wwPDB NMR Structure Validation Summary Report (i)

Apr 26, 2016 – 02:33 PM BST

PDB ID	:	1F68
Title	:	NMR SOLUTION STRUCTURE OF THE BROMODOMAIN FROM HUMAN GCN5
Authors	:	Wright, P.E.; Hudson, B.P.; Dyson, H.J.
Deposited on	:	2000-06-20

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:

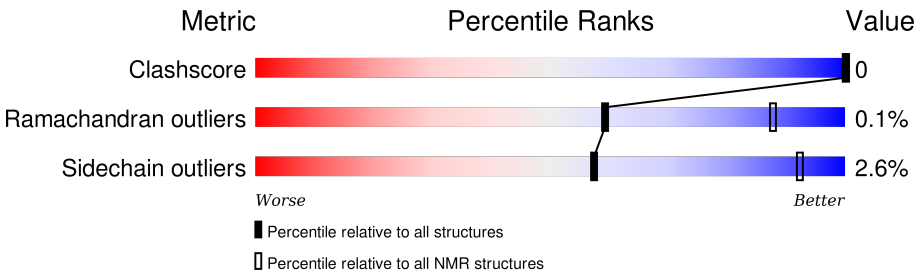
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	103	93% • 5%

2 Ensemble composition and analysis (i)

This entry contains 30 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 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 21 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:732-A:829 (98)	0.32	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 2 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1724 atoms, of which 861 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HISTONE ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	103	1724	558	861	145	155	5	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	GLY	PRO	ENGINEERED	UNP Q92830

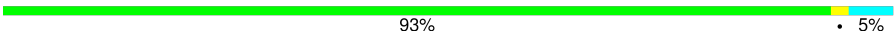
4 Residue-property plots (i)

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: HISTONE ACETYLTRANSFERASE

Chain A:



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: HISTONE ACETYLTRANSFERASE

Chain A:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Torsion angle dynamics (DYANA) for generation of initial structures; Structure-mediated assignment of ambiguous experimental restraints (SANE); Iteration between DYANA and SANE; Simulated Annealing and Energy Minimization in AMBER using full restraint set..*

Of the 185 calculated structures, 30 were deposited, based on the following criterion: *NO DISTANCE OR ANGLE VIOLATIONS GREATER THAN 0.15 A OR 5 DEGREES.*

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

Software name	Classification	Version
DYANA	refinement	1.5
SANE	refinement	1.0
AMBER	structure solution	6.0

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	0.63±0.00	0±0/852 (0.0±0.0%)	0.83±0.02	0±1/1154 (0.0±0.0%)
All	All	0.63	0/25560 (0.0%)	0.83	12/34620 (0.0%)

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	2.7±1.2
All	All	0	80

There are no bond-length outliers.

5 of 6 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	770	ARG	NE-CZ-NH2	-5.83	117.39	120.30	17	4
1	A	826	TYR	CB-CG-CD2	-5.60	117.64	121.00	18	1
1	A	816	ARG	NE-CZ-NH2	-5.53	117.53	120.30	4	2
1	A	785	ARG	NE-CZ-NH1	5.42	123.01	120.30	21	2
1	A	799	ARG	NE-CZ-NH2	-5.25	117.67	120.30	24	2

There are no chirality outliers.

5 of 14 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	766	TYR	Sidechain	18
1	A	787	TYR	Sidechain	16
1	A	786	TYR	Sidechain	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	814	TYR	Sidechain	10
1	A	781	ARG	Sidechain	6

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
All	All	24840	24960	24960	-

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 -.

There are no clashes.

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	98/103 (95%)	92±2 (93±2%)	6±2 (6±2%)	0±0 (0±0%)	59 88
All	All	2940/3090 (95%)	2745 (93%)	191 (6%)	4 (0%)	59 88

All 3 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	757	VAL	2
1	A	749	SER	1
1	A	770	ARG	1

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	91/94 (97%)	89±1 (97±1%)	2±1 (3±1%)	57 92
All	All	2730/2820 (97%)	2658 (97%)	72 (3%)	57 92

5 of 17 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	749	SER	11
1	A	776	LYS	7
1	A	770	ARG	7
1	A	785	ARG	6
1	A	791	LYS	6

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