



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 08:16 AM EST

PDB ID : 6BCU
EMDB ID : EMD-7086
Title : Cryo-EM structure of the activated RHEB-mTORC1 refined to 3.4 angstrom
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2017-10-20
Resolution : 3.43 Å(reported)

This is a wwPDB EM Validation Summary 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

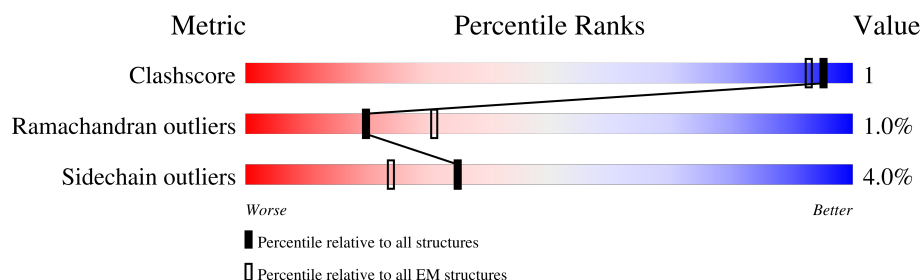
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	2549	<div> <div>21%</div> <div>80%</div> <div>6%</div> <div>14%</div> </div>
1	B	2549	<div> <div>21%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>
2	D	326	<div> <div>71%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
2	E	326	<div> <div>73%</div> <div>90%</div> <div>7%</div> <div>•</div> </div>
3	W	1343	<div> <div>43%</div> <div>72%</div> <div>6%</div> <div>22%</div> </div>
3	Y	1343	<div> <div>43%</div> <div>72%</div> <div>6%</div> <div>22%</div> </div>
4	X	122	<div> <div>6%</div> <div>•</div> <div>93%</div> </div>
4	Z	122	<div> <div>6%</div> <div>•</div> <div>93%</div> </div>

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Mol	Chain	Length	Quality of chain
5	R	188	<div><div>66%</div><div><div></div><div></div><div></div></div><div>84%</div><div>•</div><div>12%</div></div>
5	S	188	<div><div>66%</div><div><div></div><div></div><div></div></div><div>84%</div><div>•</div><div>12%</div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 119740 atoms, of which 60078 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,Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2204	Total	C	H	N	O	S	0	0
			35397	11194	17859	3074	3157	113		
1	B	2204	Total	C	H	N	O	S	0	0
			35397	11194	17859	3074	3157	113		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		
2	E	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		

- Molecule 3 is a protein called Regulatory-associated protein of mTOR,Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	W	1052	Total	C	H	N	O	S	0	0
			16791	5361	8406	1450	1518	56		
3	Y	1052	Total	C	H	N	O	S	0	0
			16791	5361	8406	1450	1518	56		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-7	MET	-	initiating methionine	UNP Q8N122
W	-6	ASP	-	expression tag	UNP Q8N122
W	-5	TYR	-	expression tag	UNP Q8N122
W	-4	LYS	-	expression tag	UNP Q8N122
W	-3	ASP	-	expression tag	UNP Q8N122
W	-2	ASP	-	expression tag	UNP Q8N122
W	-1	ASP	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
W	0	ASP	-	expression tag	UNP Q8N122
W	1	LYS	-	expression tag	UNP Q8N122
Y	-7	MET	-	initiating methionine	UNP Q8N122
Y	-6	ASP	-	expression tag	UNP Q8N122
Y	-5	TYR	-	expression tag	UNP Q8N122
Y	-4	LYS	-	expression tag	UNP Q8N122
Y	-3	ASP	-	expression tag	UNP Q8N122
Y	-2	ASP	-	expression tag	UNP Q8N122
Y	-1	ASP	-	expression tag	UNP Q8N122
Y	0	ASP	-	expression tag	UNP Q8N122
Y	1	LYS	-	expression tag	UNP Q8N122

- Molecule 4 is a protein called Eukaryotic translation initiation factor 4E-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	X	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		
4	Z	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-3	GLY	-	expression tag	UNP Q13541
X	-2	SER	-	expression tag	UNP Q13541
X	-1	GLY	-	expression tag	UNP Q13541
X	0	ARG	-	expression tag	UNP Q13541
Z	-3	GLY	-	expression tag	UNP Q13541
Z	-2	SER	-	expression tag	UNP Q13541
Z	-1	GLY	-	expression tag	UNP Q13541
Z	0	ARG	-	expression tag	UNP Q13541

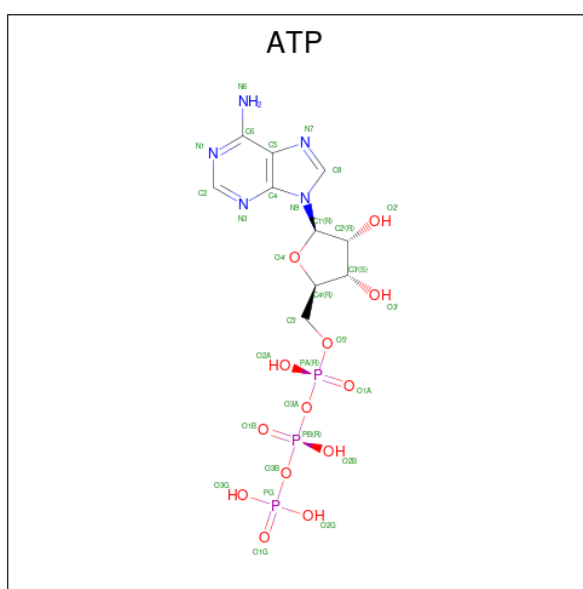
- Molecule 5 is a protein called GTP-binding protein Rheb.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	S	166	Total	C	H	N	O	S	0	0
			2657	846	1339	215	254	3		
5	R	166	Total	C	H	N	O	S	0	0
			2657	846	1339	215	254	3		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-3	GLY	-	expression tag	UNP Q15382
S	-2	SER	-	expression tag	UNP Q15382
S	-1	GLY	-	expression tag	UNP Q15382
S	0	ARG	-	expression tag	UNP Q15382
R	-3	GLY	-	expression tag	UNP Q15382
R	-2	SER	-	expression tag	UNP Q15382
R	-1	GLY	-	expression tag	UNP Q15382
R	0	ARG	-	expression tag	UNP Q15382

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

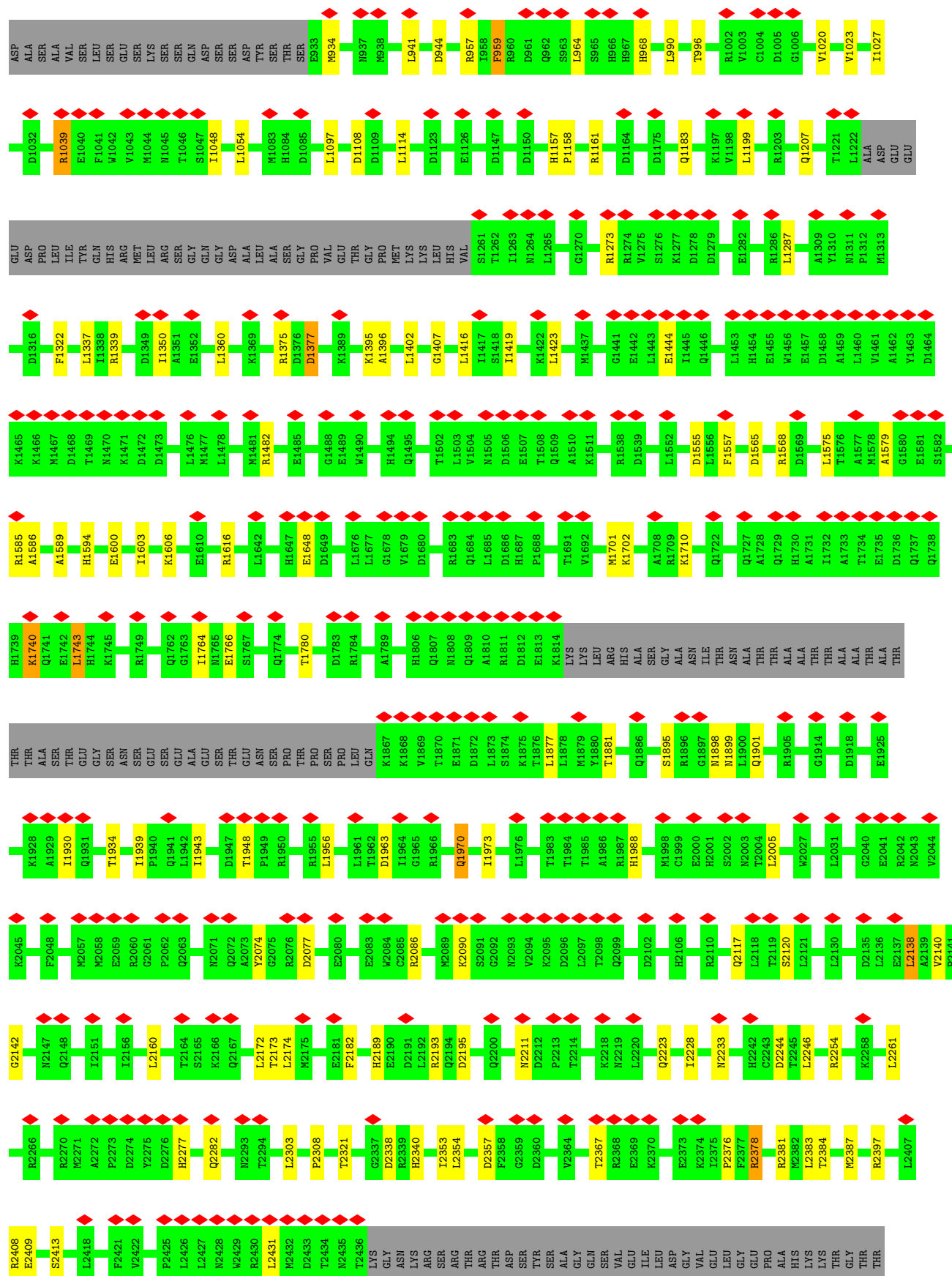
Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Mg	0
			2	2	
7	S	1	Total	Mg	0
			1	1	
7	B	2	Total	Mg	0
			2	2	

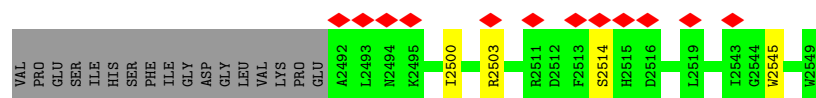
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Mol	Chain	Residues	Atoms	AltConf
7	R	1	Total Mg 1 1	0

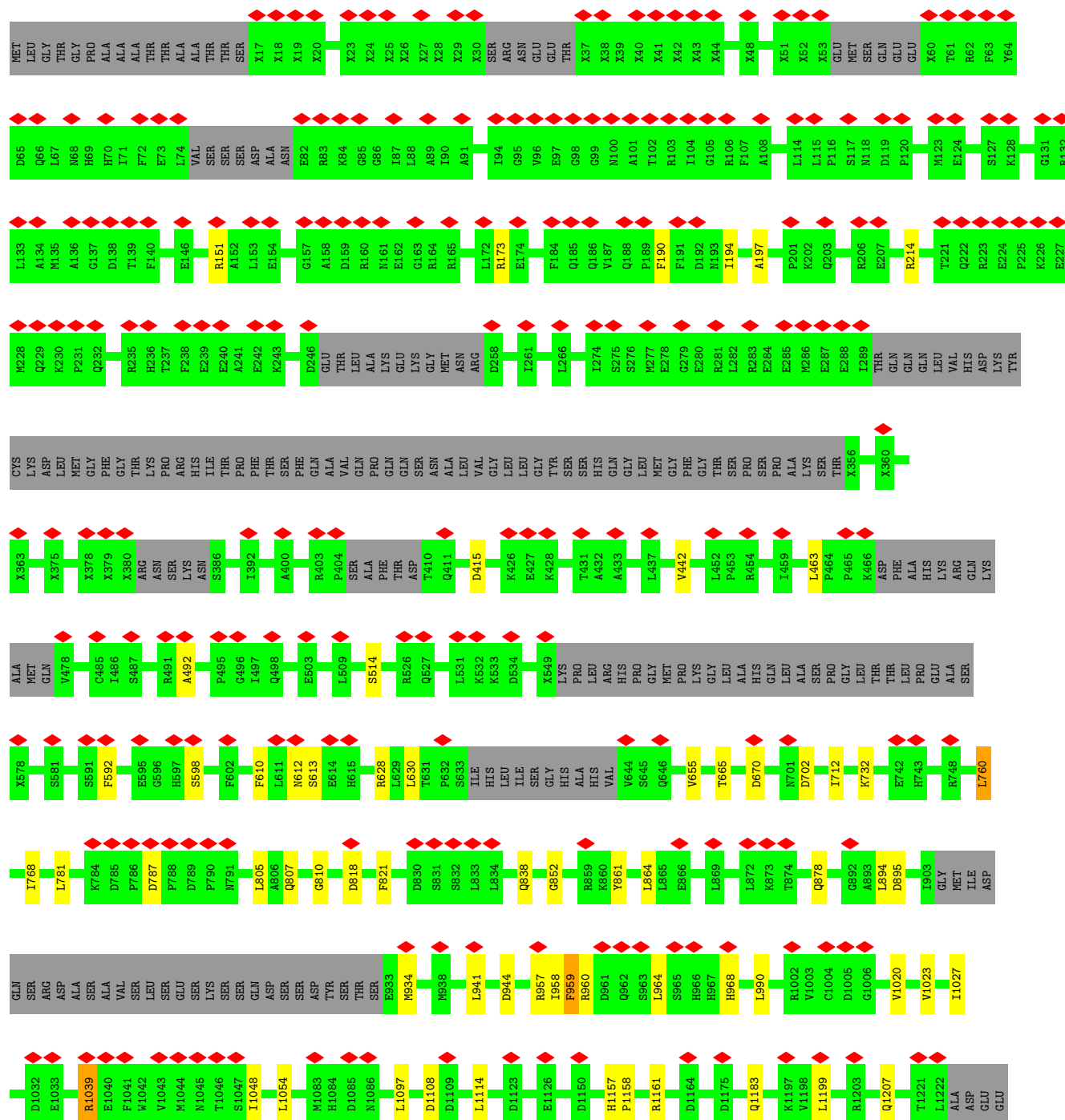
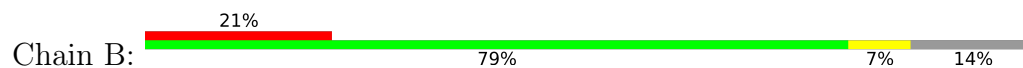
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- The image displays the chemical structure of Guanosine Triphosphate (GTP). It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar via a glycosidic bond. The ribose sugar is further linked to three phosphate groups (labeled 1, 2, and 3) via phosphodiester bonds. The structure is shown in a 3D representation with stereochemistry indicated by wedges and dashes. The atoms are labeled with their respective element symbols and numbers (e.g., N1, C2, O3, P1, O1A, etc.).

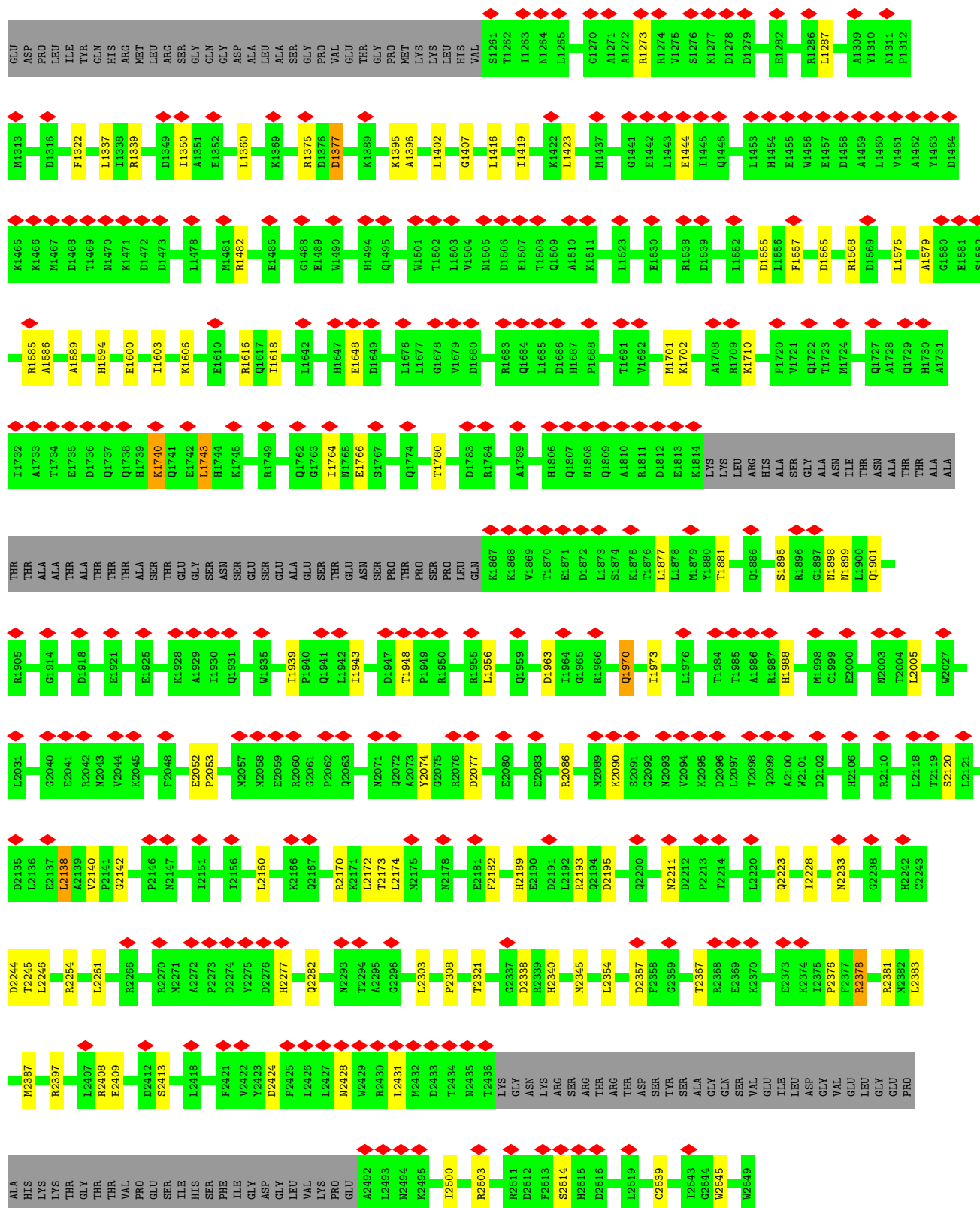
Mol	Chain	Residues	Atoms						AltConf
8	S	1	Total 44	C 10	H 12	N 5	O 14	P 3	0
8	R	1	Total 44	C 10	H 12	N 5	O 14	P 3	0





