



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:47 AM UTC

PDB ID : 6QG6 / pdb_00006qg6
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 : 10.40 Å (reported)
Based on initial models : 6FYX, 5B04

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

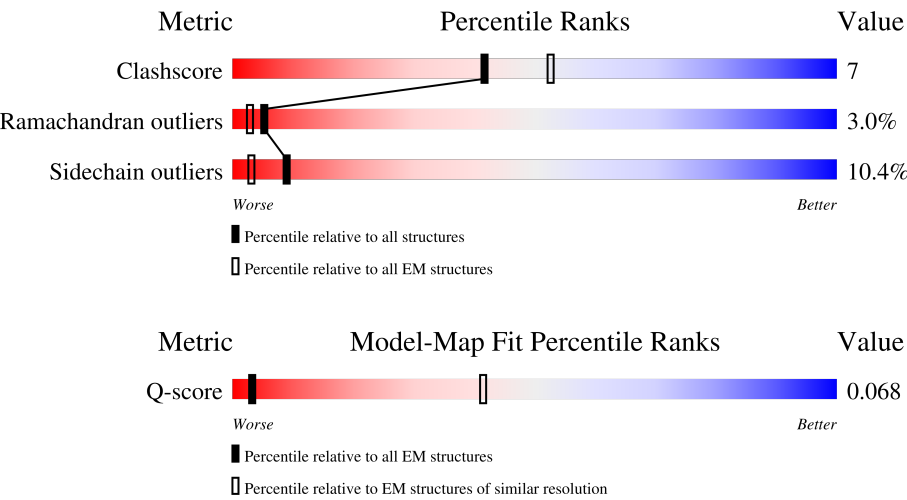
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 10.40 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.



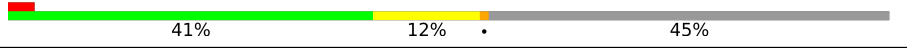
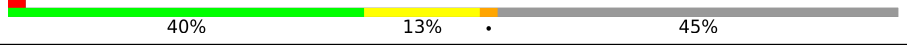
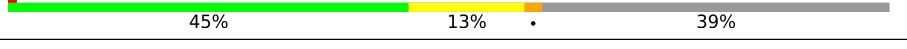
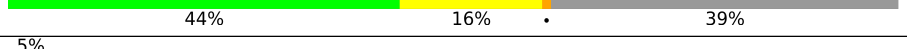
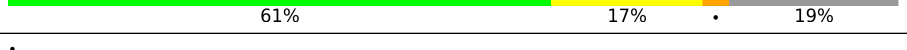
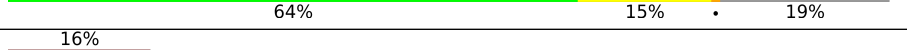
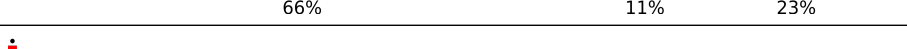
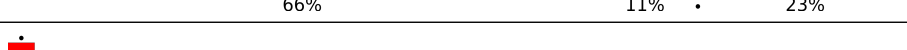
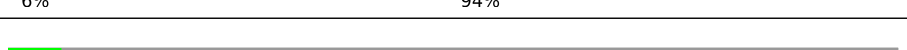
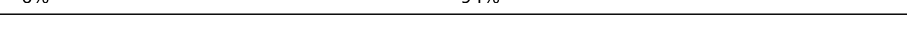
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	109 (9.90 - 10.90)

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	58%34%6%..
1	B	305	64%28%7%..
2	C	381	65%22%•9%
2	D	381	67%21%•9%

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Mol	Chain	Length	Quality of chain
3	E	578	
3	F	578	
4	G	651	
4	H	651	
5	I	712	
5	J	712	
6	K	304	
6	L	304	
7	M	527	
7	N	527	
8	O	285	
8	P	285	

2 Entry composition

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
1	A	302	Total	C	N	O	S	0	0
			2351	1504	394	443	10		
1	B	302	Total	C	N	O	S	0	0
			2351	1504	394	443	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	345	Total	C	N	O	S	0	0
			2665	1694	463	502	6		
2	D	345	Total	C	N	O	S	0	0
			2665	1694	463	502	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	267	Total	C	N	O	S	0	0
			2164	1391	363	400	10		
3	F	267	Total	C	N	O	S	0	0
			2164	1391	363	400	10		

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

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

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

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

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

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

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

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

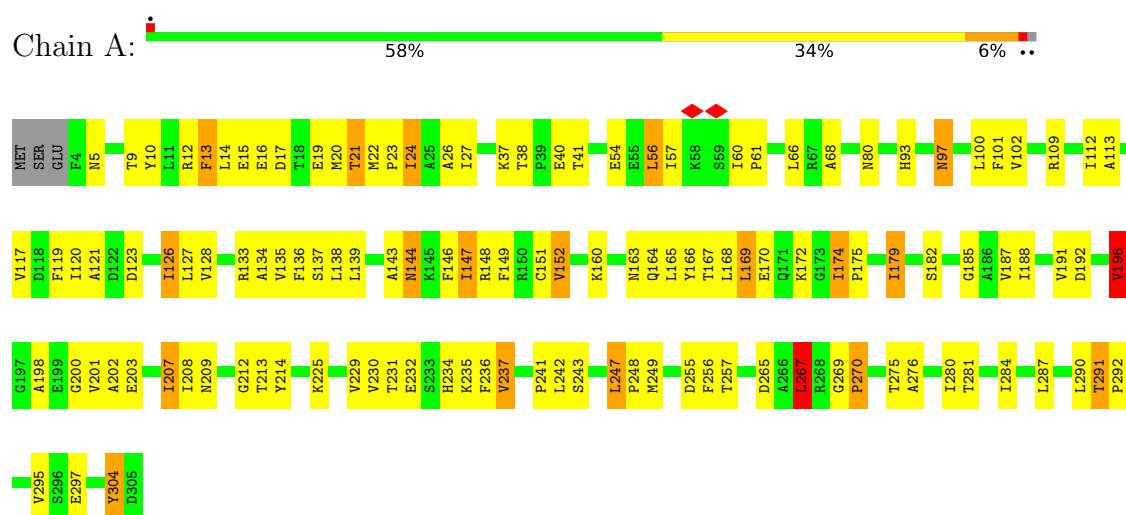
- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

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

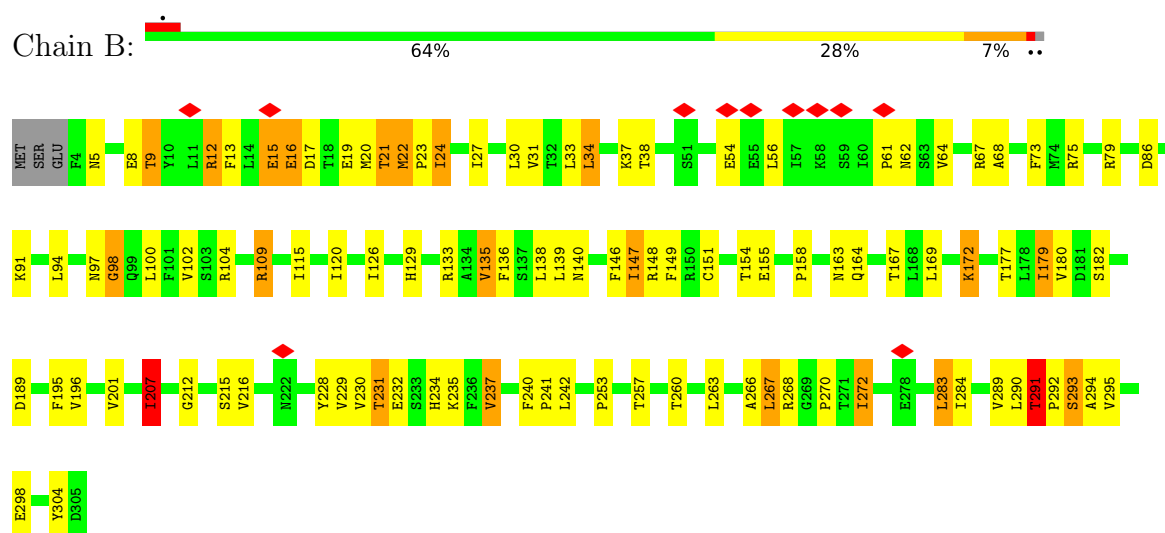
3 Residue-property plots

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

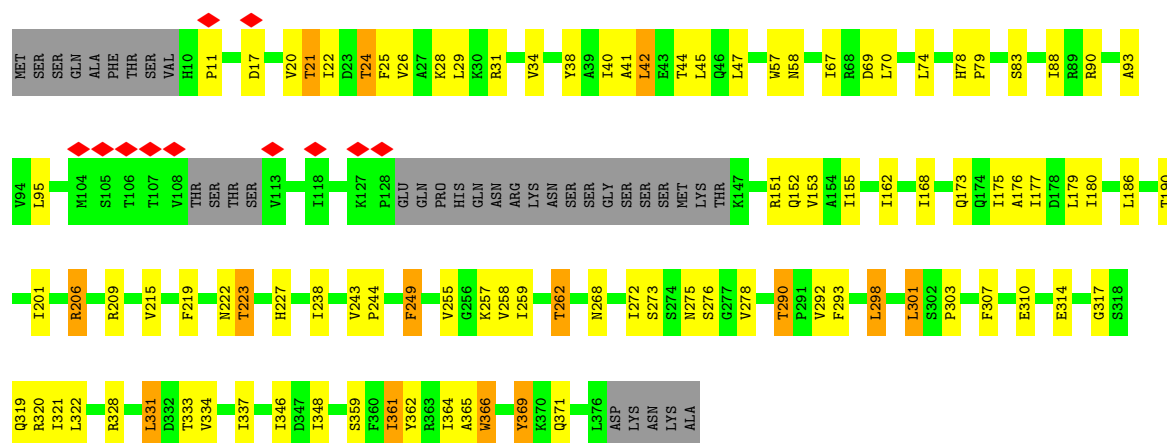


- Molecule 1: Translation initiation factor eIF-2B subunit alpha



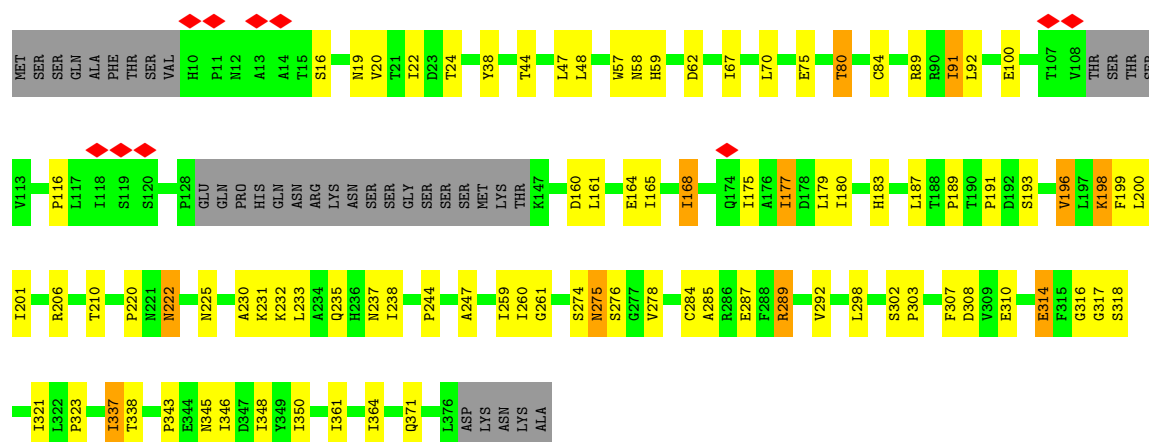
- Molecule 2: Translation initiation factor eIF-2B subunit beta





