wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:19 PM BST

PDB ID	:	5FLC
EMDB ID:	:	EMD-3213
Title	:	Architecture of human mTOR Complex 1 - 5.9 Angstrom reconstruction
Authors	:	Aylett, C.H.S.; Sauer, E.; Imseng, S.; Boehringer, D.; Hall, M.N.; Ban, N.; Maier, T.
Deposited on	:	2015-10-23
Resolution	:	5.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

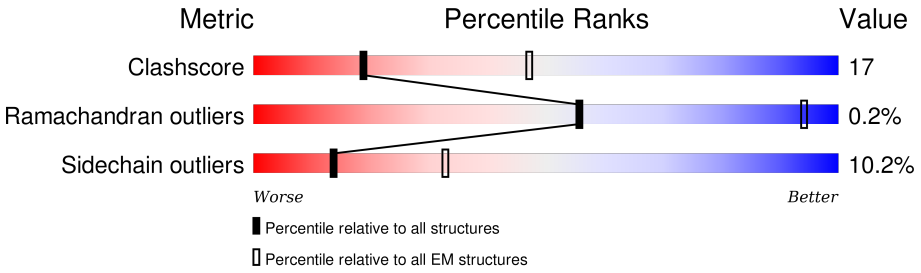
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 5.90 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	1	615	62% 38%
1	3	615	62% 38%
2	2	365	57% 43%
2	4	365	58% 42%
3	A	1029	76% 24%
3	E	1029	77% 23%
4	B	1168	53% 32% 5% 10%
4	F	1168	53% 32% 5% 10%
5	C	107	76% 24%

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Mol	Chain	Length	Quality of chain
5	G	107	
6	D	326	
6	H	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	RAP	C	999	X	-	-	-
7	RAP	G	999	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 47536 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	1	615	Total 3690	C 2460	N 615	O 615	0	0
1	3	615	Total 3690	C 2460	N 615	O 615	0	0

- Molecule 2 is a protein called SERINE/THREONINE-PROTEIN KINASE MTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	365	Total 2190	C 1460	N 365	O 365	0	0
2	4	365	Total 2190	C 1460	N 365	O 365	0	0

- Molecule 3 is a protein called REGULATORY-ASSOCIATED PROTEIN OF MTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	1029	Total 6174	C 4116	N 1029	O 1029	0	0
3	E	1029	Total 6174	C 4116	N 1029	O 1029	0	0

- Molecule 4 is a protein called SERINE/THREONINE-PROTEIN KINASE MTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1050	Total 8551	C 5439	N 1506	O 1544	S 62	1	0
4	F	1050	Total 8551	C 5439	N 1506	O 1544	S 62	1	0

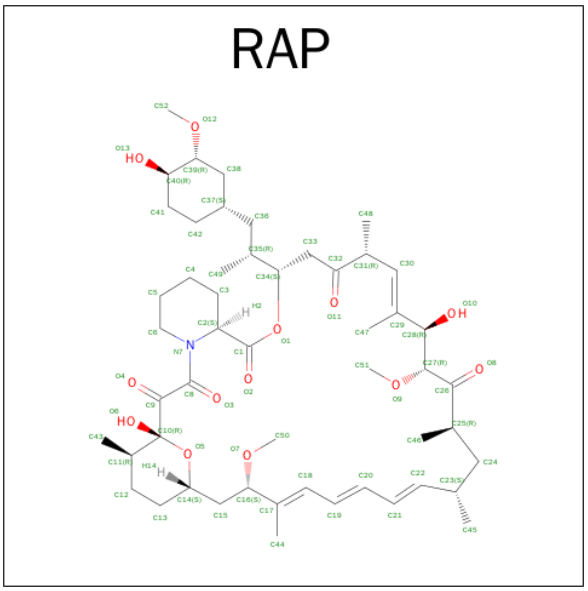
- Molecule 5 is a protein called FKBP.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	107	Total 642	C 428	N 107	O 107	0	0
5	G	107	Total 642	C 428	N 107	O 107	0	0

- Molecule 6 is a protein called TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8.

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

- Molecule 7 is RAPAMYCIN IMMUNOSUPPRESSANT DRUG (three-letter code: RAP) (formula: $C_{51}H_{79}NO_{13}$).



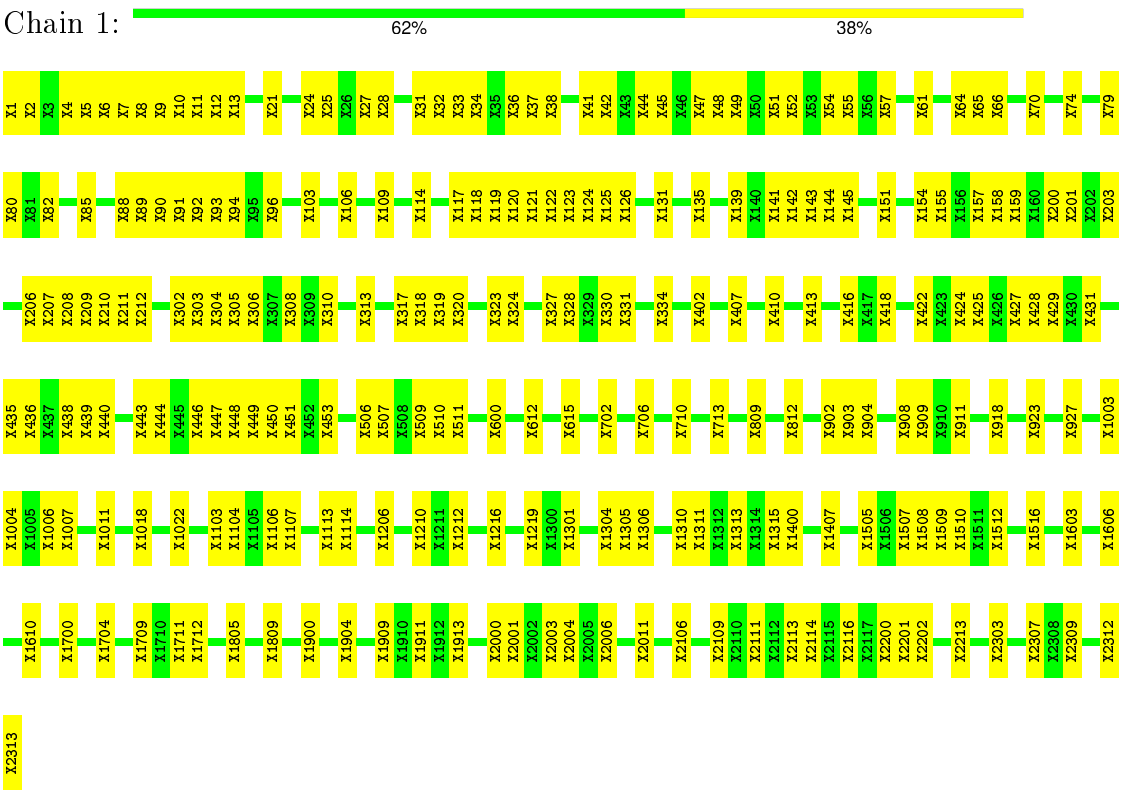
Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total 65	C 51	N 1	O 13	0
7	G	1	Total 65	C 51	N 1	O 13	0

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.

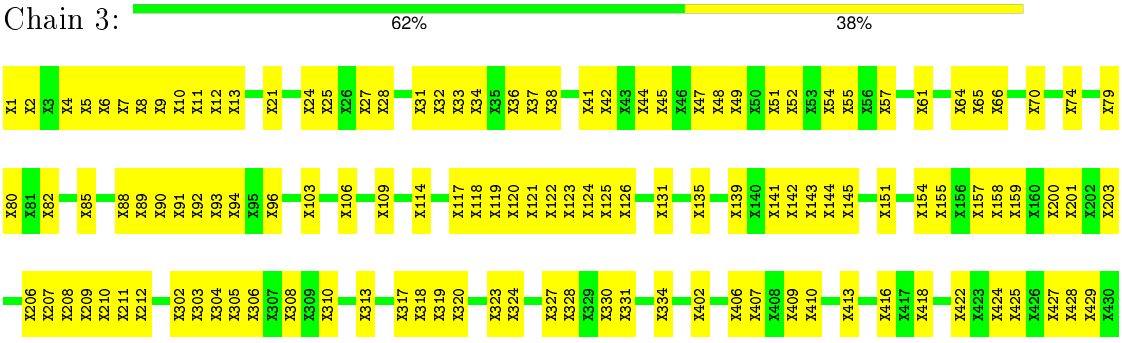
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE MTOR

Chain 1:



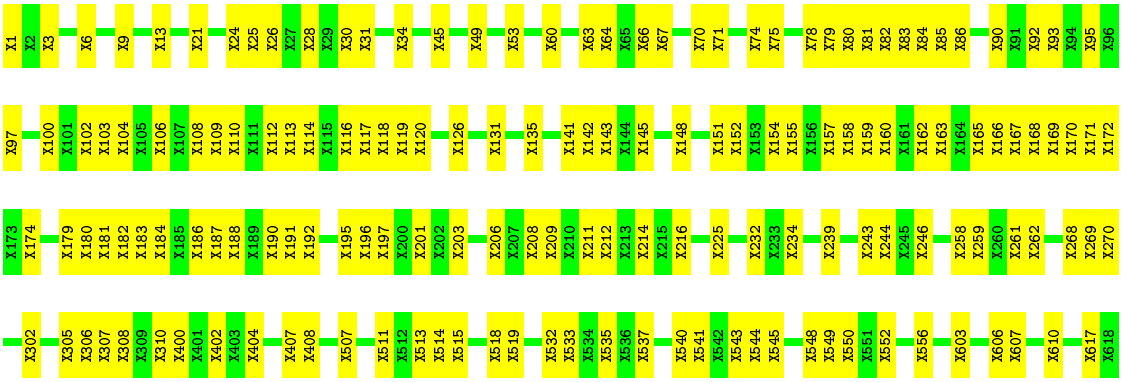
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE MTOR

Chain 3:



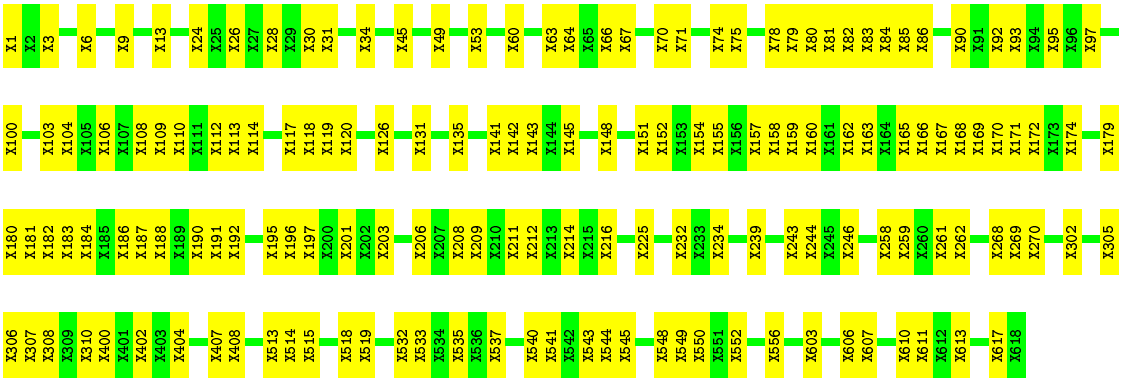
• Molecule 2: SERINE/THREONINE-PROTEIN KINASE MTOR

Chain 2:



