wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2I2Y
Title	:	Solution structure of the RRM of SRp20 bound to the RNA CAUC
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Deposited on	:	2006-08-17

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:

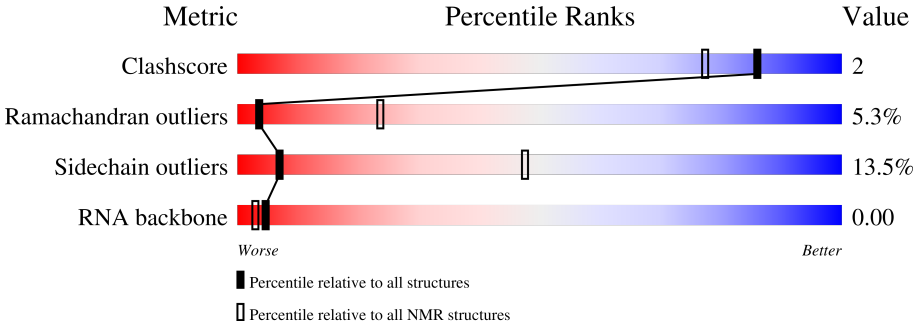
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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
RNA backbone	4643	676

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	4	50% 50%
2	A	150	57% 14% • 27%

2 Ensemble composition and analysis (i)

This entry contains 28 models. Model 9 is the overall representative, medoid model (most similar to other models).

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:2-A:8, A:13-A:55 (50)	0.14	18
2	A:75-A:79, A:87-A:106, A:112-A:145 (59)	0.37	9

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 8 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 6, 12, 15, 18, 21
2	9, 14, 26, 28
3	3, 5, 16, 24
4	8, 11
5	13, 19
Single-model clusters	7; 10; 17; 20; 22; 23; 25; 27

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2429 atoms, of which 1165 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	4	124	37	45	13	26	3	0

- Molecule 2 is a protein called Fusion protein consists of immunoglobulin G-Binding Protein G and Splicing factor, arginine/serine-rich 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	150	2305	733	1120	216	230	6	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P19909
A	2	GLN	-	cloning artifact	UNP P19909
A	57	GLY	-	cloning artifact	UNP P19909
A	58	SER	-	cloning artifact	UNP P19909
A	59	HIS	-	expression tag	UNP P84103
A	60	HIS	-	expression tag	UNP P84103
A	61	HIS	-	expression tag	UNP P84103
A	62	HIS	-	expression tag	UNP P84103
A	63	HIS	-	expression tag	UNP P84103
A	64	HIS	-	expression tag	UNP P84103

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

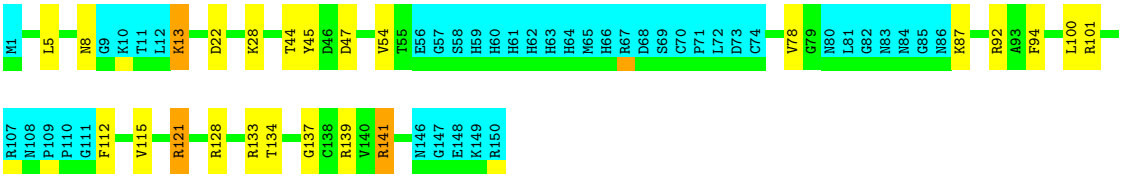
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: (5'-R(*CP*AP*UP*C)-3')

Chain B: 50% 50%

• Molecule 2: Fusion protein consists of immunoglobulin G-Binding Protein G and Splicing factor, arginine/serine-rich 3

Chain A: 57% 14% • 27%



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

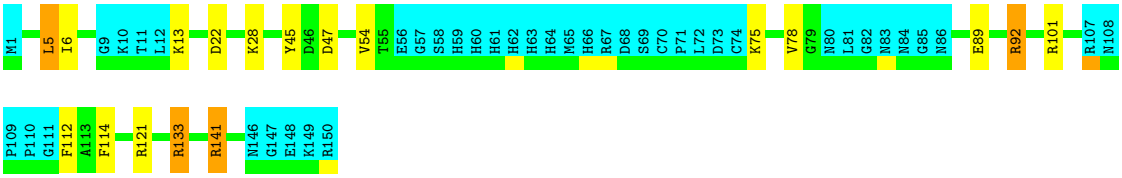
The representative model is number 9. Colouring as in section 4.1 above.