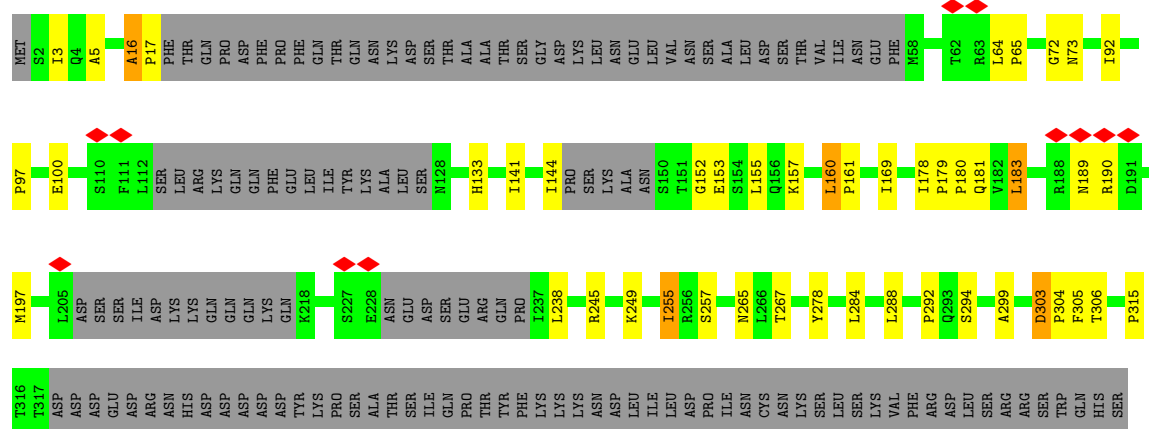
• Molecule 2: Translation initiation factor eIF-2B subunit beta

Chain D: 67% 21% 9%



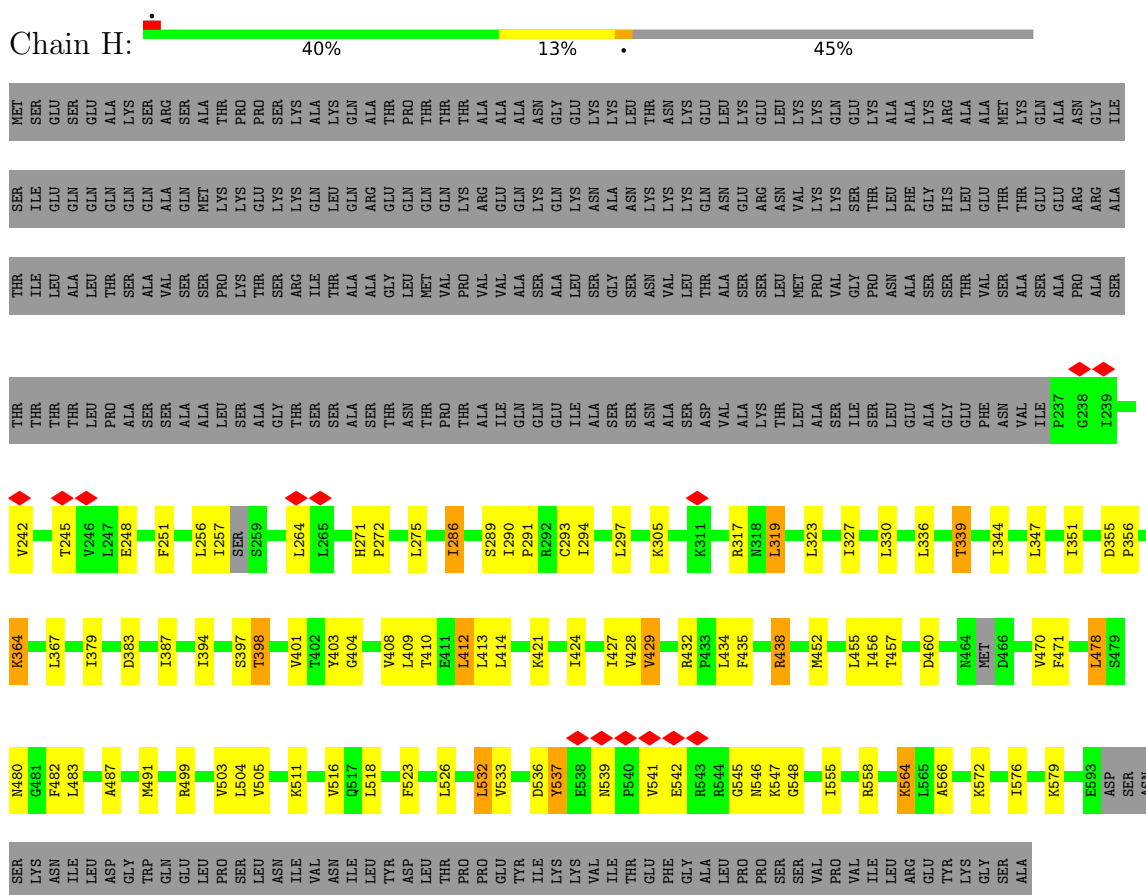
• Molecule 3: Translation initiation factor eIF-2B subunit gamma

