



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:35 AM UTC

PDB ID : 6I3M / pdb_00006i3m
EMDB ID : EMD-4404
Title : eIF2B:eIF2 complex, phosphorylated on eIF2 alpha serine 52.
Authors : Adomavicius, T.; Roseman, A.M.; Pavitt, G.D.
Deposited on : 2018-11-06
Resolution : 3.93 Å(reported)
Based on initial models : 5B04, 3JAP

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

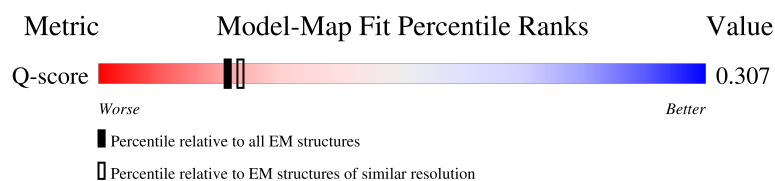
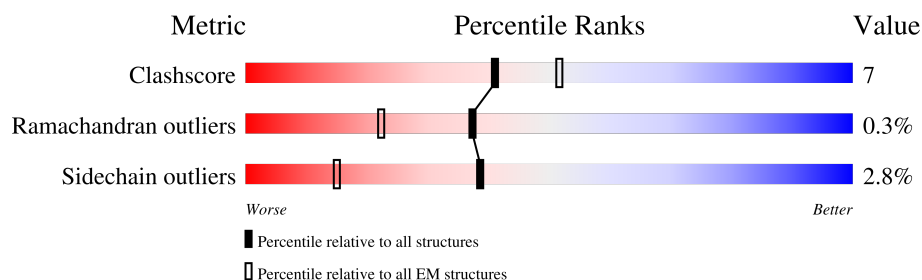
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7811 (3.43 - 4.43)

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 $\leq 5\%$. 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	 7% 82% 18%
1	B	305	 7% 80% 20%
2	C	651	 6% 43% 10% 47%
2	D	651	 6% 43% 10% 47%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	381	
3	F	381	
4	G	712	
4	H	712	
5	I	578	
5	J	578	
6	K	304	
6	L	304	
7	M	285	
7	N	285	
8	O	527	
8	P	527	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 37012 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	305	Total	C	N	O	S	0	0
			2393	1526	400	456	11		
1	B	305	Total	C	N	O	S	0	0
			2393	1526	400	456	11		

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

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

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

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

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

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

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

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

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

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

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

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

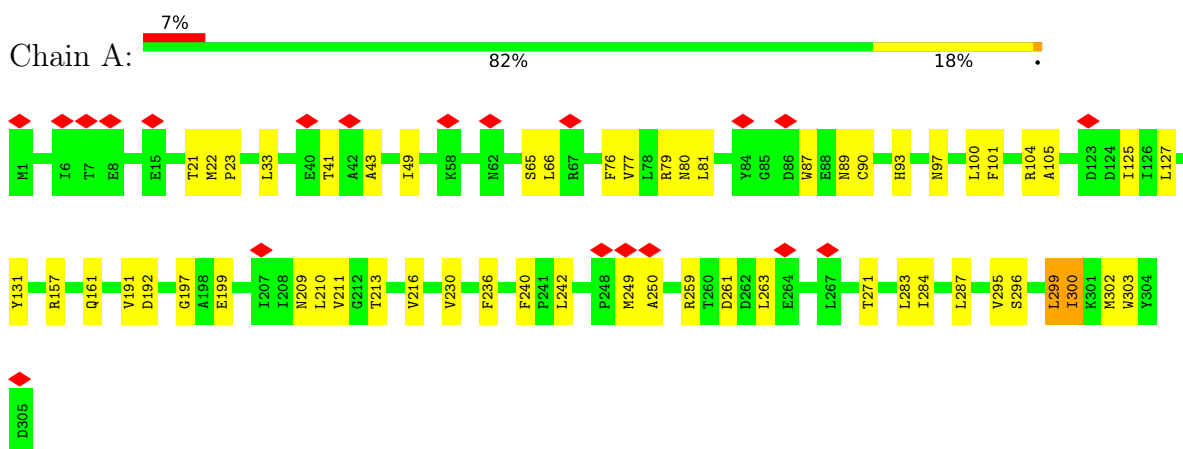
- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

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

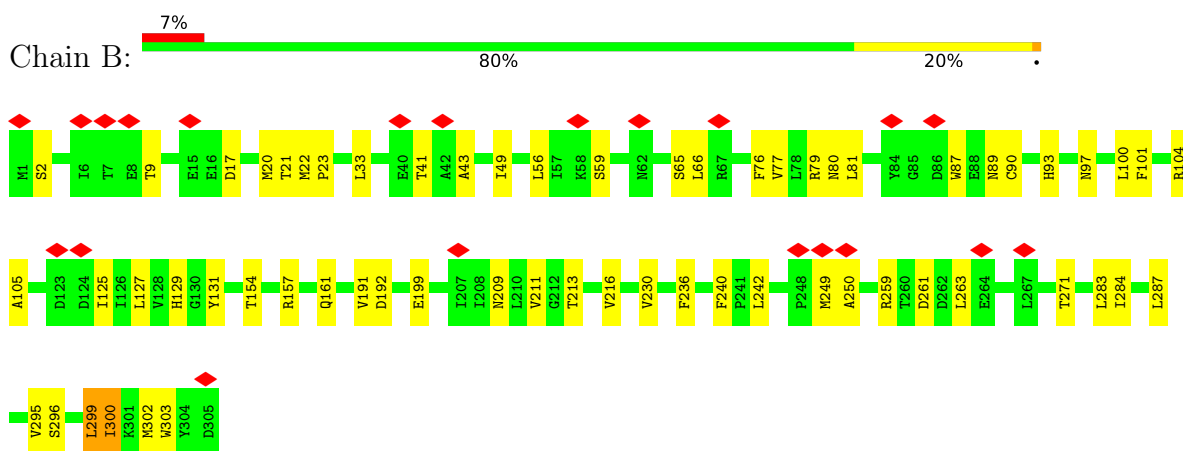
3 Residue-property plots

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.

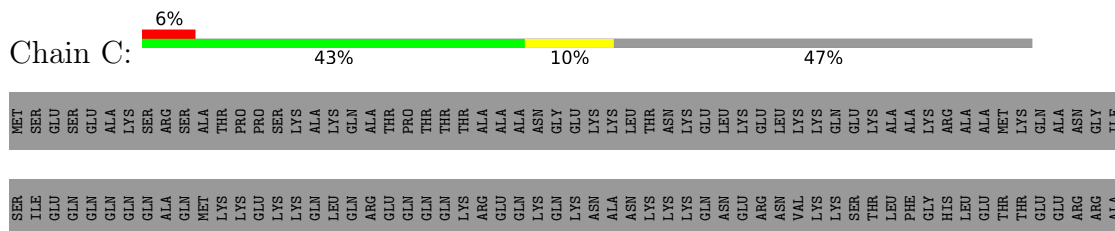
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

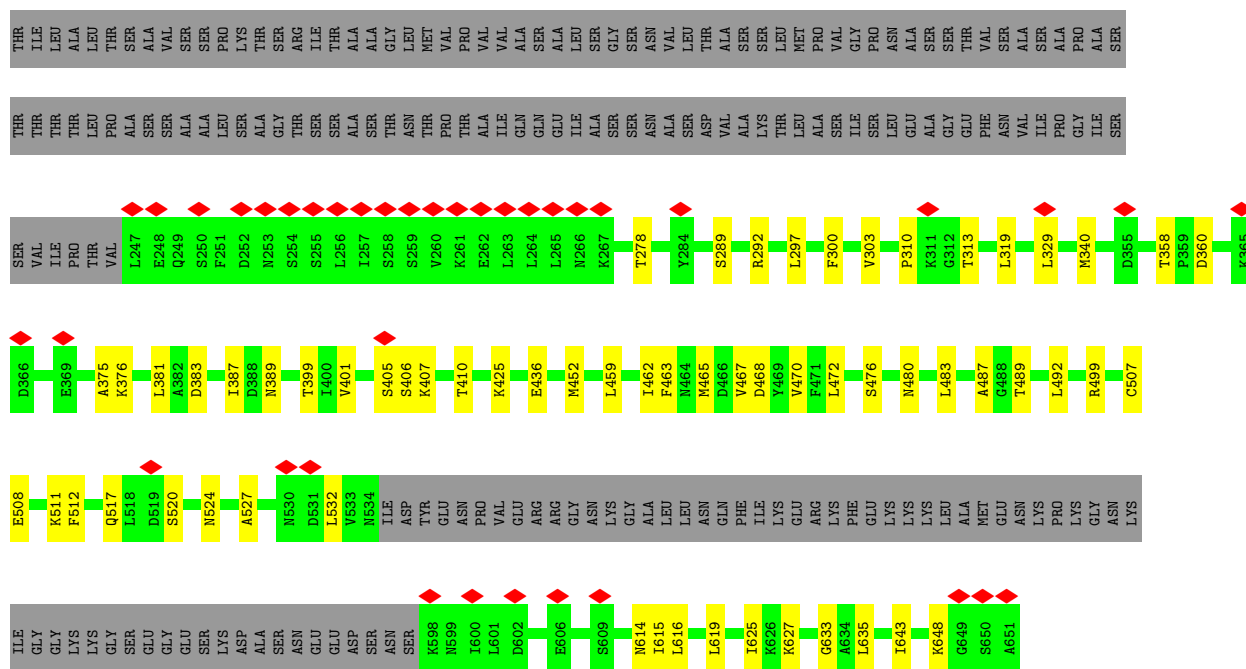


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

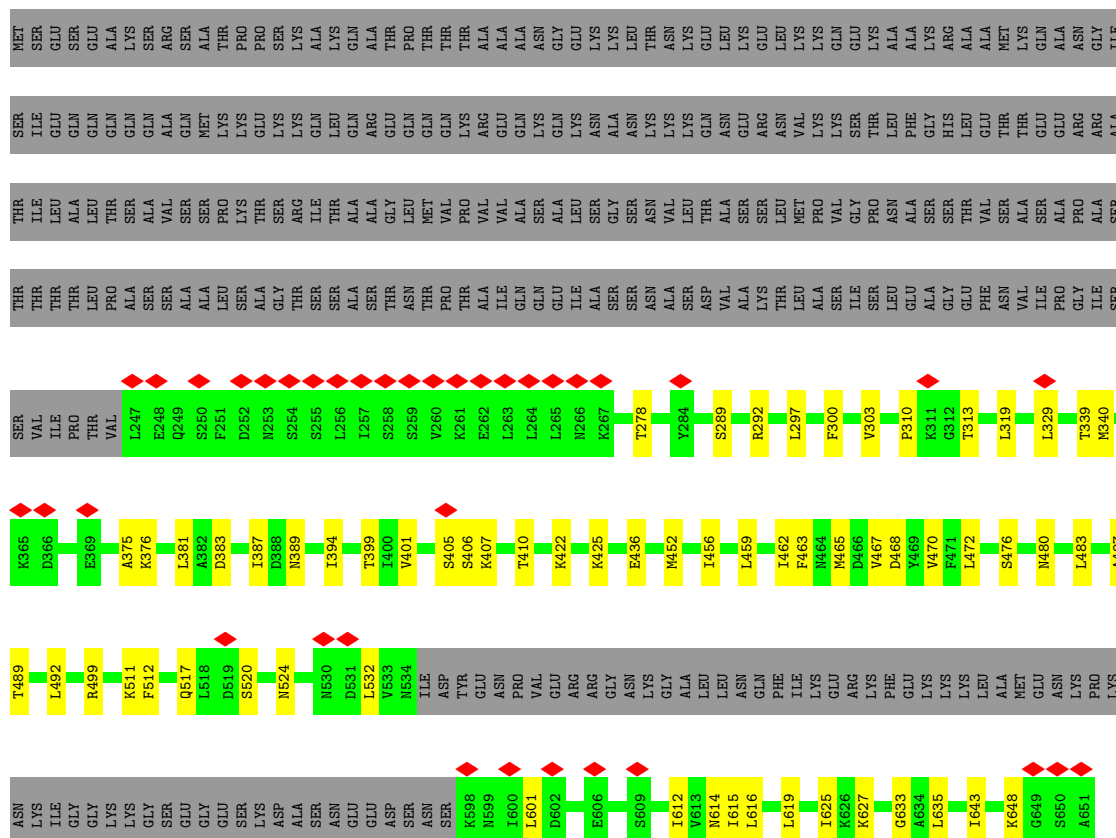
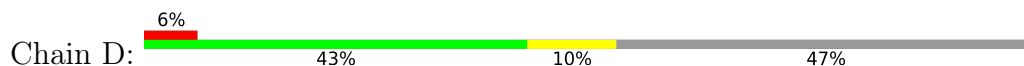


