



## Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 11:02 am GMT

PDB ID : 6QG6  
EMDB ID : EMD-4548  
Title : Structure of eIF2B-eIF2 (phosphorylated at Ser51) complex (model D)  
Authors : Llacer, J.L.; Gordiyenko, Y.; Ramakrishnan, V.  
Deposited on : 2019-01-10  
Resolution : 4.65 Å(reported)  
Based on initial models : 6FYX, 5B04

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

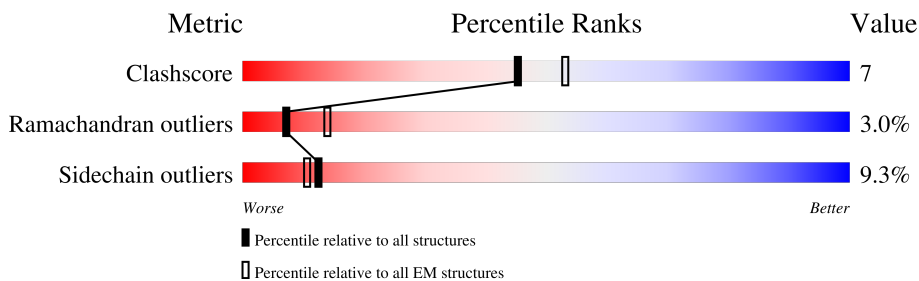
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.65 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.



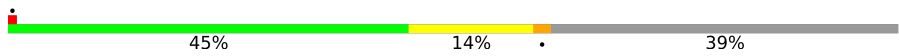
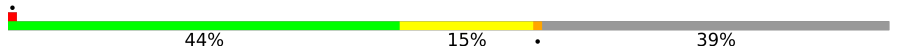




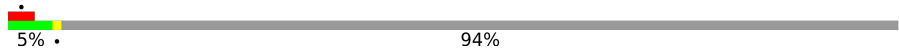
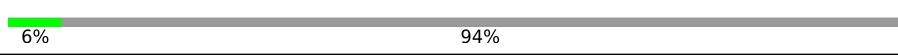
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	305	
2	C	381	
2	D	381	
3	E	578	
3	F	578	
4	G	651	
4	H	651	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	I	712	 45% 14% 39%
5	J	712	 44% 15% 39%
6	K	304	 5% 61% 18% 19%
6	L	304	 66% 14% 19%
7	M	527	 16% 66% 11% 23%
7	N	527	 68% 9% 23%
8	O	285	 5% 94%
8	P	285	 6% 94%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 36982 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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
3	E	267	Total	C	N	O	S	0	0
			2164	1391	363	400	10		
3	F	267	Total	C	N	O	S	0	0
			2164	1391	363	400	10		

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

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

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

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

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

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

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

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

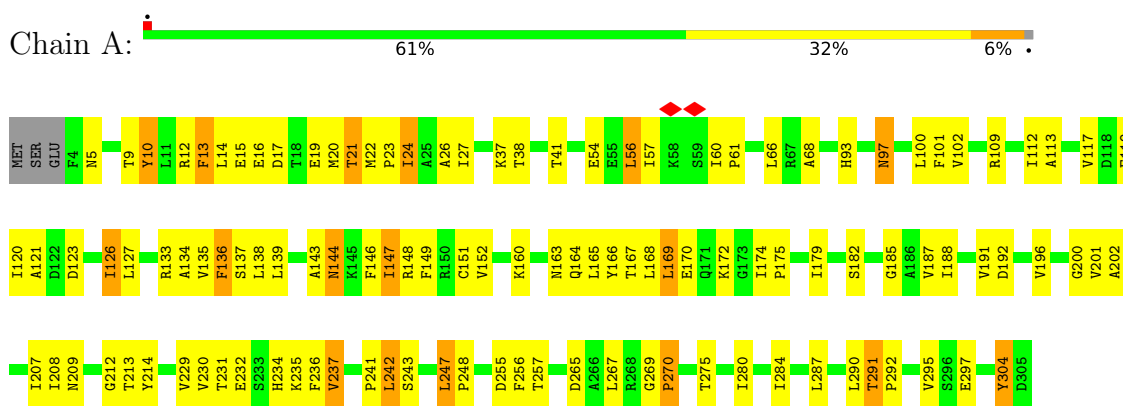
- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

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

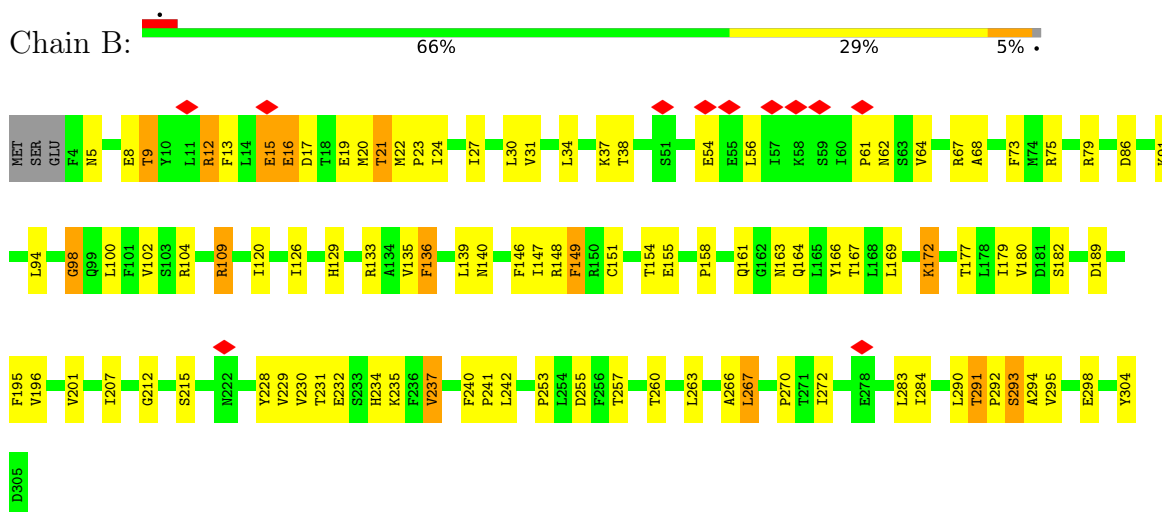
### 3 Residue-property plots i

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.

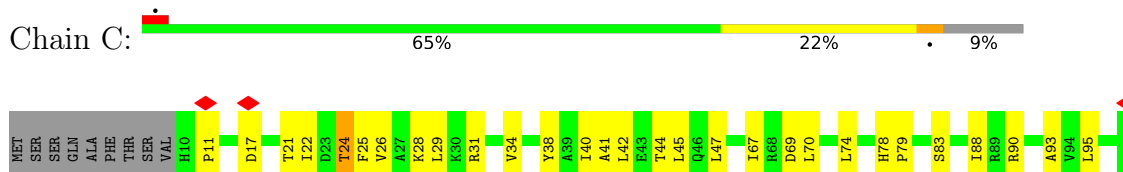
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



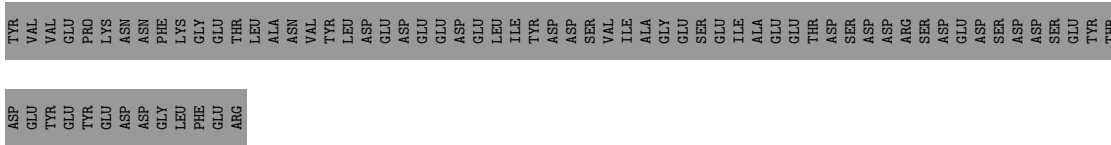
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



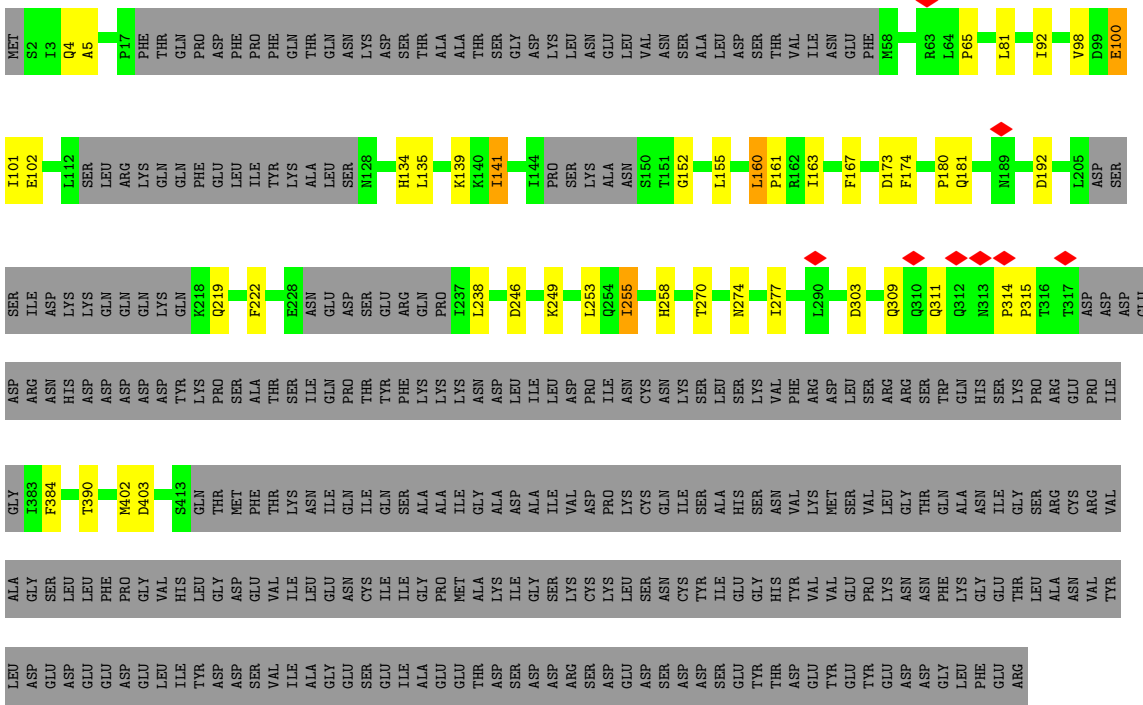
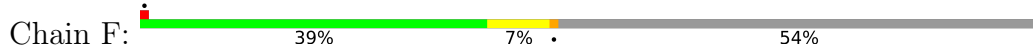
- Molecule 2: Translation initiation factor eIF-2B subunit beta



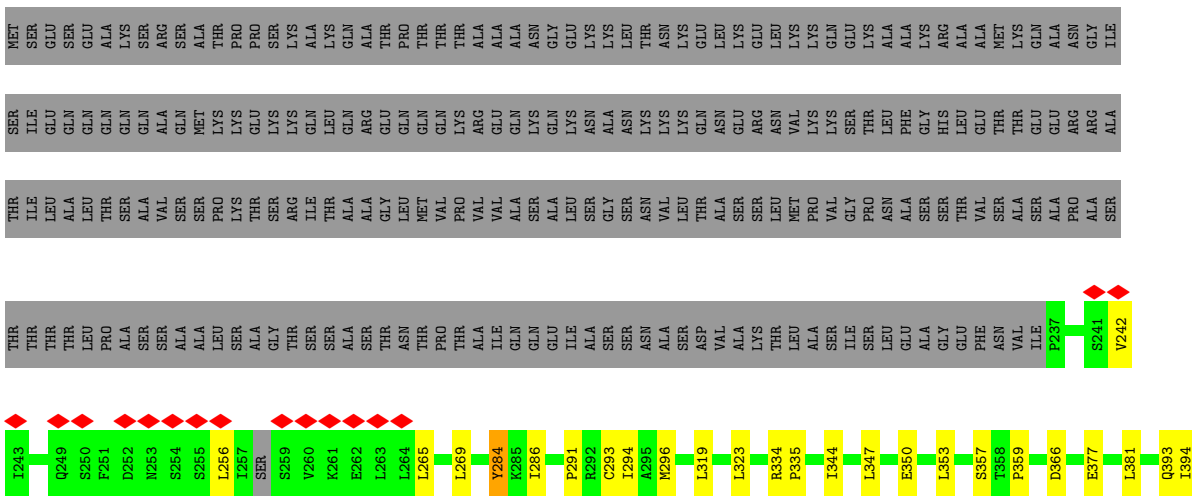




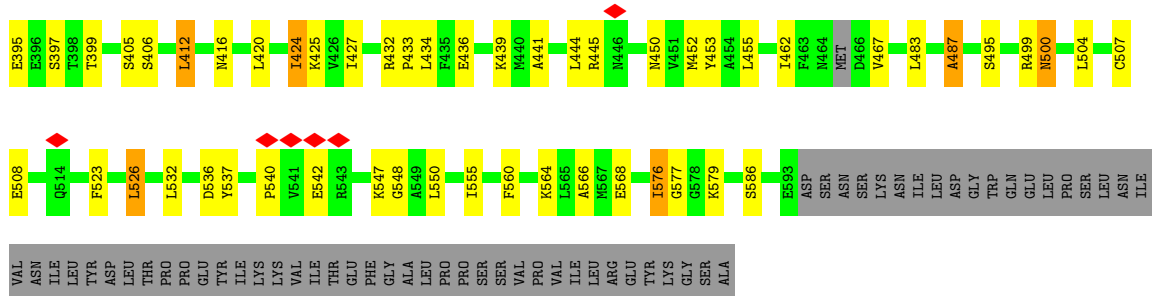
● Molecule 3: Translation initiation factor eIF-2B subunit gamma



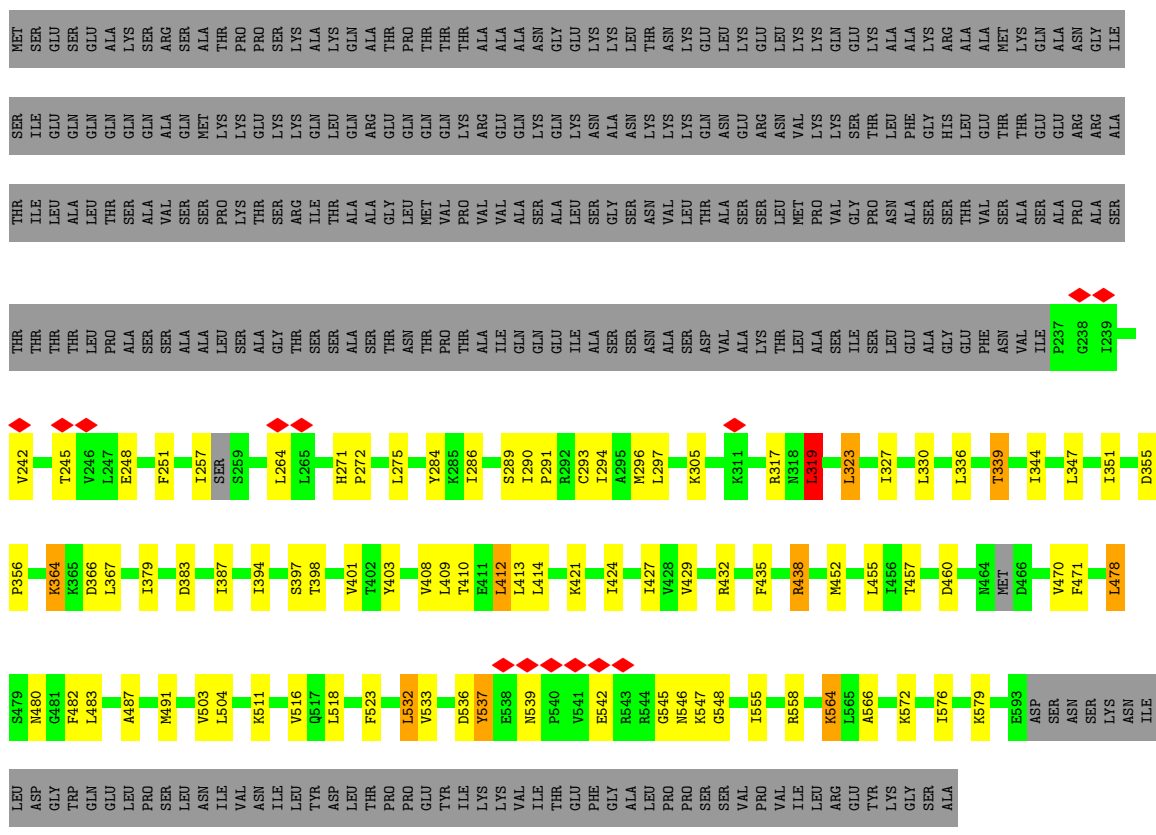
● Molecule 4: Translation initiation factor eIF-2B subunit delta



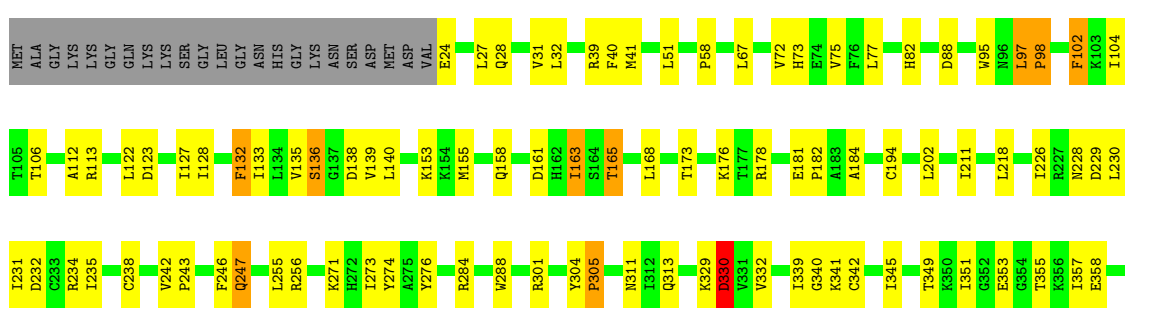
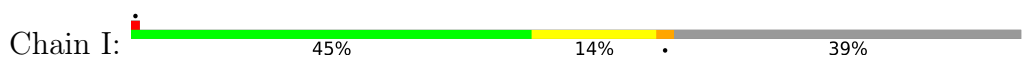




• Molecule 4: Translation initiation factor eIF-2B subunit delta



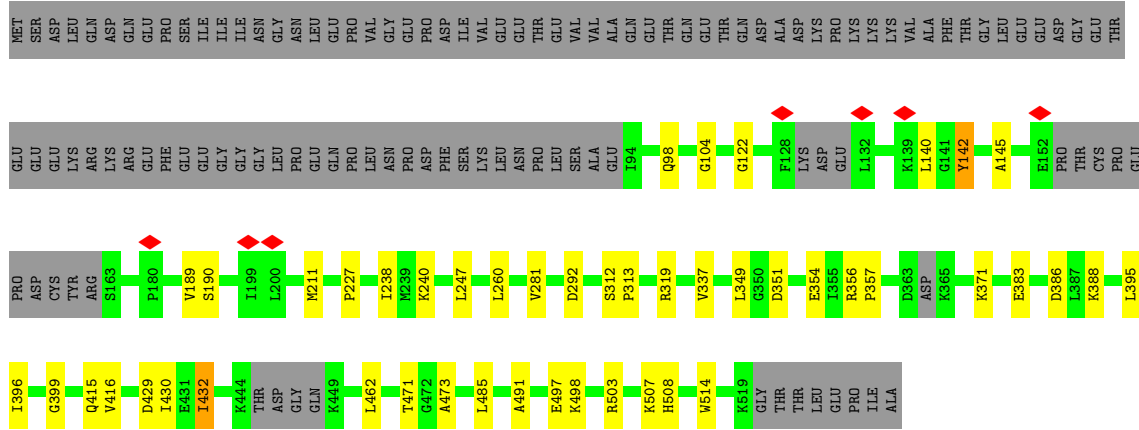
• Molecule 5: Translation initiation factor eIF-2B subunit epsilon







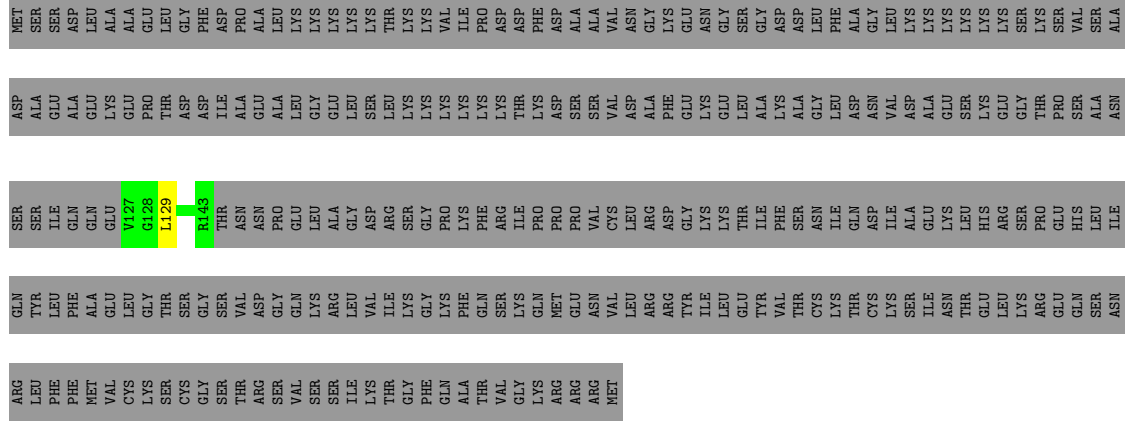
• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma



• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta



• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12575	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	0.079	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0125	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	0.41	0/2395	0.66	0/3251
1	B	0.43	0/2395	0.65	0/3251
2	C	0.42	0/2714	0.72	1/3693 (0.0%)
2	D	0.41	0/2714	0.69	0/3693
3	E	0.47	0/2209	0.64	1/2989 (0.0%)
3	F	0.48	0/2209	0.64	1/2989 (0.0%)
4	G	0.41	0/2781	0.69	1/3747 (0.0%)
4	H	0.42	0/2781	0.69	2/3747 (0.1%)
5	I	0.44	0/3468	0.68	0/4704
5	J	0.43	0/3468	0.65	0/4704
6	K	0.45	0/1989	0.69	0/2675
6	L	0.44	0/1989	0.68	0/2675
7	M	0.44	0/3087	0.62	0/4173
7	N	0.44	0/3087	0.62	0/4173
8	O	0.54	0/146	0.72	0/196
8	P	0.51	0/146	0.71	0/196
All	All	0.43	0/37578	0.67	6/50856 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	412	LEU	CA-CB-CG	6.66	130.62	115.30
3	F	135	LEU	CA-CB-CG	5.92	128.91	115.30
2	C	298	LEU	CA-CB-CG	5.60	128.18	115.30
4	H	323	LEU	CA-CB-CG	5.33	127.55	115.30
3	E	135	LEU	CA-CB-CG	5.14	127.12	115.30
4	H	319	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	94	0
1	B	2351	0	2367	118	0
2	C	2665	0	2625	43	0
2	D	2665	0	2626	28	0
3	E	2164	0	2154	21	0
3	F	2164	0	2154	14	0
4	G	2744	0	2819	28	0
4	H	2744	0	2819	38	0
5	I	3406	0	3359	46	0
5	J	3406	0	3359	50	0
6	K	1974	0	2019	17	0
6	L	1974	0	2019	10	0
7	M	3044	0	3126	22	0
7	N	3044	0	3126	20	0
8	O	143	0	148	0	0
8	P	143	0	148	0	0
All	All	36982	0	37235	499	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 (499) 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:149:PHE:CE1	1:A:174:ILE:CD1	2.26	1.17
1:A:149:PHE:CE1	1:A:174:ILE:HD13	1.80	1.16
1:B:283:LEU:HB3	1:B:291:THR:OG1	1.42	1.16
1:A:149:PHE:HE1	1:A:174:ILE:CD1	1.58	1.14
1:B:291:THR:H	1:B:292:PRO:CD	1.65	1.09
7:M:142:TYR:HB2	7:M:319:ARG:HH22	1.14	1.07
1:A:149:PHE:CZ	1:A:174:ILE:HD11	1.90	1.06
1:B:20:MET:SD	1:B:102:VAL:HG13	1.93	1.06

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:HE1	1:A:174:ILE:HD13	0.90	1.04
1:B:20:MET:CE	1:B:102:VAL:HG13	1.89	1.02
1:B:21:THR:HB	1:B:24:ILE:HD13	1.39	1.02
1:B:291:THR:H	1:B:292:PRO:HD2	1.27	0.99
1:B:283:LEU:HD23	1:B:291:THR:HA	1.48	0.93
1:B:294:ALA:O	1:B:298:GLU:HG3	1.71	0.91
1:A:149:PHE:CE1	1:A:174:ILE:HD11	2.01	0.89
1:B:20:MET:CE	1:B:102:VAL:CG1	2.51	0.89
1:B:21:THR:HB	1:B:24:ILE:CD1	2.04	0.88
7:M:142:TYR:HB2	7:M:319:ARG:NH2	1.87	0.88
7:M:142:TYR:CB	7:M:319:ARG:HH22	1.86	0.87
1:A:136:PHE:CZ	1:A:168:LEU:HB3	2.09	0.87
1:A:113:ALA:HA	1:A:138:LEU:HD22	1.57	0.86
1:A:146:PHE:HB2	5:J:332:VAL:HG13	1.54	0.86
1:B:21:THR:CB	1:B:24:ILE:HD13	2.05	0.86
1:B:290:LEU:HD23	2:C:366:TRP:HH2	1.39	0.85
1:B:172:LYS:HE2	1:B:172:LYS:HA	1.60	0.84
1:B:292:PRO:HG3	2:C:268:ASN:HA	1.60	0.83
1:B:293:SER:HB3	2:C:362:TYR:CE1	2.14	0.83
1:B:291:THR:N	1:B:292:PRO:CD	2.41	0.82
1:B:23:PRO:HG2	1:B:234:HIS:NE2	1.95	0.81
1:A:21:THR:HG22	1:A:23:PRO:HD2	1.61	0.81
1:B:283:LEU:CB	1:B:291:THR:OG1	2.27	0.80
1:B:9:THR:O	1:B:12:ARG:HB2	1.81	0.79
1:B:21:THR:HG21	1:B:234:HIS:HE1	1.46	0.79
1:B:21:THR:HG22	1:B:23:PRO:HD2	1.65	0.78
1:A:113:ALA:HB2	1:A:138:LEU:HD23	1.67	0.75
1:A:149:PHE:HZ	1:A:174:ILE:HD11	1.50	0.75
1:B:240:PHE:HZ	4:H:572:LYS:HB3	1.52	0.74
1:A:20:MET:HG2	1:A:24:ILE:HG22	1.67	0.73
1:A:136:PHE:CZ	1:A:168:LEU:CB	2.71	0.73
5:J:414:ILE:HG12	5:J:432:ILE:HD12	1.70	0.72
6:K:149:ILE:HG21	6:K:173:ILE:HG21	1.71	0.72
3:F:160:LEU:H	3:F:161:PRO:HD2	1.54	0.72
1:A:148:ARG:HD3	5:J:337:CYS:SG	2.30	0.72
1:A:20:MET:CG	1:A:24:ILE:HG22	2.19	0.72
1:B:292:PRO:HG2	2:C:362:TYR:HB3	1.70	0.72
1:B:139:LEU:HD11	1:B:151:CYS:SG	2.30	0.71
1:A:20:MET:CG	1:A:24:ILE:CG2	2.69	0.71
1:B:294:ALA:O	1:B:298:GLU:CG	2.40	0.70
1:B:129:HIS:HD2	1:B:196:VAL:HG13	1.57	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:387:ILE:HD13	4:H:412:LEU:HD22	1.73	0.69
1:B:146:PHE:HB3	5:I:332:VAL:CG1	2.23	0.69
1:B:164:GLN:O	1:B:167:THR:OG1	2.11	0.68
1:B:283:LEU:HB3	1:B:291:THR:HG1	1.56	0.68
1:B:293:SER:HB3	2:C:362:TYR:HE1	1.59	0.68
1:B:139:LEU:C	1:B:139:LEU:HD23	2.15	0.67
1:A:22:MET:HB2	1:A:23:PRO:HD3	1.75	0.67
1:B:22:MET:HB2	1:B:23:PRO:HD3	1.77	0.67
5:I:161:ASP:HB3	5:I:271:LYS:HG2	1.77	0.67
1:A:291:THR:H	1:A:292:PRO:HD3	1.59	0.66
1:A:127:LEU:HB2	1:A:191:VAL:HG11	1.77	0.66
1:A:136:PHE:CE2	1:A:168:LEU:HB3	2.30	0.66
6:K:207:SER:HB2	6:K:250:LYS:HD2	1.77	0.66
1:B:9:THR:HA	1:B:12:ARG:HD2	1.78	0.65
1:A:164:GLN:O	1:A:167:THR:OG1	2.11	0.65
5:I:304:TYR:HB3	5:I:305:PRO:HD3	1.77	0.65
1:B:129:HIS:HB3	1:B:196:VAL:HG22	1.77	0.65
1:B:20:MET:HE2	1:B:102:VAL:CG1	2.25	0.65
1:A:23:PRO:O	1:A:27:ILE:HD12	1.97	0.64
4:G:487:ALA:HA	4:G:564:LYS:HG2	1.80	0.64
1:B:290:LEU:HD23	2:C:366:TRP:CH2	2.28	0.64
2:C:258:VAL:HB	2:C:292:VAL:HA	1.79	0.64
1:A:144:ASN:N	1:A:144:ASN:HD22	1.95	0.64
2:C:317:GLY:HA2	5:I:301:ARG:HB3	1.80	0.64
1:B:19:GLU:HA	1:B:19:GLU:OE1	1.97	0.64
1:B:292:PRO:HB2	2:C:362:TYR:CD1	2.32	0.64
1:B:293:SER:CB	2:C:362:TYR:CE1	2.80	0.63
1:A:121:ALA:O	1:A:147:ILE:HG22	1.99	0.63
1:B:135:VAL:HG22	1:B:230:VAL:HB	1.79	0.63
2:D:183:HIS:H	2:D:210:THR:HB	1.63	0.63
5:J:464:VAL:HB	5:J:467:VAL:HG23	1.80	0.63
4:H:435:PHE:HB3	4:H:438:ARG:HD2	1.80	0.63
5:I:459:ASP:H	5:I:466:ILE:HD12	1.63	0.63
1:A:170:GLU:HG2	1:B:260:THR:O	1.99	0.62
1:B:146:PHE:HB3	5:I:332:VAL:HG13	1.81	0.62
1:B:139:LEU:HD23	1:B:139:LEU:O	2.00	0.62
1:B:146:PHE:CB	5:I:332:VAL:CG1	2.78	0.62
1:B:20:MET:HE1	1:B:102:VAL:CG1	2.29	0.61
1:A:175:PRO:HG2	5:J:335:GLN:NE2	2.14	0.61
4:H:339:THR:HG23	4:H:511:LYS:HA	1.83	0.61
1:A:123:ASP:OD1	1:A:148:ARG:O	2.18	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:160:LEU:H	3:E:161:PRO:HD2	1.66	0.60
1:B:21:THR:HG21	1:B:234:HIS:CE1	2.32	0.60
4:H:432:ARG:HB3	4:H:532:LEU:HD11	1.83	0.60
4:G:483:LEU:HB3	4:G:566:ALA:HB3	1.84	0.60
1:A:256:PHE:HA	1:B:177:THR:HB	1.83	0.59
2:C:90:ARG:HH22	2:C:298:LEU:HD13	1.66	0.59
6:L:146:LYS:O	6:L:149:ILE:HG13	2.02	0.59
5:J:385:ILE:HG12	5:J:402:LEU:HD12	1.85	0.59
2:C:333:THR:HG22	4:G:453:TYR:HB3	1.85	0.59
1:B:172:LYS:HA	1:B:172:LYS:CE	2.24	0.59
2:D:67:ILE:HA	2:D:70:LEU:HD12	1.83	0.59
4:H:383:ASP:O	4:H:387:ILE:HG12	2.03	0.59
1:B:283:LEU:N	1:B:291:THR:OG1	2.36	0.59
1:B:20:MET:CE	1:B:102:VAL:HG11	2.33	0.59
5:J:414:ILE:HA	5:J:432:ILE:HB	1.84	0.58
1:A:120:ILE:HG12	1:A:126:ILE:HG12	1.84	0.58
4:H:403:TYR:HD2	4:H:429:VAL:HB	1.68	0.58
1:A:152:VAL:HG13	1:A:179:ILE:HD13	1.86	0.58
1:B:9:THR:HA	1:B:12:ARG:CD	2.33	0.58
2:D:198:LYS:O	2:D:201:ILE:HG22	2.04	0.57
1:B:120:ILE:HG21	1:B:147:ILE:CG2	2.33	0.57
1:B:126:ILE:HD12	1:B:149:PHE:HD2	1.68	0.57
1:B:291:THR:H	1:B:292:PRO:HD3	1.63	0.57
4:H:427:ILE:HG12	4:H:452:MET:HB2	1.86	0.57
1:A:247:LEU:HD23	1:A:248:PRO:HD2	1.86	0.57
4:H:487:ALA:HA	4:H:564:LYS:HE3	1.86	0.57
7:N:462:LEU:HD22	7:N:503:ARG:HG2	1.85	0.57
1:B:23:PRO:HG2	1:B:235:LYS:NZ	2.20	0.57
5:I:32:LEU:HB2	5:I:136:SER:HA	1.86	0.57
2:C:74:LEU:HD12	2:C:88:ILE:HD11	1.86	0.57
2:D:317:GLY:HA2	5:J:301:ARG:HB3	1.85	0.57
4:H:394:ILE:HG23	4:H:398:THR:HG21	1.86	0.57
4:H:432:ARG:CZ	4:H:532:LEU:HG	2.34	0.57
2:C:219:PHE:HA	2:C:223:THR:HG23	1.85	0.57
7:M:237:GLU:HB3	7:M:274:ILE:HD12	1.86	0.57
1:B:146:PHE:CB	5:I:332:VAL:HG11	2.35	0.57
5:I:128:ILE:HG21	5:I:243:PRO:HG3	1.85	0.57
5:J:83:ALA:HA	5:J:86:ILE:HD12	1.87	0.57
7:M:140:LEU:HA	7:M:193:ASP:O	2.05	0.57
1:B:120:ILE:CG2	1:B:147:ILE:HG21	2.34	0.56
1:B:21:THR:O	1:B:24:ILE:HB	2.04	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:ASN:HA	2:D:338:THR:HA	1.86	0.56
1:A:113:ALA:CA	1:A:138:LEU:HD22	2.33	0.56
2:C:173:GLN:HA	2:C:176:ALA:HB3	1.87	0.56
5:I:40:PHE:HA	5:I:288:TRP:HE1	1.70	0.56
5:J:357:ILE:HA	5:J:374:ILE:HB	1.87	0.56
6:K:71:ALA:HB3	6:K:85:LEU:HD23	1.88	0.56
6:K:174:SER:O	6:K:235:LEU:O	2.24	0.56
1:A:139:LEU:HD11	1:A:151:CYS:SG	2.46	0.56
1:B:230:VAL:HA	1:B:284:ILE:HB	1.88	0.56
3:E:267:THR:HG23	5:J:225:VAL:HA	1.88	0.56
1:B:20:MET:HE2	1:B:102:VAL:HG13	1.84	0.55
2:C:42:LEU:HA	2:C:45:LEU:HD12	1.87	0.55
4:G:495:SER:HB2	4:G:499:ARG:HH21	1.71	0.55
1:B:283:LEU:HB3	1:B:291:THR:CB	2.35	0.55
2:D:187:LEU:HG	2:D:189:PRO:HD3	1.88	0.55
3:E:257:SER:HB3	5:J:209:THR:HA	1.88	0.55
3:E:152:GLY:HA2	3:E:155:LEU:HD12	1.88	0.55
1:B:109:ARG:HH22	1:B:133:ARG:HB3	1.71	0.55
1:B:290:LEU:HD13	1:B:294:ALA:HB3	1.89	0.55
1:B:22:MET:CB	1:B:23:PRO:HD3	2.37	0.55
2:C:301:LEU:HD21	2:C:365:ALA:HA	1.89	0.55
1:A:20:MET:HG3	1:A:24:ILE:CG2	2.35	0.54
4:H:319:LEU:HD21	4:H:351:ILE:HG12	1.89	0.54
1:A:20:MET:HG3	1:A:24:ILE:HG21	1.90	0.54
1:B:126:ILE:CD1	1:B:149:PHE:HD2	2.20	0.54
1:B:257:THR:HG21	1:B:266:ALA:HA	1.88	0.54
3:F:238:LEU:HD13	3:F:390:THR:HG23	1.89	0.54
1:B:20:MET:HE1	1:B:102:VAL:HG11	1.90	0.54
6:L:149:ILE:HG21	6:L:173:ILE:HD13	1.89	0.54
7:M:113:LYS:HE3	7:M:195:PRO:HA	1.89	0.54
1:A:112:ILE:HG22	1:A:138:LEU:HD11	1.90	0.54
5:I:123:ASP:HB3	5:I:247:GLN:HE21	1.72	0.54
1:A:56:LEU:HD11	1:A:66:LEU:HD22	1.90	0.54
5:I:432:ILE:HG12	5:I:459:ASP:HB2	1.89	0.54
4:H:547:LYS:HE2	4:H:558:ARG:HH21	1.73	0.53
5:I:238:CYS:HB3	5:I:242:VAL:HG21	1.90	0.53
7:M:98:GLN:HE22	7:M:396:ILE:HD11	1.73	0.53
5:I:67:LEU:HB3	5:I:72:VAL:HG21	1.89	0.53
5:J:188:ASP:HB3	5:J:193:ARG:H	1.73	0.53
1:A:202:ALA:HB2	1:A:208:ILE:HD11	1.91	0.53
1:B:290:LEU:HD12	1:B:290:LEU:O	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD22	1:B:73:PHE:HZ	1.72	0.53
1:B:163:ASN:O	1:B:167:THR:HG23	2.09	0.53
4:G:377:GLU:HA	4:G:381:LEU:HD12	1.91	0.53
7:N:142:TYR:CE2	7:N:190:SER:HB2	2.44	0.53
4:H:272:PRO:HA	4:H:275:LEU:HD12	1.92	0.52
1:A:143:ALA:HA	1:A:149:PHE:CE2	2.45	0.52
3:F:219:GLN:HE22	3:F:249:LYS:HD2	1.74	0.52
5:J:186:VAL:O	5:J:194:CYS:HA	2.09	0.52
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.10	0.52
1:A:113:ALA:HA	1:A:138:LEU:CD2	2.33	0.52
4:G:416:ASN:HD22	4:G:424:ILE:HG12	1.73	0.52
1:B:189:ASP:HB3	4:G:500:ASN:HB2	1.90	0.52
4:H:330:LEU:HB3	4:H:336:LEU:HD21	1.92	0.52
1:A:113:ALA:HB2	1:A:138:LEU:CD2	2.39	0.52
1:A:160:LYS:HB3	1:A:163:ASN:HD22	1.73	0.52
1:A:113:ALA:CA	1:A:138:LEU:CD2	2.88	0.52
1:B:68:ALA:HB2	1:B:237:VAL:HG22	1.92	0.52
1:B:146:PHE:CB	5:I:332:VAL:HG13	2.38	0.52
1:B:64:VAL:HA	1:B:67:ARG:HD2	1.92	0.52
1:A:109:ARG:HH12	1:A:133:ARG:HB3	1.74	0.52
5:I:75:VAL:HG23	5:I:102:PHE:HB2	1.92	0.52
5:I:31:VAL:HB	5:I:77:LEU:HD23	1.91	0.52
1:A:165:LEU:O	1:A:169:LEU:HD12	2.10	0.51
4:G:394:ILE:HD13	4:G:416:ASN:HD21	1.76	0.51
7:N:471:THR:HG21	7:N:491:ALA:HB2	1.91	0.51
5:J:343:THR:HG22	5:J:360:SER:H	1.74	0.51
1:B:120:ILE:HG21	1:B:147:ILE:HG21	1.91	0.51
4:H:305:LYS:HA	4:H:364:LYS:HE3	1.93	0.51
5:I:28:GLN:HE21	5:I:132:PHE:HB2	1.75	0.51
1:A:9:THR:O	1:A:13:PHE:CE2	2.63	0.51
1:B:27:ILE:HA	1:B:30:LEU:HD12	1.91	0.51
1:B:154:THR:HA	1:B:179:ILE:O	2.09	0.51
1:B:291:THR:N	1:B:292:PRO:HD3	2.22	0.51
5:J:396:ILE:HG13	5:J:414:ILE:HD12	1.92	0.51
6:L:7:ARG:HD2	6:L:12:LYS:HG2	1.92	0.51
7:M:356:ARG:HH22	7:M:423:LEU:HD23	1.76	0.51
1:B:23:PRO:CG	1:B:235:LYS:NZ	2.73	0.51
2:D:89:ARG:HA	2:D:92:LEU:HD12	1.91	0.51
2:D:19:ASN:HB2	2:D:22:ILE:HD11	1.91	0.51
5:J:300:GLY:HA2	5:J:324:HIS:HE1	1.76	0.50
6:K:92:SER:HA	6:K:95:ILE:HD12	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:206:ARG:HG3	2:C:209:ARG:HD2	1.94	0.50
2:D:220:PRO:HD3	4:H:457:THR:HG21	1.93	0.50
1:A:109:ARG:NH2	1:A:137:SER:HB3	2.26	0.50
5:J:410:ASP:HB2	5:J:428:ARG:HE	1.76	0.50
1:A:22:MET:CB	1:A:23:PRO:HD3	2.41	0.50
2:D:48:LEU:HD13	2:D:91:ILE:HD13	1.93	0.50
1:A:136:PHE:HZ	1:A:168:LEU:CB	2.21	0.50
2:D:244:PRO:HG2	2:D:247:ALA:HB3	1.94	0.50
3:F:152:GLY:HA2	3:F:155:LEU:HD12	1.93	0.50
5:J:168:LEU:HB3	5:J:230:LEU:HD22	1.92	0.50
1:A:291:THR:H	1:A:292:PRO:CD	2.25	0.50
2:D:323:PRO:HD3	4:H:537:TYR:HD1	1.77	0.50
5:J:94:LYS:HB3	5:J:99:TRP:HZ2	1.77	0.50
5:I:329:LYS:O	5:I:330:ASP:HB2	2.12	0.49
1:A:112:ILE:HG22	1:A:138:LEU:HD21	1.93	0.49
4:G:405:SER:HB3	4:G:436:GLU:HB3	1.94	0.49
5:J:324:HIS:HB3	5:J:342:CYS:H	1.77	0.49
2:C:93:ALA:HB2	2:C:369:TYR:HA	1.94	0.49
4:G:399:THR:HB	4:G:467:VAL:HA	1.95	0.49
4:G:441:ALA:HA	4:G:444:LEU:HD12	1.94	0.49
4:H:319:LEU:O	4:H:323:LEU:HG	2.12	0.49
5:I:353:GLU:H	5:I:370:GLU:HG2	1.77	0.49
1:A:134:ALA:O	1:A:138:LEU:HG	2.12	0.49
1:A:136:PHE:CZ	1:A:168:LEU:HB2	2.46	0.49
2:C:29:LEU:HD13	2:C:78:HIS:HB2	1.94	0.49
4:H:364:LYS:HA	4:H:367:LEU:HB2	1.93	0.49
1:A:185:GLY:H	1:B:215:SER:HB2	1.78	0.49
4:H:403:TYR:CD2	4:H:429:VAL:HB	2.47	0.49
5:I:357:ILE:HG12	5:I:374:ILE:HD12	1.95	0.49
3:E:72:GLY:HA3	3:E:411:ILE:HD13	1.94	0.49
4:H:291:PRO:HA	4:H:294:ILE:HD12	1.95	0.49
5:J:195:ILE:HG12	5:J:264:ILE:HG21	1.94	0.49
5:J:296:GLN:HA	5:J:299:LEU:HD12	1.95	0.49
7:N:238:ILE:HG12	7:N:514:TRP:HB3	1.95	0.49
2:C:244:PRO:HG3	4:G:560:PHE:HB2	1.94	0.48
1:B:240:PHE:CZ	4:H:572:LYS:HB3	2.42	0.48
5:I:97:LEU:HD23	5:I:98:PRO:HD2	1.95	0.48
1:B:120:ILE:CG2	1:B:147:ILE:CG2	2.90	0.48
1:B:293:SER:HB3	2:C:362:TYR:CZ	2.47	0.48
1:B:91:LYS:HA	1:B:94:LEU:HD12	1.96	0.48
4:H:344:ILE:HA	4:H:347:LEU:HD12	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:195:ILE:HA	5:J:264:ILE:HD13	1.95	0.48
7:N:473:ALA:HB1	7:N:485:LEU:HB3	1.95	0.48
2:C:186:LEU:HD22	2:C:259:ILE:HD11	1.95	0.48
2:D:231:LYS:HD2	4:H:546:ASN:HD21	1.77	0.48
6:K:19:ILE:HD13	6:K:19:ILE:H	1.79	0.48
2:C:319:GLN:HA	2:C:328:ARG:HH22	1.77	0.48
1:A:24:ILE:HG23	1:A:102:VAL:HG22	1.96	0.48
5:J:349:THR:HG22	5:J:366:CYS:HB2	1.96	0.48
6:K:133:PRO:HG2	6:K:134:LEU:HD12	1.94	0.48
1:A:170:GLU:OE2	1:B:260:THR:CB	2.62	0.48
3:F:5:ALA:HB3	3:F:92:ILE:HG12	1.96	0.48
1:A:200:GLY:HA2	1:A:235:LYS:HB3	1.96	0.48
1:B:195:PHE:HA	1:B:228:TYR:HB2	1.96	0.48
1:B:230:VAL:HG22	1:B:284:ILE:HD12	1.95	0.48
6:L:75:ARG:H	6:L:84:ASP:HB2	1.78	0.48
1:A:144:ASN:N	1:A:144:ASN:ND2	2.60	0.47
2:C:44:THR:HA	2:C:47:LEU:HD12	1.96	0.47
1:A:182:SER:HB2	1:B:212:GLY:HA3	1.96	0.47
1:A:23:PRO:O	1:A:27:ILE:CD1	2.62	0.47
2:C:186:LEU:HD23	2:C:257:LYS:HB2	1.96	0.47
5:I:163:ILE:HD11	5:I:271:LYS:HB3	1.96	0.47
5:I:178:ARG:HH22	5:I:229:ASP:HA	1.78	0.47
5:J:59:LEU:HA	5:J:62:TYR:CE2	2.49	0.47
6:K:27:ILE:HG22	6:K:64:ARG:HE	1.79	0.47
1:A:68:ALA:HB2	1:A:237:VAL:HG22	1.97	0.47
5:J:255:LEU:HA	5:J:259:PHE:HB3	1.96	0.47
2:C:28:LYS:HB3	2:C:34:VAL:HB	1.96	0.47
3:E:190:ARG:HH12	3:E:238:LEU:HD12	1.79	0.47
4:G:350:GLU:HA	4:G:353:LEU:HD12	1.95	0.47
4:H:294:ILE:HG12	4:H:379:ILE:HD13	1.95	0.47
5:J:128:ILE:H	5:J:128:ILE:HG13	1.59	0.47
3:E:169:ILE:HB	3:E:278:TYR:HB2	1.97	0.47
5:I:27:LEU:HB3	5:I:133:ILE:HD11	1.97	0.47
6:K:146:LYS:O	6:K:149:ILE:HG13	2.15	0.47
1:A:208:ILE:HD12	1:A:247:LEU:HD21	1.97	0.47
3:E:315:PRO:HB3	3:E:385:ILE:HD11	1.96	0.47
7:M:142:TYR:HD1	7:M:319:ARG:NH2	2.13	0.47
7:N:240:LYS:HG3	7:N:498:LYS:HE3	1.97	0.47
1:B:23:PRO:CG	1:B:234:HIS:NE2	2.74	0.47
5:J:43:LEU:HD12	5:J:288:TRP:HH2	1.80	0.47
5:J:304:TYR:HB3	5:J:305:PRO:HD3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:157:LYS:HG2	3:E:288:LEU:HB3	1.96	0.47
5:I:194:CYS:H	5:I:273:ILE:HD11	1.80	0.47
7:N:142:TYR:HE2	7:N:190:SER:HB2	1.79	0.46
2:D:302:SER:HA	2:D:303:PRO:HD3	1.79	0.46
5:I:340:GLY:HA3	5:I:358:GLU:HG2	1.96	0.46
5:I:355:THR:HG22	5:I:372:ILE:H	1.80	0.46
6:L:119:PHE:HB3	6:L:121:ILE:HG12	1.96	0.46
2:D:292:VAL:HB	2:D:346:ILE:HA	1.97	0.46
6:K:20:VAL:HG12	6:K:38:GLU:HB3	1.96	0.46
1:A:56:LEU:HD21	1:A:66:LEU:HB3	1.98	0.46
4:H:410:THR:HA	4:H:413:LEU:HD12	1.97	0.46
2:D:361:ILE:HD12	2:D:364:ILE:HD13	1.97	0.46
3:E:303:ASP:N	3:E:304:PRO:HD2	2.30	0.46
3:E:385:ILE:H	3:E:385:ILE:HG13	1.61	0.46
5:I:184:ALA:HA	5:I:228:ASN:HA	1.97	0.46
1:A:147:ILE:HG22	1:A:147:ILE:O	2.16	0.46
3:E:255:ILE:HD11	5:J:213:ILE:HD11	1.97	0.46
4:H:483:LEU:HB3	4:H:566:ALA:HB3	1.97	0.46
5:I:255:LEU:HD12	5:I:256:ARG:HG2	1.98	0.46
7:N:430:ILE:HD12	7:N:432:ILE:HD12	1.97	0.46
1:A:135:VAL:HG22	1:A:230:VAL:HB	1.97	0.46
1:A:230:VAL:HG22	1:A:284:ILE:HD12	1.98	0.46
3:E:157:LYS:HD3	3:E:292:PRO:HB3	1.96	0.46
5:I:165:THR:HA	5:I:274:TYR:HB2	1.97	0.46
1:A:149:PHE:CZ	1:A:174:ILE:CD1	2.65	0.46
1:A:196:VAL:HG12	1:A:229:VAL:HG13	1.98	0.46
6:L:100:GLU:HA	6:L:103:GLN:HE21	1.81	0.46
6:L:111:ILE:HG23	6:L:169:LEU:HD21	1.97	0.46
1:B:15:GLU:H	1:B:15:GLU:HG2	1.61	0.46
1:B:139:LEU:HD11	1:B:151:CYS:HG	1.80	0.46
4:G:576:ILE:HG22	4:G:577:GLY:H	1.81	0.46
5:I:168:LEU:HD22	5:I:230:LEU:HB3	1.98	0.45
2:C:45:LEU:HD22	2:C:162:ILE:HG13	1.97	0.45
5:I:24:GLU:HG2	5:I:153:LYS:HD3	1.97	0.45
1:A:212:GLY:HA3	1:B:182:SER:HB2	1.97	0.45
1:B:13:PHE:N	1:B:13:PHE:CD1	2.85	0.45
1:B:126:ILE:HD12	1:B:149:PHE:CD2	2.50	0.45
2:D:222:ASN:HA	2:D:225:ASN:HD22	1.82	0.45
2:D:230:ALA:HA	2:D:233:LEU:HD12	1.97	0.45
7:N:337:VAL:HA	7:N:399:GLY:HA2	1.97	0.45
1:B:155:GLU:HB3	1:B:180:VAL:HA	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:HB3	1:A:213:THR:HG21	1.99	0.45
2:D:318:SER:HA	2:D:321:ILE:HD12	1.99	0.45
6:L:224:ALA:HB3	6:L:227:LEU:HB2	1.98	0.45
1:B:21:THR:OG1	1:B:24:ILE:HD13	2.16	0.45
3:F:160:LEU:HA	3:F:163:ILE:HD12	1.99	0.45
4:G:344:ILE:HA	4:G:347:LEU:HD12	1.99	0.45
4:G:427:ILE:HG12	4:G:452:MET:HB2	1.98	0.45
4:H:471:PHE:HA	4:H:504:LEU:O	2.16	0.45
1:A:117:VAL:HG12	1:A:138:LEU:HB3	1.98	0.45
1:B:8:GLU:O	1:B:12:ARG:HD2	2.16	0.45
1:B:62:ASN:HB2	1:B:272:ILE:HD11	1.99	0.45
1:A:257:THR:HG21	1:A:265:ASP:HB3	1.98	0.45
5:I:95:TRP:HB2	5:I:104:ILE:HD11	1.99	0.45
7:M:337:VAL:HA	7:M:399:GLY:HA2	1.98	0.45
5:I:416:PHE:CD2	5:I:434:ALA:HB1	2.52	0.45
4:H:478:LEU:HB3	4:H:516:VAL:HA	1.99	0.44
5:J:173:THR:HB	5:J:174:TYR:H	1.62	0.44
5:J:338:LYS:HG3	5:J:356:LYS:HG2	1.99	0.44
6:K:46:ILE:HG13	6:K:85:LEU:HB2	1.98	0.44
7:M:462:LEU:HD22	7:M:503:ARG:HG2	2.00	0.44
1:A:24:ILE:HG12	1:A:102:VAL:HA	1.98	0.44
3:E:5:ALA:HB3	3:E:92:ILE:HG12	1.99	0.44
3:E:179:PRO:HA	3:E:180:PRO:HD3	1.80	0.44
7:N:145:ALA:HB3	7:N:189:VAL:HG23	1.99	0.44
1:A:136:PHE:HE1	1:A:165:LEU:HD12	1.83	0.44
5:I:351:ILE:HG12	5:I:368:ILE:HD12	1.99	0.44
1:A:214:TYR:HA	1:A:275:THR:HB	1.99	0.44
4:G:319:LEU:O	4:G:323:LEU:HG	2.17	0.44
5:I:139:VAL:HG11	5:I:235:ILE:HD11	1.99	0.44
1:A:21:THR:HG21	1:A:234:HIS:NE2	2.32	0.44
1:A:187:VAL:HG23	1:B:270:PRO:HG3	1.99	0.44
2:D:285:ALA:O	2:D:289:ARG:N	2.51	0.44
3:E:178:ILE:HG23	3:E:396:ASN:HD21	1.83	0.44
4:G:432:ARG:N	4:G:433:PRO:HD2	2.33	0.44
4:G:284:TYR:HE1	4:G:286:ILE:HB	1.83	0.44
1:A:201:VAL:HG11	1:A:295:VAL:HG21	1.99	0.44
1:A:241:PRO:HB3	1:A:247:LEU:HG	2.00	0.44
7:M:165:LYS:HA	7:M:296:GLU:OE1	2.18	0.44
5:J:37:GLU:HG2	5:J:49:ARG:HB2	2.00	0.44
5:J:418:VAL:HG22	5:J:461:THR:HG22	1.99	0.44
7:N:247:LEU:HD23	7:N:281:VAL:HB	2.00	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLU:OE2	1:B:260:THR:C	2.57	0.43
1:B:23:PRO:CG	1:B:235:LYS:HZ3	2.31	0.43
5:I:234:ARG:HB2	5:I:284:ARG:HD2	2.00	0.43
5:I:339:ILE:H	5:I:339:ILE:HG13	1.67	0.43
7:N:98:GLN:HE22	7:N:396:ILE:HD11	1.83	0.43
3:E:294:SER:HA	3:E:299:ALA:HB3	2.00	0.43
2:C:26:VAL:HA	2:C:29:LEU:HD12	1.99	0.43
2:D:196:VAL:HG21	2:D:261:GLY:HA3	2.00	0.43
1:A:170:GLU:CG	1:B:260:THR:O	2.66	0.43
3:E:16:ALA:HB3	3:E:17:PRO:HD3	2.00	0.43
3:F:98:VAL:HG12	3:F:139:LYS:HG2	2.00	0.43
4:G:291:PRO:HA	4:G:294:ILE:HD12	2.00	0.43
5:J:163:ILE:HD11	5:J:271:LYS:HB3	2.01	0.43
6:L:119:PHE:HE1	6:L:164:ASP:HB3	1.83	0.43
7:M:339:GLY:HA2	7:M:397:GLY:HA2	2.00	0.43
1:A:10:TYR:HE1	1:A:26:ALA:HB2	1.82	0.43
1:B:23:PRO:HG2	1:B:235:LYS:HZ2	1.84	0.43
1:B:120:ILE:HD13	1:B:147:ILE:HD12	2.01	0.43
2:C:328:ARG:HA	2:C:331:LEU:HB2	1.99	0.43
1:B:290:LEU:HD22	1:B:294:ALA:HB1	2.00	0.43
2:C:67:ILE:HA	2:C:70:LEU:HD12	2.00	0.43
4:H:401:VAL:HB	4:H:470:VAL:HG22	1.99	0.43
5:I:135:VAL:HG22	5:I:235:ILE:HG23	2.01	0.43
4:G:450:ASN:HB3	5:I:341:LYS:NZ	2.34	0.43
1:A:170:GLU:OE2	1:B:260:THR:HB	2.19	0.43
3:F:101:ILE:HG23	3:F:102:GLU:HG3	2.01	0.43
1:B:16:GLU:HB3	1:B:17:ASP:H	1.70	0.43
1:B:21:THR:HB	1:B:24:ILE:HD12	1.97	0.43
1:B:201:VAL:HG22	1:B:207:ILE:HG13	2.01	0.43
4:G:507:CYS:SG	4:G:508:GLU:N	2.91	0.43
2:D:316:GLY:CA	2:D:337:ILE:HG13	2.49	0.43
5:J:64:LEU:HA	5:J:67:LEU:HD12	2.00	0.43
7:M:142:TYR:CD1	7:M:319:ARG:NH2	2.87	0.43
1:A:242:LEU:HB2	4:G:504:LEU:HD11	2.00	0.42
4:H:327:ILE:HA	4:H:330:LEU:HD12	2.01	0.42
4:H:409:LEU:O	4:H:413:LEU:HG	2.19	0.42
1:B:139:LEU:C	1:B:139:LEU:CD2	2.86	0.42
4:G:399:THR:HA	4:G:425:LYS:HB2	2.01	0.42
1:B:283:LEU:CA	1:B:291:THR:OG1	2.67	0.42
2:C:152:GLN:HA	2:C:155:ILE:HD12	2.00	0.42
5:I:155:MET:HB3	5:I:274:TYR:CE1	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ALA:HB2	2:C:83:SER:HB2	2.02	0.42
4:G:256:LEU:HB3	4:G:526:LEU:HB3	2.01	0.42
4:H:480:ASN:HB2	4:H:482:PHE:HD1	1.83	0.42
5:J:327:LYS:HE2	5:J:331:VAL:HG11	2.02	0.42
5:J:370:GLU:HB3	5:J:371:ASN:HD22	1.85	0.42
6:K:25:GLN:H	6:K:34:VAL:HG11	1.85	0.42
7:M:313:PRO:HA	7:M:345:GLY:HA3	2.01	0.42
2:D:168:ILE:H	2:D:168:ILE:HG13	1.72	0.42
5:I:27:LEU:H	5:I:73:HIS:CD2	2.37	0.42
7:M:179:CYS:HA	7:M:180:PRO:HD3	1.94	0.42
1:A:139:LEU:C	1:A:139:LEU:HD23	2.40	0.42
1:B:31:VAL:HG21	1:B:98:GLY:CA	2.49	0.42
2:C:151:ARG:H	2:C:151:ARG:HD2	1.85	0.42
7:N:356:ARG:HB2	7:N:416:VAL:HG23	2.02	0.42
2:C:25:PHE:CE2	2:C:29:LEU:HD11	2.54	0.42
3:E:64:LEU:HA	3:E:65:PRO:HD3	1.84	0.42
3:F:253:LEU:HD11	5:I:218:LEU:HD21	2.01	0.42
3:F:160:LEU:H	3:F:161:PRO:CD	2.29	0.42
5:J:76:PHE:HD2	5:J:107:ILE:HD11	1.85	0.42
6:K:126:LEU:O	6:K:129:THR:HG22	2.20	0.42
5:J:308:LEU:HB2	5:J:326:TYR:CE1	2.55	0.42
7:N:312:SER:HA	7:N:313:PRO:HD3	1.84	0.42
1:A:97:ASN:HA	1:A:100:LEU:HB2	2.02	0.41
6:K:198:ILE:HG13	7:M:404:PRO:HD3	2.02	0.41
2:C:21:THR:O	2:C:24:THR:HG22	2.20	0.41
5:J:159:ASP:HB3	5:J:162:HIS:CD2	2.55	0.41
1:A:41:THR:HA	6:L:75:ARG:HH11	1.85	0.41
1:B:146:PHE:HB2	5:I:332:VAL:CG1	2.50	0.41
2:C:255:VAL:HG12	2:C:290:THR:HG21	2.02	0.41
2:C:262:THR:HA	2:C:273:SER:HA	2.01	0.41
3:F:246:ASP:HA	3:F:249:LYS:HB2	2.01	0.41
4:G:334:ARG:HA	4:G:335:PRO:HD3	1.96	0.41
7:M:440:LEU:HD12	7:M:451:ALA:HB3	2.03	0.41
7:N:140:LEU:O	7:N:319:ARG:NH1	2.54	0.41
1:B:136:PHE:CZ	1:B:169:LEU:HG	2.55	0.41
2:C:243:VAL:HA	2:C:244:PRO:HD2	1.92	0.41
5:J:37:GLU:C	5:J:39:ARG:H	2.24	0.41
6:K:247:ALA:HA	6:K:250:LYS:HE3	2.02	0.41
7:M:149:LYS:HD3	7:M:151:GLN:HE21	1.85	0.41
1:A:57:ILE:HA	1:A:60:ILE:HD12	2.03	0.41
1:B:31:VAL:HG21	1:B:98:GLY:HA2	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:97:PRO:HA	3:E:141:ILE:HD13	2.03	0.41
3:E:265:ASN:HD21	5:J:227:ARG:HG2	1.86	0.41
4:H:271:HIS:HA	4:H:272:PRO:HD3	1.84	0.41
4:H:533:VAL:HG13	4:H:558:ARG:HH22	1.85	0.41
6:K:104:LYS:O	6:K:108:VAL:HG23	2.20	0.41
7:N:357:PRO:HG2	7:N:415:GLN:HA	2.02	0.41
1:B:207:ILE:HD13	1:B:229:VAL:HG21	2.02	0.41
2:C:361:ILE:HA	2:C:364:ILE:HD13	2.03	0.41
2:D:232:LYS:O	2:D:235:GLN:HB2	2.21	0.41
4:H:355:ASP:HA	4:H:356:PRO:HD3	1.93	0.41
5:J:349:THR:HA	5:J:366:CYS:H	1.84	0.41
5:J:435:SER:HA	5:J:436:PRO:HD3	1.94	0.41
1:A:113:ALA:CB	1:A:138:LEU:HD23	2.43	0.41
4:H:410:THR:O	4:H:414:LEU:HG	2.21	0.41
1:A:9:THR:O	1:A:12:ARG:HB2	2.20	0.41
1:A:269:GLY:HA2	1:A:270:PRO:HD2	1.90	0.41
2:C:293:PHE:CZ	2:C:348:ILE:HD13	2.56	0.41
5:J:194:CYS:SG	5:J:195:ILE:N	2.93	0.41
7:N:104:GLY:HA3	7:N:211:MET:HG2	2.03	0.41
7:N:142:TYR:CD1	7:N:142:TYR:C	2.95	0.41
7:N:430:ILE:HG13	7:N:485:LEU:HB2	2.02	0.41
1:A:304:TYR:HB3	2:D:116:PRO:HB3	2.02	0.41
2:D:80:THR:HG21	2:D:314:GLU:HB2	2.03	0.41
2:D:233:LEU:HA	2:D:238:ILE:HD12	2.03	0.41
5:J:155:MET:HB3	5:J:274:TYR:CE1	2.56	0.41
7:N:349:LEU:HD12	7:N:388:LYS:HG2	2.02	0.41
2:D:193:SER:HB2	2:D:196:VAL:HG23	2.03	0.40
2:C:227:HIS:ND1	4:G:547:LYS:HD2	2.37	0.40
6:K:33:TYR:HB3	6:K:45:MET:HB3	2.04	0.40
7:M:245:ILE:HG12	7:M:279:PRO:HG2	2.03	0.40
1:B:240:PHE:HA	1:B:241:PRO:HD3	1.92	0.40
4:G:416:ASN:HA	4:G:420:LEU:HD12	2.03	0.40
3:F:4:GLN:HG3	3:F:167:PHE:HB3	2.03	0.40
5:J:300:GLY:HA2	5:J:324:HIS:CE1	2.56	0.40
7:M:194:CYS:HA	7:M:195:PRO:HD3	1.91	0.40
1:B:293:SER:HB2	2:C:359:SER:O	2.22	0.40
3:F:141:ILE:H	3:F:141:ILE:HG13	1.67	0.40
3:F:314:PRO:HA	3:F:315:PRO:HD3	1.98	0.40
5:J:268:ILE:HD13	5:J:271:LYS:HD2	2.03	0.40
7:M:106:ILE:HD13	7:M:232:HIS:HB3	2.04	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%)	240 (80%)	52 (17%)	8 (3%)	5	34
1	B	300/305 (98%)	245 (82%)	44 (15%)	11 (4%)	3	27
2	C	339/381 (89%)	296 (87%)	36 (11%)	7 (2%)	7	38
2	D	339/381 (89%)	296 (87%)	33 (10%)	10 (3%)	4	32
3	E	253/578 (44%)	206 (81%)	41 (16%)	6 (2%)	6	36
3	F	253/578 (44%)	204 (81%)	42 (17%)	7 (3%)	5	33
4	G	349/651 (54%)	277 (79%)	58 (17%)	14 (4%)	3	25
4	H	349/651 (54%)	293 (84%)	41 (12%)	15 (4%)	2	25
5	I	427/712 (60%)	358 (84%)	51 (12%)	18 (4%)	3	25
5	J	427/712 (60%)	357 (84%)	49 (12%)	21 (5%)	2	23
6	K	237/304 (78%)	198 (84%)	33 (14%)	6 (2%)	5	35
6	L	237/304 (78%)	200 (84%)	34 (14%)	3 (1%)	12	48
7	M	398/527 (76%)	329 (83%)	61 (15%)	8 (2%)	7	40
7	N	398/527 (76%)	341 (86%)	52 (13%)	5 (1%)	12	48
8	O	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	18
8	P	15/285 (5%)	12 (80%)	2 (13%)	1 (7%)	1	18
All	All	4636/7486 (62%)	3865 (83%)	630 (14%)	141 (3%)	7	31

