

# wwPDB NMR Structure Validation Summary Report (i)

#### Feb 16, 2022 – 08:57 AM EST

PDB ID	:	1MNT
Title	:	SOLUTION STRUCTURE OF DIMERIC MNT REPRESSOR (1-76)
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Deposited on	:	1994-06-28

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:

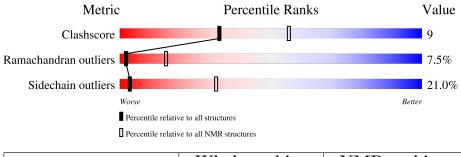
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${f NMR}  { m archive} \ (\#{ m Entries})$
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	А	76	13%	25%	7% •	41%	13%			
1	В	76	18%	25%	5% •	37%	13%			



# 2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 4 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:4-A:24, A:28-A:41, B:5-	0.30	4							
	B:42 (73)									

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 5 single-model clusters were found.

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



# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1064 atoms, of which 0 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called MNT REPRESSOR.

Mol	Chain	Residues	Atoms					Trace
1 A	Δ	66	Total	С	Ν	0	S	0
	A	00	532	326	99	104	3	0
1	1 B	66	Total	С	Ν	0	S	0
		00	532	326	99	104	3	U



# 4 Residue-property plots (i)

#### 4.1 Average score per residue in the NMR ensemble

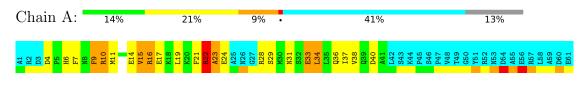
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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.

- Chain A: 13% 41% 13% 25% 7% 423 1224 1225 1227 1227 1228 1229 1328 1328 1332 1333 1332 E64 L65 LYS LYS LYS MET VAL PHE PHE PHE LYS LYS ASP • Molecule 1: MNT REPRESSOR Chain B: 18% 37% 25% 5% • 13% L65 V66 LYS LYS MET VAL VAL PHE ASP LEU LYS ASP
- Molecule 1: MNT REPRESSOR

# 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.

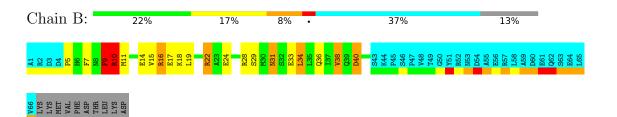
• Molecule 1: MNT REPRESSOR



#### Q62 S63 E64 LYS LYS MET VAL PHE ASP LFU LEU LS

• Molecule 1: MNT REPRESSOR







## 5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 15 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or 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	B	ond lengths	Bond angles		
	Ullaill	RMSZ	$\#Z{>}5$	RMSZ	#Z > 5	
1	А	$1.67 {\pm} 0.02$	$4{\pm}0/303~(~1.3{\pm}~0.0\%)$	$2.21{\pm}0.07$	$16{\pm}3/405~(~3.9{\pm}~0.6\%)$	
1	В	$1.64{\pm}0.01$	$4{\pm}0/320~(~1.3{\pm}~0.1\%)$	$2.12 \pm 0.07$	$14{\pm}2/427~(~3.3{\pm}~0.5\%)$	
All	All	1.65	123/9345~(~1.3%)	2.17	445/12480 ( $3.6%$ )	

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	А	$0.0{\pm}0.0$	$5.1 \pm 2.1$
1	В	$0.0{\pm}0.0$	$4.5 \pm 1.5$
All	All	0	145

5 of 18 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Mol Chain		Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
	Ullaili	$\operatorname{Res}$	Type	Atoms		Observeu(A)	Iueai(A)	Worst	Total
1	А	33	GLU	CD-OE1	10.40	1.37	1.25	12	8
1	А	14	GLU	CD-OE2	10.33	1.37	1.25	12	6
1	В	14	GLU	CD-OE2	10.32	1.37	1.25	14	8
1	А	14	GLU	CD-OE1	10.30	1.36	1.25	5	9
1	А	24	GLU	CD-OE1	10.26	1.36	1.25	14	13

5 of 73 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Mol Chain	Chain Bog	Chain Res	Type	Atoms	7	Observed(°)	$Ideal(^{o})$	Moo	dels
10101	Unain	nes	туре	Atoms		Observed()	Ideal(*)	Worst	Total	
1	А	23	ALA	CB-CA-C	11.71	127.67	110.10	1	7	
1	В	28	ARG	NE-CZ-NH1	11.05	125.83	120.30	12	15	
1	А	34	LEU	CB-CA-C	10.87	130.85	110.20	15	5	

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	Mol Chain	1	10		7	Observed(0)	Ideal(°)	Mod	dels
IVIOI	Chain	nes	Type	Atoms	L	$Observed(^{o})$	Ideal(*)	Worst	Total
1	А	22	ARG	NE-CZ-NH1	10.62	125.61	120.30	12	15
1	В	34	LEU	CB-CA-C	9.95	129.10	110.20	10	4

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There are no chirality outliers.

5 of 31 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	А	31	ASN	Peptide	15
1	В	29	SER	Peptide	15
1	А	29	SER	Peptide	14
1	В	31	ASN	Peptide	13
1	А	6	HIS	Peptide,Sidechain	12

#### 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	А	297	0	295	9±3
1	В	314	0	316	8±3
All	All	9165	0	9165	168

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 9.

5 of 65 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom 2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Atom-2 Clash(A)		Worst	Total
1:A:7:PHE:CZ	1:B:34:LEU:HD12	0.73	2.19	6	11
1:A:34:LEU:HD12	1:B:7:PHE:CZ	0.73	2.19	3	10
1:A:19:LEU:HB3	1:A:30:MET:CE	0.63	2.23	8	5
1:A:34:LEU:HD23	1:B:7:PHE:CZ	0.62	2.28	12	5
1:A:9:PHE:CD2	1:B:34:LEU:HD13	0.59	2.33	11	11



#### 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	А	35/76~(46%)	$27 \pm 1 (78 \pm 4\%)$	$5\pm1 (14\pm4\%)$	$3\pm1$ (8±3%)	2	13
1	В	38/76~(50%)	$30\pm2$ (78 $\pm5\%$ )	$6\pm2~(15\pm5\%)$	$3\pm1$ (7±2%)	2	17
All	All	1095/2280~(48%)	851 (78%)	162~(15%)	82 (7%)	2	15

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	В	22	ARG	15
1	А	22	ARG	14
1	А	23	ALA	11
1	В	23	ALA	10
1	А	10	ARG	8

#### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	33/68~(49%)	$27 \pm 1 (82 \pm 4\%)$	$6\pm1 (18\pm4\%)$	4	37	
1	В	34/68~(50%)	$26\pm2$ (76 $\pm6\%$ )	$8\pm2~(24\pm6\%)$	2	27	
All	All	1005/2040~(49%)	794 (79%)	211 (21%)	3	32	

5 of 39 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	34	LEU	15
1	А	36	GLN	15

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#### 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)

There are no chain breaks in this entry.



Mol Chain  $\operatorname{Res}$ Models (Total) Type VAL В 1515 1 В LEU 1 3415В 36  $\operatorname{GLN}$ 1 15

# 7 Chemical shift validation (i)

No chemical shift data were provided