Chain E: 37% 9% 54%

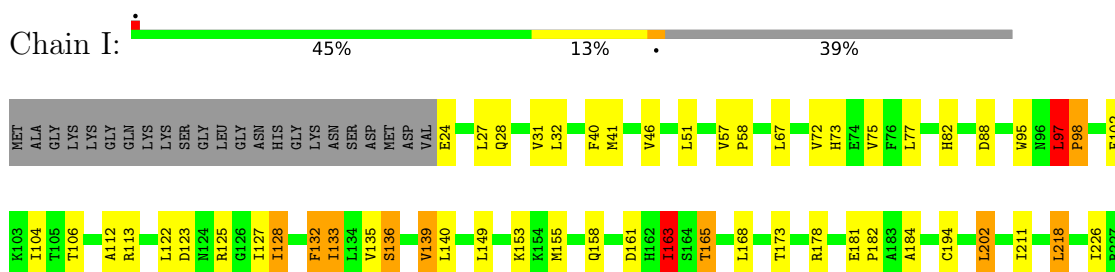


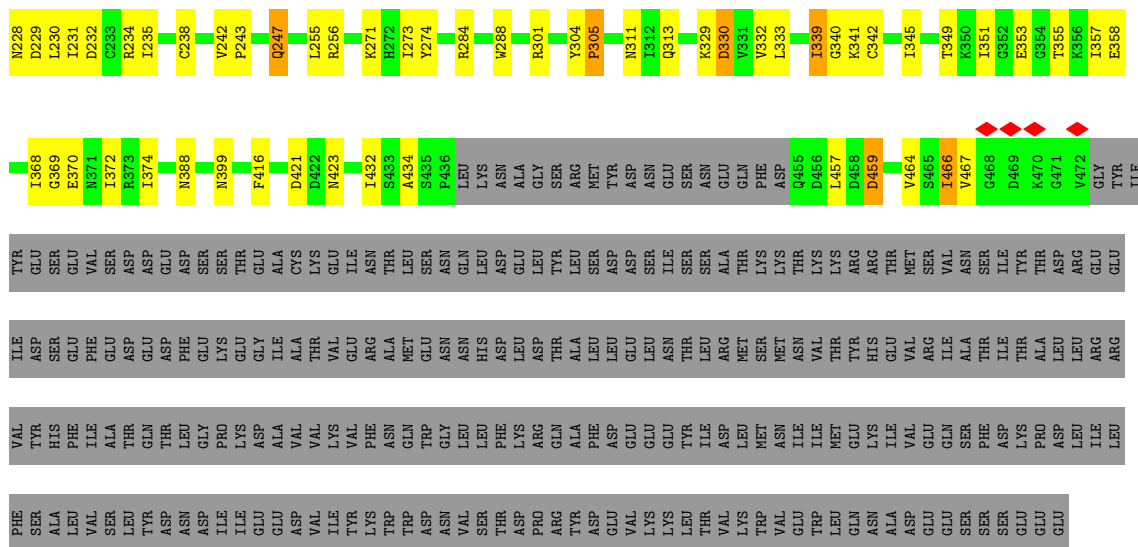


- Molecule 4: Translation initiation factor eIF-2B subunit delta

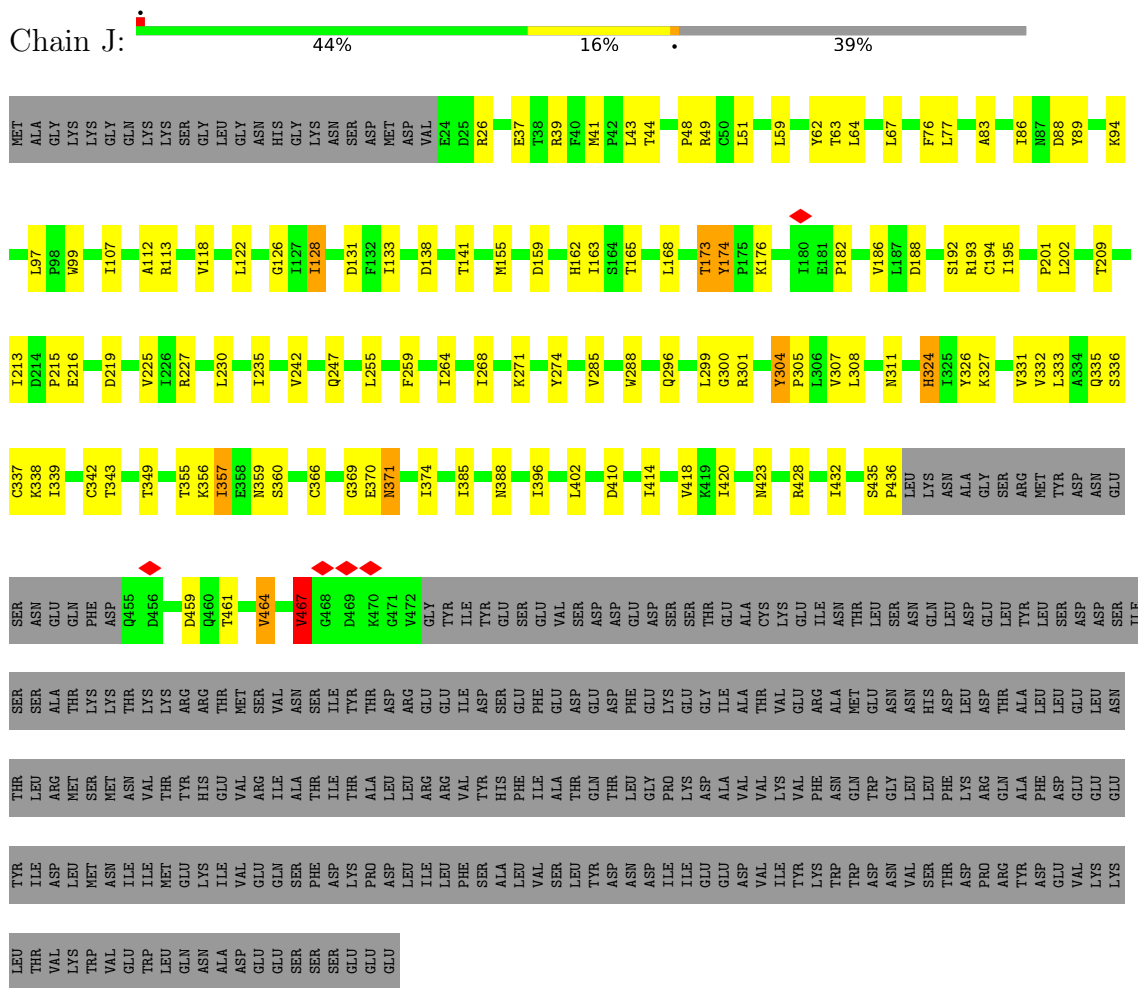


- Molecule 5: Translation initiation factor eIF-2B subunit epsilon



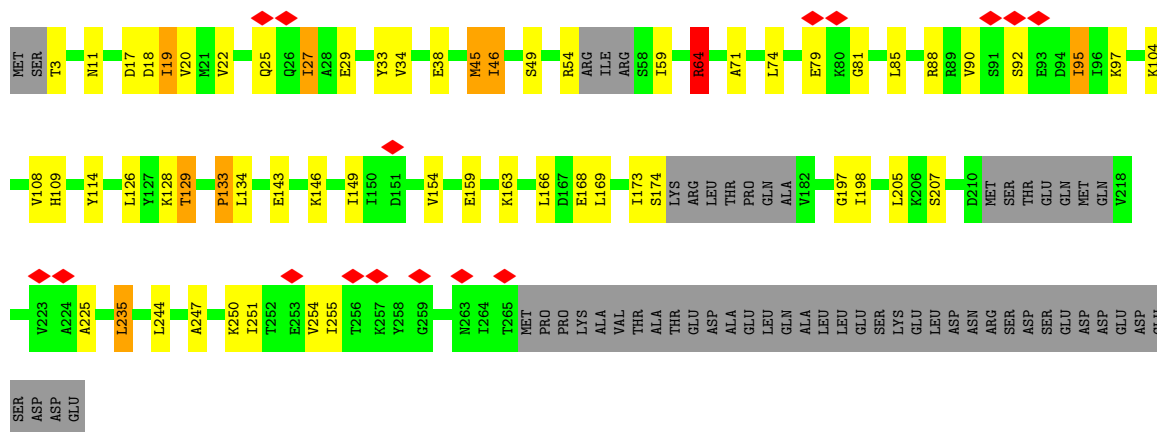


- Molecule 5: Translation initiation factor eIF-2B subunit epsilon

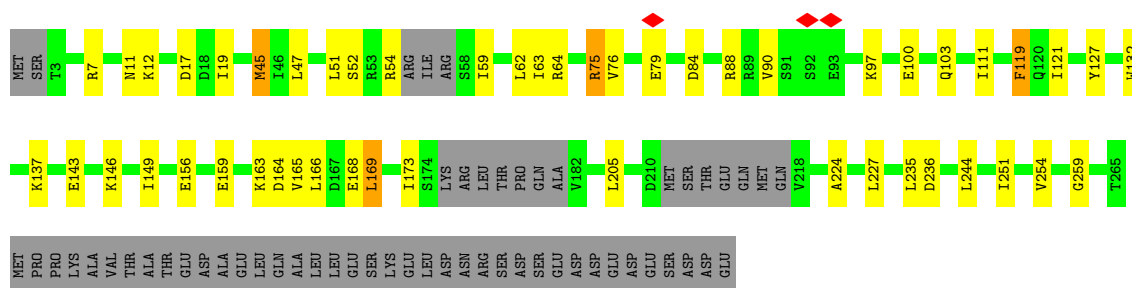


- Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

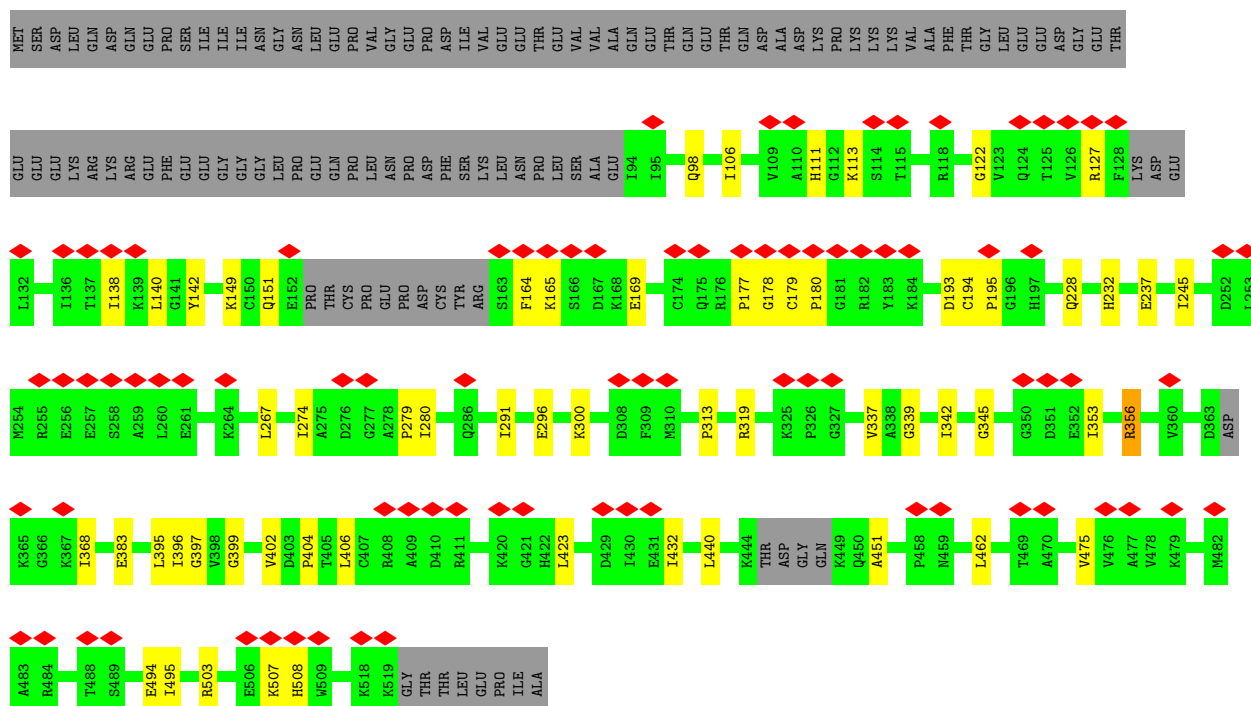




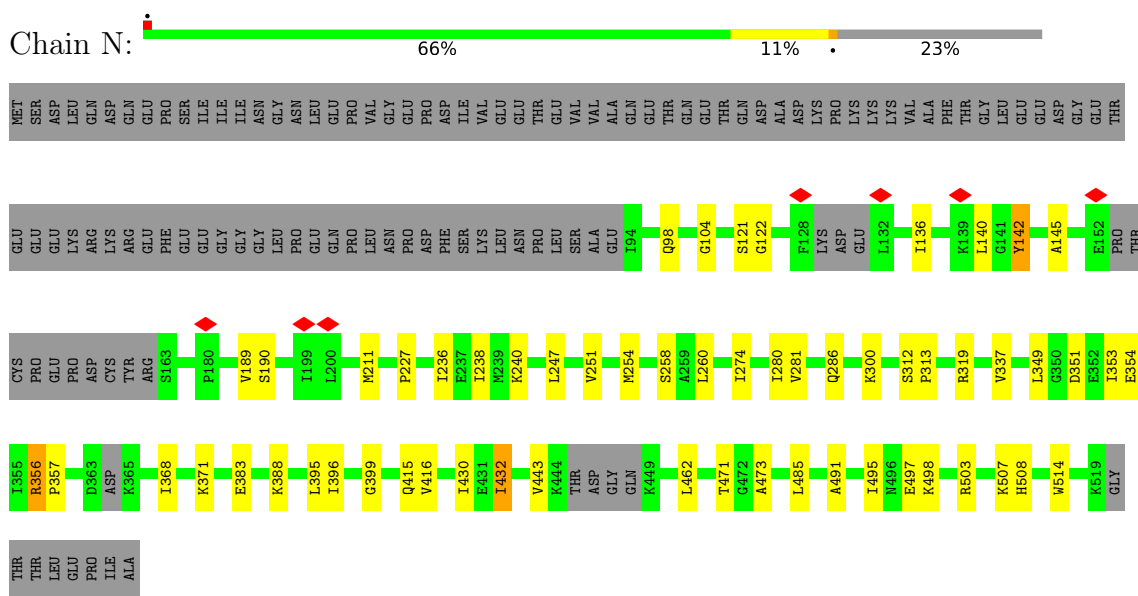
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha



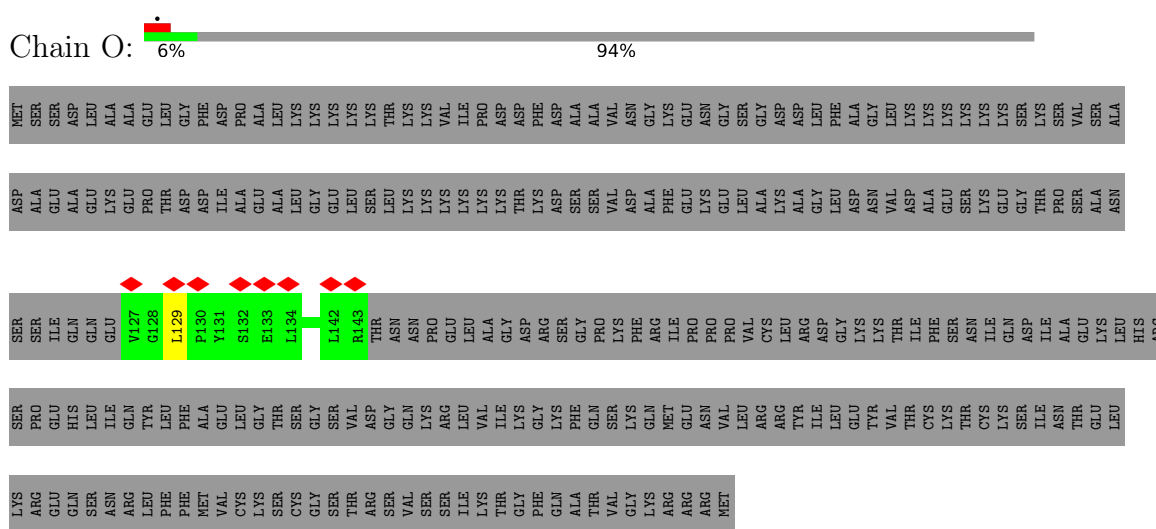
• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma



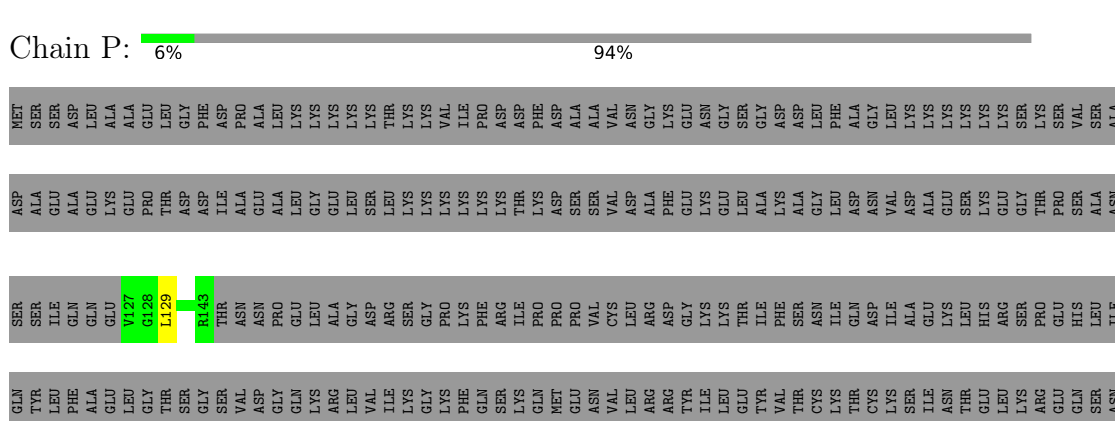
- Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma



- Molecule 8: Eukaryotic translation initiation factor 2 subunit beta



- Molecule 8: Eukaryotic translation initiation factor 2 subunit beta



ARG
LEU
PHE
PHE
MET
VAL
VAL
CYS
LYS
SER
CYS
GLY
SER
THR
THR
ARG
SER
VAL
SER
SER
ILE
LYS
THR
GLY
PHE
GLN
ALA
THR
VAL
GLY
LYS
ARG
ARG
MET

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 ($\text{\AA}$)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	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	0.59	0/2395	1.04	7/3251 (0.2%)
1	B	0.63	0/2395	1.02	4/3251 (0.1%)
2	C	0.62	0/2714	1.12	3/3693 (0.1%)
2	D	0.59	0/2714	1.05	1/3693 (0.0%)
3	E	0.66	0/2209	0.96	2/2989 (0.1%)
3	F	0.68	0/2209	0.98	1/2989 (0.0%)
4	G	0.61	0/2781	1.06	3/3747 (0.1%)
4	H	0.59	0/2781	1.09	3/3747 (0.1%)
5	I	0.63	0/3468	1.02	5/4704 (0.1%)
5	J	0.64	1/3468 (0.0%)	0.98	1/4704 (0.0%)
6	K	0.65	0/1989	1.03	1/2675 (0.0%)
6	L	0.66	0/1989	1.02	2/2675 (0.1%)
7	M	0.70	0/3087	0.97	2/4173 (0.0%)
7	N	0.70	0/3087	0.98	4/4173 (0.1%)
8	O	0.75	0/146	1.05	0/196
8	P	0.61	0/146	1.05	0/196
All	All	0.64	1/37578 (0.0%)	1.02	39/50856 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	242	VAL	CA-CB	5.42	1.56	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	404	GLY	N-CA-C	7.62	119.14	111.21
7	M	300	LYS	N-CA-C	7.41	119.05	110.97
5	I	57	VAL	CA-C-N	7.16	128.79	119.84
5	I	57	VAL	C-N-CA	7.16	128.79	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	121	SER	N-CA-C	7.12	114.62	108.78
7	M	356	ARG	N-CA-C	7.05	121.76	112.17
5	I	97	LEU	CA-C-N	6.83	128.37	119.84
5	I	97	LEU	C-N-CA	6.83	128.37	119.84
4	G	260	VAL	N-CA-C	6.82	113.50	106.21
6	K	254	VAL	N-CA-C	6.36	117.04	110.36
7	N	300	LYS	N-CA-C	6.09	117.60	110.97
3	F	98	VAL	N-CA-C	5.87	116.05	110.42
4	G	268	ASP	N-CA-C	5.73	117.24	109.11
3	E	189	ASN	N-CA-C	5.70	117.35	111.03
4	H	541	VAL	N-CA-C	5.56	116.02	111.62
5	I	202	LEU	N-CA-C	5.54	122.06	109.81
1	B	97	ASN	N-CA-C	5.52	118.17	109.39
1	A	198	ALA	N-CA-C	5.52	115.40	108.45
3	E	397	ASN	N-CA-C	5.51	115.30	108.19
1	A	207	ILE	N-CA-C	5.45	115.80	108.17
1	A	276	ALA	N-CA-C	5.42	116.92	110.19
1	A	80	ASN	N-CA-C	5.40	117.58	111.11
1	B	231	THR	N-CA-C	5.36	115.32	108.24
1	A	225	LYS	CA-C-N	5.31	125.30	119.89
1	A	225	LYS	C-N-CA	5.31	125.30	119.89
6	L	254	VAL	N-CA-C	5.31	115.93	110.36
6	L	45	MET	N-CA-C	5.29	117.71	108.76
4	H	286	ILE	N-CA-C	5.29	115.55	110.74
7	N	356	ARG	N-CA-C	5.28	121.47	109.81
2	D	20	VAL	N-CA-C	5.28	115.94	110.82
1	A	196	VAL	N-CA-C	5.27	115.72	108.12
2	C	290	THR	CA-C-N	5.20	125.49	119.93
2	C	290	THR	C-N-CA	5.20	125.49	119.93
2	C	371	GLN	N-CA-C	5.18	116.93	111.28
1	B	207	ILE	N-CA-C	5.11	115.47	108.12
7	N	136	ILE	N-CA-C	5.05	115.56	108.89
5	J	359	ASN	N-CA-C	5.05	117.33	111.02
4	G	455	LEU	N-CA-C	5.05	115.70	108.74
1	B	268	ARG	N-CA-C	5.04	116.73	108.52

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	96	0
1	B	2351	0	2367	117	0
2	C	2665	0	2625	45	0
2	D	2665	0	2626	30	0
3	E	2164	0	2154	23	0
3	F	2164	0	2154	15	0
4	G	2744	0	2819	29	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	2020	17	0
6	L	1974	0	2019	10	0
7	M	3044	0	3126	22	0
7	N	3044	0	3126	21	0
8	O	143	0	148	0	0
8	P	143	0	148	0	0
All	All	36982	0	37236	508	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 (508) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:20:MET:HE2	1:B:102:VAL:CG1	2.04	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
1:B:139:LEU:C	1:B:139:LEU:HD23	2.15	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
4:H:387:ILE:HD13	4:H:412:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:293:SER:HB3	2:C:362:TYR:HE1	1.59	0.68
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:20:MET:HE2	1:B:102:VAL:HG13	1.66	0.65
1:B:129:HIS:HB3	1:B:196:VAL:HG22	1.77	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:20:MET:HE2	1:B:102:VAL:HG11	1.83	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:23:PRO:HG2	1:B:235:LYS:HZ3	1.70	0.56
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:E:183:LEU:HB3	3:E:197:MET:HE3	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.10	0.52
2:C:249:PHE:CZ	4:G:494:MET:HE3	2.45	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
3:F:183:LEU:HD22	3:F:197:MET:HE3	1.91	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
1:B:23:PRO:CG	1:B:235:LYS:HZ3	2.23	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

