wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2CR4
Title	:	Solution structure of the SH2 domain of human SH3BP2 protein
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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:

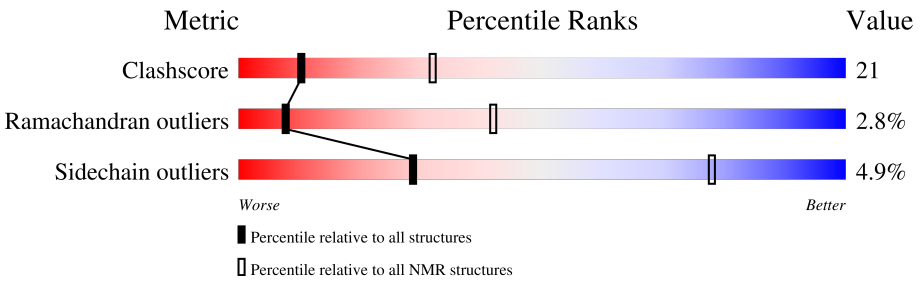
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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	126	48% 29% • 21%

2 Ensemble composition and analysis (i)

This entry contains 20 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:14-A:51, A:58-A:119 (100)	0.21	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 4 clusters and 7 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1943 atoms, of which 954 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SH3 domain-binding protein 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	126	1943	621	954	169	196	3	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P78314
A	2	SER	-	cloning artifact	UNP P78314
A	3	SER	-	cloning artifact	UNP P78314
A	4	GLY	-	cloning artifact	UNP P78314
A	5	SER	-	cloning artifact	UNP P78314
A	6	SER	-	cloning artifact	UNP P78314
A	7	GLY	-	cloning artifact	UNP P78314
A	121	SER	-	cloning artifact	UNP P78314
A	122	GLY	-	cloning artifact	UNP P78314
A	123	PRO	-	cloning artifact	UNP P78314
A	124	SER	-	cloning artifact	UNP P78314
A	125	SER	-	cloning artifact	UNP P78314
A	126	GLY	-	cloning artifact	UNP P78314

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: SH3 domain-binding protein 2

Chain A: 48% 29% • 21%

G1 S2 S3 G4 S5 S6 G7 E8 D9 Y10 E11 K12 V13 V19 F20 V21 N22 T23 V29 L32 F33 T36 P42 Q43 D44 G45 L46 Y47 C48 S52 S53 T54 K55 S56 G57 V62 W63 D64 N68 R74 I75 F76 Y83 L84 E85 G86 E87 V88 L89 F90

V91 S92 M96 Y100 H101 T102 H103 V104 L105 L111 L112 L113 R114 Y117 G118 Y119 T120 S121 G122 P123 S124 S125 G126

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: SH3 domain-binding protein 2

Chain A: 49% 28% • 21%

G1 S2 S3 G4 S5 S6 G7 E8 D9 Y10 E11 K12 V13 N17 S18 V19 F20 T24 E30 R31 L32 F33 K34 A35 T36 P42 L46 Y47 C48 N51 S52 S53 T54 K55 S56 G57 V62 W63 D64 N68 R71 F76 E77 K78 Y83 L84 E85 G86

L89 F90 V93 M96 V97 Y100 H101 T102 H103 V104 L105 L111 L112 Y117 G118 Y119 T120 S121 G122 P123 S124 S125 G126

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: *target function,structures with the lowest energy,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	2.0.17
CYANA	refinement	2.0.17

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	821	805	800	34±6
All	All	16420	16100	16000	690

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 21.

5 of 183 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG21	1:A:50:ARG:HD3	0.78	1.54	14	5
1:A:33:PHE:CD2	1:A:46:LEU:HD23	0.76	2.16	17	11
1:A:62:VAL:HG21	1:A:105:LEU:CD1	0.75	2.11	11	17
1:A:59:VAL:HG22	1:A:74:ARG:HA	0.71	1.61	8	4
1:A:29:VAL:HG21	1:A:50:ARG:CD	0.71	2.14	14	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	100/126 (79%)	83±2 (83±2%)	14±2 (14±2%)	3±1 (3±1%)	8 42
All	All	2000/2520 (79%)	1656 (83%)	288 (14%)	56 (3%)	8 42

5 of 8 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	101	HIS	16
1	A	91	VAL	11
1	A	104	VAL	10
1	A	119	TYR	8
1	A	87	GLU	6

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	94/114 (82%)	89±1 (95±2%)	5±1 (5±2%)	29 78
All	All	1880/2280 (82%)	1787 (95%)	93 (5%)	29 78

5 of 25 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	89	LEU	20
1	A	95	SER	8
1	A	48	CYS	7
1	A	64	ASP	7
1	A	74	ARG	7

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