wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2G2B
Title	:	NMR structure of the human allograft inflammatory factor 1
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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:

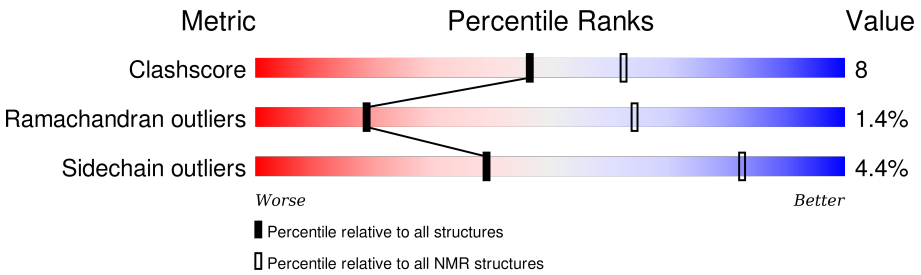
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 86%.

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	150	58% 16% 26%

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: *closest to the average*.

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:128 (111)	0.72	4

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 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2407 atoms, of which 1218 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Allograft inflammatory factor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	150	2407	753	1218	197	232	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P55008
A	2	PRO	-	CLONING ARTIFACT	UNP P55008
A	3	LEU	-	CLONING ARTIFACT	UNP P55008
A	4	GLU	-	CLONING ARTIFACT	UNP P55008

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: Allograft inflammatory factor 1

Chain A: 58% 16% 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 K20 Q23 R26 L27 D28 E29 K39 D43 L46 K54 F60 D61 L62 I70 M71 K74 R75 M76 E88 L92 I93 Y106 P107 L110 R111 M112 M113 L114

E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

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: Allograft inflammatory factor 1

Chain A: 52% 20% • 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 L18 L19 K20 Q23 E24 E25 R26 L27 D28 E29 K39 D43 E44 D45 L46 G52 F53 K54 E55 K56 Y57 G66 I70 M71 K74 R75 M76 L80 K84 T85 H86 L87 E88

L92 Y106 P107 R111 M112 G115 I120 L121 K122 M126 E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics,simulated annealing,distance geometry.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
Xplor-NIH	refinement	2.9.3

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 6980
Number of chemical shift lists	1
Total number of shifts	1595
Number of shifts mapped to atoms	1595
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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.

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	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	117	ARG	Sidechain	1

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	897	915	914	14±3
All	All	17940	18300	18280	285

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 8.

5 of 136 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:LEU:O	1:A:114:LEU:HG	0.68	1.88	9	9
1:A:93:ILE:HG12	1:A:104:PHE:CZ	0.65	2.26	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LYS:O	1:A:24:GLU:HG3	0.65	1.91	9	6
1:A:76:MET:O	1:A:80:LEU:HG	0.62	1.95	9	9
1:A:43:ASP:HB2	1:A:46:LEU:HB2	0.60	1.74	4	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	111/150 (74%)	103±2 (93±2%)	7±2 (6±2%)	2±1 (1±1%)	19	64
All	All	2220/3000 (74%)	2056 (93%)	132 (6%)	32 (1%)	19	64

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	61	ASP	6
1	A	98	SER	5
1	A	116	LYS	3
1	A	62	LEU	3
1	A	115	GLY	2

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	101/131 (77%)	97±2 (96±2%)	4±2 (4±2%)	39	82
All	All	2020/2620 (77%)	1932 (96%)	88 (4%)	39	82

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	54	LYS	15
1	A	74	LYS	12
1	A	39	LYS	12
1	A	112	MET	7
1	A	56	LYS	5

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 86% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6980

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	1595
Number of shifts mapped to atoms	1595
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	146	-0.30 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	134	0.18 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	137	-0.50 ± 0.06	Should be applied
^{15}N	138	0.18 ± 0.20	None needed (< 0.5 ppm)

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 86%, i.e. 1218 atoms were assigned a chemical shift out of a possible 1424. 1 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	536/547 (98%)	214/218 (98%)	216/222 (97%)	106/107 (99%)
Sidechain	651/792 (82%)	403/468 (86%)	242/293 (83%)	6/31 (19%)

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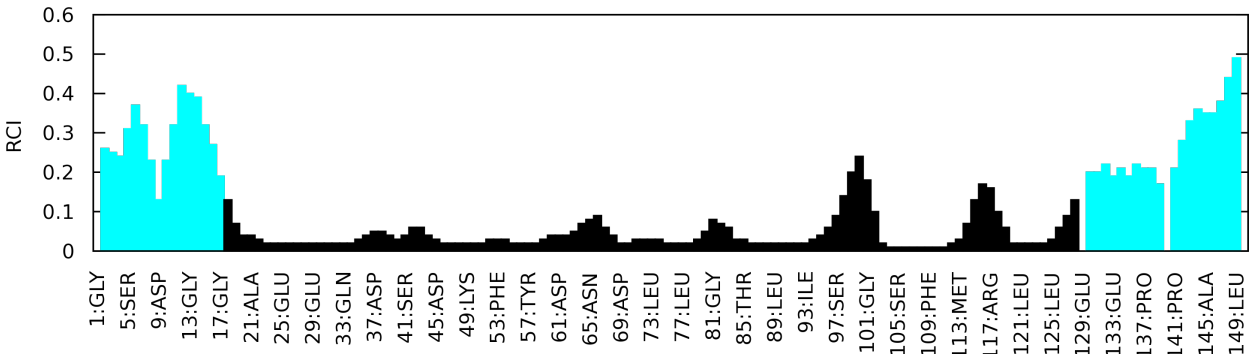
	Total	^{1}H	^{13}C	^{15}N
Aromatic	31/85 (36%)	31/45 (69%)	0/38 (0%)	0/2 (0%)
Overall	1218/1424 (86%)	648/731 (89%)	458/553 (83%)	112/140 (80%)

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	68	ILE	HB	0.06	3.24 – 0.34	-6.0

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: