



Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 04:39 pm BST

PDB ID : 9TDS / pdb_00009tds
EMDB ID : EMD-55803
Title : cryo-EM structure of dephosphorylated mTOR complex 2, overall refinement
Authors : Hay, I.M.; Anandapadamanaban, M.; Williams, R.L.
Deposited on : 2025-11-24
Resolution : 3.30 Å(reported)

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:

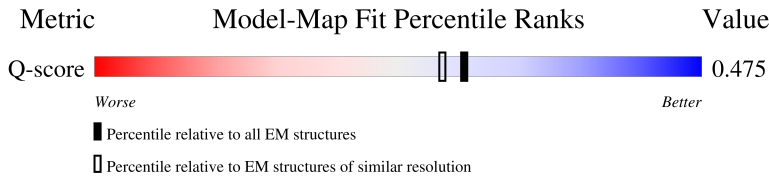
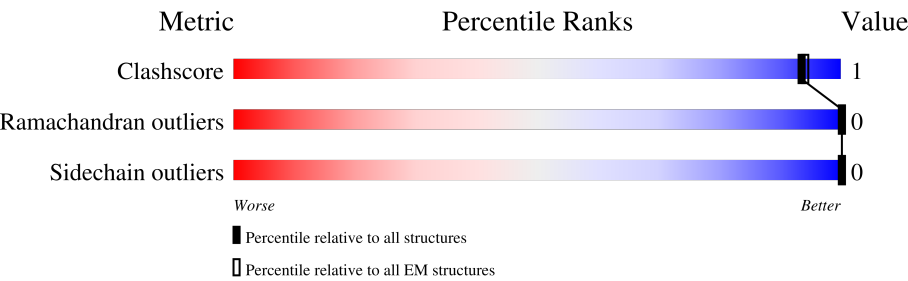
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 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	15087 (2.80 - 3.80)

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	2590	
1	B	2590	
2	C	326	
2	D	326	

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Mol	Chain	Length	Quality of chain
3	E	1734	
3	F	1734	
4	G	522	
4	H	522	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 52832 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	A	1747	Total	C	N	O	S	0	0
			14131	9029	2476	2529	97		
1	B	1749	Total	C	N	O	S	0	0
			14145	9037	2478	2532	98		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP P42345
A	-39	ALA	-	expression tag	UNP P42345
A	-38	SER	-	expression tag	UNP P42345
A	-37	TRP	-	expression tag	UNP P42345
A	-36	SER	-	expression tag	UNP P42345
A	-35	HIS	-	expression tag	UNP P42345
A	-34	PRO	-	expression tag	UNP P42345
A	-33	GLN	-	expression tag	UNP P42345
A	-32	PHE	-	expression tag	UNP P42345
A	-31	GLU	-	expression tag	UNP P42345
A	-30	LYS	-	expression tag	UNP P42345
A	-29	GLY	-	expression tag	UNP P42345
A	-28	GLY	-	expression tag	UNP P42345
A	-27	GLY	-	expression tag	UNP P42345
A	-26	ALA	-	expression tag	UNP P42345
A	-25	ARG	-	expression tag	UNP P42345
A	-24	GLY	-	expression tag	UNP P42345
A	-23	GLY	-	expression tag	UNP P42345
A	-22	SER	-	expression tag	UNP P42345
A	-21	GLY	-	expression tag	UNP P42345
A	-20	GLY	-	expression tag	UNP P42345
A	-19	GLY	-	expression tag	UNP P42345
A	-18	SER	-	expression tag	UNP P42345
A	-17	TRP	-	expression tag	UNP P42345
A	-16	SER	-	expression tag	UNP P42345
A	-15	HIS	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PRO	-	expression tag	UNP P42345
A	-13	GLN	-	expression tag	UNP P42345
A	-12	PHE	-	expression tag	UNP P42345
A	-11	GLU	-	expression tag	UNP P42345
A	-10	LYS	-	expression tag	UNP P42345
A	-9	GLY	-	expression tag	UNP P42345
A	-8	GLU	-	expression tag	UNP P42345
A	-7	ASN	-	expression tag	UNP P42345
A	-6	LEU	-	expression tag	UNP P42345
A	-5	TYR	-	expression tag	UNP P42345
A	-4	PHE	-	expression tag	UNP P42345
A	-3	GLN	-	expression tag	UNP P42345
A	-2	GLY	-	expression tag	UNP P42345
A	-1	GLY	-	expression tag	UNP P42345
A	0	THR	-	expression tag	UNP P42345
B	-40	MET	-	initiating methionine	UNP P42345
B	-39	ALA	-	expression tag	UNP P42345
B	-38	SER	-	expression tag	UNP P42345
B	-37	TRP	-	expression tag	UNP P42345
B	-36	SER	-	expression tag	UNP P42345
B	-35	HIS	-	expression tag	UNP P42345
B	-34	PRO	-	expression tag	UNP P42345
B	-33	GLN	-	expression tag	UNP P42345
B	-32	PHE	-	expression tag	UNP P42345
B	-31	GLU	-	expression tag	UNP P42345
B	-30	LYS	-	expression tag	UNP P42345
B	-29	GLY	-	expression tag	UNP P42345
B	-28	GLY	-	expression tag	UNP P42345
B	-27	GLY	-	expression tag	UNP P42345
B	-26	ALA	-	expression tag	UNP P42345
B	-25	ARG	-	expression tag	UNP P42345
B	-24	GLY	-	expression tag	UNP P42345
B	-23	GLY	-	expression tag	UNP P42345
B	-22	SER	-	expression tag	UNP P42345
B	-21	GLY	-	expression tag	UNP P42345
B	-20	GLY	-	expression tag	UNP P42345
B	-19	GLY	-	expression tag	UNP P42345
B	-18	SER	-	expression tag	UNP P42345
B	-17	TRP	-	expression tag	UNP P42345
B	-16	SER	-	expression tag	UNP P42345
B	-15	HIS	-	expression tag	UNP P42345
B	-14	PRO	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	GLN	-	expression tag	UNP P42345
B	-12	PHE	-	expression tag	UNP P42345
B	-11	GLU	-	expression tag	UNP P42345
B	-10	LYS	-	expression tag	UNP P42345
B	-9	GLY	-	expression tag	UNP P42345
B	-8	GLU	-	expression tag	UNP P42345
B	-7	ASN	-	expression tag	UNP P42345
B	-6	LEU	-	expression tag	UNP P42345
B	-5	TYR	-	expression tag	UNP P42345
B	-4	PHE	-	expression tag	UNP P42345
B	-3	GLN	-	expression tag	UNP P42345
B	-2	GLY	-	expression tag	UNP P42345
B	-1	GLY	-	expression tag	UNP P42345
B	0	THR	-	expression tag	UNP P42345

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	315	Total	C	N	O	S	0	0
			2443	1518	434	473	18		
2	D	315	Total	C	N	O	S	0	0
			2443	1518	434	473	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1119	Total	C	N	O	S	0	0
			8990	5732	1584	1625	49		
3	F	1119	Total	C	N	O	S	0	0
			8990	5732	1584	1625	49		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-25	MET	-	initiating methionine	UNP Q6R327
E	-24	ALA	-	expression tag	UNP Q6R327
E	-23	ASP	-	expression tag	UNP Q6R327
E	-22	TYR	-	expression tag	UNP Q6R327
E	-21	LYS	-	expression tag	UNP Q6R327
E	-20	ASP	-	expression tag	UNP Q6R327
E	-19	HIS	-	expression tag	UNP Q6R327
E	-18	ASP	-	expression tag	UNP Q6R327

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	GLY	-	expression tag	UNP Q6R327
E	-16	ASP	-	expression tag	UNP Q6R327
E	-15	TYR	-	expression tag	UNP Q6R327
E	-14	LYS	-	expression tag	UNP Q6R327
E	-13	ASP	-	expression tag	UNP Q6R327
E	-12	HIS	-	expression tag	UNP Q6R327
E	-11	ASP	-	expression tag	UNP Q6R327
E	-10	ILE	-	expression tag	UNP Q6R327
E	-9	ASP	-	expression tag	UNP Q6R327
E	-8	TYR	-	expression tag	UNP Q6R327
E	-7	LYS	-	expression tag	UNP Q6R327
E	-6	ASP	-	expression tag	UNP Q6R327
E	-5	ASP	-	expression tag	UNP Q6R327
E	-4	ASP	-	expression tag	UNP Q6R327
E	-3	ASP	-	expression tag	UNP Q6R327
E	-2	LYS	-	expression tag	UNP Q6R327
E	-1	GLY	-	expression tag	UNP Q6R327
E	0	THR	-	expression tag	UNP Q6R327
F	-25	MET	-	initiating methionine	UNP Q6R327
F	-24	ALA	-	expression tag	UNP Q6R327
F	-23	ASP	-	expression tag	UNP Q6R327
F	-22	TYR	-	expression tag	UNP Q6R327
F	-21	LYS	-	expression tag	UNP Q6R327
F	-20	ASP	-	expression tag	UNP Q6R327
F	-19	HIS	-	expression tag	UNP Q6R327
F	-18	ASP	-	expression tag	UNP Q6R327
F	-17	GLY	-	expression tag	UNP Q6R327
F	-16	ASP	-	expression tag	UNP Q6R327
F	-15	TYR	-	expression tag	UNP Q6R327
F	-14	LYS	-	expression tag	UNP Q6R327
F	-13	ASP	-	expression tag	UNP Q6R327
F	-12	HIS	-	expression tag	UNP Q6R327
F	-11	ASP	-	expression tag	UNP Q6R327
F	-10	ILE	-	expression tag	UNP Q6R327
F	-9	ASP	-	expression tag	UNP Q6R327
F	-8	TYR	-	expression tag	UNP Q6R327
F	-7	LYS	-	expression tag	UNP Q6R327
F	-6	ASP	-	expression tag	UNP Q6R327
F	-5	ASP	-	expression tag	UNP Q6R327
F	-4	ASP	-	expression tag	UNP Q6R327
F	-3	ASP	-	expression tag	UNP Q6R327
F	-2	LYS	-	expression tag	UNP Q6R327

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP Q6R327
F	0	THR	-	expression tag	UNP Q6R327

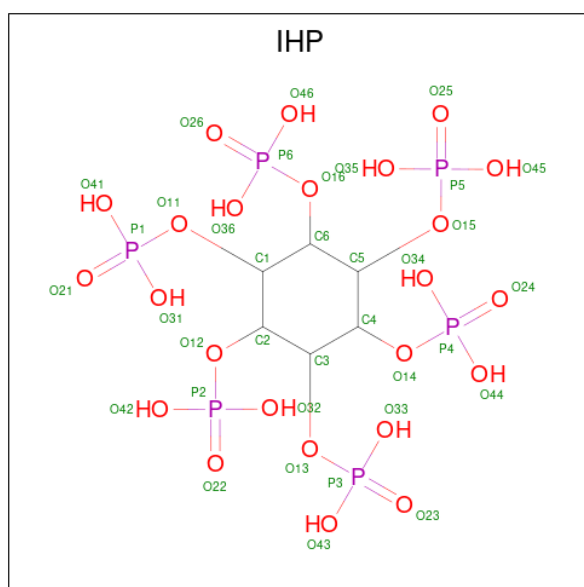
- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	100	Total	C	N	O	S	0	0
			808	499	154	151	4		
4	H	100	Total	C	N	O	S	0	0
			808	499	154	151	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ACE	-	acetylation	UNP Q9BPZ7
H	1	ACE	-	acetylation	UNP Q9BPZ7

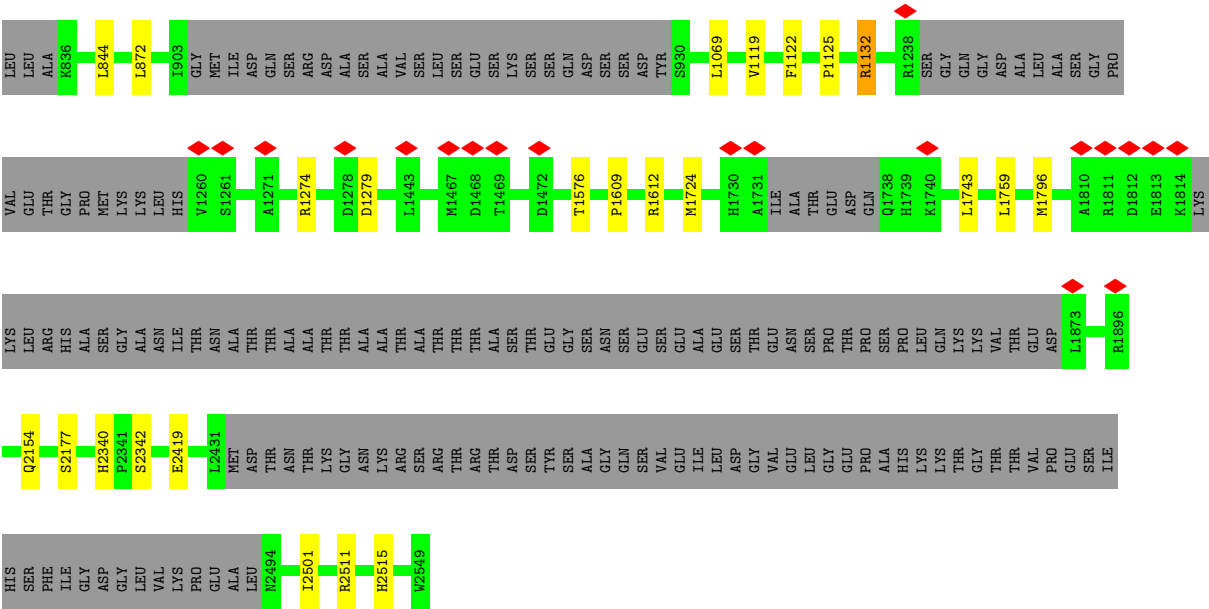
- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



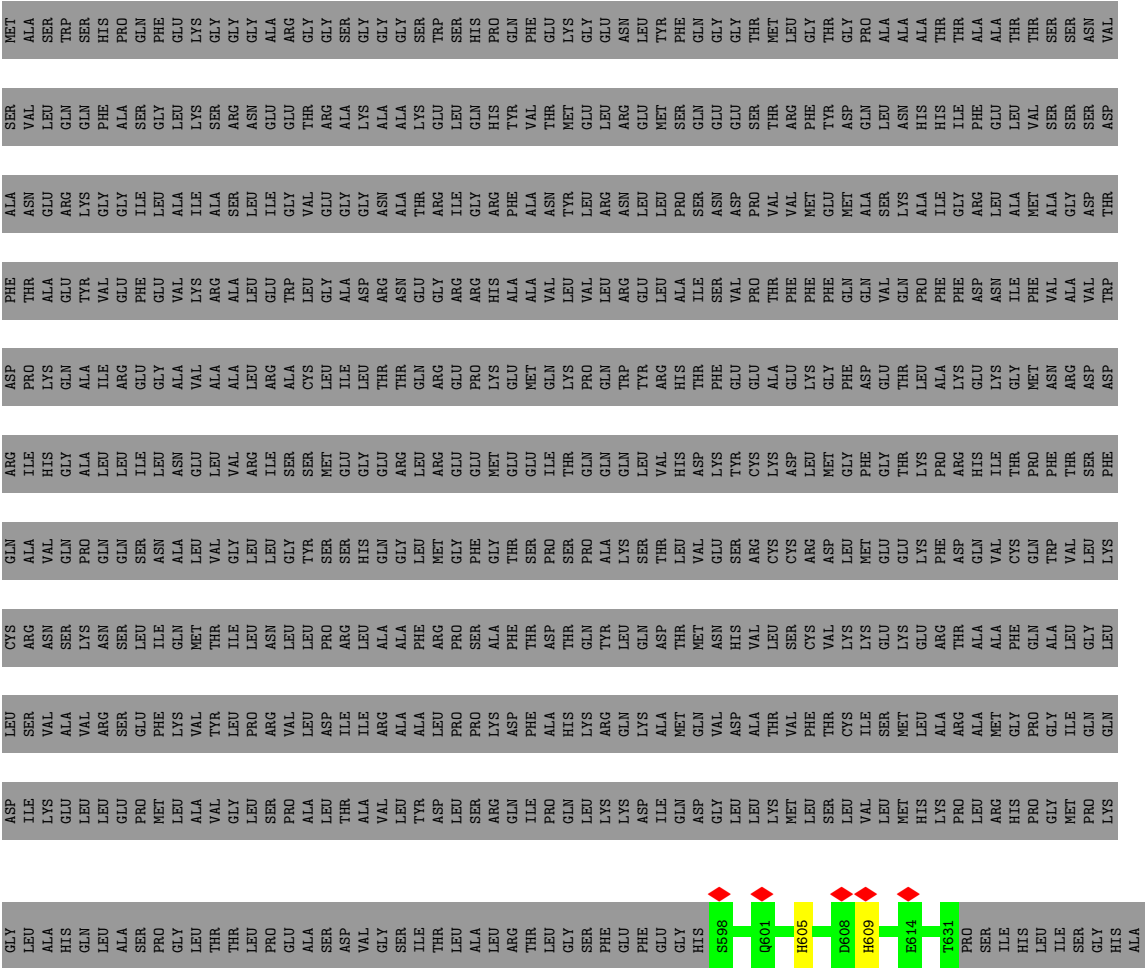
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			36	6	24	6	
5	B	1	Total	C	O	P	0
			36	6	24	6	

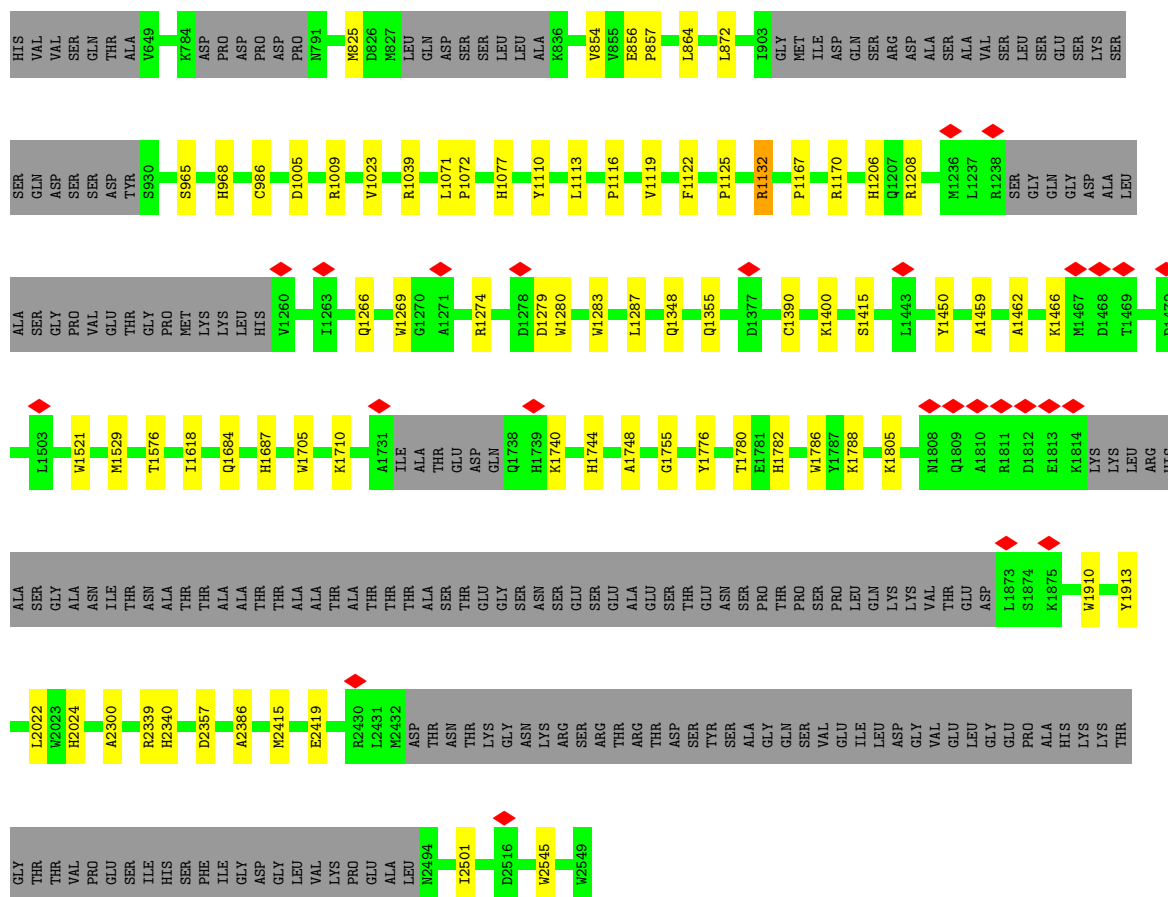
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