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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
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
5:I:329:LYS:O	5:I:330:ASP:HB2	2.12	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:A:170:GLU:OE2	1:B:260:THR:C	2.57	0.48
1:B:91:LYS:HA	1:B:94:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:344:ILE:HA	4:H:347:LEU:HD12	1.94	0.48
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
1:A:139:LEU:C	1:A:139:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:J:37:GLU:C	5:J:39:ARG:H	2.24	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:C	1:B:139:LEU:CD2	2.86	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
7:N:142:TYR:CD1	7:N:142:TYR:C	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:57:TRP:CD1	2:C:58:ASN:H	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:267:LEU:C	1:A:269:GLY:H	2.26	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
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: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
7:N:254:MET:HE3	7:N:258:SER:HB3	2.00	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
4:G:399:THR:HA	4:G:425:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:343:PRO:C	2:D:345:ASN:H	2.28	0.42
5:I:155:MET:HB3	5:I:274:TYR:CE1	2.54	0.42
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: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
1:B:22:MET:C	1:B:24:ILE:N	2.77	0.42
1:B:22:MET:C	1:B:24:ILE:H	2.27	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
2:D:57:TRP:C	2:D:59:HIS:H	2.27	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
1:A:247:LEU:H	1:A:249:MET:HE2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:E:303:ASP:C	3:E:305:PHE:H	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	4	25
1	B	300/305 (98%)	245 (82%)	44 (15%)	11 (4%)	2	20
2	C	339/381 (89%)	296 (87%)	36 (11%)	7 (2%)	5	30
2	D	339/381 (89%)	296 (87%)	33 (10%)	10 (3%)	3	23
3	E	253/578 (44%)	206 (81%)	41 (16%)	6 (2%)	4	27
3	F	253/578 (44%)	204 (81%)	42 (17%)	7 (3%)	4	24
4	G	349/651 (54%)	277 (79%)	58 (17%)	14 (4%)	2	18
4	H	349/651 (54%)	293 (84%)	41 (12%)	15 (4%)	2	17
5	I	427/712 (60%)	358 (84%)	51 (12%)	18 (4%)	2	17
5	J	427/712 (60%)	357 (84%)	49 (12%)	21 (5%)	1	16
6	K	237/304 (78%)	198 (84%)	33 (14%)	6 (2%)	4	26
6	L	237/304 (78%)	200 (84%)	34 (14%)	3 (1%)	9	42
7	M	398/527 (76%)	329 (83%)	61 (15%)	8 (2%)	6	31
7	N	398/527 (76%)	341 (86%)	52 (13%)	5 (1%)	9	42
8	O	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	12
8	P	15/285 (5%)	12 (80%)	2 (13%)	1 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4636/7486 (62%)	3865 (83%)	630 (14%)	141 (3%)	5	23

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	215 (84%)	42 (16%)	2	10
1	B	257/265 (97%)	219 (85%)	38 (15%)	3	13
2	C	286/338 (85%)	245 (86%)	41 (14%)	3	13
2	D	286/338 (85%)	248 (87%)	38 (13%)	4	14
3	E	249/529 (47%)	233 (94%)	16 (6%)	16	37
3	F	249/529 (47%)	230 (92%)	19 (8%)	12	33
4	G	305/561 (54%)	277 (91%)	28 (9%)	8	27
4	H	305/561 (54%)	272 (89%)	33 (11%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	389/649 (60%)	353 (91%)	36 (9%)	8	26
5	J	389/649 (60%)	358 (92%)	31 (8%)	11	31
6	K	219/273 (80%)	184 (84%)	35 (16%)	2	11
6	L	219/273 (80%)	187 (85%)	32 (15%)	3	13
7	M	319/449 (71%)	302 (95%)	17 (5%)	20	41
7	N	319/449 (71%)	302 (95%)	17 (5%)	20	41
8	O	16/246 (6%)	16 (100%)	0	100	100
8	P	16/246 (6%)	16 (100%)	0	100	100
All	All	4080/6620 (62%)	3657 (90%)	423 (10%)	9	22

All (423) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	40	GLU
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	128	VAL
1	A	144	ASN
1	A	147	ILE
1	A	152	VAL
1	A	166	TYR
1	A	169	LEU
1	A	172	LYS
1	A	174	ILE
1	A	179	ILE
1	A	188	ILE
1	A	192	ASP
1	A	196	VAL

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Mol	Chain	Res	Type
1	A	203	GLU
1	A	207	ILE
1	A	231	THR
1	A	232	GLU
1	A	236	PHE
1	A	237	VAL
1	A	243	SER
1	A	247	LEU
1	A	255	ASP
1	A	267	LEU
1	A	280	ILE
1	A	281	THR
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	22	MET
1	B	24	ILE
1	B	33	LEU
1	B	34	LEU
1	B	37	LYS
1	B	54	GLU
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	115	ILE
1	B	135	VAL
1	B	138	LEU
1	B	140	ASN
1	B	147	ILE
1	B	148	ARG
1	B	172	LYS
1	B	179	ILE
1	B	207	ILE

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Mol	Chain	Res	Type
1	B	216	VAL
1	B	231	THR
1	B	232	GLU
1	B	237	VAL
1	B	242	LEU
1	B	267	LEU
1	B	272	ILE
1	B	283	LEU
1	B	289	VAL
1	B	291	THR
1	B	293	SER
1	B	295	VAL
2	C	17	ASP
2	C	20	VAL
2	C	21	THR
2	C	22	ILE
2	C	24	THR
2	C	31	ARG
2	C	38	TYR
2	C	40	ILE
2	C	42	LEU
2	C	69	ASP
2	C	95	LEU
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	201	ILE
2	C	206	ARG
2	C	215	VAL
2	C	222	ASN
2	C	223	THR
2	C	238	ILE
2	C	249	PHE
2	C	262	THR
2	C	272	ILE
2	C	278	VAL
2	C	298	LEU
2	C	301	LEU
2	C	307	PHE

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Mol	Chain	Res	Type
2	C	310	GLU
2	C	314	GLU
2	C	320	ARG
2	C	321	ILE
2	C	322	LEU
2	C	331	LEU
2	C	334	VAL
2	C	346	ILE
2	C	361	ILE
2	C	366	TRP
2	C	369	TYR
2	D	24	THR
2	D	38	TYR
2	D	44	THR
2	D	47	LEU
2	D	62	ASP
2	D	75	GLU
2	D	80	THR
2	D	84	CYS
2	D	91	ILE
2	D	100	GLU
2	D	160	ASP
2	D	161	LEU
2	D	164	GLU
2	D	165	ILE
2	D	168	ILE
2	D	175	ILE
2	D	177	ILE
2	D	179	LEU
2	D	180	ILE
2	D	196	VAL
2	D	198	LYS
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	278	VAL
2	D	284	CYS
2	D	287	GLU
2	D	298	LEU

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Mol	Chain	Res	Type
2	D	307	PHE
2	D	308	ASP
2	D	310	GLU
2	D	314	GLU
2	D	348	ILE
2	D	350	ILE
2	D	371	GLN
3	E	3	ILE
3	E	133	HIS
3	E	144	ILE
3	E	153	GLU
3	E	181	GLN
3	E	183	LEU
3	E	249	LYS
3	E	255	ILE
3	E	284	LEU
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	F	3	ILE
3	F	81	LEU
3	F	100	GLU
3	F	134	HIS
3	F	141	ILE
3	F	173	ASP
3	F	181	GLN
3	F	192	ASP
3	F	239	LEU
3	F	255	ILE
3	F	258	HIS
3	F	260	LEU
3	F	270	THR
3	F	274	ASN
3	F	277	ILE
3	F	303	ASP
3	F	402	MET
3	F	403	ASP
3	F	409	LEU

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Mol	Chain	Res	Type
4	G	269	LEU
4	G	284	TYR
4	G	293	CYS
4	G	296	MET
4	G	315	LEU
4	G	366	ASP
4	G	393	GLN
4	G	395	GLU
4	G	400	ILE
4	G	406	SER
4	G	412	LEU
4	G	416	ASN
4	G	424	ILE
4	G	434	LEU
4	G	439	LYS
4	G	445	ARG
4	G	455	LEU
4	G	456	ILE
4	G	462	ILE
4	G	503	VAL
4	G	518	LEU
4	G	521	VAL
4	G	522	THR
4	G	526	LEU
4	G	532	LEU
4	G	550	LEU
4	G	568	GLU
4	G	576	ILE
4	H	256	LEU
4	H	257	ILE
4	H	264	LEU
4	H	286	ILE
4	H	290	ILE
4	H	293	CYS
4	H	297	LEU
4	H	317	ARG
4	H	319	LEU
4	H	339	THR
4	H	364	LYS
4	H	398	THR
4	H	408	VAL
4	H	412	LEU

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Mol	Chain	Res	Type
4	H	424	ILE
4	H	428	VAL
4	H	429	VAL
4	H	434	LEU
4	H	438	ARG
4	H	455	LEU
4	H	456	ILE
4	H	460	ASP
4	H	478	LEU
4	H	491	MET
4	H	499	ARG
4	H	503	VAL
4	H	505	VAL
4	H	518	LEU
4	H	523	PHE
4	H	526	LEU
4	H	532	LEU
4	H	564	LYS
4	H	576	ILE
5	I	41	MET
5	I	46	VAL
5	I	51	LEU
5	I	88	ASP
5	I	97	LEU
5	I	106	THR
5	I	113	ARG
5	I	122	LEU
5	I	125	ARG
5	I	127	ILE
5	I	128	ILE
5	I	132	PHE
5	I	133	ILE
5	I	136	SER
5	I	139	VAL
5	I	140	LEU
5	I	149	LEU
5	I	158	GLN
5	I	163	ILE
5	I	165	THR
5	I	173	THR
5	I	181	GLU
5	I	211	ILE

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Mol	Chain	Res	Type
5	I	218	LEU
5	I	226	ILE
5	I	231	ILE
5	I	232	ASP
5	I	247	GLN
5	I	313	GLN
5	I	333	LEU
5	I	339	ILE
5	I	345	ILE
5	I	349	THR
5	I	388	ASN
5	I	457	LEU
5	I	467	VAL
5	J	41	MET
5	J	51	LEU
5	J	63	THR
5	J	77	LEU
5	J	88	ASP
5	J	89	TYR
5	J	97	LEU
5	J	113	ARG
5	J	118	VAL
5	J	122	LEU
5	J	128	ILE
5	J	131	ASP
5	J	133	ILE
5	J	138	ASP
5	J	141	THR
5	J	165	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	285	VAL
5	J	307	VAL
5	J	324	HIS
5	J	333	LEU
5	J	339	ILE
5	J	357	ILE