- Molecule 2: Translation initiation factor eIF-2B subunit delta



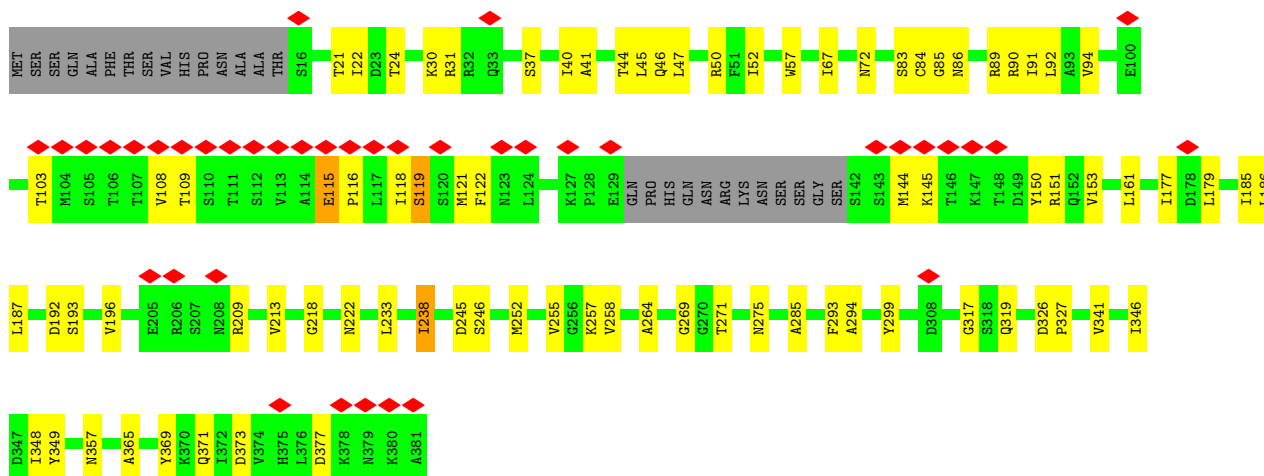


• Molecule 2: Translation initiation factor eIF-2B subunit delta

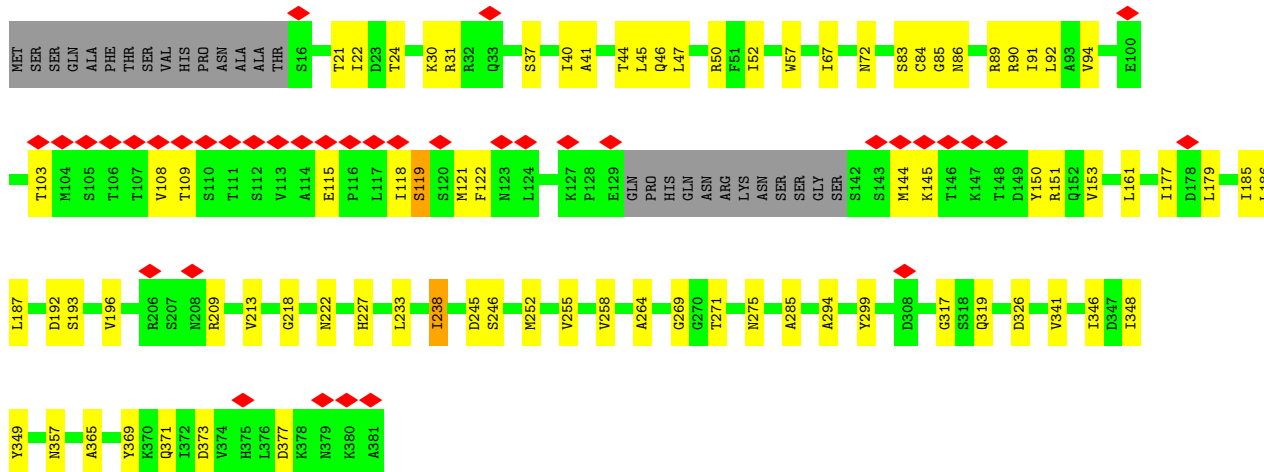


• Molecule 3: Translation initiation factor eIF-2B subunit beta

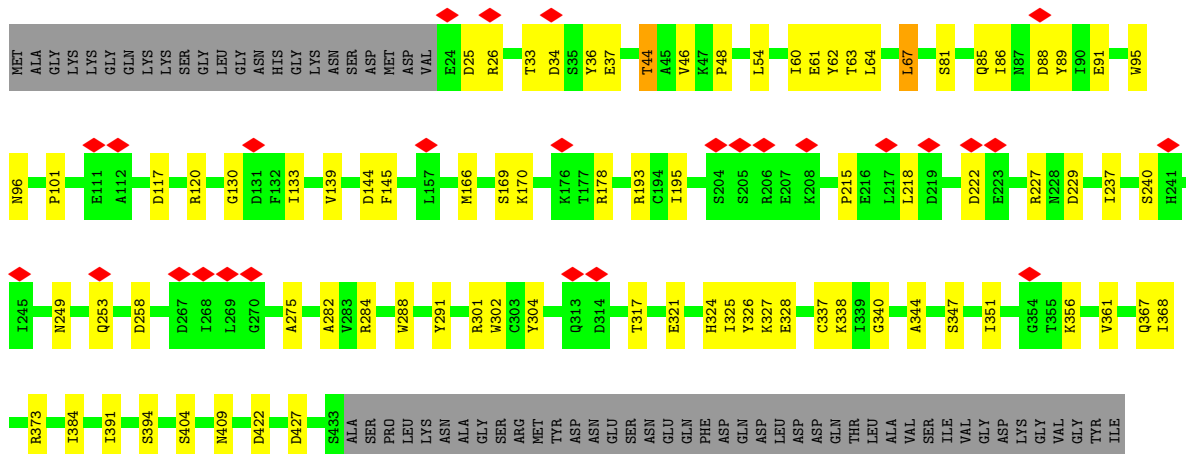


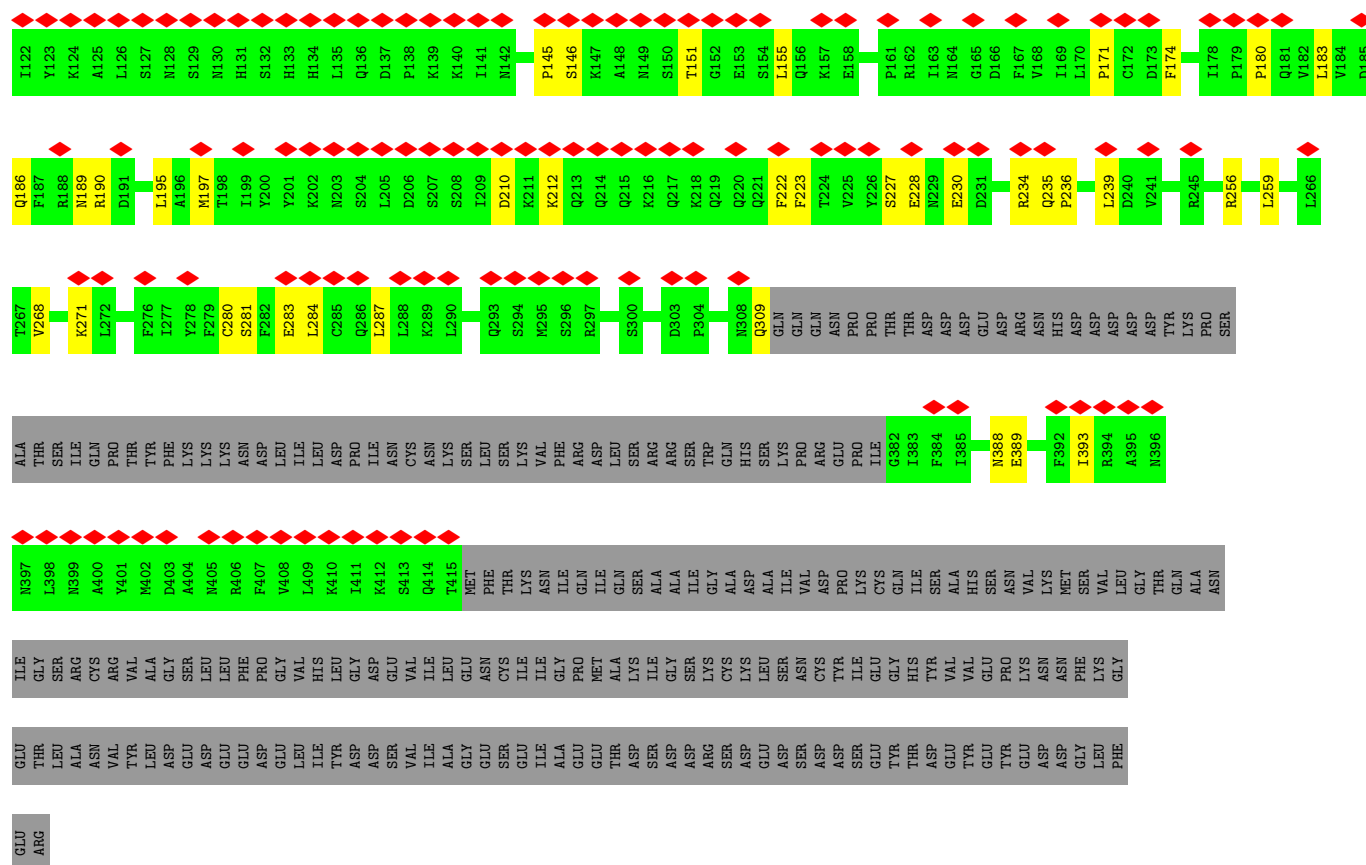


• Molecule 3: Translation initiation factor eIF-2B subunit beta

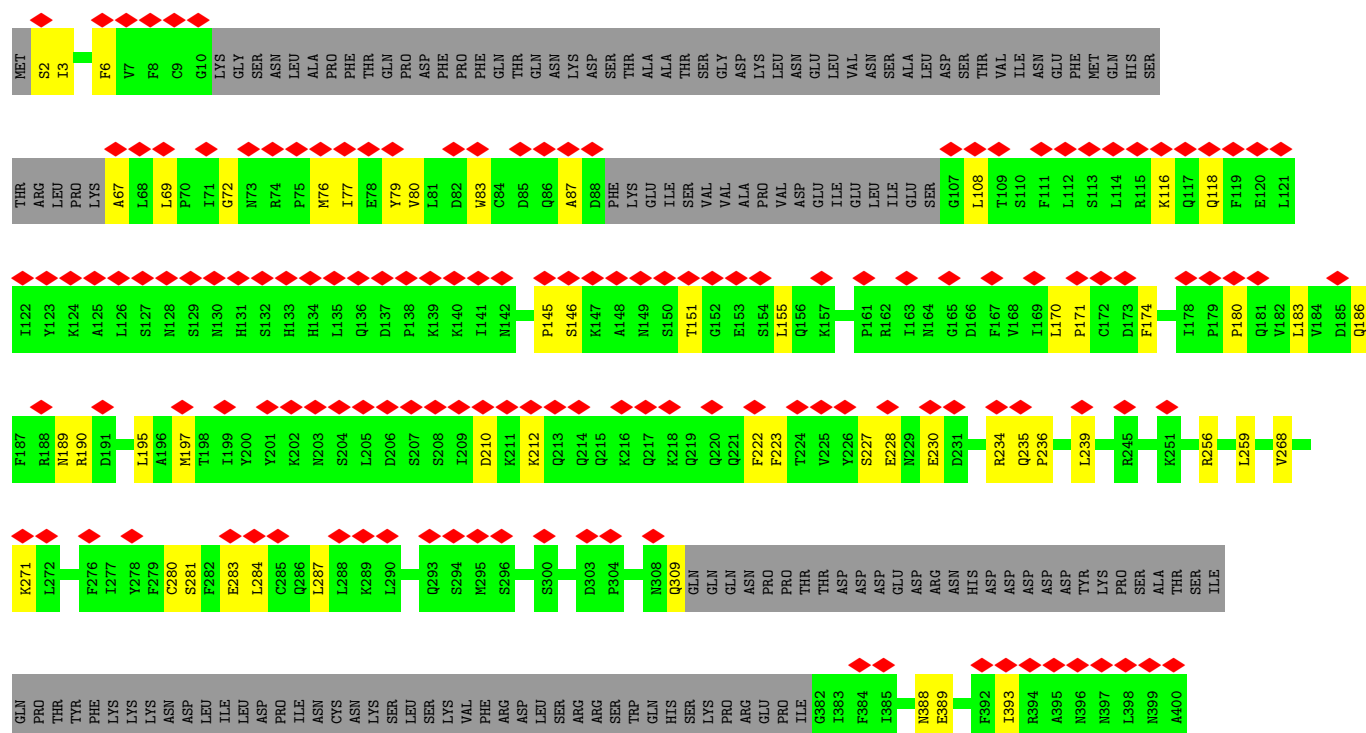
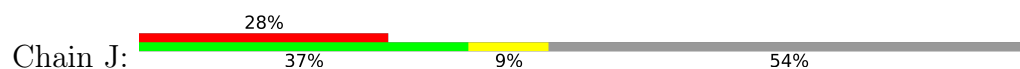


• Molecule 4: Translation initiation factor eIF-2B subunit epsilon





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





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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64541	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF determination was performed per micrograph initially. After particle picking and initial reconstruction, per particle CTF determination was performed.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	37313	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.304	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.055	Depositor
Map size ($\text{\AA}$)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.27	0/2437	0.60	0/3304
1	B	0.27	0/2437	0.60	0/3304
2	C	0.28	0/2720	0.62	2/3685 (0.1%)
2	D	0.28	0/2720	0.63	2/3685 (0.1%)
3	E	0.31	0/2846	0.72	7/3857 (0.2%)
3	F	0.31	0/2846	0.72	7/3857 (0.2%)
4	G	0.28	0/3327	0.65	1/4512 (0.0%)
4	H	0.28	0/3327	0.65	1/4512 (0.0%)
5	I	0.27	0/2232	0.71	2/3015 (0.1%)
5	J	0.27	0/2232	0.71	2/3015 (0.1%)
6	K	0.41	0/2027	0.81	2/2726 (0.1%)
6	L	0.41	0/2027	0.81	2/2726 (0.1%)
7	M	0.60	0/146	0.98	0/196
7	N	0.60	0/146	0.98	0/196
8	O	0.71	0/3079	1.03	3/4157 (0.1%)
8	P	0.71	0/3079	1.03	3/4157 (0.1%)
All	All	0.40	0/37628	0.75	34/50904 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	1
4	H	0	1
6	K	0	2
6	L	0	2
All	All	0	6

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	109	THR	N-CA-C	8.65	120.32	111.07
3	F	109	THR	N-CA-C	8.62	120.29	111.07
3	E	238	ILE	N-CA-C	6.79	113.47	106.21
3	F	238	ILE	N-CA-C	6.78	113.47	106.21
3	F	115	GLU	CA-C-N	6.62	126.40	119.05
3	F	115	GLU	C-N-CA	6.62	126.40	119.05
6	K	194	SER	N-CA-C	6.59	117.16	108.07
6	L	194	SER	N-CA-C	6.59	117.16	108.07
3	E	115	GLU	CA-C-N	6.58	126.36	119.05
3	E	115	GLU	C-N-CA	6.58	126.36	119.05
8	P	356	ARG	N-CA-C	6.05	123.19	109.81
8	O	356	ARG	N-CA-C	6.05	123.18	109.81
3	E	103	THR	N-CA-C	5.76	117.24	111.07
3	F	108	VAL	N-CA-C	5.75	116.53	110.72
8	P	430	ILE	N-CA-C	5.74	116.75	108.48
3	E	108	VAL	N-CA-C	5.73	116.51	110.72
8	O	430	ILE	N-CA-C	5.72	116.72	108.48
3	F	103	THR	N-CA-C	5.49	117.26	111.28
5	J	72	GLY	CA-C-N	5.23	131.54	121.54
5	J	72	GLY	C-N-CA	5.23	131.54	121.54
5	I	72	GLY	CA-C-N	5.22	131.50	121.54
5	I	72	GLY	C-N-CA	5.22	131.50	121.54
8	O	223	SER	N-CA-C	5.21	117.25	110.43
8	P	223	SER	N-CA-C	5.18	117.22	110.43
6	L	192	CYS	N-CA-C	5.16	116.94	110.24
4	H	324	HIS	N-CA-C	5.15	118.69	111.74
6	K	192	CYS	N-CA-C	5.14	116.92	110.24
2	C	499	ARG	CA-C-N	5.11	129.67	122.46
2	C	499	ARG	C-N-CA	5.11	129.67	122.46
4	G	324	HIS	N-CA-C	5.11	118.64	111.74
2	D	499	ARG	CA-C-N	5.10	129.65	122.46
2	D	499	ARG	C-N-CA	5.10	129.65	122.46
3	F	119	SER	N-CA-C	-5.07	102.35	109.96
3	E	119	SER	N-CA-C	-5.05	102.38	109.96

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	178	ARG	Peptide
4	H	178	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
6	K	140	HIS	Peptide
6	K	39	TYR	Peptide
6	L	140	HIS	Peptide
6	L	39	TYR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2393	0	2416	39	0
1	B	2393	0	2416	41	0
2	C	2677	0	2787	38	0
2	D	2677	0	2787	40	0
3	E	2797	0	2835	53	0
3	F	2797	0	2835	48	0
4	G	3265	0	3229	47	0
4	H	3265	0	3229	51	0
5	I	2187	0	2173	31	0
5	J	2187	0	2173	32	0
6	K	2010	0	2064	28	0
6	L	2010	0	2064	27	0
7	M	143	0	148	0	0
7	N	143	0	148	0	0
8	O	3034	0	3195	44	0
8	P	3034	0	3195	44	0
All	All	37012	0	37694	518	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 (518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:499:ILE:HD11	8:P:517:ILE:HG13	1.63	0.81
8:O:499:ILE:HD11	8:O:517:ILE:HG13	1.63	0.79
5:J:79:TYR:O	5:J:83:TRP:HB2	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:79:TYR:O	5:I:83:TRP:HB2	1.89	0.71
6:L:201:ILE:HG22	8:P:330:ILE:HG21	1.73	0.69
4:G:301:ARG:HB3	3:F:317:GLY:HA2	1.73	0.69
6:K:201:ILE:HG22	8:O:330:ILE:HG21	1.73	0.69
8:O:116:VAL:HG21	8:O:217:LEU:HD21	1.75	0.69
5:I:171:PRO:HG2	5:I:174:PHE:HB2	1.75	0.68
6:K:248:ILE:HG12	6:K:264:ILE:HG21	1.74	0.68
8:P:116:VAL:HG21	8:P:217:LEU:HD21	1.75	0.68
5:J:171:PRO:HG2	5:J:174:PHE:HB2	1.75	0.68
6:L:248:ILE:HG12	6:L:264:ILE:HG21	1.74	0.68
4:H:61:GLU:HA	4:H:64:LEU:HB2	1.77	0.67
4:G:61:GLU:HA	4:G:64:LEU:HB2	1.77	0.66
1:B:259:ARG:HG3	1:B:263:LEU:HG	1.78	0.66
3:F:218:GLY:H	3:F:222:ASN:HB2	1.60	0.66
3:E:218:GLY:H	3:E:222:ASN:HB2	1.59	0.66
3:E:317:GLY:HA2	4:H:301:ARG:HB3	1.77	0.66
5:J:222:PHE:H	5:J:268:VAL:HG12	1.61	0.66
5:I:222:PHE:H	5:I:268:VAL:HG12	1.61	0.65
1:A:259:ARG:HG3	1:A:263:LEU:HG	1.78	0.64
1:A:157:ARG:HH11	1:B:157:ARG:HH11	1.44	0.64
5:J:256:ARG:HH21	5:J:309:GLN:HE22	1.47	0.62
4:G:222:ASP:HB3	5:J:271:LYS:HZ2	1.64	0.61
2:C:532:LEU:HD11	2:C:614:ASN:HB3	1.83	0.61
1:B:79:ARG:HB3	3:F:122:PHE:CE2	2.36	0.61
8:P:426:ILE:HG22	8:P:490:PRO:HB2	1.82	0.61
5:I:256:ARG:HH21	5:I:309:GLN:HE22	1.47	0.61
2:D:532:LEU:HD11	2:D:614:ASN:HB3	1.83	0.61
8:O:426:ILE:HG22	8:O:490:PRO:HB2	1.82	0.61
2:C:459:LEU:HD11	2:C:492:LEU:HB3	1.83	0.60
3:E:269:GLY:O	3:E:349:TYR:OH	2.20	0.60
6:L:205:LEU:HG	8:P:330:ILE:HB	1.84	0.60
5:I:151:THR:O	5:I:155:LEU:HB2	2.02	0.59
8:O:320:SER:HB3	8:O:412:LEU:H	1.68	0.59
3:E:37:SER:HG	3:E:83:SER:HG	1.49	0.59
3:F:269:GLY:O	3:F:349:TYR:OH	2.20	0.59
1:A:79:ARG:HB3	3:E:122:PHE:CE2	2.38	0.59
4:H:91:GLU:HA	4:H:96:ASN:HD22	1.67	0.59
6:K:226:PRO:HG3	8:O:408:ARG:HD2	1.85	0.59
1:B:287:LEU:HD11	3:F:121:MET:HG2	1.84	0.59
6:K:24:VAL:HG23	6:K:65:VAL:HA	1.85	0.59
2:D:459:LEU:HD11	2:D:492:LEU:HB3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:151:THR:O	5:J:155:LEU:HB2	2.03	0.59
8:O:358:GLY:HA2	8:O:372:PRO:HA	1.84	0.59
8:P:358:GLY:HA2	8:P:372:PRO:HA	1.84	0.59
5:I:271:LYS:HZ2	4:H:222:ASP:HB3	1.67	0.58
4:G:91:GLU:HA	4:G:96:ASN:HD22	1.67	0.58
6:K:205:LEU:HG	8:O:330:ILE:HB	1.84	0.58
6:L:226:PRO:HG3	8:P:408:ARG:HD2	1.85	0.58
8:O:346:VAL:HG22	8:O:392:PRO:HD3	1.84	0.58
8:O:313:PRO:HA	8:O:344:ASN:O	2.03	0.58
8:P:320:SER:HB3	8:P:412:LEU:H	1.68	0.58
8:P:313:PRO:HA	8:P:344:ASN:O	2.03	0.58
6:K:51:LEU:HG	6:K:87:LYS:HE2	1.85	0.58
8:P:346:VAL:HG22	8:P:392:PRO:HD3	1.84	0.58
2:C:292:ARG:HB3	2:C:340:MET:HE2	1.86	0.58
3:F:233:LEU:HD22	3:F:238:ILE:HD11	1.85	0.58
6:L:24:VAL:HG23	6:L:65:VAL:HA	1.85	0.58
6:L:51:LEU:HG	6:L:87:LYS:HE2	1.85	0.58
5:J:186:GLN:O	5:J:190:ARG:NH2	2.31	0.58
3:E:233:LEU:HD22	3:E:238:ILE:HD11	1.85	0.57
2:D:292:ARG:HB3	2:D:340:MET:HE2	1.86	0.57
4:G:170:LYS:HD2	5:J:228:GLU:OE2	2.04	0.57
8:P:307:ARG:HG2	8:P:392:PRO:HB2	1.87	0.57
5:J:230:GLU:HG3	5:J:234:ARG:HH21	1.70	0.57
5:J:197:MET:HA	5:J:388:ASN:HB2	1.87	0.57
3:F:41:ALA:HB2	3:F:83:SER:HB3	1.86	0.57
1:A:287:LEU:HD11	3:E:121:MET:HG2	1.86	0.56
1:A:127:LEU:HB2	1:A:191:VAL:HG11	1.87	0.56
2:C:512:PHE:O	2:C:648:LYS:NZ	2.39	0.56
2:D:381:LEU:HB2	6:K:62:LEU:HD23	1.87	0.56
8:P:140:LEU:HD12	8:P:319:ARG:HH21	1.70	0.56
4:G:391:ILE:HG23	4:G:394:SER:HB2	1.87	0.56
1:B:127:LEU:HB2	1:B:191:VAL:HG11	1.87	0.56
3:F:85:GLY:O	3:F:89:ARG:NH1	2.39	0.56
8:O:140:LEU:HD12	8:O:319:ARG:HH21	1.70	0.56
2:D:512:PHE:O	2:D:648:LYS:NZ	2.39	0.56
3:E:85:GLY:O	3:E:89:ARG:NH1	2.39	0.56
5:I:230:GLU:HG3	5:I:234:ARG:HH21	1.70	0.56
5:I:228:GLU:OE2	4:H:170:LYS:HD2	2.05	0.56
1:B:76:PHE:HA	3:F:122:PHE:CZ	2.41	0.56
4:H:351:ILE:HA	4:H:368:ILE:HB	1.87	0.56
3:E:41:ALA:HB2	3:E:83:SER:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:192:ASP:OD2	3:E:275:ASN:ND2	2.39	0.56
3:F:192:ASP:OD2	3:F:275:ASN:ND2	2.39	0.56
5:I:197:MET:HA	5:I:388:ASN:HB2	1.87	0.56
1:A:230:VAL:HG22	1:A:284:ILE:HD12	1.88	0.56
2:C:627:LYS:HZ1	1:B:242:LEU:HB3	1.71	0.56
5:J:118:GLN:NE2	5:J:146:SER:OG	2.39	0.56
1:B:101:PHE:O	1:B:105:ALA:N	2.38	0.56
4:G:351:ILE:HA	4:G:368:ILE:HB	1.87	0.55
1:A:259:ARG:NH1	1:A:261:ASP:O	2.40	0.55
2:D:517:GLN:HG3	2:D:619:LEU:HD21	1.88	0.55
3:F:37:SER:HG	3:F:83:SER:HG	1.52	0.55
4:H:391:ILE:HG23	4:H:394:SER:HB2	1.87	0.55
8:O:307:ARG:HG2	8:O:392:PRO:HB2	1.87	0.55
8:P:503:ARG:HD3	8:P:512:ILE:HG21	1.89	0.55
3:F:44:THR:HG21	3:F:84:CYS:HA	1.89	0.55
8:O:503:ARG:HD3	8:O:512:ILE:HG21	1.88	0.55
3:E:326:ASP:OD1	3:E:326:ASP:N	2.40	0.55
2:C:517:GLN:HG3	2:C:619:LEU:HD21	1.88	0.55
4:H:120:ARG:NH2	4:H:249:ASN:O	2.40	0.55
4:G:120:ARG:NH2	4:G:249:ASN:O	2.40	0.54
5:I:118:GLN:NE2	5:I:146:SER:OG	2.39	0.54
1:B:259:ARG:NH1	1:B:261:ASP:O	2.40	0.54
1:B:81:LEU:HD21	6:L:47:LEU:HD12	1.89	0.54
3:E:52:ILE:O	3:E:151:ARG:NH1	2.41	0.54
5:I:186:GLN:O	5:I:190:ARG:NH2	2.31	0.54
1:A:22:MET:HE3	1:A:66:LEU:HD21	1.88	0.54
5:I:180:PRO:HA	5:I:183:LEU:HD13	1.90	0.54
3:F:90:ARG:HD3	3:F:161:LEU:HD11	1.90	0.54
6:L:149:ILE:HD12	6:L:150:ILE:HG23	1.90	0.54
1:A:90:CYS:HA	1:A:93:HIS:HB3	1.90	0.54
1:B:22:MET:HE3	1:B:66:LEU:HD21	1.88	0.54
1:B:230:VAL:HG22	1:B:284:ILE:HD12	1.88	0.54
3:E:44:THR:HG21	3:E:84:CYS:HA	1.89	0.53
1:A:101:PHE:O	1:A:105:ALA:N	2.38	0.53
5:I:271:LYS:NZ	4:H:222:ASP:O	2.40	0.53
4:H:344:ALA:HB3	4:H:361:VAL:HG23	1.89	0.53
5:J:87:ALA:H	5:J:108:LEU:HD22	1.74	0.53
1:B:90:CYS:HA	1:B:93:HIS:HB3	1.90	0.53
2:C:463:PHE:HA	2:C:467:VAL:HG11	1.91	0.53
3:F:86:ASN:ND2	3:F:299:TYR:O	2.41	0.53
4:H:25:ASP:OD2	4:H:26:ARG:NH2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PHE:HA	3:E:122:PHE:CZ	2.43	0.53
3:E:86:ASN:ND2	3:E:299:TYR:O	2.41	0.53
3:F:52:ILE:O	3:F:151:ARG:NH1	2.41	0.53
1:A:213:THR:HA	1:A:216:VAL:HG12	1.91	0.53
1:A:296:SER:O	1:A:300:ILE:HB	2.09	0.53
5:J:180:PRO:HA	5:J:183:LEU:HD13	1.90	0.53
1:B:296:SER:O	1:B:300:ILE:HB	2.09	0.53
6:K:149:ILE:HD12	6:K:150:ILE:HG23	1.90	0.53
1:A:131:TYR:H	1:A:161:GLN:HB3	1.74	0.52
2:D:463:PHE:HA	2:D:467:VAL:HG11	1.91	0.52
5:I:87:ALA:H	5:I:108:LEU:HD22	1.74	0.52
1:B:213:THR:HA	1:B:216:VAL:HG12	1.90	0.52
4:H:64:LEU:HA	4:H:67:LEU:HD23	1.91	0.52
8:O:109:VAL:HG23	8:O:136:ILE:HG21	1.92	0.52
1:A:100:LEU:O	1:A:104:ARG:CB	2.58	0.52
6:K:236:ASP:C	6:K:238:GLN:H	2.17	0.52
4:G:344:ALA:HB3	4:G:361:VAL:HG23	1.89	0.52
1:B:100:LEU:O	1:B:104:ARG:CB	2.58	0.52
6:L:236:ASP:C	6:L:238:GLN:H	2.17	0.52
6:L:117:GLU:O	6:L:120:GLN:NE2	2.43	0.52
3:E:90:ARG:HD3	3:E:161:LEU:HD11	1.90	0.52
3:E:40:ILE:HG12	3:E:84:CYS:HB3	1.91	0.52
8:O:98:GLN:HE22	8:O:396:ILE:HD11	1.75	0.52
8:P:109:VAL:HG23	8:P:136:ILE:HG21	1.92	0.52
8:P:456:LEU:HD23	8:P:503:ARG:HD2	1.92	0.52
2:D:300:PHE:HA	2:D:303:VAL:HG12	1.92	0.52
4:G:64:LEU:HA	4:G:67:LEU:HD23	1.91	0.52
4:H:60:ILE:HG22	4:H:64:LEU:HD13	1.91	0.52
3:F:40:ILE:HG12	3:F:84:CYS:HB3	1.91	0.52
6:K:117:GLU:O	6:K:120:GLN:NE2	2.43	0.52
2:D:376:LYS:HG2	2:D:381:LEU:HD23	1.92	0.51
4:G:48:PRO:HG2	4:G:86:ILE:HD11	1.92	0.51
1:B:131:TYR:H	1:B:161:GLN:HB3	1.74	0.51
6:K:35:LYS:HA	6:K:43:GLU:HA	1.93	0.51
2:C:520:SER:HA	2:C:619:LEU:HD13	1.91	0.51
3:F:91:ILE:HA	3:F:94:VAL:HG12	1.92	0.51
8:O:349:LEU:HD12	8:O:388:LYS:HA	1.93	0.51
5:I:271:LYS:NZ	4:H:222:ASP:HB3	2.25	0.51
1:B:129:HIS:ND1	1:B:154:THR:OG1	2.42	0.51
6:K:183:LYS:HB3	6:K:231:THR:HB	1.92	0.51
4:G:25:ASP:OD2	4:G:26:ARG:NH2	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:35:LYS:HA	6:L:43:GLU:HA	1.92	0.51
3:E:91:ILE:HA	3:E:94:VAL:HG12	1.92	0.51
6:L:183:LYS:HB3	6:L:231:THR:HB	1.92	0.51
8:P:98:GLN:HE22	8:P:396:ILE:HD11	1.75	0.51
1:A:209:ASN:HD21	1:A:213:THR:HG21	1.75	0.51
2:C:300:PHE:HA	2:C:303:VAL:HG12	1.92	0.51
2:D:520:SER:HA	2:D:619:LEU:HD13	1.91	0.51
4:G:36:TYR:OH	4:G:284:ARG:NH1	2.44	0.51
4:H:326:TYR:HB2	4:H:344:ALA:HA	1.93	0.51
8:P:349:LEU:HD12	8:P:388:LYS:HA	1.93	0.51
2:C:376:LYS:HG2	2:C:381:LEU:HD23	1.92	0.51
4:G:60:ILE:HG22	4:G:64:LEU:HD13	1.91	0.51
1:B:80:ASN:HD21	1:B:97:ASN:HD22	1.59	0.51
4:H:36:TYR:OH	4:H:284:ARG:NH1	2.44	0.51
1:A:80:ASN:HD21	1:A:97:ASN:HD22	1.59	0.50
4:G:222:ASP:O	5:J:271:LYS:NZ	2.44	0.50
1:A:81:LEU:HD21	6:K:47:LEU:HD12	1.94	0.50
8:P:216:LEU:HD23	8:P:246:ILE:HG12	1.92	0.50
5:I:210:ASP:HB2	5:I:212:LYS:HE2	1.94	0.50
4:H:48:PRO:HG2	4:H:86:ILE:HD11	1.92	0.50
4:H:166:MET:H	4:H:275:ALA:HA	1.76	0.50
2:D:406:SER:HB3	2:D:410:THR:HG23	1.94	0.50
8:O:237:GLU:HB3	8:O:274:ILE:HD12	1.94	0.50
8:P:320:SER:HB2	8:P:407:CYS:HA	1.94	0.50
2:C:406:SER:HB3	2:C:410:THR:HG23	1.94	0.50
4:G:326:TYR:HB2	4:G:344:ALA:HA	1.93	0.50
1:B:209:ASN:HD21	1:B:213:THR:HG21	1.75	0.50
8:P:237:GLU:HB3	8:P:274:ILE:HD12	1.94	0.50
8:O:216:LEU:HD23	8:O:246:ILE:HG12	1.92	0.50
4:H:404:SER:N	4:H:422:ASP:OD1	2.44	0.50
4:H:34:ASP:OD2	4:H:81:SER:N	2.45	0.50
8:O:320:SER:HB2	8:O:407:CYS:HA	1.94	0.50
4:G:288:TRP:HA	4:G:291:TYR:HB3	1.92	0.50
8:O:456:LEU:HD23	8:O:503:ARG:HD2	1.92	0.50
4:G:95:TRP:HZ3	4:G:101:PRO:HD2	1.77	0.49
5:J:189:ASN:OD1	5:J:190:ARG:NH2	2.45	0.49
1:A:125:ILE:HG23	1:A:192:ASP:H	1.77	0.49
5:J:284:LEU:HA	5:J:287:LEU:HD22	1.93	0.49
4:H:54:LEU:HB3	4:H:62:TYR:HE2	1.77	0.49
4:H:288:TRP:HA	4:H:291:TYR:HB3	1.92	0.49
1:A:77:VAL:O	1:A:81:LEU:HB2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:284:LEU:HA	5:I:287:LEU:HD22	1.93	0.49
5:I:189:ASN:OD1	5:I:190:ARG:NH2	2.45	0.49
5:J:210:ASP:HB2	5:J:212:LYS:HE2	1.94	0.49
4:H:193:ARG:HE	4:H:195:ILE:HD13	1.78	0.49
4:H:409:ASN:HD21	4:H:427:ASP:HA	1.77	0.49
2:C:399:THR:HG22	2:C:425:LYS:HB2	1.94	0.49
3:E:45:LEU:HD11	3:E:161:LEU:HB3	1.95	0.49
4:G:54:LEU:HB3	4:G:62:TYR:HE2	1.77	0.49
4:G:166:MET:H	4:G:275:ALA:HA	1.76	0.49
3:F:118:ILE:HG22	3:F:119:SER:O	2.13	0.49
3:F:271:THR:HG22	3:F:341:VAL:HG22	1.95	0.49
8:P:187:ARG:HH21	8:P:299:VAL:HG13	1.78	0.49
3:E:317:GLY:HA3	4:H:304:TYR:HB2	1.95	0.49
1:B:125:ILE:HG23	1:B:192:ASP:H	1.77	0.49
4:H:95:TRP:HZ3	4:H:101:PRO:HD2	1.77	0.49
3:F:45:LEU:HD11	3:F:161:LEU:HB3	1.95	0.49
3:E:118:ILE:HG22	3:E:119:SER:O	2.13	0.49
5:J:223:PHE:HZ	5:J:227:SER:HB3	1.78	0.49
3:F:177:ILE:O	3:F:209:ARG:NH1	2.35	0.49
6:L:115:CYS:HB3	6:L:165:VAL:HG13	1.95	0.49
8:P:390:ALA:HB1	8:P:396:ILE:HD13	1.95	0.49
1:A:236:PHE:HD1	1:A:299:LEU:HD12	1.78	0.49
2:D:399:THR:HG22	2:D:425:LYS:HB2	1.94	0.49
4:G:409:ASN:HD21	4:G:427:ASP:HA	1.77	0.49
8:O:355:ILE:HG12	8:O:417:VAL:HG22	1.95	0.49
4:H:337:CYS:SG	4:H:338:LYS:N	2.86	0.48
3:F:326:ASP:N	3:F:326:ASP:OD1	2.40	0.48
8:O:444:LYS:HB2	8:O:449:LYS:HB2	1.95	0.48
1:A:23:PRO:HG3	1:A:65:SER:HB2	1.95	0.48
1:A:242:LEU:HB3	2:D:627:LYS:HZ1	1.76	0.48
4:G:337:CYS:SG	4:G:338:LYS:N	2.86	0.48
5:I:223:PHE:HZ	5:I:227:SER:HB3	1.78	0.48
4:G:193:ARG:HE	4:G:195:ILE:HD13	1.78	0.48
4:H:130:GLY:N	4:H:240:SER:OG	2.46	0.48
8:O:320:SER:HB3	8:O:412:LEU:HB2	1.94	0.48
2:C:462:ILE:HA	2:C:465:MET:HE2	1.96	0.48
2:D:462:ILE:HA	2:D:465:MET:HE2	1.96	0.48
4:G:34:ASP:OD2	4:G:81:SER:N	2.45	0.48
5:J:76:MET:HA	5:J:79:TYR:HD2	1.78	0.48
1:B:236:PHE:HD1	1:B:299:LEU:HD12	1.79	0.48
8:O:357:PRO:HD3	8:O:416:VAL:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:355:ILE:HG12	8:P:417:VAL:HG22	1.95	0.48
1:B:79:ARG:HB3	3:F:122:PHE:HE2	1.77	0.48
2:D:524:ASN:HD21	2:D:615:ILE:HG23	1.79	0.48
5:I:76:MET:HA	5:I:79:TYR:HD2	1.78	0.48
6:K:50:GLU:OE2	6:K:86:SER:OG	2.32	0.48
8:P:444:LYS:HB2	8:P:449:LYS:HB2	1.95	0.48
4:G:404:SER:N	4:G:422:ASP:OD1	2.44	0.48
1:B:23:PRO:HG3	1:B:65:SER:HB2	1.95	0.48
1:B:77:VAL:O	1:B:81:LEU:HB2	2.12	0.48
8:O:187:ARG:HH21	8:O:299:VAL:HG13	1.78	0.48
1:A:100:LEU:O	1:A:104:ARG:HB3	2.14	0.48
3:E:179:LEU:HD21	3:E:348:ILE:HG21	1.96	0.48
4:G:130:GLY:N	4:G:240:SER:OG	2.46	0.48
3:E:245:ASP:OD1	3:E:246:SER:N	2.47	0.48
1:B:100:LEU:O	1:B:104:ARG:HB3	2.14	0.47
3:F:179:LEU:HD21	3:F:348:ILE:HG21	1.96	0.47
8:P:320:SER:HB3	8:P:412:LEU:HB2	1.94	0.47
8:O:390:ALA:HB1	8:O:396:ILE:HD13	1.95	0.47
1:A:41:THR:HG22	1:A:43:ALA:H	1.79	0.47
1:A:240:PHE:HE2	2:D:627:LYS:HG3	1.79	0.47
3:F:245:ASP:OD1	3:F:246:SER:N	2.47	0.47
2:C:389:ASN:HD21	2:C:633:GLY:HA2	1.80	0.47
5:I:116:LYS:HD2	5:I:145:PRO:HG2	1.96	0.47
5:J:280:CYS:SG	5:J:281:SER:N	2.87	0.47
6:L:69:ASP:OD2	6:L:87:LYS:NZ	2.37	0.47
2:C:524:ASN:HD21	2:C:615:ILE:HG23	1.79	0.47
2:D:289:SER:OG	2:D:511:LYS:NZ	2.48	0.47
3:E:271:THR:HG22	3:E:341:VAL:HG22	1.95	0.47
6:K:69:ASP:OD2	6:K:87:LYS:NZ	2.37	0.47
6:K:115:CYS:HB3	6:K:165:VAL:HG13	1.95	0.47
3:E:294:ALA:HB2	3:E:346:ILE:HD11	1.97	0.47
6:L:236:ASP:HB2	6:L:239:LYS:HG3	1.96	0.47
5:I:239:LEU:HB3	5:I:259:LEU:HD21	1.96	0.47
8:P:297:PHE:HA	8:P:300:LYS:HB2	1.96	0.47
8:P:357:PRO:HD3	8:P:416:VAL:HG22	1.95	0.47
1:A:199:GLU:HB2	1:A:209:ASN:HA	1.96	0.47
2:C:289:SER:OG	2:C:511:LYS:NZ	2.48	0.47
5:J:239:LEU:HB3	5:J:259:LEU:HD21	1.96	0.47
1:B:33:LEU:HD23	1:B:49:ILE:HG22	1.97	0.47
3:F:150:TYR:HA	3:F:153:VAL:HG12	1.97	0.47
6:K:236:ASP:HB2	6:K:239:LYS:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:46:VAL:O	4:G:85:GLN:NE2	2.42	0.47
4:H:133:ILE:HA	4:H:237:ILE:HG22	1.97	0.47
6:L:50:GLU:OE2	6:L:86:SER:OG	2.32	0.47
3:F:294:ALA:HB2	3:F:346:ILE:HD11	1.97	0.46
2:D:389:ASN:HD21	2:D:633:GLY:HA2	1.80	0.46
4:H:328:GLU:OE1	4:H:347:SER:N	2.47	0.46
8:O:357:PRO:HB2	8:O:415:GLN:HE21	1.79	0.46
8:O:375:SER:HB2	8:O:400:THR:HB	1.98	0.46
3:E:177:ILE:O	3:E:209:ARG:NH1	2.35	0.46
4:G:215:PRO:HA	4:G:218:LEU:HD23	1.97	0.46
4:H:215:PRO:HA	4:H:218:LEU:HD23	1.97	0.46
3:F:92:LEU:HD22	3:F:373:ASP:HB3	1.98	0.46
3:E:72:ASN:ND2	3:E:377:ASP:OD1	2.43	0.46
5:J:2:SER:OG	5:J:3:ILE:N	2.43	0.46
1:B:199:GLU:HB2	1:B:209:ASN:HA	1.96	0.46
8:O:297:PHE:HA	8:O:300:LYS:HB2	1.96	0.46
2:D:480:ASN:O	3:E:357:ASN:ND2	2.45	0.46
4:G:328:GLU:OE1	4:G:347:SER:N	2.47	0.46
5:I:280:CYS:SG	5:I:281:SER:N	2.87	0.46
2:D:483:LEU:HB2	2:D:625:ILE:HD11	1.97	0.46
3:E:92:LEU:HD22	3:E:373:ASP:HB3	1.97	0.46
5:J:116:LYS:HD2	5:J:145:PRO:HG2	1.96	0.46
3:F:57:TRP:HH2	3:F:151:ARG:HB2	1.80	0.46
3:F:264:ALA:O	3:F:271:THR:OG1	2.32	0.46
8:P:357:PRO:HB2	8:P:415:GLN:HE21	1.79	0.46
3:E:57:TRP:HH2	3:E:151:ARG:HB2	1.81	0.46
3:E:150:TYR:HA	3:E:153:VAL:HG12	1.97	0.46
4:G:133:ILE:HA	4:G:237:ILE:HG22	1.97	0.46
1:B:41:THR:HG22	1:B:43:ALA:H	1.79	0.46
6:K:201:ILE:HG22	8:O:330:ILE:CG2	2.43	0.46
2:C:472:LEU:HD22	2:C:489:THR:HG23	1.98	0.46
3:F:365:ALA:O	3:F:369:TYR:N	2.49	0.46
2:C:358:THR:HG22	2:C:360:ASP:H	1.81	0.46
2:D:358:THR:HG22	2:D:360:ASP:H	1.81	0.46
2:D:468:ASP:N	2:D:468:ASP:OD1	2.47	0.46
3:E:118:ILE:HG22	3:E:119:SER:N	2.31	0.46
5:I:2:SER:OG	5:I:3:ILE:N	2.43	0.46
8:O:174:CYS:HB2	8:O:182:ARG:HA	1.98	0.46
5:I:151:THR:O	5:I:155:LEU:CB	2.64	0.45
5:J:151:THR:O	5:J:155:LEU:CB	2.64	0.45
1:A:33:LEU:HD23	1:A:49:ILE:HG22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:472:LEU:HD22	2:D:489:THR:HG23	1.98	0.45
1:B:2:SER:HG	1:B:9:THR:HG1	1.61	0.45
8:O:351:ASP:HB2	8:O:377:ILE:HD12	1.98	0.45
3:E:187:LEU:HB3	3:E:258:VAL:HG12	1.97	0.45
3:E:365:ALA:O	3:E:369:TYR:N	2.49	0.45
4:G:302:TRP:O	3:F:319:GLN:NE2	2.50	0.45
3:F:187:LEU:HB3	3:F:258:VAL:HG12	1.97	0.45
8:P:351:ASP:HB2	8:P:377:ILE:HD12	1.98	0.45
1:A:249:MET:HG3	1:A:250:ALA:H	1.81	0.45
2:C:381:LEU:HB2	6:L:62:LEU:HD23	1.97	0.45
3:E:264:ALA:O	3:E:271:THR:OG1	2.32	0.45
1:B:249:MET:HG3	1:B:250:ALA:H	1.81	0.45
2:C:310:PRO:HG2	2:C:313:THR:HB	1.98	0.45
2:C:483:LEU:HB2	2:C:625:ILE:HD11	1.97	0.45
2:D:310:PRO:HG2	2:D:313:THR:HB	1.98	0.45
4:H:46:VAL:O	4:H:85:GLN:NE2	2.42	0.45
1:A:197:GLY:O	1:A:209:ASN:ND2	2.39	0.45
2:C:406:SER:OG	2:C:407:LYS:N	2.49	0.45
8:P:375:SER:HB2	8:P:400:THR:HB	1.98	0.45
5:J:87:ALA:HB3	5:J:108:LEU:HD13	1.98	0.45
2:D:406:SER:OG	2:D:407:LYS:N	2.49	0.45
6:K:126:LEU:HA	6:K:129:THR:HG22	1.99	0.45
4:H:144:ASP:OD1	4:H:144:ASP:N	2.50	0.45
1:A:79:ARG:HB3	3:E:122:PHE:HE2	1.82	0.44
4:H:367:GLN:HB2	4:H:384:ILE:HG12	1.99	0.44
5:I:87:ALA:HB3	5:I:108:LEU:HD13	1.98	0.44
5:J:195:LEU:HD12	5:J:283:GLU:HB3	2.00	0.44
6:K:192:CYS:HA	6:K:261:VAL:H	1.82	0.44
4:G:304:TYR:HB2	3:F:317:GLY:HA3	1.99	0.44
5:J:80:VAL:HG11	5:J:174:PHE:HB3	1.99	0.44
4:H:88:ASP:OD1	4:H:89:TYR:N	2.50	0.44
2:C:278:THR:HG21	2:C:329:LEU:HG	2.00	0.44
2:C:480:ASN:O	3:F:357:ASN:ND2	2.46	0.44
4:H:37:GLU:OE1	4:H:44:THR:OG1	2.31	0.44
3:F:118:ILE:HG22	3:F:119:SER:N	2.31	0.44
8:P:174:CYS:HB2	8:P:182:ARG:HA	1.99	0.44
4:G:117:ASP:OD1	4:G:120:ARG:NH1	2.50	0.44
4:G:367:GLN:HB2	4:G:384:ILE:HG12	1.99	0.44
5:I:195:LEU:HD12	5:I:283:GLU:HB3	2.00	0.44
6:L:192:CYS:HA	6:L:261:VAL:H	1.83	0.44
4:G:144:ASP:OD1	4:G:144:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:80:VAL:HG11	5:I:174:PHE:HB3	1.99	0.44
8:P:315:LEU:HB3	8:P:417:VAL:HB	1.99	0.44
2:D:394:ILE:O	2:D:422:LYS:NZ	2.39	0.44
4:G:63:THR:HG22	4:G:139:VAL:H	1.83	0.44
4:G:88:ASP:OD1	4:G:89:TYR:N	2.50	0.44
4:H:253:GLN:N	4:H:258:ASP:OD2	2.48	0.44
8:O:315:LEU:HB3	8:O:417:VAL:HB	1.99	0.44
4:H:117:ASP:OD1	4:H:120:ARG:NH1	2.50	0.44
6:L:126:LEU:HA	6:L:129:THR:HG22	1.99	0.44
3:F:193:SER:HB3	3:F:196:VAL:HG22	2.00	0.43
6:L:201:ILE:HG22	8:P:330:ILE:CG2	2.43	0.43
3:E:319:GLN:NE2	4:H:302:TRP:O	2.50	0.43
8:P:466:ILE:HG12	8:P:499:ILE:HG12	2.01	0.43
3:E:22:ILE:HG22	3:E:47:LEU:HD11	2.00	0.43
6:K:188:VAL:HG22	6:K:264:ILE:HG23	2.01	0.43
8:O:176:ARG:HB2	8:O:177:PRO:HD3	2.00	0.43
8:O:466:ILE:HG12	8:O:499:ILE:HG12	2.01	0.43
6:L:19:ILE:HG13	6:L:72:VAL:HG23	2.00	0.43
8:P:176:ARG:HB2	8:P:177:PRO:HD3	2.00	0.43
1:A:87:TRP:HA	1:A:90:CYS:HB2	2.00	0.43
4:G:37:GLU:OE1	4:G:44:THR:OG1	2.31	0.43
3:F:22:ILE:HG22	3:F:47:LEU:HD11	2.00	0.43
6:K:19:ILE:HG13	6:K:72:VAL:HG23	2.00	0.43
2:C:468:ASP:OD1	2:C:468:ASP:N	2.47	0.43
2:D:339:THR:HG21	2:D:511:LYS:HZ3	1.83	0.43
3:E:30:LYS:HB2	3:E:31:ARG:HD2	2.01	0.43
3:F:30:LYS:HB2	3:F:31:ARG:HD2	2.01	0.43
2:C:627:LYS:HG3	1:B:240:PHE:HE2	1.83	0.43
5:I:190:ARG:NH1	5:I:235:GLN:OE1	2.52	0.43
5:J:190:ARG:NH1	5:J:235:GLN:OE1	2.52	0.43
8:P:432:ILE:HD11	8:P:499:ILE:HD13	2.01	0.43
6:K:247:ALA:HA	6:K:250:LYS:HE3	2.01	0.43
8:O:432:ILE:HD11	8:O:499:ILE:HD13	2.01	0.43
2:C:383:ASP:O	2:C:387:ILE:HG12	2.19	0.42
2:D:278:THR:HG21	2:D:329:LEU:HG	2.00	0.42
2:D:383:ASP:O	2:D:387:ILE:HG12	2.19	0.42
3:E:185:ILE:HG13	3:E:255:VAL:HA	2.01	0.42
3:E:115:GLU:HA	3:E:116:PRO:HD3	1.80	0.42
3:E:144:MET:HG2	3:E:145:LYS:HD2	2.01	0.42
3:F:52:ILE:HD11	3:F:67:ILE:HD12	2.01	0.42
6:L:188:VAL:HG22	6:L:264:ILE:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:33:THR:OG1	4:G:34:ASP:N	2.52	0.42
4:H:33:THR:OG1	4:H:34:ASP:N	2.52	0.42
3:F:144:MET:HG2	3:F:145:LYS:HD2	2.01	0.42
8:O:312:SER:HA	8:O:313:PRO:HD3	1.84	0.42
6:L:52:SEP:HB2	6:L:53:ARG:H	1.68	0.42
3:E:252:MET:HE2	3:E:285:ALA:HA	2.02	0.42
1:B:87:TRP:HA	1:B:90:CYS:HB2	2.00	0.42
4:H:287:SER:O	4:H:291:TYR:N	2.48	0.42
3:F:72:ASN:ND2	3:F:377:ASP:OD1	2.43	0.42
6:K:5:HIS:HD1	6:K:40:ASP:HB2	1.85	0.42
1:B:283:LEU:HD21	1:B:295:VAL:HG11	2.02	0.42
8:O:132:LEU:HD13	8:O:137:THR:HA	2.02	0.42
6:L:5:HIS:HD1	6:L:40:ASP:HB2	1.85	0.42
1:A:21:THR:OG1	1:A:22:MET:N	2.52	0.42
3:E:327:PRO:HG3	4:H:174:TYR:HB3	2.01	0.42
6:L:202:LYS:HG3	8:P:333:LEU:HD12	2.01	0.42
1:A:89:ASN:O	1:A:93:HIS:N	2.40	0.42
2:C:401:VAL:HB	2:C:470:VAL:HG22	2.02	0.42
3:E:193:SER:HB3	3:E:196:VAL:HG22	2.00	0.42
1:B:56:LEU:O	1:B:59:SER:OG	2.31	0.42
4:H:356:LYS:HD2	4:H:373:ARG:HG2	2.01	0.42
1:A:283:LEU:HD21	1:A:295:VAL:HG11	2.02	0.42
1:A:76:PHE:HD1	3:E:122:PHE:HZ	1.67	0.42
4:G:227:ARG:NH2	4:G:229:ASP:OD2	2.52	0.42
3:F:21:THR:HA	3:F:24:THR:HG22	2.02	0.42
8:P:260:LEU:O	8:P:264:LYS:HG2	2.20	0.42
2:D:401:VAL:HB	2:D:470:VAL:HG22	2.02	0.42
3:E:21:THR:HA	3:E:24:THR:HG22	2.02	0.42
4:G:145:PHE:HZ	4:G:237:ILE:HG21	1.84	0.42
4:G:317:THR:O	4:G:328:GLU:HA	2.20	0.42
5:I:67:ALA:HB3	5:I:69:LEU:HG	2.02	0.42
4:H:57:VAL:HA	4:H:58:PRO:HD3	1.90	0.42
4:H:145:PHE:HZ	4:H:237:ILE:HG21	1.84	0.42
2:C:405:SER:HB2	2:C:436:GLU:HB2	2.02	0.41
1:B:17:ASP:HB3	1:B:20:MET:HE3	2.01	0.41
1:B:21:THR:OG1	1:B:22:MET:N	2.52	0.41
8:P:132:LEU:HD13	8:P:137:THR:HA	2.02	0.41
3:E:186:LEU:HB2	3:E:213:VAL:HG12	2.02	0.41
4:H:60:ILE:O	4:H:63:THR:OG1	2.36	0.41
4:H:63:THR:HG22	4:H:139:VAL:H	1.83	0.41
4:H:227:ARG:NH2	4:H:229:ASP:OD2	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:247:ALA:HA	6:L:250:LYS:HE3	2.01	0.41
4:G:169:SER:OG	4:G:282:ALA:O	2.30	0.41
6:K:22:VAL:HG12	6:K:36:LEU:HA	2.02	0.41
3:E:52:ILE:HD11	3:E:67:ILE:HD12	2.01	0.41
3:F:46:GLN:OE1	3:F:50:ARG:NH1	2.54	0.41
2:D:476:SER:HA	2:D:511:LYS:HG2	2.02	0.41
2:D:601:LEU:HD23	3:F:227:HIS:HB3	2.01	0.41
1:B:302:MET:HG3	1:B:303:TRP:CD1	2.56	0.41
4:H:163:ILE:HG23	4:H:242:VAL:HG11	2.03	0.41
6:K:202:LYS:HG3	8:O:333:LEU:HD12	2.02	0.41
8:P:101:ILE:HG13	8:P:212:ASP:HB2	2.02	0.41
8:P:312:SER:HA	8:P:313:PRO:HD3	1.84	0.41
2:C:487:ALA:N	2:C:616:LEU:O	2.54	0.41
2:D:456:ILE:HG13	2:D:459:LEU:HD12	2.02	0.41
3:E:192:ASP:OD1	3:E:192:ASP:N	2.50	0.41
4:H:317:THR:O	4:H:328:GLU:HA	2.20	0.41
4:H:325:ILE:HD11	4:H:340:GLY:O	2.21	0.41
3:F:185:ILE:HG13	3:F:255:VAL:HA	2.01	0.41
2:C:476:SER:HA	2:C:511:LYS:HG2	2.02	0.41
2:D:635:LEU:HD22	2:D:643:ILE:HD12	2.03	0.41
4:G:356:LYS:HD2	4:G:373:ARG:HG2	2.01	0.41
5:J:234:ARG:HD3	5:J:234:ARG:HA	1.85	0.41
1:B:211:VAL:HG22	1:B:271:THR:HA	2.03	0.41
8:O:260:LEU:O	8:O:264:LYS:HG2	2.20	0.41
6:L:22:VAL:HG12	6:L:36:LEU:HA	2.02	0.41
8:P:355:ILE:HD12	8:P:373:ILE:HB	2.02	0.41
1:A:211:VAL:HG22	1:A:271:THR:HA	2.03	0.41
2:C:297:LEU:HD23	2:C:375:ALA:HB2	2.03	0.41
2:C:527:ALA:O	2:C:614:ASN:ND2	2.41	0.41
2:D:487:ALA:N	2:D:616:LEU:O	2.54	0.41
5:I:236:PRO:O	5:I:389:GLU:N	2.54	0.41
3:F:186:LEU:HB2	3:F:213:VAL:HG12	2.02	0.41
3:F:252:MET:HE2	3:F:285:ALA:HA	2.02	0.41
2:C:452:MET:HE1	2:C:465:MET:HE1	2.02	0.41
2:C:472:LEU:HD21	2:C:492:LEU:HD11	2.03	0.41
2:D:405:SER:HB2	2:D:436:GLU:HB2	2.02	0.41
5:J:67:ALA:HB3	5:J:69:LEU:HG	2.02	0.41
2:C:507:CYS:SG	2:C:508:GLU:N	2.94	0.40
2:D:452:MET:HE1	2:D:465:MET:HE1	2.02	0.40
3:E:46:GLN:OE1	3:E:50:ARG:NH1	2.54	0.40
3:E:257:LYS:HD3	3:E:293:PHE:CE2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:6:PHE:O	5:J:170:LEU:N	2.54	0.40
1:A:302:MET:HG3	1:A:303:TRP:CD1	2.56	0.40
2:D:472:LEU:HD21	2:D:492:LEU:HD11	2.03	0.40
3:E:373:ASP:OD1	3:E:373:ASP:N	2.53	0.40
4:G:325:ILE:HD11	4:G:340:GLY:O	2.21	0.40
5:J:236:PRO:O	5:J:389:GLU:N	2.54	0.40
8:O:116:VAL:HG21	8:O:217:LEU:CD2	2.47	0.40
1:A:210:LEU:HG	1:A:211:VAL:H	1.87	0.40
2:C:289:SER:HG	2:C:511:LYS:NZ	2.19	0.40
2:D:601:LEU:HD11	2:D:612:ILE:HD11	2.04	0.40
1:B:21:THR:HG23	1:B:23:PRO:HD2	2.04	0.40
8:P:142:TYR:CE1	8:P:395:LEU:HB3	2.56	0.40
2:D:297:LEU:HD23	2:D:375:ALA:HB2	2.03	0.40
4:G:253:GLN:N	4:G:258:ASP:OD2	2.48	0.40
4:G:321:GLU:OE2	4:G:327:LYS:NZ	2.55	0.40
6:K:141:ALA:HA	6:K:144:ALA:HB3	2.03	0.40
6:K:155:TRP:HH2	6:K:169:LEU:HB3	1.87	0.40
8:O:355:ILE:HD12	8:O:373:ILE:HB	2.02	0.40
8:P:436:LEU:HD23	8:P:513:GLY:HA3	2.04	0.40
2:C:635:LEU:HD22	2:C:643:ILE:HD12	2.03	0.40
1:B:89:ASN:O	1:B:93:HIS:N	2.40	0.40
8:O:101:ILE:HG13	8:O:212:ASP:HB2	2.02	0.40
8:O:506:GLU:HB2	8:O:510:ARG:NE	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/305 (99%)	264 (87%)	39 (13%)	0	100	100
1	B	303/305 (99%)	265 (88%)	38 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	338/651 (52%)	303 (90%)	35 (10%)	0	100	100
2	D	338/651 (52%)	303 (90%)	35 (10%)	0	100	100
3	E	350/381 (92%)	327 (93%)	23 (7%)	0	100	100
3	F	350/381 (92%)	327 (93%)	23 (7%)	0	100	100
4	G	408/712 (57%)	364 (89%)	44 (11%)	0	100	100
4	H	408/712 (57%)	364 (89%)	44 (11%)	0	100	100
5	I	260/578 (45%)	214 (82%)	46 (18%)	0	100	100
5	J	260/578 (45%)	215 (83%)	45 (17%)	0	100	100
6	K	242/304 (80%)	212 (88%)	29 (12%)	1 (0%)	30	65
6	L	242/304 (80%)	212 (88%)	29 (12%)	1 (0%)	30	65
7	M	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	15
7	N	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	15
8	O	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	8	38
8	P	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	8	38
All	All	4608/7486 (62%)	4074 (88%)	518 (11%)	16 (0%)	37	70

All (16) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/265 (100%)	263 (99%)	2 (1%)	73	77
1	B	265/265 (100%)	263 (99%)	2 (1%)	73	77
2	C	308/561 (55%)	307 (100%)	1 (0%)	86	86
2	D	308/561 (55%)	307 (100%)	1 (0%)	86	86
3	E	315/338 (93%)	314 (100%)	1 (0%)	86	86
3	F	315/338 (93%)	314 (100%)	1 (0%)	86	86
4	G	375/649 (58%)	373 (100%)	2 (0%)	81	82
4	H	375/649 (58%)	373 (100%)	2 (0%)	81	82
5	I	250/529 (47%)	248 (99%)	2 (1%)	73	77
5	J	250/529 (47%)	248 (99%)	2 (1%)	73	77
6	K	223/273 (82%)	211 (95%)	12 (5%)	20	45
6	L	223/273 (82%)	211 (95%)	12 (5%)	20	45
7	M	16/246 (6%)	15 (94%)	1 (6%)	16	42
7	N	16/246 (6%)	15 (94%)	1 (6%)	16	42
8	O	332/449 (74%)	294 (89%)	38 (11%)	5	22
8	P	332/449 (74%)	294 (89%)	38 (11%)	5	22
All	All	4168/6620 (63%)	4050 (97%)	118 (3%)	38	60

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	LEU
1	A	300	ILE
2	C	319	LEU
2	D	319	LEU
3	E	371	GLN
4	G	44	THR
4	G	67	LEU
5	I	77	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	I	393	ILE
5	J	77	ILE
5	J	393	ILE
1	B	299	LEU
1	B	300	ILE
4	H	44	THR
4	H	67	LEU
3	F	371	GLN
6	K	85	LEU
6	K	185	ARG
6	K	195	TYR
6	K	203	ASP
6	K	230	LEU
6	K	235	LEU
6	K	236	ASP
6	K	244	LEU
6	K	251	ILE
6	K	255	ILE
6	K	261	VAL
6	K	264	ILE
7	M	141	ILE
8	O	116	VAL
8	O	117	VAL
8	O	130	ASP
8	O	132	LEU
8	O	133	GLU
8	O	192	VAL
8	O	210	VAL
8	O	224	CYS
8	O	228	GLN
8	O	236	ILE
8	O	251	VAL
8	O	253	LEU
8	O	257	GLU
8	O	291	ILE
8	O	307	ARG
8	O	318	ILE
8	O	332	ASP
8	O	353	ILE
8	O	354	GLU
8	O	355	ILE
8	O	359	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	O	373	ILE
8	O	380	LEU
8	O	395	LEU
8	O	402	VAL
8	O	403	ASP
8	O	406	LEU
8	O	412	LEU
8	O	426	ILE
8	O	432	ILE
8	O	440	LEU
8	O	443	VAL
8	O	462	LEU
8	O	466	ILE
8	O	495	ILE
8	O	502	SER
8	O	508	HIS
8	O	512	ILE
6	L	85	LEU
6	L	185	ARG
6	L	195	TYR
6	L	203	ASP
6	L	230	LEU
6	L	235	LEU
6	L	236	ASP
6	L	244	LEU
6	L	251	ILE
6	L	255	ILE
6	L	261	VAL
6	L	264	ILE
7	N	141	ILE
8	P	116	VAL
8	P	117	VAL
8	P	130	ASP
8	P	132	LEU
8	P	133	GLU
8	P	192	VAL
8	P	210	VAL
8	P	224	CYS
8	P	228	GLN
8	P	236	ILE
8	P	251	VAL
8	P	253	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	P	257	GLU
8	P	291	ILE
8	P	307	ARG
8	P	318	ILE
8	P	332	ASP
8	P	353	ILE
8	P	354	GLU
8	P	355	ILE
8	P	359	ILE
8	P	373	ILE
8	P	380	LEU
8	P	395	LEU
8	P	402	VAL
8	P	403	ASP
8	P	406	LEU
8	P	412	LEU
8	P	426	ILE
8	P	432	ILE
8	P	440	LEU
8	P	443	VAL
8	P	462	LEU
8	P	466	ILE
8	P	495	ILE
8	P	502	SER
8	P	508	HIS
8	P	512	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	93	HIS
2	C	271	HIS
2	C	325	HIS
2	C	384	GLN
2	C	389	ASN
2	C	415	HIS
2	C	416	ASN
2	C	464	ASN
2	C	517	GLN
2	D	271	HIS
2	D	325	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	342	ASN
2	D	384	GLN
2	D	389	ASN
2	D	415	HIS
2	D	416	ASN
2	D	464	ASN
2	D	517	GLN
3	E	221	ASN
3	E	227	HIS
3	E	368	ASN
4	G	82	HIS
4	G	85	GLN
4	G	87	ASN
4	G	96	ASN
4	G	241	HIS
4	G	253	GLN
4	G	371	ASN
4	G	409	ASN
5	I	118	GLN
5	I	215	GLN
5	I	309	GLN
5	I	388	ASN
5	J	118	GLN
5	J	215	GLN
5	J	309	GLN
5	J	388	ASN
1	B	80	ASN
1	B	93	HIS
4	H	82	HIS
4	H	85	GLN
4	H	87	ASN
4	H	96	ASN
4	H	253	GLN
4	H	371	ASN
4	H	409	ASN
3	F	221	ASN
3	F	227	HIS
3	F	319	GLN
3	F	368	ASN
6	K	60	GLN
6	K	103	GLN
6	K	120	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	M	140	ASN
8	O	98	GLN
8	O	111	HIS
8	O	226	GLN
8	O	249	ASN
8	O	290	ASN
8	O	415	GLN
8	O	433	ASN
8	O	496	ASN
8	O	508	HIS
6	L	60	GLN
6	L	103	GLN
6	L	109	HIS
6	L	120	GLN
7	N	140	ASN
8	P	98	GLN
8	P	111	HIS
8	P	144	ASN
8	P	226	GLN
8	P	249	ASN
8	P	415	GLN
8	P	433	ASN
8	P	496	ASN
8	P	508	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SEP	L	52	6	8,9,10	1.59	1 (12%)	7,12,14	1.26	1 (14%)
6	SEP	K	52	6	8,9,10	1.60	1 (12%)	7,12,14	1.25	1 (14%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	52	SEP	P-O1P	3.47	1.61	1.50
6	K	52	SEP	P-O1P	3.47	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	52	SEP	OG-CB-CA	2.80	110.87	108.14
6	K	52	SEP	OG-CB-CA	2.79	110.86	108.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

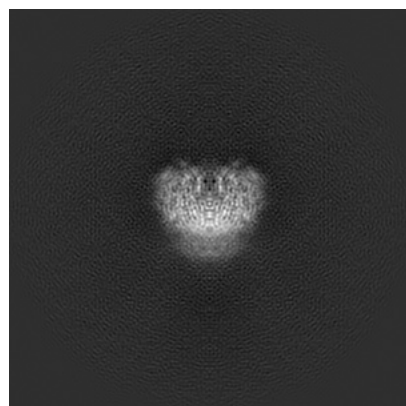
6 Map visualisation [i](#)

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

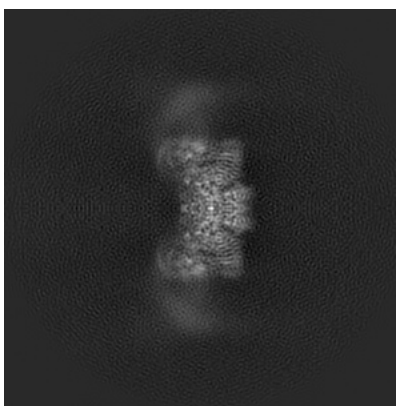
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

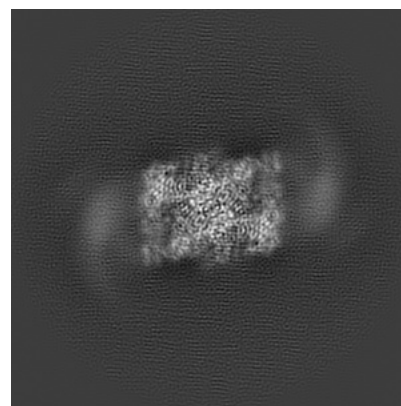
6.1.1 Primary map



X

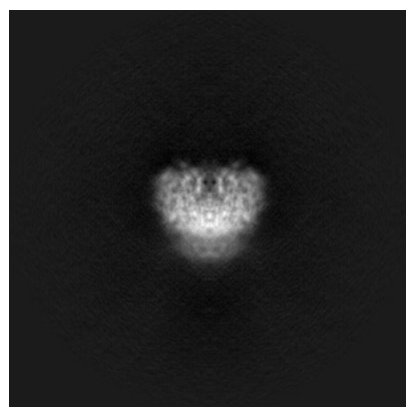


Y

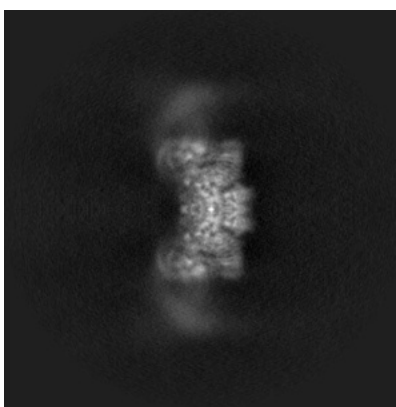


Z

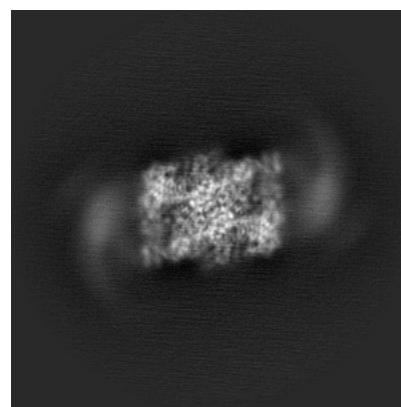
6.1.2 Raw map



X



Y

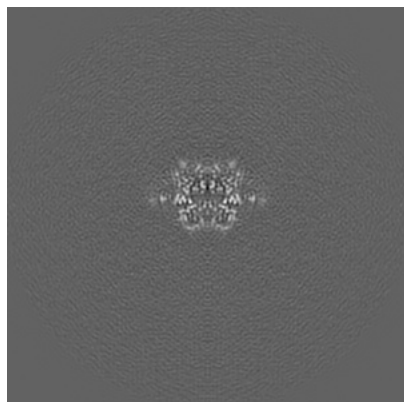


Z

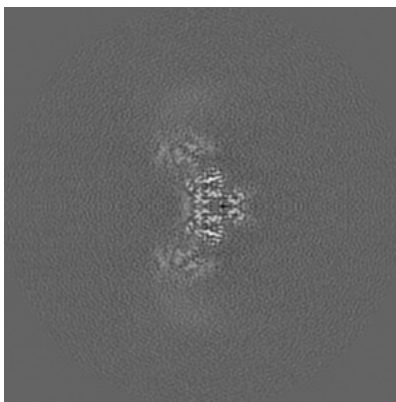
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

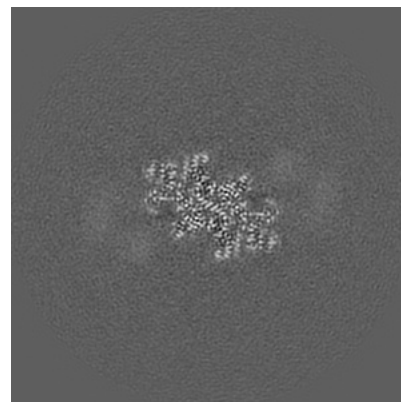
6.2.1 Primary map



X Index: 160

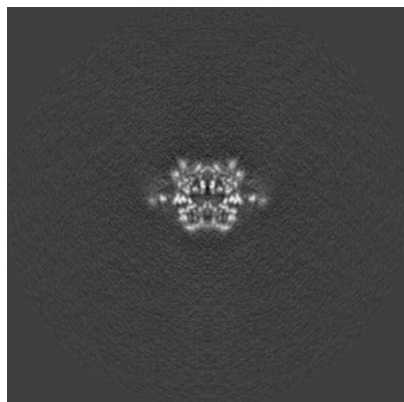


Y Index: 160

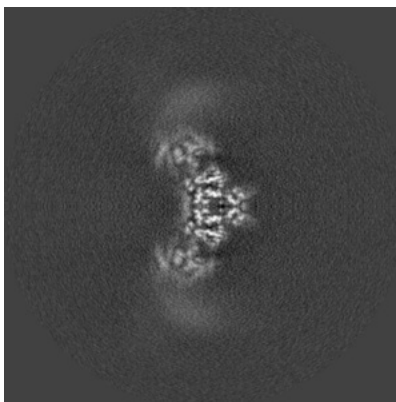


Z Index: 160

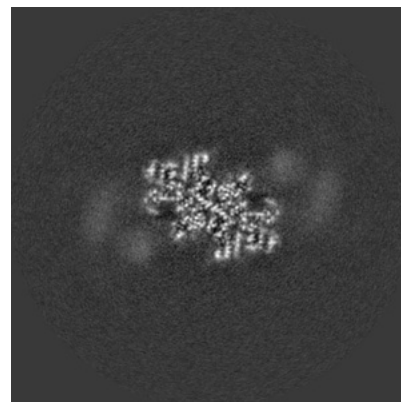
6.2.2 Raw map



X Index: 160



Y Index: 160

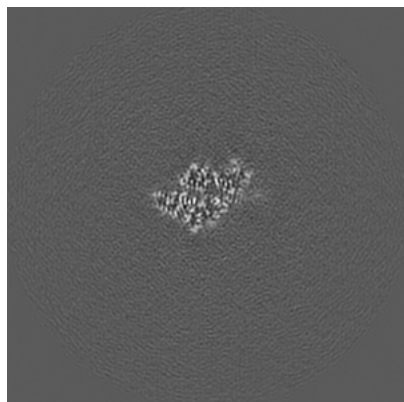


Z Index: 160

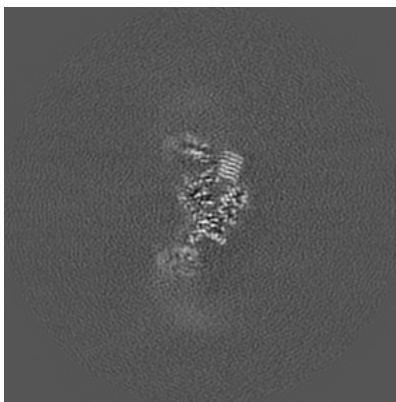
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

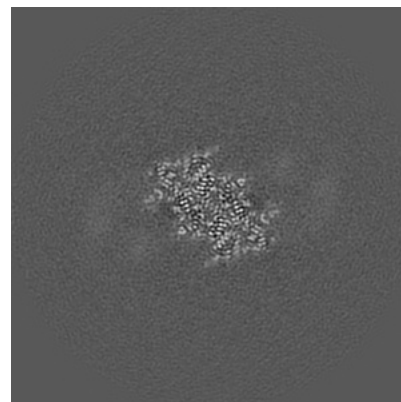
6.3.1 Primary map



X Index: 167

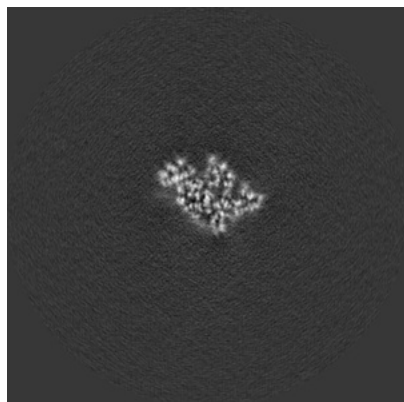


Y Index: 151

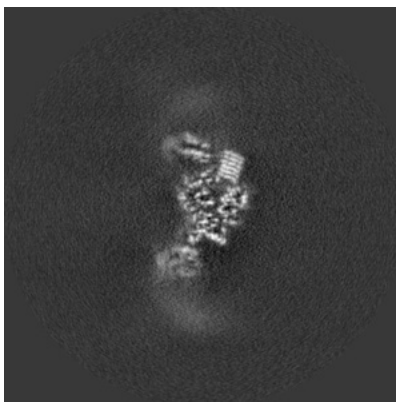


Z Index: 163

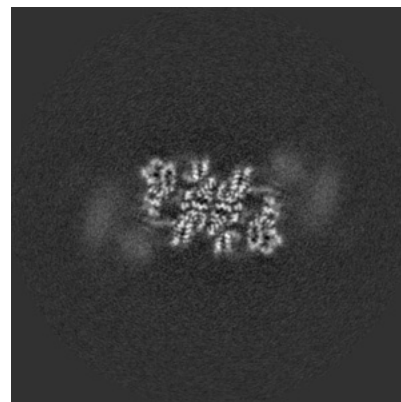
6.3.2 Raw map



X Index: 149



Y Index: 151

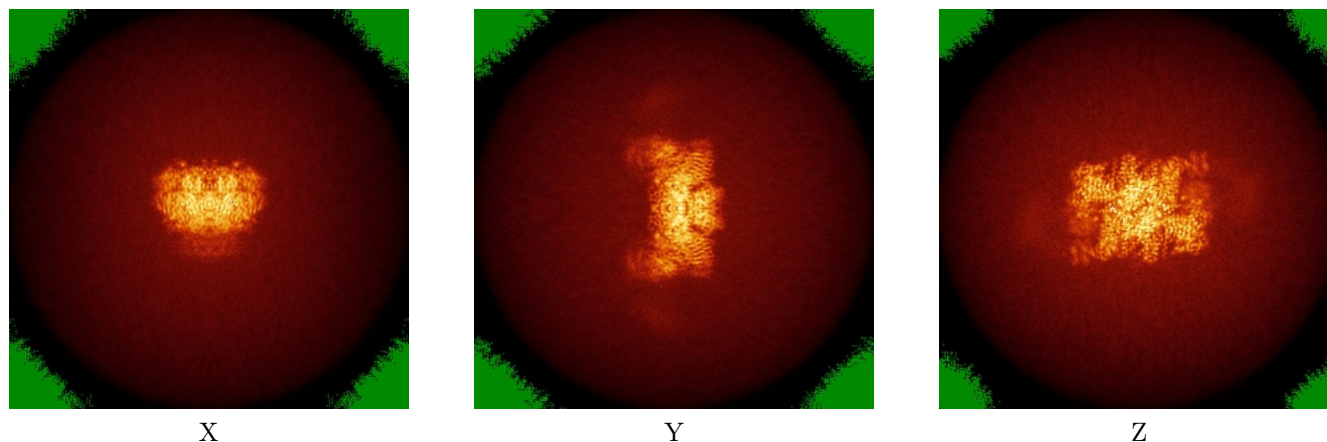


Z Index: 156

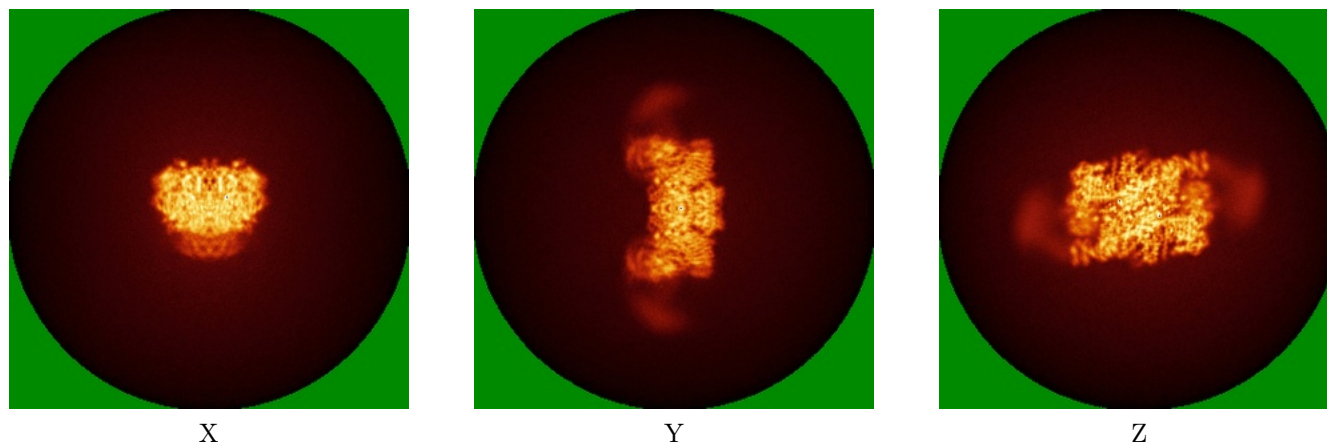
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

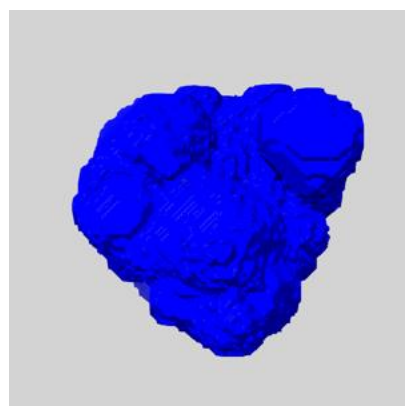
6.6 Mask visualisation [i](#)

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

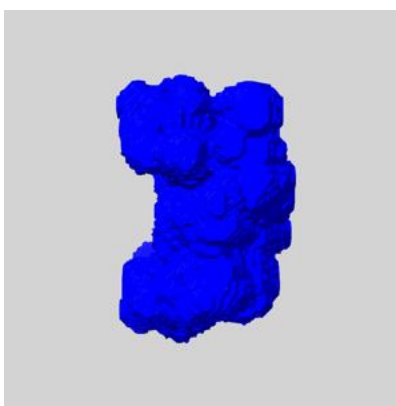
A mask typically either:

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

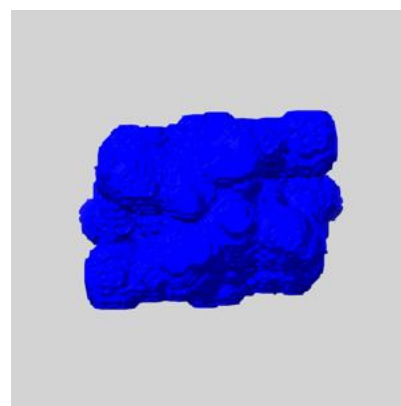
6.6.1 emd_4404_msk_1.map [i](#)



X



Y

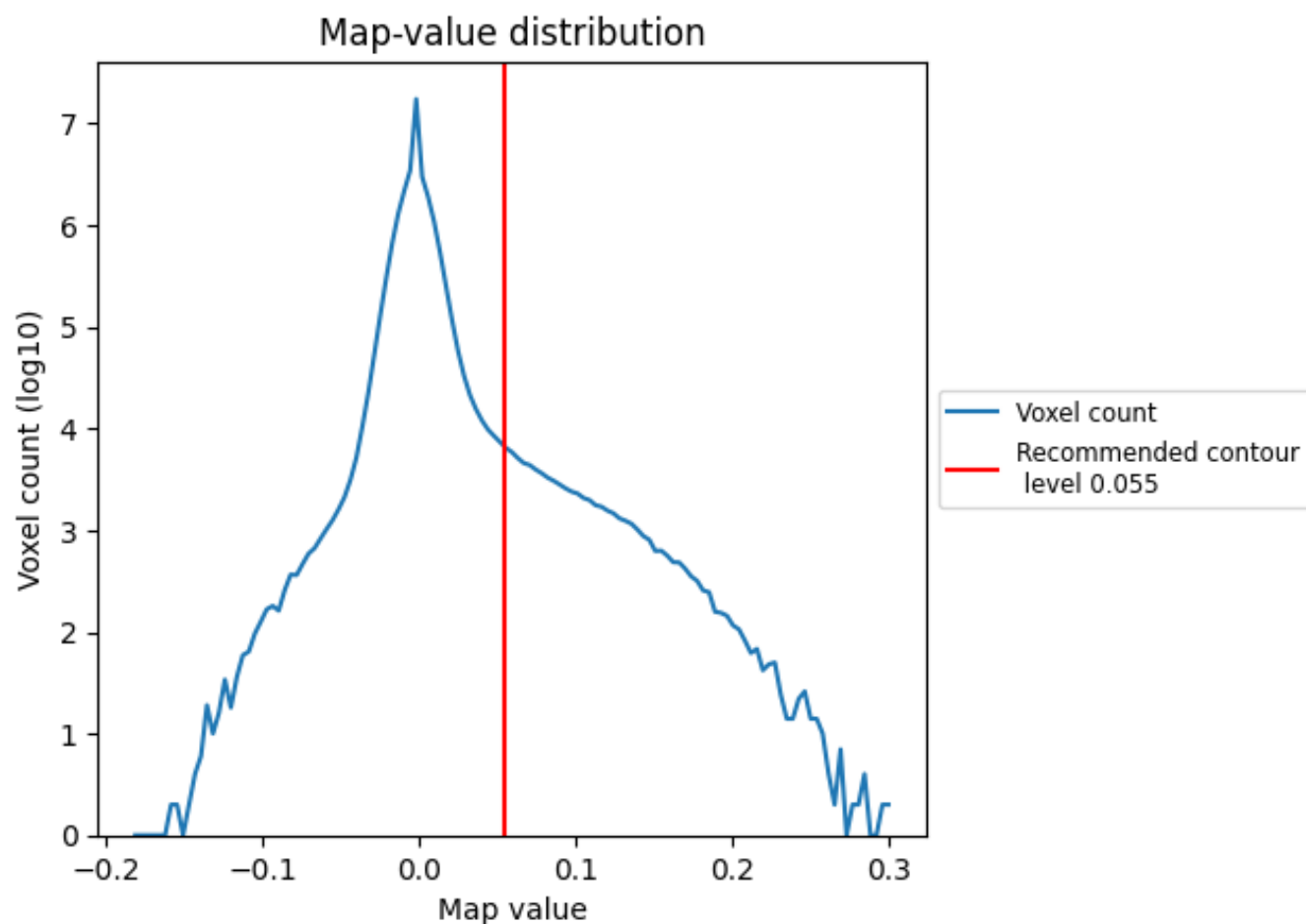


Z

7 Map analysis [i](#)

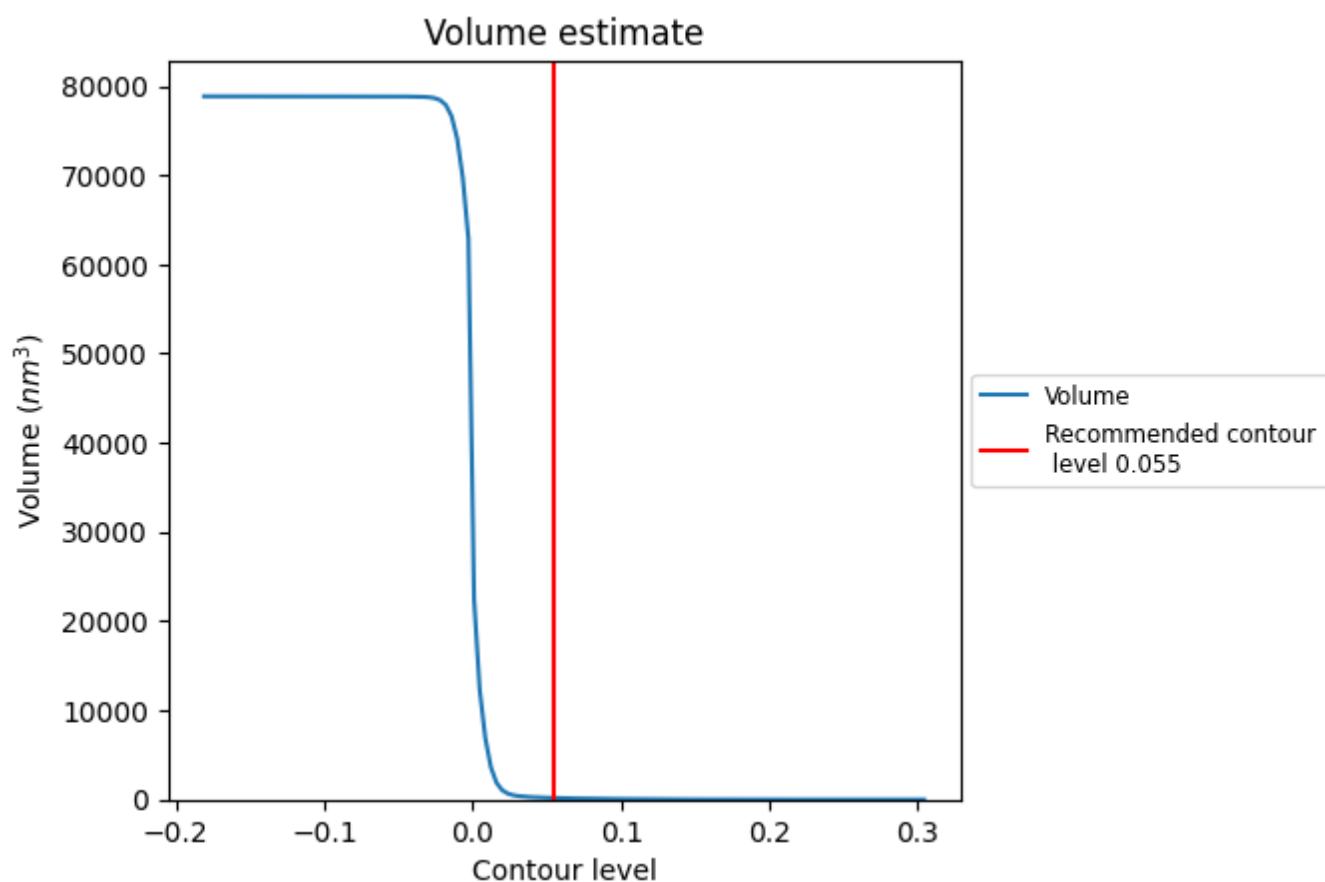
This section contains the results of statistical analysis of the map.

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.