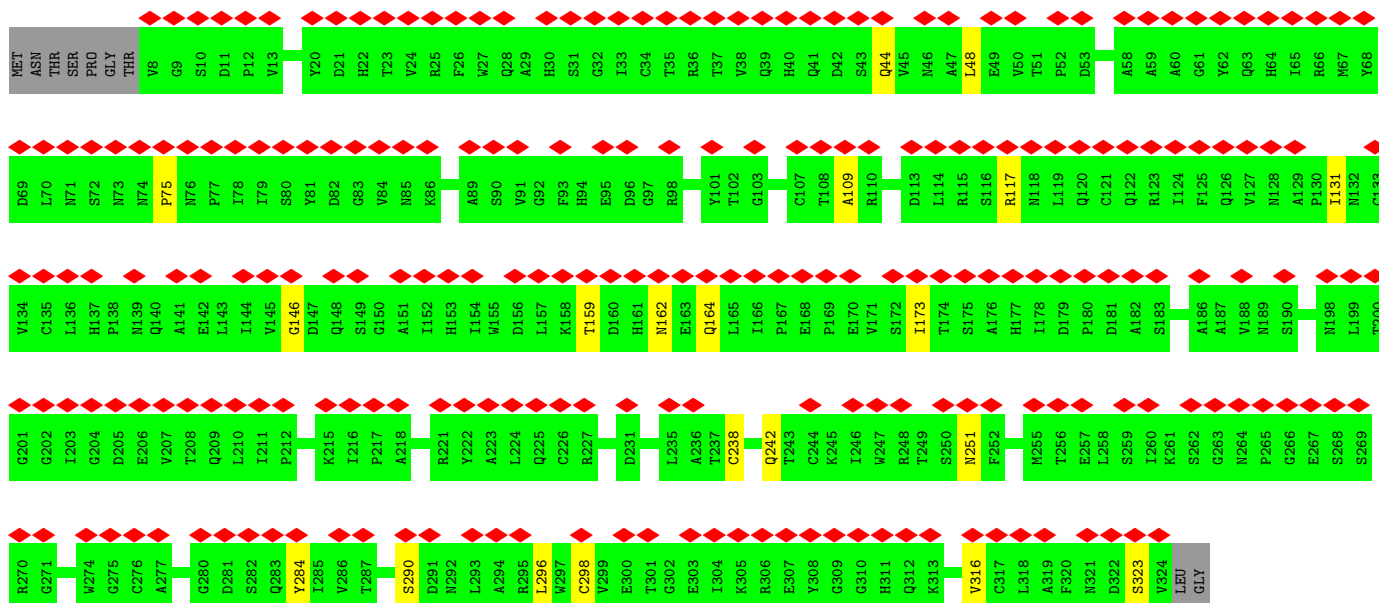
- Molecule 1: Serine/threonine-protein kinase mTOR, Serine/threonine-protein kinase mTOR



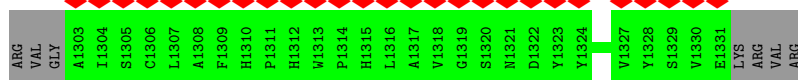


• Molecule 2: Target of rapamycin complex subunit LST8



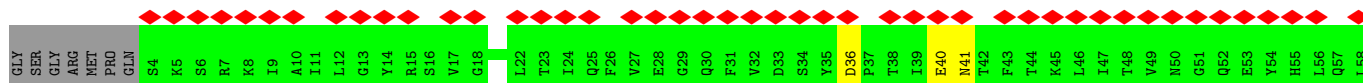


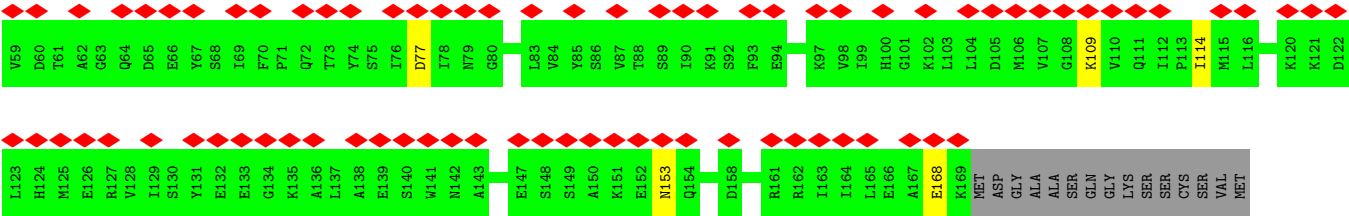




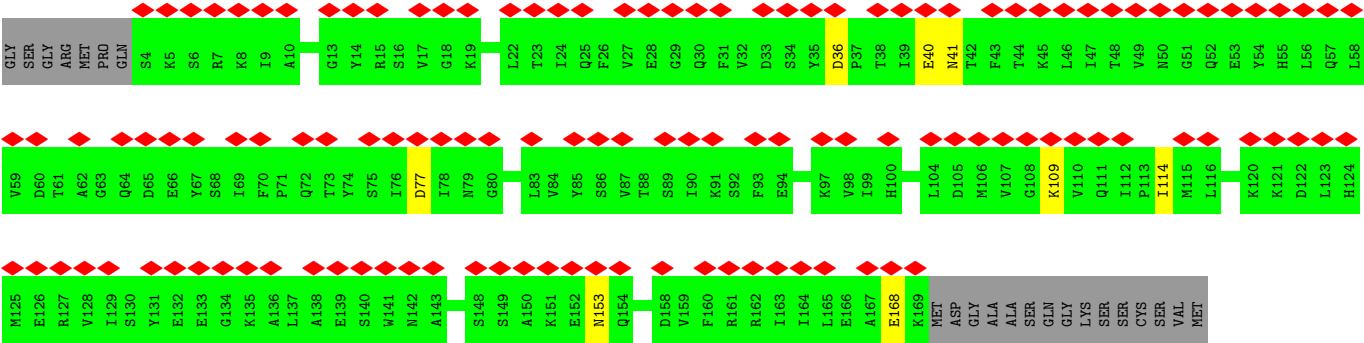
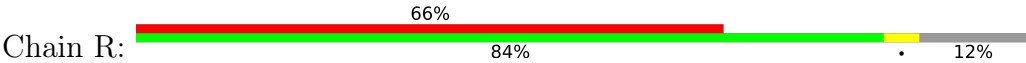
- Chain Y:  43% 72% 6% 22%







• Molecule 5: GTP-binding protein Rheb



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	198237	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 ($e^-/\text{\AA}^2$)	56	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	0.167	Depositor
Minimum map value	-0.086	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	497.6444, 497.6444, 497.6444	wwPDB
Map dimensions	374, 374, 374	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3306, 1.3306, 1.3306	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GTP, MG

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	0/17599	0.84	17/23827 (0.1%)
1	B	0.59	0/17599	0.84	17/23827 (0.1%)
2	D	0.56	0/2514	0.78	2/3426 (0.1%)
2	E	0.56	0/2514	0.78	2/3426 (0.1%)
3	W	0.55	0/8584	0.78	4/11677 (0.0%)
3	Y	0.55	0/8584	0.78	4/11677 (0.0%)
4	X	0.62	0/68	0.70	0/89
4	Z	0.62	0/68	0.70	0/89
5	R	0.59	0/1340	0.73	0/1809
5	S	0.59	0/1340	0.73	0/1809
All	All	0.57	0/60210	0.81	46/81656 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
2	D	0	1
2	E	0	1
3	Y	0	2
5	R	0	2
5	S	0	2
All	All	0	18

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1743	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	1743	LEU	CA-CB-CG	6.46	130.17	115.30
1	A	2138	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	2138	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	1273	ARG	NE-CZ-NH1	5.70	123.15	120.30

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1377	ASP	Peptide
1	A	197	ALA	Peptide
1	A	878	GLN	Peptide
1	A	894	LEU	Peptide
1	A	941	LEU	Peptide

5.2 Too-close contacts [i](#)

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	17538	17859	17553	38	0
1	B	17538	17859	17553	41	0
2	D	2456	2353	2341	5	0
2	E	2456	2353	2341	6	0
3	W	8385	8406	8374	19	0
3	Y	8385	8406	8374	18	0
4	X	68	58	57	0	0
4	Z	68	58	57	0	0
5	R	1318	1339	1334	0	0
5	S	1318	1339	1333	0	0
6	A	31	12	12	0	0
6	B	31	12	12	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
8	R	32	12	12	0	0
8	S	32	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59662	60078	59365	121	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.

The worst 5 of 121 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:B:190:PHE:CZ	1:B:194:ILE:HD11	2.32	0.64
1:A:190:PHE:CZ	1:A:194:ILE:HD11	2.32	0.64
1:A:1970:GLN:HE21	1:A:1970:GLN:HA	1.63	0.63
1:B:1970:GLN:HE21	1:B:1970:GLN:HA	1.64	0.63
1:B:964:LEU:HD13	1:B:968:HIS:CD2	2.35	0.62

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	2124/2549 (83%)	1934 (91%)	170 (8%)	20 (1%)	17 54
1	B	2124/2549 (83%)	1933 (91%)	171 (8%)	20 (1%)	17 54
2	D	315/326 (97%)	263 (84%)	50 (16%)	2 (1%)	25 62
2	E	315/326 (97%)	263 (84%)	50 (16%)	2 (1%)	25 62
3	W	1038/1343 (77%)	936 (90%)	89 (9%)	13 (1%)	12 46
3	Y	1038/1343 (77%)	934 (90%)	91 (9%)	13 (1%)	12 46
4	X	6/122 (5%)	5 (83%)	1 (17%)	0	100 100
4	Z	6/122 (5%)	5 (83%)	1 (17%)	0	100 100
5	R	164/188 (87%)	152 (93%)	11 (7%)	1 (1%)	25 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	S	164/188 (87%)	152 (93%)	11 (7%)	1 (1%)	25 62
All	All	7294/9056 (80%)	6577 (90%)	645 (9%)	72 (1%)	20 52

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	959	PHE
1	A	1444	GLU
1	A	1766	GLU
3	W	1115	LEU
3	W	1212	ALA

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	1881/2166 (87%)	1800 (96%)	81 (4%)	29 61
1	B	1881/2166 (87%)	1801 (96%)	80 (4%)	29 61
2	D	269/276 (98%)	262 (97%)	7 (3%)	46 74
2	E	269/276 (98%)	262 (97%)	7 (3%)	46 74
3	W	928/1171 (79%)	893 (96%)	35 (4%)	33 64
3	Y	928/1171 (79%)	893 (96%)	35 (4%)	33 64
4	X	8/104 (8%)	7 (88%)	1 (12%)	4 21
4	Z	8/104 (8%)	7 (88%)	1 (12%)	4 21
5	R	147/163 (90%)	142 (97%)	5 (3%)	37 68
5	S	147/163 (90%)	142 (97%)	5 (3%)	37 68
All	All	6466/7760 (83%)	6209 (96%)	257 (4%)	35 63

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Y	331	ASP

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Mol	Chain	Res	Type
3	Y	548	THR
3	W	246	CYS
3	W	138	ARG
3	Y	1011	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	153	ASN
5	R	153	ASN
1	B	1941	GLN
5	R	41	ASN
3	Y	565	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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
6	ATP	A	3000	7	26,33,33	1.49	3 (11%)	31,52,52	1.77	7 (22%)
6	ATP	B	3000	7	26,33,33	1.59	5 (19%)	31,52,52	1.89	8 (25%)
8	GTP	S	201	7	26,34,34	0.84	0	32,54,54	1.37	5 (15%)
8	GTP	R	201	7	26,34,34	0.85	0	32,54,54	1.36	5 (15%)

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	ATP	A	3000	7	-	0/18/38/38	0/3/3/3
6	ATP	B	3000	7	-	0/18/38/38	0/3/3/3
8	GTP	S	201	7	-	3/18/38/38	0/3/3/3
8	GTP	R	201	7	-	4/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3000	ATP	C5-C4	4.24	1.52	1.40
6	B	3000	ATP	C2-N3	4.06	1.38	1.32
6	B	3000	ATP	C5-C4	3.92	1.51	1.40
6	A	3000	ATP	C2-N1	3.47	1.40	1.33
6	A	3000	ATP	C2'-C1'	2.30	1.57	1.53

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3000	ATP	C3'-C2'-C1'	4.38	107.57	100.98
6	B	3000	ATP	O4'-C4'-C3'	4.32	113.66	105.11
6	A	3000	ATP	C3'-C2'-C1'	3.85	106.78	100.98
8	S	201	GTP	PA-O3A-PB	-3.30	121.50	132.83
6	A	3000	ATP	PB-O3B-PG	-3.24	121.70	132.83

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	S	201	GTP	PB-O3A-PA-O1A
8	R	201	GTP	PB-O3A-PA-O1A

Continued on next page...

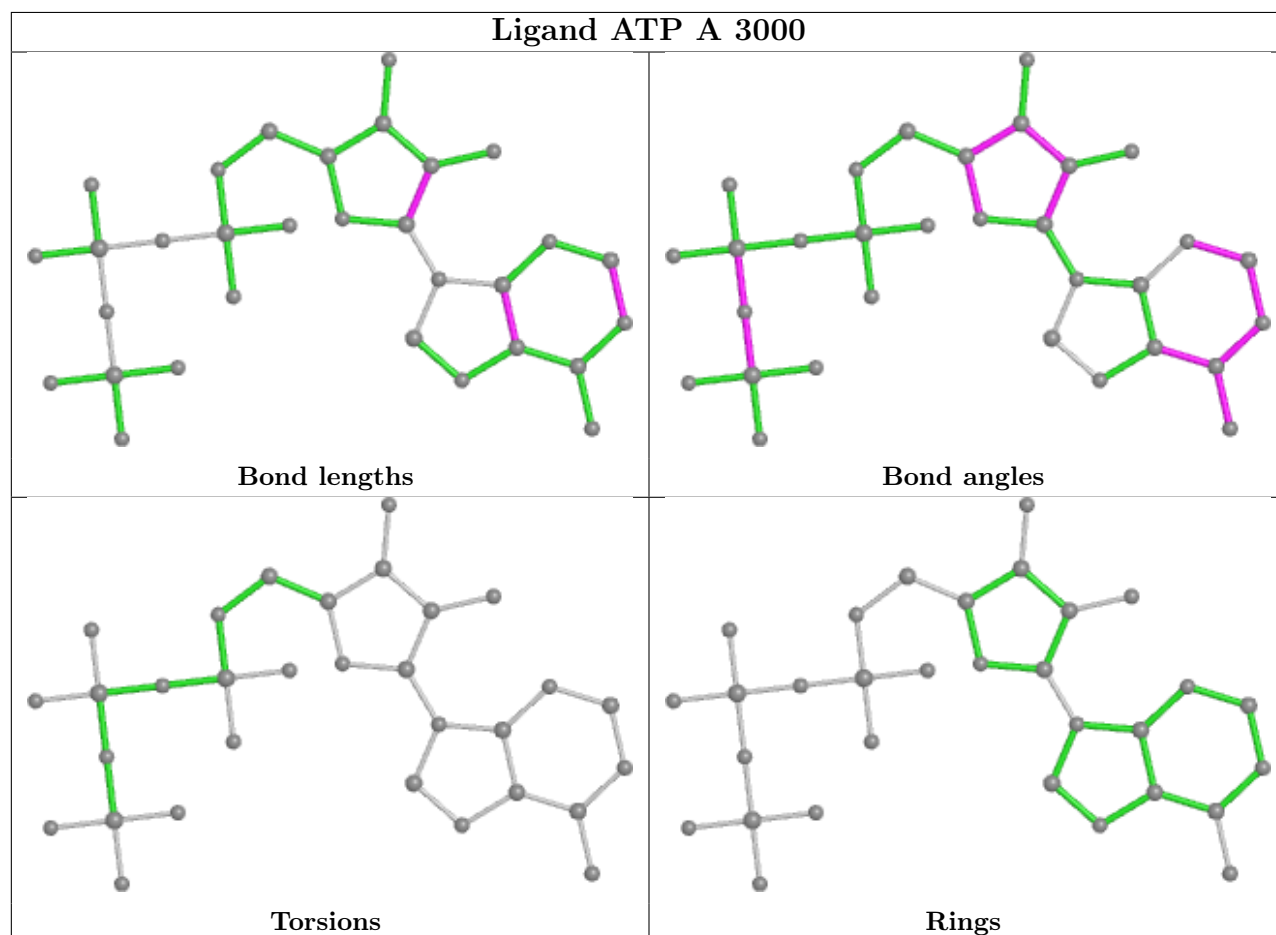
Continued from previous page...

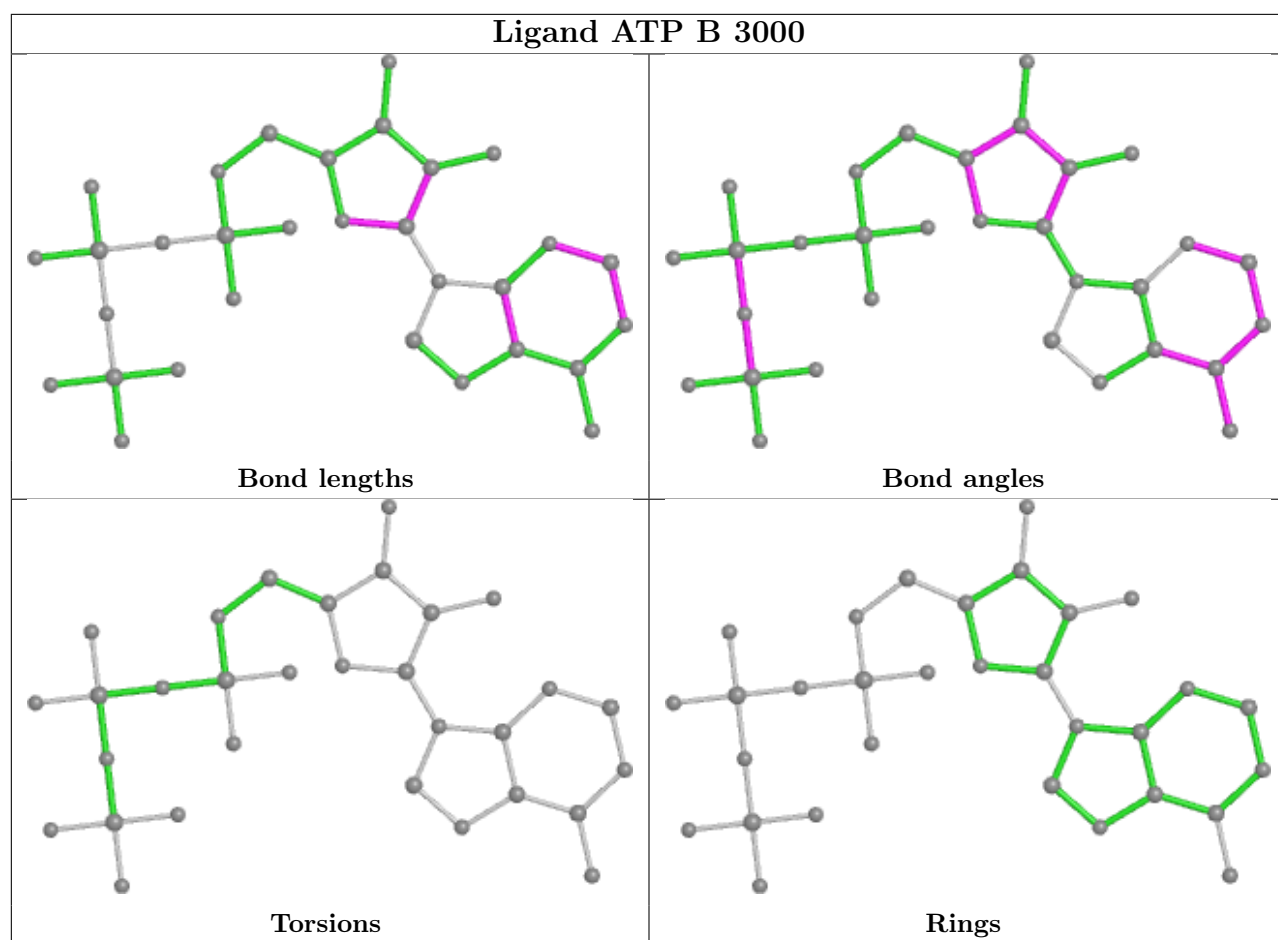
Mol	Chain	Res	Type	Atoms
8	S	201	GTP	PB-O3A-PA-O2A
8	S	201	GTP	C4'-C5'-O5'-PA
8	R	201	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

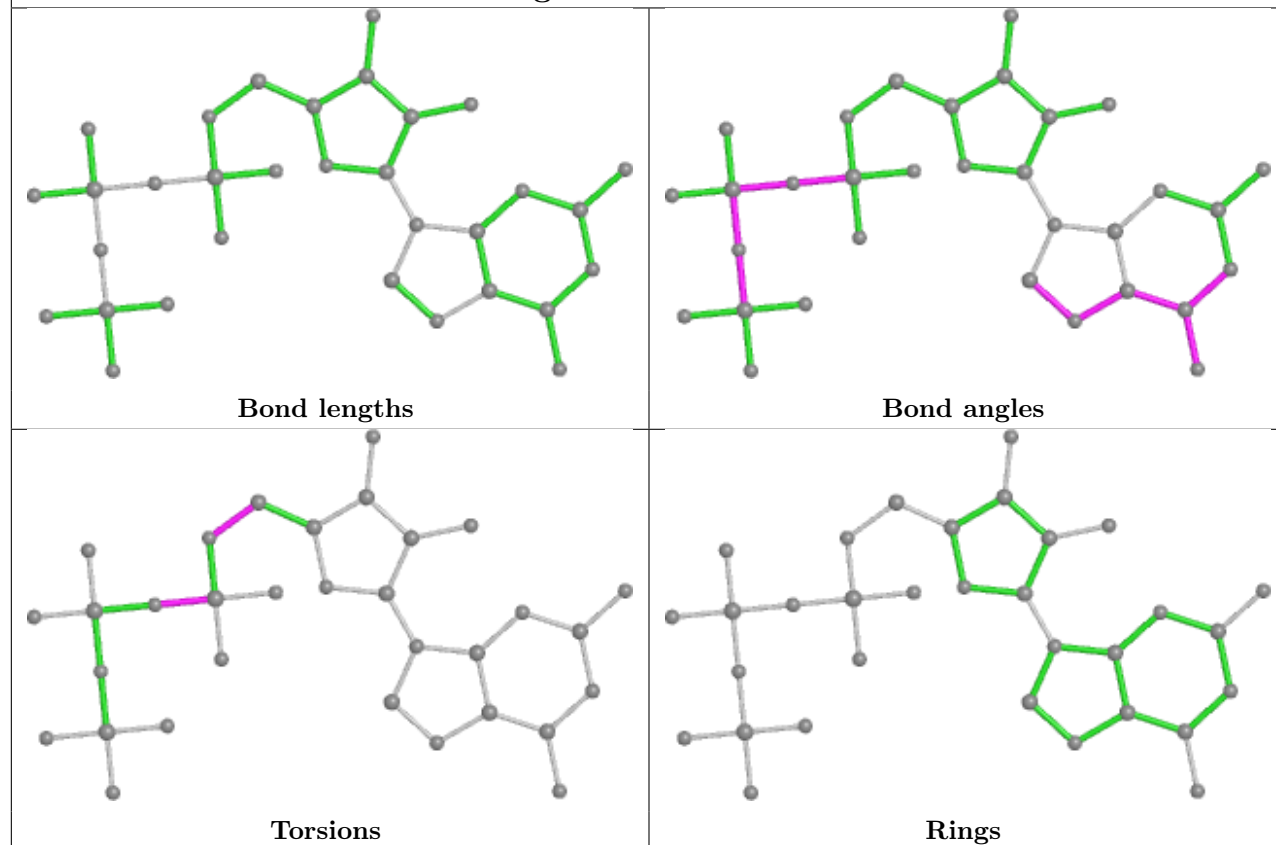
No monomer is involved in short contacts.

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.

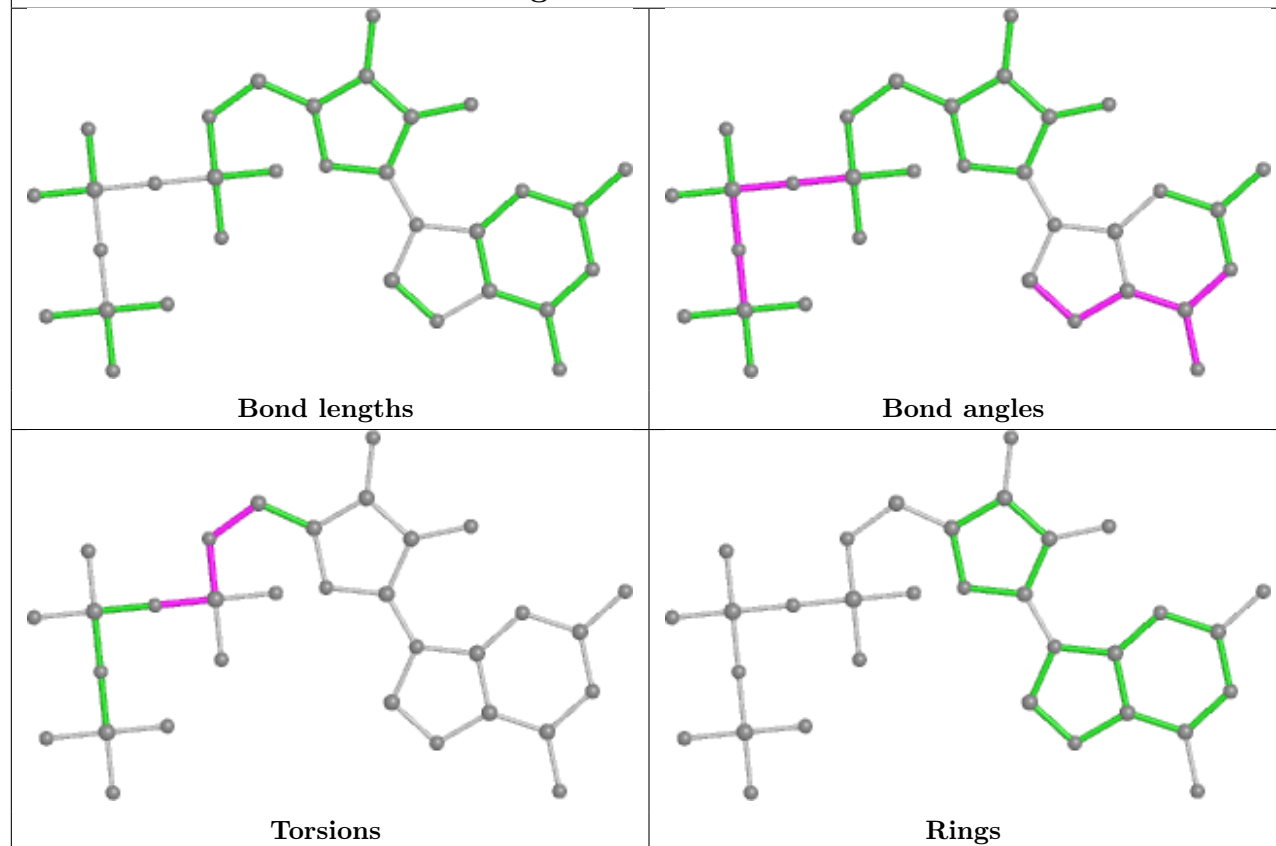




Ligand GTP S 201



Ligand GTP R 201



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	Y	1
3	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	40:GLU	C	41:GLY	N	3.34
1	W	40:GLU	C	41:GLY	N	3.22

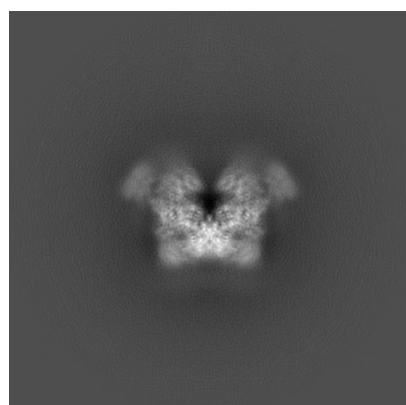
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7086. These allow visual inspection of the internal detail of the map and identification of artifacts.

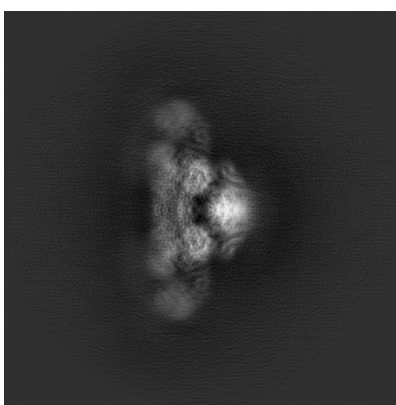
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

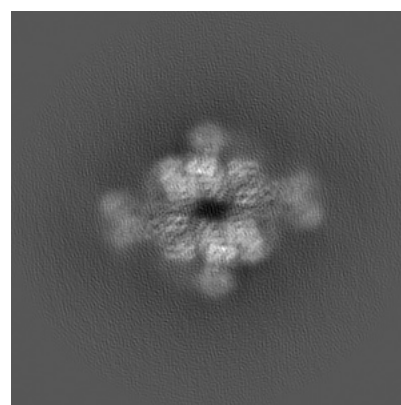
6.1.1 Primary map



X



Y

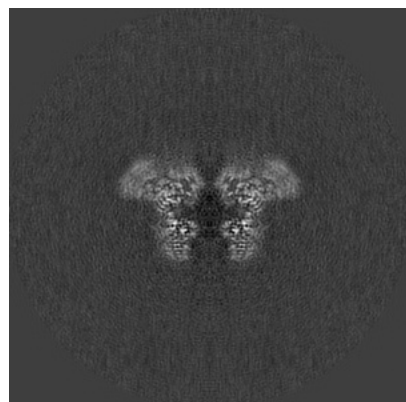


Z

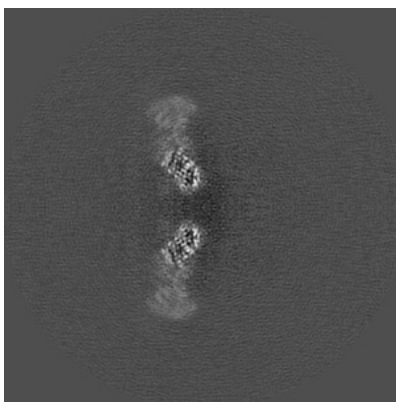
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

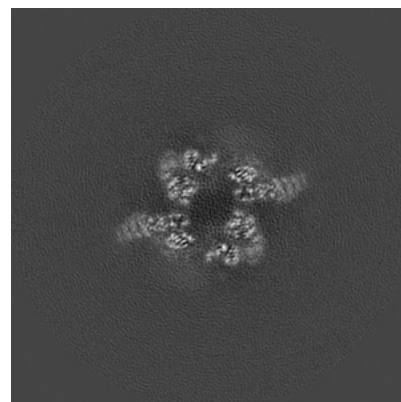
6.2.1 Primary map



X Index: 187



Y Index: 187

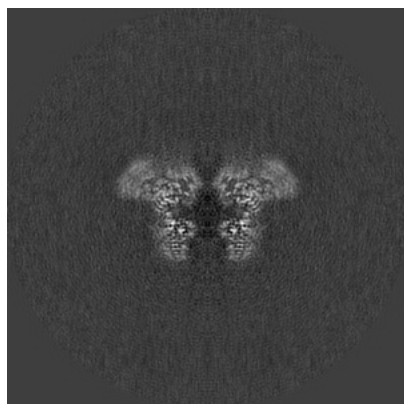


Z Index: 187

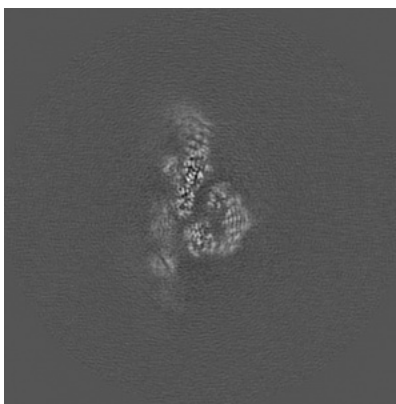
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

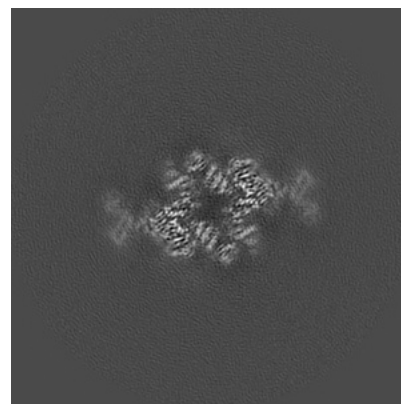
6.3.1 Primary map



X Index: 187



Y Index: 207



Z Index: 174

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

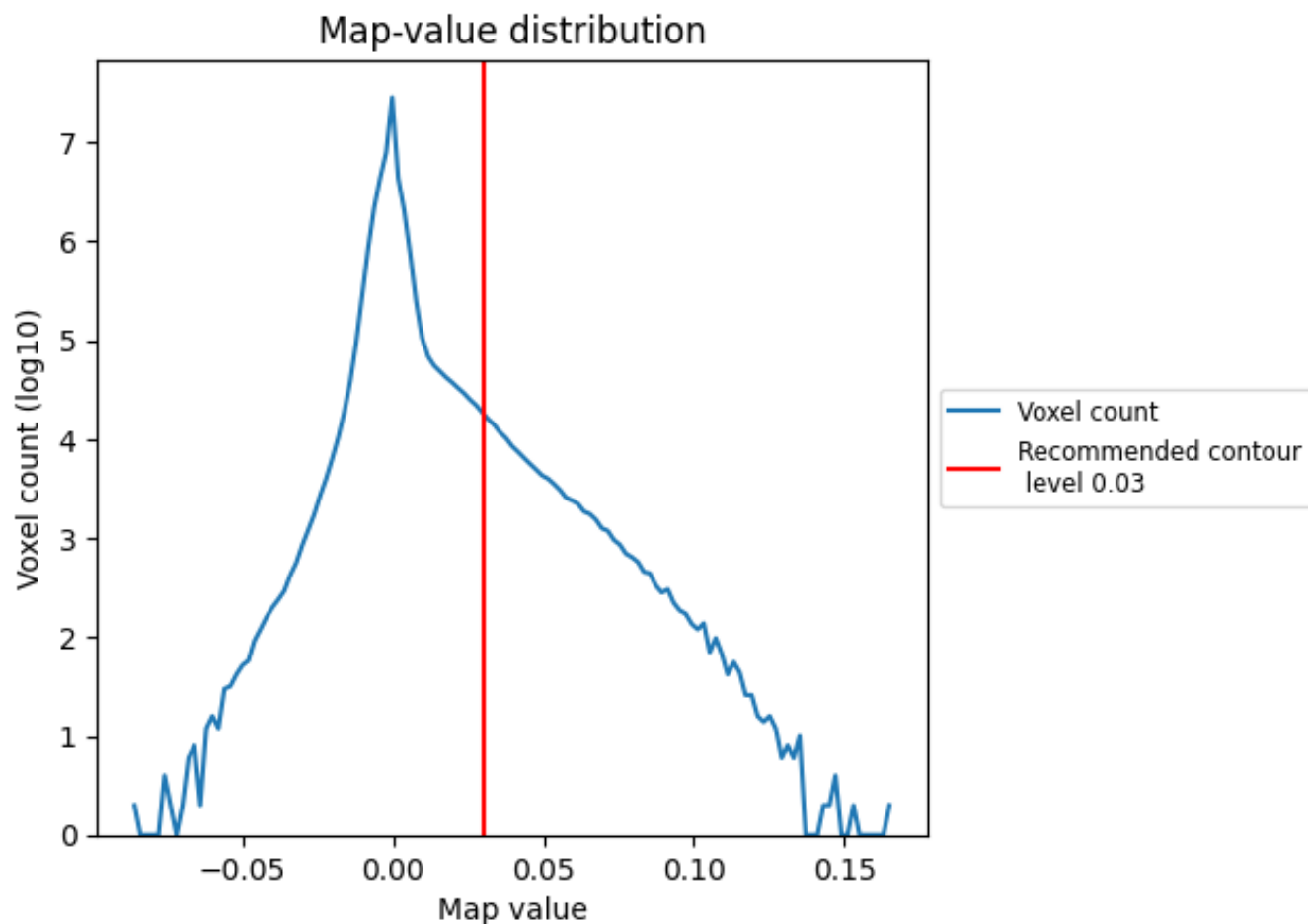
6.5 Mask visualisation

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

7 Map analysis [i](#)

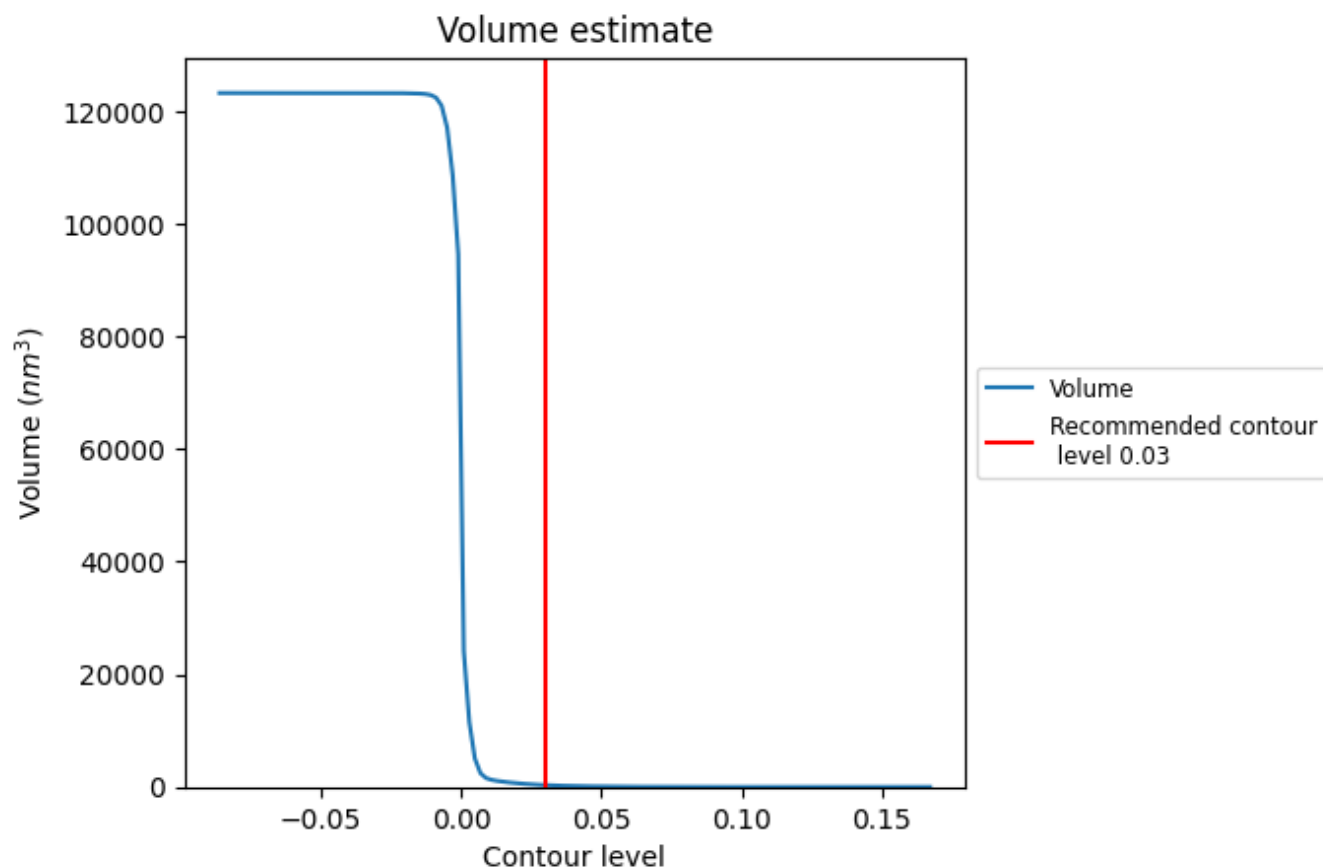
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

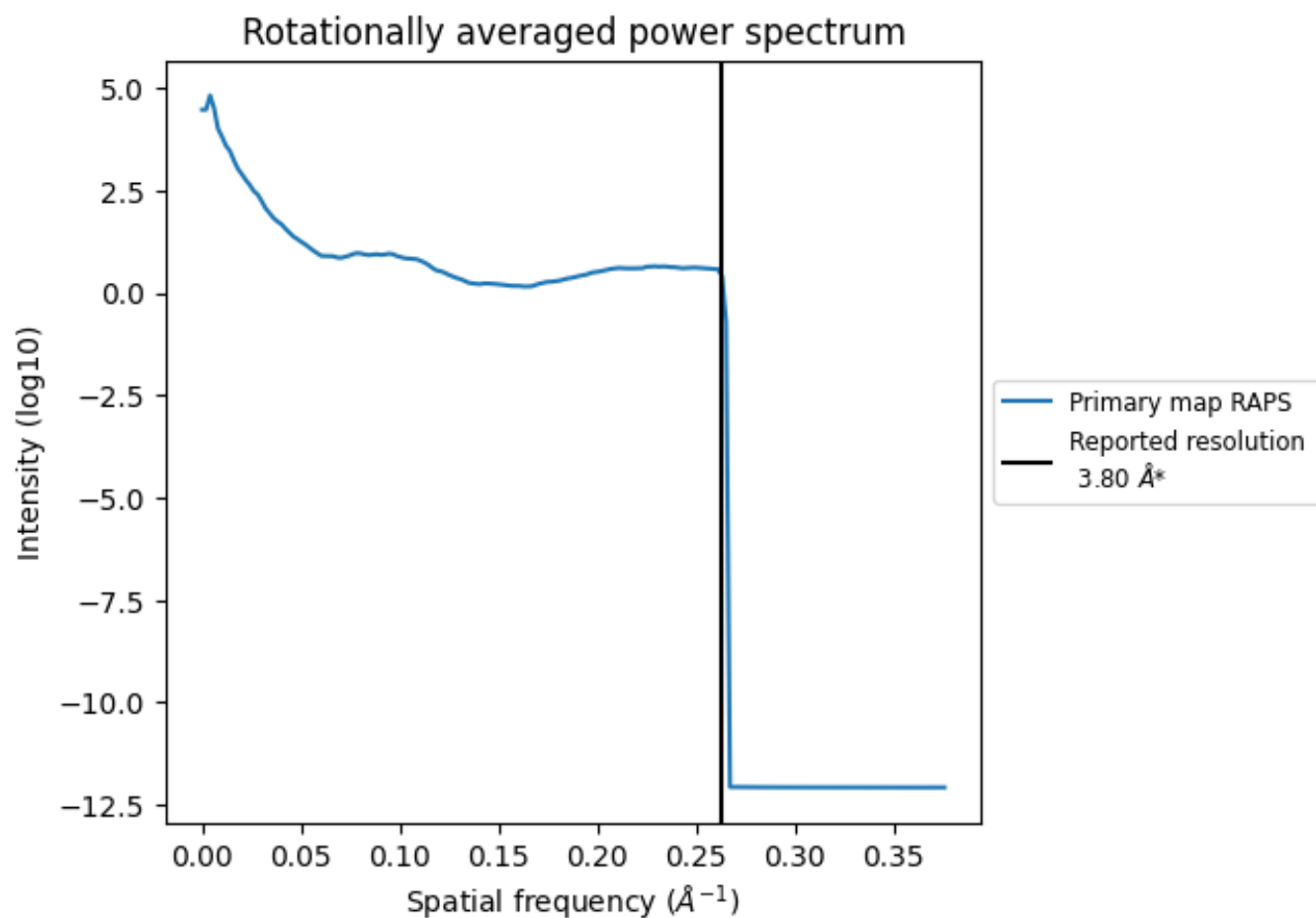
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm³; this corresponds to an approximate mass of 289 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 0.263 Å⁻¹

