Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 02:34 AM BST

PDB ID	:	2M7S
Title	:	NMR structure of RNA recognition motif 2 (RRM2) of Homo sapiens splicing factor, arginine/serine-rich 1
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Deposited on	:	2013-04-29

This is a Full wwPDB NMR Structure Validation 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:

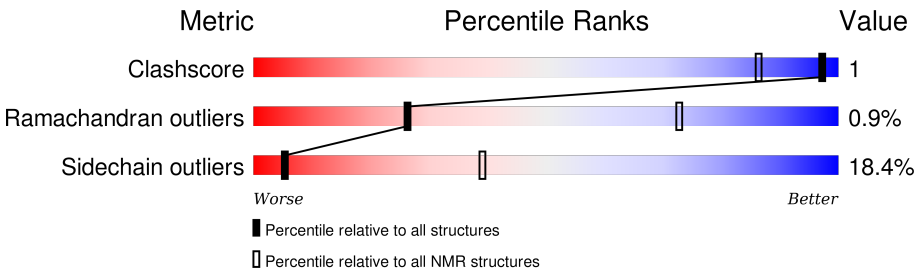
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 is 80%.

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

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	90	73% 12% 14%

2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:14-A:90 (77)	0.36	10

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1293 atoms, of which 577 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine/arginine-rich splicing factor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	90	1293	441	577	136	136	3	0

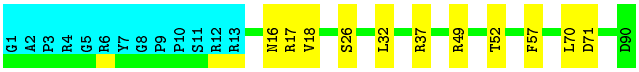
4 Residue-property plots (i)

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: Serine/arginine-rich splicing factor 1

Chain A:



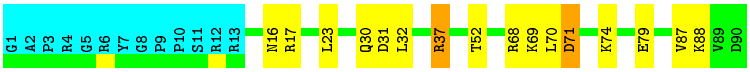
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Serine/arginine-rich splicing factor 1

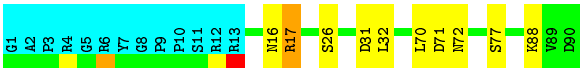
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 68% 16% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 S14 E15 N16 R17 V18 S26 D31 L32 K33 D34 V42 C43 Y44 T52 F57 V58 R59 L70 S77 Y84 D90

4.2.4 Score per residue for model 4

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 66% 20% 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 V18 S26 Q30 D31 L32 M36 R37 Y44 R49 T52 D62 L70 D71 H78 V87 K88 V89 D90

4.2.5 Score per residue for model 5

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 69% 16% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 V20 S21 S26 L32 C43 G53 R59 K69 L70 D71 N72 E79 R86 D90

4.2.6 Score per residue for model 6

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 60% 23% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 V18 S21 G22 L23 P24 S28 W29 Q30 D31 L32 K33 D34 H35 M36 R37 D41 V42 Y48 T52 R59 L70 E81 T82 A83 K88 V89 D90

4.2.7 Score per residue for model 7

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 68% 18% 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 V18 S21 S26 Q30 D31 L32 K33 D34 R37 D41 Y48 R49 T52 L70 K74 H78 E81 D90

4.2.8 Score per residue for model 8

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 73% 11% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 M36 R49 T52 F57 L70 K74 E79 A83 K88 V89 D90

4.2.9 Score per residue for model 9

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 69% 16% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 S14 E15 N16 R17 V18 S26 D34 R37 R49 M63 K69 L70 S77 E81 Y84 K88 V89 D90

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 71% 14% 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 S14 E15 N16 R17 S26 L32 H35 F57 V58 R59 L70 D71 K74 E79 Y84 D90

4.2.11 Score per residue for model 11

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 73% 12% 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 S26 Q30 D31 L32 R37 R68 D71 R76 E79 R86 D90

4.2.12 Score per residue for model 12

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 60% 23% •• 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 V18 S21 S26 L32 K33 D34 H35 M36 R37 G40 D41 V42 C43 Y44 Y48 R49 D50 G51 T52 E56 F57 M63 L70 D71 E81 K88 V89 D90

