



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:52 PM UTC

PDB ID : 7PE7 / pdb_00007pe7
EMDB ID : EMD-13347
Title : cryo-EM structure of DEPTOR bound to human mTOR complex 2, overall refinement
Authors : Waelchli, M.; Maier, T.
Deposited on : 2021-08-09
Resolution : 3.41 Å(reported)
Based on initial model : 6ZWM

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:

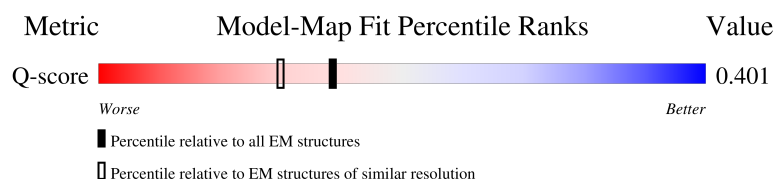
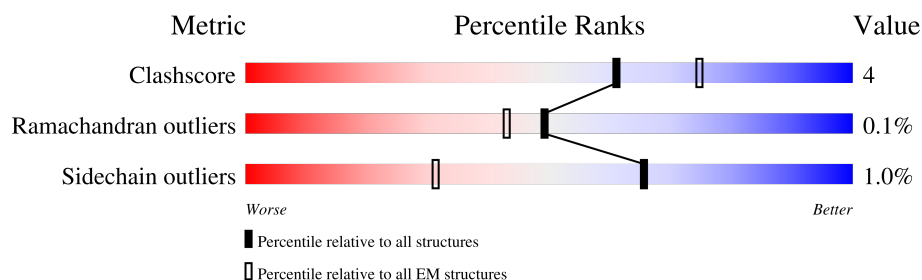
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.41 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	13997 (2.91 - 3.91)

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	2571	
1	B	2571	
2	C	326	
2	D	326	

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Mol	Chain	Length	Quality of chain
3	E	1708	57%8%35%
3	F	1708	57%8%35%
4	G	522	17%81%
4	H	522	17%81%
5	I	409	20%6%74%
5	J	409	20%6%74%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58582 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	2194	Total	C	N	O	S	0	0
			16419	10414	2922	2984	99		
1	A	2194	Total	C	N	O	S	0	0
			16419	10414	2922	2984	99		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	246M	GLY	-	insertion	UNP P42345
B	246N	SER	-	insertion	UNP P42345
B	246O	THR	-	insertion	UNP P42345
B	246P	SER	-	insertion	UNP P42345
B	246Q	GLY	-	insertion	UNP P42345
B	246R	SER	-	insertion	UNP P42345
B	246S	GLY	-	insertion	UNP P42345
B	246T	ASP	-	insertion	UNP P42345
B	246U	TYR	-	insertion	UNP P42345
B	246V	LYS	-	insertion	UNP P42345
B	246W	ASP	-	insertion	UNP P42345
B	246X	ASP	-	insertion	UNP P42345
B	246Y	ASP	-	insertion	UNP P42345
B	246Z	ASP	-	insertion	UNP P42345
B	247A	LYS	-	insertion	UNP P42345
B	247B	GLY	-	insertion	UNP P42345
B	247C	SER	-	insertion	UNP P42345
B	247D	THR	-	insertion	UNP P42345
B	247E	SER	-	insertion	UNP P42345
B	247F	GLY	-	insertion	UNP P42345
B	247G	SER	-	insertion	UNP P42345
B	247H	GLY	-	insertion	UNP P42345
A	246M	GLY	-	insertion	UNP P42345
A	246N	SER	-	insertion	UNP P42345
A	246O	THR	-	insertion	UNP P42345
A	246P	SER	-	insertion	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	246Q	GLY	-	insertion	UNP P42345
A	246R	SER	-	insertion	UNP P42345
A	246S	GLY	-	insertion	UNP P42345
A	246T	ASP	-	insertion	UNP P42345
A	246U	TYR	-	insertion	UNP P42345
A	246V	LYS	-	insertion	UNP P42345
A	246W	ASP	-	insertion	UNP P42345
A	246X	ASP	-	insertion	UNP P42345
A	246Y	ASP	-	insertion	UNP P42345
A	246Z	ASP	-	insertion	UNP P42345
A	247A	LYS	-	insertion	UNP P42345
A	247B	GLY	-	insertion	UNP P42345
A	247C	SER	-	insertion	UNP P42345
A	247D	THR	-	insertion	UNP P42345
A	247E	SER	-	insertion	UNP P42345
A	247F	GLY	-	insertion	UNP P42345
A	247G	SER	-	insertion	UNP P42345
A	247H	GLY	-	insertion	UNP P42345

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	319	Total	C	N	O	S	0	0
			2465	1533	437	477	18		
2	C	319	Total	C	N	O	S	0	0
			2465	1533	437	477	18		

- Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	1115	Total	C	N	O	S	0	0
			8917	5680	1582	1608	47		
3	E	1115	Total	C	N	O	S	0	0
			8917	5680	1582	1608	47		

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	98	Total	C	N	O	S	0	0
			655	399	125	127	4		
4	G	98	Total	C	N	O	S	0	0
			655	399	125	127	4		

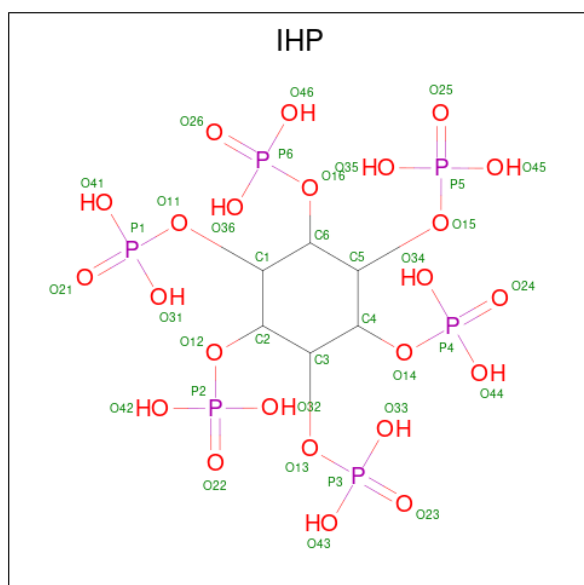
- Molecule 5 is a protein called DEP domain-containing mTOR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	106	Total	C	N	O	S	0	0
			795	504	138	146	7		
5	J	106	Total	C	N	O	S	0	0
			795	504	138	146	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	204	SER	ASN	variant	UNP Q8TB45
I	389	ASN	SER	variant	UNP Q8TB45
J	204	SER	ASN	variant	UNP Q8TB45
J	389	ASN	SER	variant	UNP Q8TB45

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

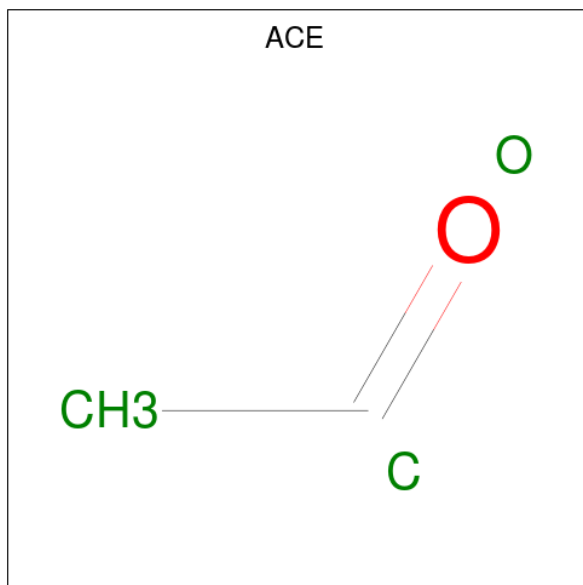


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	O	P	0
			36	6	24	6	
6	A	1	Total	C	O	P	0
			36	6	24	6	

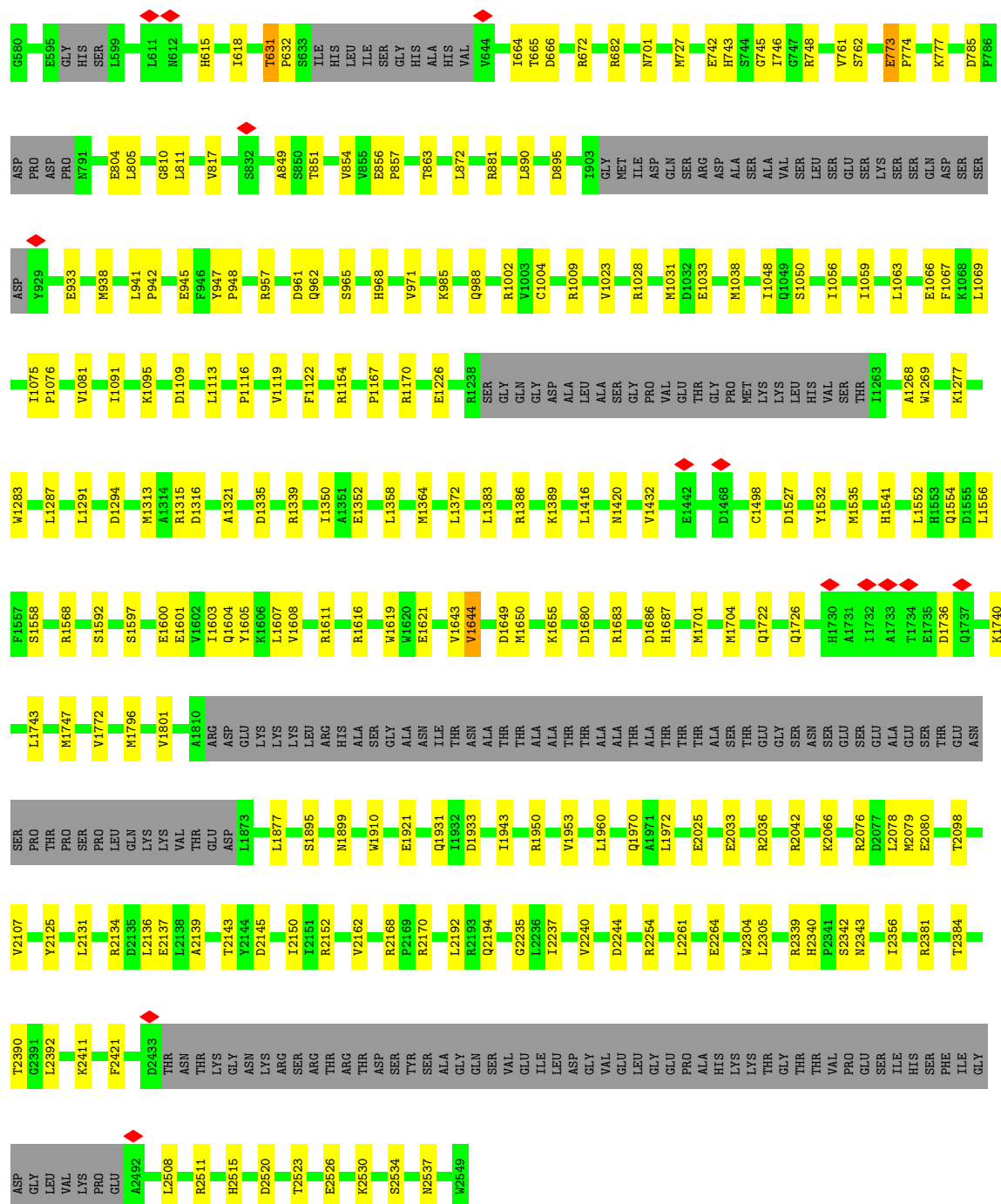
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	F	1	Total	Zn	0
			1	1	
7	E	1	Total	Zn	0
			1	1	

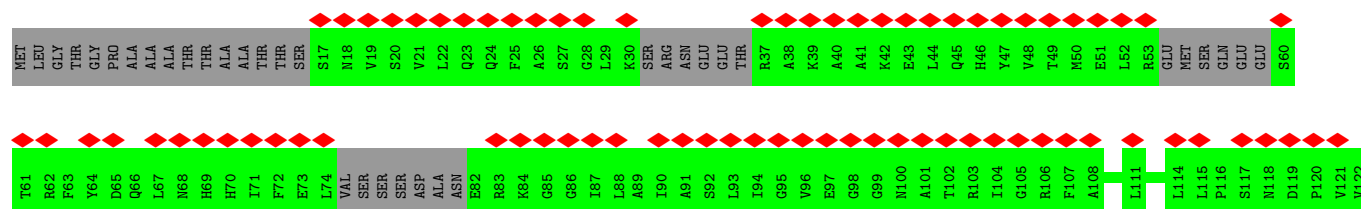
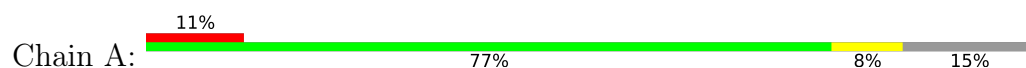
- Molecule 8 is ACETYL GROUP (CCD ID: ACE) (formula: C_2H_4O).



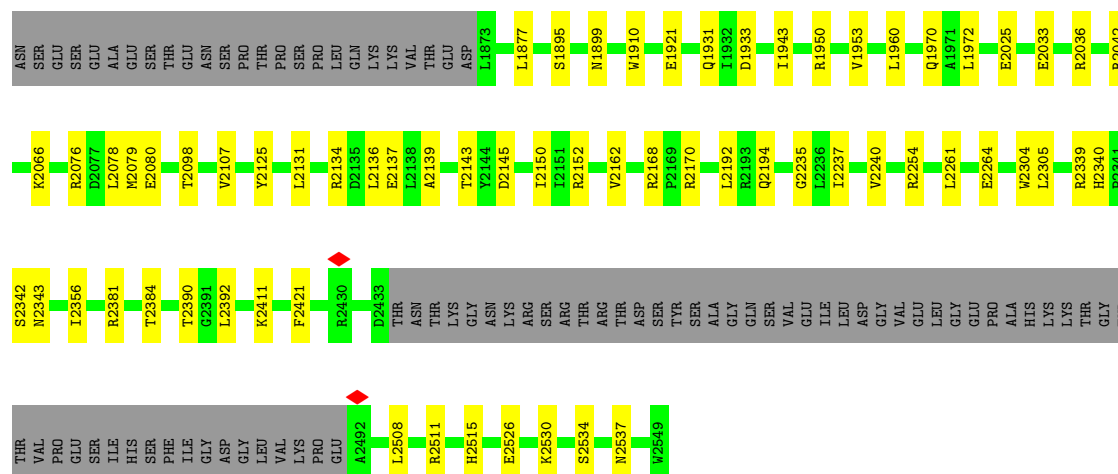
Mol	Chain	Residues	Atoms			AltConf
8	H	1	Total	C	O	0
			3	2	1	
8	G	1	Total	C	O	0
			3	2	1	



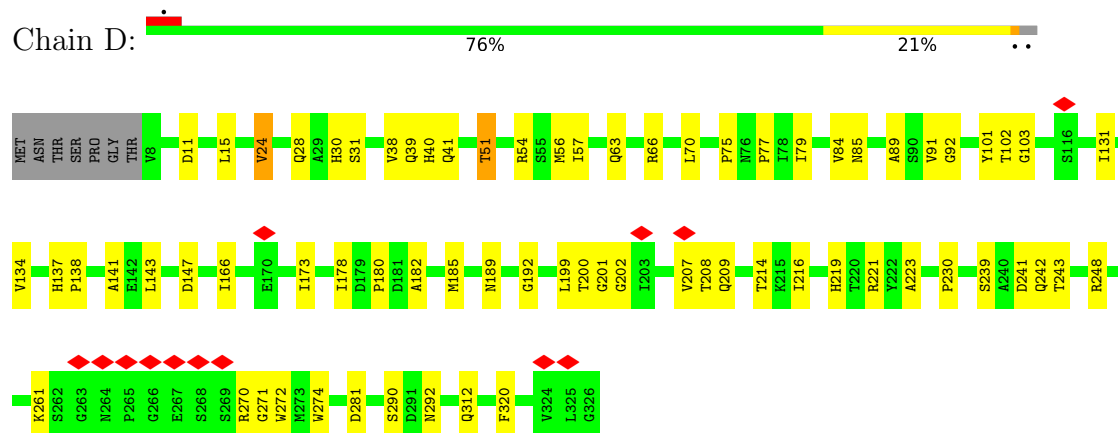
• Molecule 1: Serine/threonine-protein kinase mTOR



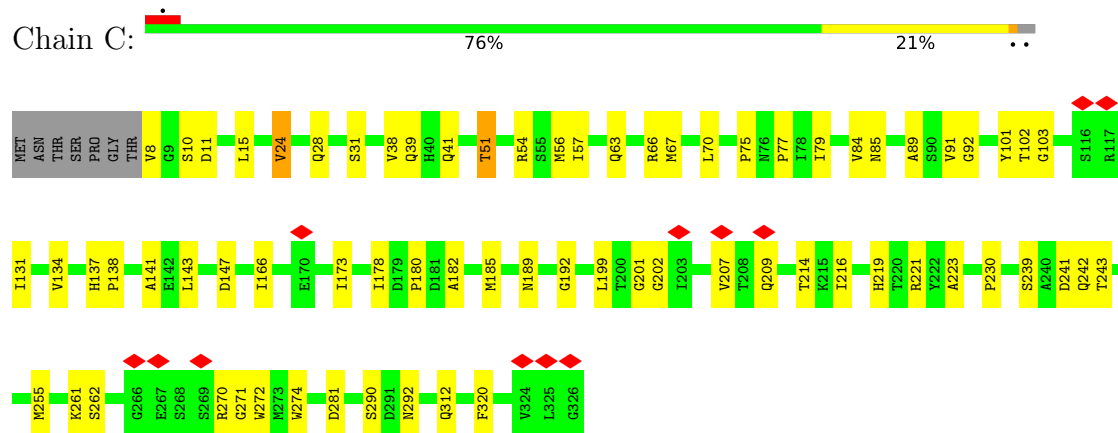




• Molecule 2: Target of rapamycin complex subunit LST8



• Molecule 2: Target of rapamycin complex subunit LST8



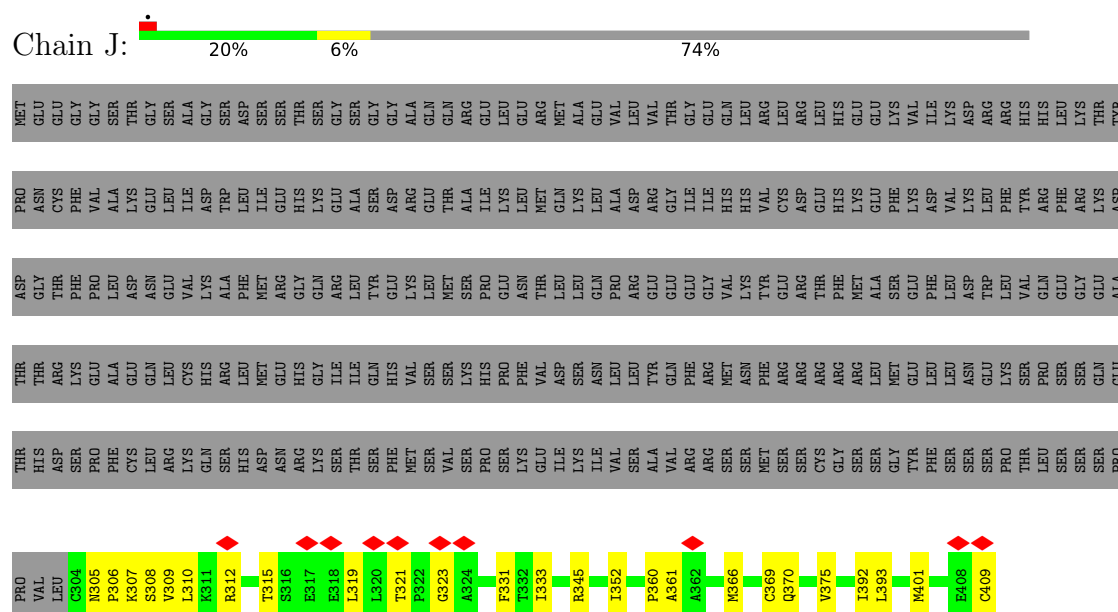
• Molecule 3: Rapamycin-insensitive companion of mTOR











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	467078	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.018	Depositor
Minimum map value	-0.956	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.206	Depositor
Map size (Å)	507.84, 507.84, 507.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IHP, ACE

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	0.09	0/16719	0.23	1/22710 (0.0%)
1	B	0.09	0/16719	0.23	1/22710 (0.0%)
2	C	0.09	0/2523	0.27	0/3438
2	D	0.09	0/2523	0.27	0/3438
3	E	0.09	0/9078	0.27	0/12281
3	F	0.09	0/9078	0.27	0/12281
4	G	0.08	0/660	0.23	0/900
4	H	0.08	0/660	0.23	0/900
5	I	0.12	0/811	0.31	0/1104
5	J	0.12	0/811	0.31	0/1104
All	All	0.09	0/59582	0.25	2/80866 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1081	VAL	N-CA-C	-5.98	107.67	113.53
1	A	1081	VAL	N-CA-C	-5.96	107.69	113.53

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	16419	0	15461	124	0
1	B	16419	0	15461	127	0
2	C	2465	0	2351	42	0
2	D	2465	0	2351	42	0
3	E	8917	0	9064	82	0
3	F	8917	0	9064	81	0
4	G	655	0	519	7	0
4	H	655	0	519	8	0
5	I	795	0	812	11	0
5	J	795	0	812	12	0
6	A	36	0	6	1	0
6	B	36	0	6	1	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	G	3	0	3	0	0
8	H	3	0	3	0	0
All	All	58582	0	56432	503	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 4.

