wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2CKN
Title	:	NMR STRUCTURE OF THE FIRST IG MODULE OF MOUSE FGFR1
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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:

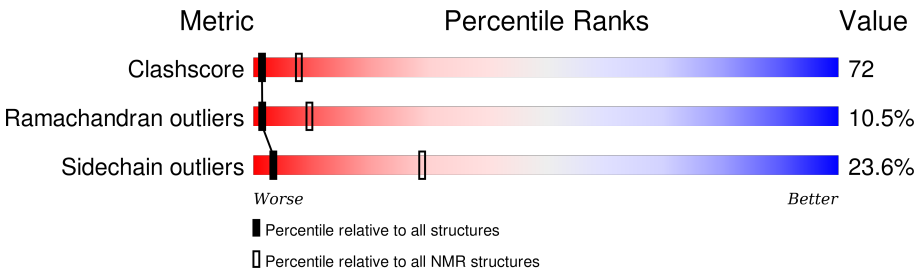
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 is 51%.

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	95	17% 41% 24% 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 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:28-A:63, A:67-A:108 (78)	0.40	14

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1445 atoms, of which 711 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1445	454	711	128	150	2	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: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1

Chain A: 17% 41% 24% 18%

P14 T15 L16 P17 E18 Q19 A20 Q21 P22 W23 G24 Y25 P26 V27 E28 V29 E30 L33 V34 H35 P36 G37 D38 L39 L40 Q41 L42 R43 C44 R45 L46 R47 D48 D49 V50 Q51 S52 I53 N54 W55 L56 R57 D58 G59 V60 Q61 L62 V63 E64 S65 N66 R67 T68 R69 I70 T71 G72 E73 E74

V75 E76 V77 R78 D79 S80 I81 P82 A83 D84 L87 Y88 A89 C90 V91 T92 S93 S94 P95 S96 T101 Y102 F103 S104 V105 N106 V107 S108

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

The representative model is number 14. Colouring as in section 4.1 above.

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1

Chain A: 17% 44% 18% • 18%

P14 T15 L16 P17 E18 Q19 A20 Q21 P22 W23 G24 Y25 P26 V27 E28 V29 E30 L33 V34 H35 P36 L39 L40 Q41 L42 R43 C44 R45 L46 R47 D48 D49 V50 Q51 S52 I53 N54 W55 L56 R57 D58 G59 V60 Q61 L62 V63 E64 S65 N66 R67 T68 R69 I70 T71 G72 E73 E74 V75

E76 V77 R78 D79 S80 I81 P82 A83 L87 Y88 A89 C90 V91 T92 S93 S94 P95 S96 G97 S98 D99 T100 T101 Y102 F103 S104 V105 N106 V107 S108

5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 20 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	

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 6885
Number of chemical shift lists	1
Total number of shifts	702
Number of shifts mapped to atoms	634
Number of unparsed shifts	0
Number of shifts with mapping errors	68
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

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	1.11±0.00	1±0/612 (0.2±0.0%)	1.42±0.02	5±1/833 (0.6±0.1%)
All	All	1.11	19/12240 (0.2%)	1.42	96/16660 (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	5.9±1.0
All	All	0	118

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	55	TRP	CG-CD2	-5.32	1.34	1.43	20	19

5 of 12 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	55	TRP	CD1-NE1-CE2	8.99	117.09	109.00	9	20
1	A	55	TRP	NE1-CE2-CZ2	7.89	139.08	130.40	9	20
1	A	55	TRP	CG-CD1-NE1	-7.45	102.66	110.10	10	20
1	A	47	ARG	NE-CZ-NH2	-7.37	116.61	120.30	10	4
1	A	57	ARG	NE-CZ-NH2	-7.17	116.72	120.30	20	1

There are no chirality outliers.

5 of 9 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	69	ARG	Sidechain	18
1	A	67	ARG	Sidechain	18
1	A	78	ARG	Sidechain	16
1	A	43	ARG	Sidechain	16
1	A	45	ARG	Sidechain	16

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	604	590	590	85±4
All	All	12080	11800	11800	1709

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 72.

5 of 496 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG21	1:A:101:THR:HB	1.04	1.27	5	18
1:A:29:VAL:HG21	1:A:101:THR:CB	0.95	1.91	5	16
1:A:29:VAL:HG11	1:A:103:PHE:CE2	0.93	1.98	10	17
1:A:63:VAL:HB	1:A:70:ILE:HD13	0.89	1.45	2	7
1:A:71:THR:O	1:A:73:GLU:N	0.84	2.10	12	18

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	77/95 (81%)	57±2 (74±2%)	12±2 (15±3%)	8±2 (11±2%)	1 9
All	All	1540/1900 (81%)	1142 (74%)	236 (15%)	162 (11%)	1 9

5 of 19 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	63	VAL	20
1	A	29	VAL	20
1	A	72	GLY	19
1	A	58	ASP	16
1	A	79	ASP	14

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	71/86 (83%)	54±2 (76±2%)	17±2 (24±2%)	3 29
All	All	1420/1720 (83%)	1085 (76%)	335 (24%)	3 29

5 of 51 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	101	THR	18
1	A	34	VAL	18
1	A	54	ASN	17
1	A	42	LEU	17
1	A	78	ARG	15

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)

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 50% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6885

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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	702
Number of shifts mapped to atoms	634
Number of unparsed shifts	0
Number of shifts with mapping errors	68
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- Residue not found in structure. First 5 (of 68) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	105	SER	HB3	3.8	0.005	2
A	107	GLU	HA	4.14	0.005	1
A	107	GLU	HG2	2.2	0.005	2
A	103	LEU	N	123.11	0.02	1
A	105	SER	HB2	3.94	0.005	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	96	-1.19 ± 0.25	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 51%, i.e. 472 atoms were assigned a chemical shift out of a possible 931. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	223/384 (58%)	149/153 (97%)	0/156 (0%)	74/75 (99%)
Sidechain	228/503 (45%)	223/291 (77%)	0/186 (0%)	5/26 (19%)
Aromatic	21/44 (48%)	20/23 (87%)	0/19 (0%)	1/2 (50%)
Overall	472/931 (51%)	392/467 (84%)	0/361 (0%)	80/103 (78%)

7.1.4 Statistically unusual chemical shifts (i)

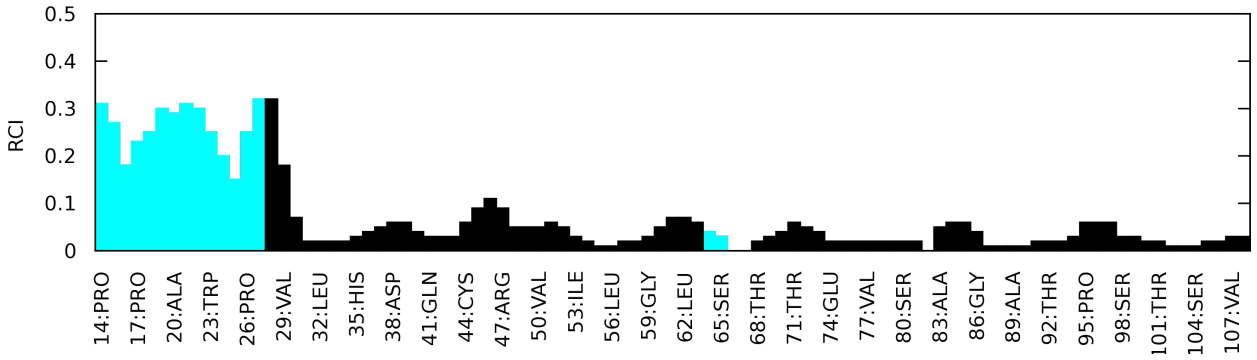
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	75	VAL	HG22	-0.70	2.20 – -0.60	-5.4
1	A	75	VAL	HG23	-0.70	2.20 – -0.60	-5.4
1	A	75	VAL	HG21	-0.70	2.20 – -0.60	-5.4

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:


RCI
0.5
0.4
0.3
0.2
0.1
0
14:PRO
17:PRO
20:ALA
23:TRP
26:PRO
29:VAL
32:LEU
35:HIS
38:ASP
41:GLN
44:CYS
47:ARG
50:VAL
53:ILE
56:LEU
59:GLY
62:LEU
65:SER
68:THR
71:THR
74:GLU
77:VAL
80:SER
83:ALA
86:GLY
89:ALA
92:THR
95:PRO
98:SER
101:THR
104:SER
107:VAL