wwPDB EM Validation Summary Report

Sep 18, 2021 – 08:06 am BST

PDB ID	:	7PEA
EMDB ID	:	EMD-13350
Title	:	cryo-EM structure of DEPTOR bound to human mTOR complex 1, overall refinement
Authors	:	Waelchli, M.; Maier, T.
Deposited on	:	2021-08-09
Resolution	:	4.07 Å(reported)
Based on initial model	:	6BCX

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

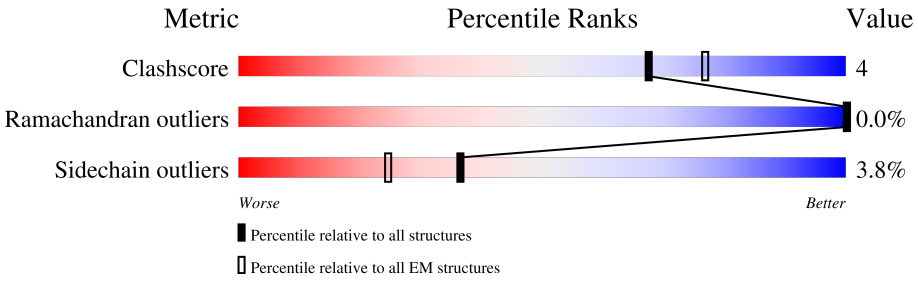
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 4.07 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2549	75% 10% • 14%
1	B	2549	75% 10% • 14%
2	C	326	82% 14% • •
2	D	326	83% 13% • •
3	E	1396	66% 8% • 25%
3	F	1396	66% 8% • 25%
4	I	409	20% 6% 74%
4	J	409	19% 6% 74%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 58252 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	2192	Total	C	N	O	S	0	0
			17454	11152	3058	3133	111		
1	A	2192	Total	C	N	O	S	0	0
			17454	11152	3058	3133	111		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	1052	Total	C	N	O	S	0	0
			8385	5361	1450	1518	56		
3	E	1052	Total	C	N	O	S	0	0
			8385	5361	1450	1518	56		

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-60	MET	-	initiating methionine	UNP Q8N122
F	-59	ALA	-	expression tag	UNP Q8N122
F	-58	HIS	-	expression tag	UNP Q8N122
F	-57	HIS	-	expression tag	UNP Q8N122
F	-56	HIS	-	expression tag	UNP Q8N122
F	-55	HIS	-	expression tag	UNP Q8N122
F	-54	HIS	-	expression tag	UNP Q8N122
F	-53	HIS	-	expression tag	UNP Q8N122
F	-52	HIS	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-51	HIS	-	expression tag	UNP Q8N122
F	-50	HIS	-	expression tag	UNP Q8N122
F	-49	HIS	-	expression tag	UNP Q8N122
F	-48	GLY	-	expression tag	UNP Q8N122
F	-47	SER	-	expression tag	UNP Q8N122
F	-46	THR	-	expression tag	UNP Q8N122
F	-45	SER	-	expression tag	UNP Q8N122
F	-44	GLY	-	expression tag	UNP Q8N122
F	-43	SER	-	expression tag	UNP Q8N122
F	-42	GLY	-	expression tag	UNP Q8N122
F	-41	GLU	-	expression tag	UNP Q8N122
F	-40	GLN	-	expression tag	UNP Q8N122
F	-39	LYS	-	expression tag	UNP Q8N122
F	-38	LEU	-	expression tag	UNP Q8N122
F	-37	ILE	-	expression tag	UNP Q8N122
F	-36	SER	-	expression tag	UNP Q8N122
F	-35	GLU	-	expression tag	UNP Q8N122
F	-34	GLU	-	expression tag	UNP Q8N122
F	-33	ASP	-	expression tag	UNP Q8N122
F	-32	LEU	-	expression tag	UNP Q8N122
F	-31	GLY	-	expression tag	UNP Q8N122
F	-30	SER	-	expression tag	UNP Q8N122
F	-29	THR	-	expression tag	UNP Q8N122
F	-28	SER	-	expression tag	UNP Q8N122
F	-27	GLY	-	expression tag	UNP Q8N122
F	-26	SER	-	expression tag	UNP Q8N122
F	-25	GLY	-	expression tag	UNP Q8N122
F	-24	ASP	-	expression tag	UNP Q8N122
F	-23	TYR	-	expression tag	UNP Q8N122
F	-22	LYS	-	expression tag	UNP Q8N122
F	-21	ASP	-	expression tag	UNP Q8N122
F	-20	ASP	-	expression tag	UNP Q8N122
F	-19	ASP	-	expression tag	UNP Q8N122
F	-18	ASP	-	expression tag	UNP Q8N122
F	-17	LYS	-	expression tag	UNP Q8N122
F	-16	LEU	-	expression tag	UNP Q8N122
F	-15	THR	-	expression tag	UNP Q8N122
F	-14	SER	-	expression tag	UNP Q8N122
F	-13	LEU	-	expression tag	UNP Q8N122
F	-12	TYR	-	expression tag	UNP Q8N122
F	-11	LYS	-	expression tag	UNP Q8N122
F	-10	LYS	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	ALA	-	expression tag	UNP Q8N122
F	-8	GLY	-	expression tag	UNP Q8N122
F	-7	LEU	-	expression tag	UNP Q8N122
F	-6	GLU	-	expression tag	UNP Q8N122
F	-5	ASN	-	expression tag	UNP Q8N122
F	-4	LEU	-	expression tag	UNP Q8N122
F	-3	TYR	-	expression tag	UNP Q8N122
F	-2	PHE	-	expression tag	UNP Q8N122
F	-1	GLN	-	expression tag	UNP Q8N122
F	0	GLY	-	expression tag	UNP Q8N122
E	-60	MET	-	initiating methionine	UNP Q8N122
E	-59	ALA	-	expression tag	UNP Q8N122
E	-58	HIS	-	expression tag	UNP Q8N122
E	-57	HIS	-	expression tag	UNP Q8N122
E	-56	HIS	-	expression tag	UNP Q8N122
E	-55	HIS	-	expression tag	UNP Q8N122
E	-54	HIS	-	expression tag	UNP Q8N122
E	-53	HIS	-	expression tag	UNP Q8N122
E	-52	HIS	-	expression tag	UNP Q8N122
E	-51	HIS	-	expression tag	UNP Q8N122
E	-50	HIS	-	expression tag	UNP Q8N122
E	-49	HIS	-	expression tag	UNP Q8N122
E	-48	GLY	-	expression tag	UNP Q8N122
E	-47	SER	-	expression tag	UNP Q8N122
E	-46	THR	-	expression tag	UNP Q8N122
E	-45	SER	-	expression tag	UNP Q8N122
E	-44	GLY	-	expression tag	UNP Q8N122
E	-43	SER	-	expression tag	UNP Q8N122
E	-42	GLY	-	expression tag	UNP Q8N122
E	-41	GLU	-	expression tag	UNP Q8N122
E	-40	GLN	-	expression tag	UNP Q8N122
E	-39	LYS	-	expression tag	UNP Q8N122
E	-38	LEU	-	expression tag	UNP Q8N122
E	-37	ILE	-	expression tag	UNP Q8N122
E	-36	SER	-	expression tag	UNP Q8N122
E	-35	GLU	-	expression tag	UNP Q8N122
E	-34	GLU	-	expression tag	UNP Q8N122
E	-33	ASP	-	expression tag	UNP Q8N122
E	-32	LEU	-	expression tag	UNP Q8N122
E	-31	GLY	-	expression tag	UNP Q8N122
E	-30	SER	-	expression tag	UNP Q8N122
E	-29	THR	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-28	SER	-	expression tag	UNP Q8N122
E	-27	GLY	-	expression tag	UNP Q8N122
E	-26	SER	-	expression tag	UNP Q8N122
E	-25	GLY	-	expression tag	UNP Q8N122
E	-24	ASP	-	expression tag	UNP Q8N122
E	-23	TYR	-	expression tag	UNP Q8N122
E	-22	LYS	-	expression tag	UNP Q8N122
E	-21	ASP	-	expression tag	UNP Q8N122
E	-20	ASP	-	expression tag	UNP Q8N122
E	-19	ASP	-	expression tag	UNP Q8N122
E	-18	ASP	-	expression tag	UNP Q8N122
E	-17	LYS	-	expression tag	UNP Q8N122
E	-16	LEU	-	expression tag	UNP Q8N122
E	-15	THR	-	expression tag	UNP Q8N122
E	-14	SER	-	expression tag	UNP Q8N122
E	-13	LEU	-	expression tag	UNP Q8N122
E	-12	TYR	-	expression tag	UNP Q8N122
E	-11	LYS	-	expression tag	UNP Q8N122
E	-10	LYS	-	expression tag	UNP Q8N122
E	-9	ALA	-	expression tag	UNP Q8N122
E	-8	GLY	-	expression tag	UNP Q8N122
E	-7	LEU	-	expression tag	UNP Q8N122
E	-6	GLU	-	expression tag	UNP Q8N122
E	-5	ASN	-	expression tag	UNP Q8N122
E	-4	LEU	-	expression tag	UNP Q8N122
E	-3	TYR	-	expression tag	UNP Q8N122
E	-2	PHE	-	expression tag	UNP Q8N122
E	-1	GLN	-	expression tag	UNP Q8N122
E	0	GLY	-	expression tag	UNP Q8N122

