

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1SZL
Title	:	F-spondin TSR domain 1
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Deposited on	:	2004-04-06

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 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:

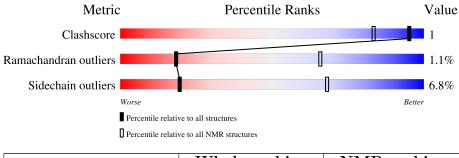
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	NMR archive
Metric	$(\# { m Entries})$	(# 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	А	61	82%	•	16%	



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 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:441-A:491 (51)	0.30	14	

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 4 clusters and 1 single-model cluster was found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 883 atoms, of which 422 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called F-spondin.

Mol	Chain	Residues	Atoms				Trace		
1	٨	61	Total	С	Η	Ν	0	S	0
	А	01	883	277	422	80	95	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	439	GLY	-	cloning artifact	UNP P35446
А	440	SER	-	cloning artifact	UNP P35446



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: F-spondin

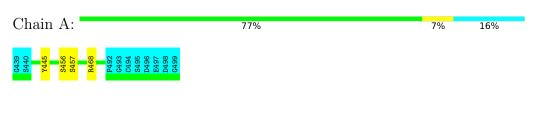
Chain	A:	82%	•	16%
G439 S440 Y445	0492 0493 0496 0496 0498 0498 0499			

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

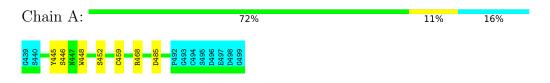
4.2.1 Score per residue for model 1

• Molecule 1: F-spondin



4.2.2 Score per residue for model 2

• Molecule 1: F-spondin





4.2.3 Score per residue for model 3

• Molecule 1: F-spondin

Chain A:	72%	11%	16%
C439 2440 W448 W451 W451 R464	04 67 14463 04 85 14 92 14 95 14 95 14 95 14 96 14 98 14 98 14 98 14 98		

4.2.4 Score per residue for model 4

• Molecule 1: F-spondin

Chain A:	77%	7%	16%
6439 8440 8440 8456 8456 8456 0482 0482 6493 6493 8495 8495	E497 D498 G499		

4.2.5 Score per residue for model 5

 \bullet Molecule 1: F-spondin

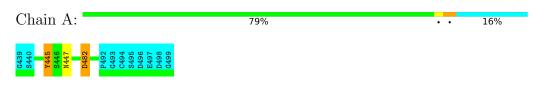
Chain A:	80%	• 16%
6439 8456 8456 8456 1470 1470 1493 6493 6493 6493 1498 1498 1498 1498 1498		

4.2.6 Score per residue for model 6

• Molecule 1: F-spondin



4.2.7 Score per residue for model 7





4.2.8 Score per residue for model 8

• Molecule 1: F-spondin

Chain A:	79%	5%	16%
0430 8440 8455 8455 8455 8456 8492 6493 6493 6493 6496 8496 6499 6499 6499			

4.2.9 Score per residue for model 9

• Molecule 1: F-spondin

Chain A:		82%	•	16%
64:39 84:40 0487 0487 0492 0494 0495 0495 0496 0496	0499			

4.2.10 Score per residue for model 10

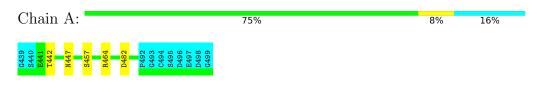
 \bullet Molecule 1: F-spondin

Chain A:				74%	10%	16%
6439 8440 1445 1448 1448 1448	0467	D485 F486 Q487	P 492 G 493 C 494 S 495 D 496 E 497 D 498 G 499			

- 4.2.11 Score per residue for model 11
- Molecule 1: F-spondin



4.2.12 Score per residue for model 12





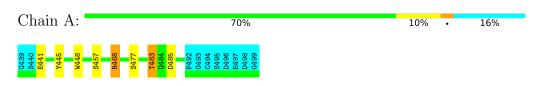
4.2.13 Score per residue for model 13

• Molecule 1: F-spondin



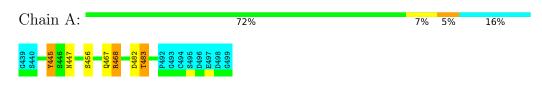
4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: F-spondin



