	236	ASP
6	K	244	LEU
6	K	251	ILE
6	L	7	ARG
6	L	17	ASP
6	L	19	ILE

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Mol	Chain	Res	Type
6	L	27	ILE
6	L	39	TYR
6	L	45	MET
6	L	47	LEU
6	L	54	ARG
6	L	59	ILE
6	L	61	LYS
6	L	62	LEU
6	L	64	ARG
6	L	69	ASP
6	L	79	GLU
6	L	97	LYS
6	L	102	TYR
6	L	127	TYR
6	L	129	THR
6	L	130	ILE
6	L	137	LYS
6	L	143	GLU
6	L	159	GLU
6	L	168	GLU
6	L	185	ARG
6	L	244	LEU
6	L	251	ILE
7	M	111	HIS
7	M	228	GLN
7	M	291	ILE
7	M	315	LEU
7	M	330	ILE
7	M	494	GLU
7	M	495	ILE
7	M	508	HIS
8	O	131	TYR
7	N	188	HIS
7	N	197	HIS
7	N	292	ASP
7	N	315	LEU
7	N	352	GLU
7	N	354	GLU
7	N	371	LYS
7	N	420	LYS
7	N	422	HIS
7	N	423	LEU

Continued on next page...

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Mol	Chain	Res	Type
7	N	510	ARG
8	P	166	LEU
8	P	168	ASP
8	P	170	LYS
8	P	171	LYS
8	P	174	PHE
8	P	180	ILE
8	P	191	LEU
8	P	221	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	B	129	HIS
1	B	209	ASN
1	B	234	HIS
2	C	156	GLN
2	C	222	ASN
2	C	237	ASN
2	D	19	ASN
2	D	173	GLN
2	D	222	ASN
2	D	225	ASN
3	E	59	GLN
3	E	265	ASN
3	E	309	GLN
3	F	221	GLN
4	G	271	HIS
4	G	416	ASN
4	G	446	ASN
4	G	500	ASN
4	H	271	HIS
4	H	349	GLN
4	H	384	GLN
4	H	450	ASN
5	I	73	HIS
5	I	92	ASN
5	J	73	HIS
6	K	11	ASN
6	K	41	ASN
6	L	11	ASN

Continued on next page...

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Mol	Chain	Res	Type
7	M	98	GLN
7	M	221	ASN
7	N	98	GLN
8	P	190	HIS

5.3.3 RNA (i)

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	0.63	0	8,12,14	1.11	0
6	SEP	K	52	6	8,9,10	0.64	0	8,12,14	1.64	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SEP	L	52	6	-	1/5/8/10	-
6	SEP	K	52	6	-	0/5/8/10	-

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	K	52	SEP	OG-CB-CA	3.56	111.61	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	413:SER	C	414:GLN	N	7.58

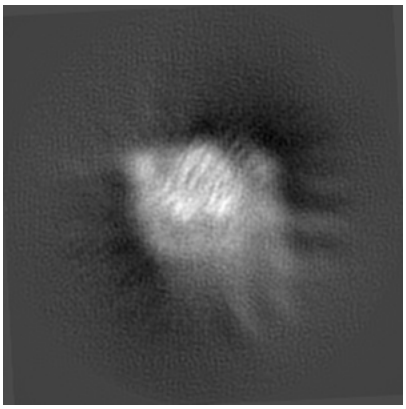
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4545. These allow visual inspection of the internal detail of the map and identification of artifacts.

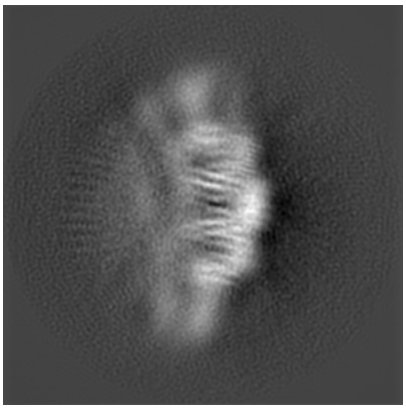
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