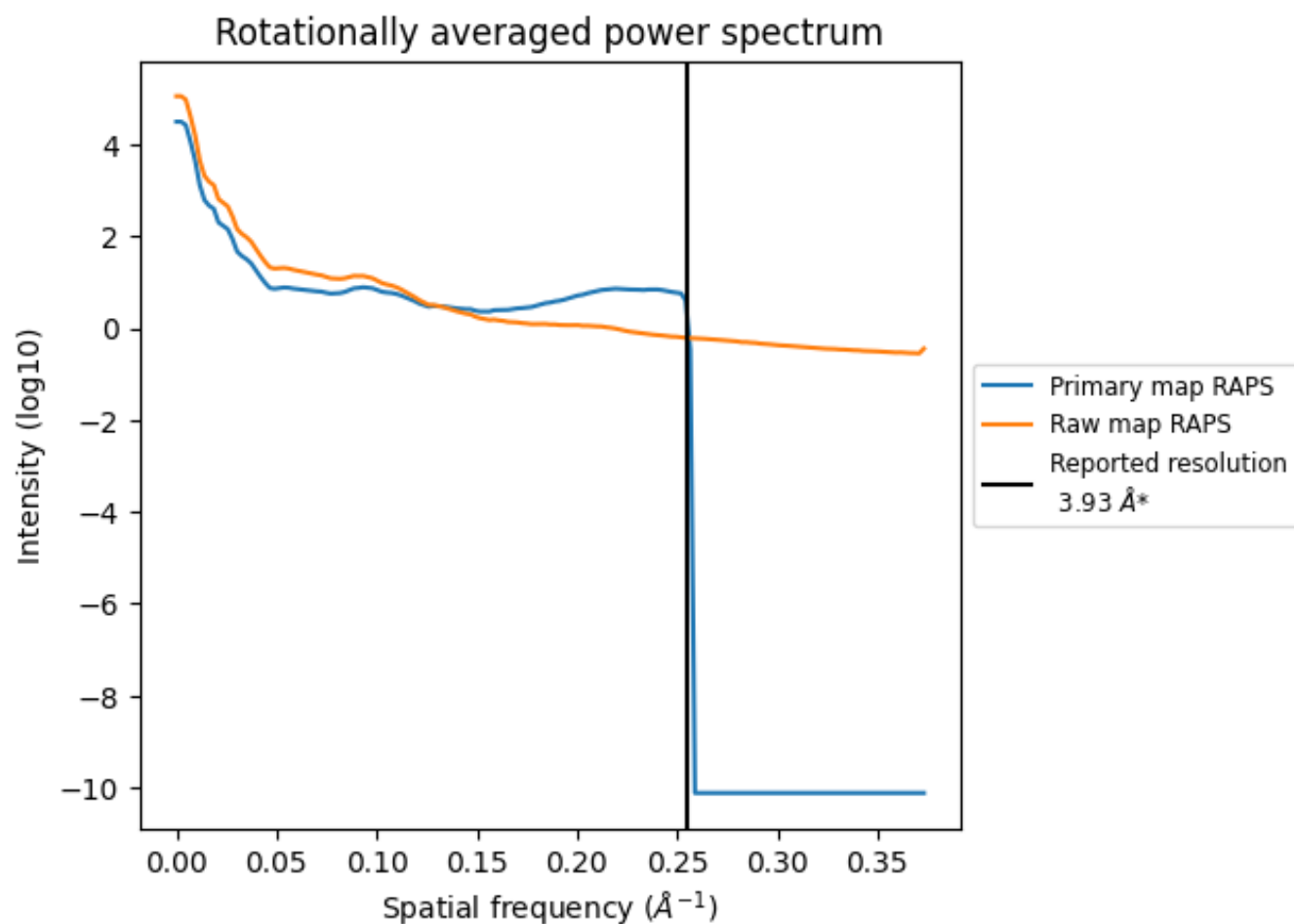
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 162 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

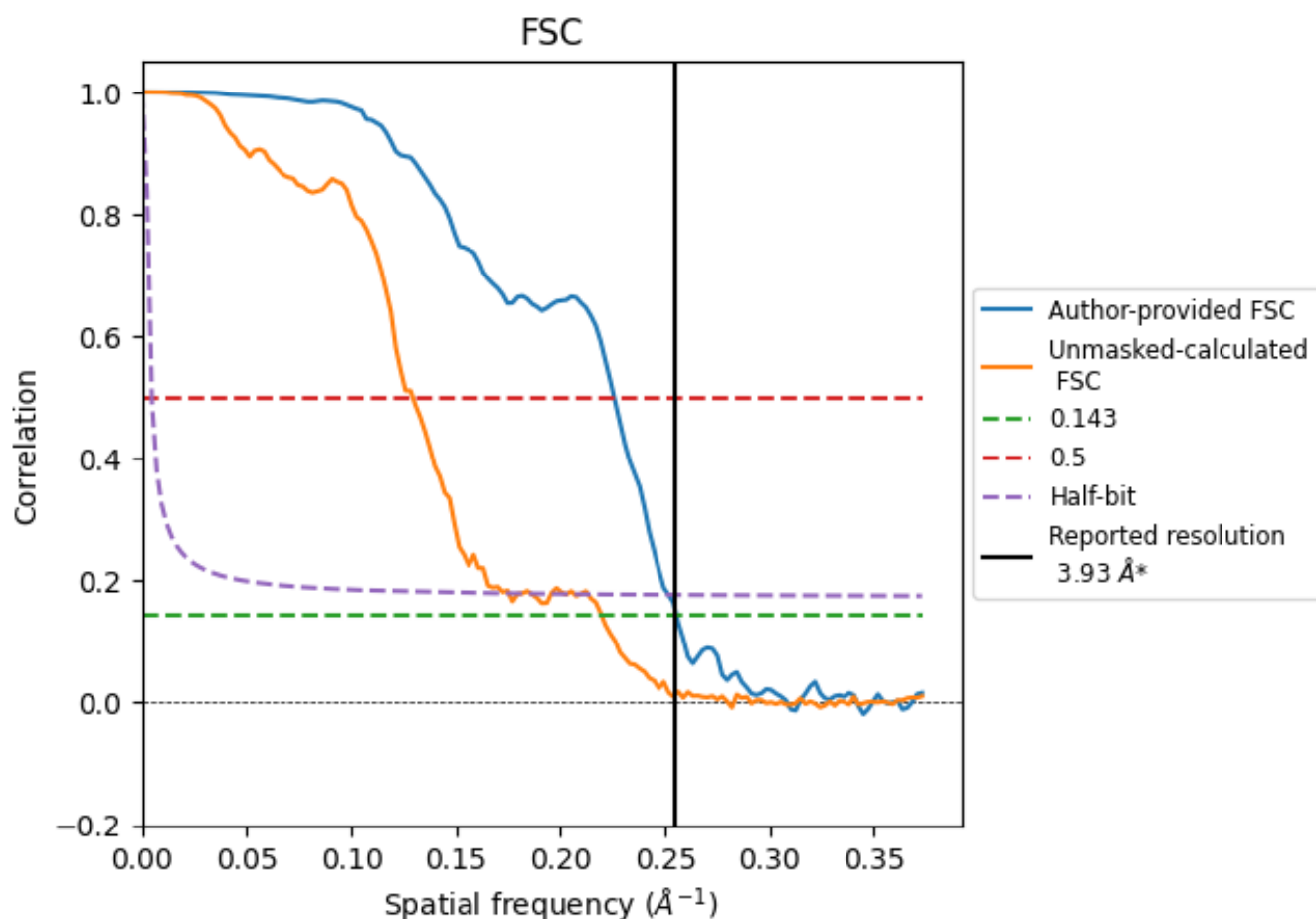


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.254 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

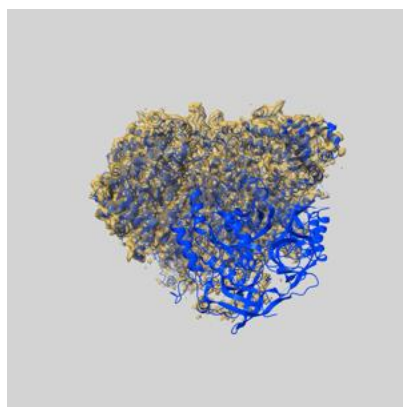
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.91	4.43	3.97
Unmasked-calculated*	4.55	7.73	5.70

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

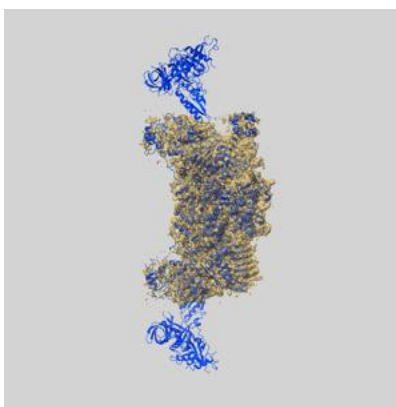
9 Map-model fit [i](#)

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

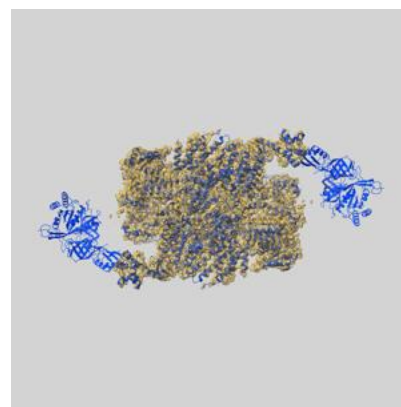
9.1 Map-model overlay [i](#)



X



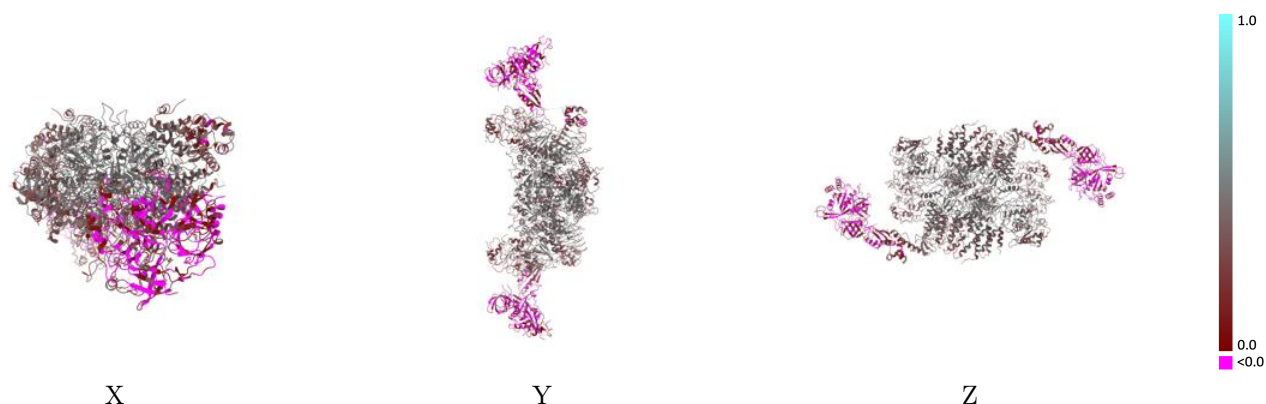
Y



Z

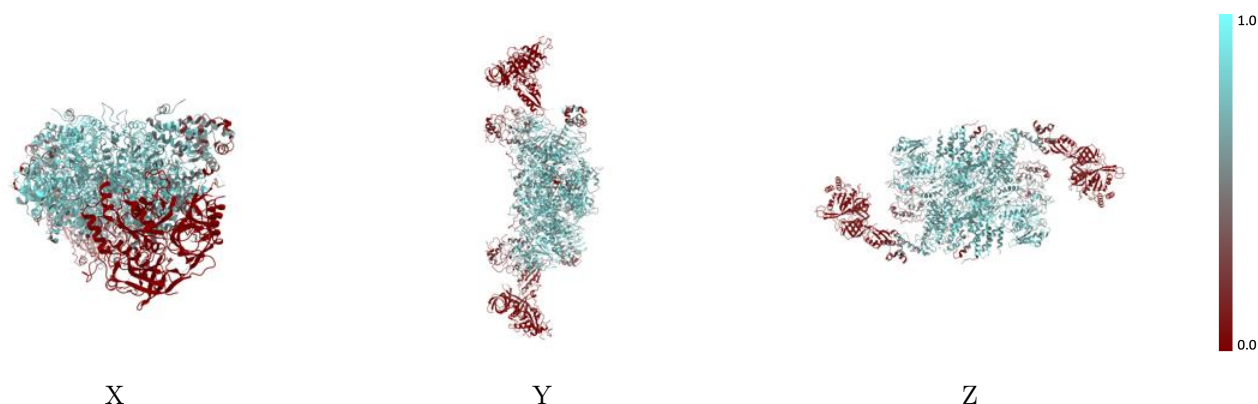
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



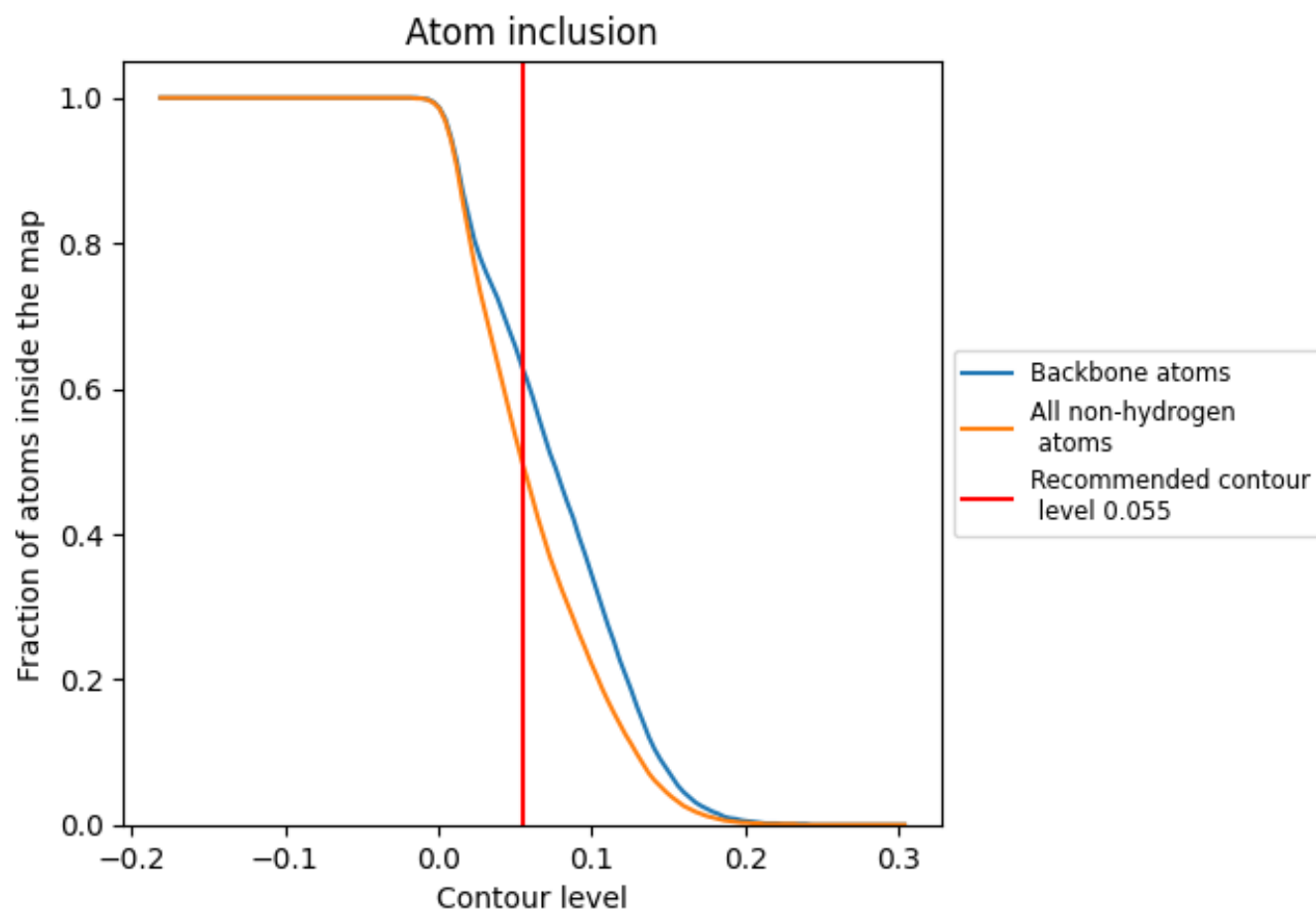
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

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

