



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2IUE
Title : PACTOLUS I-DOMAIN: FUNCTIONAL SWITCHING OF THE ROSS-MANN FOLD
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Deposited on : 2006-06-02

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

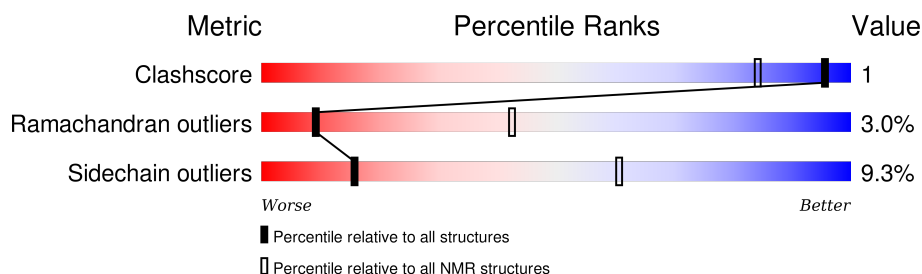
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 28%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	212	 67% 5% 28%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 20 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:3-A:13, A:40-A:60, A:75-A:194 (152)	0.22	20

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2813 atoms, of which 1168 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PACTOLUS I-DOMAIN.

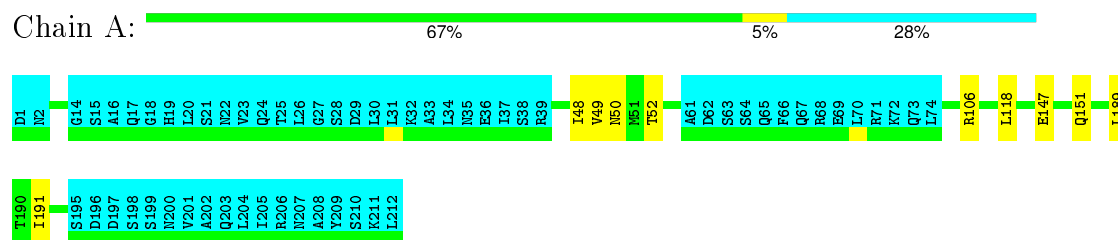
Mol	Chain	Residues	Atoms						Trace
1	A	212	Total	C	H	N	O	S	0
			2813	1029	1168	293	317	6	

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.

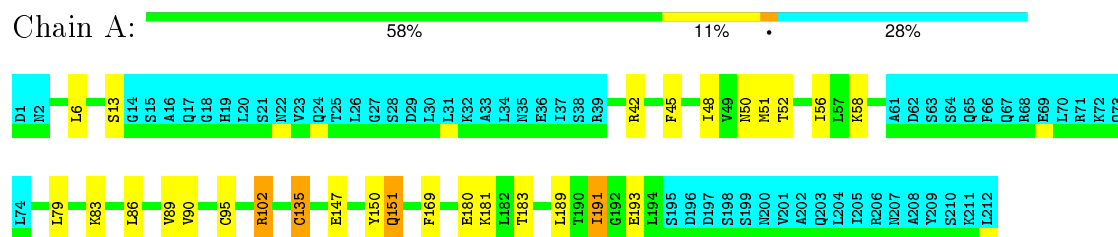
- Molecule 1: PACTOLUS I-DOMAIN



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

The representative model is number 20. Colouring as in section 4.1 above.

- Molecule 1: PACTOLUS I-DOMAIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DYANA AMBER 8.0 AND MODELLER8V2*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST POTENTIAL ENERGY ENSEMBLES*.

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

Software name	Classification	Version
AMBER 8.0	refinement	
NMRPIPE	structure solution	
NMRVIEW	structure solution	
DYANA	structure solution	
AMBER 8.0	structure solution	
MOLMOL	structure solution	
MODELLER8V2	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 7313
Number of chemical shift lists	1
Total number of shifts	804
Number of shifts mapped to atoms	799
Number of unparsed shifts	0
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	28%

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	0.68±0.01	0±0/1203 (0.0±0.0%)	1.14±0.03	2±1/1627 (0.1±0.1%)
All	All	0.68	0/24060 (0.0%)	1.14	36/32540 (0.1%)

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	1.1±1.0
All	All	0	22

There are no bond-length outliers.

5 of 22 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	127	ARG	NE-CZ-NH1	8.67	124.64	120.30	16	1
1	A	183	THR	CA-CB-CG2	6.25	121.15	112.40	7	1
1	A	51	MET	C-N-CA	6.25	137.32	121.70	15	4
1	A	145	ARG	NE-CZ-NH1	6.03	123.32	120.30	7	3
1	A	102	ARG	NE-CZ-NH1	6.03	123.32	120.30	16	2

There are no chirality outliers.

5 of 11 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	45	PHE	Sidechain	6
1	A	145	ARG	Sidechain	4
1	A	106	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	116	PHE	Sidechain	2
1	A	7	TYR	Sidechain	2

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	1182	856	1210	3±2
All	All	23640	17123	24200	60

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 1.

5 of 49 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:HG12	1:A:170:VAL:HG22	0.70	1.63	4	1
1:A:90:VAL:HG21	1:A:156:LEU:HD22	0.65	1.69	15	1
1:A:86:LEU:HD23	1:A:156:LEU:HD21	0.62	1.72	8	1
1:A:85:GLN:CG	1:A:110:LEU:HD21	0.55	2.32	11	1
1:A:181:LYS:O	1:A:184:THR:HG22	0.54	2.02	19	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	152/212 (72%)	133±2 (87±1%)	15±2 (10±1%)	5±2 (3±1%)	9	42
All	All	3040/4240 (72%)	2655 (87%)	294 (10%)	91 (3%)	9	42

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	147	GLU	19
1	A	52	THR	14
1	A	49	VAL	14
1	A	50	ASN	13
1	A	191	ILE	7

6.3.2 Protein sidechains ⓘ

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	132/184 (72%)	120±3 (91±2%)	12±3 (9±2%)	16	61
All	All	2640/3680 (72%)	2394 (91%)	246 (9%)	16	61

5 of 78 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	48	ILE	16
1	A	151	GLN	9
1	A	58	LYS	7
1	A	118	LEU	7
1	A	184	THR	6

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 28% for the well-defined parts and 31% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 7313

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	804
Number of shifts mapped to atoms	799
Number of unparsed shifts	0
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 5 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	230	SER	CA	59.6	0.1	1
A	230	SER	C	175.5	0.1	1
A	230	SER	N	121.6	0.02	1
A	230	SER	CB	64.8	0.1	1
A	230	SER	H	7.6	0.02	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	167	0.20 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	152	0.84 ± 0.10	Should be applied
$^{13}\text{C}'$	163	2.97 ± 0.12	Should be applied

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
^{15}N	161	-0.90 \pm 0.35	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 28%, i.e. 516 atoms were assigned a chemical shift out of a possible 1861. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	420/750 (56%)	104/299 (35%)	212/304 (70%)	104/147 (71%)
Sidechain	96/983 (10%)	0/572 (0%)	96/365 (26%)	0/46 (0%)
Aromatic	0/128 (0%)	0/69 (0%)	0/55 (0%)	0/4 (0%)
Overall	516/1861 (28%)	104/940 (11%)	308/724 (43%)	104/197 (53%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