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Mol	Chain	Res	Type
5	J	420	ILE
5	J	467	VAL
6	K	3	THR
6	K	11	ASN
6	K	17	ASP
6	K	18	ASP
6	K	19	ILE
6	K	22	VAL
6	K	27	ILE
6	K	29	GLU
6	K	45	MET
6	K	46	ILE
6	K	54	ARG
6	K	59	ILE
6	K	64	ARG
6	K	74	LEU
6	K	79	GLU
6	K	88	ARG
6	K	90	VAL
6	K	95	ILE
6	K	97	LYS
6	K	109	HIS
6	K	114	TYR
6	K	128	LYS
6	K	129	THR
6	K	143	GLU
6	K	154	VAL
6	K	159	GLU
6	K	163	LYS
6	K	166	LEU
6	K	168	GLU
6	K	169	LEU
6	K	205	LEU
6	K	235	LEU
6	K	244	LEU
6	K	251	ILE
6	K	255	ILE
6	L	11	ASN
6	L	17	ASP
6	L	19	ILE
6	L	45	MET
6	L	47	LEU

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Mol	Chain	Res	Type
6	L	51	LEU
6	L	54	ARG
6	L	59	ILE
6	L	62	LEU
6	L	64	ARG
6	L	75	ARG
6	L	76	VAL
6	L	79	GLU
6	L	88	ARG
6	L	90	VAL
6	L	97	LYS
6	L	119	PHE
6	L	127	TYR
6	L	137	LYS
6	L	143	GLU
6	L	156	GLU
6	L	159	GLU
6	L	163	LYS
6	L	165	VAL
6	L	166	LEU
6	L	168	GLU
6	L	169	LEU
6	L	205	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	228	GLN
7	M	267	LEU
7	M	280	ILE
7	M	291	ILE
7	M	342	ILE
7	M	353	ILE
7	M	368	ILE
7	M	395	LEU
7	M	402	VAL
7	M	406	LEU
7	M	432	ILE
7	M	475	VAL
7	M	494	GLU

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Mol	Chain	Res	Type
7	M	495	ILE
7	M	508	HIS
7	N	142	TYR
7	N	236	ILE
7	N	251	VAL
7	N	260	LEU
7	N	274	ILE
7	N	280	ILE
7	N	286	GLN
7	N	351	ASP
7	N	353	ILE
7	N	354	GLU
7	N	368	ILE
7	N	371	LYS
7	N	395	LEU
7	N	432	ILE
7	N	443	VAL
7	N	495	ILE
7	N	508	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	62	ASN
1	A	82	HIS
1	A	97	ASN
1	A	144	ASN
1	A	163	ASN
1	A	171	GLN
1	A	222	ASN
1	A	277	GLN
1	B	47	ASN
1	B	82	HIS
1	B	129	HIS
1	B	144	ASN
1	B	161	GLN
1	B	209	ASN
1	B	222	ASN
2	C	19	ASN
2	C	221	ASN
2	C	222	ASN

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Mol	Chain	Res	Type
2	C	268	ASN
2	C	275	ASN
2	C	335	ASN
2	C	352	ASN
2	C	357	ASN
2	D	19	ASN
2	D	167	ASN
2	D	174	GLN
2	D	221	ASN
2	D	222	ASN
2	D	225	ASN
2	D	275	ASN
2	D	336	GLN
2	D	371	GLN
3	E	134	HIS
3	E	164	ASN
3	E	258	HIS
3	E	265	ASN
3	E	396	ASN
3	F	59	GLN
3	F	164	ASN
3	F	181	GLN
3	F	186	GLN
3	F	274	ASN
3	F	313	ASN
3	F	399	ASN
4	G	384	GLN
4	G	416	ASN
4	G	446	ASN
4	G	574	ASN
4	H	450	ASN
5	I	28	GLN
5	I	73	HIS
5	I	96	ASN
5	I	228	ASN
5	I	247	GLN
5	I	249	ASN
5	I	272	HIS
5	I	289	GLN
5	I	296	GLN
5	I	313	GLN
5	I	335	GLN

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Mol	Chain	Res	Type
5	I	365	ASN
5	I	423	ASN
5	I	455	GLN
5	J	73	HIS
5	J	96	ASN
5	J	212	GLN
5	J	228	ASN
5	J	241	HIS
5	J	316	GLN
5	J	359	ASN
6	K	23	ASN
6	K	41	ASN
6	L	23	ASN
6	L	41	ASN
6	L	103	GLN
7	M	98	GLN
7	M	151	GLN
7	M	248	GLN
7	M	286	GLN
7	M	295	ASN
7	M	324	ASN
7	M	376	ASN
7	M	415	GLN
7	M	465	ASN
8	O	140	ASN
7	N	98	GLN
7	N	111	HIS
7	N	226	GLN
7	N	248	GLN
7	N	295	ASN
7	N	324	ASN
7	N	376	ASN
7	N	415	GLN
7	N	450	GLN
8	P	140	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SEP	L	52	6	8,9,10	0.67	0	7,12,14	1.41	1 (14%)
6	SEP	K	52	6	8,9,10	0.63	0	7,12,14	1.15	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	-	2/6/8/10	-
6	SEP	K	52	6	-	2/6/8/10	-

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 (4) 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	L	52	SEP	N-CA-CB-OG
6	L	52	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

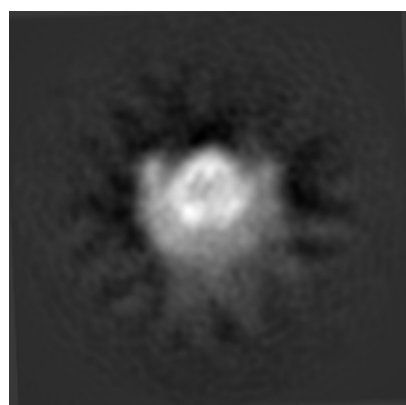
6 Map visualisation [i](#)

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.

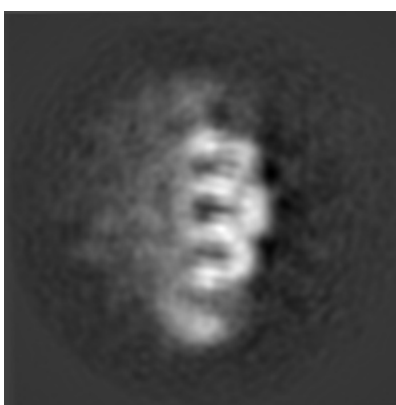
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

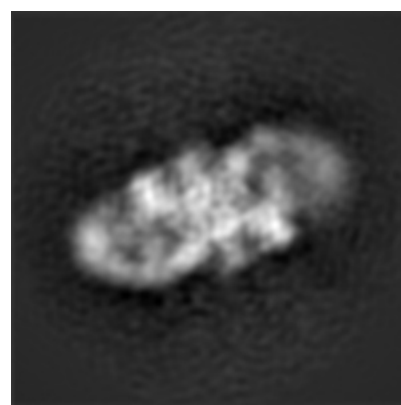
6.1.1 Primary map



X



Y

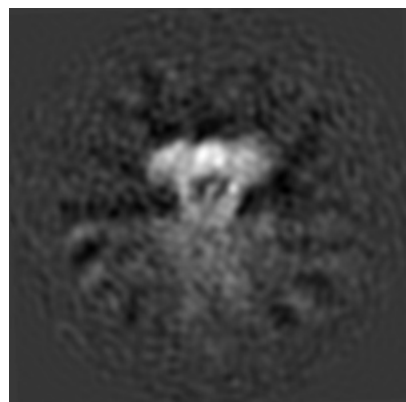


Z

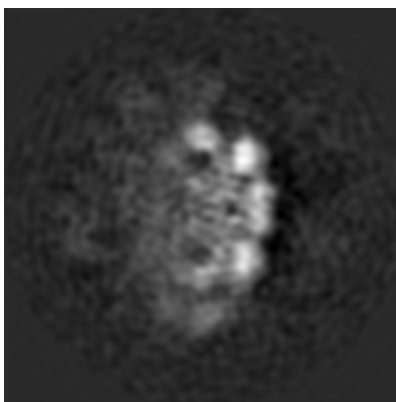
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

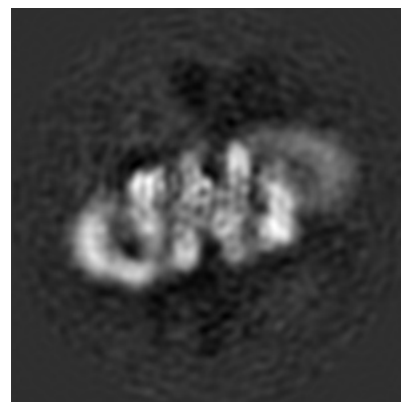
6.2.1 Primary map



X Index: 140



Y Index: 140

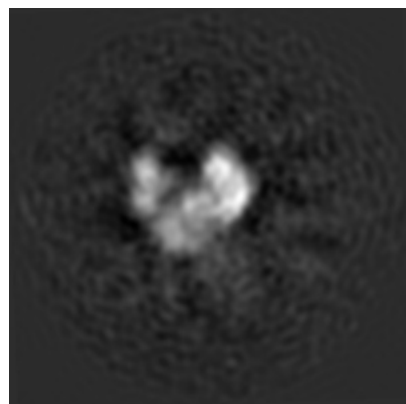


Z Index: 140

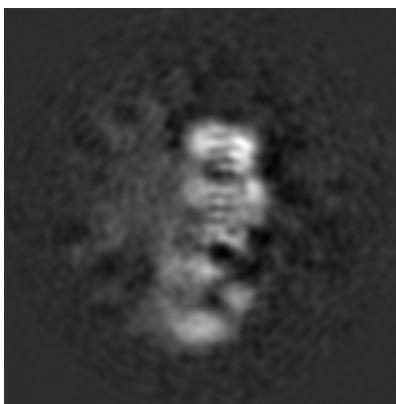
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

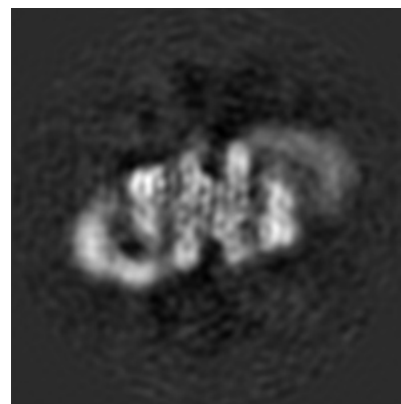
6.3.1 Primary map



X Index: 96



Y Index: 126

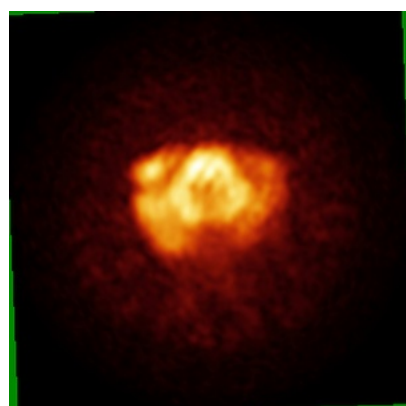


Z Index: 143

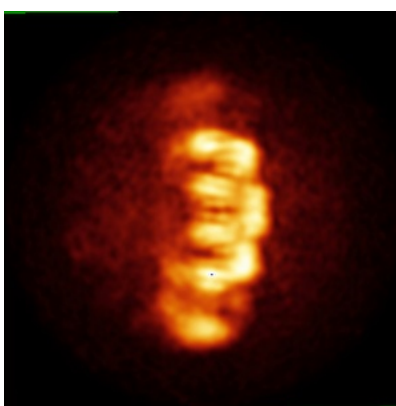
The images above show the largest variance slices of the map in three orthogonal directions.

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

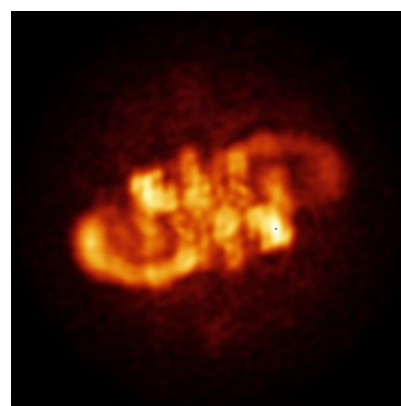
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

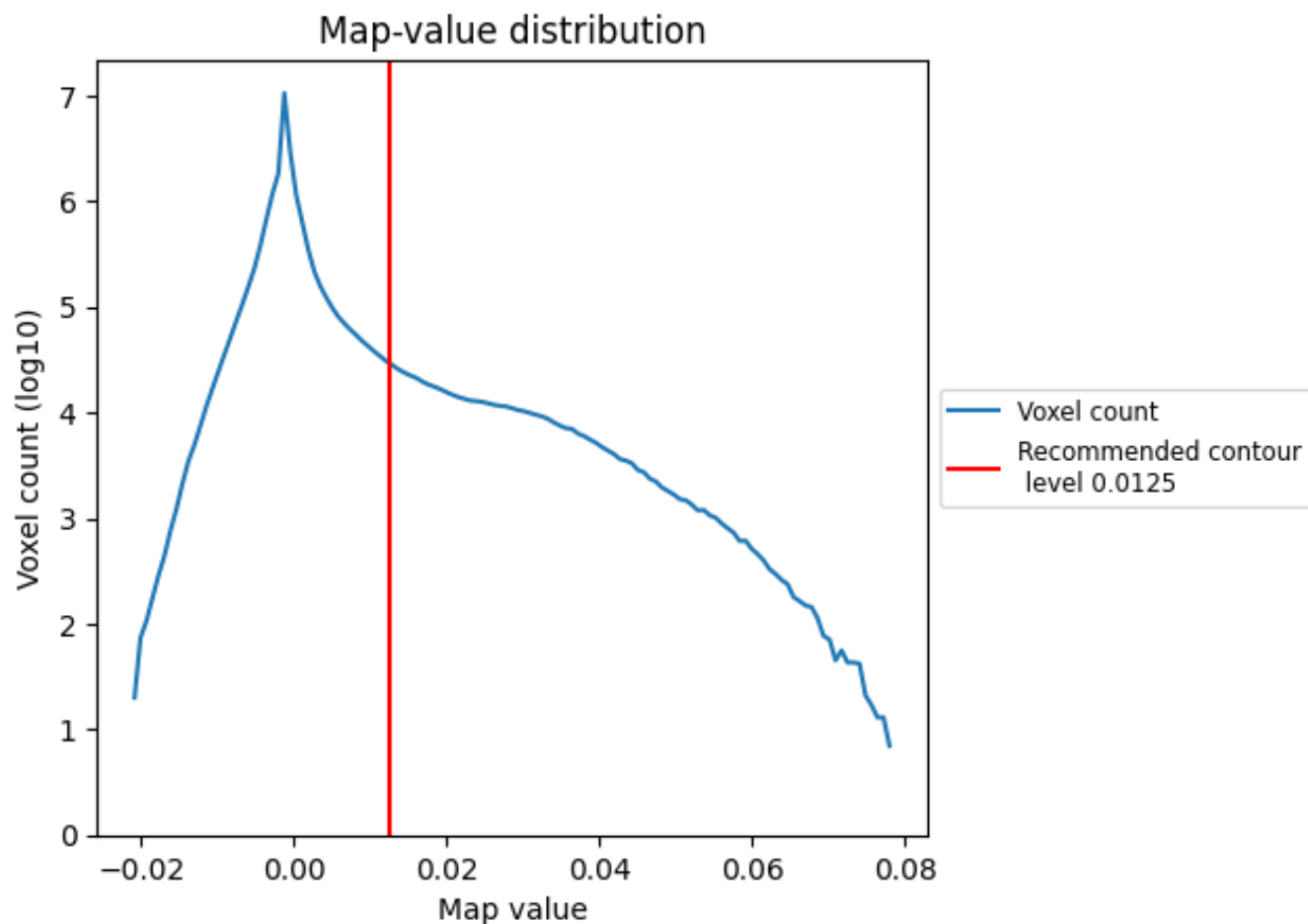
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

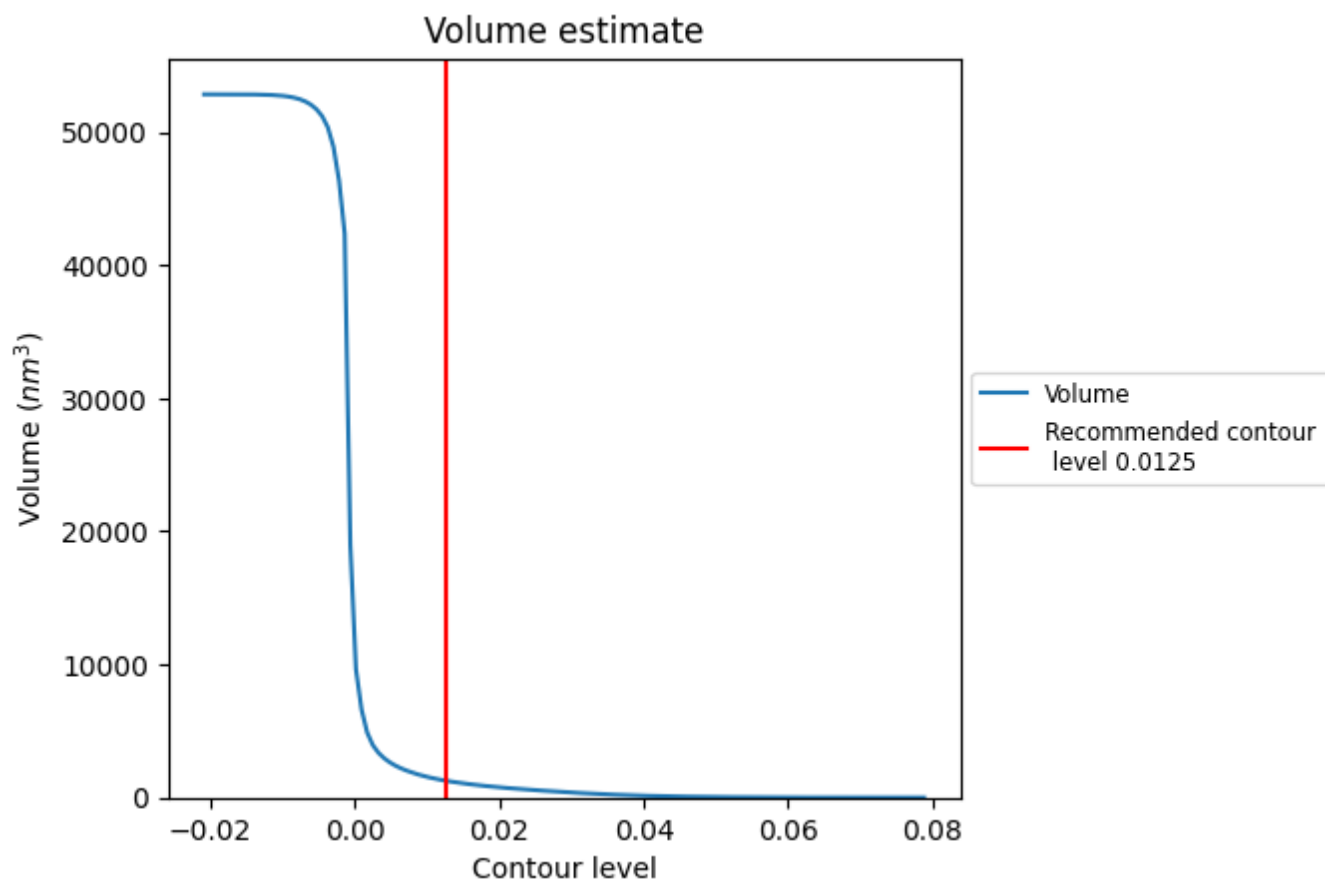
This section contains the results of statistical analysis of the map.

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.