All (503) 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:1031:MET:HE1	1:A:1059:ILE:HD13	1.68	0.76
1:B:1031:MET:HE1	1:B:1059:ILE:HD13	1.68	0.76
3:E:556:LYS:HB2	3:E:607:GLN:HE21	1.54	0.73
3:F:556:LYS:HB2	3:F:607:GLN:HE21	1.54	0.73
1:A:2192:LEU:HD22	1:A:2235:GLY:HA3	1.72	0.72
1:B:2192:LEU:HD22	1:B:2235:GLY:HA3	1.72	0.72
3:F:447:HIS:HB2	1:A:727:MET:HE3	1.72	0.71
1:A:1722:GLN:O	1:A:1726:GLN:NE2	2.24	0.70
1:A:1069:LEU:HD23	3:E:467:LEU:HD12	1.74	0.69
1:B:1722:GLN:O	1:B:1726:GLN:NE2	2.24	0.69
1:A:2526:GLU:OE2	1:A:2530:LYS:NZ	2.23	0.69
1:B:631:THR:HA	1:B:682:ARG:HH22	1.57	0.69
1:A:631:THR:HA	1:A:682:ARG:HH22	1.57	0.68
1:B:2526:GLU:OE2	1:B:2530:LYS:NZ	2.23	0.68
2:D:178:ILE:HG12	2:D:185:MET:HG2	1.76	0.68
1:B:1069:LEU:HD23	3:F:467:LEU:HD12	1.76	0.68
2:D:173:ILE:HA	2:D:189:ASN:HA	1.76	0.68
2:C:178:ILE:HG12	2:C:185:MET:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:ILE:HA	2:C:189:ASN:HA	1.76	0.67
3:F:566:LYS:NZ	3:F:618:ASP:OD2	2.28	0.67
3:E:566:LYS:NZ	3:E:618:ASP:OD2	2.28	0.66
3:E:296:ALA:O	3:E:300:ASN:ND2	2.29	0.66
3:E:155:THR:HG21	4:G:36:VAL:HG23	1.78	0.66
3:F:296:ALA:O	3:F:300:ASN:ND2	2.28	0.66
1:B:1028:ARG:NH1	1:B:1066:GLU:OE1	2.29	0.66
1:B:1950:ARG:HB2	1:B:1953:VAL:HG12	1.78	0.66
3:E:293:ARG:HD3	3:E:851:LEU:HD12	1.78	0.65
3:F:155:THR:HG21	4:H:36:VAL:HG23	1.78	0.65
1:A:2194:GLN:HG3	1:A:2421:PHE:HZ	1.61	0.65
3:F:293:ARG:HD3	3:F:851:LEU:HD12	1.78	0.65
1:A:1028:ARG:NH1	1:A:1066:GLU:OE1	2.29	0.65
1:B:2194:GLN:HG3	1:B:2421:PHE:HZ	1.61	0.65
2:C:131:ILE:HA	2:C:147:ASP:HA	1.77	0.65
2:D:131:ILE:HA	2:D:147:ASP:HA	1.77	0.65
1:B:1004:CYS:O	1:B:1009:ARG:NH2	2.30	0.65
1:A:1004:CYS:O	1:A:1009:ARG:NH2	2.30	0.64
1:A:1950:ARG:HB2	1:A:1953:VAL:HG12	1.78	0.64
1:B:1416:LEU:O	1:B:1420:ASN:ND2	2.28	0.64
1:B:311:ARG:HE	1:B:315:PRO:HD2	1.63	0.64
1:A:1416:LEU:O	1:A:1420:ASN:ND2	2.28	0.63
1:A:311:ARG:HE	1:A:315:PRO:HD2	1.63	0.63
3:F:726:ASP:OD1	3:F:729:ARG:NH2	2.27	0.62
3:E:726:ASP:OD1	3:E:729:ARG:NH2	2.27	0.62
1:B:1604:GLN:OE1	1:B:1611:ARG:NH1	2.33	0.61
3:F:543:ASN:HD22	3:F:580:PHE:HE1	1.48	0.61
3:E:543:ASN:HD22	3:E:580:PHE:HE1	1.48	0.61
2:D:201:GLY:H	2:D:209:GLN:HE22	1.49	0.61
1:A:1604:GLN:OE1	1:A:1611:ARG:NH1	2.33	0.61
4:H:32:ILE:HG22	4:H:34:HIS:H	1.66	0.61
2:D:248:ARG:HH21	2:D:255:MET:HA	1.66	0.61
3:F:398:ALA:O	3:F:402:ASN:ND2	2.35	0.60
4:G:32:ILE:HG22	4:G:34:HIS:H	1.66	0.60
1:B:1315:ARG:NH1	1:B:1352:GLU:OE2	2.35	0.60
2:D:11:ASP:O	2:D:54:ARG:NH1	2.35	0.60
2:C:201:GLY:H	2:C:209:GLN:HE22	1.49	0.60
1:B:727:MET:HE3	3:E:447:HIS:HB2	1.84	0.60
3:F:380:ARG:NH2	3:F:780:ASP:OD2	2.35	0.60
1:A:1050:SER:OG	1:A:1095:LYS:NZ	2.33	0.60
1:A:1315:ARG:NH1	1:A:1352:GLU:OE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:ASP:O	2:C:54:ARG:NH1	2.35	0.60
2:C:248:ARG:HH21	2:C:255:MET:HA	1.66	0.60
1:A:1364:MET:HG3	1:A:1372:LEU:HD23	1.84	0.59
3:E:380:ARG:NH2	3:E:780:ASP:OD2	2.35	0.59
1:B:1364:MET:HG3	1:B:1372:LEU:HD23	1.84	0.59
3:E:398:ALA:O	3:E:402:ASN:ND2	2.35	0.59
1:B:2042:ARG:NH1	3:F:1485:GLN:OE1	2.36	0.59
2:C:51:THR:OG1	2:C:56:MET:O	2.20	0.59
3:E:810:SER:OG	3:E:888:HIS:ND1	2.27	0.58
3:E:557:TRP:HB3	3:E:560:VAL:HG22	1.85	0.58
2:D:51:THR:OG1	2:D:56:MET:O	2.21	0.58
1:B:761:VAL:HG21	1:B:805:LEU:HD23	1.85	0.57
1:B:1050:SER:OG	1:B:1095:LYS:NZ	2.33	0.57
3:F:557:TRP:HB3	3:F:560:VAL:HG22	1.85	0.57
1:A:761:VAL:HG21	1:A:805:LEU:HD23	1.85	0.57
3:E:324:ARG:NH1	3:E:415:SER:OG	2.38	0.57
3:F:324:ARG:NH1	3:F:415:SER:OG	2.38	0.57
1:A:985:LYS:O	1:A:988:GLN:NE2	2.37	0.56
1:B:2139:ALA:HB2	1:B:2150:ILE:HD11	1.87	0.56
1:A:817:VAL:HG21	1:A:851:THR:HG21	1.87	0.56
1:A:2139:ALA:HB2	1:A:2150:ILE:HD11	1.87	0.56
3:F:771:LEU:HD11	3:F:797:LEU:HD13	1.88	0.56
3:F:810:SER:OG	3:F:888:HIS:ND1	2.27	0.56
3:E:755:LEU:HD21	3:E:773:ILE:HD11	1.87	0.56
3:F:755:LEU:HD21	3:F:773:ILE:HD11	1.87	0.56
3:E:771:LEU:HD11	3:E:797:LEU:HD13	1.88	0.56
1:B:817:VAL:HG21	1:B:851:THR:HG21	1.87	0.56
1:B:1736:ASP:HA	1:B:1740:LYS:HB3	1.88	0.56
1:A:2137:GLU:HA	1:A:2152:ARG:HD2	1.87	0.56
1:B:985:LYS:O	1:B:988:GLN:NE2	2.37	0.56
1:B:2137:GLU:HA	1:B:2152:ARG:HD2	1.87	0.56
1:A:2042:ARG:NH1	3:E:1485:GLN:OE1	2.38	0.55
3:E:360:ASP:O	3:E:363:ARG:NE	2.40	0.55
1:B:2079:MET:HE3	3:F:245:ARG:HD3	1.88	0.55
1:A:1736:ASP:HA	1:A:1740:LYS:HB3	1.88	0.55
3:F:360:ASP:O	3:F:363:ARG:NE	2.40	0.55
1:B:762:SER:HB2	1:B:804:GLU:HG2	1.88	0.55
1:A:773:GLU:HG2	1:A:774:PRO:HD3	1.89	0.55
1:A:2079:MET:HE3	3:E:245:ARG:HD3	1.89	0.55
1:B:773:GLU:HG2	1:B:774:PRO:HD3	1.89	0.54
5:J:333:ILE:HD11	5:J:360:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1605:TYR:OH	1:B:1616:ARG:NH1	2.40	0.54
1:A:762:SER:HB2	1:A:804:GLU:HG2	1.88	0.54
1:A:1605:TYR:OH	1:A:1616:ARG:NH1	2.40	0.54
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.89	0.54
1:A:1343:LEU:O	1:A:1347:SER:OG	2.22	0.53
1:B:1432:VAL:HG22	1:B:2390:THR:HG21	1.89	0.53
1:A:2131:LEU:O	1:A:2134:ARG:NH1	2.41	0.53
2:C:24:VAL:HG13	2:C:38:VAL:HB	1.89	0.53
1:B:1568:ARG:NH2	1:B:1600:GLU:OE2	2.38	0.53
1:B:2131:LEU:O	1:B:2134:ARG:NH1	2.41	0.53
3:F:831:TRP:NE1	3:F:835:TYR:OH	2.41	0.53
1:A:2254:ARG:NH2	1:A:2264:GLU:OE2	2.42	0.53
2:C:292:ASN:ND2	2:C:312:GLN:O	2.41	0.53
2:D:292:ASN:ND2	2:D:312:GLN:O	2.41	0.53
3:E:831:TRP:NE1	3:E:835:TYR:OH	2.41	0.53
1:B:615:HIS:HB2	1:B:618:ILE:HG22	1.91	0.53
5:I:333:ILE:HD11	5:I:360:PRO:HB2	1.89	0.53
2:D:24:VAL:HG13	2:D:38:VAL:HB	1.89	0.52
3:F:121:LEU:HD13	3:F:162:PRO:HG3	1.92	0.52
1:A:615:HIS:HB2	1:A:618:ILE:HG22	1.91	0.52
1:A:1109:ASP:OD1	3:E:474:ASN:ND2	2.39	0.52
3:F:167:ASN:ND2	3:F:1660:LEU:O	2.42	0.52
1:A:1568:ARG:NH2	1:A:1600:GLU:OE2	2.38	0.52
1:B:2078:LEU:HD21	1:B:2107:VAL:HG11	1.90	0.52
3:F:1607:MET:SD	3:F:1607:MET:N	2.83	0.52
2:D:38:VAL:HG13	2:D:75:PRO:HA	1.92	0.52
3:F:916:LYS:HB2	3:F:919:GLU:HG2	1.92	0.52
3:E:1607:MET:SD	3:E:1607:MET:N	2.83	0.52
2:D:180:PRO:HG2	2:D:230:PRO:HA	1.92	0.52
1:A:2078:LEU:HD21	1:A:2107:VAL:HG11	1.90	0.52
5:I:375:VAL:HG21	5:I:392:ILE:HG22	1.92	0.52
5:J:312:ARG:NH2	5:J:409:CYS:OXT	2.43	0.52
2:C:38:VAL:HG13	2:C:75:PRO:HA	1.92	0.52
2:C:39:GLN:HE22	2:C:41:GLN:HB2	1.75	0.52
3:E:121:LEU:HD13	3:E:162:PRO:HG3	1.92	0.52
1:A:1226:GLU:O	3:E:485:ARG:NH1	2.41	0.52
3:E:916:LYS:HB2	3:E:919:GLU:HG2	1.91	0.52
5:I:312:ARG:NH2	5:I:409:CYS:OXT	2.43	0.52
2:D:39:GLN:HE22	2:D:41:GLN:HB2	1.75	0.52
3:F:889:HIS:CD2	3:F:892:GLY:H	2.28	0.52
3:E:641:LYS:O	3:E:643:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2511:ARG:NH2	1:B:2515:HIS:O	2.43	0.52
3:F:532:LEU:HD12	3:F:554:ILE:HD13	1.92	0.52
3:F:541:LYS:HA	3:F:576:ARG:HH21	1.75	0.52
2:C:180:PRO:HG2	2:C:230:PRO:HA	1.92	0.52
3:E:167:ASN:ND2	3:E:1660:LEU:O	2.42	0.52
3:E:532:LEU:HD12	3:E:554:ILE:HD13	1.92	0.52
3:E:889:HIS:CD2	3:E:892:GLY:H	2.28	0.51
5:J:375:VAL:HG21	5:J:392:ILE:HG22	1.92	0.51
1:B:1226:GLU:O	3:F:485:ARG:NH1	2.41	0.51
1:A:2511:ARG:NH2	1:A:2515:HIS:O	2.43	0.51
3:E:541:LYS:HA	3:E:576:ARG:HH21	1.75	0.51
1:B:777:LYS:NZ	3:E:460:ASP:OD2	2.28	0.51
3:F:1622:ASN:HB3	3:F:1632:HIS:CE1	2.46	0.51
2:D:192:GLY:HA2	2:D:223:ALA:HB2	1.93	0.51
1:A:2304:TRP:HE3	1:A:2305:LEU:HD12	1.76	0.51
5:J:310:LEU:HD21	5:J:369:CYS:HA	1.93	0.51
3:F:641:LYS:O	3:F:643:GLU:N	2.43	0.51
3:F:835:TYR:HB2	3:F:838:LYS:HE3	1.93	0.51
2:C:192:GLY:HA2	2:C:223:ALA:HB2	1.93	0.51
1:B:2411:LYS:NZ	1:B:2508:LEU:O	2.44	0.51
5:I:310:LEU:HD21	5:I:369:CYS:HA	1.93	0.51
3:F:36:ASP:HA	3:F:39:ARG:HH11	1.76	0.50
1:A:631:THR:HG23	1:A:632:PRO:HD3	1.93	0.50
1:B:631:THR:HG23	1:B:632:PRO:HD3	1.93	0.50
1:B:1601:GLU:OE1	1:B:1619:TRP:NE1	2.41	0.50
1:B:1655:LYS:NZ	6:B:2601:IHP:O42	2.44	0.50
1:A:1498:CYS:SG	1:A:1532:TYR:OH	2.69	0.50
1:A:1655:LYS:NZ	6:A:2601:IHP:O42	2.44	0.50
2:C:89:ALA:N	2:C:103:GLY:O	2.43	0.50
3:E:536:GLN:OE1	3:E:539:GLN:NE2	2.39	0.50
3:E:781:LYS:O	3:E:785:HIS:ND1	2.44	0.50
3:E:1622:ASN:HB3	3:E:1632:HIS:CE1	2.46	0.50
2:D:272:TRP:N	2:D:290:SER:OG	2.44	0.50
1:B:2304:TRP:HE3	1:B:2305:LEU:HD12	1.76	0.50
1:A:2411:LYS:NZ	1:A:2508:LEU:O	2.44	0.50
1:B:1268:ALA:O	1:B:1283:TRP:NE1	2.44	0.50
1:B:742:GLU:OE1	1:B:743:HIS:ND1	2.45	0.50
1:B:1109:ASP:OD1	3:F:474:ASN:ND2	2.38	0.50
1:A:933:GLU:HG3	1:A:938:MET:HB3	1.94	0.50
1:A:1268:ALA:O	1:A:1283:TRP:NE1	2.44	0.50
2:C:272:TRP:N	2:C:290:SER:OG	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:835:TYR:HB2	3:E:838:LYS:HE3	1.93	0.50
1:A:742:GLU:OE1	1:A:743:HIS:ND1	2.45	0.50
3:E:36:ASP:HA	3:E:39:ARG:HH11	1.76	0.50
1:A:941:LEU:HD12	1:A:942:PRO:HD2	1.94	0.50
1:A:1335:ASP:OD2	1:A:1339:ARG:NH1	2.38	0.50
1:A:2145:ASP:N	1:A:2145:ASP:OD1	2.45	0.49
1:B:933:GLU:HG3	1:B:938:MET:HB3	1.94	0.49
1:B:1552:LEU:HD11	1:B:1603:ILE:HG12	1.94	0.49
1:B:2254:ARG:NH2	1:B:2264:GLU:OE2	2.42	0.49
1:B:1801:VAL:HG23	1:B:1877:LEU:HD22	1.95	0.49
3:F:763:ASN:ND2	3:F:765:THR:OG1	2.45	0.49
3:F:1001:TRP:CG	1:A:725:PHE:HE2	2.30	0.49
1:A:1552:LEU:HD11	1:A:1603:ILE:HG12	1.94	0.49
1:A:1680:ASP:HB3	1:A:1683:ARG:HG2	1.94	0.49
3:E:557:TRP:CG	3:E:558:PRO:HD2	2.48	0.49
1:B:1680:ASP:HB3	1:B:1683:ARG:HG2	1.94	0.49
3:F:746:PHE:HB3	3:F:749:ASN:HD21	1.78	0.49
3:E:48:LEU:HD22	3:E:1681:GLN:HG3	1.94	0.49
3:E:746:PHE:HB3	3:E:749:ASN:HD21	1.77	0.49
1:B:941:LEU:HD12	1:B:942:PRO:HD2	1.94	0.49
1:B:1686:ASP:OD1	1:B:1687:HIS:ND1	2.46	0.49
1:B:2076:ARG:NH1	1:B:2080:GLU:OE1	2.46	0.49
1:A:1686:ASP:OD1	1:A:1687:HIS:ND1	2.46	0.49
3:F:557:TRP:CG	3:F:558:PRO:HD2	2.48	0.49
3:E:236:ASN:HD21	3:E:963:SER:HG	1.58	0.49
1:B:872:LEU:O	1:B:881:ARG:NH2	2.42	0.49
1:A:1801:VAL:HG23	1:A:1877:LEU:HD22	1.95	0.49
1:A:2076:ARG:NH1	1:A:2080:GLU:OE1	2.46	0.49
3:E:763:ASN:ND2	3:E:765:THR:OG1	2.45	0.49
1:B:1498:CYS:SG	1:B:1532:TYR:OH	2.69	0.49
4:G:27:CYS:HA	4:G:30:VAL:HG12	1.94	0.49
3:F:48:LEU:HD22	3:F:1681:GLN:HG3	1.94	0.49
1:A:961:ASP:OD1	1:A:961:ASP:N	2.45	0.49
2:D:182:ALA:HB1	2:D:199:LEU:HD11	1.94	0.48
3:F:1520:CYS:HB3	3:F:1523:CYS:HB2	1.95	0.48
1:B:1554:GLN:HG3	1:B:1556:LEU:HD13	1.95	0.48
2:C:182:ALA:HB1	2:C:199:LEU:HD11	1.94	0.48
5:I:331:PHE:N	5:I:401:MET:O	2.41	0.48
5:I:352:ILE:HD12	5:I:370:GLN:HB2	1.94	0.48
3:F:693:ASN:OD1	3:F:693:ASN:N	2.46	0.48
4:H:27:CYS:HA	4:H:30:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:ALA:HB2	4:H:127:LYS:HA	1.96	0.48
1:A:308:THR:O	1:A:1558:SER:OG	2.32	0.48
2:C:141:ALA:HB2	4:G:127:LYS:HA	1.96	0.48
3:E:134:ASP:OD1	3:E:134:ASP:N	2.47	0.48
1:B:1556:LEU:HD21	5:J:393:LEU:HD22	1.94	0.48
1:A:2254:ARG:NH1	1:A:2261:LEU:O	2.47	0.48
1:B:1910:TRP:HH2	1:B:1960:LEU:HD21	1.78	0.48
1:B:2033:GLU:OE2	1:B:2036:ARG:NH2	2.47	0.48
1:A:310:PRO:HD2	1:A:1607:LEU:HD11	1.96	0.48
5:J:352:ILE:HD12	5:J:370:GLN:HB2	1.94	0.48
1:B:310:PRO:HD2	1:B:1607:LEU:HD11	1.96	0.47
1:B:1335:ASP:OD2	1:B:1339:ARG:NH1	2.38	0.47
1:A:1554:GLN:HG3	1:A:1556:LEU:HD13	1.95	0.47
1:A:1910:TRP:HH2	1:A:1960:LEU:HD21	1.78	0.47
1:A:2033:GLU:OE2	1:A:2036:ARG:NH2	2.47	0.47
1:A:962:GLN:O	1:A:965:SER:OG	2.30	0.47
2:C:63:GLN:NE2	2:C:85:ASN:O	2.47	0.47
2:C:91:VAL:HG12	2:C:102:THR:HG22	1.96	0.47
3:E:809:LEU:HD23	3:E:886:LEU:HD13	1.96	0.47
1:B:308:THR:O	1:B:1558:SER:OG	2.32	0.47
1:B:1527:ASP:O	5:J:345:ARG:NH1	2.35	0.47
2:D:91:VAL:HG12	2:D:102:THR:HG22	1.96	0.47
1:A:1601:GLU:OE1	1:A:1619:TRP:NE1	2.41	0.47
3:E:220:LEU:HD12	3:E:223:ILE:HD12	1.97	0.47
5:J:331:PHE:N	5:J:401:MET:O	2.41	0.47
3:E:1520:CYS:HB3	3:E:1523:CYS:HB2	1.95	0.47
1:B:962:GLN:O	1:B:965:SER:OG	2.30	0.47
1:B:1701:MET:HA	1:B:1704:MET:HE2	1.97	0.47
1:B:2136:LEU:O	1:B:2152:ARG:NH1	2.47	0.47
1:B:2254:ARG:NH1	1:B:2261:LEU:O	2.47	0.47
2:D:63:GLN:NE2	2:D:85:ASN:O	2.47	0.47
2:D:89:ALA:N	2:D:103:GLY:O	2.43	0.47
3:F:134:ASP:OD1	3:F:134:ASP:N	2.47	0.47
3:F:809:LEU:HD23	3:F:886:LEU:HD13	1.96	0.47
3:E:693:ASN:OD1	3:E:693:ASN:N	2.46	0.47
3:F:220:LEU:HD12	3:F:223:ILE:HD12	1.97	0.47
1:B:1038:MET:HE1	1:B:1056:ILE:HD11	1.96	0.47
3:F:285:LYS:HG3	3:F:330:VAL:HG22	1.96	0.47
1:A:664:ILE:HG13	1:A:665:THR:HG23	1.97	0.47
1:B:961:ASP:OD1	1:B:961:ASP:N	2.45	0.46
1:A:1038:MET:HE1	1:A:1056:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ILE:HG13	1:B:665:THR:HG23	1.98	0.46
3:F:737:ARG:HE	3:F:773:ILE:HG22	1.80	0.46
2:C:28:GLN:OE1	2:C:31:SER:OG	2.33	0.46
2:C:137:HIS:CG	2:C:138:PRO:HD2	2.50	0.46
3:E:586:LYS:HB3	3:E:590:ASN:OD1	2.15	0.46
3:F:435:ASN:HB3	3:F:447:HIS:NE2	2.31	0.46
1:A:1701:MET:HA	1:A:1704:MET:HE2	1.97	0.46
1:A:2136:LEU:O	1:A:2152:ARG:NH1	2.47	0.46
3:F:586:LYS:HB3	3:F:590:ASN:OD1	2.15	0.46
3:F:660:PHE:HA	3:F:663:ILE:HG22	1.97	0.46
1:A:872:LEU:O	1:A:881:ARG:NH2	2.42	0.46
1:B:2145:ASP:OD1	1:B:2145:ASP:N	2.45	0.46
3:E:285:LYS:HG3	3:E:330:VAL:HG22	1.96	0.46
3:E:435:ASN:HB3	3:E:447:HIS:NE2	2.31	0.46
1:B:2392:LEU:HD23	1:B:2392:LEU:H	1.81	0.46
1:A:2340:HIS:CE1	1:A:2342:SER:HB2	2.51	0.46
1:B:849:ALA:HB2	1:B:890:LEU:HD13	1.97	0.46
2:D:28:GLN:OE1	2:D:31:SER:OG	2.33	0.46
3:E:245:ARG:H	3:E:249:GLU:HG3	1.80	0.46
3:E:737:ARG:HE	3:E:773:ILE:HG22	1.80	0.46
1:B:1116:PRO:HA	1:B:1119:VAL:HG12	1.98	0.46
2:D:137:HIS:CG	2:D:138:PRO:HD2	2.50	0.46
3:F:245:ARG:H	3:F:249:GLU:HG3	1.80	0.46
3:E:537:VAL:HG12	3:E:546:TRP:CG	2.51	0.46
3:E:660:PHE:HA	3:E:663:ILE:HG22	1.97	0.46
1:B:2340:HIS:CE1	1:B:2342:SER:HB2	2.51	0.46
3:F:393:ALA:HB2	3:F:437:ILE:HG22	1.98	0.46
3:E:235:LEU:HA	3:E:241:ARG:HG2	1.98	0.46
3:F:537:VAL:HG12	3:F:546:TRP:CG	2.51	0.45
1:A:849:ALA:HB2	1:A:890:LEU:HD13	1.97	0.45
2:C:242:GLN:HE21	2:C:271:GLY:H	1.64	0.45
1:A:1556:LEU:HD21	5:I:393:LEU:HD22	1.97	0.45
3:E:835:TYR:HB2	3:E:838:LYS:HB3	1.99	0.45
3:F:235:LEU:HA	3:F:241:ARG:HG2	1.98	0.45
3:F:830:LYS:HG2	3:F:835:TYR:HE1	1.81	0.45
1:A:1643:VAL:HG23	1:A:1644:VAL:HG12	1.98	0.45
3:E:557:TRP:CD2	3:E:558:PRO:HD2	2.51	0.45
2:D:39:GLN:NE2	2:D:41:GLN:HB2	2.32	0.45
3:F:835:TYR:HB2	3:F:838:LYS:HB3	1.99	0.45
5:I:361:ALA:HB1	5:I:366:MET:HG2	1.99	0.45
1:B:895:ASP:N	1:B:895:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2534:SER:OG	1:B:2537:ASN:OD1	2.34	0.45
1:A:957:ARG:NH1	1:A:1316:ASP:OD2	2.49	0.45
1:B:1277:LYS:HG2	1:B:1350:ILE:HD11	1.99	0.45
1:A:1116:PRO:HA	1:A:1119:VAL:HG12	1.98	0.45
1:A:2098:THR:HG23	3:E:1625:SER:HB3	1.99	0.45
1:A:2392:LEU:HD23	1:A:2392:LEU:H	1.81	0.45
1:A:2534:SER:OG	1:A:2537:ASN:OD1	2.34	0.45
2:C:39:GLN:NE2	2:C:41:GLN:HB2	2.32	0.45
5:J:361:ALA:HB1	5:J:366:MET:HG2	1.99	0.45
2:D:242:GLN:HE21	2:D:271:GLY:H	1.64	0.45
3:F:557:TRP:CD2	3:F:558:PRO:HD2	2.51	0.45
3:F:781:LYS:O	3:F:785:HIS:ND1	2.44	0.45
1:A:1277:LYS:HG2	1:A:1350:ILE:HD11	1.99	0.45
2:C:261:LYS:HA	2:C:270:ARG:HH12	1.82	0.45
3:E:393:ALA:HB2	3:E:437:ILE:HG22	1.98	0.45
1:B:957:ARG:NH1	1:B:1316:ASP:OD2	2.49	0.45
1:B:1063:LEU:HD12	1:B:1067:PHE:HD1	1.82	0.45
3:E:1521:LEU:HD12	3:E:1650:ILE:HD11	1.98	0.45
2:D:261:LYS:HA	2:D:270:ARG:HH12	1.81	0.45
1:A:1386:ARG:HD3	1:A:1389:LYS:HE3	1.99	0.45
2:C:92:GLY:HA3	2:C:101:TYR:CZ	2.53	0.45
1:B:1643:VAL:HG23	1:B:1644:VAL:HG12	1.98	0.44
1:A:1541:HIS:NE2	1:A:1592:SER:OG	2.50	0.44
3:E:454:ASN:O	3:E:458:SER:OG	2.28	0.44
1:B:785:ASP:OD1	1:B:785:ASP:N	2.51	0.44
1:B:2381:ARG:HA	1:B:2384:THR:HG22	1.98	0.44
3:F:1521:LEU:HD12	3:F:1650:ILE:HD11	1.98	0.44
3:E:959:CYS:H	3:E:965:ARG:HH21	1.64	0.44
5:I:321:THR:O	5:I:323:GLY:N	2.49	0.44
5:J:321:THR:O	5:J:323:GLY:N	2.49	0.44
1:B:1541:HIS:NE2	1:B:1592:SER:OG	2.50	0.44
1:A:1063:LEU:HD12	1:A:1067:PHE:HD1	1.82	0.44
1:A:1211:VAL:HA	3:E:553:THR:HG21	1.99	0.44
2:D:92:GLY:HA3	2:D:101:TYR:CZ	2.53	0.44
1:A:2192:LEU:HD21	1:A:2237:ILE:HG13	1.99	0.44
5:I:305:ASN:HB2	5:I:306:PRO:HD3	2.00	0.44
1:B:1386:ARG:HD3	1:B:1389:LYS:HE3	1.99	0.44
3:F:617:GLU:OE1	3:F:617:GLU:N	2.37	0.44
3:F:959:CYS:H	3:F:965:ARG:HH21	1.64	0.44
1:A:1943:ILE:HD11	1:A:1972:LEU:HD11	2.00	0.44
3:E:830:LYS:HG2	3:E:835:TYR:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:305:ASN:HB2	5:J:306:PRO:HD3	2.00	0.44
1:B:1943:ILE:HD11	1:B:1972:LEU:HD11	2.00	0.44
1:A:2381:ARG:HA	1:A:2384:THR:HG22	1.98	0.44
3:E:562:LEU:O	3:E:566:LYS:NZ	2.39	0.44
3:E:617:GLU:OE1	3:E:617:GLU:N	2.37	0.44
1:A:1772:VAL:HG21	1:A:1796:MET:HE2	2.00	0.44
1:B:2131:LEU:H	1:B:2131:LEU:HD23	1.83	0.43
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.51	0.43
2:D:281:ASP:HB3	4:H:139:GLN:HA	1.99	0.43
3:F:41:ILE:HG13	3:F:1693:LEU:HD21	1.99	0.43
1:B:2192:LEU:HD21	1:B:2237:ILE:HG13	1.99	0.43
3:F:957:LYS:HG3	3:F:958:GLN:HG3	1.99	0.43
3:E:41:ILE:HG13	3:E:1693:LEU:HD21	1.99	0.43
3:F:942:LEU:HD23	3:F:942:LEU:H	1.83	0.43
1:A:2339:ARG:NH2	1:A:2356:ILE:O	2.51	0.43
1:B:1091:ILE:HG22	1:B:1095:LYS:HE2	2.01	0.43
1:A:895:ASP:OD1	1:A:895:ASP:N	2.48	0.43
1:A:1091:ILE:HG22	1:A:1095:LYS:HE2	2.01	0.43
2:C:201:GLY:H	2:C:209:GLN:NE2	2.15	0.43
1:B:1291:LEU:HB3	1:B:1321:ALA:HB1	2.00	0.43
1:B:2520:ASP:OD1	1:B:2523:THR:OG1	2.33	0.43
2:D:57:ILE:HB	2:D:70:LEU:HD11	2.01	0.43
2:D:201:GLY:H	2:D:209:GLN:NE2	2.15	0.43
1:A:2025:GLU:OE1	1:A:2168:ARG:NH1	2.52	0.43
2:C:57:ILE:HB	2:C:70:LEU:HD11	2.01	0.43
2:C:281:ASP:HB3	4:G:139:GLN:HA	1.99	0.43
3:F:536:GLN:OE1	3:F:539:GLN:NE2	2.39	0.43
1:A:2131:LEU:HD23	1:A:2131:LEU:H	1.82	0.43
3:E:592:ASP:OD1	3:E:593:LEU:N	2.50	0.43
3:E:957:LYS:HG3	3:E:958:GLN:HG3	1.99	0.43
1:B:2078:LEU:HD13	1:B:2078:LEU:HA	1.88	0.43
1:A:1294:ASP:OD1	1:A:1294:ASP:N	2.52	0.43
1:B:745:GLY:H	1:A:1076:PRO:HB3	1.84	0.43
1:B:1002:ARG:NH2	1:B:1033:GLU:OE2	2.52	0.43
1:B:1116:PRO:HG3	1:B:1154:ARG:HH11	1.84	0.43
1:B:1772:VAL:HG21	1:B:1796:MET:HE2	2.00	0.43
1:B:2162:VAL:HG22	1:B:2170:ARG:HG3	2.01	0.43
2:D:15:LEU:HD13	2:D:320:PHE:HD1	1.84	0.43
3:E:942:LEU:H	3:E:942:LEU:HD23	1.83	0.43
1:B:1294:ASP:OD1	1:B:1294:ASP:N	2.52	0.42
3:F:560:VAL:HG12	3:F:565:TYR:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ILE:HG22	1:A:748:ARG:H	1.84	0.42
1:B:2025:GLU:OE1	1:B:2168:ARG:NH1	2.52	0.42
2:D:192:GLY:HA3	2:D:219:HIS:O	2.19	0.42
3:F:562:LEU:O	3:F:566:LYS:NZ	2.39	0.42
1:A:1291:LEU:HB3	1:A:1321:ALA:HB1	2.00	0.42
1:A:2162:VAL:HG22	1:A:2170:ARG:HG3	2.01	0.42
3:F:592:ASP:OD1	3:F:593:LEU:N	2.50	0.42
1:B:746:ILE:HG22	1:B:748:ARG:H	1.84	0.42
1:B:810:GLY:O	1:B:811:LEU:HG	2.19	0.42
1:A:1002:ARG:NH2	1:A:1033:GLU:OE2	2.52	0.42
3:E:269:ALA:HB3	3:E:272:GLN:HE22	1.85	0.42
1:A:810:GLY:O	1:A:811:LEU:HG	2.19	0.42
1:A:1116:PRO:HG3	1:A:1154:ARG:HH11	1.84	0.42
1:A:1931:GLN:HG2	1:A:1933:ASP:H	1.84	0.42
2:C:15:LEU:HD13	2:C:320:PHE:HD1	1.84	0.42
3:E:588:TYR:HA	3:E:591:LEU:HD23	2.01	0.42
1:B:2066:LYS:HD3	1:B:2125:TYR:CE2	2.55	0.42
1:A:308:THR:OG1	1:A:1558:SER:OG	2.24	0.42
2:C:242:GLN:NE2	2:C:271:GLY:H	2.18	0.42
1:B:2339:ARG:HH21	1:B:2343:ASN:HB3	1.85	0.42
2:D:79:ILE:HG13	4:H:104:LYS:HB3	2.02	0.42
3:F:269:ALA:HB3	3:F:272:GLN:HE22	1.85	0.42
4:H:23:ASP:N	4:H:23:ASP:OD1	2.52	0.42
1:B:631:THR:CA	1:B:682:ARG:HH22	2.28	0.42
1:B:1313:MET:HE2	1:B:1313:MET:HB2	1.97	0.42
1:B:2098:THR:HG23	3:F:1625:SER:HB3	2.02	0.42
2:D:134:VAL:HG13	2:D:143:LEU:HD21	2.01	0.42
2:C:192:GLY:HA3	2:C:219:HIS:O	2.20	0.42
1:B:1895:SER:HB3	1:B:1899:ASN:HB3	2.00	0.42
1:B:2244:ASP:N	1:B:2244:ASP:OD1	2.52	0.42
1:A:631:THR:CA	1:A:682:ARG:HH22	2.28	0.42
1:A:1743:LEU:O	1:A:1747:MET:HG2	2.20	0.42
1:B:1931:GLN:HG2	1:B:1933:ASP:H	1.84	0.41
3:F:453:MET:HE1	1:A:731:ARG:O	2.19	0.41
3:F:889:HIS:HD2	3:F:891:THR:HB	1.85	0.41
3:E:136:GLN:OE1	3:E:143:ARG:NH1	2.53	0.41
3:E:561:ASN:O	3:E:615:SER:HB3	2.20	0.41
1:B:1075:ILE:N	1:B:1076:PRO:HD2	2.34	0.41
2:D:242:GLN:NE2	2:D:271:GLY:H	2.18	0.41
2:C:239:SER:OG	2:C:243:THR:O	2.38	0.41
1:B:1743:LEU:O	1:B:1747:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:SER:OG	2:D:243:THR:O	2.38	0.41
3:F:561:ASN:O	3:F:615:SER:HB3	2.20	0.41
1:A:1075:ILE:N	1:A:1076:PRO:HD2	2.34	0.41
2:C:79:ILE:HG13	4:G:104:LYS:HB3	2.02	0.41
3:E:560:VAL:HG12	3:E:565:TYR:HD2	1.83	0.41
1:A:785:ASP:N	1:A:785:ASP:OD1	2.51	0.41
1:A:1650:MET:SD	1:A:1650:MET:N	2.93	0.41
1:A:2339:ARG:HH21	1:A:2343:ASN:HB3	1.85	0.41
1:B:2194:GLN:HG3	1:B:2421:PHE:CZ	2.49	0.41
2:D:66:ARG:HB3	2:D:77:PRO:HB3	2.02	0.41
3:F:136:GLN:OE1	3:F:143:ARG:NH1	2.53	0.41
1:A:1119:VAL:HA	1:A:1122:PHE:CE1	2.56	0.41
1:A:1895:SER:HB3	1:A:1899:ASN:HB3	2.00	0.41
3:E:237:HIS:ND1	3:E:239:LYS:HG2	2.36	0.41
1:B:968:HIS:HA	1:B:971:VAL:HG12	2.03	0.41
2:D:202:GLY:HA3	2:D:207:VAL:HG22	2.01	0.41
3:F:588:TYR:HA	3:F:591:LEU:HD23	2.01	0.41
1:A:2066:LYS:HD3	1:A:2125:TYR:CE2	2.55	0.41
2:C:66:ARG:HB3	2:C:77:PRO:HB3	2.02	0.41
1:A:1358:LEU:HD23	1:A:1383:LEU:HD12	2.03	0.41
1:A:1423:LEU:HD12	1:A:1423:LEU:HA	1.90	0.41
2:C:134:VAL:HG13	2:C:143:LEU:HD21	2.01	0.41
1:B:1075:ILE:HD13	1:B:1113:LEU:HD11	2.03	0.41
1:B:1649:ASP:N	1:B:1649:ASP:OD1	2.52	0.41
3:F:505:HIS:NE2	3:F:743:ASN:O	2.47	0.41
2:C:202:GLY:HA3	2:C:207:VAL:HG22	2.01	0.41
3:E:889:HIS:HD2	3:E:891:THR:HB	1.86	0.41
1:B:308:THR:OG1	1:B:1558:SER:OG	2.24	0.41
1:B:856:GLU:N	1:B:857:PRO:HD2	2.36	0.41
1:B:1167:PRO:HA	1:B:1170:ARG:NE	2.36	0.41
1:B:1358:LEU:HD23	1:B:1383:LEU:HD12	2.03	0.41
2:D:30:HIS:ND1	4:H:145:ARG:O	2.53	0.41
2:D:63:GLN:HA	2:D:84:VAL:HG23	2.02	0.41
2:D:200:THR:OG1	2:D:208:THR:HA	2.21	0.41
3:F:299:ILE:HG23	3:F:1437:PHE:HA	2.03	0.41
1:A:947:TYR:HB2	1:A:948:PRO:HD3	2.03	0.41
1:A:968:HIS:HA	1:A:971:VAL:HG12	2.03	0.41
2:C:67:MET:HB3	2:C:79:ILE:HB	2.03	0.41
3:E:628:LYS:O	3:E:632:GLN:HG2	2.20	0.41
3:E:959:CYS:O	3:E:965:ARG:NH2	2.54	0.41
1:B:701:ASN:HA	1:A:1154:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:LEU:HD23	1:B:1597:SER:HB2	2.03	0.41
1:B:947:TYR:HB2	1:B:948:PRO:HD3	2.03	0.41
2:D:274:TRP:HE1	2:D:290:SER:HB3	1.85	0.41
3:F:968:CYS:HA	3:F:971:VAL:HG22	2.03	0.41
3:E:299:ILE:HG23	3:E:1437:PHE:HA	2.03	0.41
3:E:968:CYS:HA	3:E:971:VAL:HG22	2.03	0.41
1:B:1650:MET:SD	1:B:1650:MET:N	2.93	0.40
1:A:1075:ILE:HD13	1:A:1113:LEU:HD11	2.03	0.40
1:A:1167:PRO:HA	1:A:1170:ARG:NE	2.36	0.40
1:A:1538:ARG:NH2	5:I:356:ASP:OD2	2.52	0.40
2:C:63:GLN:HA	2:C:84:VAL:HG23	2.02	0.40
5:J:307:LYS:HE2	5:J:307:LYS:HB2	1.88	0.40
2:D:40:HIS:CE1	2:D:66:ARG:HH11	2.40	0.40
3:F:237:HIS:ND1	3:F:239:LYS:HG2	2.36	0.40
4:G:23:ASP:OD1	4:G:23:ASP:N	2.52	0.40
1:B:1119:VAL:HA	1:B:1122:PHE:CE1	2.56	0.40
2:D:221:ARG:HG3	2:D:241:ASP:HB3	2.04	0.40
3:F:1000:LEU:HD23	3:F:1000:LEU:H	1.87	0.40
1:A:856:GLU:N	1:A:857:PRO:HD2	2.36	0.40
1:A:890:LEU:HD23	1:A:1597:SER:HB2	2.03	0.40
3:F:45:VAL:HG22	3:F:90:LEU:HD12	2.02	0.40
3:F:653:THR:HG23	3:F:654:THR:HG23	2.03	0.40
1:A:601:GLN:H	1:A:601:GLN:CD	2.30	0.40
2:C:8:VAL:HG12	2:C:10:SER:H	1.87	0.40
2:C:262:SER:H	2:C:270:ARG:HH22	1.70	0.40
3:E:505:HIS:NE2	3:E:743:ASN:O	2.47	0.40
1:B:666:ASP:HB3	1:B:672:ARG:HG3	2.04	0.40
1:B:945:GLU:OE1	1:B:945:GLU:N	2.54	0.40
1:B:1269:TRP:CZ2	1:B:1287:LEU:HD21	2.57	0.40
3:F:628:LYS:O	3:F:632:GLN:HG2	2.20	0.40
1:A:1313:MET:HE2	1:A:1313:MET:HB2	1.97	0.40
2:C:221:ARG:HG3	2:C:241:ASP:HB3	2.04	0.40
2:C:274:TRP:HE1	2:C:290:SER:HB3	1.85	0.40
3:E:45:VAL:HG22	3:E:90:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2152/2571 (84%)	2101 (98%)	51 (2%)	0	100	100
1	B	2152/2571 (84%)	2100 (98%)	52 (2%)	0	100	100
2	C	317/326 (97%)	301 (95%)	16 (5%)	0	100	100
2	D	317/326 (97%)	301 (95%)	16 (5%)	0	100	100
3	E	1101/1708 (64%)	1056 (96%)	44 (4%)	1 (0%)	48	78
3	F	1101/1708 (64%)	1056 (96%)	44 (4%)	1 (0%)	48	78
4	G	94/522 (18%)	91 (97%)	3 (3%)	0	100	100
4	H	94/522 (18%)	91 (97%)	3 (3%)	0	100	100
5	I	104/409 (25%)	92 (88%)	11 (11%)	1 (1%)	12	39
5	J	104/409 (25%)	92 (88%)	11 (11%)	1 (1%)	12	39
All	All	7536/11072 (68%)	7281 (97%)	251 (3%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	642	PRO
3	E	642	PRO
5	I	308	SER
5	J	308	SER

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	1571/2236 (70%)	1556 (99%)	15 (1%)	68	74
1	B	1571/2236 (70%)	1556 (99%)	15 (1%)	68	74
2	C	269/276 (98%)	264 (98%)	5 (2%)	50	66
2	D	269/276 (98%)	264 (98%)	5 (2%)	50	66
3	E	985/1539 (64%)	980 (100%)	5 (0%)	81	80
3	F	985/1539 (64%)	980 (100%)	5 (0%)	81	80
4	G	50/471 (11%)	49 (98%)	1 (2%)	48	65
4	H	50/471 (11%)	49 (98%)	1 (2%)	48	65
5	I	89/364 (24%)	86 (97%)	3 (3%)	32	56
5	J	89/364 (24%)	86 (97%)	3 (3%)	32	56
All	All	5928/9772 (61%)	5870 (99%)	58 (1%)	65	74

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	314	THR
1	B	631	THR
1	B	773	GLU
1	B	854	VAL
1	B	863	THR
1	B	1023	VAL
1	B	1048	ILE
1	B	1535	MET
1	B	1608	VAL
1	B	1621	GLU
1	B	1644	VAL
1	B	1921	GLU
1	B	1970	GLN
1	B	2143	THR
1	B	2240	VAL
2	D	24	VAL
2	D	51	THR
2	D	166	ILE
2	D	214	THR
2	D	216	ILE
3	F	240	THR
3	F	446	LEU
3	F	1003	VAL
3	F	1621	ILE

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Mol	Chain	Res	Type
3	F	1664	THR
4	H	36	VAL
1	A	314	THR
1	A	631	THR
1	A	773	GLU
1	A	854	VAL
1	A	863	THR
1	A	1023	VAL
1	A	1048	ILE
1	A	1535	MET
1	A	1608	VAL
1	A	1621	GLU
1	A	1644	VAL
1	A	1921	GLU
1	A	1970	GLN
1	A	2143	THR
1	A	2240	VAL
2	C	24	VAL
2	C	51	THR
2	C	166	ILE
2	C	214	THR
2	C	216	ILE
3	E	240	THR
3	E	446	LEU
3	E	1003	VAL
3	E	1621	ILE
3	E	1664	THR
4	G	36	VAL
5	I	309	VAL
5	I	315	THR
5	I	319	LEU
5	J	309	VAL
5	J	315	THR
5	J	319	LEU

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

Mol	Chain	Res	Type
1	B	1049	GLN
1	B	1319	ASN
1	B	1355	GLN
1	B	1561	GLN

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Mol	Chain	Res	Type
1	B	1624	GLN
1	B	1726	GLN
1	B	2265	HIS
1	B	2282	GLN
2	D	87	ASN
2	D	120	GLN
3	F	480	HIS
3	F	607	GLN
3	F	648	ASN
3	F	658	HIS
3	F	758	GLN
3	F	763	ASN
3	F	827	GLN
3	F	889	HIS
3	F	1434	ASN
3	F	1632	HIS
3	F	1678	GLN
1	A	1049	GLN
1	A	1355	GLN
1	A	1561	GLN
1	A	1617	GLN
1	A	1624	GLN
1	A	1726	GLN
1	A	2282	GLN
2	C	87	ASN
2	C	120	GLN
3	E	214	ASN
3	E	480	HIS
3	E	543	ASN
3	E	607	GLN
3	E	648	ASN
3	E	658	HIS
3	E	748	ASN
3	E	758	GLN
3	E	763	ASN
3	E	827	GLN
3	E	889	HIS
3	E	1632	HIS
3	E	1678	GLN
5	I	389	ASN
5	J	389	ASN
5	J	390	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
8	ACE	G	601	4	1,2,2	0.76	0	0,1,1	-	-
6	IHP	B	2601	-	36,36,36	0.78	1 (2%)	60,60,60	0.57	1 (1%)
8	ACE	H	601	4	1,2,2	0.77	0	0,1,1	-	-
6	IHP	A	2601	-	36,36,36	0.78	1 (2%)	60,60,60	0.57	1 (1%)

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	IHP	B	2601	-	-	1/30/54/54	0/1/1/1
6	IHP	A	2601	-	-	1/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2601	IHP	P3-O13	3.11	1.65	1.59
6	A	2601	IHP	P3-O13	3.10	1.65	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2601	IHP	P2-O12-C2	2.89	131.16	123.43
6	A	2601	IHP	P2-O12-C2	2.88	131.13	123.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

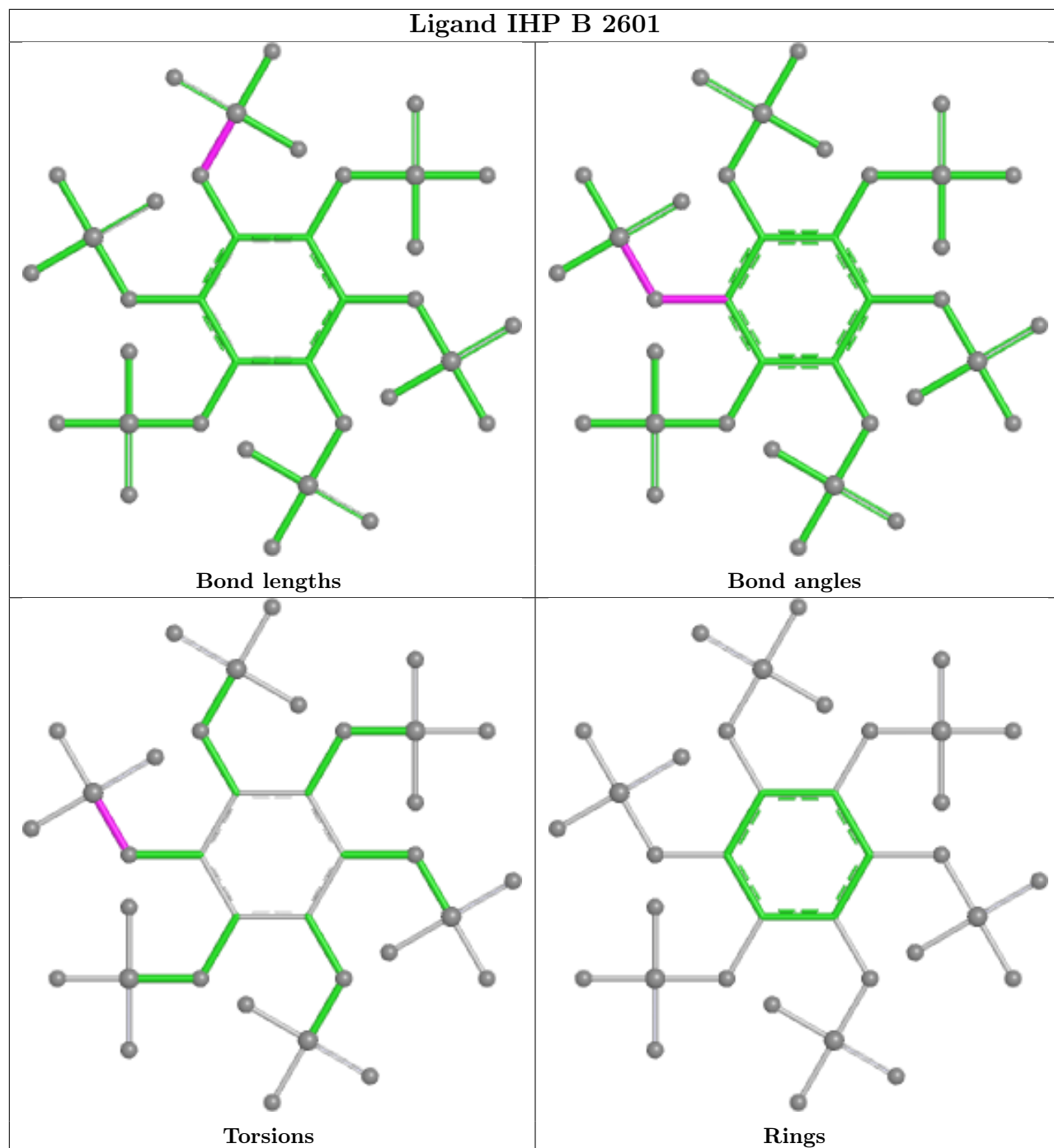
Mol	Chain	Res	Type	Atoms
6	B	2601	IHP	C2-O12-P2-O22
6	A	2601	IHP	C2-O12-P2-O22

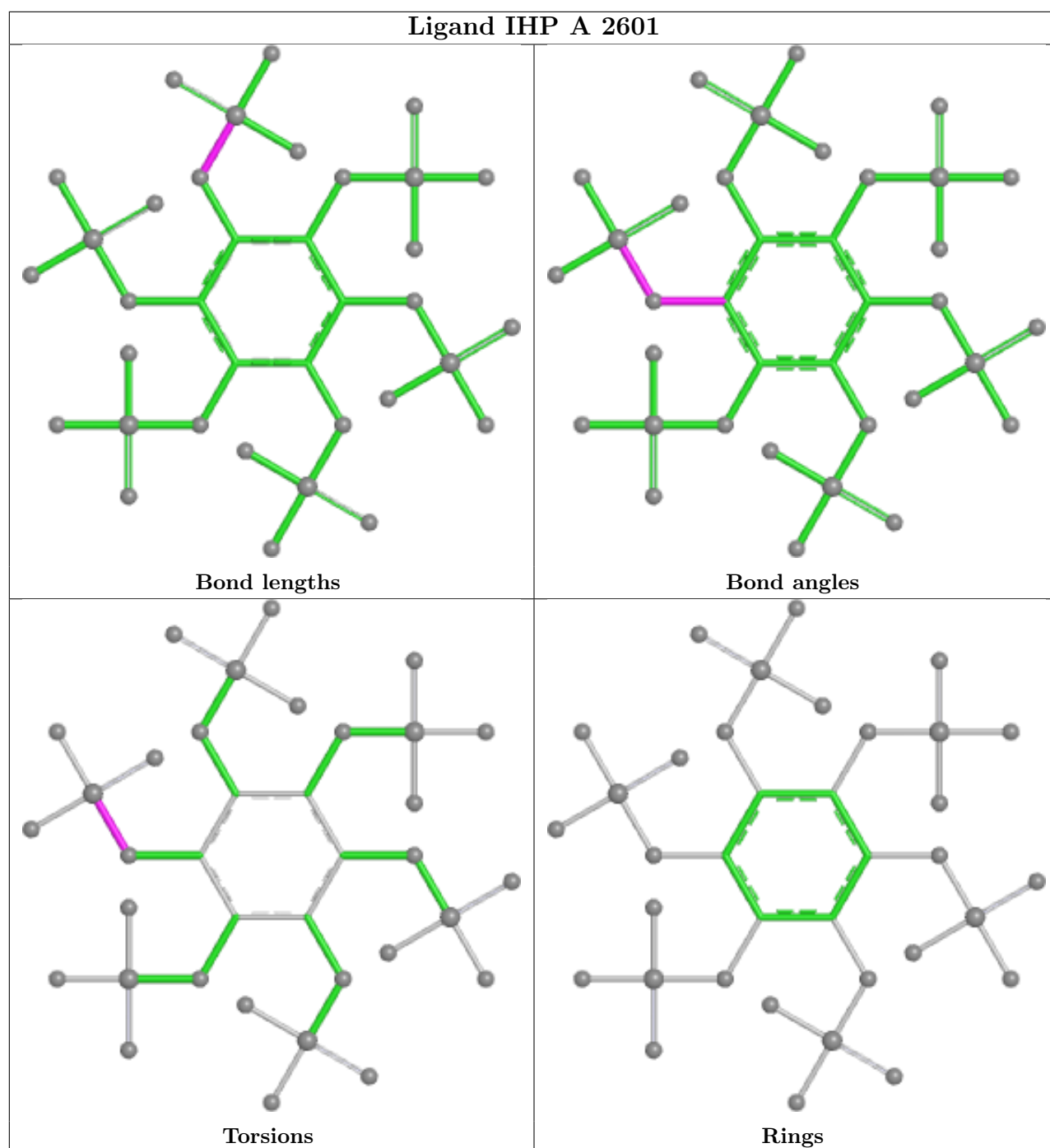
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2601	IHP	1	0
6	A	2601	IHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

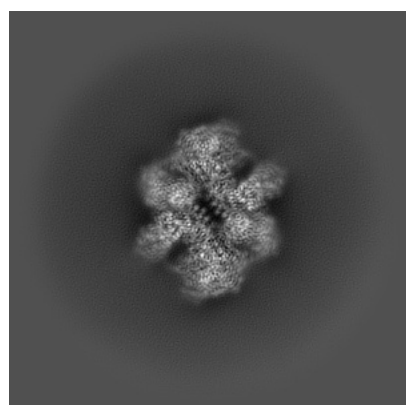
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13347. These allow visual inspection of the internal detail of the map and identification of artifacts.

