

# Full wwPDB NMR Structure Validation Report (i)

#### Feb 17, 2022 – 10:41 AM EST

PDB ID	:	1PBZ
Title	:	DE NOVO DESIGNED PEPTIDE-METALLOPORPHYRIN COMPLEX,
		SOLUTION STRUCTURE
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Deposited on	:	2003-05-15

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:

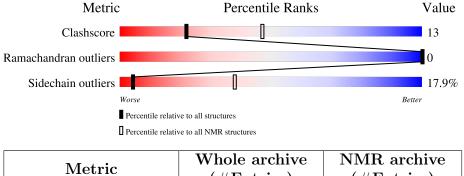
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	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 $(\#Entries)$	(#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	19	37%	11%	53%
1	В	19		100%	



# 2 Ensemble composition and analysis (i)

This entry contains 14 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 9 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 mode					
1	A:3-A:11 (9)	0.06	9		

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 2 clusters and 1 single-model cluster was found.

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



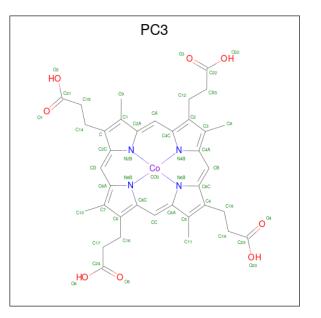
# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 509 atoms, of which 240 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called De novo designed cyclic peptide.

Mol	Chain	Residues	Atoms				Trace		
1	٨	10	Total	С	Н	Ν	0	$\mathbf{S}$	1
	I A	19	214	64	104	22	22	2	
1	D	10	Total	С	Η	Ν	Ο	S	1
	ГВ	19	214	64	104	22	22	2	

• Molecule 2 is COPROPORPHYRIN I CONTAINING CO(III) (three-letter code: PC3) (formula:  $C_{36}H_{36}CoN_4O_8$ ).



Mol	Chain	Residues	Atoms					
0	٨	1	Total	С	Co	Η	Ν	0
	A	1	81	36	1	32	4	8



# 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: De novo designed cyclic peptide

Chain A:	37%	11%	53%	
ACE0 C1 C2 C2 C2 C1 A10 A12 A12 A15 A15 C17 C17 C17 C17 C17				
• Molecule 1: De n	ovo designed	cyclic peptide		
Chain B:		100%		
ACEO C1 C2 C2 C2 C2 C2 A3 A3 A1 A1 A12 A12 A12 A12 A12 A12 A12	E14 A15 G16 C17 NH218			

## 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

• Molecule 1: De novo designed cyclic peptide

Chain A:	32%	16%	53%
ACE0 C1 C2 G2 H9 A10 A11 A12 E14 E14	A15 G16 C17 M1218		
• Molecule 1:	De novo designe	ed cyclic peptic	le
Chain B:		100%	
ACEO C1 G2 A3 A5 A5 A8 A8 H9	A10 K11 A12 A13 E14 A15 G16 G16 C17 C17 NH218		
		W_	ORLDWIDE

#### 4.2.2 Score per residue for model 2

• Molecule 1: De novo designed cyclic peptide

Chain A:	32%	16%	53%	
ACE0 C1 C2 C2 C2 C2 A8 A10 A12 A12 A13 A13	A15 G16 C17 NH218			
• Molecule 1: D	e novo designe	d cyclic peptide		
Chain B:		100%		

#### 4.2.3 Score per residue for model 3

• Molecule 1: De novo designed cyclic peptide

Chain A:	37%	11%	53%
ACE0 C1 C2 C2 A10 A12 A12 A12 A12 A12 A12 A12 A12 A12 A12			

• Molecule 1: De novo designed cyclic peptide

Chain B:		100%	/ 0	
្ព	0 7 8 7 10 9 7 0 18			

### 4.2.4 Score per residue for model 4

• Molecule 1: De novo designed cyclic peptide

Chain A: 37% 11% 53%

 $\bullet$  Molecule 1: De novo designed cyclic peptide

Chain B:

100%



#### ACE0 C1 C1 C2 A2 A5 A5 A5 A5 A1 A10 A10 A112 A13 C115 C17 C17 C17

#### 4.2.5 Score per residue for model 5

• Molecule 1: De novo designed cyclic peptide

Chain A:	42%	5%	53%
ACE0 C1 C2 C2 C2 A10 A13 A13 A13 A13 A13 A13 C17 C17 C17 C17			

• Molecule 1: De novo designed cyclic peptide

Chain B:	100%
ACE0 C 1 C 1 C 1 C 1 C 1 A 2 A 3 A 4 A 10 A 12 A 12 A 12 A 12 A 12 A 12 A 12 A 12	NH218

#### 4.2.6 Score per residue for model 6

• Molecule 1: De novo designed cyclic peptide

Chain A:	37%	11%	53%	
ACE0 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	NH218			
• Molecule 1. D	e novo desig	ned cyclic peptide		
• Molecule 1. D	e novo desigi	ieu cycne pepilde		
Chain B:		100%		
Unann D.		100%		
ACE0 C1 C2 C3 C3 A3 A3 A3 A3 A1 A1 A11 A11 A11	A12 A13 E14 A15 G16 C17 NH218			
4.2.7 Score p	oer residue	for model 7		
• Molecule 1: D	e novo desigr	ned cyclic peptide		
Chain A:	42%	5%	53%	



• Molecule 1: De novo designed cyclic peptide



Chain B:

100%



#### 4.2.8 Score per residue for model 8

• Molecule 1: De novo designed cyclic peptide

Chain A: 37% 11% 53%

• Molecule 1: De novo designed cyclic peptide

Chain B:	100%	
ACE0 G1 G2 G2 G1 G3 A3 A5 A1 A1 A12 A12 A15 A15 A15 C15 G16 G16 G16 C15 C17 C17 C17		

#### 4.2.9 Score per residue for model 9 (medoid)

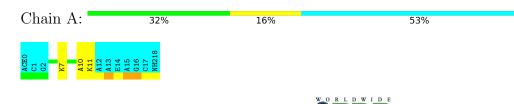
• Molecule 1: De novo designed cyclic peptide

Chain A:	42%	5%	53%	
ACE0 C1 C2 C2 C2 A10 A12 A12 A12 A12 A12 A12 A12 A12 A12 C17 C17 C17 C17				
• Molecule 1: De :	novo designed	l cyclic peptide		
Chain B:		100%		



#### 4.2.10 Score per residue for model 10

• Molecule 1: De novo designed cyclic peptide



• Molecule 1: De novo designed cyclic peptide

Chain B:	100%	
ACE0 C1 C1 C2 C2 A3 A5 A6 A15 A10 A112 A112 A112 A112 A112 A112 A112		

#### 4.2.11 Score per residue for model 11

• Molecule 1: De novo designed cyclic peptide

Chain A: 37% 11% 53%

• Molecule 1: De novo designed cyclic peptide

Chain B:		100%	
ACEO C1 C2 C2 C2 A3 A5 A5 A5 A8 A8 A8 A8 A8 A8 A8 A8 A8 A8 A8 A8 A8	A10 K11 A12 A13 E14 A15 G16 G16 C17 C17		

### 4.2.12 Score per residue for model 12

• Molecule 1: De novo designed cyclic peptide

Chain A: 42% 5% 53%

 $\bullet$  Molecule 1: De novo designed cyclic peptide

Chain B: 100%

### 4.2.13 Score per residue for model 13

• Molecule 1: De novo designed cyclic peptide

Chain A: 42% 5% 53%





• Molecule 1: De novo designed cyclic peptide

Chain B: 100%

#### 4.2.14 Score per residue for model 14

• Molecule 1: De novo designed cyclic peptide

Chain A:	37%	11%	53%
ACE0 C1 C1 C1 C2 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1			

 $\bullet$  Molecule 1: De novo designed cyclic peptide

Chain B:	100%	
ACE0 C1 C1 C2 C2 C1 A2 A5 A5 A15 A10 A12 A13 A12 A13 A12 C17 C17 A12 A12 C17 A12 A12 C17 A12 A13 A13 A13 A13 A13 A13 A13 A13 A13 A13		



# 5 Refinement protocol and experimental data overview (i)

Of the 40 calculated structures, 14 were deposited, based on the following criterion: NO RE-STRAINT VIOLATIONS GREATER THAN 0.3 ANGSTROMS.