4.2.13 Score per residue for model 13

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 63% 21% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 V18 S26 Q30 D31 L32 K33 D34 H35 M36 Y44 R49 T52 V55 E56 F57 V58 R59 Y65 K69 L70 D71 K74 E79 K88 V89 D90

4.2.14 Score per residue for model 14

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 67% 17% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 V18 S21 S26 Q30 D31 L32 H35 M36 R37 V42 T52 F57 L70 D71 K74 E79 G80 E81 D90

4.2.15 Score per residue for model 15

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 70% 14% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 R17 V18 S21 S26 Q30 D31 L32 R37 D41 L70 S77 H78 E79 R86 D90

4.2.16 Score per residue for model 16

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A: 70% 13% • 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 S14 E15 N16 R17 V18 S28 L32 R37 E38 D41 V47 T52 L70 E79 G80 E81 D90

4.2.17 Score per residue for model 17

- Molecule 1: Serine/arginine-rich splicing factor 1

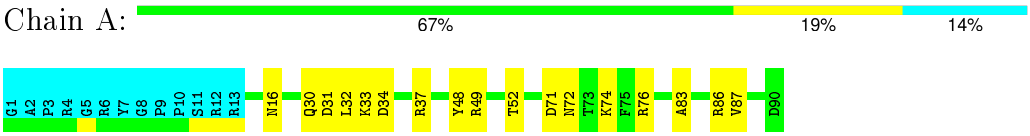
Chain A: 71% 12% •• 14%

G1 A2 P3 R4 G5 R6 Y7 G8 P9 P10 S11 R12 R13 N16 L32 K33 D34 H35 M36 R37 R49 D50 F57 V58 R59 K69 L70 D71 H78 E81 D90

4.2.18 Score per residue for model 18

- Molecule 1: Serine/arginine-rich splicing factor 1

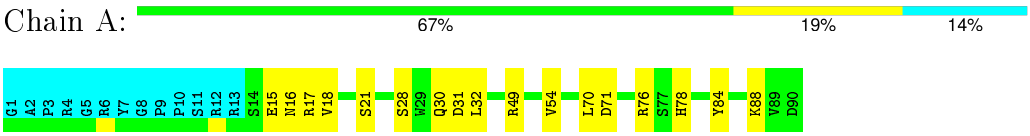
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Serine/arginine-rich splicing factor 1

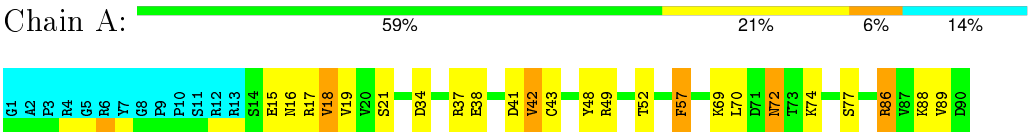
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Serine/arginine-rich splicing factor 1

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
OPAL	refinement	
j-UNIO	structure solution	
CYANA	structure solution	3.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2m7s_cs.str
Number of chemical shift lists	1
Total number of shifts	961
Number of shifts mapped to atoms	961
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	A	0.61±0.01	0±0/627 (0.0±0.0%)	1.13±0.04	2±1/845 (0.2±0.1%)
All	All	0.61	0/12540 (0.0%)	1.13	30/16900 (0.2%)

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	1.5±1.0
All	All	0	30

There are no bond-length outliers.

All 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	20	VAL	CA-CB-CG2	7.74	122.51	110.90	5	1
1	A	57	PHE	CB-CG-CD2	-6.80	116.04	120.80	20	3
1	A	17	ARG	NE-CZ-NH2	-6.66	116.97	120.30	2	2
1	A	76	ARG	NE-CZ-NH2	-6.39	117.10	120.30	19	2
1	A	17	ARG	NE-CZ-NH1	6.31	123.46	120.30	2	1
1	A	59	ARG	NE-CZ-NH2	-6.31	117.14	120.30	5	2
1	A	49	ARG	NE-CZ-NH2	-6.20	117.20	120.30	17	4
1	A	57	PHE	CB-CG-CD1	6.05	125.04	120.80	10	3
1	A	18	VAL	CA-CB-CG2	5.76	119.54	110.90	4	1
1	A	68	ARG	NE-CZ-NH2	-5.75	117.42	120.30	1	1
1	A	42	VAL	CA-CB-CG1	5.48	119.12	110.90	20	3
1	A	86	ARG	NE-CZ-NH1	5.47	123.03	120.30	11	1
1	A	49	ARG	NE-CZ-NH1	5.34	122.97	120.30	9	2
1	A	87	VAL	CA-CB-CG1	5.33	118.89	110.90	4	2
1	A	84	TYR	CB-CG-CD2	-5.27	117.84	121.00	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	59	ARG	NE-CZ-NH1	5.14	122.87	120.30	6	1