- Molecule 4 is a protein called DEP domain-containing mTOR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	106	Total	C	N	O	S	0	0
			795	504	138	146	7		
4	I	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
J	204	SER	ASN	variant	UNP Q8TB45

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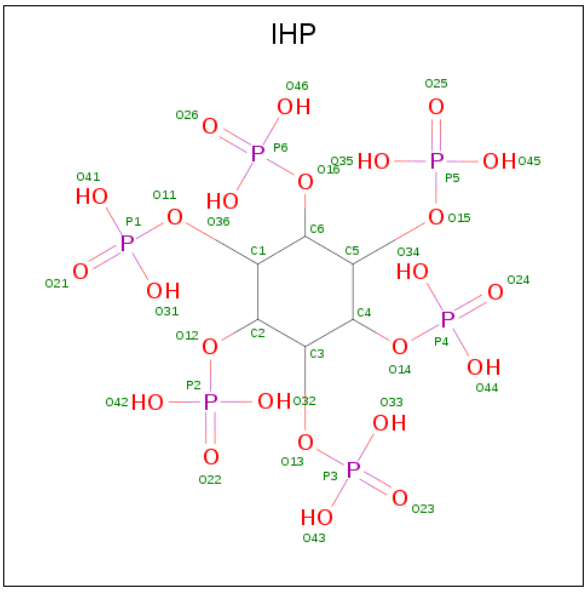
Chain	Residue	Modelled	Actual	Comment	Reference
J	389	ASN	SER	variant	UNP Q8TB45
I	204	SER	ASN	variant	UNP Q8TB45
I	389	ASN	SER	variant	UNP Q8TB45

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



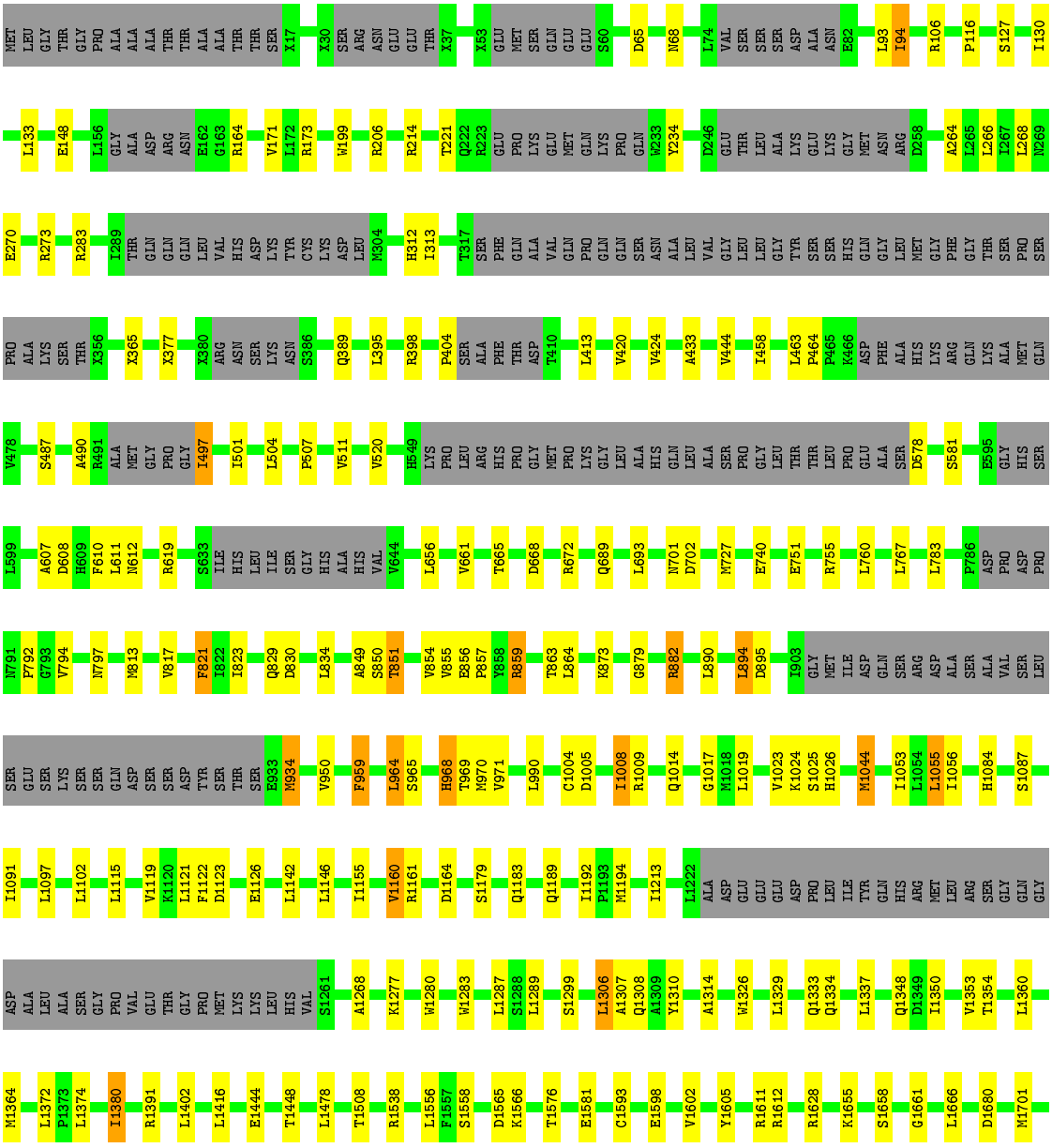
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	O	P	0
			36	6	24	6	
5	A	1	Total	C	O	P	0
			36	6	24	6	

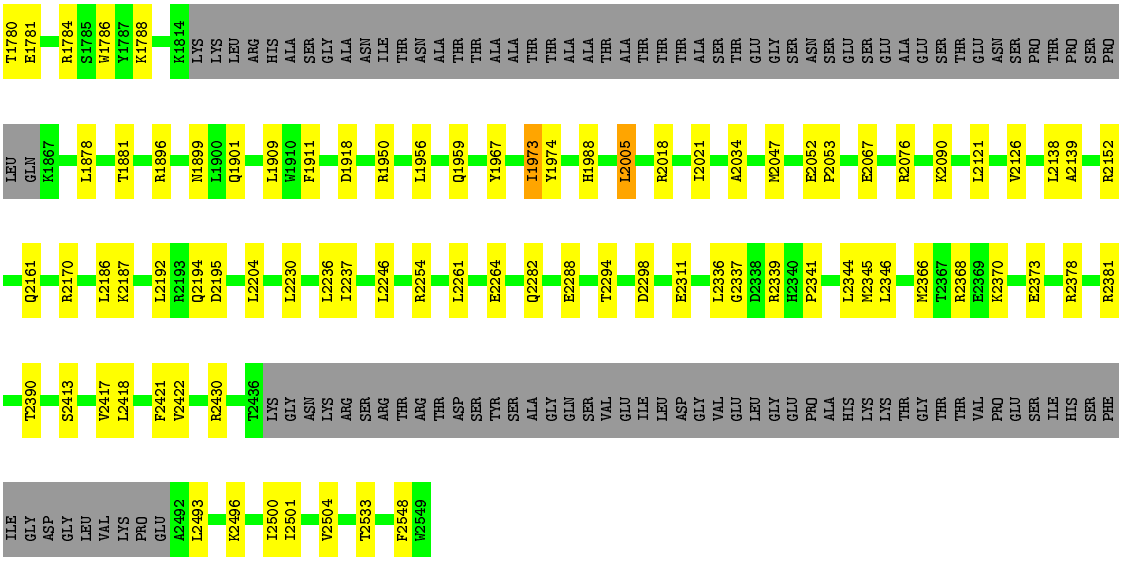
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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

