wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Feb 22, 2017 – 11:44 AM EST

PDB ID	:	5H64
EMDB ID:	:	EMD-6668
Title	:	Cryo-EM structure of mTORC1
Authors	:	Yang, H.; Wang, J.; Liu, M.; Chen, X.; Huang, M.; Tan, D.; Dong, M.; Wong, C.C.L.; Wang, J.; Xu, Y.; Wang, H.
Deposited on	:	2016-11-10
Resolution	:	4.40 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

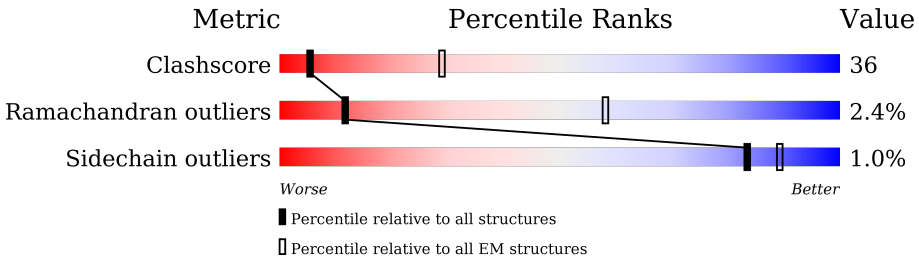
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2549	19% 59% • 18%
1	a	2549	77% 5% 18%
2	B	1335	30% 27% • 40%
2	b	1335	55% • • 40%
3	C	326	14% 82% • •
3	c	326	95% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 45252 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	2101	Total	C	N	O	S	0	0
			15617	9886	2788	2849	94		
1	a	2101	Total	C	N	O	S	0	0
			15617	9886	2788	2849	94		

- Molecule 2 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	797	Total	C	N	O	S	0	0
			4553	2817	832	894	10		
2	b	797	Total	C	N	O	S	0	0
			4553	2817	832	894	10		

- Molecule 3 is a protein called Target of rapamycin complex subunit LST8.

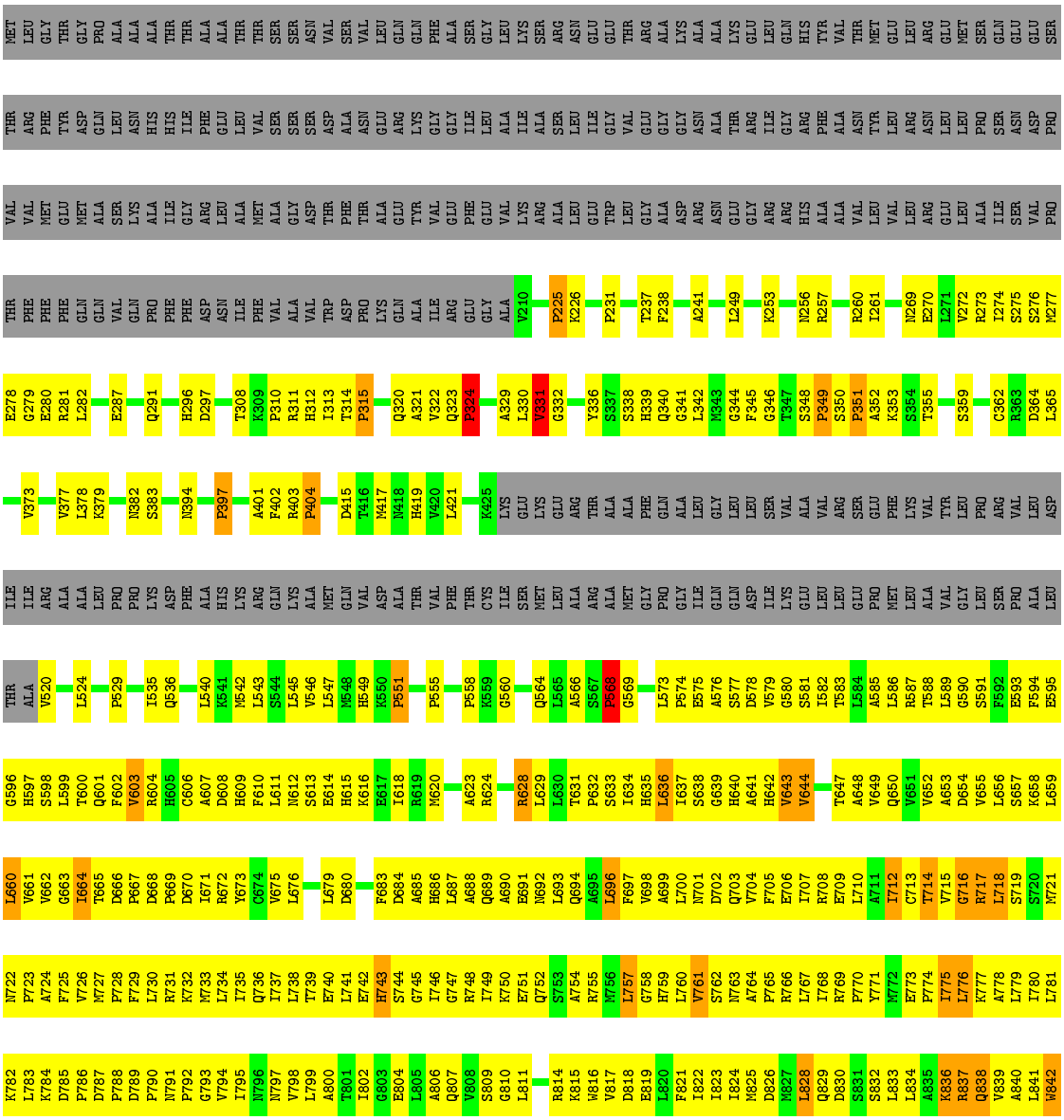
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		
3	c	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		