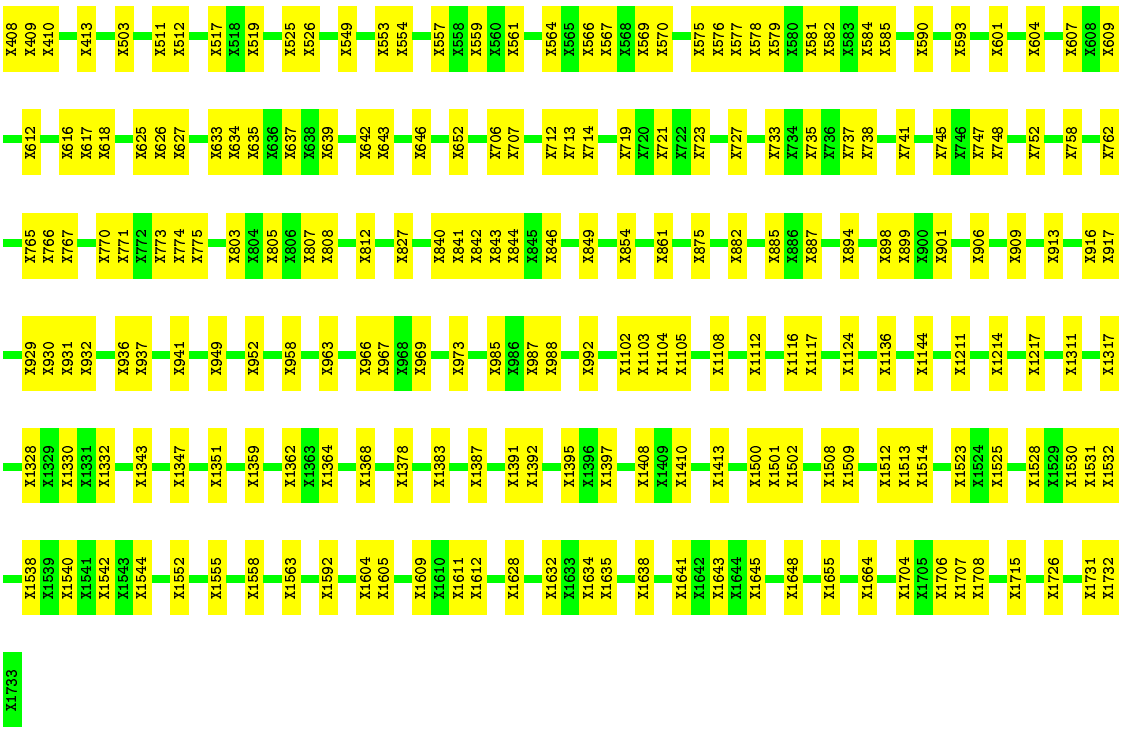
• Molecule 2: SERINE/THREONINE-PROTEIN KINASE MTOR

Chain 4:



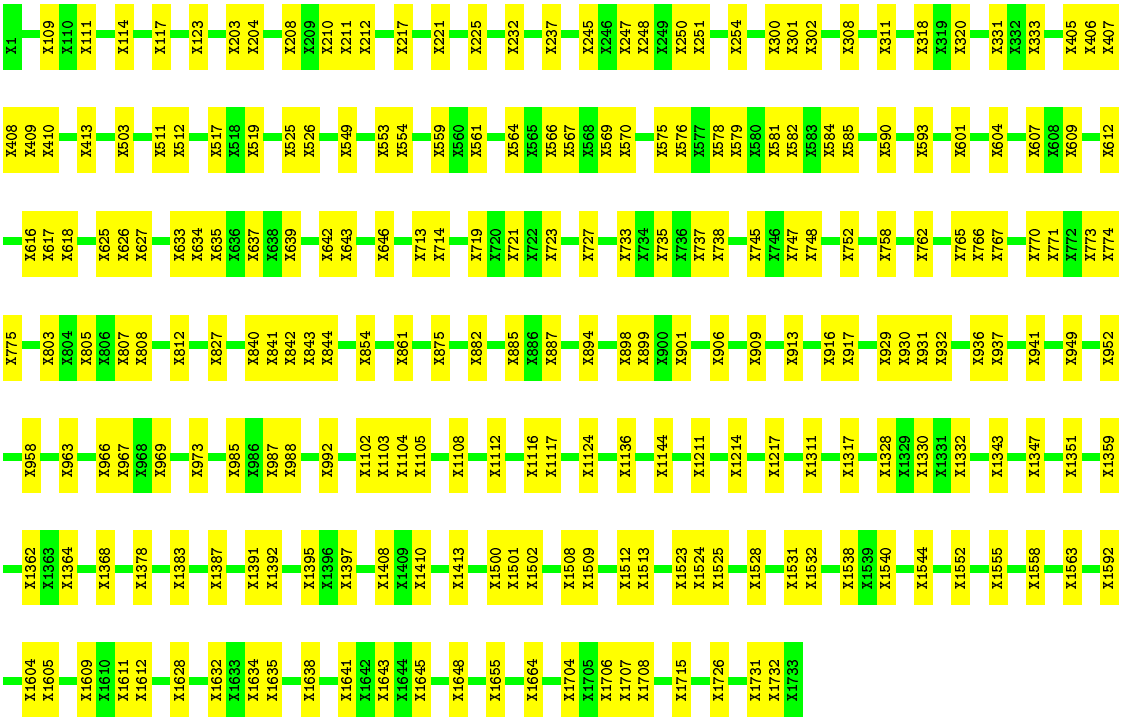
• Molecule 3: REGULATORY-ASSOCIATED PROTEIN OF MTOR

