wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2ADB
Title	:	Solution structure of Polypyrimidine Tract Binding protein RBD2 complexed with CUCUCU RNA
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Deposited on	:	2005-07-20

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
http://wwpdb.org/validation/2016/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:

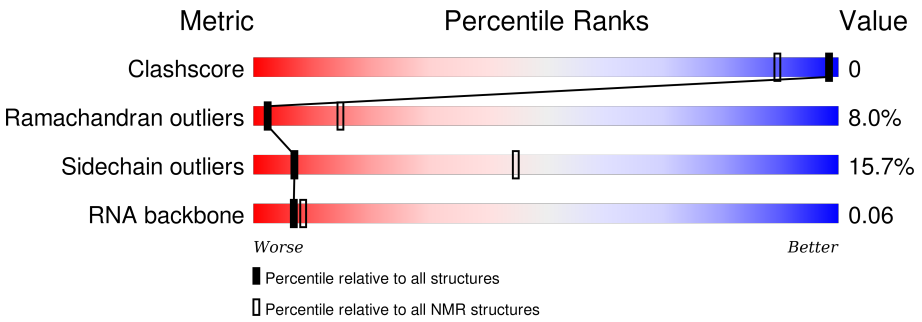
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958
RNA backbone	3027	600

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	B	6	17% 67% 17%
2	A	148	60% 16% • 9% 14%

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: *lowest energy*.

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:180-A:282 (103)	0.50	2
2	A:287-A:297 (11)	0.21	1

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2154 atoms, of which 1048 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(*CP*UP*CP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	6	182	54	65	15	43	5	0

- Molecule 2 is a protein called Polypyrimidine tract-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	127	1972	627	983	167	190	5	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	MET	-	EXPRESSION TAG	UNP P26599
A	152	GLY	-	EXPRESSION TAG	UNP P26599
A	153	SER	-	EXPRESSION TAG	UNP P26599
A	154	SER	-	EXPRESSION TAG	UNP P26599
A	155	HIS	-	EXPRESSION TAG	UNP P26599
A	156	HIS	-	EXPRESSION TAG	UNP P26599
A	157	HIS	-	EXPRESSION TAG	UNP P26599
A	158	HIS	-	EXPRESSION TAG	UNP P26599
A	159	HIS	-	EXPRESSION TAG	UNP P26599
A	160	HIS	-	EXPRESSION TAG	UNP P26599
A	161	SER	-	EXPRESSION TAG	UNP P26599
A	162	SER	-	EXPRESSION TAG	UNP P26599
A	163	GLY	-	EXPRESSION TAG	UNP P26599
A	164	LEU	-	EXPRESSION TAG	UNP P26599
A	165	VAL	-	EXPRESSION TAG	UNP P26599
A	166	PRO	-	EXPRESSION TAG	UNP P26599
A	167	ARG	-	EXPRESSION TAG	UNP P26599
A	168	GLY	-	EXPRESSION TAG	UNP P26599
A	169	SER	-	EXPRESSION TAG	UNP P26599
A	170	HIS	-	EXPRESSION TAG	UNP P26599
A	171	MET	-	EXPRESSION TAG	UNP P26599

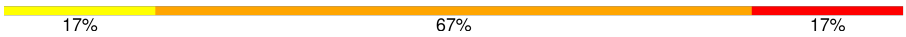
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

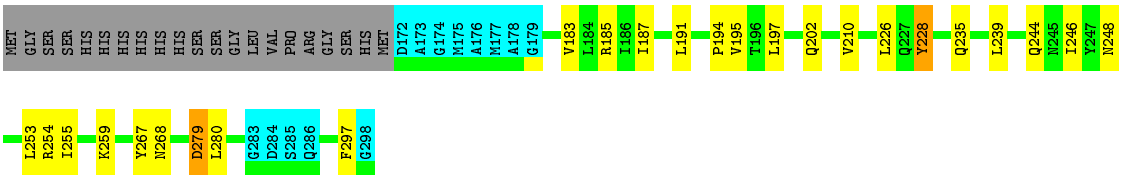
- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*U)-3'