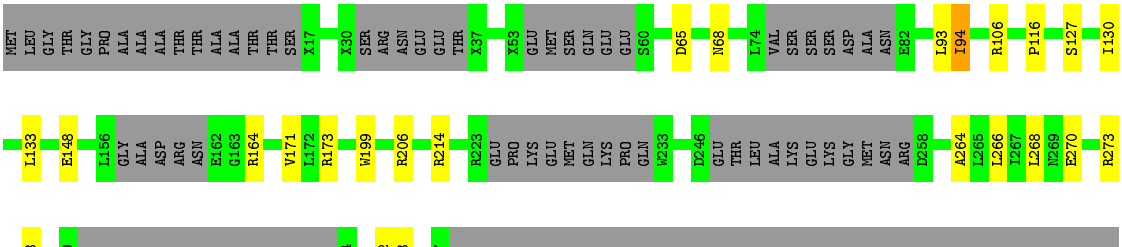
Chain B:

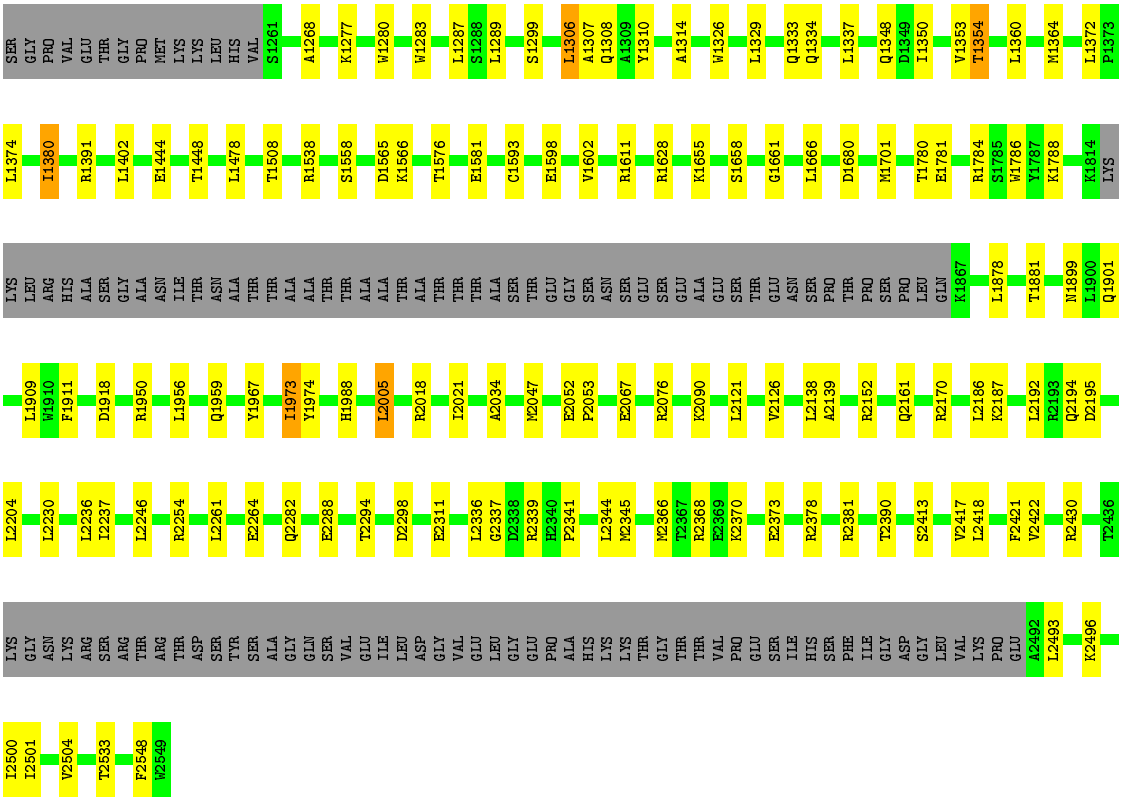




- Molecule 1: Serine/threonine-protein kinase mTOR

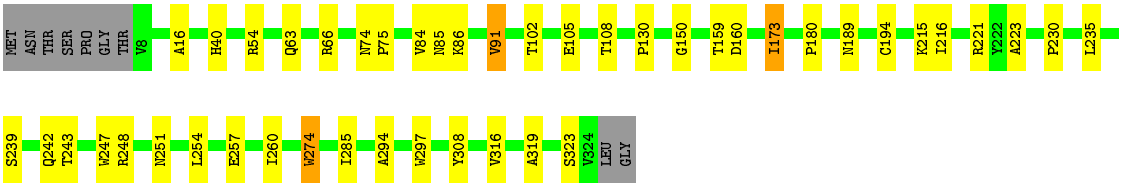
Chain A:





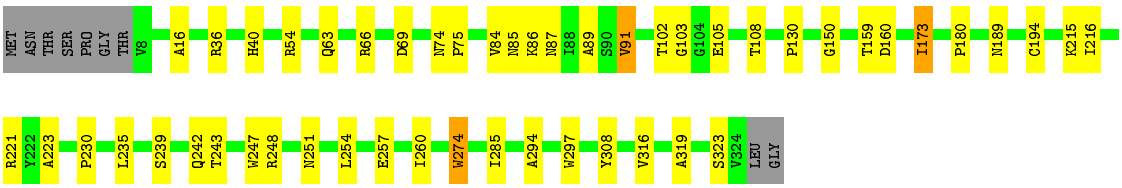
• Molecule 2: Target of rapamycin complex subunit LST8

Chain D:



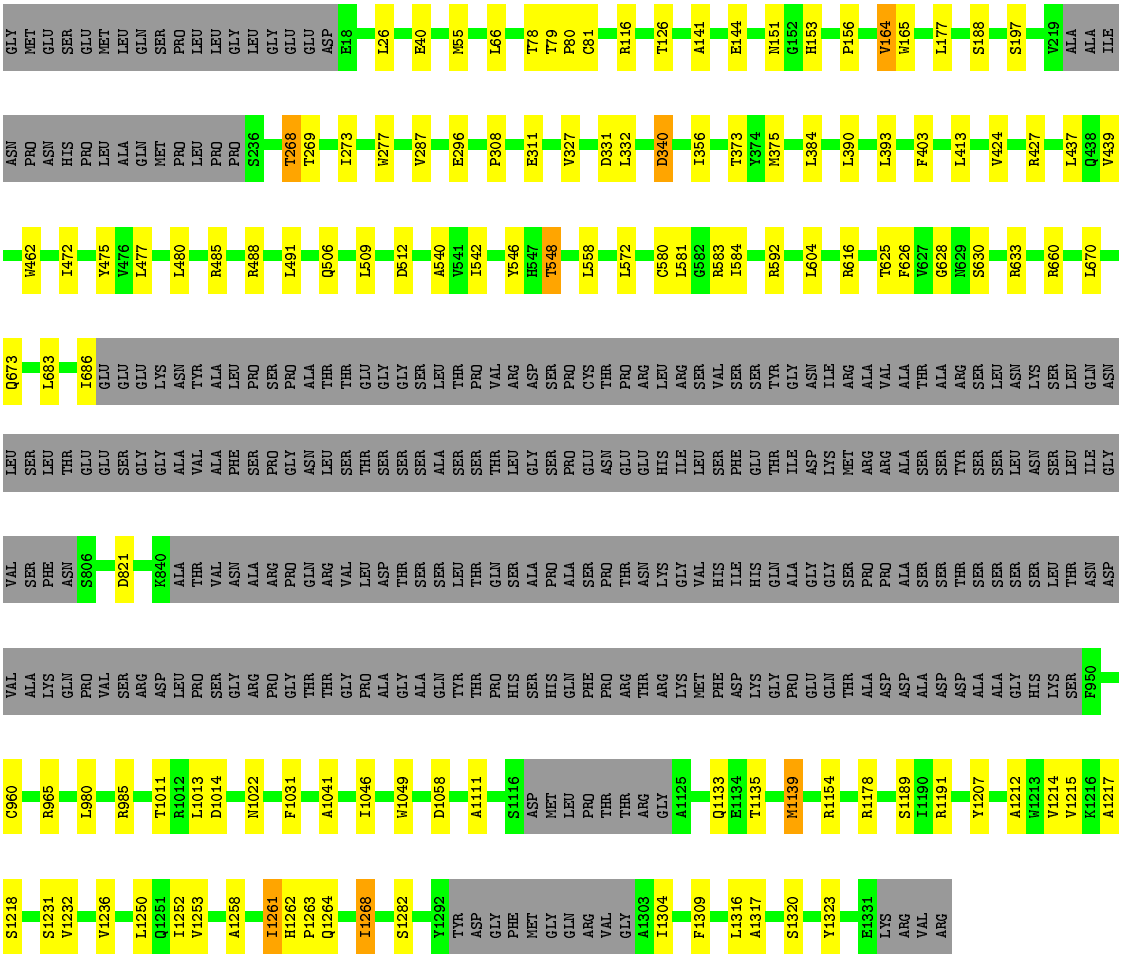
• Molecule 2: Target of rapamycin complex subunit LST8

Chain C:



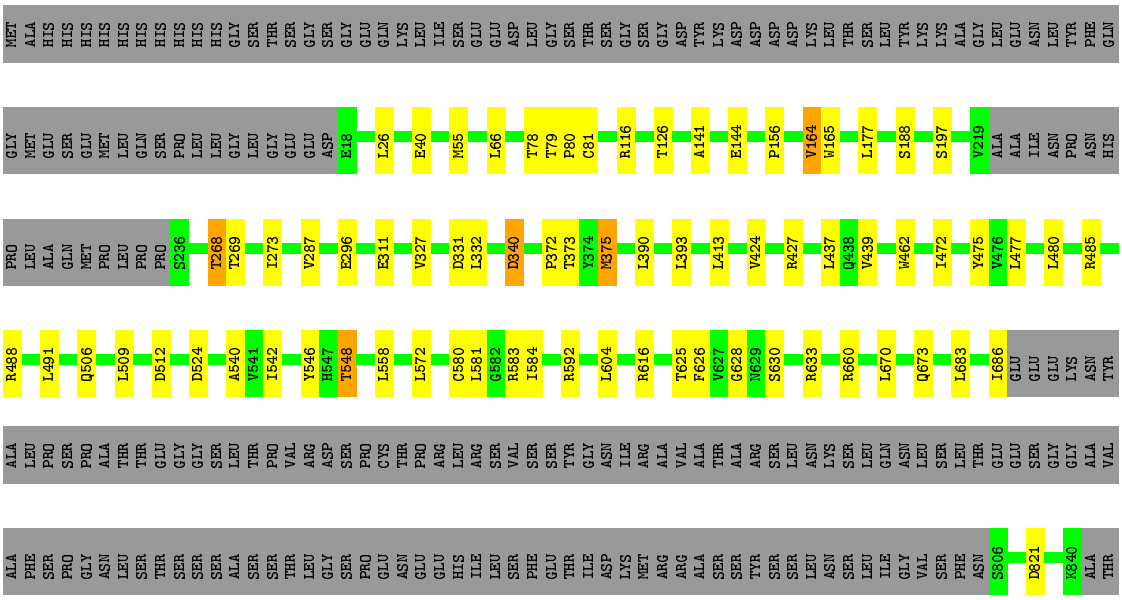
• Molecule 3: Regulatory-associated protein of mTOR

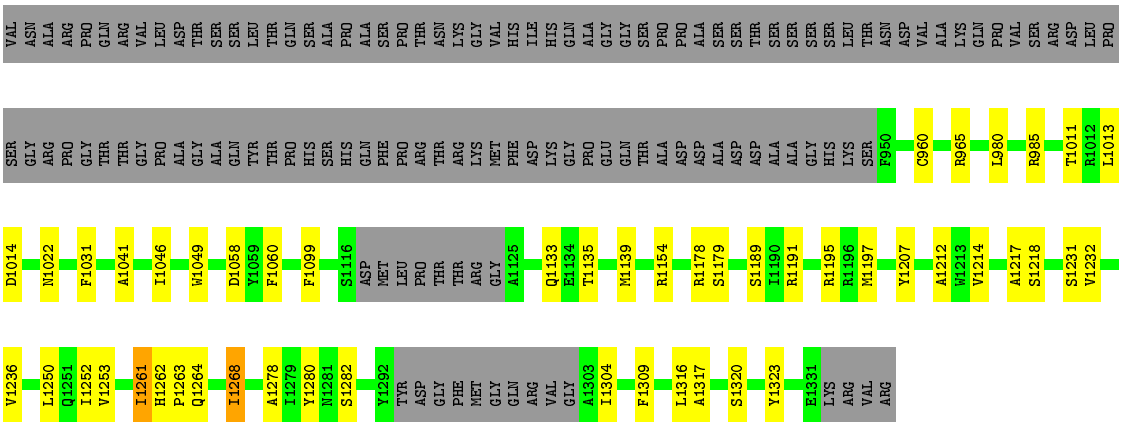
Chain F:



• Molecule 3: Regulatory-associated protein of mTOR

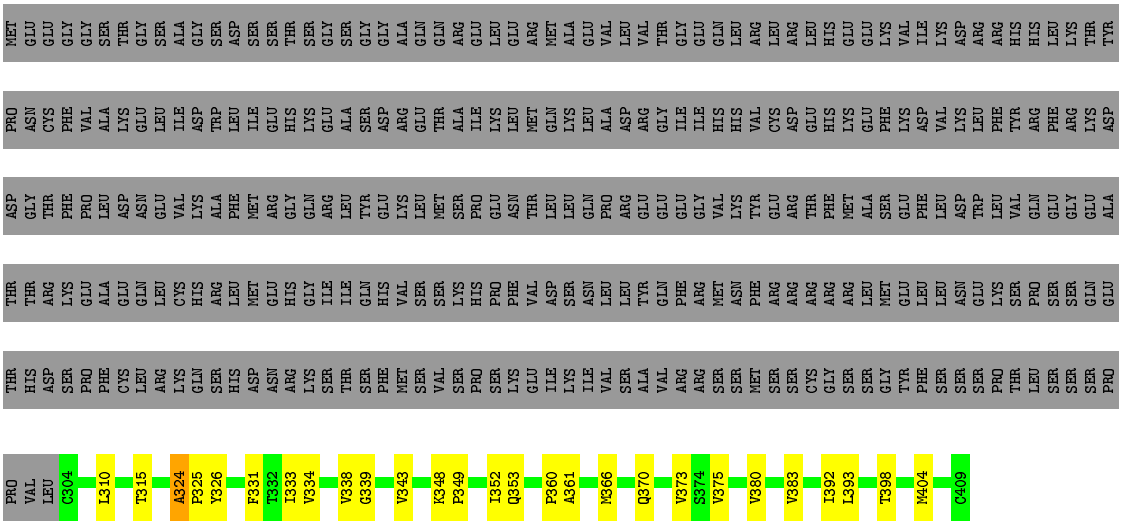
Chain E:





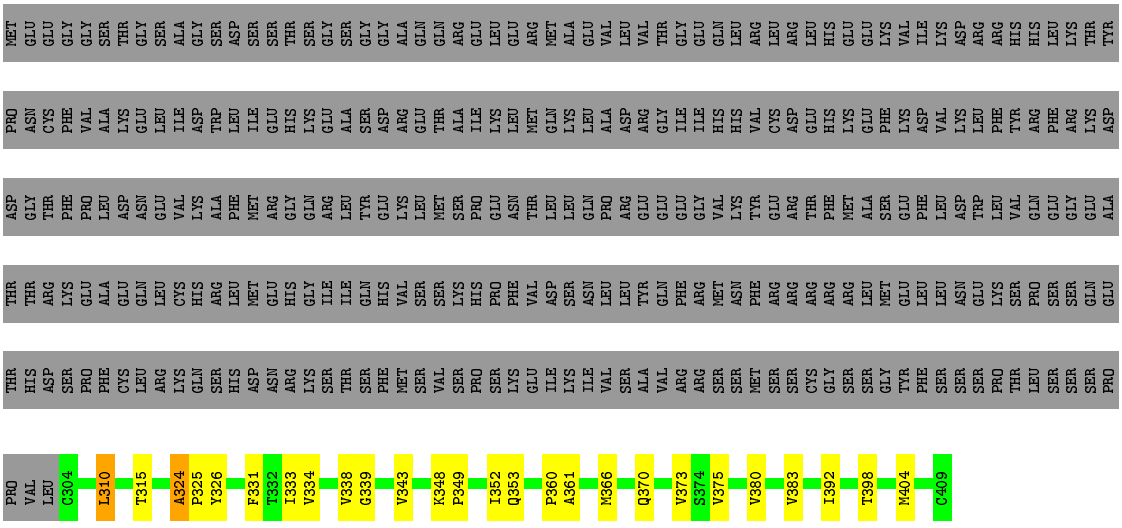
• Molecule 4: DEP domain-containing mTOR-interacting protein

Chain J:



• Molecule 4: DEP domain-containing mTOR-interacting protein

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	425076	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/17523	0.44	0/23716
1	B	0.23	0/17523	0.44	0/23716
2	C	0.24	0/2514	0.48	0/3426
2	D	0.24	0/2514	0.48	0/3426
3	E	0.23	0/8585	0.46	0/11680
3	F	0.23	0/8585	0.46	0/11680
4	I	0.24	0/811	0.51	0/1104
4	J	0.24	0/811	0.51	0/1104
All	All	0.23	0/58866	0.45	0/79852

There are no bond length outliers.

There are no bond angle outliers.

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	17454	0	17471	136	0
1	B	17454	0	17471	142	0
2	C	2456	0	2341	25	0
2	D	2456	0	2341	23	0
3	E	8385	0	8375	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	8385	0	8375	59	0
4	I	795	0	812	13	0
4	J	795	0	812	13	0
5	A	36	0	6	2	0
5	B	36	0	6	2	0
All	All	58252	0	58010	449	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.

The worst 5 of 449 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:1268:ALA:O	1:A:1283:TRP:NE1	2.25	0.68
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.27	0.68
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.27	0.67
3:E:1252:ILE:HG22	3:E:1253:VAL:HG23	1.77	0.67
3:F:1252:ILE:HG22	3:F:1253:VAL:HG23	1.77	0.66

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	2100/2549 (82%)	2031 (97%)	69 (3%)	0	100	100
1	B	2100/2549 (82%)	2031 (97%)	69 (3%)	0	100	100
2	C	315/326 (97%)	290 (92%)	25 (8%)	0	100	100
2	D	315/326 (97%)	289 (92%)	26 (8%)	0	100	100
3	E	1040/1396 (74%)	975 (94%)	65 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	1040/1396 (74%)	975 (94%)	65 (6%)	0	100	100
4	I	104/409 (25%)	95 (91%)	8 (8%)	1 (1%)	15	52
4	J	104/409 (25%)	95 (91%)	8 (8%)	1 (1%)	15	52
All	All	7118/9360 (76%)	6781 (95%)	335 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	324	ALA
4	I	324	ALA

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	1871/2169 (86%)	1798 (96%)	73 (4%)	32	58
1	B	1871/2169 (86%)	1797 (96%)	74 (4%)	31	57
2	C	269/276 (98%)	260 (97%)	9 (3%)	38	62
2	D	269/276 (98%)	260 (97%)	9 (3%)	38	62
3	E	928/1214 (76%)	895 (96%)	33 (4%)	35	60
3	F	928/1214 (76%)	895 (96%)	33 (4%)	35	60
4	I	89/364 (24%)	85 (96%)	4 (4%)	27	54
4	J	89/364 (24%)	85 (96%)	4 (4%)	27	54
All	All	6314/8046 (78%)	6075 (96%)	239 (4%)	36	59

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	1323	TYR
3	E	572	LEU
1	A	1044	MET
3	E	512	ASP

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Mol	Chain	Res	Type
4	I	315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	968	HIS
1	A	968	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	IHP	A	2601	-	36,36,36	0.79	2 (5%)	54,60,60	0.31	0
5	IHP	B	2601	-	36,36,36	0.79	2 (5%)	54,60,60	0.31	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	-	-	3/30/54/54	0/1/1/1
5	IHP	B	2601	-	-	3/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2601	IHP	P3-O13	3.05	1.65	1.59
5	B	2601	IHP	P3-O13	3.00	1.65	1.59
5	B	2601	IHP	P1-O11	2.07	1.63	1.59
5	A	2601	IHP	P1-O11	2.05	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2601	IHP	C2-O12-P2-O22
5	A	2601	IHP	C2-O12-P2-O22
5	B	2601	IHP	C3-O13-P3-O23
5	A	2601	IHP	C3-O13-P3-O23
5	B	2601	IHP	C6-O16-P6-O36

There are no ring outliers.

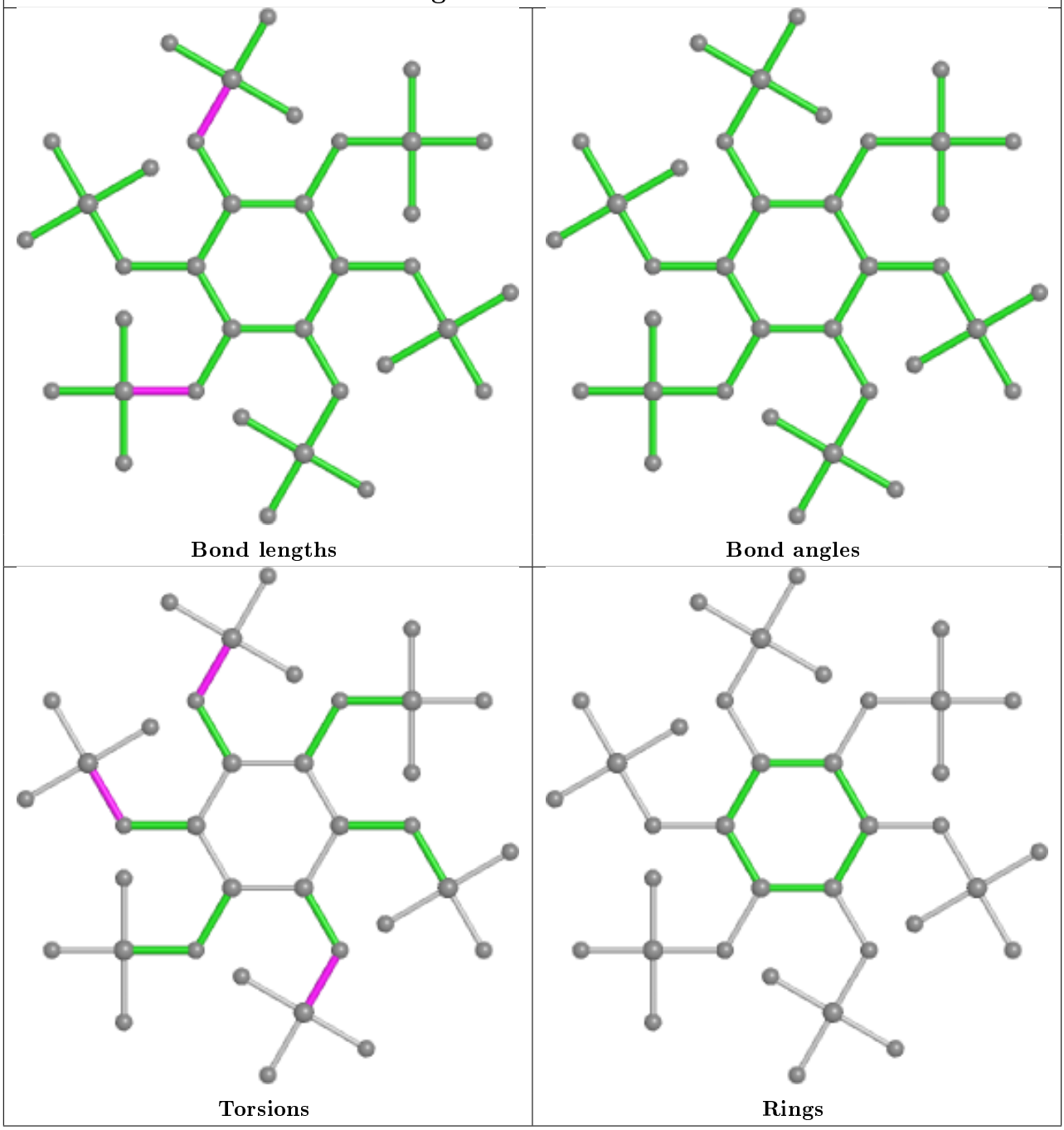
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2601	IHP	2	0
5	B	2601	IHP	2	0

