wwPDB NMR Structure Validation Summary Report (i)

Feb 28, 2022 – 02:33 PM EST

PDB ID	:	2EE8
Title	:	Solution structure of three zf-C2H2 domains from mouse protein odd-skipped-related 2 splicing isoform 2
Authors	:	Tomizawa, T.; Koshiba, S.; Watanabe, S.; Harada, T.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-02-15

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:

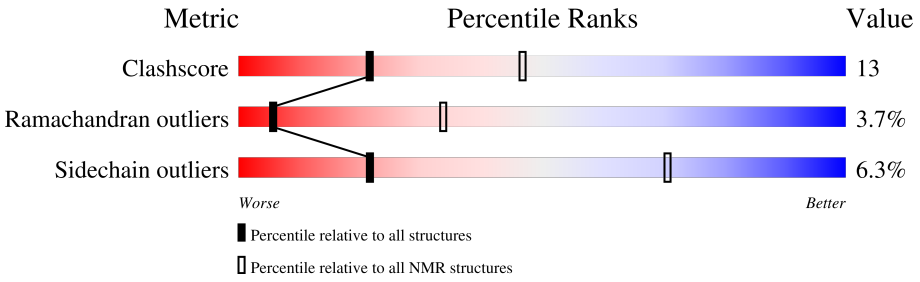
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	106	47% 17% • 35%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:18-A:40 (23)	0.20	4
2	A:46-A:68 (23)	0.20	16
3	A:74-A:96 (23)	0.40	3

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1688 atoms, of which 832 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein odd-skipped-related 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	106	1685	526	832	167	152	8	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q91ZD1
A	2	SER	-	expression tag	UNP Q91ZD1
A	3	SER	-	expression tag	UNP Q91ZD1
A	4	GLY	-	expression tag	UNP Q91ZD1
A	5	SER	-	expression tag	UNP Q91ZD1
A	6	SER	-	expression tag	UNP Q91ZD1
A	7	GLY	-	expression tag	UNP Q91ZD1
A	99	THR	GLU	SEE REMARK 999	UNP Q91ZD1
A	101	SER	-	expression tag	UNP Q91ZD1
A	102	PRO	-	expression tag	UNP Q91ZD1
A	103	THR	-	expression tag	UNP Q91ZD1
A	104	ALA	-	expression tag	UNP Q91ZD1
A	105	ALA	-	expression tag	UNP Q91ZD1
A	106	SER	-	expression tag	UNP Q91ZD1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	3	3	3

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: Protein odd-skipped-related 2

Chain A: 47% 17% • 35%

G1 S2 S3 G4 S5 S6 G7 G8 R9 L10 P11 S12 K13 T14 K15 K16 E17 F18 I19 C20 R25 H26 F27 Y31 N32 L33 L34 T39 H40 T41 D42 E43 R44 P45 Y46 H52 F55 L61 H64 I67 H68 S69 K70 E71 K72 P73 K81 G82 F83 K93

T94 L95 H96 M97 Q98 T99 S100 S101 P102 T103 A104 A105 S106

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

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: Protein odd-skipped-related 2

Chain A: 49% 15% • 35%

G1 S2 S3 G4 S5 S6 G7 G8 R9 L10 P11 S12 K13 T14 K15 K16 E17 F18 I19 C20 R25 H26 L33 L34 T35 H36 T39 H40 T41 D42 E43 R44 P45 F55 Q58 D59 D63 H64 R65 Y66 S69 K70 E71 K72 P73 H92 K93 M97 Q98 T99 S100

S101 P102 T103 A104 A105 S106

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics, restrainted molecular dynamics.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function.*

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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	590	568	568	15±5
All	All	11860	11360	11360	303

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 13.

5 of 129 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:ALA:O	1:A:94:THR:HG23	0.78	1.77	20	1
1:A:19:ILE:HG23	1:A:25:ARG:O	0.74	1.81	18	10
1:A:36:HIS:O	1:A:39:THR:HG22	0.74	1.83	4	8
1:A:95:LEU:HD12	1:A:95:LEU:C	0.71	2.07	20	1
1:A:34:LEU:C	1:A:34:LEU:HD12	0.69	2.08	2	16

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	69/106 (65%)	54±3 (79±5%)	12±3 (18±4%)	3±1 (4±2%)	6	34
All	All	1380/2120 (65%)	1086 (79%)	243 (18%)	51 (4%)	6	34

5 of 15 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	20	CYS	14
1	A	48	CYS	7
1	A	65	ARG	6
1	A	76	CYS	4
1	A	83	PHE	4

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	64/95 (67%)	60±1 (94±2%)	4±1 (6±2%)	21	70
All	All	1280/1900 (67%)	1199 (94%)	81 (6%)	21	70

5 of 26 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	34	LEU	20
1	A	63	ASP	7
1	A	95	LEU	5
1	A	21	LYS	5
1	A	31	TYR	4

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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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