wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1MPZ
Title	:	NMR solution structure of native Viperidae lebetina obtusa protein
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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
https://www.wwpdb.org/validation/2017/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:

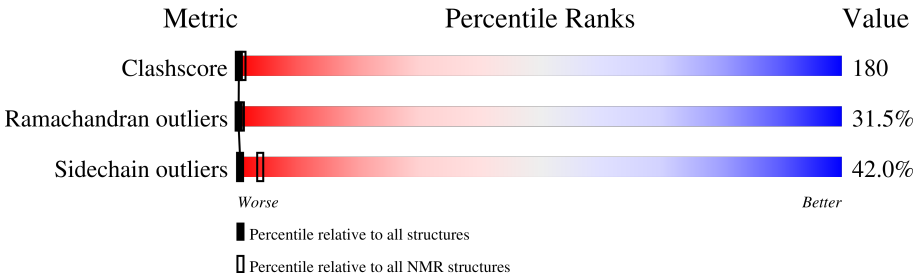
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	41	41% 51% 7%

2 Ensemble composition and analysis (i)

This entry contains 22 models. Model 22 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2-A:39 (38)	0.46	22

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 588 atoms, of which 288 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Obtustatin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	41	588	184	288	52	56	8	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Obtustatin

Chain A: 41% 51% 7%

C1 T2 T3 G4 P5 C6 C7 R8 Q9 C10 K11 L12 K13 P14 A15 G16 T17 T18 C19 W20 K21 T22 S23 L24 T25 S26 H27 Y28 C29 T30 G31 K32 S33 C34 D35 C36 P37 L38 Y39 P40 G41

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

The representative model is number 22. Colouring as in section 4.1 above.

- Molecule 1: Obtustatin

Chain A: 5% 12% 32% 44% 7%

C1 T2 T3 G4 P5 C6 C7 R8 Q9 C10 K11 L12 K13 P14 A15 G16 T17 T18 C19 W20 K21 T22 S23 L24 T25 S26 H27 Y28 C29 T30 G31 K32 S33 C34 D35 C36 P37 L38 Y39 P40 G41

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Manual assignment by Wuthrich protocols and automatic NOESY assignment extension by NOAH.*

Of the 500 calculated structures, 22 were deposited, based on the following criterion: *structures with the lowest energy,target function.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	

No chemical shift data was provided.

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	1.54±3.85	6±26/291 (1.9± 8.8%)	1.69±3.05	5±24/397 (1.3± 6.0%)
All	All	4.14	123/6402 (1.9%)	3.48	114/8734 (1.3%)

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	0.1±0.6	0.0±0.0
All	All	3	0

5 of 123 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	39	TYR	CE2-CZ	-71.67	0.45	1.38	22	1
1	A	39	TYR	CG-CD1	-70.27	0.47	1.39	22	1
1	A	20	TRP	NE1-CE2	-69.48	0.47	1.37	22	1
1	A	20	TRP	CD2-CE3	-61.09	0.48	1.40	22	1
1	A	39	TYR	CE1-CZ	-59.71	0.60	1.38	22	1

5 of 114 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	28	TYR	CD1-CG-CD2	-82.41	27.25	117.90	22	1
1	A	28	TYR	CB-CG-CD1	75.72	166.43	121.00	22	1
1	A	28	TYR	CB-CG-CD2	75.54	166.32	121.00	22	1
1	A	20	TRP	CD1-CG-CD2	-71.57	49.05	106.30	22	1
1	A	27	HIS	ND1-CG-CD2	-65.12	14.83	106.00	22	1

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	2	THR	CA,CB	1
1	A	30	THR	CB	1

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	283	274	250	100±15
All	All	6226	6028	5974	2192

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 180.

5 of 818 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LYS:NZ	1:A:21:LYS:CD	1.50	1.74	22	1
1:A:32:LYS:CB	1:A:32:LYS:CE	1.47	1.93	22	1
1:A:11:LYS:NZ	1:A:11:LYS:CD	1.44	1.75	22	1
1:A:28:TYR:CZ	1:A:28:TYR:CD2	1.43	2.07	22	1
1:A:28:TYR:CZ	1:A:28:TYR:CD1	1.42	2.06	22	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	38/41 (93%)	12±3 (31±9%)	14±3 (37±7%)	12±3 (31±7%)	0 0
All	All	836/902 (93%)	260 (31%)	313 (37%)	263 (31%)	0 0

5 of 33 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	35	ASP	20
1	A	26	SER	19
1	A	21	LYS	18
1	A	7	CYS	16
1	A	15	ALA	16

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	34/36 (94%)	20±2 (58±6%)	14±2 (42±6%)	0 4
All	All	748/792 (94%)	434 (58%)	314 (42%)	0 4

5 of 30 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	11	LYS	22
1	A	13	LYS	22
1	A	32	LYS	18
1	A	21	LYS	16
1	A	23	SER	16

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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	22-A	17

The worst 5 of 17 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
22	A	17:THR	C	18:THR	N	1.18
22	A	24:LEU	C	25:THR	N	1.08
22	A	33:SER	C	34:CYS	N	1.08
22	A	39:TYR	C	40:PRO	N	1.08
22	A	1:CYS	C	2:THR	N	1.04

7 Chemical shift validation (i)

No chemical shift data were provided