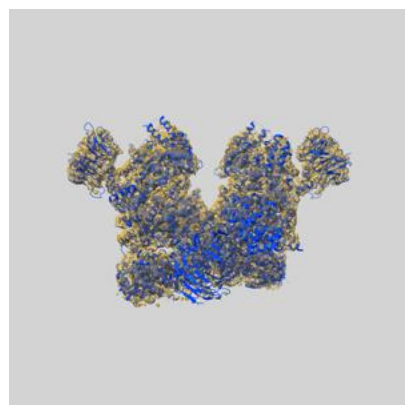
8 Fourier-Shell correlation ⓘ

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

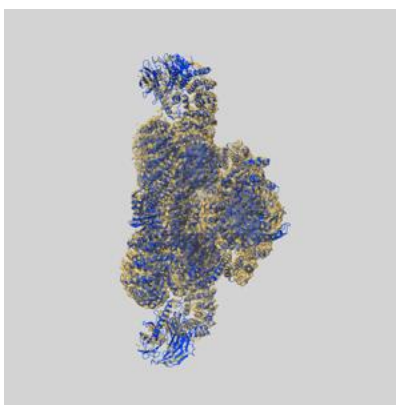
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7086 and PDB model 6BCU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

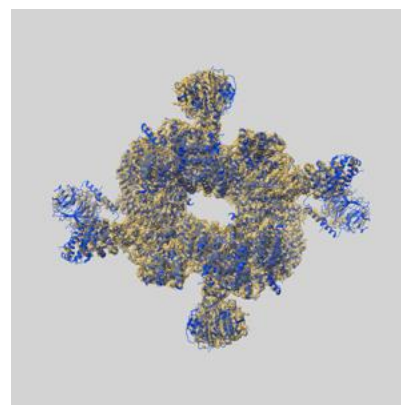
9.1 Map-model overlay [i](#)



X



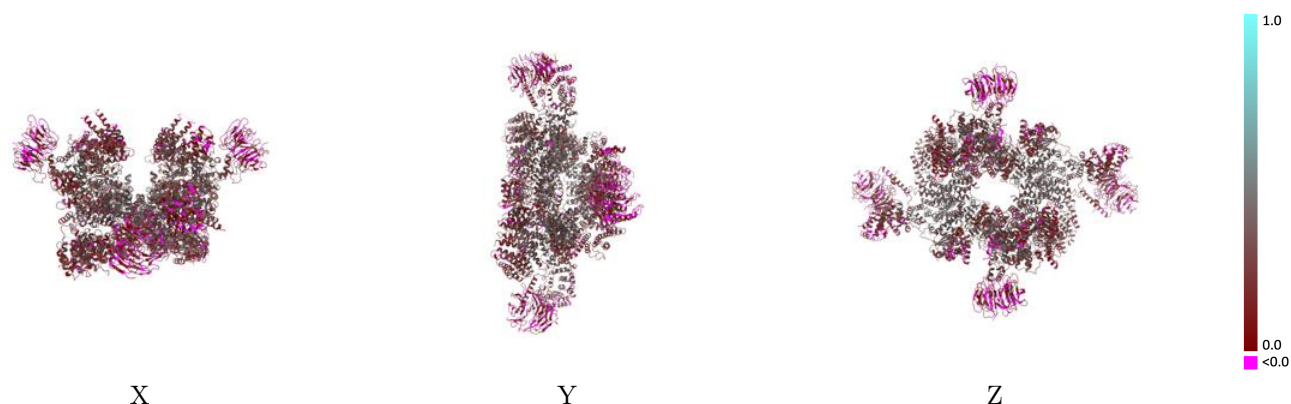
Y



Z

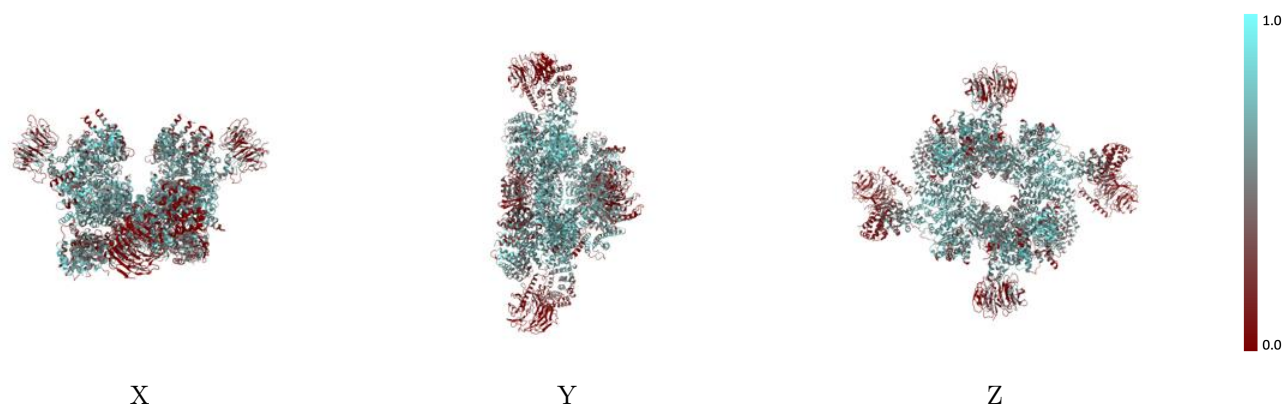
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



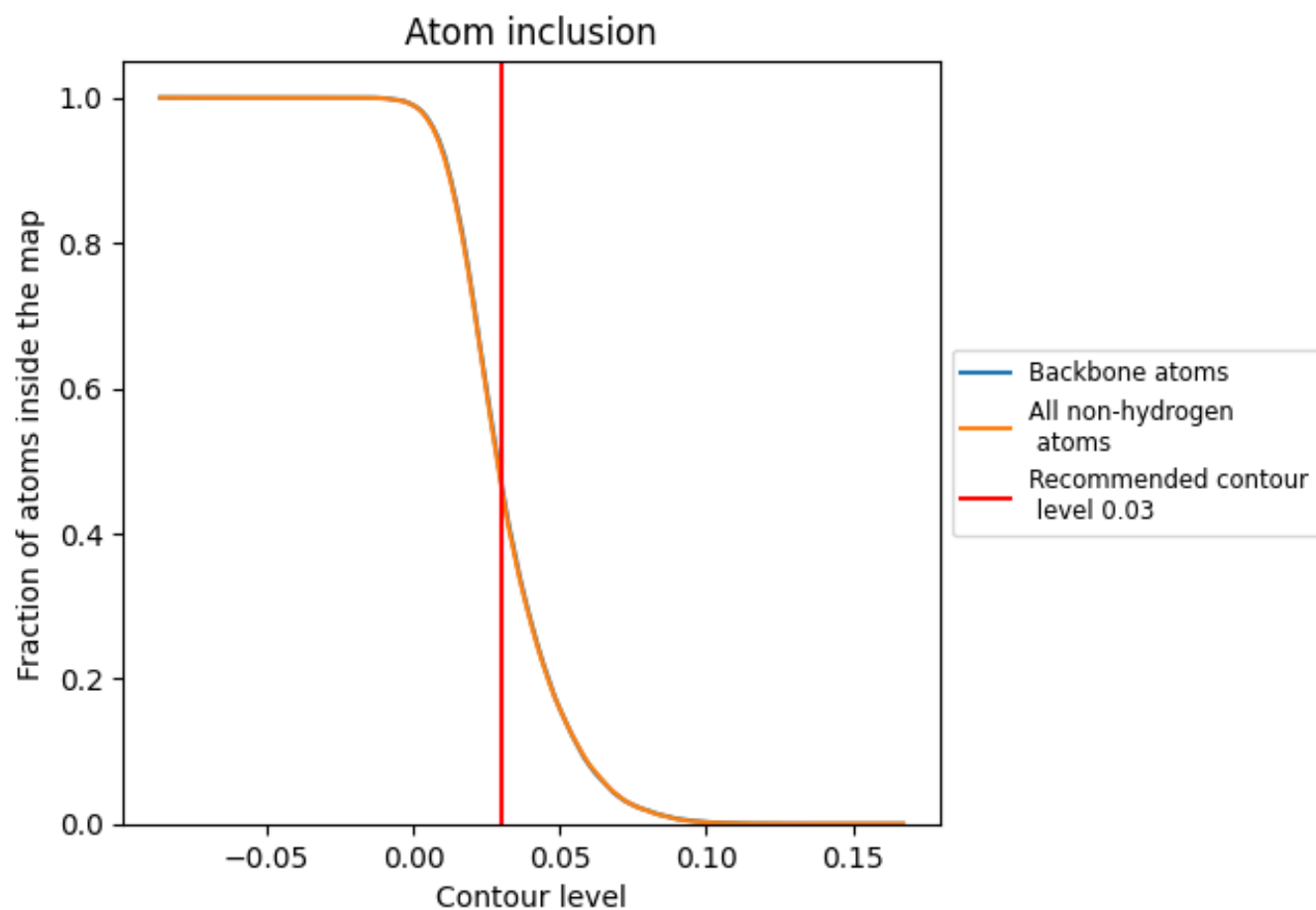
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 47% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4677	<div></div> 0.2500
A	<div></div> 0.5790	<div></div> 0.2870
B	<div></div> 0.5805	<div></div> 0.2870
D	<div></div> 0.2592	<div></div> 0.0710
E	<div></div> 0.2592	<div></div> 0.0680
R	<div></div> 0.2545	<div></div> 0.2150
S	<div></div> 0.2568	<div></div> 0.2230
W	<div></div> 0.3742	<div></div> 0.2280
X	<div></div> 0.4706	<div></div> 0.3660
Y	<div></div> 0.3706	<div></div> 0.2270
Z	<div></div> 0.5000	<div></div> 0.3750

1.0
0.0
<0.0