wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2EV8
Title	:	Solution structure of the erythroid p55 PDZ domain
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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:

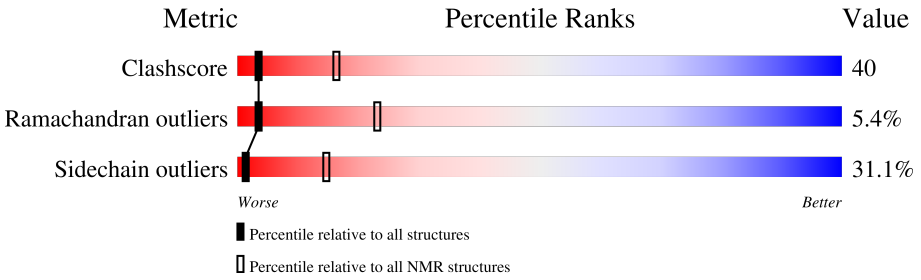
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	97	24% 40% 9% • 13% 12%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 19 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:69-A:75, A:83-A:100, A:105-A:151 (72)	0.28	19

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1357 atoms, of which 694 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 55 kDa erythrocyte membrane protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	85	1357	411	694	121	126	5	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MET	-	expression tag	UNP Q00013
A	58	GLY	-	expression tag	UNP Q00013
A	59	HIS	-	expression tag	UNP Q00013
A	60	HIS	-	expression tag	UNP Q00013
A	61	HIS	-	expression tag	UNP Q00013
A	62	HIS	-	expression tag	UNP Q00013
A	63	HIS	-	expression tag	UNP Q00013
A	64	HIS	-	expression tag	UNP Q00013
A	65	SER	-	expression tag	UNP Q00013
A	66	GLY	-	expression tag	UNP Q00013
A	67	HIS	-	expression tag	UNP Q00013
A	68	MET	-	expression tag	UNP Q00013

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: 55 kDa erythrocyte membrane protein

Chain A: 24% 40% 9% • 13% 12%

MET GLY HIS HIS HIS HIS HIS HIS SER GLY HIS MET V69 R70 L71 I72 Q73 F74 E75 K76 V77 T78 E79 E80 P81 M82 G83 I84 T85 L86 K87 L88 N89 E90 K91 Q92 S93 C94 T95 V96 A97 R98 I99 L100 H101 G102 G103 M104 I105 L111 H112 V113 E116 I117 L118 E119 I120 N121

G122 T123 N124 V125 H128 S129 V130 L133 A136 E139 T140 K141 G142 M143 I144 S145 L146 K147 V148 I149 P150 N151 Q152 Q153

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

The representative model is number 19. Colouring as in section 4.1 above.

• Molecule 1: 55 kDa erythrocyte membrane protein

Chain A: 23% 40% 10% • 13% 12%

MET GLY HIS HIS HIS HIS HIS HIS SER GLY HIS MET V69 R70 L71 I72 Q73 F74 E75 K76 V77 T78 E79 E80 P81 M82 G83 I84 T85 L86 K87 L88 N89 E90 K91 Q92 S93 C94 T95 V96 A97 R98 I99 L100 H101 G102 G103 M104 I105 H106 R107 L111 H112 V113 G114 D115 E116 I117 L118

E119 I120 N121 G122 T123 N124 V125 T126 N127 H128 S129 V130 D131 Q132 L133 Q134 K135 A136 M137 K138 E139 T140 K141 G142 M143 I144 S145 L146 K147 V148 I149 P150 N151 Q152 Q153

5 Refinement protocol and experimental data overview (i)

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

Of the 100 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
CNS	structure solution	1.1
CNS	refinement	1.1

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	562	598	594	46±6
All	All	11240	11960	11880	922

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 40.

5 of 260 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:LEU:HD21	1:A:130:VAL:HG21	0.95	1.34	2	3
1:A:120:ILE:CG2	1:A:146:LEU:HD23	0.89	1.98	4	12
1:A:120:ILE:HG21	1:A:146:LEU:HD23	0.86	1.48	4	9
1:A:105:ILE:HG23	1:A:111:LEU:HD13	0.84	1.50	11	1
1:A:99:ILE:HD13	1:A:113:VAL:HG22	0.82	1.51	15	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	71/97 (73%)	56±2 (79±3%)	11±2 (16±4%)	4±2 (5±3%)	3 23
All	All	1420/1940 (73%)	1116 (79%)	227 (16%)	77 (5%)	3 23

5 of 13 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	94	CYS	19
1	A	96	VAL	9
1	A	142	GLY	8
1	A	89	ASN	6
1	A	124	ASN	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	65/86 (76%)	45±2 (69±3%)	20±2 (31±3%)	1 15
All	All	1300/1720 (76%)	896 (69%)	404 (31%)	1 15

5 of 47 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	70	ARG	20
1	A	71	LEU	20
1	A	93	SER	20
1	A	118	LEU	20
1	A	116	GLU	19

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