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

Software name	Classification	Version
Felix	refinement	98

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: ACE, PC3, NH2  $\,$ 

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	Bond lengths		Bond angles	
	Chain	RMSZ	$\#Z{>}5$	RMSZ	#Z>5
1	А	$1.29 {\pm} 0.03$	$0{\pm}0/63~(~0.0{\pm}~0.0\%)$	$1.70{\pm}0.08$	$1{\pm}1/84~(~1.3{\pm}~0.7\%)$
All	All	1.29	0/882~(~0.0%)	1.70	15/1176~(~1.3%)

There are no bond-length outliers.

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

Mol	Chain	n Res	Turne	Atoms	7	Observed(°)	$Ideal(^{o})$	Models	
	Unam	nes	Type	Atoms		Observed()	Iueai()	Worst	Total
1	А	10	ALA	N-CA-CB	-5.81	101.96	110.10	8	12
1	А	9	HIS	CA-CB-CG	5.36	122.71	113.60	1	1
1	А	7	LYS	N-CA-CB	-5.33	101.01	110.60	2	2

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	62	64	64	$0\pm 0$
1	В	0	0	0	$0\pm 0$
2	А	49	32	32	$3\pm 2$
All	All	1553	1344	1344	37



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 13.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Mo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
2:A:20:PC3:O4	2:A:20:PC3:CB	1.29	1.80	13	3
2:A:20:PC3:H191	2:A:20:PC3:HB	1.08	1.26	1	4
2:A:20:PC3:HB	2:A:20:PC3:C19	0.95	1.91	5	3
2:A:20:PC3:O4	2:A:20:PC3:HB	0.90	1.63	13	1
2:A:20:PC3:O4	2:A:20:PC3:C6C	0.89	2.19	13	3
2:A:20:PC3:O23	2:A:20:PC3:C6C	0.81	2.29	6	3
2:A:20:PC3:C4	2:A:20:PC3:O23	0.80	2.29	10	1
2:A:20:PC3:H191	2:A:20:PC3:CB	0.76	2.01	5	2
2:A:20:PC3:O23	2:A:20:PC3:CB	0.72	2.38	6	1
2:A:20:PC3:HB	2:A:20:PC3:C23	0.69	2.16	13	1
2:A:20:PC3:H192	2:A:20:PC3:HB	0.69	1.64	2	1
2:A:20:PC3:O4	2:A:20:PC3:C4	0.69	2.41	14	3
2:A:20:PC3:H192	2:A:20:PC3:CB	0.68	2.18	2	1
2:A:20:PC3:C19	2:A:20:PC3:CB	0.63	2.69	1	3
2:A:20:PC3:O23	2:A:20:PC3:C5	0.55	2.54	10	1
2:A:20:PC3:HC	2:A:20:PC3:H171	0.55	1.79	2	1
2:A:20:PC3:CB	2:A:20:PC3:C23	0.54	2.75	13	1
2:A:20:PC3:O23	2:A:20:PC3:C4	0.54	2.55	6	1
2:A:20:PC3:H171	2:A:20:PC3:CC	0.51	2.35	2	1
2:A:20:PC3:C6C	2:A:20:PC3:C23	0.42	2.98	12	1
1:A:8:ALA:HB1	2:A:20:PC3:C21	0.40	2.46	2	1

All unique clashes are listed below, sorted by their clash magnitude.

## 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	9/19~(47%)	$9\pm0$ (99±3%)	0±0 (1±3%)	0±0 (0±0%)	100 100
1	В	0	-	-	-	-
All	All	126/532~(24%)	125~(99%)	1 (1%)	0  (0%)	100 100

There are no Ramachandran outliers.



#### 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	А	4/7~(57%)	$3\pm1$ (82 $\pm15\%$ )	$1\pm1 (18\pm15\%)$	4 38		
1	В	0	-	-	-		
All	All	56/196~(29%)	46 (82%)	10 (18%)	4 38		

All 2 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	11	LYS	8
1	А	7	LYS	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)

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)

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.



ſ	Mol	Turne	Chain	Res	Tink	Bond lengths			
		Type	Chain		LIIIK	Counts	RMSZ	#Z>2	
	2	PC3	А	20	1	36, 56, 56	$1.38 {\pm} 0.05$	6±1 (17±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.

