

# Full wwPDB NMR Structure Validation Report (i)

#### Feb 23, 2022 - 01:56 PM EST

PDB ID	:	1YL9
Title	:	3D Solution Structure of [Tyr3]Octreotate derivatives in DMSO
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Deposited on	:	2005-01-19

This is a Full wwPDB NMR Structure Validation 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:

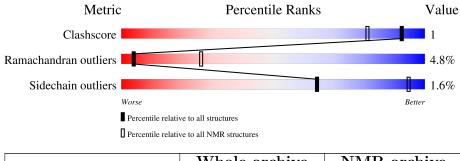
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
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	8	100%



# 2 Ensemble composition and analysis (i)

This entry contains 21 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (6) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust



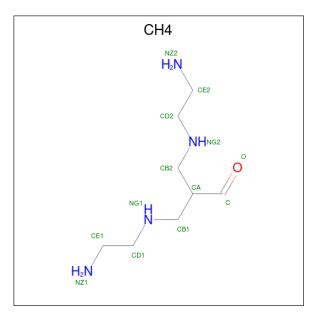
# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 168 atoms, of which 82 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called [Tyr3]Octreotate.

Mol	Chain	Residues	Atoms					Trace	
1	۸	0	Total	С	Η	Ν	Ο	S	0
	A	A o	136	49	63	10	12	2	0

• Molecule 2 is 3-[(2-AMINOETHYL)AMINO]-2-{[(2-AMINOETHYL)AMINO]METHYL}P ROPANAL (three-letter code: CH4) (formula:  $C_8H_{20}N_4O$ ).



Mol	Chain	Residues	Atoms				
2	Λ	1	Total	С	Η	Ν	0
2	A	1	32	8	19	4	1



# 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: [Tyr3]Octreotate

Chain A:

100%

There are no outlier residues in this chain.

## 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

• Mole	cule 1: [Tyr3]Octreotate	
Chain	A: 88%	12%
2 8 <u>8</u>		
4.2.2	Score per residue for model 2	
• Mole	cule 1: [Tyr3]Octreotate	
Chain	A: 100%	
<b>T</b> 1		

### There are no outlier residues in this chain.

### 4.2.3 Score per residue for model 3

• Molecule 1: [Tyr3]Octreotate



Chain A: 100% There are no outlier residues in this chain. 4.2.4Score per residue for model 4 • Molecule 1: [Tyr3]Octreotate Chain A: 100% There are no outlier residues in this chain. 4.2.5Score per residue for model 5 • Molecule 1: [Tyr3]Octreotate Chain A: 100% There are no outlier residues in this chain. Score per residue for model 6 4.2.6• Molecule 1: [Tyr3]Octreotate Chain A: 100% There are no outlier residues in this chain. 4.2.7Score per residue for model 7 • Molecule 1: [Tyr3]Octreotate Chain A: 75% 25% 4.2.8Score per residue for model 8 • Molecule 1: [Tyr3]Octreotate

Chain A:

100%

There are no outlier residues in this chain.



### 4.2.9 Score per residue for model 9

• Molecule 1: [Tyr3]Octreotate

Chain A:

There are no outlier residues in this chain.

### 4.2.10 Score per residue for model 10

• Molecule 1: [Tyr3]Octreotate

Chain A.	1000/
Unam A.	100%

100%

There are no outlier residues in this chain.

### 4.2.11 Score per residue for model 11

• Molecule 1: [Tyr3]Octreotate

Chain A: 100%

There are no outlier residues in this chain.

## 4.2.12 Score per residue for model 12

• Molecule 1: [Tyr3]Octreotate

Chain A: 88% 12%

## 4.2.13 Score per residue for model 13

• Molecule 1: [Tyr3]Octreotate

Chain A:

100%

There are no outlier residues in this chain.



