

# wwPDB NMR Structure Validation Summary Report (i)

### May 28, 2020 – 09:42 pm BST

PDB ID	:	2 E Q T
$\operatorname{Title}$	:	Micelle-bound structure of growth-blocking peptide of the armyworm, Pseu-
		daletia separata
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Deposited on	:	2007-03-30

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 (1)) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
$\operatorname{NmrClust}$	:	Kelley et al. (1996)
$\operatorname{MolProbity}$	:	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. $(2010)$
${ m ShiftChecker}$	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

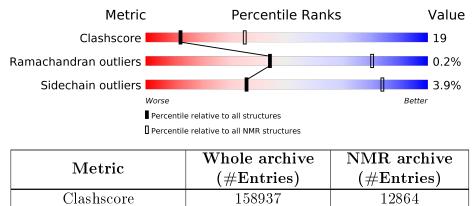
Ramachandran outliers

# 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.



154571

Sidechai	n outliers	154315	11428	
The table be	elow summar	ises the geometric iss	ues observed across	the polymeric chains and their
fit to the ex	perimental d	ata. The red, orange	e, yellow and green	segments indicate the fraction
of residues t	hat contain o	outliers for $>=3, 2, 1$	and 0 types of geor	metric quality criteria. A cyan
segment indi	cates the frac	tion of residues that a	are not part of the we	ell-defined cores, and a grey seg-
ment represe	nts the fracti	on of residues that ar	e not modelled. The	numeric value for each fraction
is indicated	below the co	cresponding segment,	with a dot represent	ting fractions $<=5\%$

11451

Mol	Chain	Length	Quality of chain				
1	А	28	50%	25%	25%		



# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues							
Well-defined core	Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model						
1	A:8-A:28 (21)	0.38	6				

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 4 single-model clusters were found.

Cluster number	Models
1	6, 7, 10, 14, 15
2	2, 4, 11, 13
3	3, 9, 12, 17
4	1, 5, 16
Single-model clusters	8; 18; 19; 20



# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 423 atoms, of which 206 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Growth-blocking peptide, long form.

Mol	Chain	Residues	Atoms					Trace	
1	٨	20	Total	С	Η	Ν	Ο	S	0
	A	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	423	136	206	37	41	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	LEU	-	EXPRESSION TAG	UNP Q27913
A	27	ILE	-	EXPRESSION TAG	UNP Q27913
A	28	THR	-	EXPRESSION TAG	UNP Q27913



# 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: Growth-blocking peptide, long form



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

The representative model is number 6. Colouring as in section 4.1 above.

• Molecule 1: Growth-blocking peptide, long form

Chain A:	39%	36%	25%
80 80 80 80 80 80 80 80 80 80 80 80 80 8	M12 114 114 115 115 112 112 112 112 112 112 112 112		



# 5 Refinement protocol and experimental data overview (i)

Of the 100 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
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

## 5.1 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	169	168	168	$6\pm 2$
All	All	3380	3360	3360	128

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 19.

5 of 43 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:24:TYR:HA	1:A:27:ILE:CG1	0.78	2.08	18	9
1:A:24:TYR:HA	1:A:27:ILE:HG12	0.69	1.61	18	7
1:A:12:MET:SD	1:A:20:LYS:HB3	0.67	2.29	6	1
1:A:20:LYS:HD3	1:A:24:TYR:HE1	0.66	1.48	1	1
1:A:20:LYS:HD3	1:A:21:PRO:HD2	0.64	1.68	3	2



# 5.2 Torsion angles (i)

### 5.2.1 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	20/28~(71%)	$18\pm1 (91\pm4\%)$	$2\pm1 (9\pm4\%)$	0±0 (0±1%)	44 80	
All	All	400/560~(71%)	364~(91%)	35~(9%)	1  (0%)	44 80	

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	А	8	VAL	1

#### 5.2.2 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	А	18/23~(78%)	$17 \pm 1 (96 \pm 4\%)$	$1\pm1 (4\pm4\%)$	36 84
All	All	360/460~(78%)	346 (96%)	14 (4%)	36 84

All 4 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	А	13	ARG	9
1	А	24	TYR	2
1	А	16	ASP	2
1	А	25	GLN	1

### 5.2.3 RNA (i)

There are no RNA molecules in this entry.



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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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 (i)

No chemical shift data were provided