• Molecule 1: (5'-R(*CP*AP*UP*C)-3')

Chain B: 25% 75%

• Molecule 2: Fusion protein consists of immunoglobulin G-Binding Protein G and Splicing factor, arginine/serine-rich 3

Chain A: 61% 9% • 27%


M1
L5
I6
G9
K10
T11
L12
K13
D22
K28
Y45
D46
D47
V54
T55
E56
G57
S58
H59
H60
H61
H62
H63
H64
M65
H66
R67
D68
S69
C70
P71
L72
D73
C74
K75
V78
G79
N80
L81
G82
N83
N84
G85
N86
E89
R92
R101
R107
N108

P109
P110
G111
F112
A113
F114
R121
R133
R141
N146
G147
E148
K149
R150

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *AMBER 7*.

Of the 50 calculated structures, 28 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
DIANA	structure solution	
Amber 7	refinement	

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	B	1.49±0.03	0±0/87 (0.0± 0.0%)	2.85±0.14	12±2/133 (9.1± 1.7%)
2	A	0.76±0.01	0±0/883 (0.0± 0.0%)	1.28±0.03	6±2/1199 (0.5± 0.1%)
All	All	0.85	0/27160 (0.0%)	1.51	513/37296 (1.4%)

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	1.4±0.8
2	A	0.0±0.0	2.0±0.8
All	All	0	96

There are no bond-length outliers.

5 of 55 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	154	C	O4'-C1'-N1	12.59	118.27	108.20	1	25
2	A	141	ARG	NE-CZ-NH1	11.15	125.88	120.30	7	24
1	B	152	A	N1-C6-N6	-10.76	112.15	118.60	8	28
2	A	121	ARG	NE-CZ-NH1	10.55	125.57	120.30	3	27
1	B	152	A	O4'-C1'-N9	10.01	116.21	108.20	16	11

There are no chirality outliers.

5 of 13 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	45	TYR	Sidechain	28

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Mol	Chain	Res	Type	Group	Models (Total)
1	B	154	C	Sidechain	24
1	B	153	U	Sidechain	11
2	A	77	TYR	Sidechain	10
1	B	152	A	Sidechain	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	B	79	45	45	0±0
2	A	865	831	831	4±2
All	All	26432	24528	24528	107

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 2.

5 of 31 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:94:PHE:CD1	2:A:130:LEU:HD23	0.64	2.28	18	2
2:A:5:LEU:HD22	2:A:30:PHE:HB3	0.58	1.74	19	12
2:A:94:PHE:CZ	2:A:115:VAL:HG11	0.55	2.36	6	3
2:A:18:THR:HG21	2:A:29:VAL:HG11	0.54	1.79	17	12
2:A:94:PHE:CE2	2:A:115:VAL:HG11	0.54	2.37	27	4

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	109/150 (73%)	92±2 (84±2%)	11±2 (10±2%)	6±2 (5±2%)	3 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3052/4200 (73%)	2571 (84%)	318 (10%)	163 (5%)	3 23

5 of 22 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	22	ASP	28
2	A	8	ASN	20
2	A	134	THR	19
2	A	137	GLY	18
2	A	54	VAL	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	89/124 (72%)	77±2 (87±3%)	12±2 (13±3%)	7 47
All	All	2492/3472 (72%)	2156 (87%)	336 (13%)	7 47

5 of 40 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	13	LYS	28
2	A	28	LYS	28
2	A	112	PHE	24
2	A	92	ARG	23
2	A	44	THR	22

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	4/4 (100%)	3±0 (75±0%)	1±1 (37±14%)	0.00±0.00
All	All	112/112 (100%)	84 (75%)	41 (37%)	0.00

The overall RNA backbone suiteness is 0.00.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	152	A	28
1	B	153	U	28
1	B	154	C	28

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	151	C	28
1	B	153	U	11
1	B	152	A	2

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