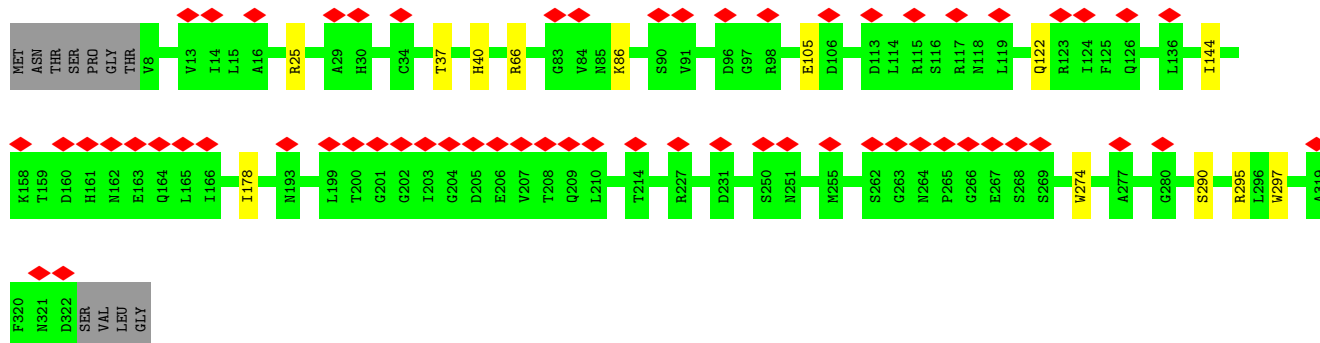
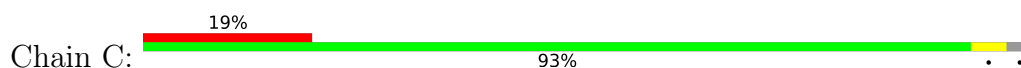


● Molecule 1: Serine/threonine-protein kinase mTOR

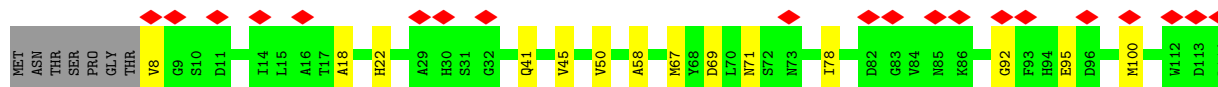
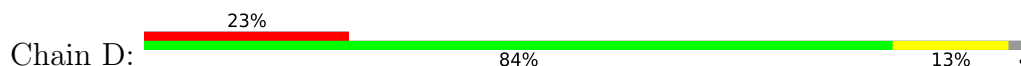


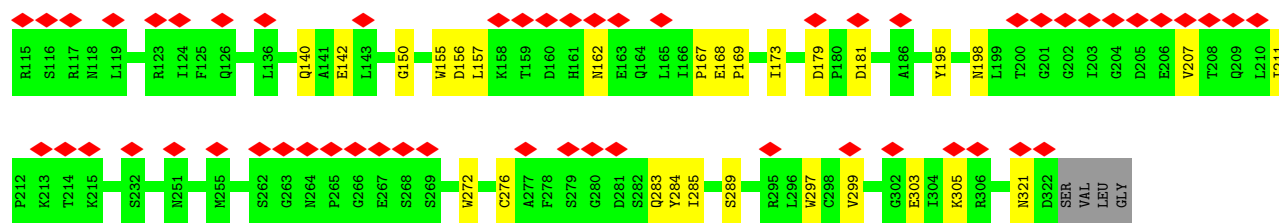


• Molecule 2: Target of rapamycin complex subunit LST8



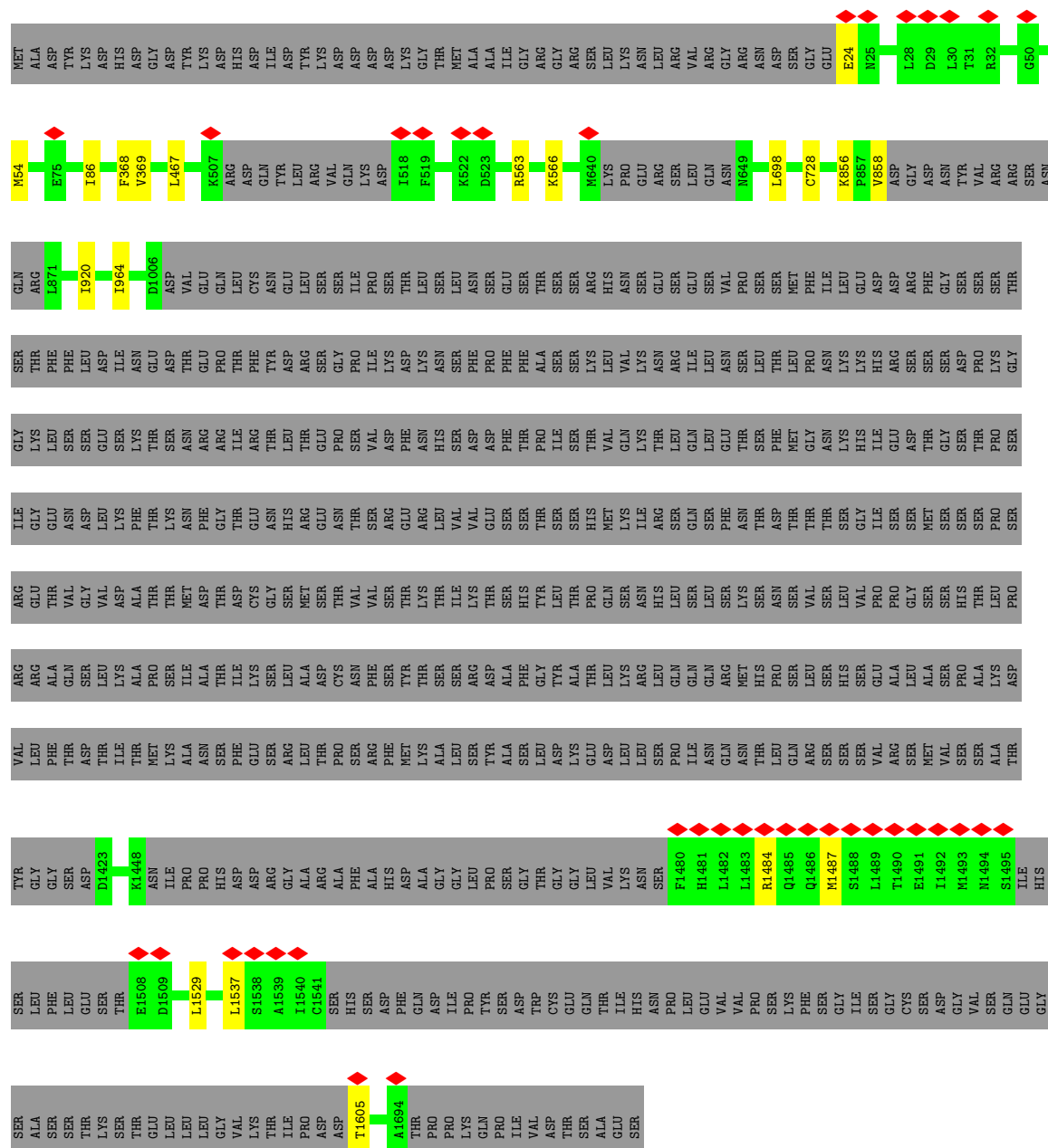
• Molecule 2: Target of rapamycin complex subunit LST8





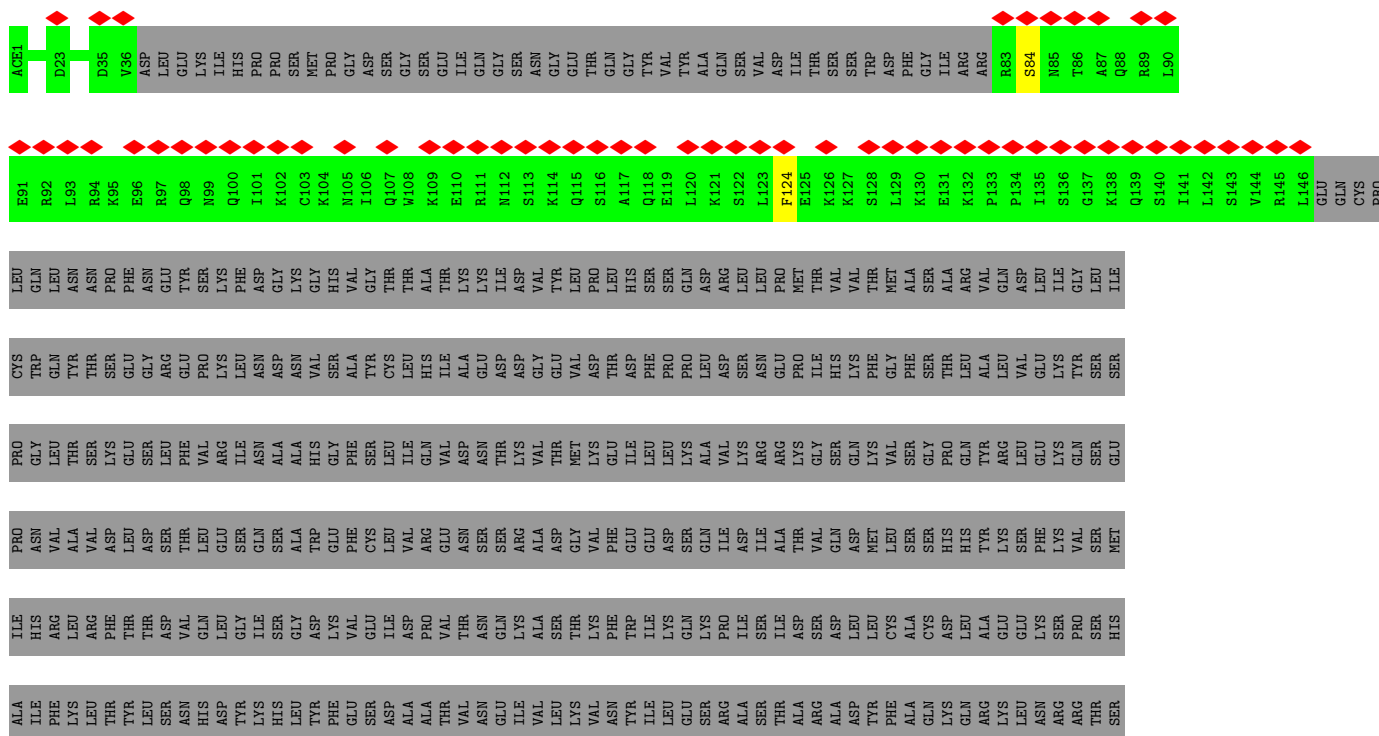
- Molecule 3: Rapamycin-insensitive companion of mTOR

Chain E: 63% 35%



- Molecule 3: Rapamycin-insensitive companion of mTOR





PHE
SER
PHE
GLN
LYS
GLU
LYS
LYS
SER
GLY
GLN
GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191304	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	488.96, 488.96, 488.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.955, 0.955, 0.955	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	0.37	0/14434	0.50	0/19544
1	B	0.29	0/14448	0.47	0/19562
2	C	0.20	0/2501	0.49	0/3408
2	D	0.16	0/2501	0.45	0/3408
3	E	0.38	0/9154	0.48	0/12384
3	F	0.22	0/9154	0.45	0/12384
4	G	0.25	0/814	0.51	0/1087
4	H	0.16	0/814	0.46	0/1087
All	All	0.31	0/53820	0.48	0/72864

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1132	ARG	Sidechain
1	B	1132	ARG	Sidechain

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	14131	0	14293	18	0
1	B	14145	0	14307	46	0
2	C	2443	0	2327	7	0
2	D	2443	0	2327	23	0
3	E	8990	0	9188	10	0
3	F	8990	0	9187	31	0
4	G	808	0	841	1	0
4	H	808	0	841	2	0
5	A	36	0	6	0	0
5	B	36	0	6	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	52832	0	53323	134	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 1.

All (134) 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)
2:D:50:VAL:HG21	2:D:321:ASN:HB2	1.80	0.64
1:B:1125:PRO:HA	1:B:1132:ARG:NH2	2.18	0.58
1:B:1400:LYS:HE2	1:B:1415:SER:HB3	1.85	0.58
2:C:122:GLN:HE21	4:G:108:TRP:CD1	2.21	0.58
1:A:2419:GLU:HG2	1:A:2501:ILE:HD13	1.86	0.58
2:C:40:HIS:CE1	2:C:66:ARG:HH21	2.21	0.57
1:A:1125:PRO:HA	1:A:1132:ARG:NH2	2.20	0.57
1:B:1119:VAL:HA	1:B:1122:PHE:CE2	2.40	0.56
1:A:872:LEU:HB3	1:A:1576:THR:HG22	1.87	0.56
2:D:69:ASP:HB2	2:D:78:ILE:HD13	1.87	0.55
3:E:86:ILE:HG13	3:E:1529:LEU:HD11	1.88	0.55
3:F:580:PHE:HA	3:F:587:LEU:HD12	1.90	0.54
1:A:1119:VAL:HA	1:A:1122:PHE:CE2	2.43	0.54
3:F:691:LEU:HB3	3:F:694:GLN:OE1	2.09	0.53
1:B:1072:PRO:HD3	1:B:1110:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:504:THR:HG21	3:F:745:GLU:HB2	1.91	0.52
1:B:965:SER:HA	1:B:968:HIS:CD2	2.46	0.51
1:B:965:SER:HA	1:B:968:HIS:CG	2.46	0.51
3:E:24:GLU:HG2	3:E:54:MET:HG2	1.93	0.51
2:D:150:GLY:HA2	2:D:173:ILE:HG13	1.92	0.51
3:F:1484:ARG:HD3	3:F:1618:ARG:NE	2.26	0.50
1:B:1274:ARG:HD3	1:B:1279:ASP:C	2.37	0.50
3:F:432:HIS:HE1	3:F:1000:LEU:HD21	1.74	0.50
1:A:761:VAL:HG22	1:A:768:ILE:HG21	1.93	0.50
3:E:1537:LEU:HB2	3:E:1605:THR:HG23	1.94	0.50
2:D:8:VAL:HG13	2:D:71:ASN:HA	1.94	0.50
3:F:117:LEU:HD23	3:F:160:LEU:HD12	1.94	0.49
1:A:1609:PRO:HA	1:A:1612:ARG:HG3	1.95	0.49
2:D:58:ALA:HA	2:D:67:MET:HG2	1.94	0.49
1:B:1786:TRP:CZ2	1:B:1788:LYS:HD2	2.48	0.48
2:D:142:GLU:HG3	2:D:156:ASP:HA	1.94	0.48
1:B:1283:TRP:CH2	1:B:1287:LEU:HD22	2.48	0.48
1:B:1521:TRP:HB2	1:B:1529:MET:SD	2.53	0.48
3:F:172:VAL:HA	3:F:1667:LEU:HD22	1.96	0.48
1:A:772:MET:HE2	1:A:809:SER:HB3	1.95	0.48
1:A:664:ILE:HD11	1:A:695:ALA:HB1	1.96	0.47
3:F:652:LEU:HD11	3:F:696:HIS:CD2	2.49	0.47
1:A:2340:HIS:CE1	1:A:2342:SER:HB2	2.49	0.47
2:C:144:ILE:HD12	2:C:178:ILE:HD11	1.97	0.47
1:B:1755:GLY:HA3	1:B:1776:TYR:CE1	2.50	0.47
1:B:2339:ARG:HH22	1:B:2357:ASP:HB3	1.80	0.47
3:F:396:LEU:HD13	3:F:430:LEU:HD22	1.97	0.47
1:B:1748:ALA:HB2	1:B:1782:HIS:HB2	1.97	0.47
1:B:1462:ALA:O	1:B:1466:LYS:HD3	2.14	0.46
3:F:593:LEU:HA	3:F:655:LEU:HD23	1.97	0.46
1:A:1724:MET:HE1	1:A:1743:LEU:HD22	1.97	0.46
1:A:709:GLU:OE2	1:A:755:ARG:HD3	2.15	0.46
3:F:698:LEU:HD12	3:F:728:CYS:SG	2.56	0.46
3:F:1522:TYR:CE1	3:F:1531:PHE:HD2	2.33	0.46
2:D:284:TYR:HE2	2:D:305:LYS:HE3	1.80	0.46
1:B:1113:LEU:O	1:B:1116:PRO:HD2	2.15	0.46
3:F:893:CYS:SG	3:F:938:TRP:HB3	2.56	0.46
3:F:930:LEU:HD23	3:F:933:ILE:HD12	1.99	0.45
2:D:167:PRO:HB2	2:D:195:TYR:CZ	2.51	0.45
3:F:1612:LEU:HD13	3:F:1646:THR:OG1	2.16	0.45
1:B:1206:HIS:HE1	1:B:1208:ARG:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2419:GLU:HG2	1:B:2501:ILE:HD13	1.99	0.45
2:D:156:ASP:HB2	2:D:207:VAL:HG12	1.97	0.45
1:A:1274:ARG:HD3	1:A:1279:ASP:HB3	1.98	0.45
1:A:2154:GLN:HG3	1:A:2177:SER:HA	1.99	0.45
1:B:2340:HIS:HA	1:B:2545:TRP:CD1	2.52	0.45
3:F:43:GLN:HG2	3:F:1693:LEU:HD13	1.99	0.45
1:B:856:GLU:N	1:B:857:PRO:HD2	2.30	0.45
1:B:1744:HIS:O	1:B:1782:HIS:HB3	2.17	0.45
1:B:872:LEU:HB3	1:B:1576:THR:HG22	2.00	0.44
1:B:1805:LYS:HD3	1:B:1913:TYR:OH	2.17	0.44
3:F:1537:LEU:HD13	3:F:1609:ARG:NH1	2.31	0.44
3:F:1687:GLU:O	3:F:1690:GLU:HB2	2.17	0.44
1:B:986:CYS:SG	1:B:1023:VAL:HG12	2.57	0.44
1:B:1206:HIS:CE1	1:B:1208:ARG:HB3	2.52	0.44
3:E:856:LYS:HG3	3:E:858:VAL:HG13	2.00	0.44
3:F:931:GLY:HA3	3:F:971:VAL:HG13	1.99	0.44
2:D:297:TRP:HA	2:D:303:GLU:O	2.18	0.44
1:B:1167:PRO:HA	1:B:1170:ARG:HG3	1.99	0.44
1:B:1684:GLN:HB3	1:B:1687:HIS:HD2	1.83	0.44
3:F:1539:ALA:H	3:F:1606:PRO:HG3	1.83	0.44
1:B:1910:TRP:C	1:B:1910:TRP:CD1	2.95	0.44
2:D:92:GLY:O	2:D:100:MET:HG3	2.17	0.44
3:E:920:ILE:HG23	3:E:964:ILE:HD11	1.99	0.44
1:A:2511:ARG:HG2	1:A:2515:HIS:HA	2.00	0.43
1:B:1266:GLN:HG2	1:B:1269:TRP:CZ3	2.53	0.43
2:C:25:ARG:HD2	2:C:37:THR:HG22	2.00	0.43
1:A:821:PHE:CZ	1:A:844:LEU:HD11	2.54	0.43
1:B:825:MET:HE1	1:B:864:LEU:HD13	2.00	0.43
3:E:698:LEU:HD12	3:E:728:CYS:SG	2.58	0.43
1:B:1266:GLN:HG2	1:B:1269:TRP:CE3	2.54	0.43
1:B:1740:LYS:HE2	1:B:1744:HIS:NE2	2.33	0.43
2:D:272:TRP:O	2:D:289:SER:HA	2.18	0.43
1:B:1355:GLN:NE2	1:B:1390:CYS:HB3	2.33	0.43
2:D:18:ALA:HB1	2:D:45:VAL:HG21	2.00	0.43
3:F:633:TRP:HE1	3:F:651:LEU:HD21	1.84	0.43
1:A:773:GLU:HB3	1:A:774:PRO:HD3	2.01	0.42
2:C:86:LYS:HB3	2:C:105:GLU:HB2	2.01	0.42
3:F:950:PRO:HA	3:F:953:LEU:HD12	2.01	0.42
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	2.01	0.42
3:F:362:TRP:CD1	3:F:362:TRP:N	2.87	0.42
1:B:605:HIS:CE1	1:B:609:HIS:CD2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:TRP:CD1	2:D:162:ASN:HD21	2.38	0.42
1:B:1280:TRP:NE1	1:B:1348:GLN:HB3	2.34	0.42
2:D:179:ASP:OD2	2:D:181:ASP:HB3	2.20	0.42
1:B:2300:ALA:HB2	1:B:2386:ALA:HA	2.02	0.42
2:D:285:ILE:HB	2:D:299:VAL:HG12	2.02	0.42
1:B:1450:TYR:HB2	1:B:1459:ALA:HB2	2.00	0.42
1:B:2415:MET:HE1	1:B:2501:ILE:HG23	2.02	0.42
3:F:1675:GLU:CD	4:H:84:SER:HB2	2.45	0.41
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.56	0.41
2:D:22:HIS:CG	2:D:41:GLN:HA	2.55	0.41
2:D:95:GLU:HB2	2:D:140:GLN:OE1	2.20	0.41
3:F:558:PRO:C	3:F:559:ASN:HD22	2.27	0.41
1:B:1005:ASP:HA	1:B:1009:ARG:NH2	2.35	0.41
2:C:295:ARG:HB2	2:C:297:TRP:HE1	1.85	0.41
3:F:41:ILE:HD13	3:F:63:PHE:HA	2.02	0.41
3:F:46:ALA:HA	3:F:90:LEU:HD12	2.01	0.41
1:B:854:VAL:HG11	1:B:1618:ILE:HG23	2.02	0.41
3:F:631:VAL:CG2	3:F:681:VAL:HG22	2.49	0.41
2:D:198:ASN:HB3	2:D:211:ILE:HG23	2.02	0.41
1:B:1776:TYR:O	1:B:1780:THR:HG23	2.20	0.41
2:D:276:CYS:SG	2:D:285:ILE:HD11	2.61	0.41
1:A:1069:LEU:HD23	3:E:467:LEU:HD12	2.02	0.41
1:B:1705:TRP:CE2	1:B:1710:LYS:HE2	2.56	0.41
1:B:2022:LEU:HD12	1:B:2024:HIS:HE1	1.86	0.41
3:E:368:PHE:CG	3:E:369:VAL:N	2.87	0.41
3:F:662:PHE:N	3:F:662:PHE:CD1	2.88	0.41
1:B:1039:ARG:HD3	1:B:1077:HIS:NE2	2.35	0.41
1:B:1071:LEU:HD23	1:B:1110:TYR:CD2	2.56	0.41
3:E:563:ARG:O	3:E:566:LYS:HE3	2.21	0.41
3:F:111:ILE:HG21	3:F:117:LEU:HD13	2.03	0.41
2:D:157:LEU:CB	4:H:124:PHE:HB3	2.52	0.40
2:D:168:GLU:HA	2:D:169:PRO:HD3	1.98	0.40
1:B:1072:PRO:HD3	1:B:1110:TYR:OH	2.21	0.40
2:C:274:TRP:CD1	2:C:290:SER:HB3	2.56	0.40
3:F:550:LEU:HD23	3:F:550:LEU:HA	1.81	0.40
2:D:283:GLN:O	2:D:299:VAL:HG22	2.21	0.40
3:E:1484:ARG:HG3	3:E:1487:MET:O	2.21	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	1729/2590 (67%)	1698 (98%)	31 (2%)	0	100	100
1	B	1731/2590 (67%)	1702 (98%)	29 (2%)	0	100	100
2	C	313/326 (96%)	301 (96%)	12 (4%)	0	100	100
2	D	313/326 (96%)	304 (97%)	9 (3%)	0	100	100
3	E	1103/1734 (64%)	1072 (97%)	31 (3%)	0	100	100
3	F	1103/1734 (64%)	1076 (98%)	27 (2%)	0	100	100
4	G	96/522 (18%)	87 (91%)	9 (9%)	0	100	100
4	H	96/522 (18%)	88 (92%)	8 (8%)	0	100	100
All	All	6484/10344 (63%)	6328 (98%)	156 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1547/2248 (69%)	1547 (100%)	0	100	100
1	B	1549/2248 (69%)	1549 (100%)	0	100	100
2	C	267/276 (97%)	267 (100%)	0	100	100
2	D	267/276 (97%)	267 (100%)	0	100	100
3	E	1005/1562 (64%)	1005 (100%)	0	100	100
3	F	1005/1562 (64%)	1005 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	93/470 (20%)	93 (100%)	0	100	100
4	H	93/470 (20%)	93 (100%)	0	100	100
All	All	5826/9112 (64%)	5826 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	HIS
1	A	736	GLN
1	A	743	HIS
1	A	759	HIS
1	A	967	HIS
1	A	1026	HIS
1	A	1106	ASN
1	A	1207	GLN
1	A	1308	GLN
1	A	1398	HIS
1	A	1420	ASN
1	A	1594	HIS
1	A	1647	HIS
1	A	1693	HIS
1	A	1758	GLN
1	A	1760	ASN
1	A	1992	ASN
1	A	2180	HIS
1	A	2233	ASN
1	A	2247	HIS
1	A	2282	GLN
1	A	2340	HIS
1	A	2401	HIS
1	A	2540	GLN
1	B	605	HIS
1	B	609	HIS
1	B	686	HIS
1	B	694	GLN
1	B	701	ASN
1	B	743	HIS
1	B	759	HIS
1	B	899	HIS

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Mol	Chain	Res	Type
1	B	967	HIS
1	B	1420	ASN
1	B	1509	GLN
1	B	1687	HIS
1	B	1693	HIS
1	B	1937	GLN
1	B	1992	ASN
1	B	2024	HIS
1	B	2154	GLN
1	B	2180	HIS
1	B	2289	HIS
1	B	2395	ASN
2	C	39	GLN
2	C	64	HIS
2	D	39	GLN
2	D	73	ASN
2	D	128	ASN
2	D	161	HIS
2	D	164	GLN
2	D	193	ASN
3	E	44	ASN
3	E	242	GLN
3	E	402	ASN
3	E	435	ASN
3	E	440	HIS
3	E	444	HIS
3	E	559	ASN
3	E	561	ASN
3	E	836	ASN
3	E	872	GLN
3	E	937	ASN
3	E	1446	GLN
3	E	1494	ASN
3	E	1519	ASN
3	F	432	HIS
3	F	435	ASN
3	F	440	HIS
3	F	454	ASN
3	F	480	HIS
3	F	505	HIS
3	F	543	ASN
3	F	559	ASN

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Mol	Chain	Res	Type
3	F	658	HIS
3	F	827	GLN
3	F	846	GLN
3	F	888	HIS
3	F	932	ASN
3	F	999	HIS
3	F	1438	GLN
4	G	13	HIS
4	G	16	GLN
4	G	18	HIS
4	H	13	HIS
4	H	118	GLN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
5	IHP	A	2601	-	36,36,36	1.85	6 (16%)	54,60,60	0.98	2 (3%)
5	IHP	B	2601	-	36,36,36	1.89	6 (16%)	54,60,60	0.80	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
5	IHP	A	2601	-	-	4/30/54/54	0/1/1/1
5	IHP	B	2601	-	-	6/30/54/54	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2601	IHP	P2-O12	4.76	1.68	1.59
5	A	2601	IHP	P2-O12	4.70	1.68	1.59
5	B	2601	IHP	P6-O16	4.44	1.67	1.59
5	B	2601	IHP	P5-O15	4.32	1.67	1.59
5	A	2601	IHP	P5-O15	4.30	1.67	1.59
5	A	2601	IHP	P6-O16	4.19	1.67	1.59
5	B	2601	IHP	P4-O14	4.16	1.67	1.59
5	B	2601	IHP	P1-O11	4.08	1.67	1.59
5	A	2601	IHP	P3-O13	4.00	1.66	1.59
5	A	2601	IHP	P4-O14	3.94	1.66	1.59
5	B	2601	IHP	P3-O13	3.78	1.66	1.59
5	A	2601	IHP	P1-O11	3.72	1.66	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2601	IHP	C5-C4-C3	-2.95	103.95	110.41
5	A	2601	IHP	C6-C1-C2	2.89	116.74	110.41

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C6-O16-P6-O26
5	B	2601	IHP	C2-C1-O11-P1
5	B	2601	IHP	C6-C1-O11-P1
5	B	2601	IHP	C1-O11-P1-O21
5	B	2601	IHP	C6-O16-P6-O46
5	A	2601	IHP	C1-O11-P1-O21
5	B	2601	IHP	C2-O12-P2-O22
5	B	2601	IHP	C6-O16-P6-O26

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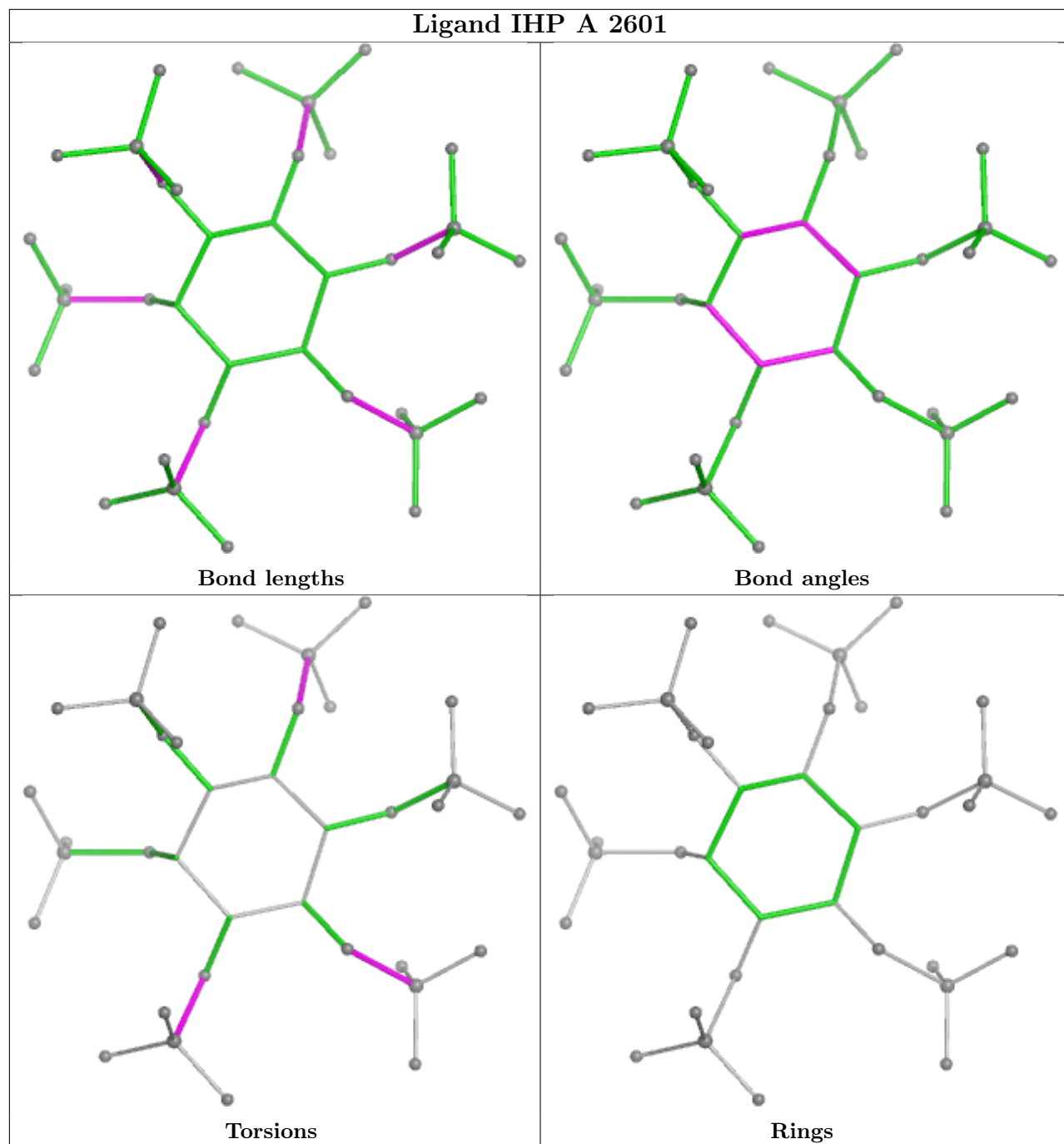
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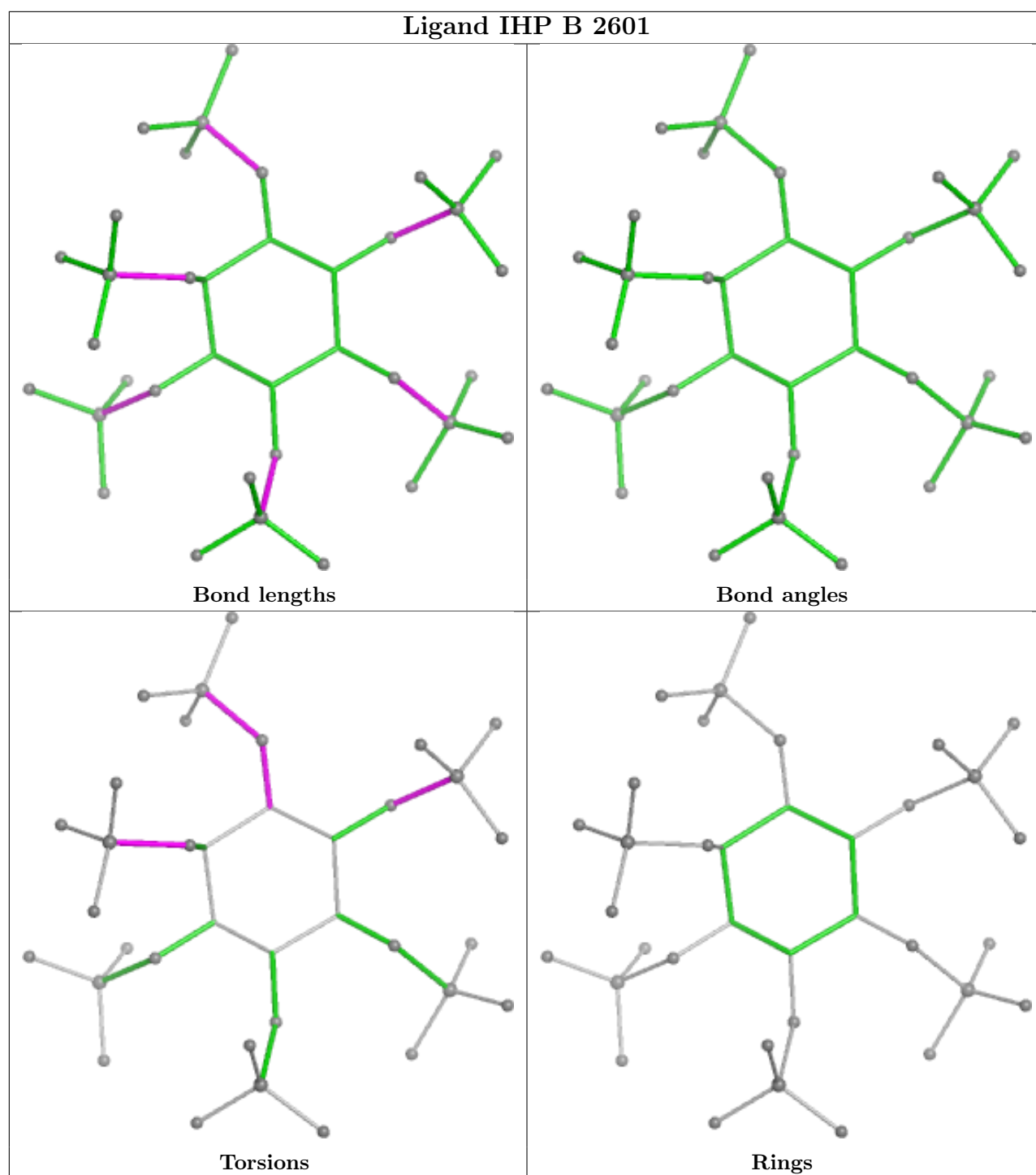
Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C4-O14-P4-O44
5	A	2601	IHP	C6-O16-P6-O46