Chain A:



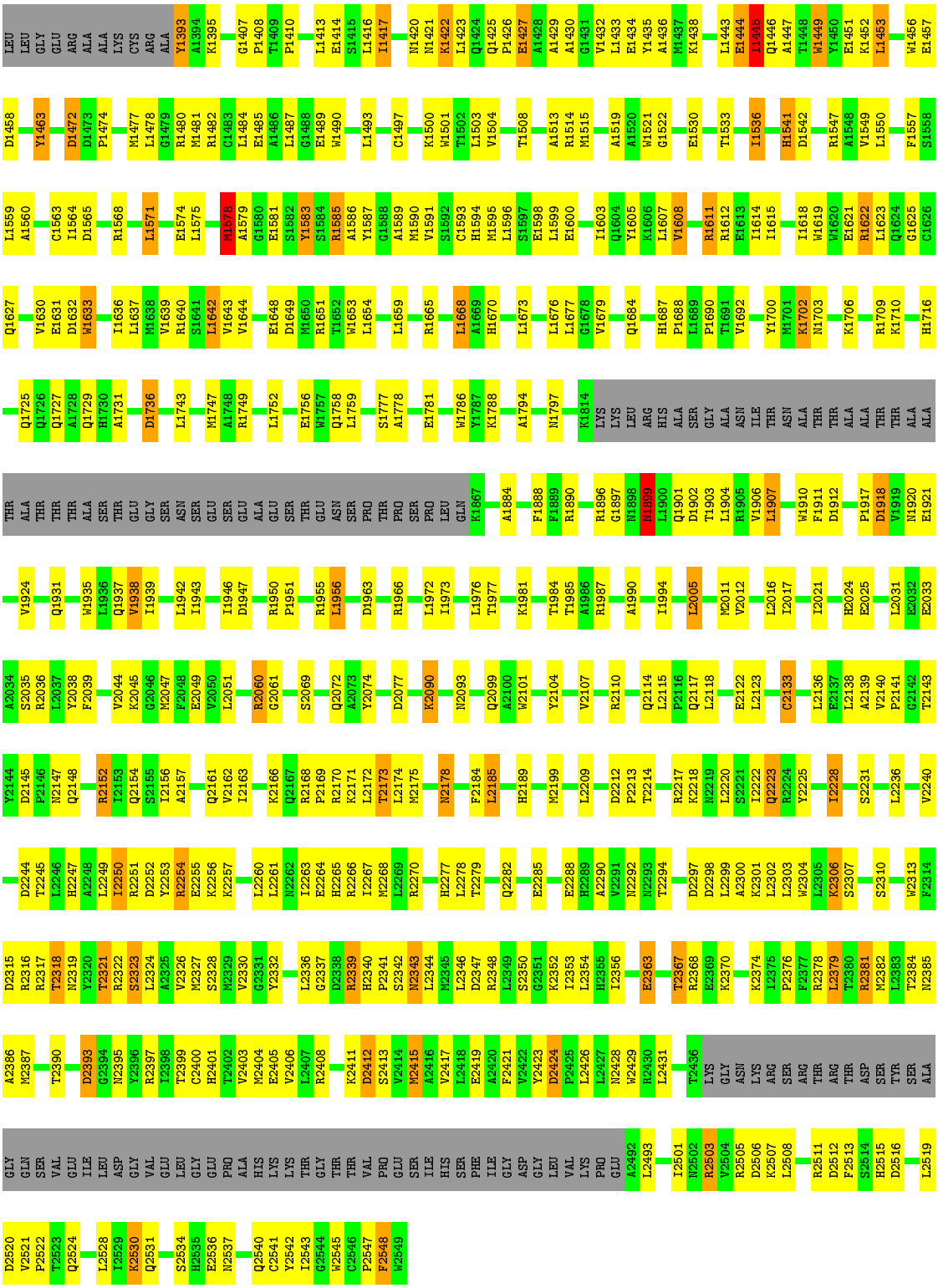
• Molecule 3: REGULATORY-ASSOCIATED PROTEIN OF MTOR

Chain E:



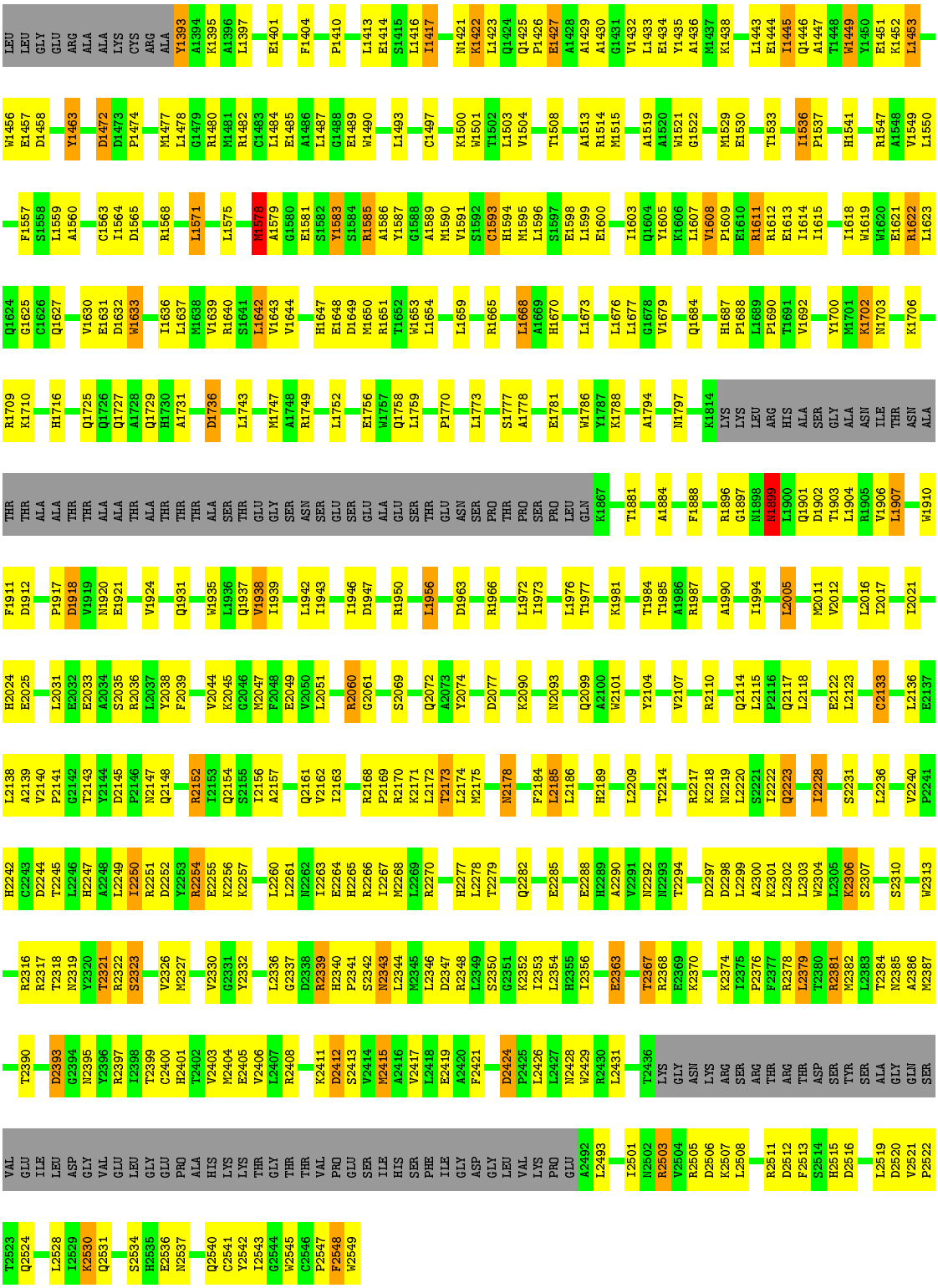
• Molecule 4: SERINE/THREONINE-PROTEIN KINASE MTOR

Chain B:



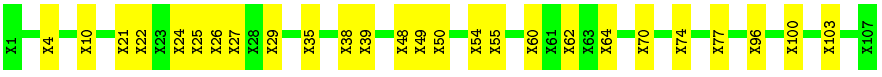
• Molecule 4: SERINE/THREONINE-PROTEIN KINASE MTOR

Chain F:



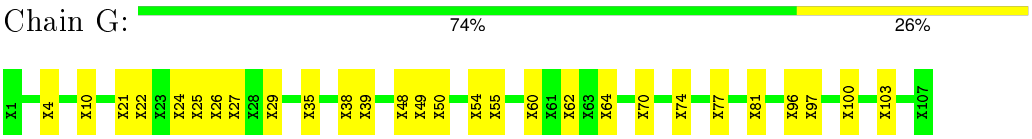
- Molecule 5: FKBP

Chain C:



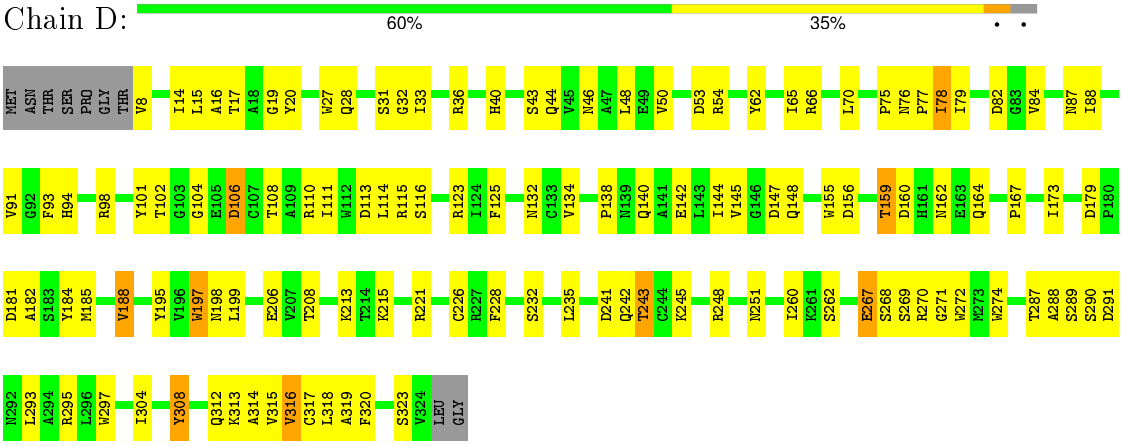
• Molecule 5: FKBP

Chain G:



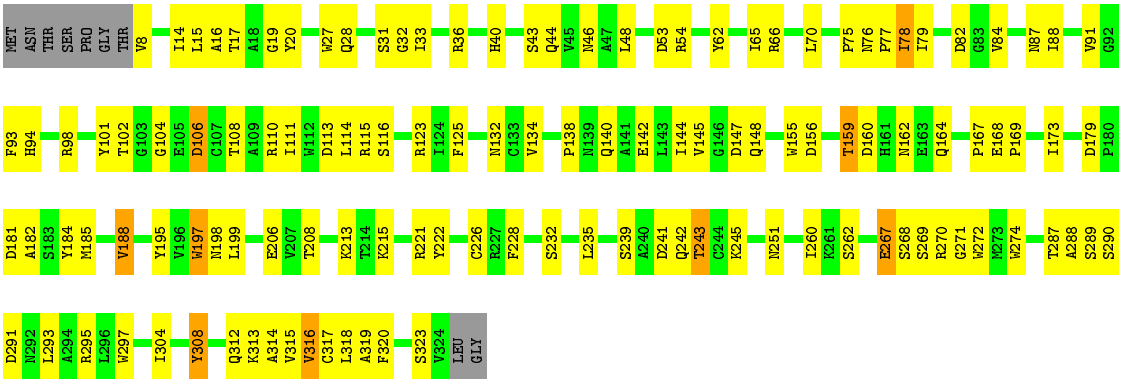
• Molecule 6: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8

Chain D:



• Molecule 6: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8

Chain H:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4K 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: RAP

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	#$\|Z\|>2$
4	B	0.36	1/8753 (0.0%)	0.55	3/11852 (0.0%)
4	F	0.36	1/8753 (0.0%)	0.54	2/11852 (0.0%)
6	D	0.26	0/2514	0.50	0/3426
6	H	0.26	0/2514	0.50	0/3426
All	All	0.34	2/22534 (0.0%)	0.54	5/30556 (0.0%)