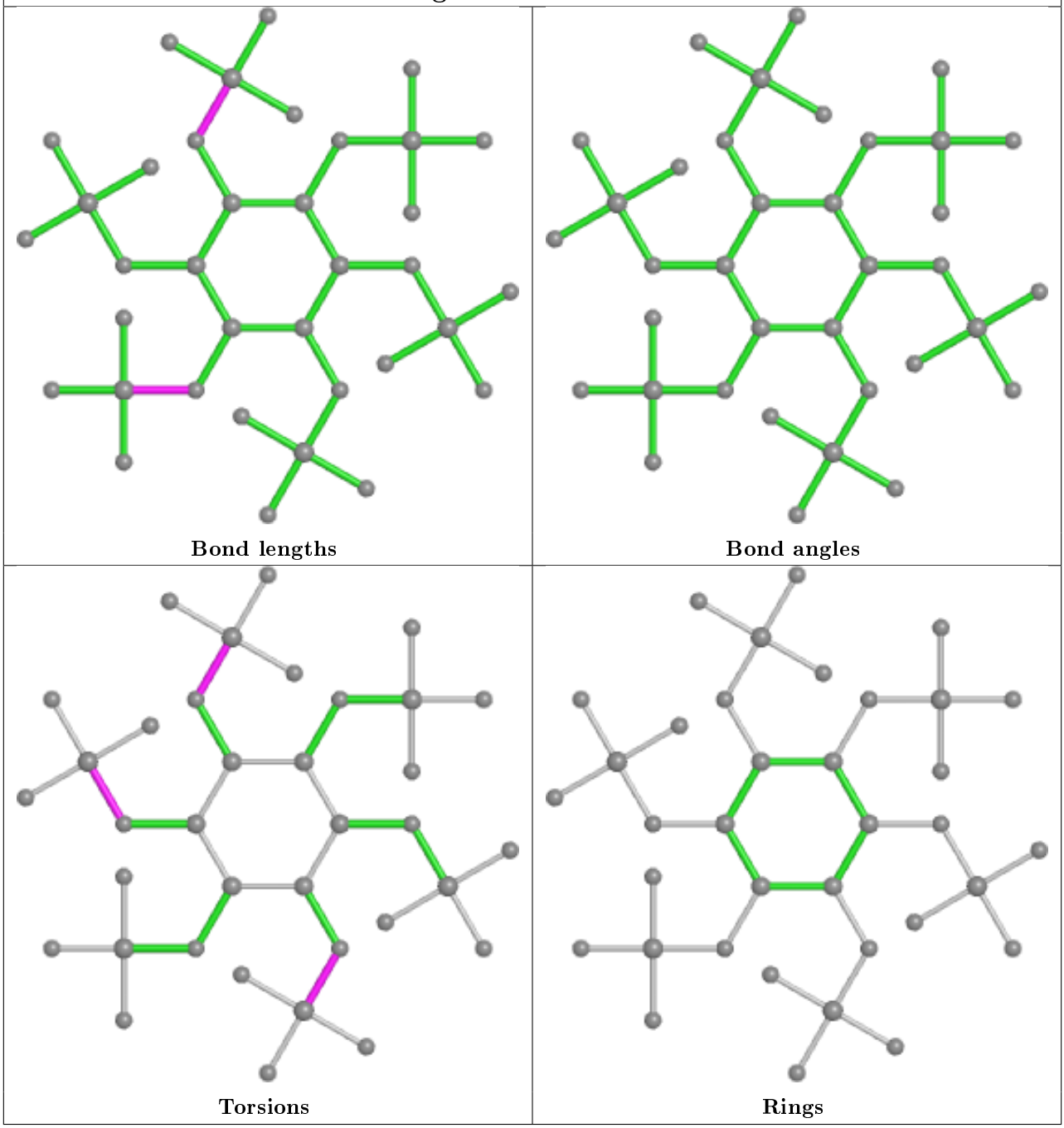
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 IHP A 2601



Ligand IHP B 2601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.