wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1ADZ
Title	:	THE SOLUTION STRUCTURE OF THE SECOND KUNITZ DOMAIN OF TISSUE FACTOR PATHWAY INHIBITOR, NMR, 30 STRUCTURES
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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
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:

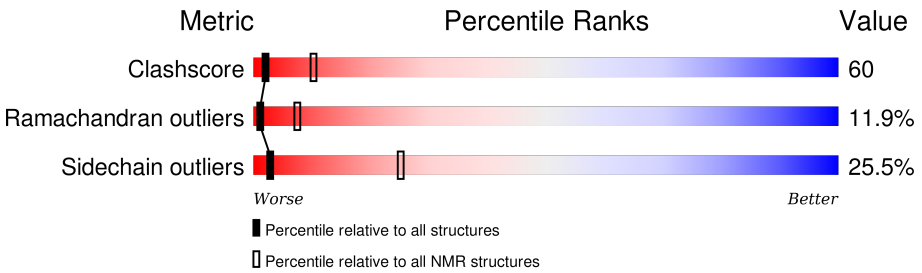
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 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	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	71	14% 44% 15% 27%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 6 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:10-A:44, A:50-A:66 (52)	0.27	6

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 5, 6, 8, 9, 10, 12, 13, 15, 17, 20, 24, 26, 27, 30
2	1, 11, 14, 16, 21, 28, 29
3	4, 7
4	23, 25
5	18, 19
Single-model clusters	22

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1111 atoms, of which 527 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TISSUE FACTOR PATHWAY INHIBITOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	71	1111	364	527	95	118	7	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	TYR	ASN	ENGINEERED	UNP P10646
A	3	LYS	ALA	CONFLICT	UNP P10646
A	4	ASP	ASN	ENGINEERED	UNP P10646
A	5	ASP	ARG	ENGINEERED	UNP P10646
A	6	ASP	ILE	ENGINEERED	UNP P10646
A	7	ASP	ILE	ENGINEERED	UNP P10646
A	?	-	THR	DELETION	UNP P10646
A	?	-	THR	DELETION	UNP P10646
A	?	-	GLN	DELETION	UNP P10646
A	?	-	GLN	DELETION	UNP P10646
A	?	-	GLU	DELETION	UNP P10646

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: TISSUE FACTOR PATHWAY INHIBITOR

Chain A: 14% 44% 15% 27%

D1 Y2 K3 D4 D5 D6 D7 K8 L9 K10 P11 D12 F13 C14 F15 L16 E17 E18 D19 P20 G21 I22 C23 R24 G25 Y26 I27 T28 R29 Y30 F31 Y32 Q35 T36 K37 Q38 C39 E40 R41 F42 K43 Y44 G45 G46 C47 L48 G49 N50 N51 N52 N53 F54 E55 T56 E59 C60 K61 N62 I63 C64 E65 D66 G67 P68 N69 G70 F71

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

The representative model is number 6. Colouring as in section 4.1 above.

- Molecule 1: TISSUE FACTOR PATHWAY INHIBITOR

Chain A: 15% 44% 11% • 27%

D1 Y2 K3 D4 D5 D6 D7 K8 L9 K10 P11 D12 F13 C14 F15 L16 E17 E18 D19 P20 G21 I22 C23 R24 G25 Y26 I27 T28 R29 Y30 F31 Y32 K37 Q38 C39 E40 R41 F42 K43 Y44 G45 G46 C47 L48 G49 N50 N51 N52 N53 F54 E55 T56 E59 C60 K61 N62 I63 C64 E65 D66 G67 P68 N69 G70 F71

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DIANA*.

Of the 300 calculated structures, 30 were deposited, based on the following criterion: *LOWEST VALUE OF VARIABLE TARGET FUNCTION*.

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

Software name	Classification	Version
DIANA	refinement	
TRIAD NMR FROM TRIPOS	structure solution	TRIPOS

No chemical shift data was provided. 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)

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	446	408	405	51±7
All	All	13380	12240	12170	1537

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 60.

5 of 289 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ARG:O	1:A:26:TYR:CD1	0.83	2.32	9	10
1:A:22:ILE:O	1:A:23:CYS:O	0.81	1.99	30	10
1:A:30:TYR:CE2	1:A:41:ARG:HG3	0.73	2.19	10	30
1:A:43:LYS:CD	1:A:43:LYS:N	0.68	2.57	22	3
1:A:26:TYR:CD1	1:A:43:LYS:CB	0.68	2.77	22	2

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	52/71 (73%)	37±2 (71±4%)	9±2 (17±4%)	6±2 (12±4%)	1 7
All	All	1560/2130 (73%)	1109 (71%)	266 (17%)	185 (12%)	1 7

5 of 21 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	65	GLU	29
1	A	23	CYS	20
1	A	52	ASN	18
1	A	66	ASP	16
1	A	25	GLY	12

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	50/64 (78%)	37±2 (75±4%)	13±2 (25±4%)	3 25
All	All	1500/1920 (78%)	1118 (75%)	382 (25%)	3 25

5 of 28 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	10	LYS	29
1	A	24	ARG	27
1	A	43	LYS	25
1	A	22	ILE	25
1	A	38	GLN	24

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)

No chemical shift data were provided