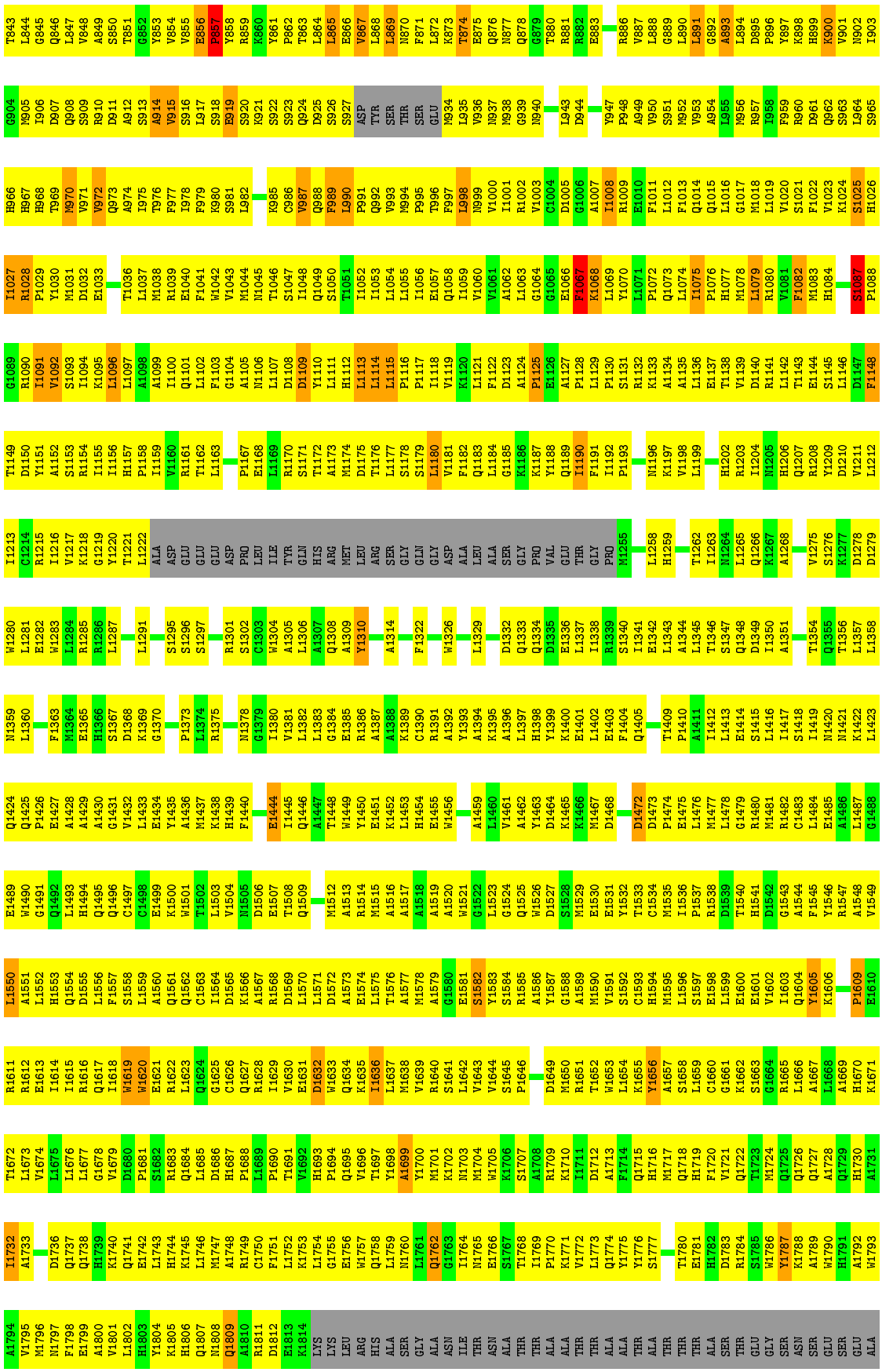
3 Residue-property plots (i)

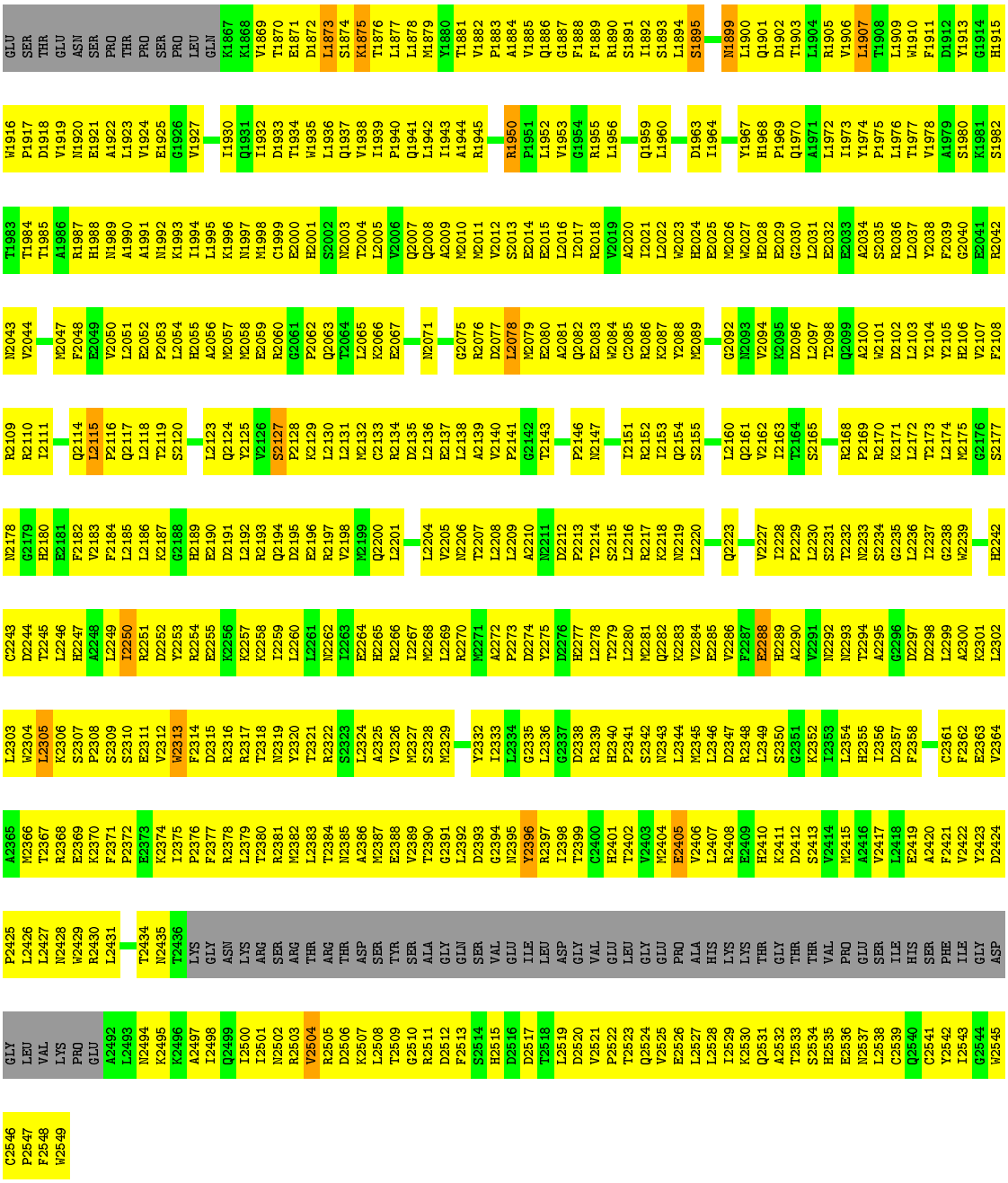
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein kinase mTOR