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
2	2	0	1
2	4	0	1
4	B	0	5
4	F	0	4
6	D	0	1
6	H	0	1
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1583	TYR	CB-CG	5.54	1.59	1.51
4	F	1583	TYR	CB-CG	5.10	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1583	TYR	CA-CB-CG	6.74	126.21	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1583	TYR	CA-CB-CG	6.59	125.93	113.40
4	B	1445	ILE	N-CA-C	-5.12	97.18	111.00
4	F	2115	LEU	C-N-CD	5.01	138.93	128.40
4	B	2115	LEU	C-N-CD	5.01	138.93	128.40

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	216	UNK	Peptide
2	4	216	UNK	Peptide
4	B	1444	GLU	Peptide
4	B	1445	ILE	Peptide
4	B	1649	ASP	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	1	3690	0	3759	178	0
1	3	3690	0	3760	177	0
2	2	2190	0	2212	116	0
2	4	2190	0	2212	111	0
3	A	6174	0	6228	150	0
3	E	6174	0	6228	141	0
4	B	8551	0	8530	306	0
4	F	8551	0	8530	309	0
5	C	642	0	649	16	0
5	G	642	0	648	16	0
6	D	2456	0	2341	72	0
6	H	2456	0	2341	71	0
7	C	65	0	79	6	0
7	G	65	0	79	4	0
All	All	47536	0	47596	1607	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 17.

The worst 5 of 1607 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)
4:B:2419:GLU:HG2	4:B:2501:ILE:HG12	1.40	1.03
4:F:2419:GLU:HG2	4:F:2501:ILE:HG12	1.39	1.02
1:1:51:UNK:O	1:1:55:UNK:N	2.06	0.89
1:3:51:UNK:O	1:3:55:UNK:N	2.06	0.88
1:3:41:UNK:HB1	1:3:79:UNK:HG1	1.58	0.86

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	
4	B	1045/1168 (90%)	996 (95%)	47 (4%)	2 (0%)	52	86
4	F	1045/1168 (90%)	997 (95%)	46 (4%)	2 (0%)	52	86
6	D	315/326 (97%)	293 (93%)	21 (7%)	1 (0%)	46	83
6	H	315/326 (97%)	293 (93%)	21 (7%)	1 (0%)	46	83
All	All	2720/2988 (91%)	2579 (95%)	135 (5%)	6 (0%)	56	86

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	268	SER
6	H	268	SER
4	B	1578	MET
4	F	1578	MET
4	B	1679	VAL

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
4	B	927/1019 (91%)	829 (89%)	98 (11%)	8 36
4	F	927/1019 (91%)	828 (89%)	99 (11%)	8 36
6	D	269/276 (98%)	246 (91%)	23 (9%)	13 47
6	H	269/276 (98%)	246 (91%)	23 (9%)	13 47
All	All	2392/2590 (92%)	2149 (90%)	243 (10%)	14 38

5 of 243 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	173	ILE
4	F	1536	ILE
6	H	84	VAL
6	D	199	LEU
4	F	1422	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	153	HIS
4	F	1647	HIS
6	H	153	HIS
6	D	161	HIS
6	D	219	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
7	RAP	C	999	-	64,68,68	1.37	6 (9%)	63,96,96	2.91	21 (33%)
7	RAP	G	999	-	64,68,68	1.37	6 (9%)	63,96,96	2.91	21 (33%)

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
7	RAP	C	999	-	1/1/23/29	2/81/124/124	0/2/4/4
7	RAP	G	999	-	1/1/23/29	2/81/124/124	0/2/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	999	RAP	C8-C9	-5.20	1.47	1.53
7	G	999	RAP	C8-C9	-5.16	1.47	1.53
7	C	999	RAP	O1-C34	-2.03	1.42	1.46
7	G	999	RAP	O1-C34	-2.02	1.42	1.46
7	C	999	RAP	C27-C28	2.61	1.56	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	999	RAP	O5-C10-C11	-11.84	94.90	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	999	RAP	O5-C10-C11	-11.82	94.94	110.23
7	C	999	RAP	C48-C31-C30	-6.67	104.58	110.75
7	G	999	RAP	C48-C31-C30	-6.66	104.59	110.75
7	C	999	RAP	C43-C11-C12	-4.90	102.51	110.44

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	999	RAP	C10
7	C	999	RAP	C10

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	999	RAP	C50-O7-C16-C15
7	C	999	RAP	C50-O7-C16-C15
7	G	999	RAP	C31-C30-C29-C28
7	C	999	RAP	C31-C30-C29-C28

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	999	RAP	6	0
7	G	999	RAP	4	0

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.