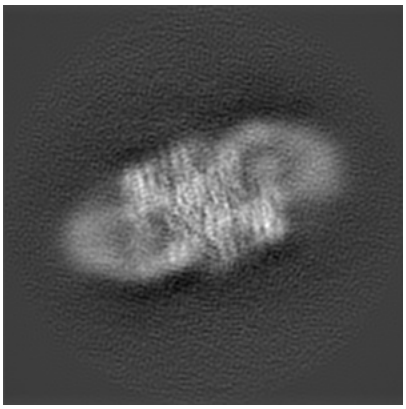
6.1.1 Primary map



X

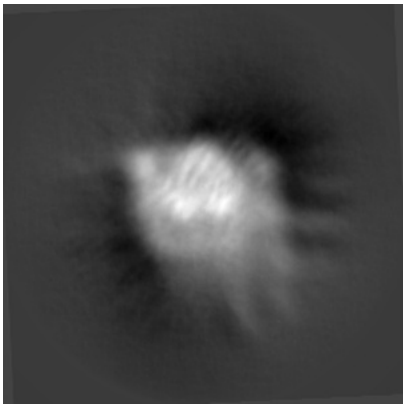


Y

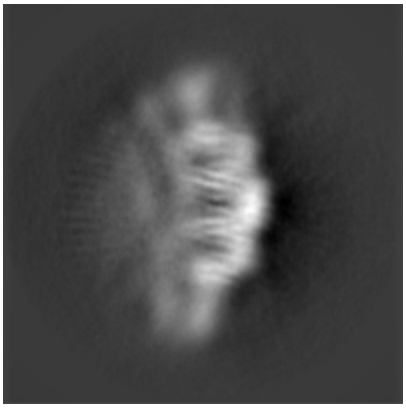


Z

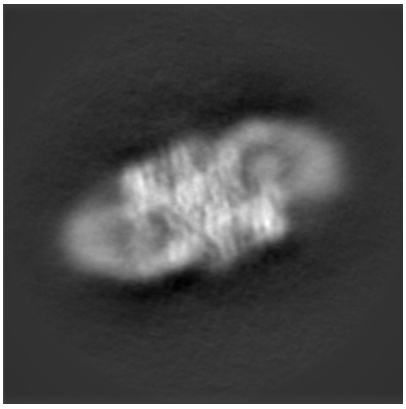
6.1.2 Raw map



X



Y

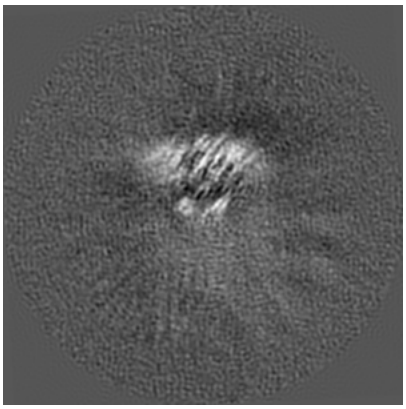


Z

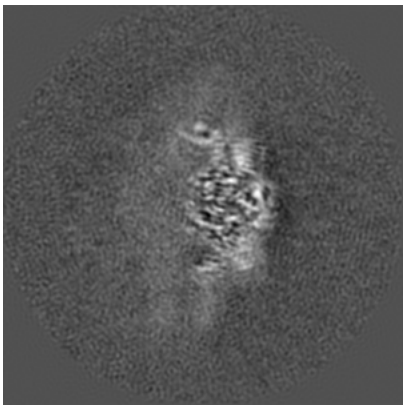
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