There are no ring outliers.

No monomer is involved in short contacts.

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.

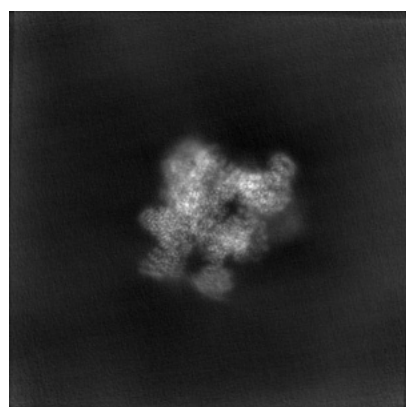
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55803. These allow visual inspection of the internal detail of the map and identification of artifacts.

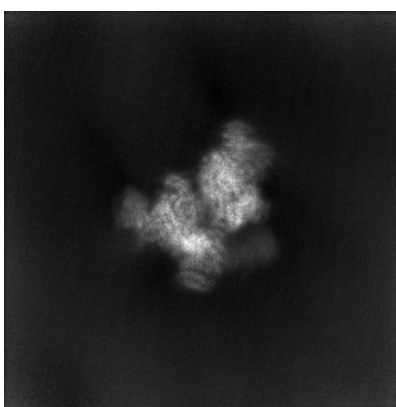
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

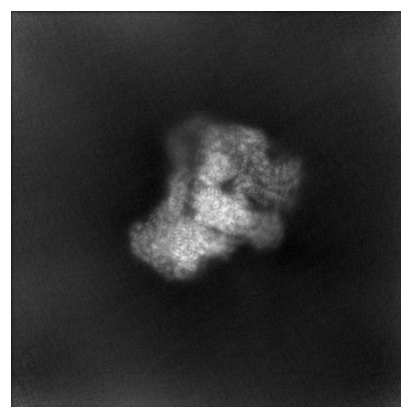
6.1.1 Primary map



X



Y

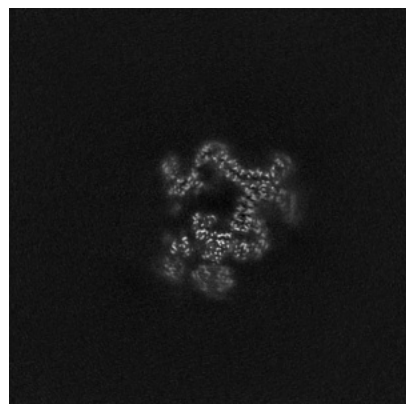


Z

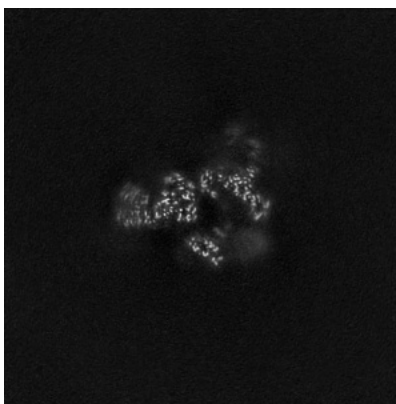
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

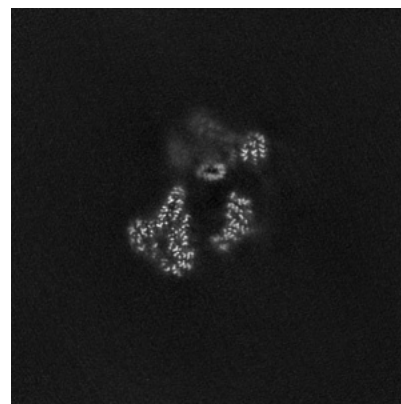
6.2.1 Primary map



X Index: 256



Y Index: 256

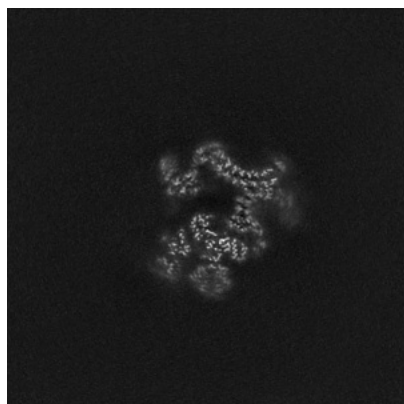


Z Index: 256

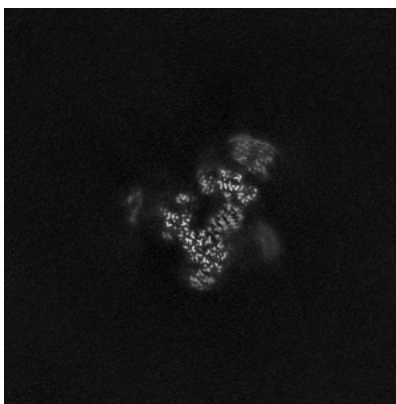
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

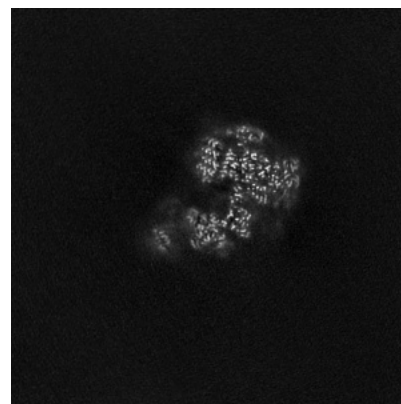
6.3.1 Primary map



X Index: 253



Y Index: 233

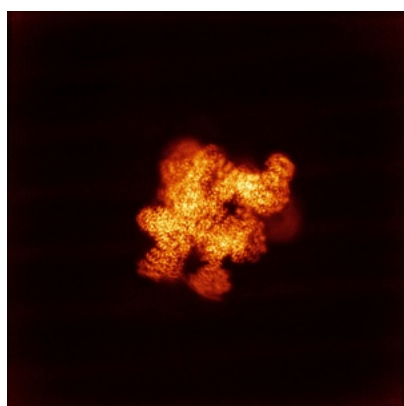


Z Index: 287

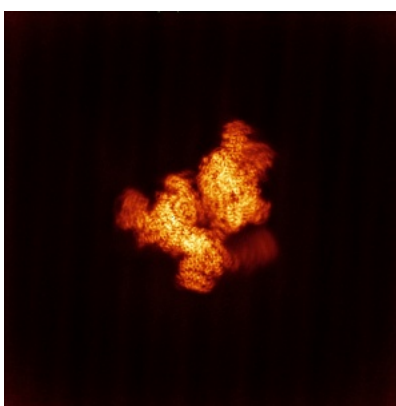
The images above show the largest variance slices of the map in three orthogonal directions.