#### 4.2.14 Score per residue for model 14

• Molecule 1: [Tyr3]Octreotate

Chain A: 75% 25%

#### 4.2.15 Score per residue for model 15

• Molecule 1: [Tyr3]Octreotate

Chain A: 75% 25%

100%

#### 4.2.16 Score per residue for model 16

• Molecule 1: [Tyr3]Octreotate

Chain A:

There are no outlier residues in this chain.

#### 4.2.17 Score per residue for model 17

• Molecule 1: [Tyr3]Octreotate

Chain A:

100%

There are no outlier residues in this chain.

## 4.2.18 Score per residue for model 18

• Molecule 1: [Tyr3]Octreotate

Chain A:

88%

12%





#### 4.2.19 Score per residue for model 19

62%

• Molecule 1: [Tyr3]Octreotate

Chain A:



#### 4.2.20 Score per residue for model 20

• Molecule 1: [Tyr3]Octreotate

Chain A:

100%

38%

There are no outlier residues in this chain.

#### 4.2.21 Score per residue for model 21

• Molecule 1: [Tyr3]Octreotate

Chain A:	88%	12%
3 3		



# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, torsion angle dynamics.* 

Of the 400 calculated structures, 21 were deposited, based on the following criterion: target function.

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

Software name	Classification	Version
DYANA	structure solution	1.5
Amber	refinement	5.0

No chemical shift data was provided.



# 6 Model quality (i)

# 6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DTR, CH4, DPN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	А	73	63	61	$0\pm 0$
2	А	13	19	19	$0\pm 0$
All	All	1806	1722	1681	5

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		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:5:DTR:CZ3	1:A:6:LYS:HE3	0.48	2.38	19	2	
2:A:0:CH4:HZ21	2:A:0:CH4:HB22	0.47	1.69	17	1	
1:A:9:THR:OXT	2:A:0:CH4:HA	0.45	2.12	18	1	
1:A:9:THR:OXT	2:A:0:CH4:HD13	0.40	2.16	14	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	А	5/8~(62%)	$3\pm1~(52\pm12\%)$	$2\pm1$ (43 $\pm15\%$ )	$0{\pm}0$ (5 ${\pm}9\%$ )	4	26
All	All	105/168~(62%)	55 (52%)	45 (43%)	5(5%)	4	26

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	8	CYS	4
1	А	3	CYS	1

#### 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	6/6~(100%)	$6\pm0$ (98 $\pm5\%$ )	$0\pm0~(2\pm5\%)$	64 9	94	
All	All	$126/126\ (100\%)$	124 (98%)	2(2%)	64 9	94	

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	А	4	TYR	2

### 6.3.3 RNA (i)

There are no RNA molecules in this entry.



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

2 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.

## 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

	Mol	Type	Chain	Chain	Chain	Chain	Chain	Chain	Bos	Link	Bond lengths			
		туре		nes		Counts	RMSZ	#Z>2						
	2	CH4	А	0	1	$10,\!12,\!12$	$0.72 {\pm} 0.06$	0±0 (1±3%)						

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Chain	Chain	Chain	Bos	Link	Bond angles		
			nes		Counts	RMSZ	#Z>2			
2	CH4	А	0	1	9,12,12	$1.12 \pm 0.24$	$1\pm1 (10\pm9\%)$			



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CH4	А	0	1	-	$0\pm0,12,12,12$	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)	Moo Worst	
2	А	0	CH4	CA-C	2.13	1.54	1.50	4	3

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

Mol	Chain	in Res	Type	Type Atoms		Observed(°)	$Ideal(^{o})$	Models	
	Ullaill		Type	Atoms	Z	Observed()	Iueai()	Worst	Total
2	А	0	CH4	CA-CB1-NG1	3.89	117.57	112.32	4	10
2	А	0	CH4	CA-CB2-NG2	3.37	107.76	112.32	12	4
2	А	0	CH4	CB2-NG2-CD2	2.63	107.54	113.42	3	3
2	А	0	CH4	CB1-NG1-CD1	2.10	118.11	113.42	19	1
2	А	0	CH4	O-C-CA	2.00	120.46	125.22	5	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

### 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