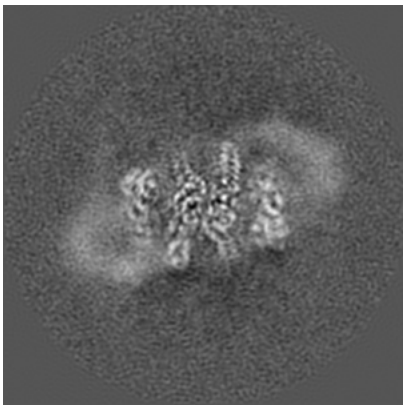
6.2.1 Primary map



X Index: 140

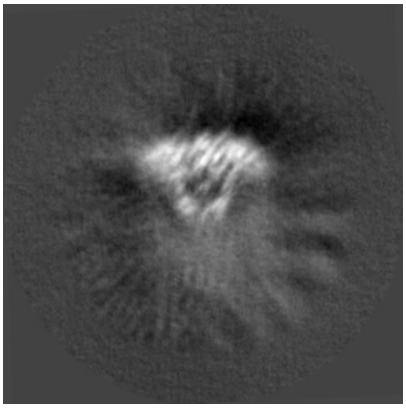


Y Index: 140

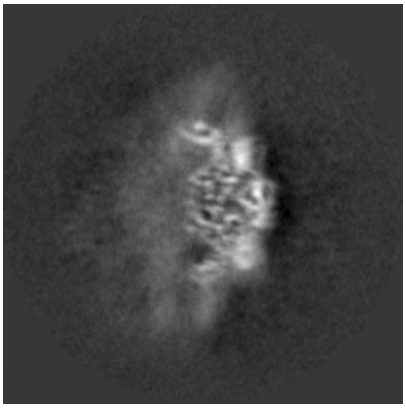


Z Index: 140

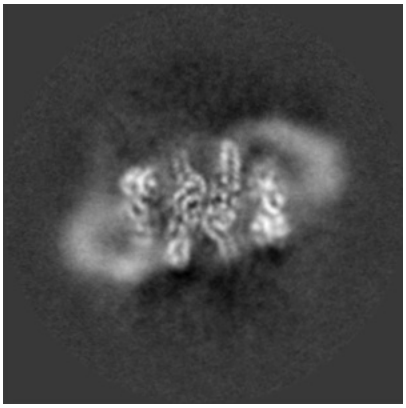
6.2.2 Raw map



X Index: 140



Y Index: 140

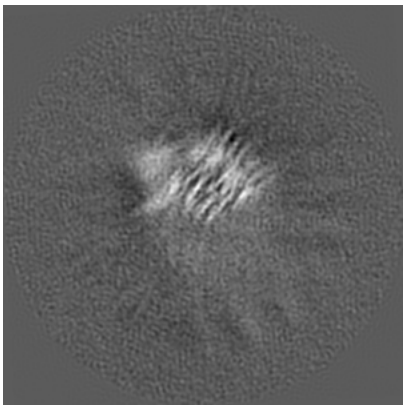


Z Index: 140

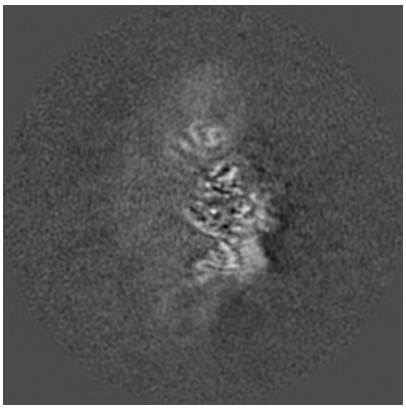
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

