wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2GAQ
Title	:	NMR SOLUTION STRUCTURE OF THE FRB DOMAIN OF mTOR
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This is a wwPDB NMR Structure 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

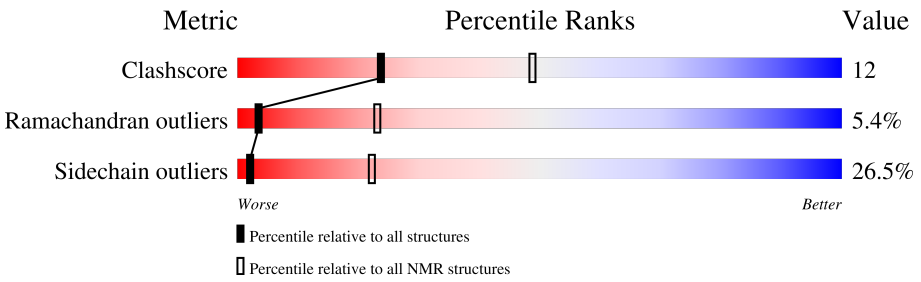
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	100	50% 39% • 7%

2 Ensemble composition and analysis (i)

This entry contains 19 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:7-A:99 (93)	0.56	19

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 6 single-model clusters were found.

Cluster number	Models
1	3, 5, 6, 14, 16, 19
2	1, 4, 7, 8, 18
3	10, 17
Single-model clusters	2; 9; 11; 12; 13; 15

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1674 atoms, of which 824 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FKBP12-rapamycin complex-associated protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	100	1674	542	824	150	151	7	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: FKBP12-rapamycin complex-associated protein

Chain A: 50% 39% • 7%

E1 L2 I3 R4 V5 A6 I7 L8 W9 H10 E11 M12 W13 H14 L17 L23 Y24 E27 V30 K31 G32 M33 F34 L37 E38 P39 L40 M44 T50 L51 K52 E53 T54 S55 F56 Y60 D63 L64 A67 Q68 E69 W70 K73 Y74 M75 L83 W87

Y90 V93 F94 R95 R96 I97 S98 K99 Q100

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 19. Colouring as in section 4.1 above.

• Molecule 1: FKBP12-rapamycin complex-associated protein

Chain A: 54% 33% • • 7%

E1 L2 I3 R4 V5 A6 I7 L8 W9 H10 E11 M12 W13 H14 E15 G16 L17 E27 F34 L37 L40 H41 A42 M43 M44 E45 R46 T50 L51 K52 E53 Q58 A59 Y60 D63 L64 A67 Q68 C71 Y74 M75 N79 L83 W87 Y90

V93 R96 I97 S98 K99 Q100

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics energy minimization.*

Of the 100 calculated structures, 19 were deposited, based on the following criterion: *structures with the least restraint violations.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DYANA	structure solution	1.5
GROMOS	refinement	96

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (average) 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	0.79±0.01	0±0/815 (0.0± 0.0%)	1.10±0.03	1±1/1096 (0.1± 0.1%)
All	All	0.79	0/15485 (0.0%)	1.10	22/20824 (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	Planarity
1	A	0.0±0.0	2.3±1.4
All	All	0	43

There are no bond-length outliers.

5 of 7 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	74	TYR	CB-CG-CD2	-6.21	117.27	121.00	12	7
1	A	90	TYR	CB-CG-CD2	-6.18	117.29	121.00	13	6
1	A	54	THR	CA-CB-CG2	5.77	120.47	112.40	6	4
1	A	34	PHE	CB-CG-CD2	-5.68	116.83	120.80	19	2
1	A	56	PHE	CB-CG-CD2	-5.39	117.03	120.80	2	1

There are no chirality outliers.

5 of 17 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	74	TYR	Sidechain	5
1	A	24	TYR	Sidechain	5
1	A	17	LEU	Mainchain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	71	CYS	Mainchain	4
1	A	13	TRP	Mainchain	4

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	792	760	760	19±4
All	All	15048	14440	14440	357

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 12.

5 of 207 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:LEU:HD12	1:A:87:TRP:CZ2	0.80	2.11	17	1
1:A:60:TYR:CZ	1:A:93:VAL:HG11	0.80	2.11	13	1
1:A:37:LEU:HD12	1:A:40:LEU:HD12	0.78	1.54	11	2
1:A:13:TRP:HB3	1:A:97:ILE:HD12	0.77	1.55	18	1
1:A:74:TYR:CD1	1:A:83:LEU:HD21	0.69	2.23	19	2

6.3 Torsion angles (i)

6.3.1 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 NMR 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	93/100 (93%)	73±2 (79±2%)	15±2 (16±2%)	5±1 (5±1%)	3 23
All	All	1767/1900 (93%)	1389 (79%)	283 (16%)	95 (5%)	3 23

5 of 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of

occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	51	LEU	19
1	A	50	THR	16
1	A	63	ASP	12
1	A	7	ILE	10
1	A	8	LEU	8

6.3.2 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 NMR 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	82/88 (93%)	60±3 (73±4%)	22±3 (27±4%)	2 22
All	All	1558/1672 (93%)	1145 (73%)	413 (27%)	2 22

5 of 67 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	7	ILE	17
1	A	13	TRP	16
1	A	10	HIS	16
1	A	27	GLU	15
1	A	37	LEU	15

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided