wwPDB NMR Structure Validation Summary Report (i)

Apr 26, 2016 – 11:56 PM BST

PDB ID	:	2KVD
Title	:	Mesencephalic astrocyte-derived neurotrophic factor (MANF)
Authors	:	Hellman, M.H.; Peranen, J.; Saarma, M.; Permi, P.
Deposited on	:	2010-03-12

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:

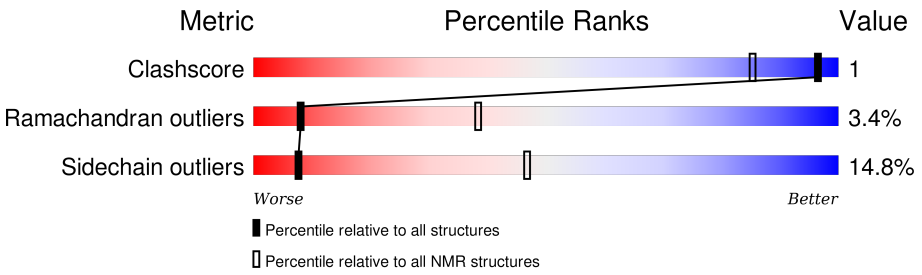
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	160	62% 11% • 26%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 1 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:8-A:60, A:64-A:94 (84)	0.29	1
2	A:108-A:125, A:132-A:148 (35)	0.13	13

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 6, 9, 10, 11, 12, 13, 14
2	4, 5, 8
3	3, 15
Single-model clusters	7

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2589 atoms, of which 1309 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mesencephalic astrocyte-derived neurotrophic factor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	160	2589	807	1309	221	243	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P55145
A	0	SER	-	EXPRESSION TAG	UNP P55145

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: Mesencephalic astrocyte-derived neurotrophic factor

Chain A: 62% 11% • 26%

G-1 S0 L1 R2 P3 G4 D5 C6 E7 F16 Y17 R23 F27 S28 P29 E33 L36 I37 K38 F39 C40 R41 R49 A61 T62 K63 I64 I65 K70 P71 L72 I76 P77 V78 L95 K96 Y97 D98 K99 Q100 I101 D102 L103 S104 T105 V106 D107 L120

T126 C127 K128 G129 C130 A131 K146 P149 K150 A151 A152 S153 A154 R155 T156 D157 L158

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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Mesencephalic astrocyte-derived neurotrophic factor

Chain A: 59% 14% •• 26%

G-1 S0 L1 R2 P3 G4 D5 C6 E7 R15 F16 Y17 Q18 R23 F27 S28 P29 E33 L36 I37 K38 F39 C40 R41 E42 A43 R49 L50 A61 T62 K63 I64 I65 L72 I76 P77 V78 I92 L95 K96 Y97 D98 K99 Q100 I101 D102 L103 S104 T105

V106 D107 L120 T126 C127 K128 G129 C130 A131 K146 P149 K150 A151 A152 S153 A154 R155 T156 D157 L158

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *TORSION ANGLE DYNAMICS, simulated annealing, TORSION ANGLE DYNAMICS.*

Of the 400 calculated structures, 15 were deposited, based on the following criterion: *STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS.*

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

Software name	Classification	Version
AMBER	structure solution	8.0
AMBER	refinement	8.0

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	0.71±0.00	0±0/998 (0.0±0.0%)	1.07±0.02	4±1/1339 (0.3±0.1%)
All	All	0.71	0/14970 (0.0%)	1.07	56/20085 (0.3%)

There are no bond-length outliers.

5 of 9 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	15	ARG	NE-CZ-NH1	7.94	124.27	120.30	6	7
1	A	23	ARG	NE-CZ-NH1	7.28	123.94	120.30	1	12
1	A	138	ARG	NE-CZ-NH1	6.84	123.72	120.30	8	7
1	A	112	ARG	NE-CZ-NH1	6.59	123.60	120.30	9	6
1	A	41	ARG	NE-CZ-NH1	6.12	123.36	120.30	13	9

There are no chirality outliers.

There are no planarity outliers.

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	981	1008	1008	2±0
All	All	14715	15120	15120	32

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.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:HG13	1:A:27:PHE:CD1	0.49	2.41	9	1
1:A:17:TYR:CD1	1:A:17:TYR:C	0.47	2.89	9	8
1:A:20:LEU:O	1:A:25:VAL:HG12	0.46	2.10	9	1
1:A:17:TYR:C	1:A:17:TYR:CD1	0.44	2.91	14	7
1:A:76:ILE:HB	1:A:77:PRO:HD3	0.43	1.91	9	15

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	119/160 (74%)	105±1 (88±1%)	10±1 (9±1%)	4±1 (3±1%)	8	38
All	All	1785/2400 (74%)	1568 (88%)	156 (9%)	61 (3%)	8	38

5 of 8 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	78	VAL	15
1	A	29	PRO	15
1	A	28	SER	15
1	A	43	ALA	6
1	A	30	ALA	5

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	109/142 (77%)	93±2 (85±2%)	16±2 (15±2%)	8	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1635/2130 (77%)	1393 (85%)	242 (15%)	8 47

5 of 35 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	33	GLU	15
1	A	16	PHE	15
1	A	27	PHE	15
1	A	76	ILE	15
1	A	36	LEU	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)

No chemical shift data were provided