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	PRO
1	B	158	PRO
1	B	291	THR
2	C	276	SER
3	E	100	GLU
3	F	100	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	G	487	ALA
4	H	536	ASP
5	I	202	LEU
5	J	202	LEU
1	B	98	GLY
1	B	304	TYR
2	D	337	ILE
3	F	180	PRO
4	G	265	LEU
4	G	357	SER
4	G	397	SER
4	G	579	LYS
4	G	586	SER
4	H	537	TYR
5	I	330	ASP
5	I	464	VAL
5	J	182	PRO
5	J	201	PRO
5	J	464	VAL
5	J	467	VAL
6	K	64	ARG
6	K	81	GLY
7	M	507	LYS
7	N	497	GLU
7	N	507	LYS
1	A	5	ASN
1	A	61	PRO
1	A	267	LEU
1	A	291	THR
1	B	38	THR
2	C	275	ASN
2	C	337	ILE
2	D	58	ASN
2	D	237	ASN
2	D	275	ASN
2	D	276	SER
3	E	160	LEU
3	F	160	LEU
3	F	311	GLN
4	H	289	SER
4	H	397	SER
5	I	58	PRO

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	I	112	ALA
5	I	421	ASP
5	I	423	ASN
5	J	112	ALA
5	J	355	THR
5	J	371	ASN
5	J	388	ASN
5	J	423	ASN
5	J	459	ASP
6	K	225	ALA
6	L	132	TRP
7	M	164	PHE
8	O	129	LEU
8	P	129	LEU
1	A	16	GLU
1	A	97	ASN
1	B	5	ASN
1	B	16	GLU
1	B	263	LEU
1	B	267	LEU
2	C	79	PRO
2	D	274	SER
3	E	73	ASN
3	E	306	THR
3	F	309	GLN
4	G	269	LEU
4	G	359	PRO
4	G	537	TYR
4	G	542	GLU
4	H	245	THR
4	H	248	GLU
4	H	542	GLU
4	H	555	ILE
4	H	579	LYS
5	I	82	HIS
5	I	305	PRO
5	I	399	ASN
5	I	459	ASP
5	J	26	ARG
5	J	48	PRO
5	J	311	ASN
5	J	336	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	K	49	SER
6	L	259	GLY
1	A	38	THR
1	B	253	PRO
2	D	16	SER
2	D	289	ARG
3	E	16	ALA
3	E	245	ARG
4	G	242	VAL
4	G	548	GLY
4	H	251	PHE
4	H	421	LYS
5	I	98	PRO
5	I	311	ASN
5	I	342	CYS
5	J	44	THR
7	M	127	ARG
7	M	177	PRO
7	M	178	GLY
7	N	122	GLY
7	N	227	PRO
7	N	383	GLU
1	A	270	PRO
2	C	303	PRO
2	D	191	PRO
4	G	540	PRO
4	H	548	GLY
5	I	369	GLY
5	J	126	GLY
5	J	192	SER
5	J	304	TYR
5	J	369	GLY
7	M	383	GLU
4	G	555	ILE
6	K	197	GLY
6	L	63	ILE
2	C	11	PRO
4	H	242	VAL
5	I	163	ILE
7	M	122	GLY
2	C	177	ILE
3	F	65	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	H	539	ASN
4	H	545	GLY
5	I	182	PRO
5	I	466	ILE
7	M	138	ILE
2	D	177	ILE
3	F	255	ILE
5	J	215	PRO
6	K	133	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%)	221 (86%)	36 (14%)	3	19
1	B	257/265 (97%)	229 (89%)	28 (11%)	6	25
2	C	286/338 (85%)	245 (86%)	41 (14%)	3	18
2	D	286/338 (85%)	255 (89%)	31 (11%)	6	26
3	E	249/529 (47%)	231 (93%)	18 (7%)	14	41
3	F	249/529 (47%)	231 (93%)	18 (7%)	14	41
4	G	305/561 (54%)	283 (93%)	22 (7%)	14	41
4	H	305/561 (54%)	278 (91%)	27 (9%)	9	33
5	I	389/649 (60%)	354 (91%)	35 (9%)	9	32
5	J	389/649 (60%)	358 (92%)	31 (8%)	12	38
6	K	219/273 (80%)	186 (85%)	33 (15%)	3	16
6	L	219/273 (80%)	189 (86%)	30 (14%)	3	19
7	M	319/449 (71%)	302 (95%)	17 (5%)	22	50
7	N	319/449 (71%)	308 (97%)	11 (3%)	37	61
8	O	16/246 (6%)	15 (94%)	1 (6%)	18	44
8	P	16/246 (6%)	16 (100%)	0	100	100
All	All	4080/6620 (62%)	3701 (91%)	379 (9%)	12	30



All (379) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	13	PHE
1	A	14	LEU
1	A	15	GLU
1	A	17	ASP
1	A	21	THR
1	A	24	ILE
1	A	37	LYS
1	A	54	GLU
1	A	56	LEU
1	A	93	HIS
1	A	101	PHE
1	A	119	PHE
1	A	126	ILE
1	A	136	PHE
1	A	144	ASN
1	A	147	ILE
1	A	166	TYR
1	A	169	LEU
1	A	172	LYS
1	A	188	ILE
1	A	192	ASP
1	A	207	ILE
1	A	231	THR
1	A	232	GLU
1	A	236	PHE
1	A	237	VAL
1	A	242	LEU
1	A	243	SER
1	A	247	LEU
1	A	255	ASP
1	A	280	ILE
1	A	287	LEU
1	A	290	LEU
1	A	297	GLU
1	A	304	TYR
1	B	9	THR
1	B	12	ARG
1	B	15	GLU
1	B	21	THR
1	B	37	LYS
1	B	54	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	56	LEU
1	B	75	ARG
1	B	79	ARG
1	B	86	ASP
1	B	100	LEU
1	B	104	ARG
1	B	109	ARG
1	B	136	PHE
1	B	140	ASN
1	B	148	ARG
1	B	149	PHE
1	B	161	GLN
1	B	166	TYR
1	B	172	LYS
1	B	231	THR
1	B	232	GLU
1	B	237	VAL
1	B	242	LEU
1	B	255	ASP
1	B	267	LEU
1	B	293	SER
1	B	295	VAL
2	C	17	ASP
2	C	22	ILE
2	C	24	THR
2	C	31	ARG
2	C	38	TYR
2	C	40	ILE
2	C	69	ASP
2	C	95	LEU
2	C	151	ARG
2	C	153	VAL
2	C	168	ILE
2	C	175	ILE
2	C	179	LEU
2	C	180	ILE
2	C	190	THR
2	C	199	PHE
2	C	201	ILE
2	C	206	ARG
2	C	222	ASN
2	C	223	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	238	ILE
2	C	249	PHE
2	C	262	THR
2	C	272	ILE
2	C	286	ARG
2	C	288	PHE
2	C	298	LEU
2	C	301	LEU
2	C	307	PHE
2	C	314	GLU
2	C	320	ARG
2	C	322	LEU
2	C	331	LEU
2	C	336	GLN
2	C	346	ILE
2	C	347	ASP
2	C	361	ILE
2	C	363	ARG
2	C	366	TRP
2	C	369	TYR
2	C	371	GLN
2	D	17	ASP
2	D	24	THR
2	D	38	TYR
2	D	44	THR
2	D	47	LEU
2	D	62	ASP
2	D	80	THR
2	D	84	CYS
2	D	160	ASP
2	D	161	LEU
2	D	164	GLU
2	D	168	ILE
2	D	180	ILE
2	D	199	PHE
2	D	200	LEU
2	D	206	ARG
2	D	222	ASN
2	D	259	ILE
2	D	260	ILE
2	D	284	CYS
2	D	286	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	287	GLU
2	D	298	LEU
2	D	307	PHE
2	D	308	ASP
2	D	330	ARG
2	D	348	ILE
2	D	350	ILE
2	D	363	ARG
2	D	366	TRP
2	D	371	GLN
3	E	3	ILE
3	E	100	GLU
3	E	133	HIS
3	E	153	GLU
3	E	174	PHE
3	E	181	GLN
3	E	183	LEU
3	E	185	ASP
3	E	249	LYS
3	E	255	ILE
3	E	303	ASP
3	E	384	PHE
3	E	385	ILE
3	E	390	THR
3	E	393	ILE
3	E	398	LEU
3	E	402	MET
3	E	406	ARG
3	F	81	LEU
3	F	100	GLU
3	F	134	HIS
3	F	141	ILE
3	F	173	ASP
3	F	174	PHE
3	F	181	GLN
3	F	192	ASP
3	F	222	PHE
3	F	255	ILE
3	F	258	HIS
3	F	270	THR
3	F	274	ASN
3	F	277	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	F	303	ASP
3	F	384	PHE
3	F	402	MET
3	F	403	ASP
4	G	284	TYR
4	G	293	CYS
4	G	296	MET
4	G	366	ASP
4	G	393	GLN
4	G	395	GLU
4	G	406	SER
4	G	412	LEU
4	G	424	ILE
4	G	434	LEU
4	G	439	LYS
4	G	445	ARG
4	G	455	LEU
4	G	462	ILE
4	G	500	ASN
4	G	523	PHE
4	G	526	LEU
4	G	532	LEU
4	G	536	ASP
4	G	550	LEU
4	G	568	GLU
4	G	576	ILE
4	H	257	ILE
4	H	264	LEU
4	H	284	TYR
4	H	286	ILE
4	H	290	ILE
4	H	293	CYS
4	H	296	MET
4	H	297	LEU
4	H	317	ARG
4	H	319	LEU
4	H	339	THR
4	H	364	LYS
4	H	366	ASP
4	H	408	VAL
4	H	412	LEU
4	H	424	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	H	438	ARG
4	H	455	LEU
4	H	460	ASP
4	H	478	LEU
4	H	491	MET
4	H	503	VAL
4	H	518	LEU
4	H	523	PHE
4	H	532	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	97	LEU
5	I	102	PHE
5	I	106	THR
5	I	113	ARG
5	I	122	LEU
5	I	127	ILE
5	I	132	PHE
5	I	136	SER
5	I	138	ASP
5	I	140	LEU
5	I	158	GLN
5	I	165	THR
5	I	173	THR
5	I	176	LYS
5	I	181	GLU
5	I	211	ILE
5	I	226	ILE
5	I	231	ILE
5	I	232	ASP
5	I	246	PHE
5	I	247	GLN
5	I	276	TYR
5	I	313	GLN
5	I	330	ASP
5	I	345	ILE
5	I	349	THR
5	I	381	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	I	388	ASN
5	I	427	ASP
5	I	457	LEU
5	I	467	VAL
5	J	41	MET
5	J	51	LEU
5	J	62	TYR
5	J	63	THR
5	J	77	LEU
5	J	88	ASP
5	J	89	TYR
5	J	97	LEU
5	J	99	TRP
5	J	113	ARG
5	J	122	LEU
5	J	128	ILE
5	J	131	ASP
5	J	138	ASP
5	J	140	LEU
5	J	141	THR
5	J	173	THR
5	J	174	TYR
5	J	176	LYS
5	J	216	GLU
5	J	219	ASP
5	J	235	ILE
5	J	247	GLN
5	J	279	ASP
5	J	324	HIS
5	J	333	LEU
5	J	341	LYS
5	J	421	ASP
5	J	436	PRO
5	J	457	LEU
5	J	467	VAL
6	K	3	THR
6	K	7	ARG
6	K	11	ASN
6	K	17	ASP
6	K	18	ASP
6	K	19	ILE
6	K	22	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	K	40	ASP
6	K	45	MET
6	K	54	ARG
6	K	59	ILE
6	K	64	ARG
6	K	75	ARG
6	K	79	GLU
6	K	88	ARG
6	K	97	LYS
6	K	109	HIS
6	K	114	TYR
6	K	128	LYS
6	K	129	THR
6	K	137	LYS
6	K	140	HIS
6	K	143	GLU
6	K	154	VAL
6	K	159	GLU
6	K	166	LEU
6	K	168	GLU
6	K	169	LEU
6	K	185	ARG
6	K	230	LEU
6	K	235	LEU
6	K	236	ASP
6	K	251	ILE
6	L	7	ARG
6	L	11	ASN
6	L	17	ASP
6	L	18	ASP
6	L	19	ILE
6	L	45	MET
6	L	47	LEU
6	L	51	LEU
6	L	54	ARG
6	L	59	ILE
6	L	62	LEU
6	L	75	ARG
6	L	79	GLU
6	L	88	ARG
6	L	97	LYS
6	L	119	PHE

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	L	127	TYR
6	L	137	LYS
6	L	143	GLU
6	L	159	GLU
6	L	165	VAL
6	L	166	LEU
6	L	168	GLU
6	L	169	LEU
6	L	185	ARG
6	L	230	LEU
6	L	235	LEU
6	L	236	ASP
6	L	244	LEU
6	L	251	ILE
7	M	111	HIS
7	M	169	GLU
7	M	267	LEU
7	M	291	ILE
7	M	292	ASP
7	M	342	ILE
7	M	353	ILE
7	M	395	LEU
7	M	402	VAL
7	M	403	ASP
7	M	406	LEU
7	M	432	ILE
7	M	475	VAL
7	M	494	GLU
7	M	495	ILE
7	M	508	HIS
7	M	510	ARG
8	O	131	TYR
7	N	142	TYR
7	N	260	LEU
7	N	292	ASP
7	N	351	ASP
7	N	354	GLU
7	N	371	LYS
7	N	386	ASP
7	N	395	LEU
7	N	429	ASP
7	N	432	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	N	508	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	144	ASN
1	A	163	ASN
1	A	277	GLN
1	B	129	HIS
1	B	144	ASN
1	B	209	ASN
2	C	12	ASN
2	C	19	ASN
2	C	221	ASN
2	C	222	ASN
2	C	335	ASN
2	C	352	ASN
2	D	19	ASN
2	D	61	ASN
2	D	66	GLN
2	D	174	GLN
2	D	221	ASN
2	D	222	ASN
2	D	225	ASN
3	E	258	HIS
3	E	265	ASN
3	F	59	GLN
4	G	271	HIS
4	G	416	ASN
4	G	446	ASN
4	H	271	HIS
4	H	450	ASN
5	I	28	GLN
5	I	73	HIS
5	I	247	GLN
5	I	249	ASN
5	I	335	GLN
5	J	87	ASN
5	J	124	ASN
5	J	316	GLN
5	J	359	ASN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
5	J	371	ASN
6	K	41	ASN
6	L	23	ASN
6	L	103	GLN
7	M	98	GLN
7	M	151	GLN
7	M	324	ASN
7	N	98	GLN
7	N	111	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SEP	L	52	6	8,9,10	0.66	0	8,12,14	1.40	1 (12%)
6	SEP	K	52	6	8,9,10	0.62	0	8,12,14	1.18	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	52	SEP	OG-CB-CA	2.74	110.81	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

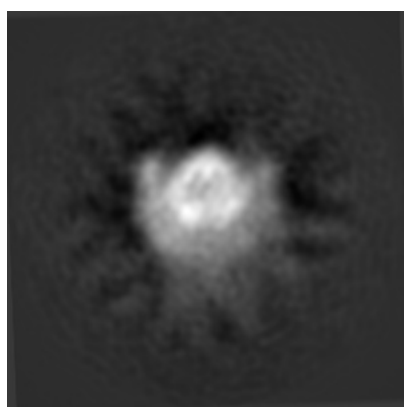
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4548. These allow visual inspection of the internal detail of the map and identification of artifacts.

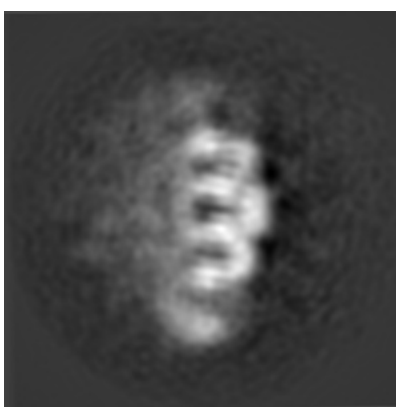
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

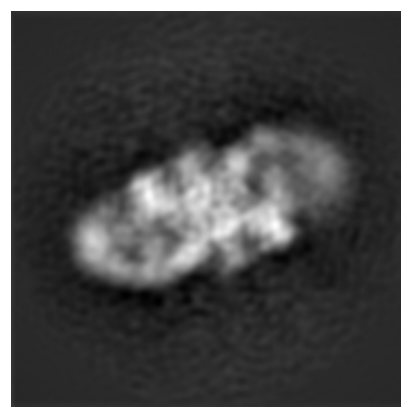
#### 6.1.1 Primary map



X



Y

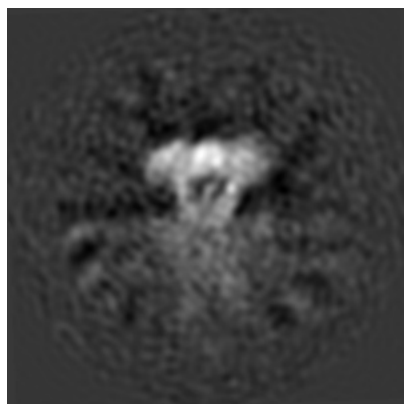


Z

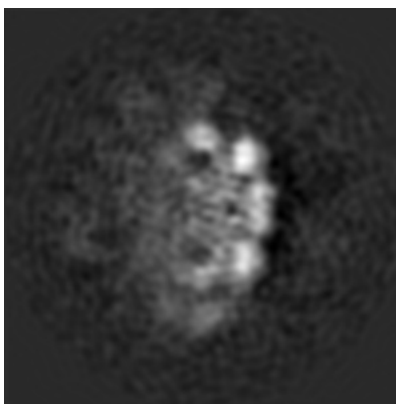
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

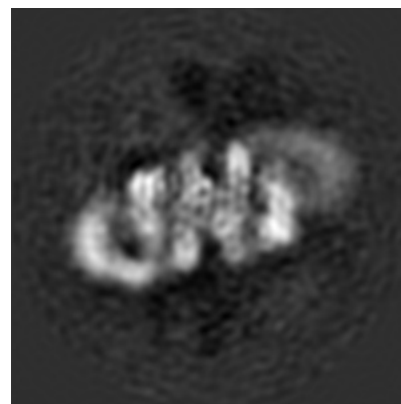
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

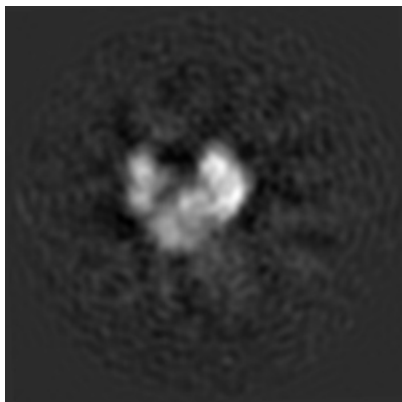


Z Index: 140

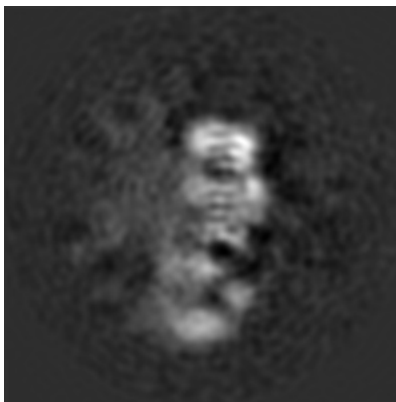
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

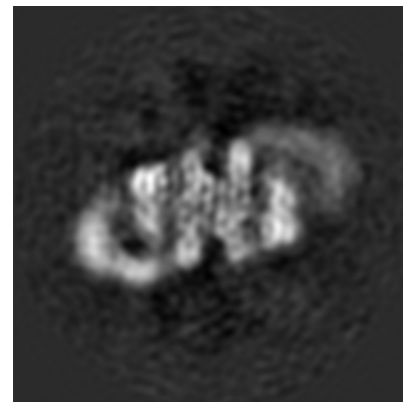
### 6.3.1 Primary map



X Index: 96



Y Index: 126

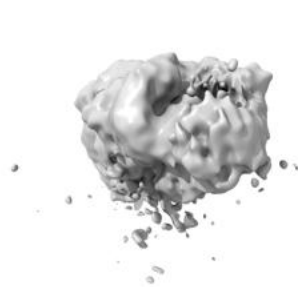


Z Index: 143

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

## 6.4 Orthogonal surface views [i](#)

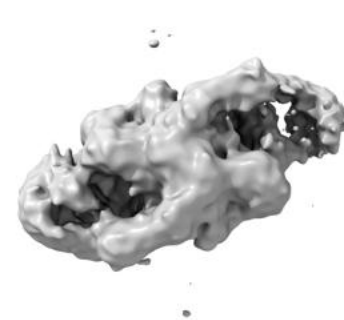
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

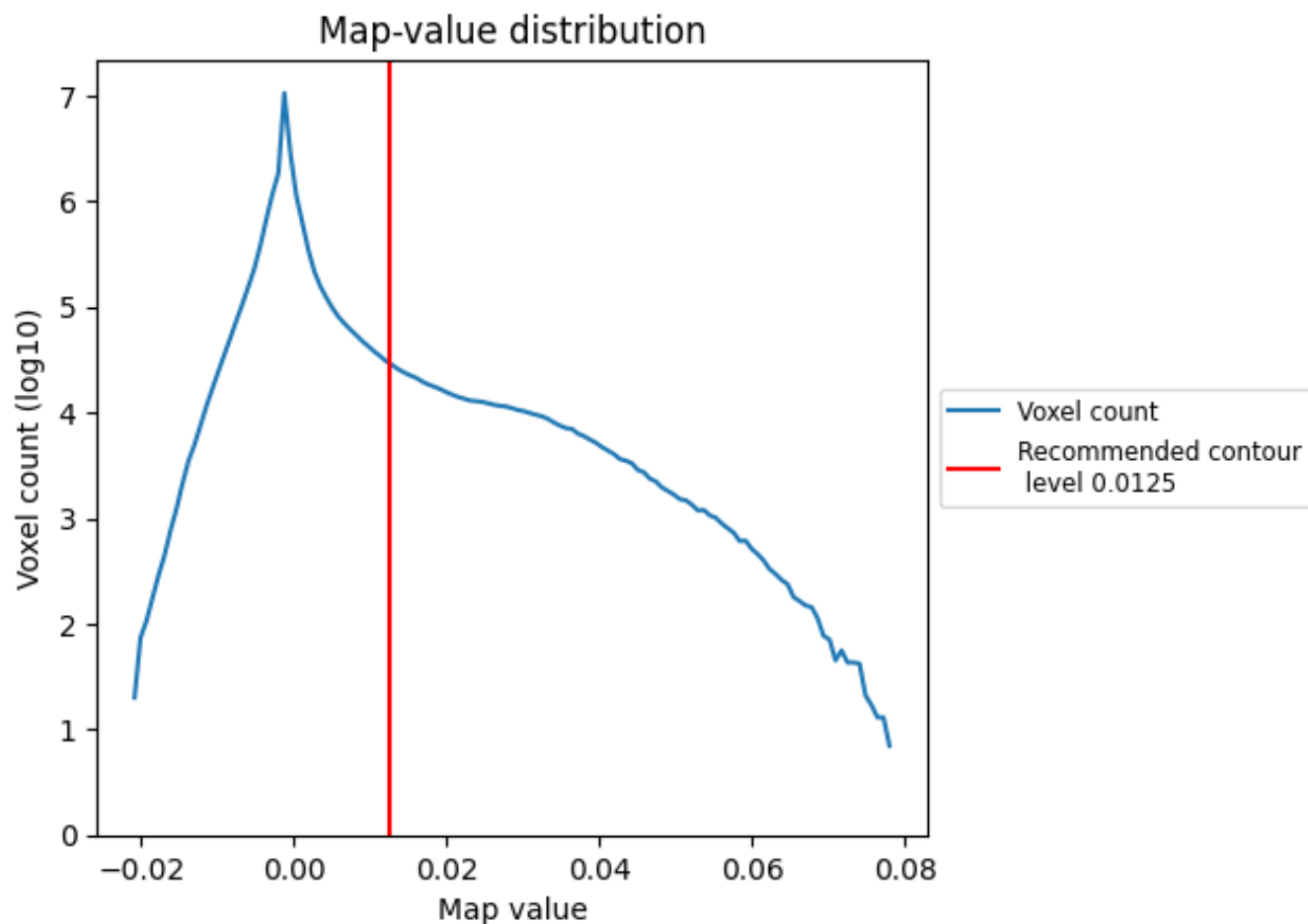
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

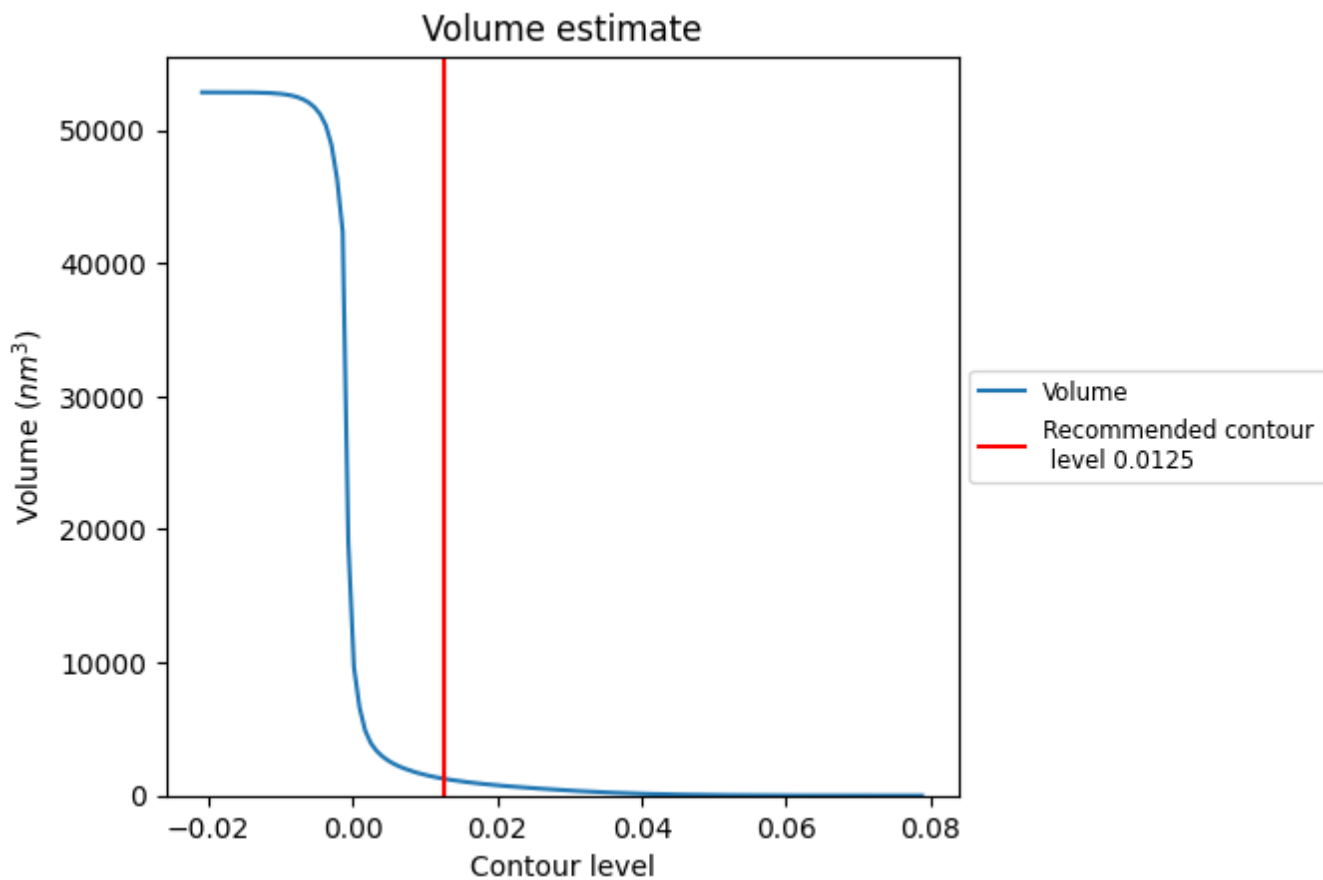
### 7.1 Map-value distribution [i](#)



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



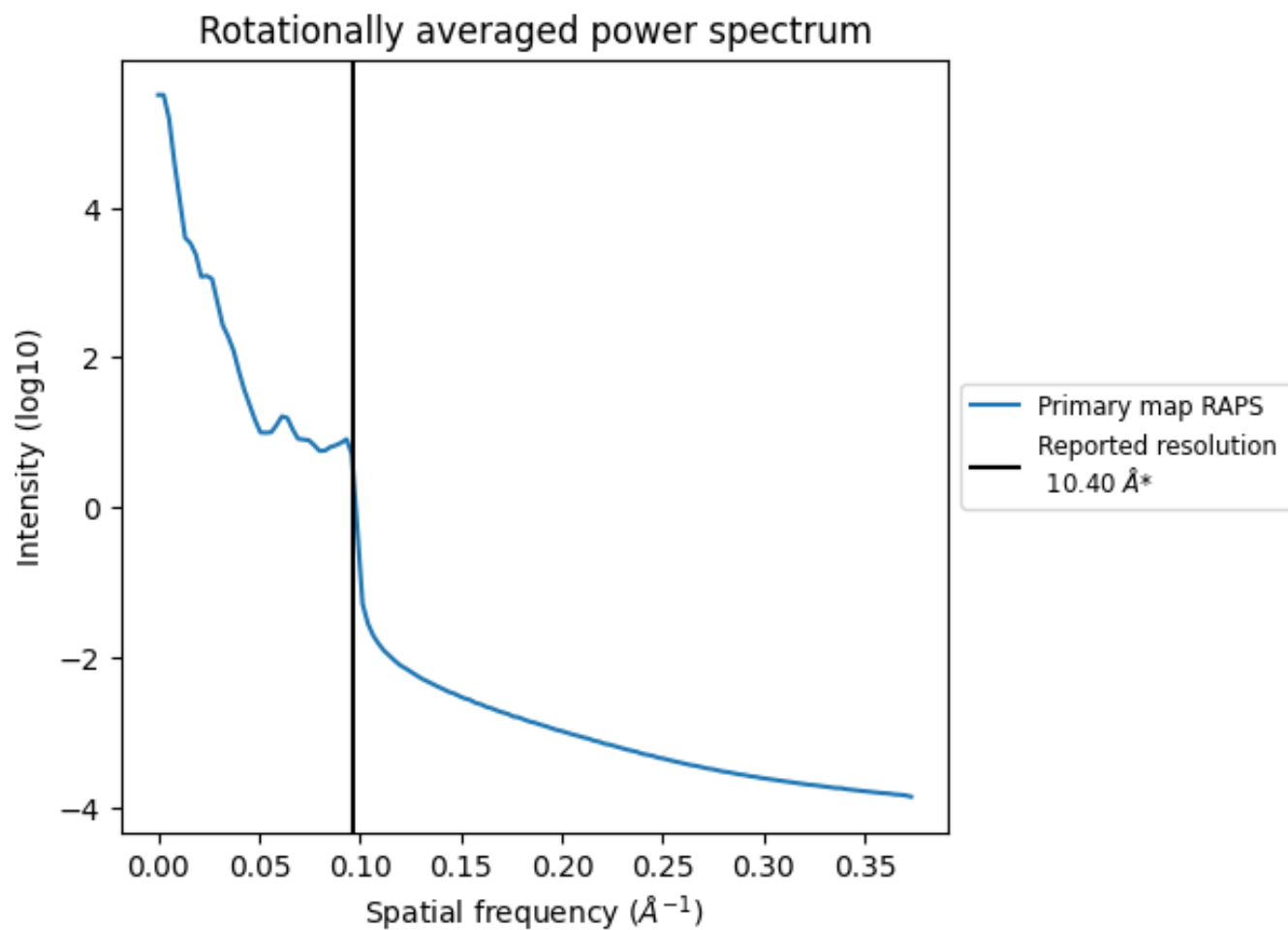
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1275 nm<sup>3</sup>; this corresponds to an approximate mass of 1151 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  $0.096 \text{\AA}^{-1}$

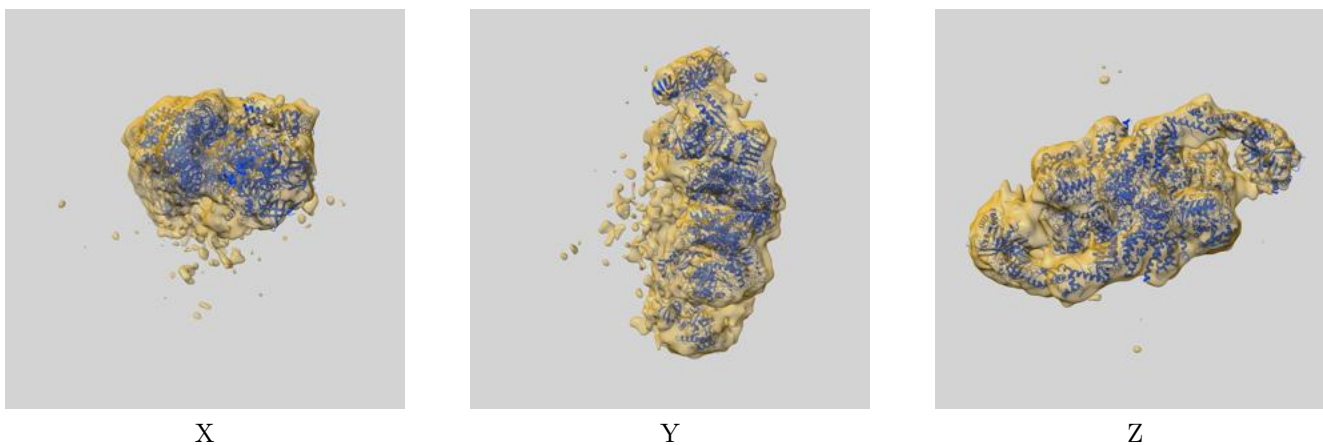
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

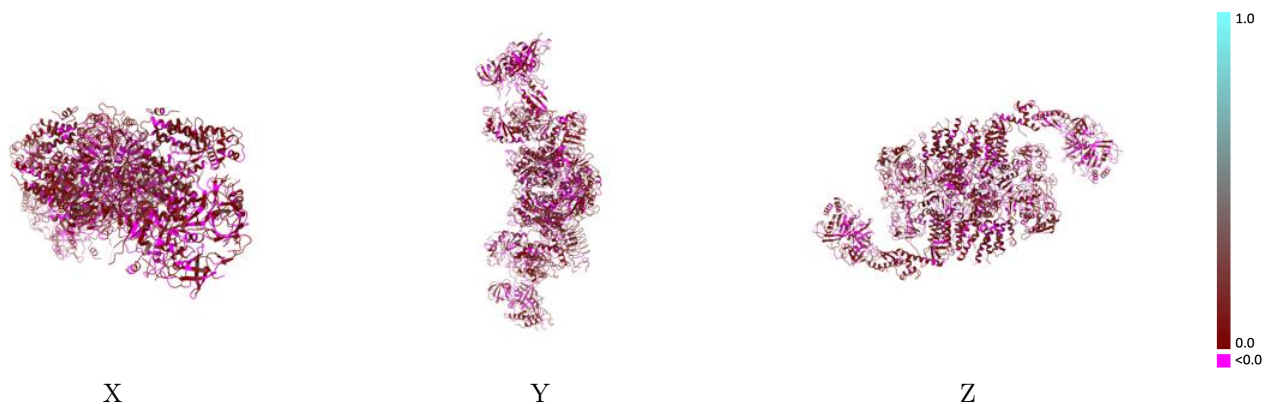
This section contains information regarding the fit between EMDB map EMD-4548 and PDB model 6QG6. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



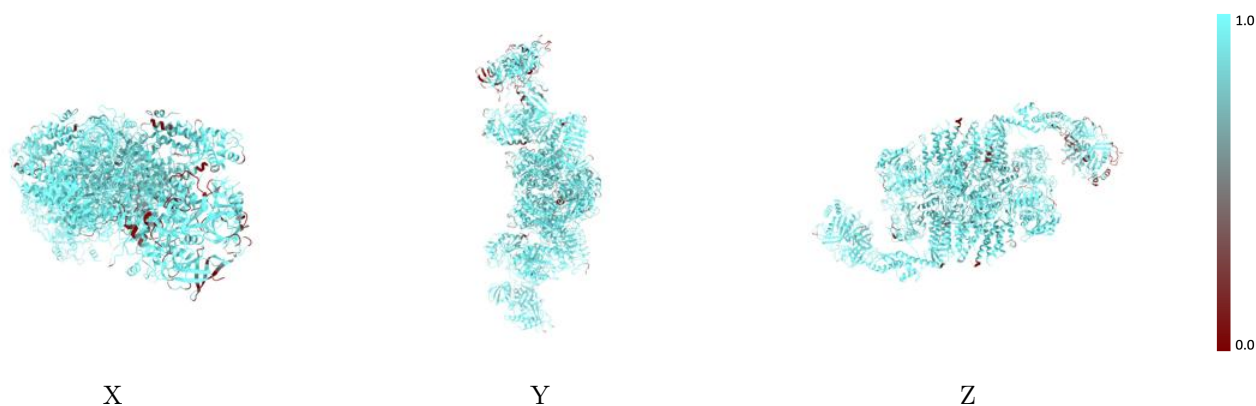
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [\(i\)](#)



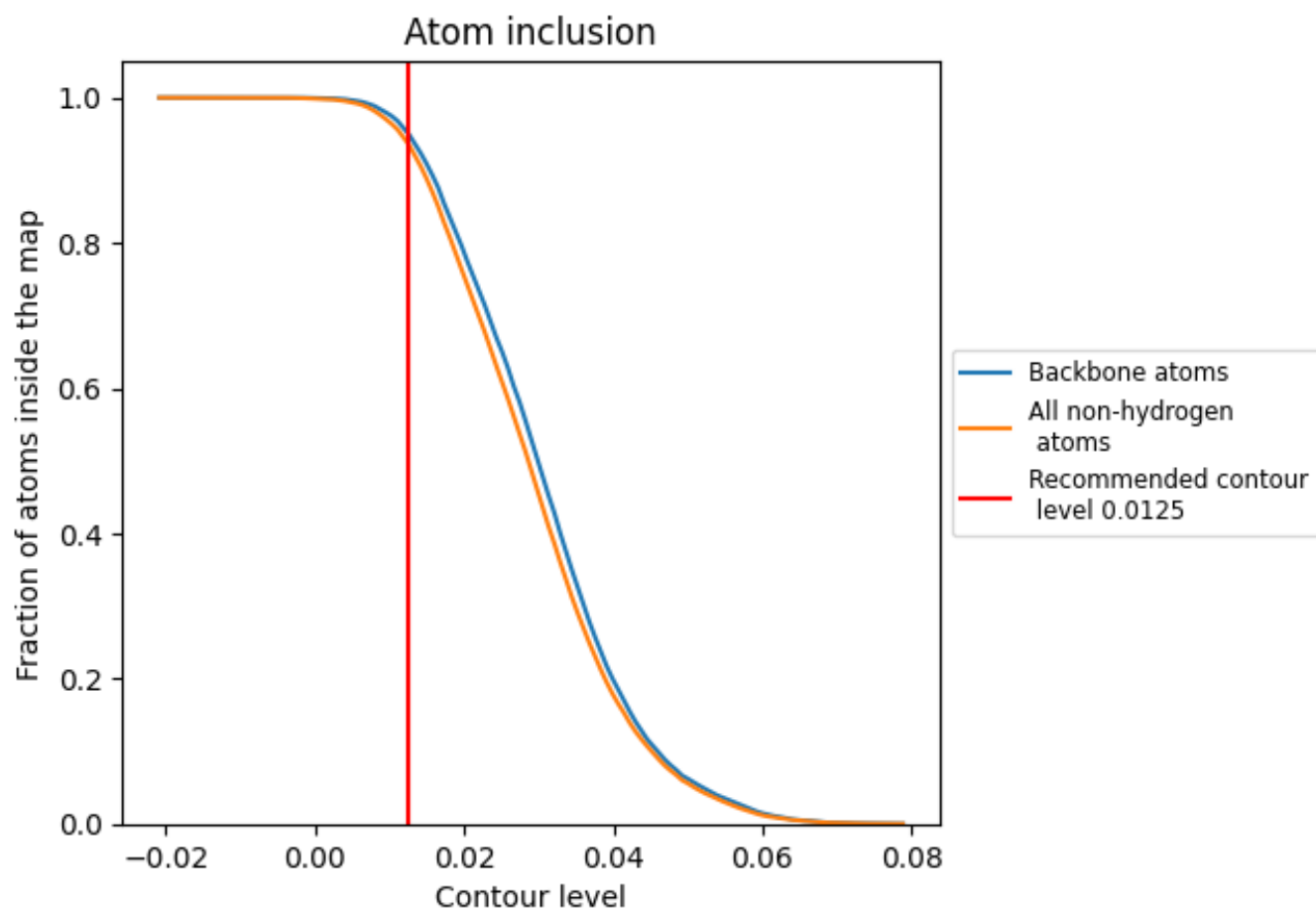
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [\(i\)](#)



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 (0.0125).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9367	 0.0680
A	 0.9775	 0.0750
B	 0.9468	 0.0500
C	 0.9595	 0.0750
D	 0.9553	 0.0730
E	 0.9330	 0.0530
F	 0.9522	 0.0620
G	 0.9287	 0.0800
H	 0.9328	 0.0830
I	 0.9809	 0.0750
J	 0.9734	 0.0820
K	 0.8814	 0.0640
L	 0.9778	 0.0780
M	 0.7611	 0.0470
N	 0.9783	 0.0470
O	 0.4275	 0.0780
P	 1.0000	 0.0400

