wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1DZD
Title	:	HIGH RESOLUTION STRUCTURE OF ACIDIC FIBROBLAST GROWTH FACTOR (27-154), 24 NMR STRUCTURES
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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:

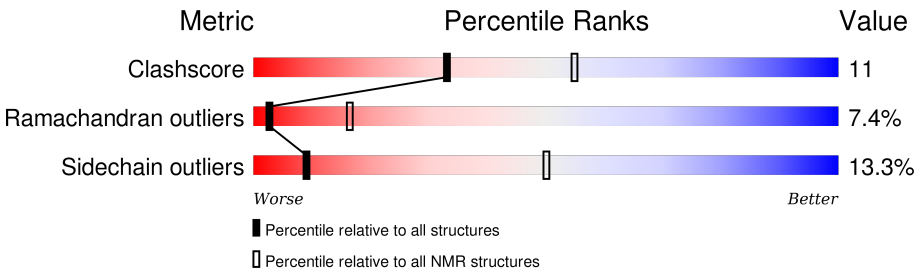
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	127	49% 39% 6% • 6%

2 Ensemble composition and analysis (i)

This entry contains 24 models. Model 24 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:30-A:148 (119)	0.48	24

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. No single-model clusters were found.

Cluster number	Models
1	3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24
2	1, 2, 5

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1010 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ACIDIC FIBROBLAST GROWTH FACTOR.

Mol	Chain	Residues	Atoms					Trace
			Total	C	N	O	S	
1	A	127	1010	633	176	197	4	0

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: ACIDIC FIBROBLAST GROWTH FACTOR

Chain A: 49% 39% 6% • 6%

L28 Y29 N32 G33 G34 H35 F36 L37 R38 I39 L40 P41 V45 T48 R49 D50 R51 S52 D53 Q54 H55 I56 Q57 L58 Q59 L60 V65 V68 Y69 T73 E74 T75 G76 Q77 Y78 L79 D82 L87 Y88 P93 L98 F99 R102 L103 E104 E105 Y108

Y111 K115 F122 V123 G124 L125 K126 K127 N128 G129 S130 C131 K132 R133 G134 P135 R136 Y139 I144 L145 F146 L147 P148 L149 P150 V151 S152 S153 D154

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

The representative model is number 24. Colouring as in section 4.1 above.

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain A: 50% 33% • 6% 6%

L28 Y29 C30 S31 N32 G33 G34 H35 F36 L37 R38 I39 L40 D46 G47 T48 R49 D50 R51 S52 D53 Q54 H55 I56 Q57 L58 Q59 L60 S61 V65 V68 Y69 T73 E74 T75 G76 Q77 Y78 L79 G85 Y88 L98 F99 L100 E101 R102 L103 H107 Y108 N109 T110 Y111

I112 S113 K114 V123 K126 K127 N128 G129 K132 R133 G134 P135 R136 Y139 K142 A143 I144 L145 F146 L147 P148 L149 P150 V151 S152 S153 D154

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *RESTRAINED MOLECULAR DYNAMICS*.

Of the 24 calculated structures, 24 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
GROMOS	refinement	
GROMOS	structure solution	

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)

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	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.82±0.01	0±0/968 (0.0±0.0%)	1.46±0.04	8±3/1306 (0.6±0.2%)
All	All	0.82	0/23232 (0.0%)	1.46	203/31344 (0.6%)

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	A	0.0±0.0	8.5±1.8
All	All	0	205

There are no bond-length outliers.

5 of 40 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	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	49	ARG	NE-CZ-NH1	-17.71	111.44	120.30	17	8
1	A	49	ARG	NE-CZ-NH2	11.90	126.25	120.30	17	2
1	A	88	TYR	CB-CG-CD2	-11.44	114.13	121.00	20	19
1	A	68	VAL	CG1-CB-CG2	-10.47	94.15	110.90	2	9
1	A	136	ARG	NE-CZ-NH1	9.14	124.87	120.30	7	8

There are no chirality outliers.

5 of 47 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	A	139	TYR	Mainchain,Sidechain	15
1	A	122	PHE	Sidechain	12
1	A	108	TYR	Sidechain,Mainchain	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	33	GLY	Peptide,Mainchain	11
1	A	78	TYR	Sidechain	11

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	947	0	917	20±4
All	All	22728	0	22008	490

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 11.

5 of 209 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:HIS:HB2	1:A:125:LEU:HD23	0.83	1.49	10	7
1:A:35:HIS:HB3	1:A:48:THR:H	0.80	1.36	5	16
1:A:38:ARG:HD2	1:A:55:HIS:HB2	0.79	1.54	12	4
1:A:99:PHE:HB3	1:A:111:TYR:HB3	0.78	1.53	20	14
1:A:126:LYS:HE3	1:A:128:ASN:HB2	0.74	1.58	6	8

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	119/127 (94%)	86±4 (72±3%)	25±4 (21±3%)	9±3 (7±2%)	3 16
All	All	2856/3048 (94%)	2053 (72%)	592 (21%)	211 (7%)	3 16

5 of 44 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	VAL	19
1	A	127	LYS	18
1	A	53	ASP	15
1	A	132	LYS	13
1	A	105	GLU	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	103/111 (93%)	89±3 (87±3%)	14±3 (13±3%)	9	50
All	All	2472/2664 (93%)	2142 (87%)	330 (13%)	9	50

5 of 62 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	139	TYR	24
1	A	75	THR	21
1	A	133	ARG	18
1	A	126	LYS	15
1	A	60	LEU	14

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