



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 09:26 am BST

PDB ID : 6BEW  
Title : Solution structure of de novo macrocycle design7.2  
Authors : Shortridge, M.D.; Hosseinzadeh, P.; Pardo-Avila, F.; Varani, G.; Baker, D.  
Deposited on : 2017-10-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

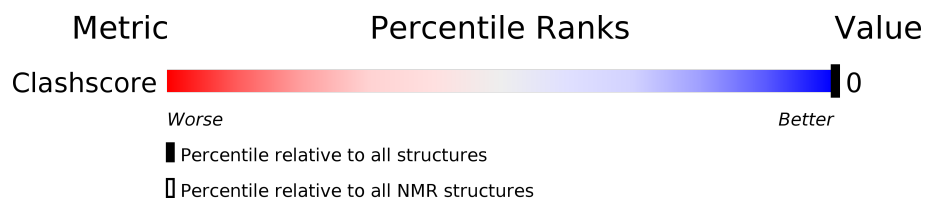
## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 58%.

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.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>NMR archive (#Entries)</b>
Clashscore	158937	12864

## WHAT HAPPENED

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 101 atoms, of which 45 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein (with D amino acids) called (DHI)P(DAS)(DGN)(DSN)(DGL)P.

Mol	Chain	Residues	Atoms					Trace
1	A	7	Total	C	H	N	O	0
			101	33	45	10	13	

## 4 Residue-property plots

### 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.

### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.2 Score per residue for model 2

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.3 Score per residue for model 3

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.4 Score per residue for model 4

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.5 Score per residue for model 5

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.6 Score per residue for model 6

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.7 Score per residue for model 7

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.8 Score per residue for model 8

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.9 Score per residue for model 9

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.10 Score per residue for model 10

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.11 Score per residue for model 11

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.12 Score per residue for model 12

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.13 Score per residue for model 13

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.14 Score per residue for model 14

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.15 Score per residue for model 15

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

#### 4.2.16 Score per residue for model 16

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

**4.2.17 Score per residue for model 17**

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

**4.2.18 Score per residue for model 18**

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

**4.2.19 Score per residue for model 19**

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

**4.2.20 Score per residue for model 20**

There is no protein, DNA or RNA molecules in this entry to show sequence plots.

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
GROMACS	refinement	2016.1
X-PLOR NIH	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	43
Number of shifts mapped to atoms	43
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 Too-close contacts

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	1120	900	807	-

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.



## 5.2 Torsion angles [i](#)

### 5.2.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.2.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

5 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.6 Other polymers [i](#)

There are no such molecules in this entry.

## 5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 58% for the well-defined parts and 58% for the entire structure.

### 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *binoculars\_bmrB.txt*

#### 6.1.1 Bookkeeping

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	43
Number of shifts mapped to atoms	43
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 6.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

#### 6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 58%, i.e. 14 atoms were assigned a chemical shift out of a possible 24. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	2/6 (33%)	2/2 (100%)	0/4 (0%)	0/0 (—%)
Sidechain	12/18 (67%)	12/12 (100%)	0/6 (0%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	14/24 (58%)	14/14 (100%)	0/10 (0%)	0/0 (—%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 58%, i.e. 14 atoms were assigned a chemical shift out of a possible 24. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	2/6 (33%)	2/2 (100%)	0/4 (0%)	0/0 (—%)
Sidechain	12/18 (67%)	12/12 (100%)	0/6 (0%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	14/24 (58%)	14/14 (100%)	0/10 (0%)	0/0 (—%)

#### 6.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

#### 6.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index* (RCI) plot could be generated from the current chemical shift list (binoculars\_bmr.txt). RCI is only applicable to proteins.