Chain B:



- Molecule 2: Polypyrimidine tract-binding protein 1

Chain A:

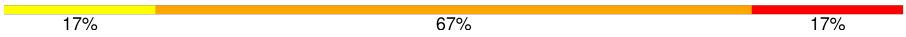


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

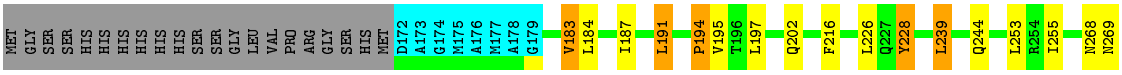
- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*U)-3'

Chain B:



- Molecule 2: Polypyrimidine tract-binding protein 1

Chain A:



R273
R277
P278
D279
L280
G283
D284
S285
Q286
A294
F297
G298

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry simulated annealing.*

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
DYANA	structure solution	3.02
AMBER	refinement	7

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	B	1.34±0.04	0±0/128 (0.0±0.0%)	2.20±0.11	7±1/196 (3.5±0.6%)
2	A	0.71±0.00	0±0/930 (0.0±0.0%)	1.22±0.03	3±2/1265 (0.2±0.1%)
All	All	0.81	0/21160 (0.0%)	1.40	188/29220 (0.6%)

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	B	0.0±0.0	2.1±0.9
2	A	0.0±0.0	5.2±2.0
All	All	0	145

There are no bond-length outliers.

5 of 36 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	B	304	U	O4'-C1'-N1	10.53	116.62	108.20	19	8
2	A	254	ARG	NE-CZ-NH1	8.14	124.37	120.30	10	13
2	A	185	ARG	NE-CZ-NH1	8.04	124.32	120.30	14	9
1	B	302	U	O4'-C1'-N1	7.58	114.26	108.20	11	16
1	B	304	U	N3-C2-O2	-7.50	116.95	122.20	12	10

There are no chirality outliers.

5 of 30 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	A	228	TYR	Sidechain	18

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Mol	Chain	Res	Type	Group	Models (Total)
1	B	300	U	Sidechain	15
2	A	279	ASP	Peptide	13
1	B	301	C	Sidechain	13
2	A	253	LEU	Peptide	12

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	B	117	65	65	0±0
2	A	910	917	917	1±1
All	All	20540	19640	19640	18

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 0.

5 of 14 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:280:LEU:HD22	2:A:281:PRO:HD2	0.59	1.74	18	4
2:A:238:LYS:HB3	2:A:255:ILE:HD13	0.53	1.80	17	1
2:A:210:VAL:HG21	2:A:213:ILE:HD11	0.49	1.83	14	1
2:A:266:LYS:HE3	2:A:267:TYR:CE2	0.48	2.44	3	1
2:A:273:ARG:HA	2:A:280:LEU:HD12	0.47	1.87	16	1

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
2	A	114/148 (77%)	83±3 (73±3%)	22±3 (19±3%)	9±2 (8±2%)	2 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2280/2960 (77%)	1657 (73%)	441 (19%)	182 (8%)	2 15

5 of 30 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	279	ASP	20
2	A	280	LEU	19
2	A	239	LEU	19
2	A	268	ASN	15
2	A	297	PHE	15

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
2	A	104/128 (81%)	88±2 (84±2%)	16±2 (16±2%)	7 45
All	All	2080/2560 (81%)	1753 (84%)	327 (16%)	7 45

5 of 51 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)
2	A	202	GLN	19
2	A	255	ILE	19
2	A	187	ILE	16
2	A	259	LYS	16
2	A	197	LEU	15

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	6/6 (100%)	4±1 (68±13%)	2±1 (27±15%)	0.07±0.10
All	All	104/120 (87%)	82 (79%)	32 (31%)	0.06

The overall RNA backbone suiteness is 0.06.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	301	C	20
1	B	300	U	18
1	B	304	U	16
1	B	303	C	16
1	B	302	U	12

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	300	U	15
1	B	301	C	7
1	B	303	C	6
1	B	299	C	4

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 carbohydrates 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