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

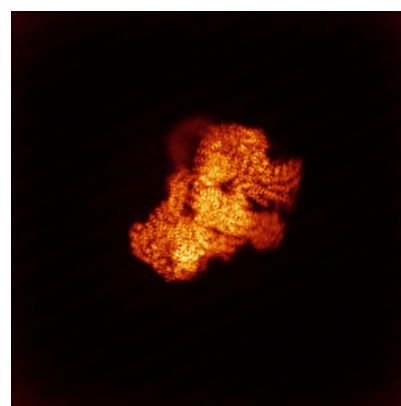
6.4.1 Primary map



X



Y

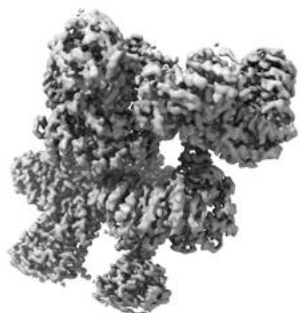


Z

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](#)

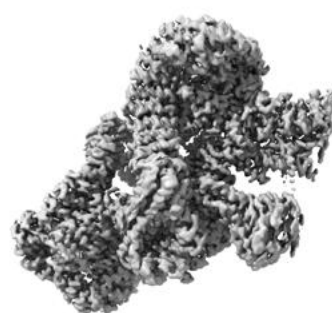
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

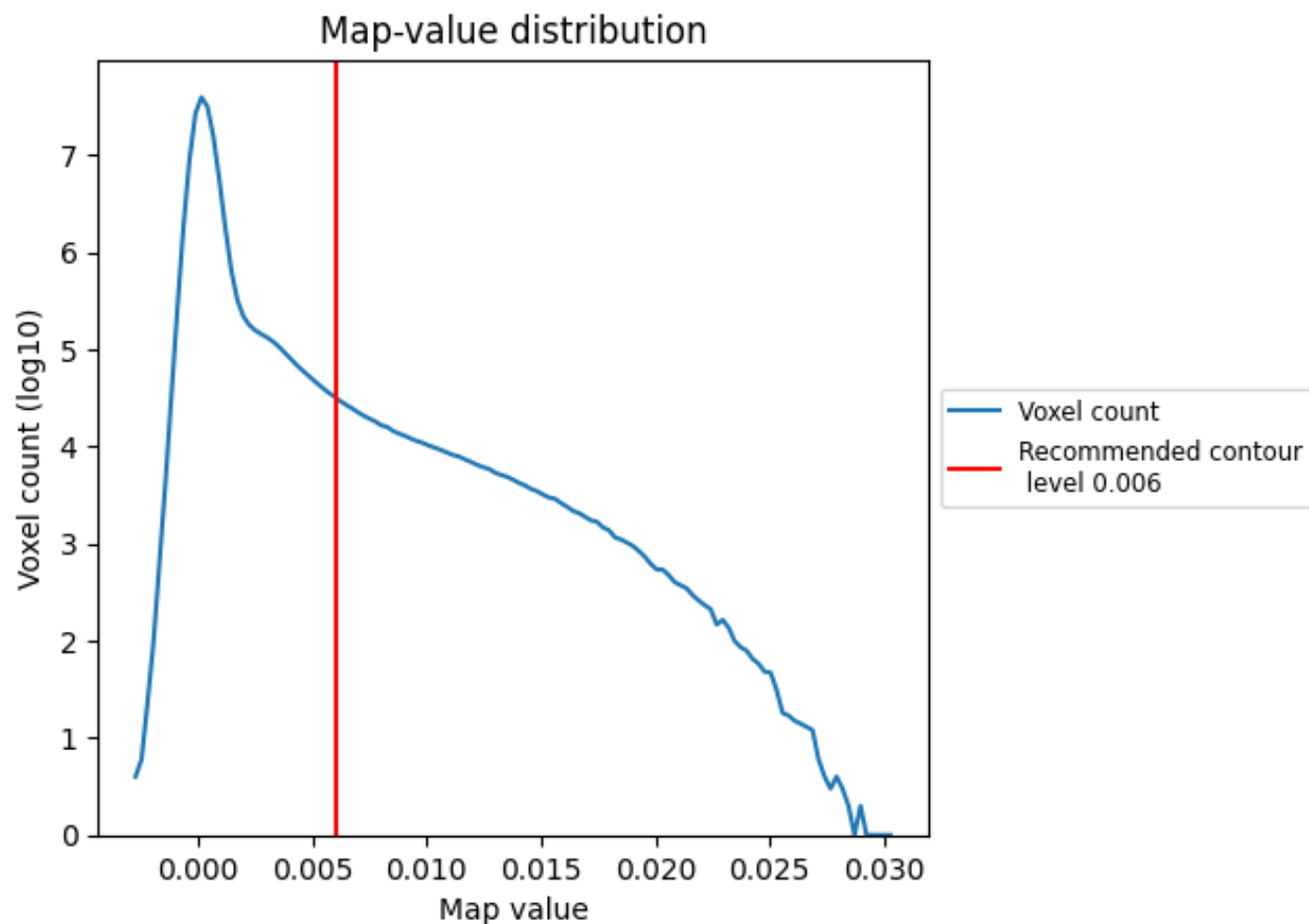
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

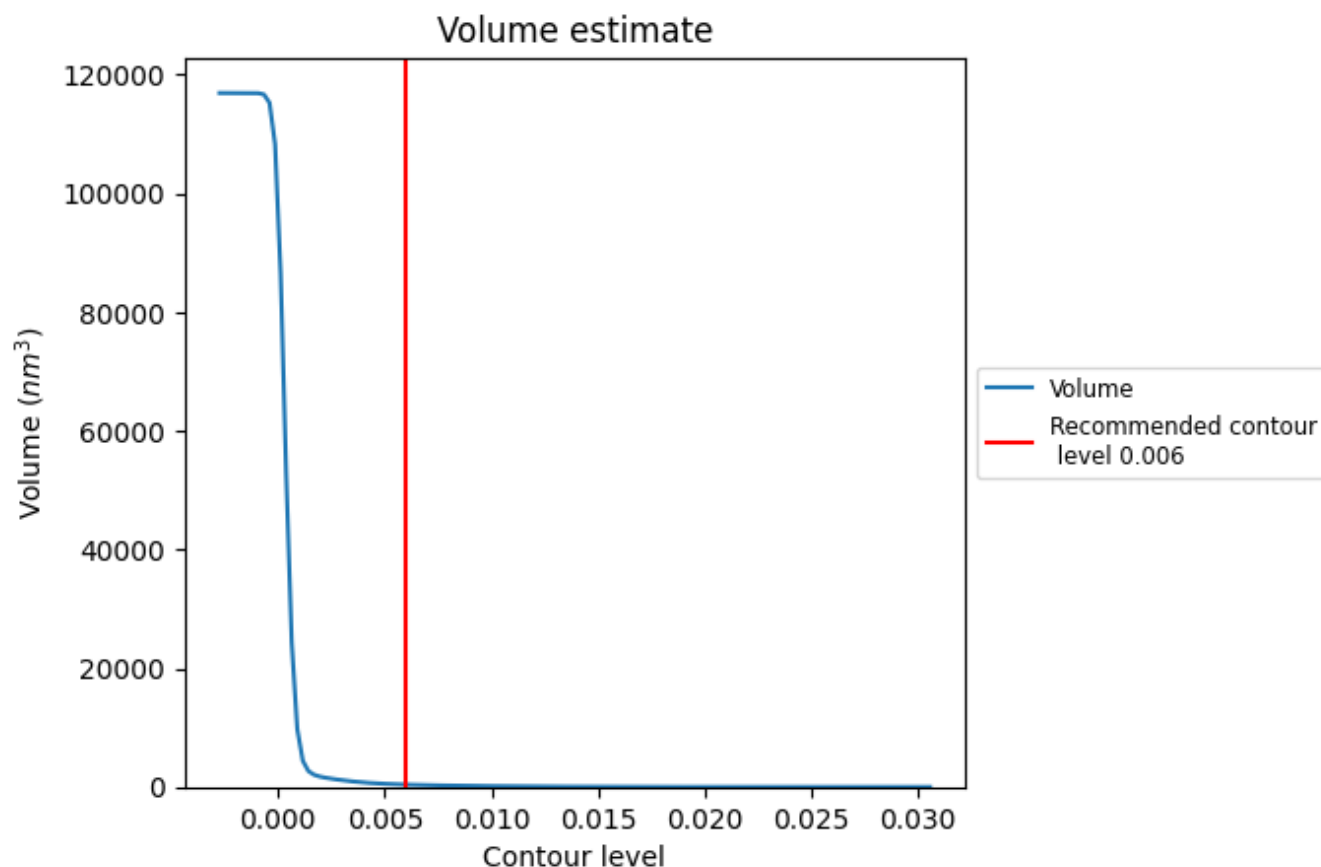
This section contains the results of statistical analysis of the map.

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.

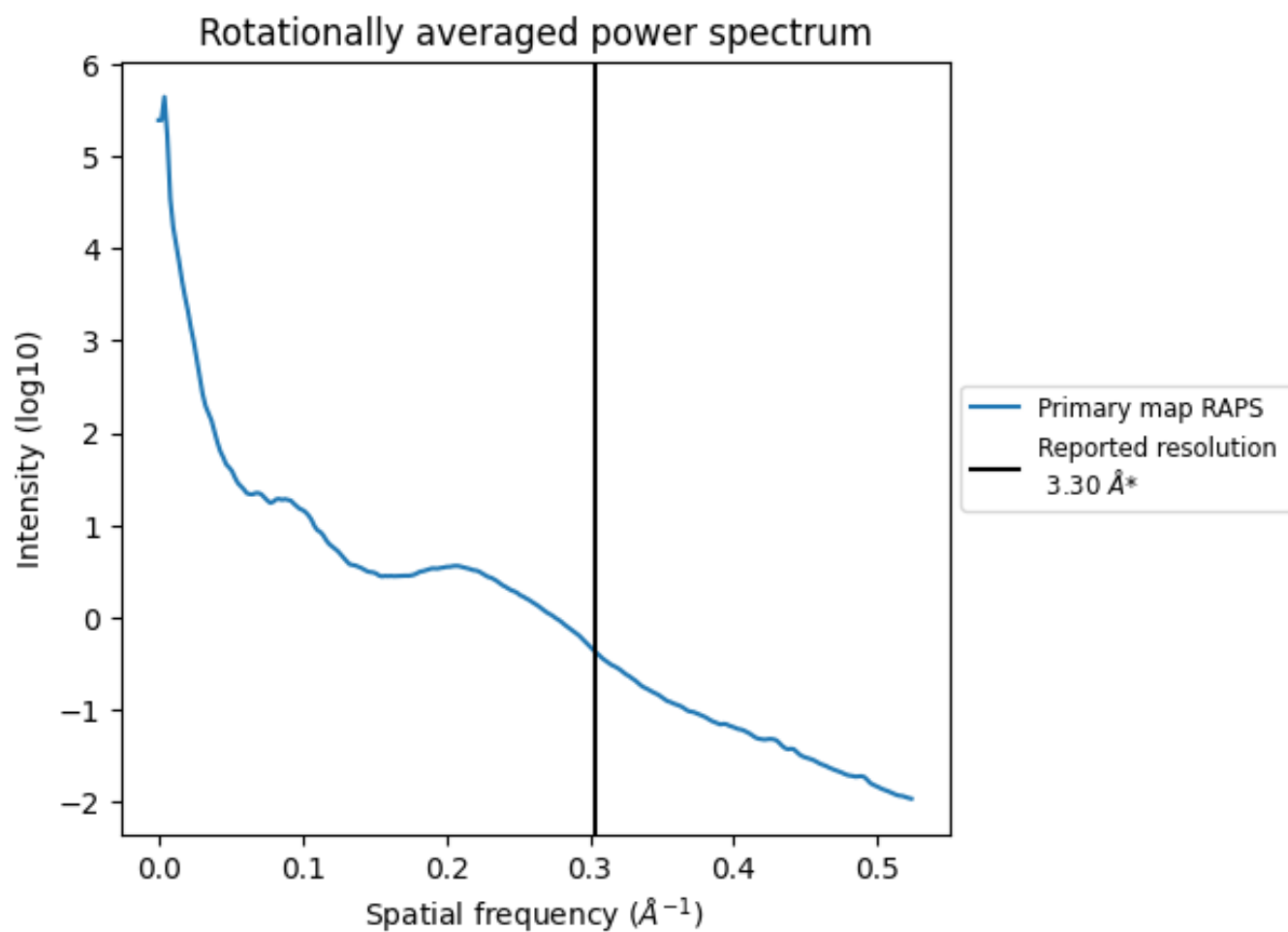
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 394 nm³; this corresponds to an approximate mass of 356 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 0.303 Å⁻¹

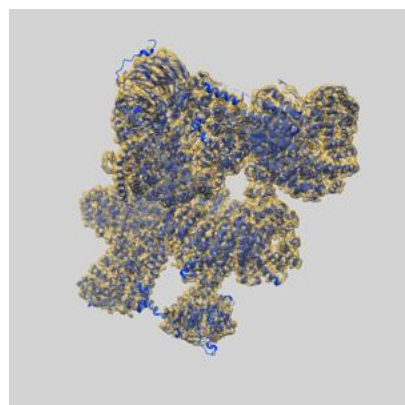
8 Fourier-Shell correlation

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

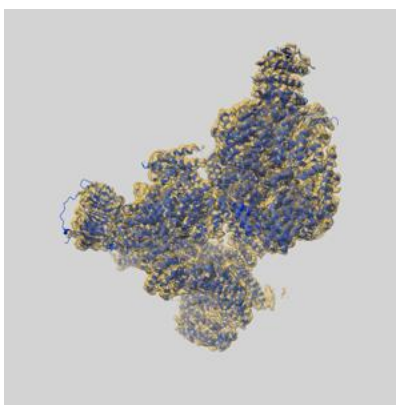
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55803 and PDB model 9TDS. Per-residue inclusion information can be found in section 3 on page 10.

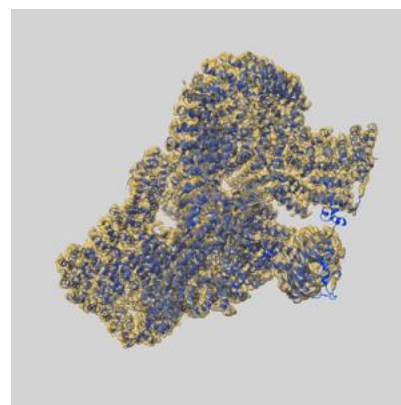
9.1 Map-model overlay [i](#)



X



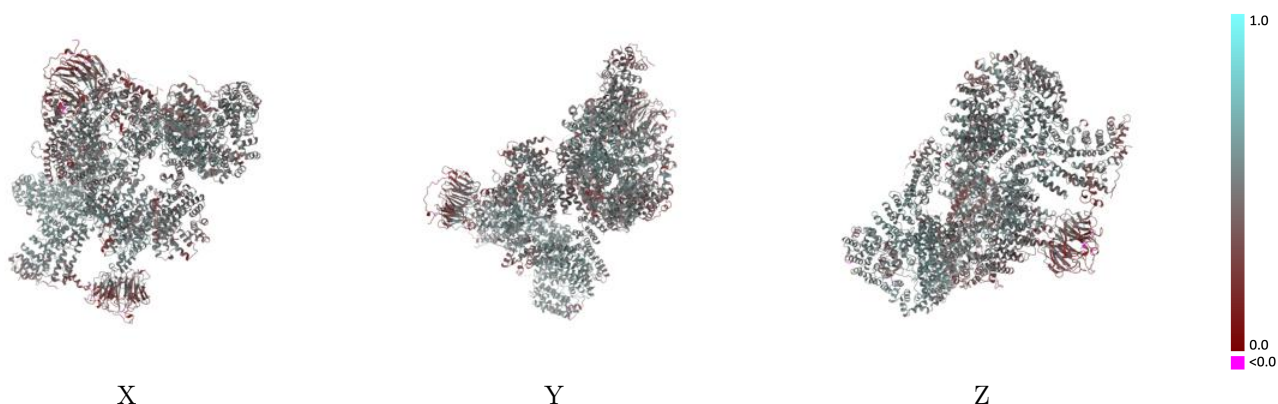
Y



Z

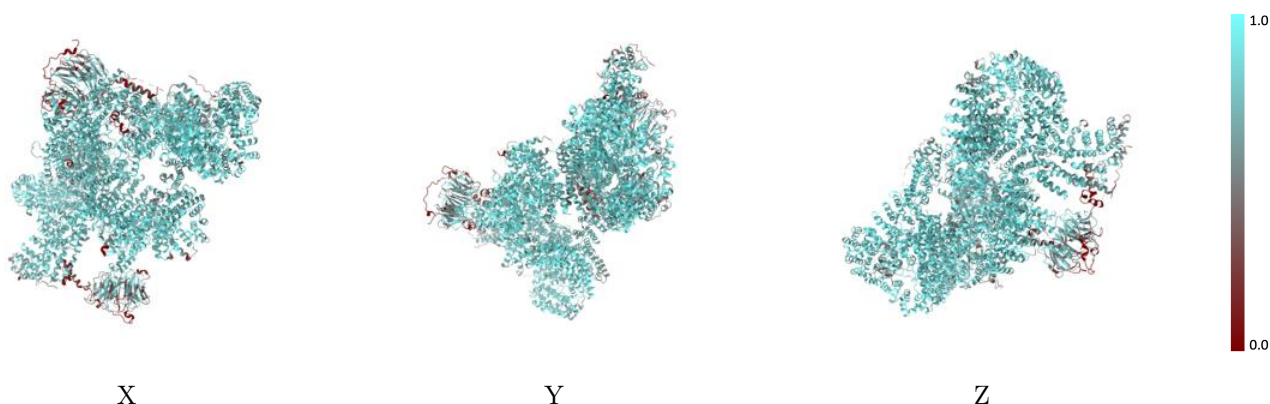
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



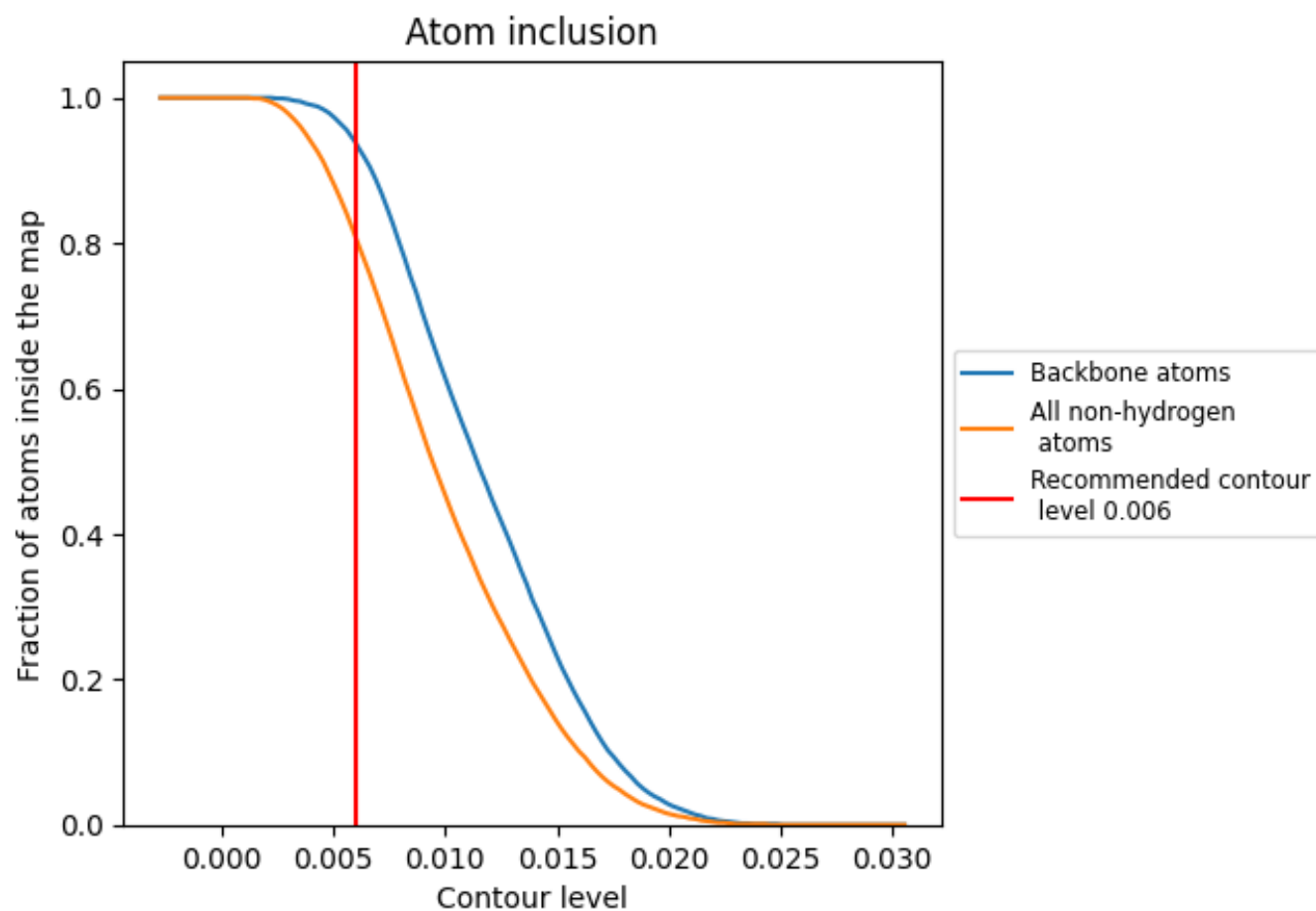
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8080	<div></div> 0.4750
A	<div></div> 0.8560	<div></div> 0.5000
B	<div></div> 0.8430	<div></div> 0.4730
C	<div></div> 0.6190	<div></div> 0.3650
D	<div></div> 0.5890	<div></div> 0.3400
E	<div></div> 0.8570	<div></div> 0.5270
F	<div></div> 0.8110	<div></div> 0.4780
G	<div></div> 0.4490	<div></div> 0.3790
H	<div></div> 0.4000	<div></div> 0.3270