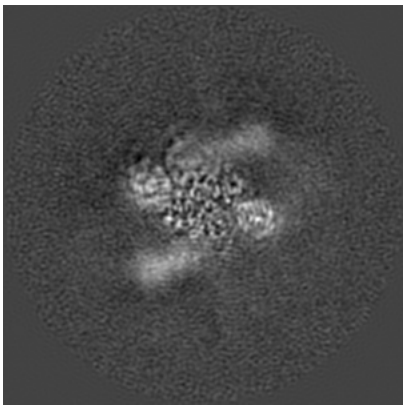
6.3.1 Primary map



X Index: 128

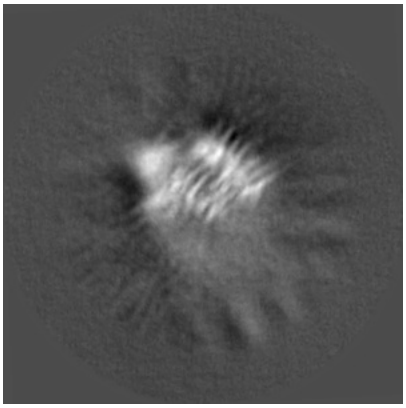


Y Index: 147

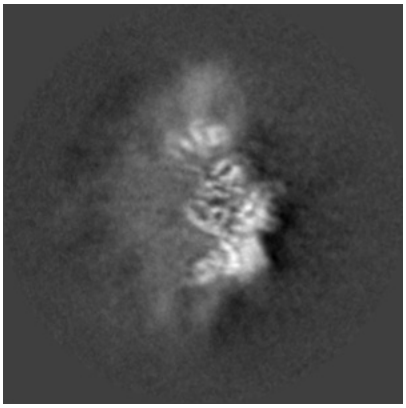


Z Index: 165

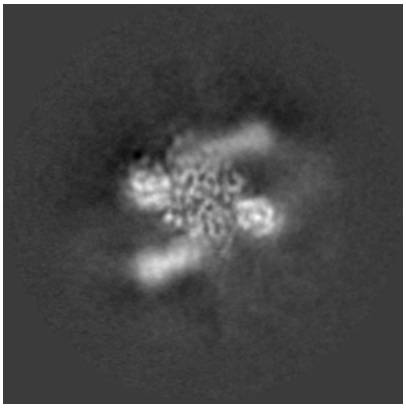
6.3.2 Raw map



X Index: 127



Y Index: 148



Z Index: 166