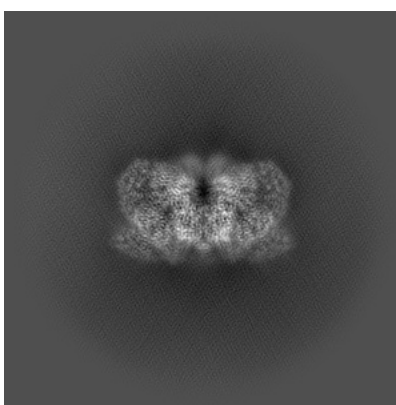
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

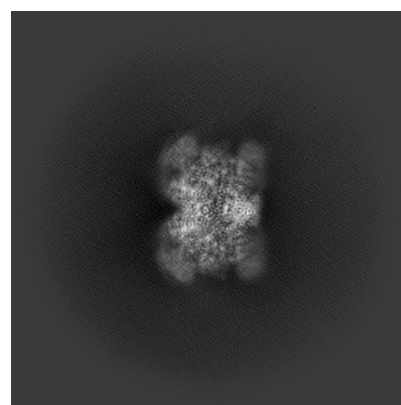
6.1.1 Primary map



X



Y

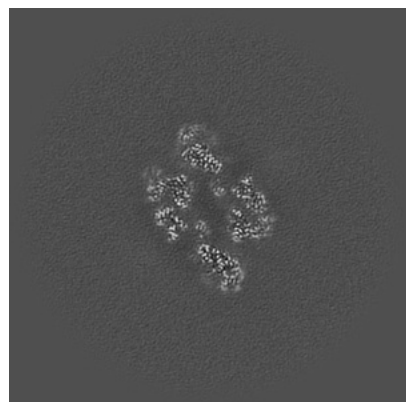


Z

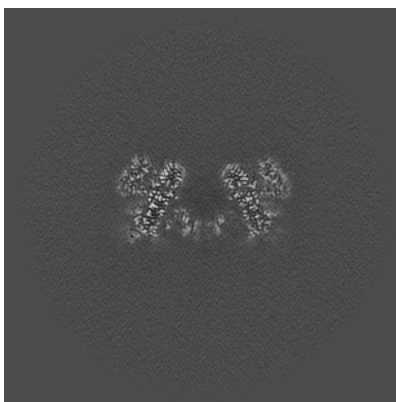
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

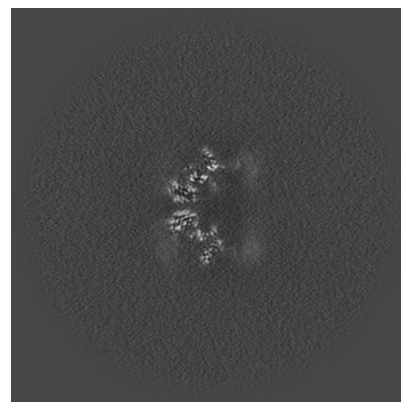
6.2.1 Primary map



X Index: 240



Y Index: 240

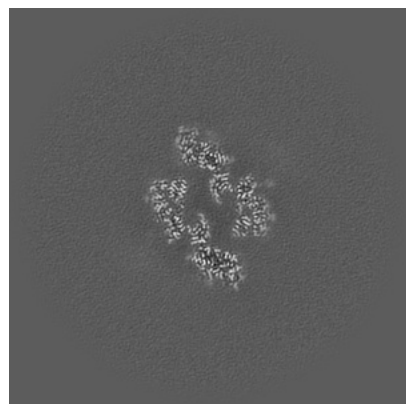


Z Index: 240

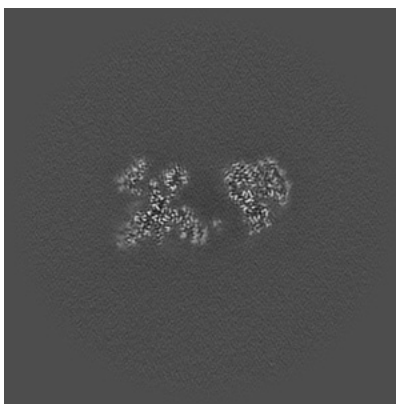
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

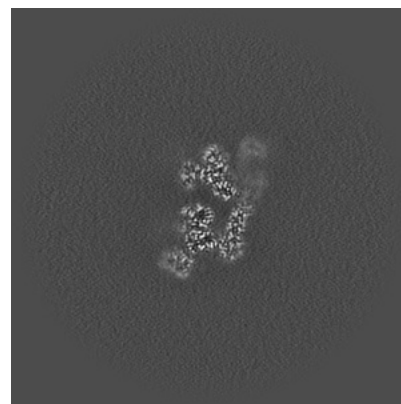
6.3.1 Primary map



X Index: 235



Y Index: 235

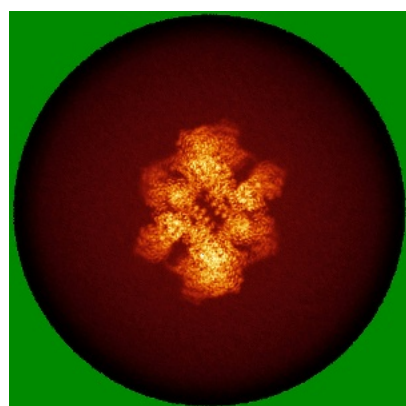


Z Index: 215

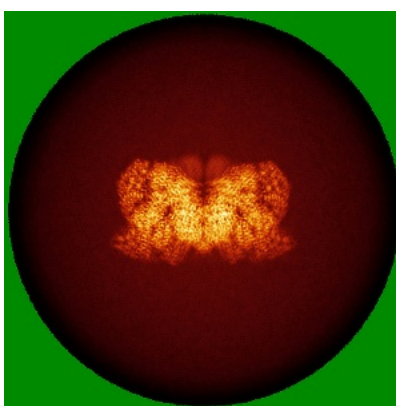
The images above show the largest variance slices of the map in three orthogonal directions.

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

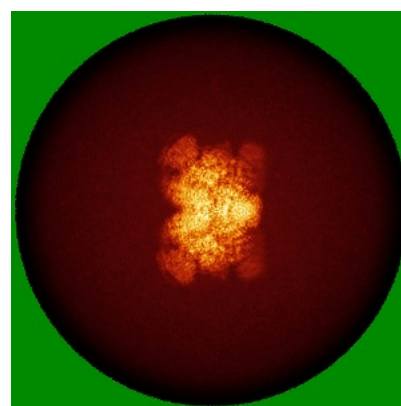
6.4.1 Primary map



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

This section was not generated.

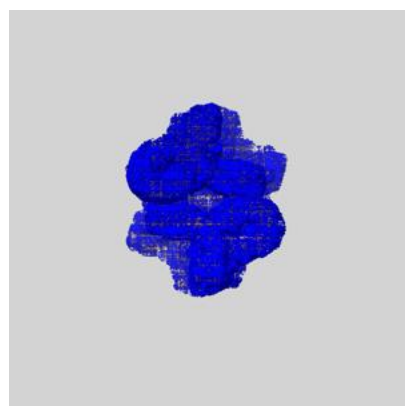
6.6 Mask visualisation [i](#)

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

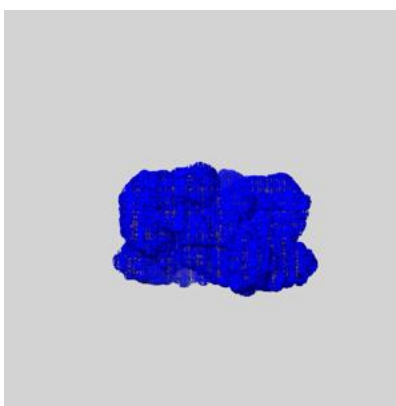
A mask typically either:

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

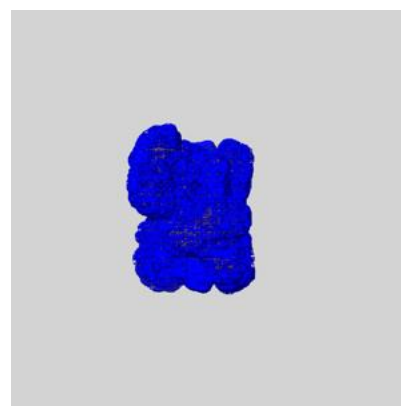
6.6.1 emd_13347_msk_1.map [i](#)



X



Y

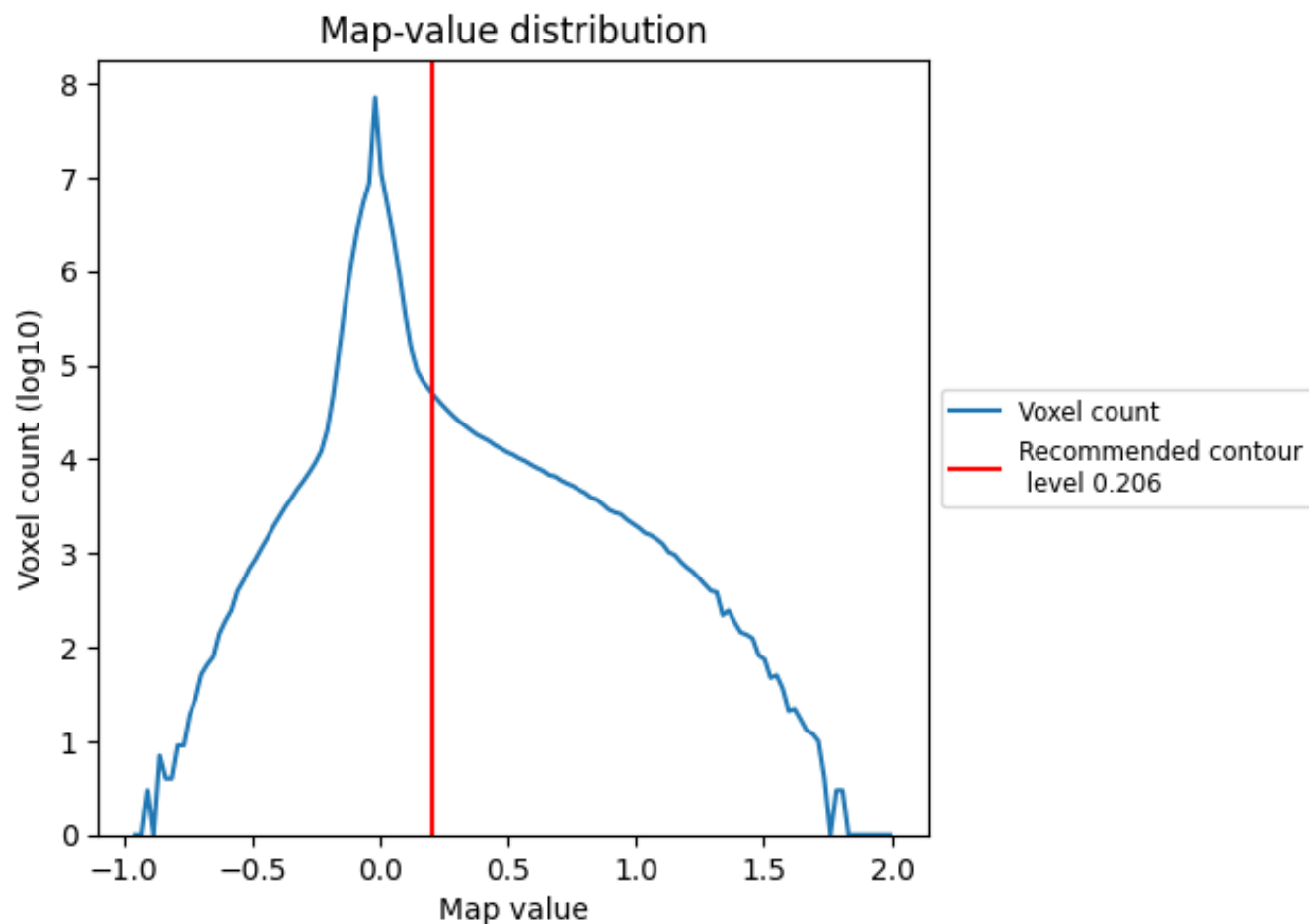


Z

7 Map analysis [i](#)

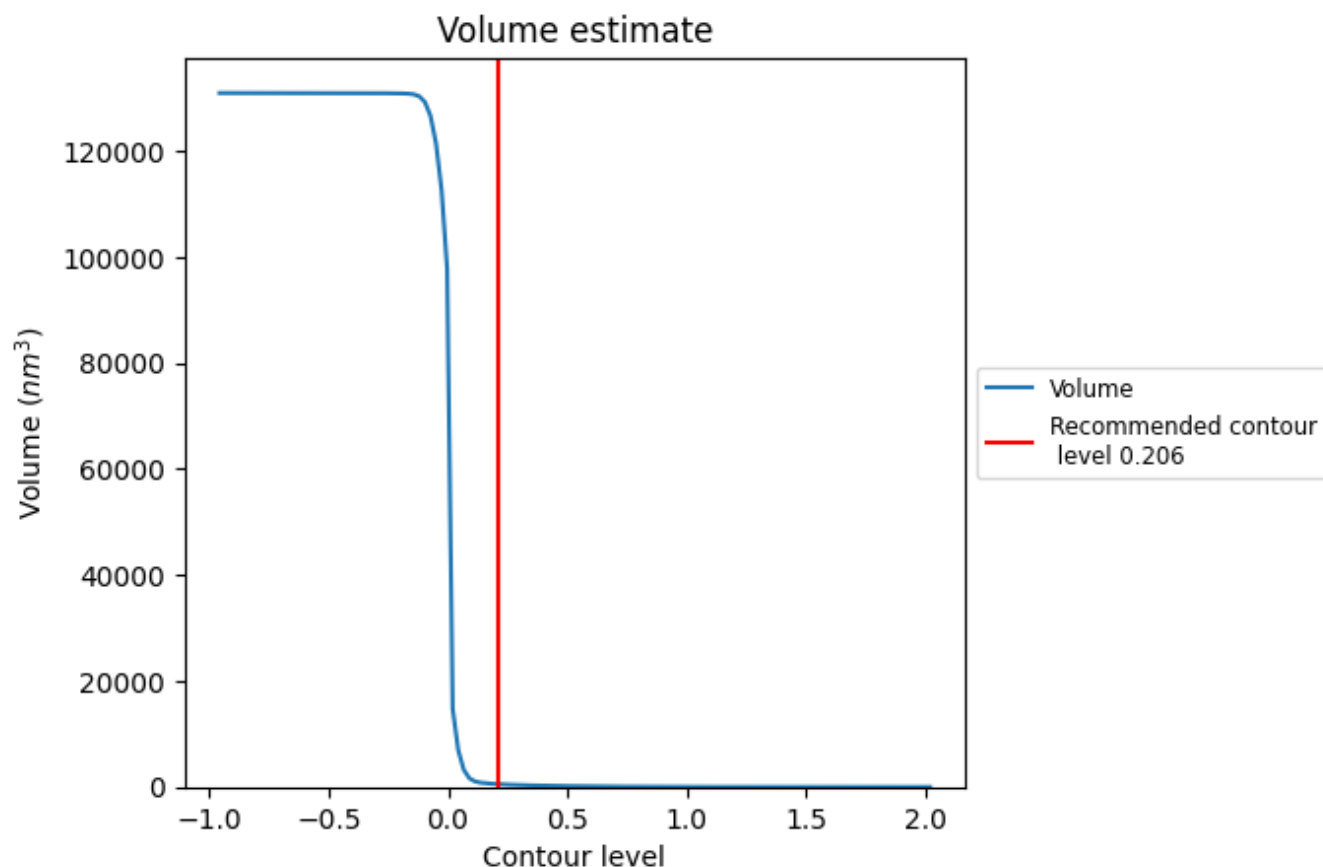
This section contains the results of statistical analysis of the map.

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.

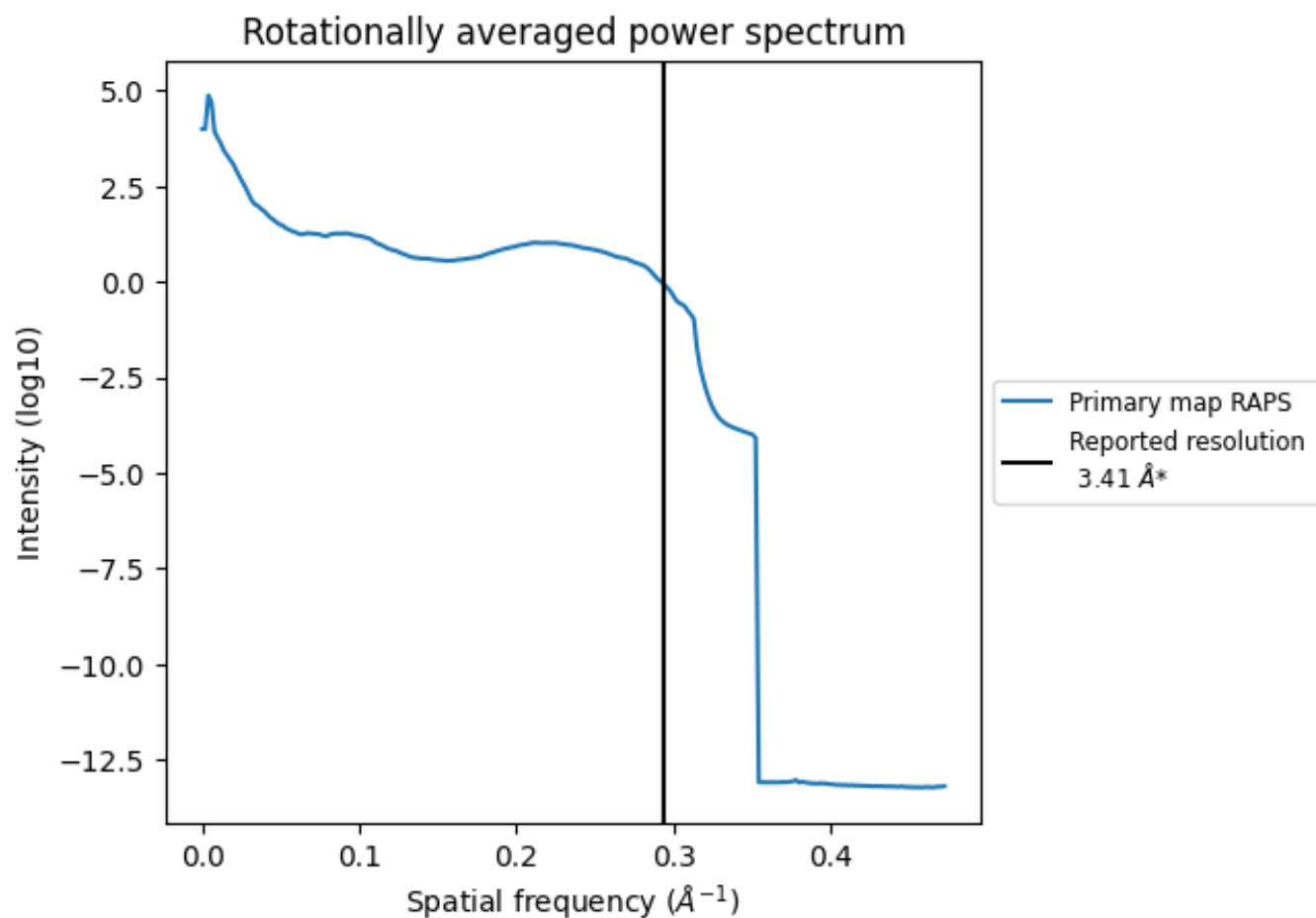
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 542 nm^3 ; this corresponds to an approximate mass of 490 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 0.293 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

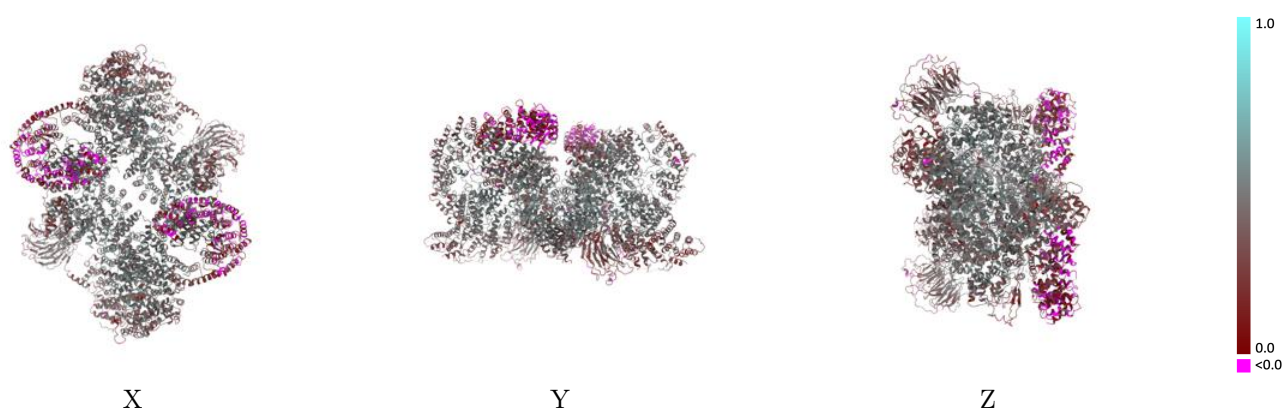
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-13347 and PDB model 7PE7. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

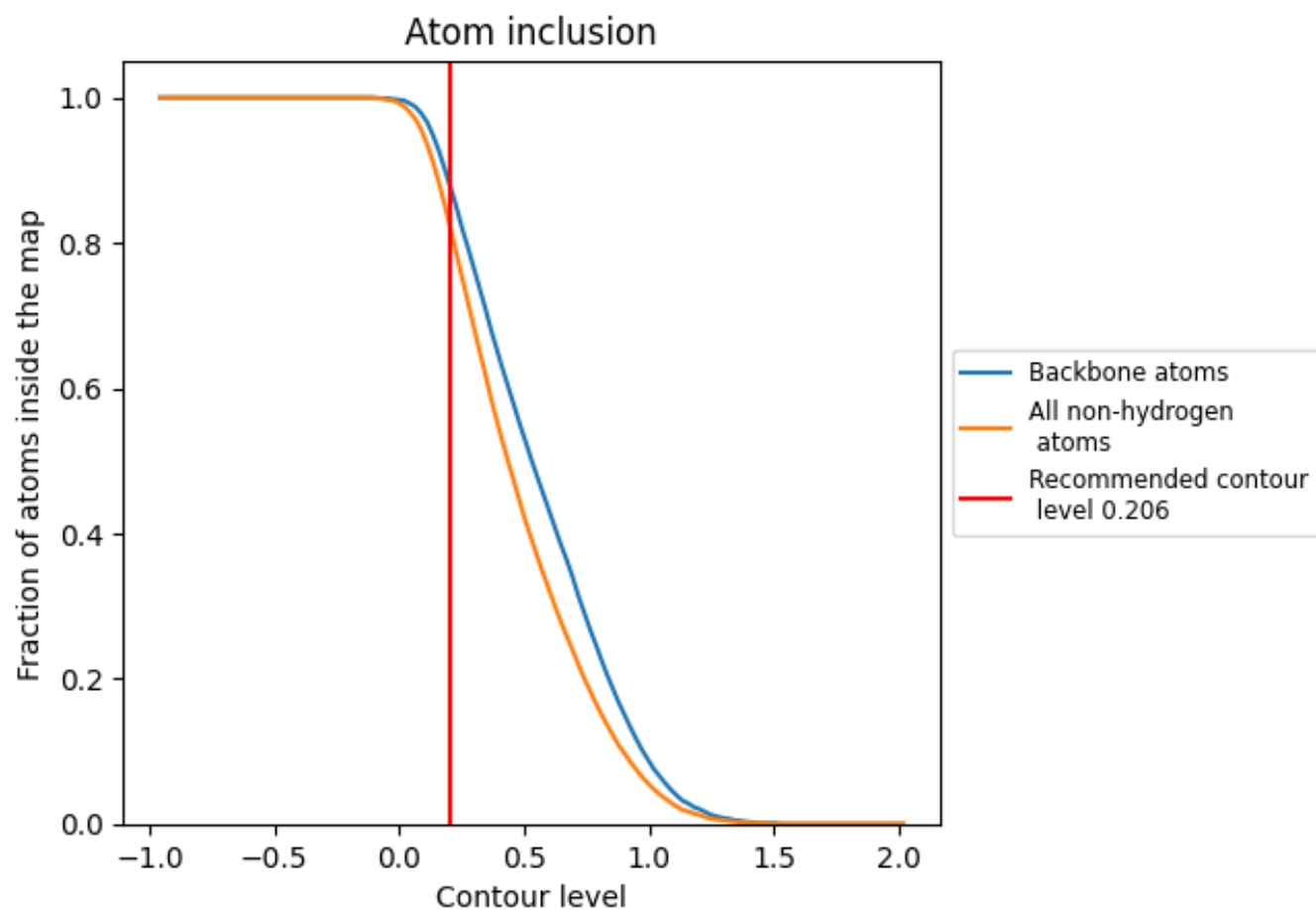


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.206) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8190	0.4010
A	0.8160	0.4110
B	0.8150	0.4080
C	0.8090	0.3230
D	0.8280	0.3390
E	0.8220	0.4090
F	0.8530	0.4260
G	0.7500	0.3380
H	0.8040	0.3450
I	0.6980	0.2890
J	0.7330	0.2880

1.0

0.0

<0.0