There are no chirality outliers.

All 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	17	ARG	Sidechain	5
1	A	49	ARG	Sidechain,Peptide	4
1	A	44	TYR	Sidechain	4
1	A	84	TYR	Sidechain	3
1	A	83	ALA	Peptide	3
1	A	37	ARG	Sidechain	3
1	A	59	ARG	Sidechain	2
1	A	86	ARG	Sidechain	2
1	A	76	ARG	Sidechain	1
1	A	57	PHE	Sidechain	1
1	A	40	GLY	Peptide	1
1	A	48	TYR	Sidechain	1

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	616	499	593	1±1
All	All	12320	9980	11860	21

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:SER:HA	1:A:47:VAL:HG13	0.58	1.74	16	1
1:A:23:LEU:HD23	1:A:24:PRO:HD2	0.57	1.77	6	1
1:A:18:VAL:HG13	1:A:63:MET:HG2	0.47	1.86	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ARG:HH21	1:A:54:VAL:CG1	0.46	2.23	19	1
1:A:36:MET:HG3	1:A:70:LEU:HD11	0.45	1.89	4	1
1:A:42:VAL:HG22	1:A:57:PHE:CE1	0.45	2.46	12	2
1:A:17:ARG:HH21	1:A:54:VAL:HG11	0.45	1.70	19	1
1:A:72:ASN:H	1:A:86:ARG:HB3	0.45	1.72	20	1
1:A:71:ASP:HB2	1:A:87:VAL:HG12	0.45	1.88	1	1
1:A:18:VAL:HG23	1:A:55:VAL:HB	0.44	1.90	13	1
1:A:28:SER:CA	1:A:47:VAL:HG13	0.43	2.43	16	1
1:A:20:VAL:HG22	1:A:53:GLY:N	0.42	2.28	5	1
1:A:65:TYR:CZ	1:A:69:LYS:HE3	0.42	2.48	13	1
1:A:70:LEU:HD13	1:A:70:LEU:O	0.41	2.15	4	2
1:A:36:MET:HE2	1:A:57:PHE:CE1	0.41	2.49	13	1
1:A:18:VAL:HG12	1:A:89:VAL:HA	0.41	1.92	20	1
1:A:19:VAL:HG23	1:A:88:LYS:HG3	0.41	1.93	20	1
1:A:42:VAL:HB	1:A:57:PHE:CD1	0.41	2.51	20	1
1:A:18:VAL:CG1	1:A:63:MET:HG2	0.41	2.46	9	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	
1	A	76/90 (84%)	69±2 (90±3%)	7±2 (9±3%)	1±1 (1±1%)	26	73
All	All	1520/1800 (84%)	1372 (90%)	134 (9%)	14 (1%)	26	73

All 4 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	49	ARG	6
1	A	15	GLU	5
1	A	37	ARG	2
1	A	36	MET	1

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	67/76 (88%)	55±3 (82±4%)	12±3 (18±4%)	5 39
All	All	1340/1520 (88%)	1094 (82%)	246 (18%)	5 39

All 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)
1	A	16	ASN	20
1	A	32	LEU	17
1	A	70	LEU	15
1	A	71	ASP	12
1	A	37	ARG	12
1	A	17	ARG	12
1	A	26	SER	12
1	A	52	THR	12
1	A	30	GLN	10
1	A	88	LYS	9
1	A	79	GLU	9
1	A	34	ASP	9
1	A	31	ASP	8
1	A	18	VAL	8
1	A	74	LYS	8
1	A	21	SER	8
1	A	81	GLU	7
1	A	48	TYR	5
1	A	41	ASP	5
1	A	35	HIS	5
1	A	77	SER	5
1	A	69	LYS	5
1	A	78	HIS	4
1	A	72	ASN	4
1	A	28	SER	3
1	A	43	CYS	2
1	A	33	LYS	2
1	A	50	ASP	2
1	A	86	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	57	PHE	2
1	A	38	GLU	2
1	A	23	LEU	2
1	A	59	ARG	1
1	A	84	TYR	1
1	A	62	ASP	1
1	A	15	GLU	1
1	A	49	ARG	1
1	A	56	GLU	1
1	A	68	ARG	1
1	A	36	MET	1

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 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)

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: 2m7s_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	961
Number of shifts mapped to atoms	961
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	87	2.81 ± 0.14	Should be applied
$^{13}C_{\beta}$	81	2.38 ± 0.20	Should be applied
$^{13}C'$	0	—	—
^{15}N	83	1.06 ± 0.57	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 760 atoms were assigned a chemical shift out of a possible 951. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	302/381 (79%)	151/152 (99%)	76/154 (49%)	75/75 (100%)
Sidechain	399/494 (81%)	249/288 (86%)	147/177 (83%)	3/29 (10%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	59/76 (78%)	30/40 (75%)	28/33 (85%)	1/3 (33%)
Overall	760/951 (80%)	430/480 (90%)	251/364 (69%)	79/107 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 876 atoms were assigned a chemical shift out of a possible 1125. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	340/440 (77%)	170/175 (97%)	87/180 (48%)	83/85 (98%)
Sidechain	470/601 (78%)	296/355 (83%)	171/205 (83%)	3/41 (7%)
Aromatic	66/84 (79%)	34/44 (77%)	31/37 (84%)	1/3 (33%)
Overall	876/1125 (78%)	500/574 (87%)	289/422 (68%)	87/129 (67%)

7.1.4 Statistically unusual chemical shifts (i)

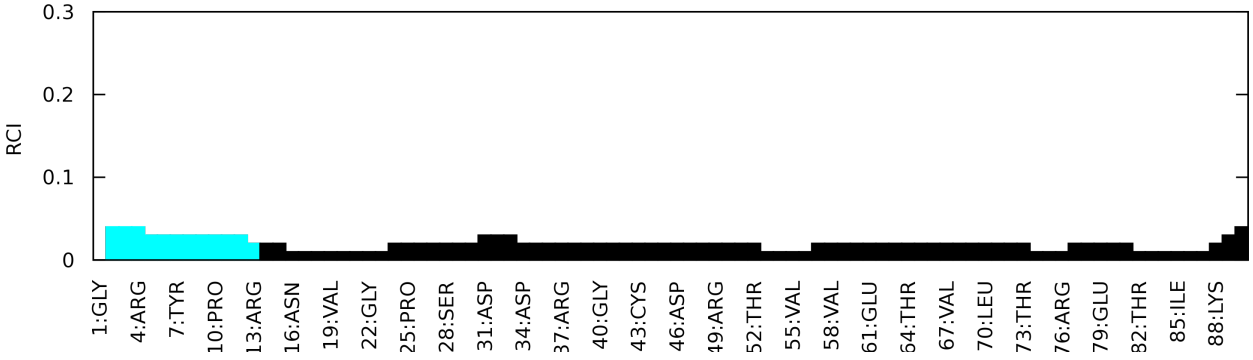
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	13	ARG	CD	37.92	47.57 – 38.77	-6.0
1	A	86	ARG	CD	38.37	47.57 – 38.77	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:


RCI
0.3
0.2
0.1
0
1:GLY
4:ARG
7:TYR
10:PRO
13:ARG
16:ASN
19:VAL
22:GLY
25:PRO
28:SER
31:ASP
34:ASP
37:ARG
40:GLY
43:CYS
46:ASP
49:ARG
52:THR
55:VAL
58:VAL
61:GLU
64:THR
67:VAL
70:LEU
73:THR
76:ARG
79:GLU
82:THR
85:ILE
88:LYS