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

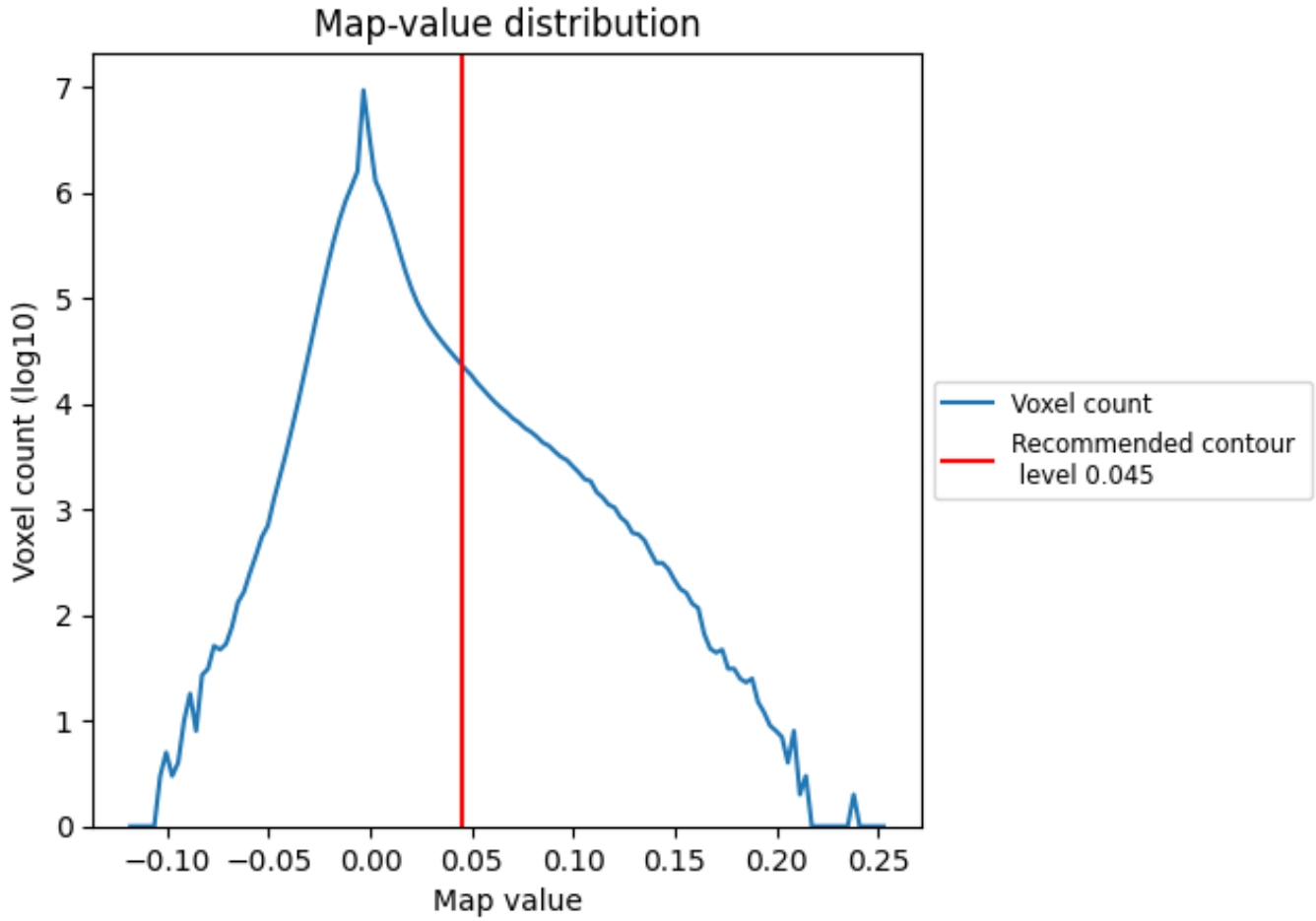
6.5 Mask visualisation (i)

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

7 Map analysis

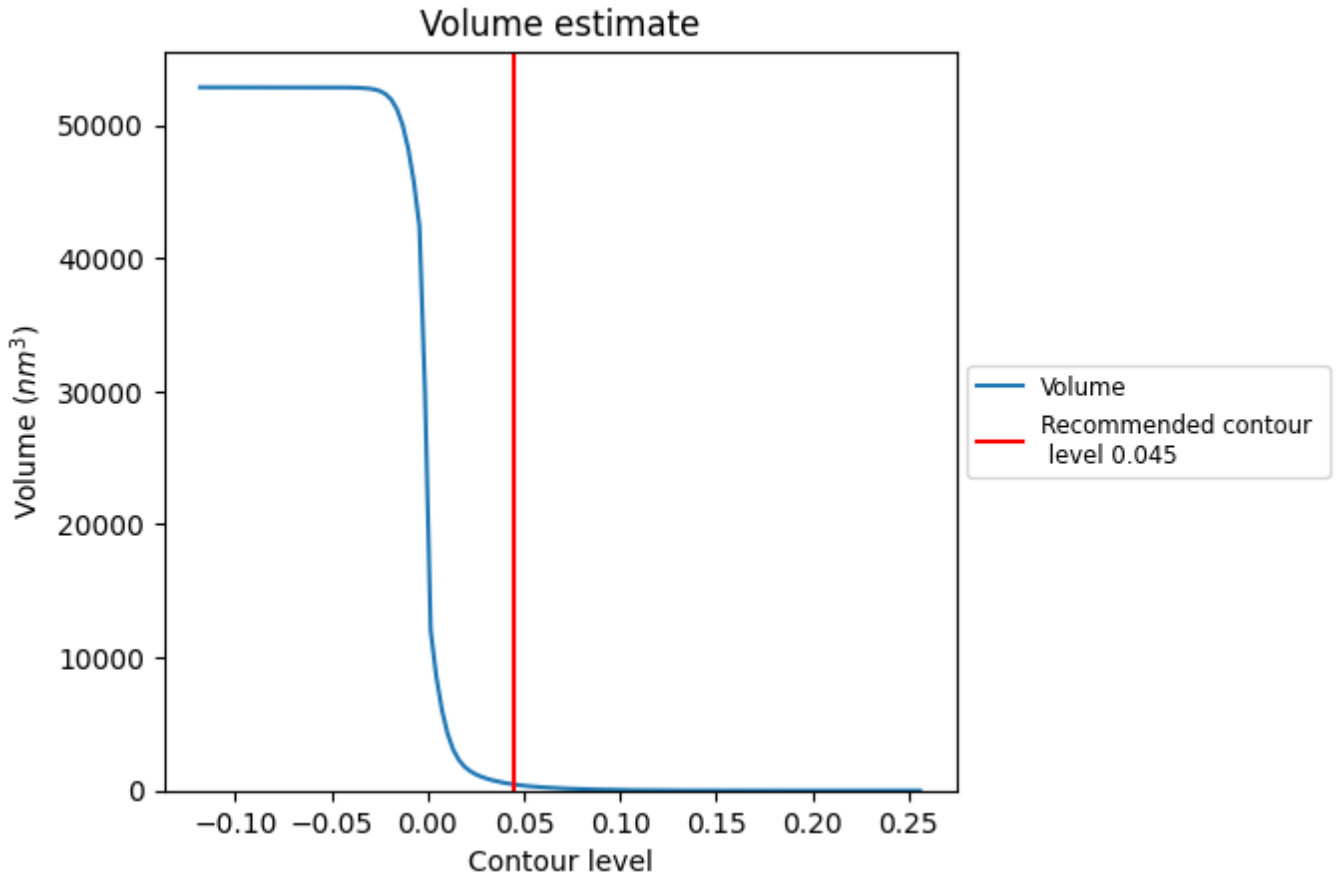
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

