wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2KM4
Title	:	Solution structure of Rtt103 CTD interacting domain
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Deposited on	:	2009-07-20

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

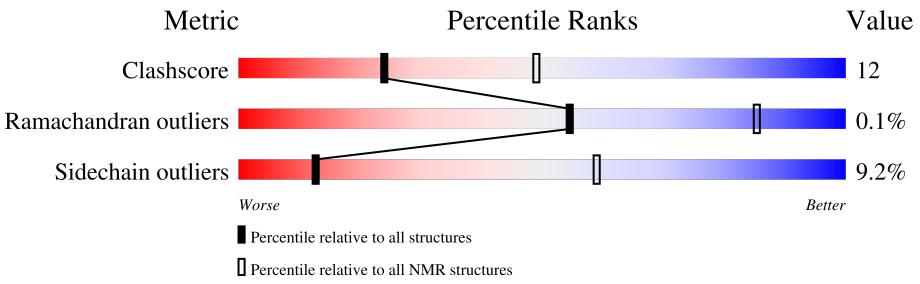
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	142	65% 23% • 7% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 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:5-A:131 (127)	0.52	2

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 7, 8, 10, 14, 17
2	6, 9, 12, 18, 20
3	11, 13, 15, 16, 19

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2268 atoms, of which 1151 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Regulator of Ty1 transposition protein 103.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	137	2268	709	1151	202	203	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	PRO	conflict	UNP Q05543
A	132	ALA	-	expression tag	UNP Q05543
A	133	ALA	-	expression tag	UNP Q05543
A	134	ALA	-	expression tag	UNP Q05543
A	135	LEU	-	expression tag	UNP Q05543
A	136	GLU	-	expression tag	UNP Q05543
A	137	HIS	-	expression tag	UNP Q05543
A	138	HIS	-	expression tag	UNP Q05543
A	139	HIS	-	expression tag	UNP Q05543
A	140	HIS	-	expression tag	UNP Q05543
A	141	HIS	-	expression tag	UNP Q05543
A	142	HIS	-	expression tag	UNP Q05543

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: Regulator of Ty1 transposition protein 103

Chain A: 65% 23% • 7% •

MET A2 F3 S4 F8 L12 L15 L29 L30 D35 A36 P37 K38 V39 Y46 V52 N53 T54 L58 L61 Y62 L63 M64 V67 V68 A71 I76 F79 F83 G84 K85 V86 A87 V90 L91 P99 L102 K105 V109 S120

V124 I127 A132 A133 A134 L135 E136 H137 H138 HIS HIS HIS HIS

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

The representative model is number 2. Colouring as in section 4.1 above.

• Molecule 1: Regulator of Ty1 transposition protein 103

Chain A: 64% 24% • 7% •

MET A2 F3 S4 F8 T9 L12 L15 A25 L29 L30 D35 A36 P37 K38 V39 E45 Y46 M47 L48 V52 N53 T54 L58 L61 Y62 L63 M64 V67 A71 I76 V86 V90 L91 P99 L102 K103 K104 K105 V109 I112

V124 I127 A132 A133 A134 L135 E136 H137 H138 HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 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
CYANA	refinement	2.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1043	1086	1086	26±2
All	All	20860	21720	21720	510

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 126 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ALA:HB3	1:A:63:LEU:HD11	0.97	1.36	10	3
1:A:29:LEU:HD13	1:A:67:VAL:HG21	0.74	1.57	15	5
1:A:91:LEU:HD13	1:A:127:ILE:HG23	0.72	1.61	19	1
1:A:8:PHE:CZ	1:A:12:LEU:HD11	0.69	2.22	13	15
1:A:13:ASN:OD1	1:A:14:THR:HG23	0.67	1.89	14	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	127/142 (89%)	124±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	54 85
All	All	2540/2840 (89%)	2483 (98%)	54 (2%)	3 (0%)	54 85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	118	ILE	3

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	117/128 (91%)	106±2 (91±2%)	11±2 (9±2%)	13 59
All	All	2340/2560 (91%)	2125 (91%)	215 (9%)	13 59

5 of 48 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	54	THR	20
1	A	64	MET	20
1	A	30	LEU	17
1	A	61	LEU	17
1	A	79	PHE	14

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