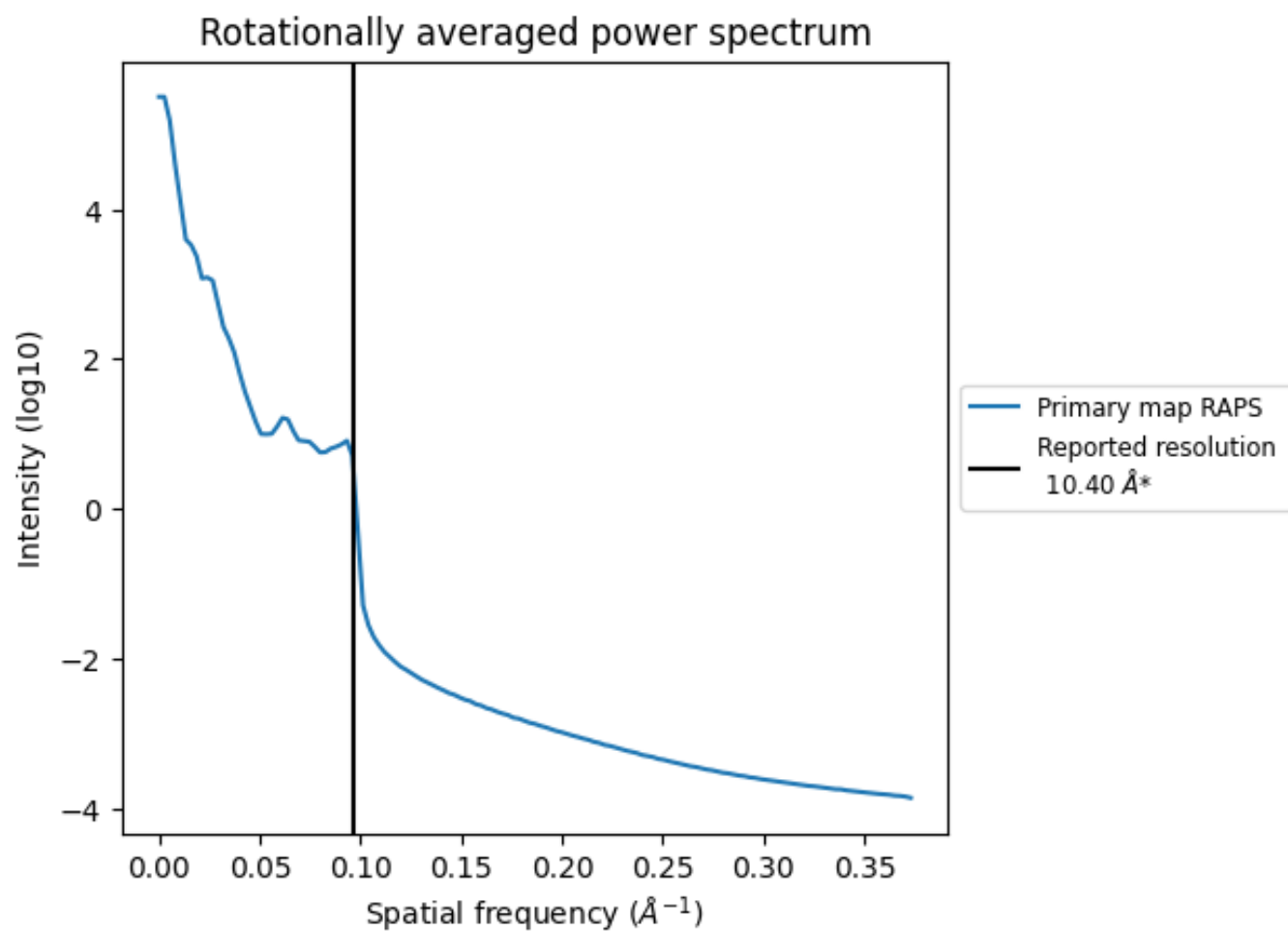
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1275 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.096 Å⁻¹

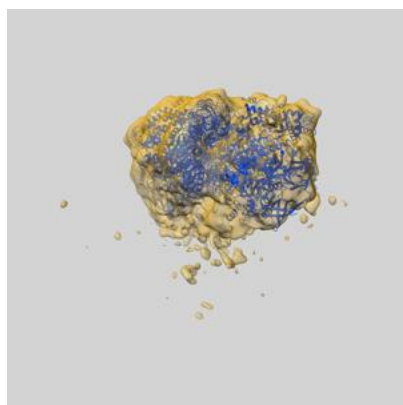
8 Fourier-Shell correlation

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

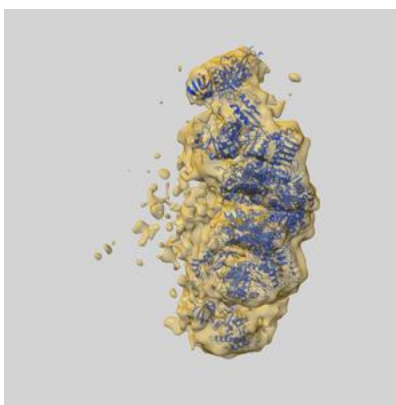
9 Map-model fit [i](#)

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.

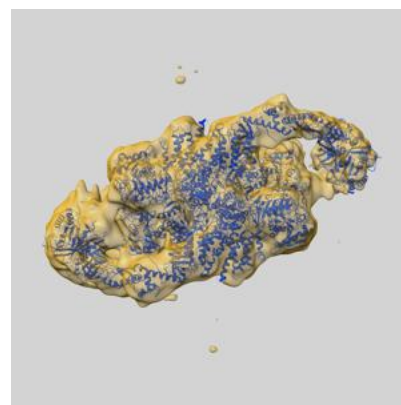
9.1 Map-model overlay [i](#)



X



Y



Z

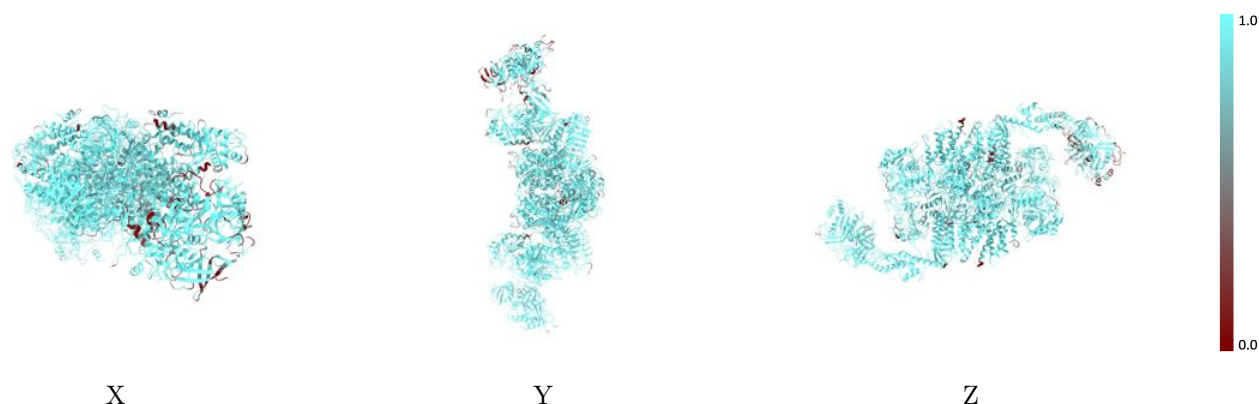
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



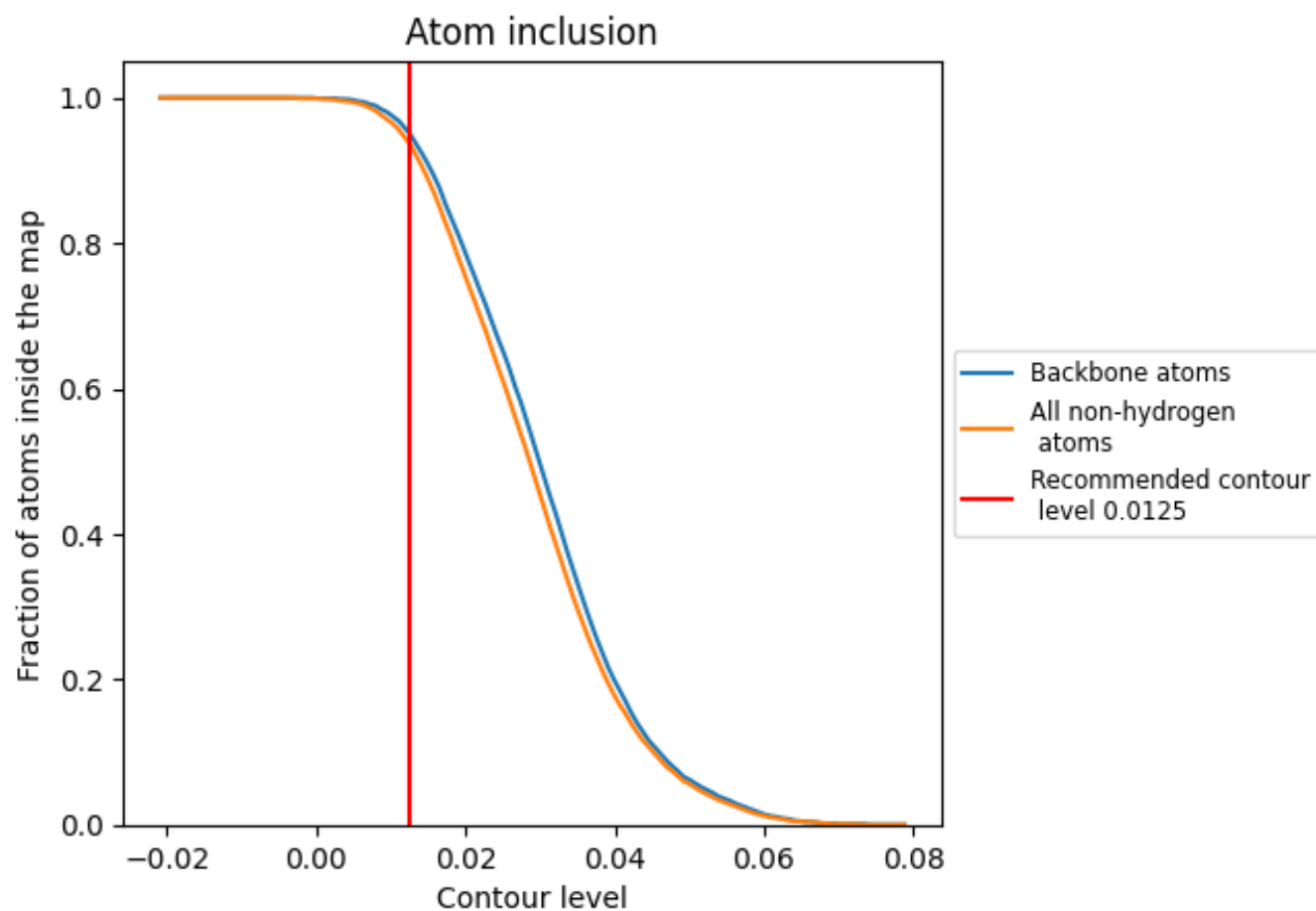
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9370	 0.0680
A	 0.9780	 0.0750
B	 0.9470	 0.0500
C	 0.9600	 0.0750
D	 0.9550	 0.0730
E	 0.9330	 0.0530
F	 0.9520	 0.0620
G	 0.9290	 0.0800
H	 0.9330	 0.0830
I	 0.9810	 0.0750
J	 0.9730	 0.0820
K	 0.8810	 0.0640
L	 0.9780	 0.0780
M	 0.7610	 0.0470
N	 0.9780	 0.0470
O	 0.4270	 0.0780
P	 1.0000	 0.0400