Chain A:

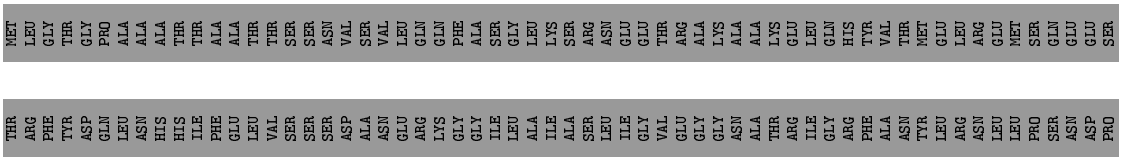


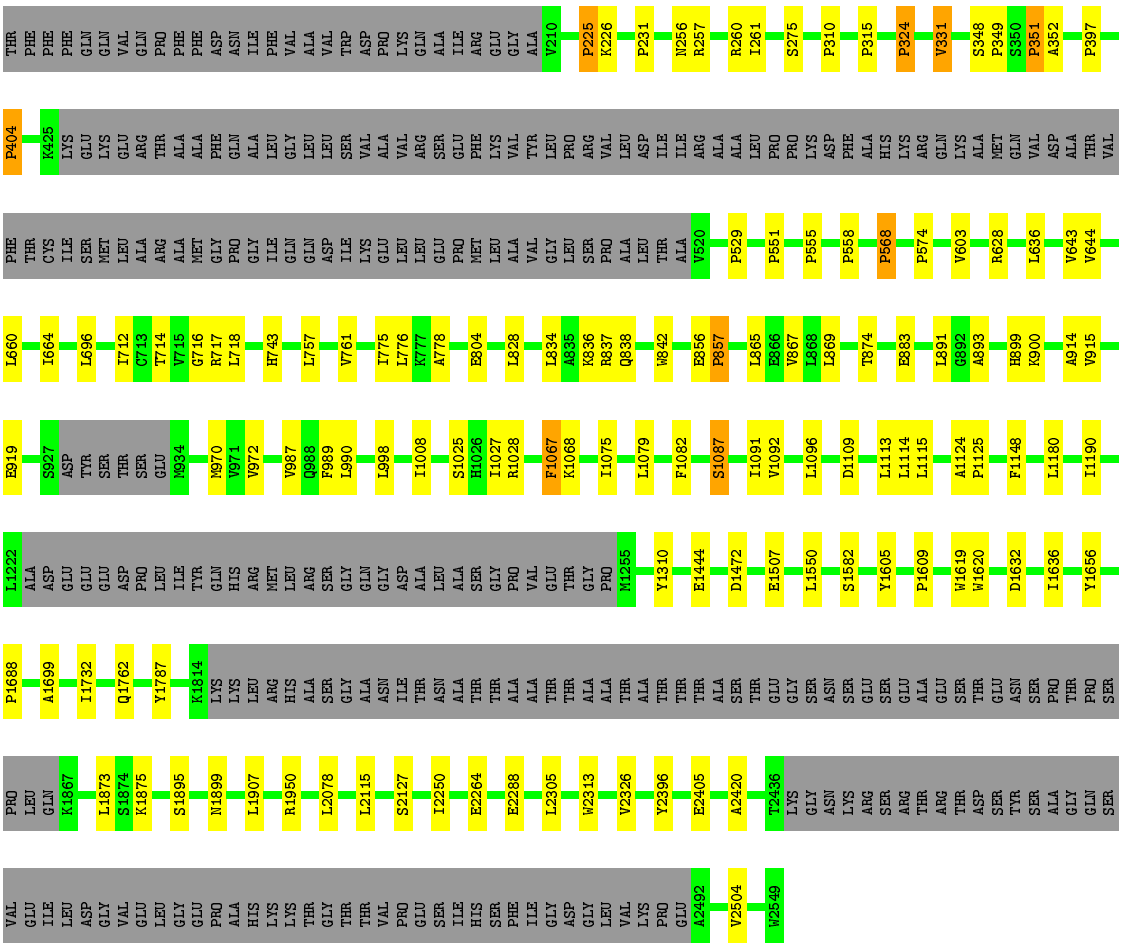




• Molecule 1: Serine/threonine-protein kinase mTOR

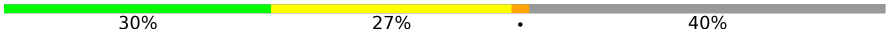
Chain a:

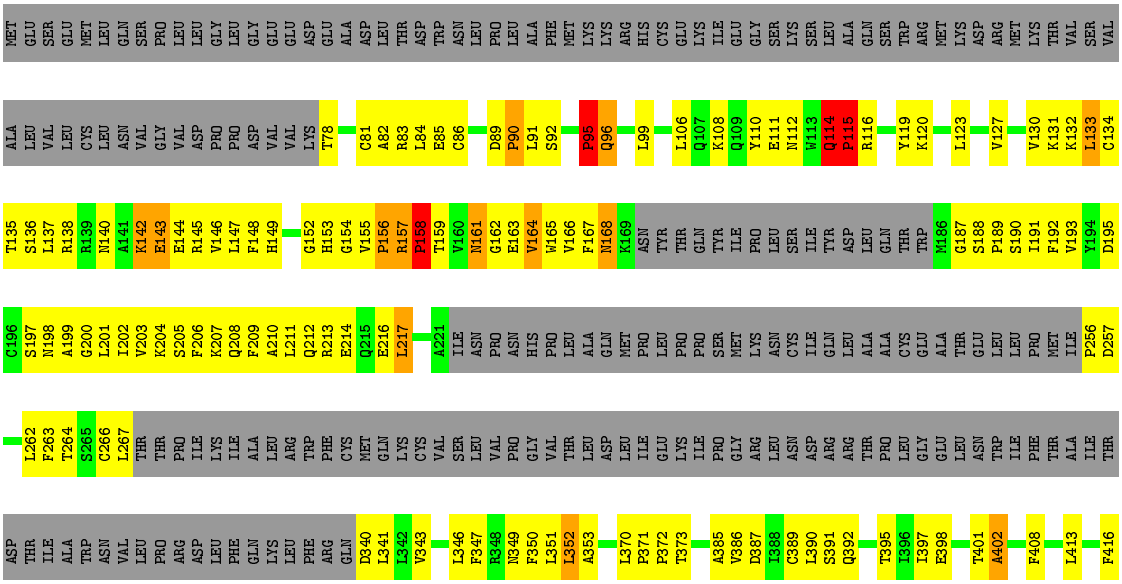


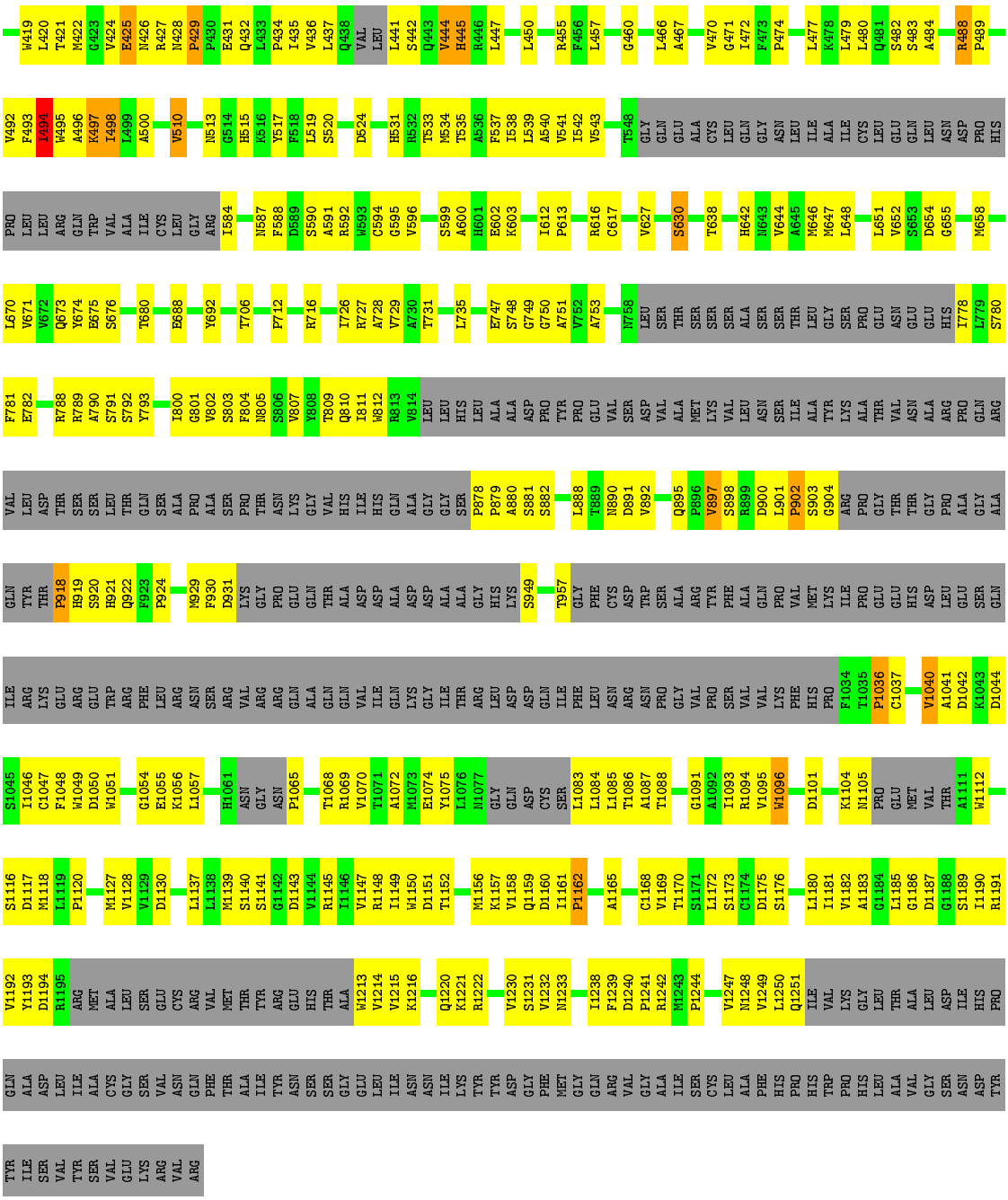


• Molecule 2: Regulatory-associated protein of mTOR

Chain B:

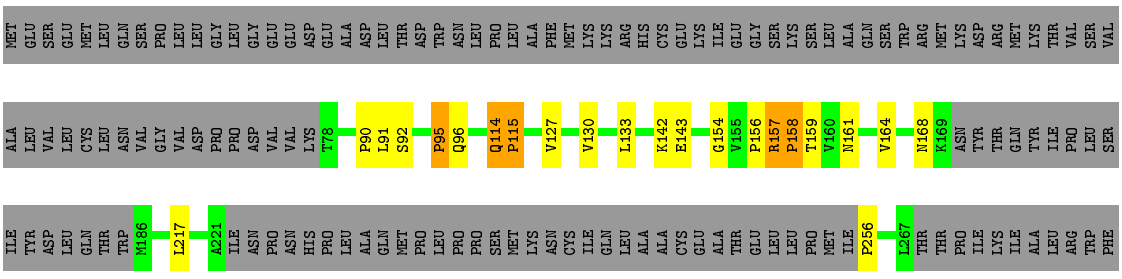


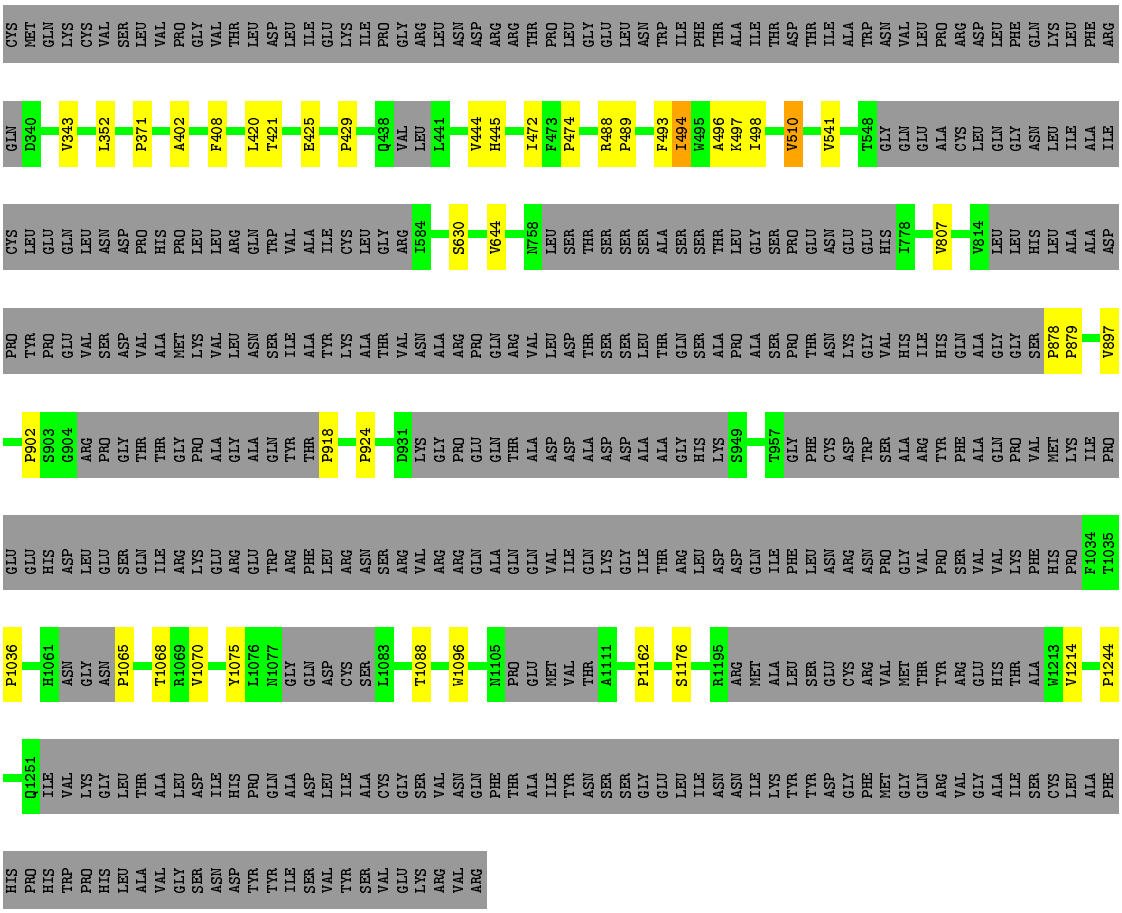




• Molecule 2: Regulatory-associated protein of mTOR

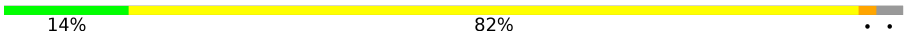
Chain b:





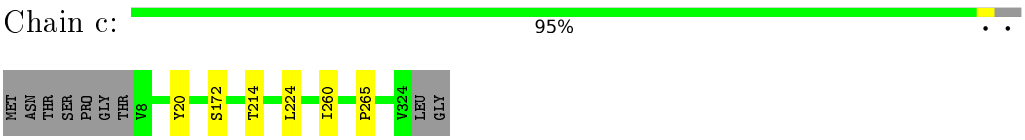
• Molecule 3: Target of rapamycin complex subunit LST8

Chain C:



• Molecule 3: Target of rapamycin complex subunit LST8

Chain c:


95%
MET
ASN
THR
SER
PRO
GLY
THR
V8
Y20
S172
T214
L224
I260
P265
V324
LEU
GLY

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	115039	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.56	4/15910 (0.0%)	0.78	38/21634 (0.2%)
1	a	0.56	4/15910 (0.0%)	0.78	38/21634 (0.2%)
2	B	0.40	1/4567 (0.0%)	0.73	13/6217 (0.2%)
2	b	0.40	1/4567 (0.0%)	0.73	13/6217 (0.2%)
3	C	0.49	0/2514	0.68	1/3426 (0.0%)
3	c	0.49	0/2514	0.68	1/3426 (0.0%)
All	All	0.53	10/45982 (0.0%)	0.76	104/62554 (0.2%)

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	47
1	a	0	46
2	B	0	14
2	b	0	14
3	C	0	4
3	c	0	4
All	All	0	129

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2313	TRP	CB-CG	-7.38	1.36	1.50
1	a	2313	TRP	CB-CG	-7.37	1.36	1.50
1	A	1619	TRP	CB-CG	-6.24	1.39	1.50
1	a	1619	TRP	CB-CG	-6.22	1.39	1.50
1	a	842	TRP	CB-CG	-5.75	1.40	1.50

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	114	GLN	C-N-CD	-17.81	81.41	120.60
2	B	114	GLN	C-N-CD	-17.81	81.41	120.60
1	a	1113	LEU	CA-CB-CG	-10.98	90.05	115.30
1	A	1113	LEU	CA-CB-CG	-10.97	90.06	115.30
2	b	115	PRO	CA-N-CD	-10.09	97.38	111.50

There are no chirality outliers.

5 of 129 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	LYS	Peptide
1	A	257	ARG	Peptide
1	A	260	ARG	Peptide
1	A	261	ILE	Peptide
1	A	275	SER	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	15617	0	14621	2309	0
1	a	15617	0	14621	0	0
2	B	4553	0	2926	333	0
2	b	4553	0	2926	0	0
3	C	2456	0	2341	423	0
3	c	2456	0	2341	0	0
All	All	45252	0	39776	3046	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 36.

The worst 5 of 3046 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:B:89:ASP:HB3	2:B:153:HIS:CB	1.53	1.38
2:B:82:ALA:O	2:B:115:PRO:HB2	1.24	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:GLU:HA	2:B:114:GLN:HA	1.27	1.14
2:B:142:LYS:O	2:B:143:GLU:O	1.73	1.07
1:A:912:ALA:O	1:A:1622:ARG:NH2	1.88	1.06

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	2089/2549 (82%)	1654 (79%)	386 (18%)	49 (2%)	8 50
1	a	2089/2549 (82%)	1656 (79%)	384 (18%)	49 (2%)	8 50
2	B	767/1335 (58%)	608 (79%)	132 (17%)	27 (4%)	4 41
2	b	767/1335 (58%)	609 (79%)	131 (17%)	27 (4%)	4 41
3	C	315/326 (97%)	281 (89%)	33 (10%)	1 (0%)	46 83
3	c	315/326 (97%)	281 (89%)	33 (10%)	1 (0%)	46 83
All	All	6342/8420 (75%)	5089 (80%)	1099 (17%)	154 (2%)	12 49

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	351	PRO
1	A	404	PRO
1	A	568	PRO
1	A	664	ILE

5.3.2 Protein sidechains (i)

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	1487/2220 (67%)	1485 (100%)	2 (0%)	95 97
1	a	1487/2220 (67%)	1485 (100%)	2 (0%)	95 97
2	B	185/1163 (16%)	167 (90%)	18 (10%)	10 43
2	b	177/1163 (15%)	160 (90%)	17 (10%)	10 43
3	C	269/276 (98%)	269 (100%)	0	100 100
3	c	269/276 (98%)	269 (100%)	0	100 100
All	All	3874/7318 (53%)	3835 (99%)	39 (1%)	83 91

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1162	PRO
1	a	1632	ASP
2	b	1162	PRO
2	B	1214	VAL
2	B	1244	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	153	HIS
1	a	694	GLN
2	b	1177	HIS
3	C	164	GLN
1	a	597	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.