Mal	Turne	Chain	Res	Link	Bond angles			
IVIOI	Type	Chain			Counts	RMSZ	#Z>2	
2	PC3	А	20	1	22,90,90	$2.68 \pm 0.25$	$10\pm2~(43\pm7\%)$	

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	PC3	А	20	1	-	$0\pm0,12,60,60$	-

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

Mol	Chain	Dec	Trune	Atoms	Z	Observed(Å)	Ideal(Å)	Moo	dels
	Unain	$\operatorname{Res}$	Type	Atoms		Observed(A)	Ideal(A)	Worst	Total
2	А	20	PC3	C16-C6	3.34	1.57	1.52	6	8
2	А	20	PC3	C12-C2	3.26	1.56	1.52	11	9
2	А	20	PC3	C6-C7	3.09	1.46	1.37	6	14
2	А	20	PC3	C-C1	3.07	1.46	1.37	1	14
2	А	20	PC3	C2-C3	2.90	1.46	1.37	9	14
2	А	20	PC3	C4-C5	2.61	1.45	1.37	11	13
2	А	20	PC3	CO3-N4B	2.54	2.12	1.97	11	3
2	А	20	PC3	C14-C	2.39	1.56	1.52	1	2
2	А	20	PC3	CO3-N2B	2.37	2.11	1.97	13	7
2	А	20	PC3	C8A-CD	2.16	1.47	1.41	6	1
2	А	20	PC3	C4C-CA	2.02	1.46	1.41	13	1
2	А	20	PC3	CO3-N6B	2.01	2.09	1.97	8	1

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



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	Observed(°)	Ideal(°)	Moo	lels
	Ullalli	nes	туре	Atoms		Observed()	Ideal()	Worst	Total
2	А	20	PC3	C5-C6A-N6B	6.76	115.15	108.72	2	14
2	А	20	PC3	CX5-C12-C2	6.50	124.48	112.49	1	10
2	А	20	PC3	C1-C2A-N2B	6.33	114.74	108.72	9	14
2	А	20	PC3	C15-C14-C	6.18	123.86	112.48	1	9
2	А	20	PC3	C12-CX5-C22	5.57	122.01	112.67	13	10
2	А	20	PC3	C16-C17-C24	5.26	121.50	112.67	2	10
2	А	20	PC3	C14-C15-C21	4.67	120.51	112.67	1	7
2	А	20	PC3	C4A-C3-C2	4.64	103.77	107.00	2	14
2	А	20	PC3	C17-C16-C6	4.39	120.58	112.49	1	8
2	А	20	PC3	C19-C18-C4	4.19	104.75	112.48	2	4
2	А	20	PC3	C8A-C7-C6	3.87	104.30	107.00	14	14
2	А	20	PC3	C11-C5-C4	3.29	131.14	124.94	6	12
2	А	20	PC3	C12-C2-C3	2.62	119.71	127.25	1	1
2	А	20	PC3	C18-C19-C23	2.56	116.97	112.67	10	5
2	А	20	PC3	C8-C3-C2	2.16	129.02	124.94	1	1

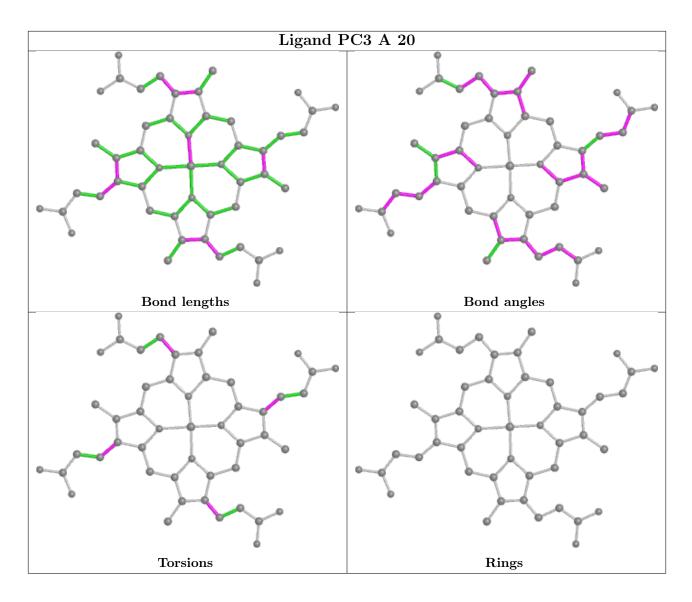
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





# 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