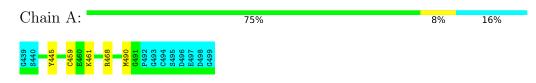
4.2.15 Score per residue for model 15

 \bullet Molecule 1: F-spondin

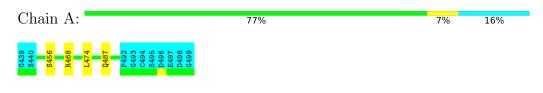


4.2.16 Score per residue for model 16

• Molecule 1: F-spondin



4.2.17 Score per residue for model 17





4.2.18 Score per residue for model 18

• Molecule 1: F-spondin



4.2.19 Score per residue for model 19

• Molecule 1: F-spondin

Chain A:		80%		•	16%
6439 8440 8456 0475	P492 6493 6494 8496 5496 5497 5497 5497 6498 6498				

$4.2.20 \quad \text{Score per residue for model } 20$

Chain A:	72%	11% 16%
6439 8440 8446 8455 8455 8455 8457 8457 8457 8457 8457	0487 0487 04932 04955 04995 04998 04998 04998	



5 Refinement protocol and experimental data overview (i)

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

Of the 200 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	structure solution	2.0.30
OPALp	refinement	1.3

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	l Chain E		Sond lengths	Bond angles		
	Unam	RMSZ	$\#Z{>}5$	RMSZ	#Z > 5	
1	А	$0.57 {\pm} 0.01$	$0{\pm}0/409~(~0.0{\pm}~0.0\%)$	1.09 ± 0.03	$0{\pm}0/554~(~0.1{\pm}~0.1\%)$	
All	All	0.57	0/8180~(~0.0%)	1.09	7/11080 ($0.1%$)	

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	А	$0.0{\pm}0.0$	0.1 ± 0.4
All	All	0	3

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	$\mathbf{Z} = \mathbf{Observed}(^{o})$			$Ideal(^{o})$	Moo	dels
	Unam	nes	туре	Atoms			Atoms Z Observed() Ideal()		Worst	Total
1	А	468	ARG	CD-NE-CZ	5.90	131.86	123.60	13	4	
1	А	466	ARG	NE-CZ-NH2	-5.43	117.58	120.30	20	1	
1	А	468	ARG	NE-CZ-NH2	-5.24	117.68	120.30	1	1	
1	А	464	ARG	NE-CZ-NH2	-5.23	117.68	120.30	8	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	А	445	TYR	Sidechain	2
1	А	468	ARG	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	А	399	378	378	1±1
All	All	7980	7560	7560	15

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.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:448:TRP:CH2	1:A:468:ARG:NH1	0.60	2.70	14	1
1:A:451:TRP:CE3	1:A:464:ARG:HB2	0.49	2.42	18	2
1:A:448:TRP:CH2	1:A:485:ASP:HB2	0.46	2.46	13	6
1:A:461:LYS:HE3	1:A:490:MET:SD	0.43	2.53	16	1
1:A:451:TRP:CH2	1:A:487:GLN:HB2	0.42	2.49	20	1
1:A:468:ARG:HH11	1:A:468:ARG:HG2	0.42	1.73	14	1
1:A:443:CYS:HB2	1:A:445:TYR:CZ	0.42	2.49	11	1
1:A:448:TRP:CZ2	1:A:468:ARG:CZ	0.41	3.04	3	1
1:A:445:TYR:CD2	1:A:468:ARG:NH1	0.41	2.88	15	1

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

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	Percentile	es
1	А	51/61~(84%)	$48 \pm 1 (94 \pm 3\%)$	$3\pm1~(5\pm3\%)$	1±1 (1±1%)	18 66	Π
All	All	1020/1220 (84%)	954 (94%)	55~(5%)	11 (1%)	18 66	

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



Mol	Chain	Res	• -	Models (Total)
1	А	482	ASP	4
1	А	452	SER	2
1	А	459	CYS	2
1	А	483	THR	2
1	А	491	GLY	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	А	47/54~(87%)	$44 \pm 1 (93 \pm 3\%)$	$3\pm1~(7\pm3\%)$	19 68
All	All	940/1080~(87%)	876 (93%)	64 (7%)	19 68

All 22 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	456	SER	8
1	А	445	TYR	8
1	А	447	ASN	6
1	А	487	GLN	6
1	А	457	SER	4
1	А	467	GLN	4
1	А	477	SER	4
1	А	482	ASP	3
1	А	455	SER	3
1	А	463	LYS	2
1	А	441	GLU	2
1	А	464	ARG	2
1	А	442	THR	2
1	А	483	THR	2
1	А	446	SER	1
1	А	470	LEU	1
1	А	452	SER	1
1	А	460	GLU	1
1	А	468	ARG	1
1	А	474	LEU	1
1	А	475	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	А	471	LYS	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 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