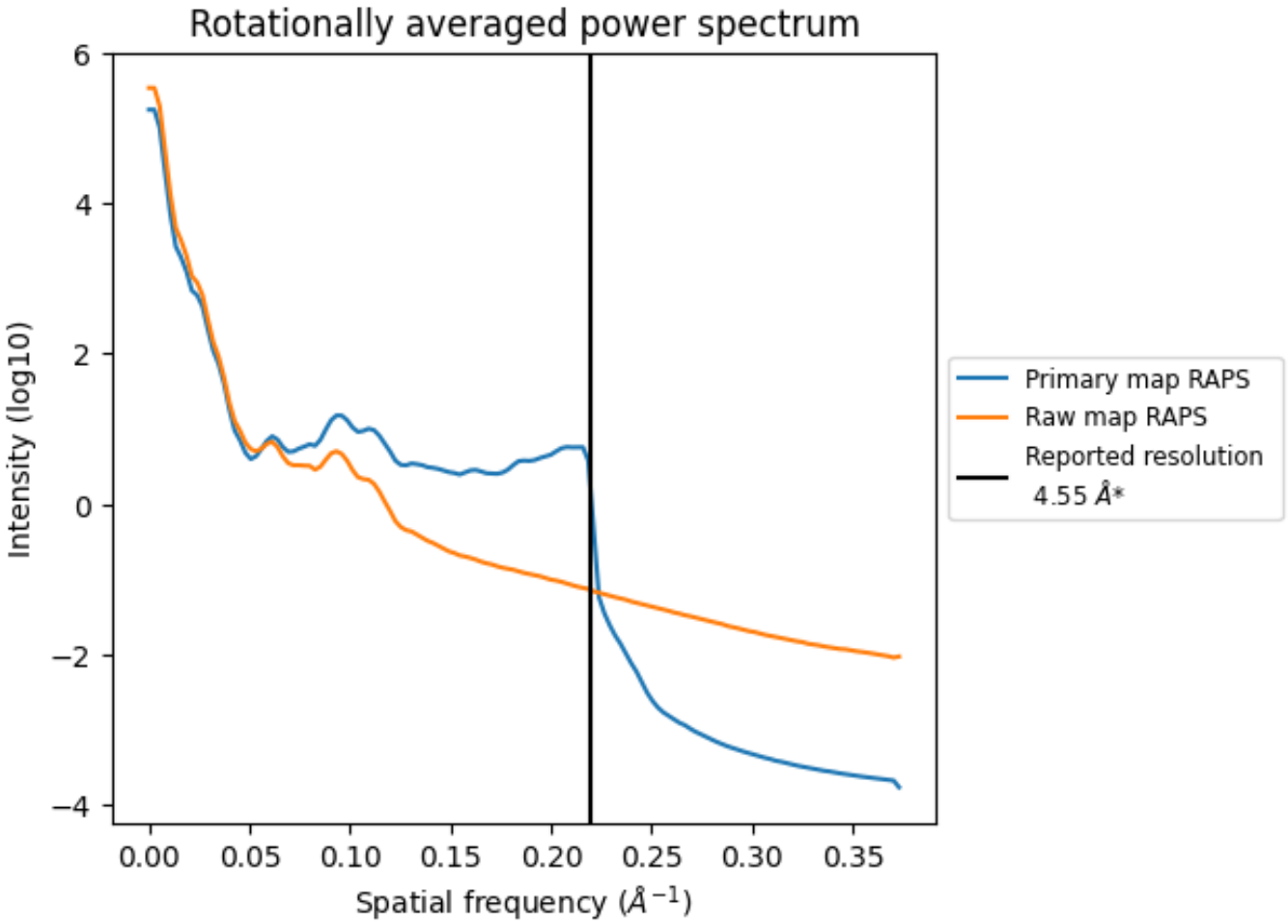
7.2 Volume estimate



The volume at the recommended contour level is 459 nm^3; this corresponds to an approximate mass of 414 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)

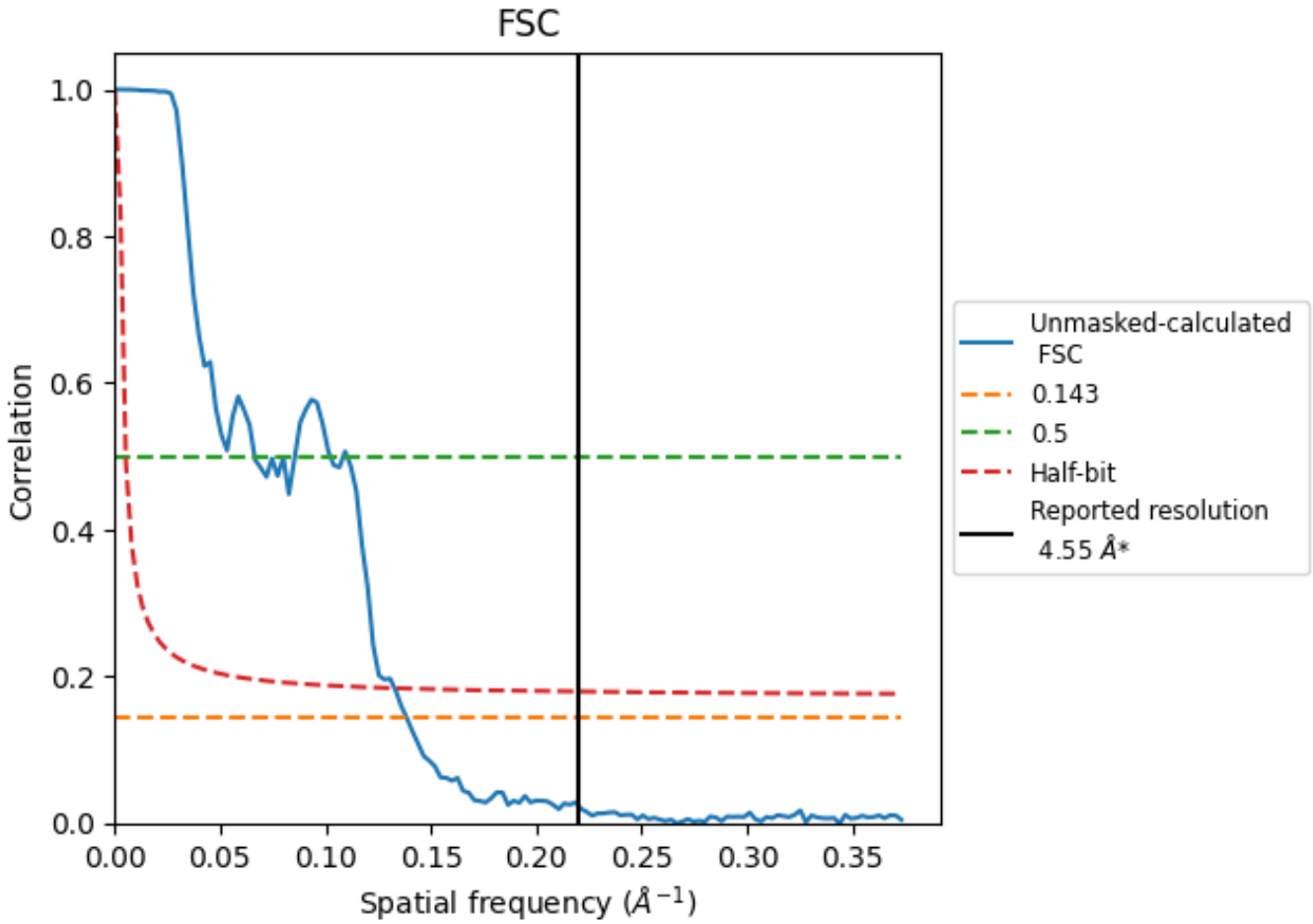


*Reported resolution corresponds to spatial frequency of 0.220 Å^{-1}

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 0.220 Å^{-1}

8.2 Resolution estimates (i)

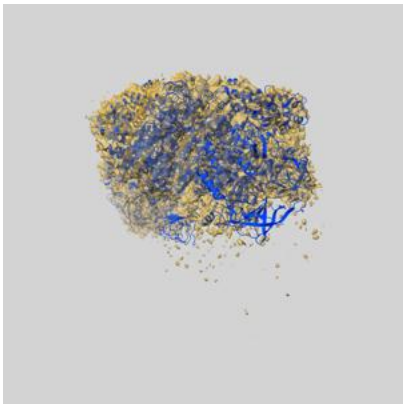
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.22	15.08	7.54

*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 7.22 differs from the reported value 4.55 by more than 10 %

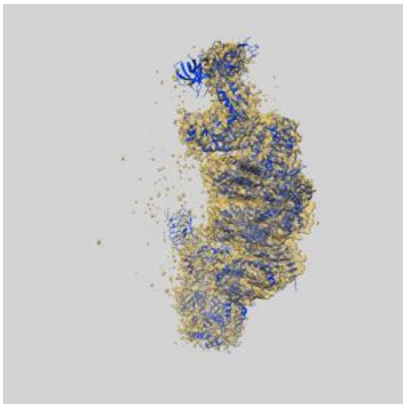
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4545 and PDB model 6QG2. Per-residue inclusion information can be found in section 3 on page 6.

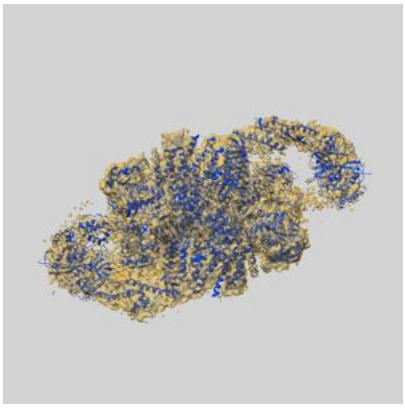
9.1 Map-model overlay



X



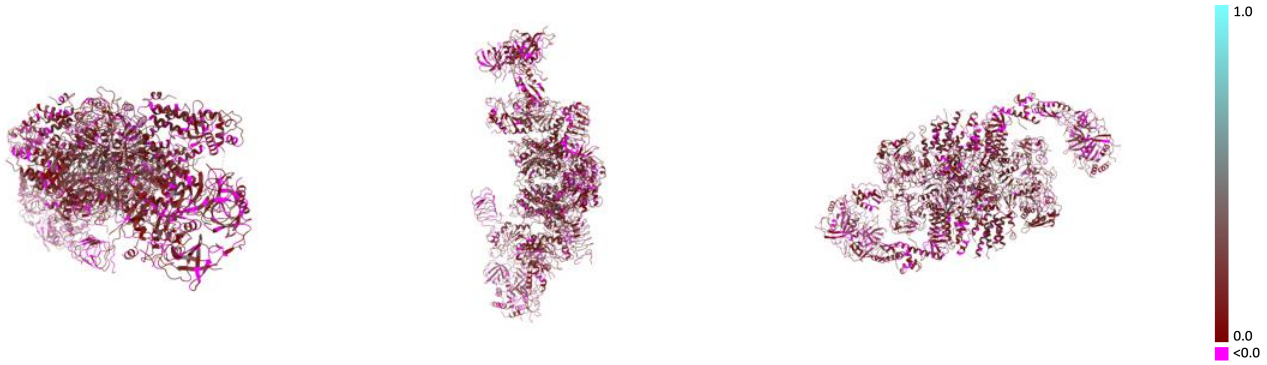
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

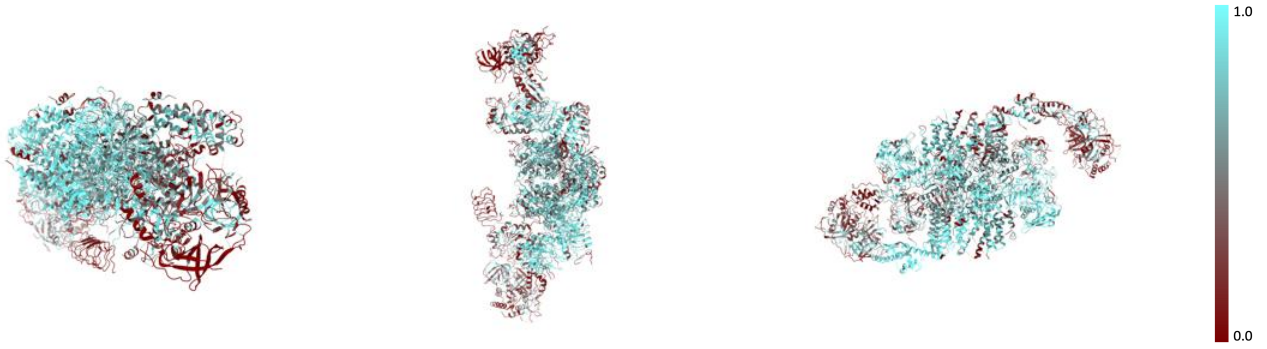
9.2 Q-score mapped to coordinate model



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.

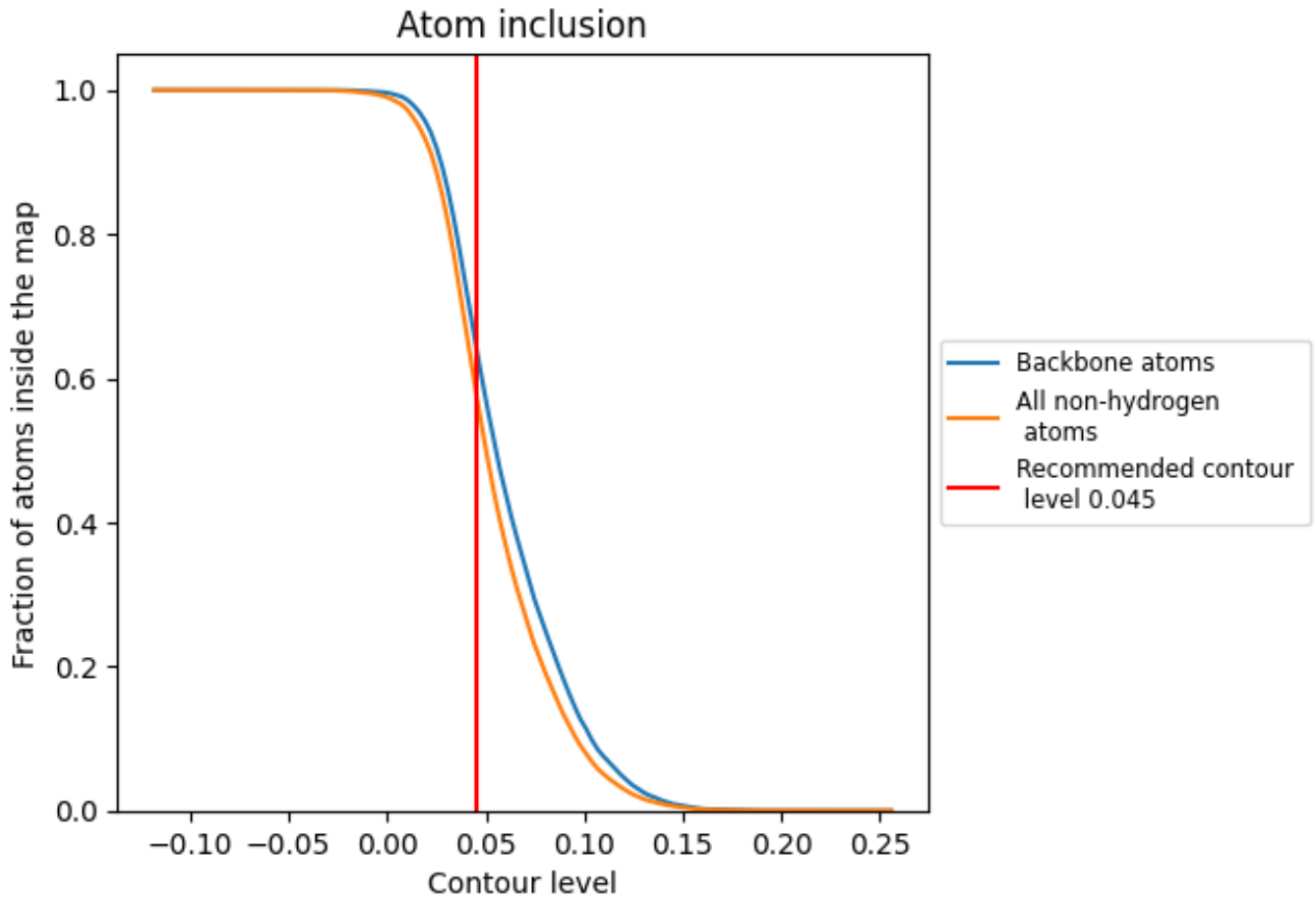
9.3 Atom inclusion mapped to coordinate model



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 58% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5816	0.1580
A	0.7758	0.1660
B	0.6528	0.1190
C	0.6686	0.1890
D	0.6838	0.2240
E	0.5560	0.1560
F	0.3341	0.1140
G	0.6531	0.2130
H	0.6136	0.2040
I	0.7745	0.1730
J	0.8333	0.2050
K	0.4095	0.1010
L	0.8170	0.1100
M	0.2416	0.1160
N	0.3353	0.1020
O	0.0942	0.1270
P	0.1891	0.1180