



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 4, 2020 – 11:44 pm BST

PDB ID : 1RRU  
Title : The influence of a chiral amino acid on the helical handedness of PNA in solution and in crystals  
Authors : Rasmussen, H.; Liljefors, T.; Petersson, B.; Nielsen, P.E.; Kastrup, J.S.  
Deposited on : 2003-12-09  
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

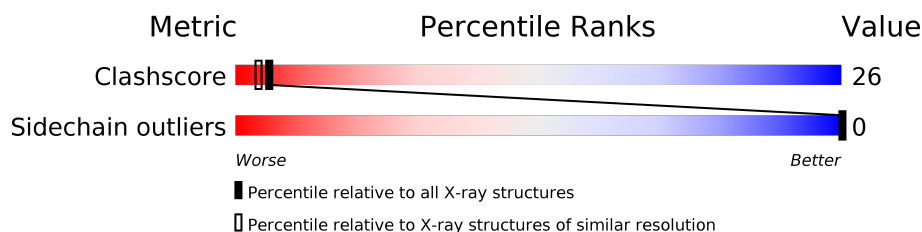
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.



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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	8	 50% 50%
1	B	8	 88% 13%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 294 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called Peptide Nucleic Acid, (H-P(\*CPN\*GPN\*TPN\*APN\*CPN\*GPN)-LYS-NH<sub>2</sub>).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	8	Total	C	N	O	0	2	1
			133	74	39	20			
1	B	8	Total	C	N	O	0	2	1
			133	74	39	20			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	13	Total	O	0	0
			13	13		

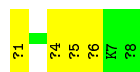
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Peptide Nucleic Acid, (H-P(\*CPN\*GPN\*TPN\*APN\*CPN\*GPN)-LYS-NH2)

Chain A: 



- Molecule 1: Peptide Nucleic Acid, (H-P(\*CPN\*GPN\*TPN\*APN\*CPN\*GPN)-LYS-NH2)

Chain B: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.75Å 44.07Å 31.22Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	6.00 – 2.35	Depositor
% Data completeness (in resolution range)	74.0 (6.00-2.35)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.219 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPN, GPN, APN, CPN, 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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.96	0/8	1.93	0/8
1	B	1.73	0/8	2.81	0/8
All	All	1.40	0/16	2.41	0/16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	133	0	80	7	0
1	B	133	0	79	1	0
2	A	15	0	0	10	0
2	B	13	0	0	0	0
All	All	294	0	159	12	0

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 26.

The worst 5 of 12 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:CPN:N1'	2:A:29:HOH:O	2.29	0.65
1:A:4[B]:APN:C3'	2:A:29:HOH:O	2.47	0.61
1:A:4[A]:APN:C3'	2:A:29:HOH:O	2.49	0.59
1:A:5:CPN:C7'	2:A:30:HOH:O	2.57	0.53
1:A:6:GPN:H8'1	2:A:30:HOH:O	2.17	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein molecules in this entry.

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

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CPN	A	1	1	15,18,19	1.25	3 (20%)	16,23,25	2.58	8 (50%)
1	APN	A	4[A]	1	18,21,22	1.31	3 (16%)	15,28,30	2.12	5 (33%)
1	TPN	B	11[B]	1	16,19,20	1.40	2 (12%)	15,25,27	3.55	6 (40%)
1	APN	B	12[A]	1	18,21,22	1.73	3 (16%)	15,28,30	2.66	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPN	B	11[A]	1	16,19,20	1.49	3 (18%)	15,25,27	3.53	6 (40%)
1	CPN	A	5	1	15,18,19	1.02	1 (6%)	16,23,25	2.61	9 (56%)
1	CPN	B	9	1	15,18,19	1.96	5 (33%)	16,23,25	2.59	6 (37%)
1	APN	A	4[B]	1	18,21,22	1.31	3 (16%)	15,28,30	2.08	4 (26%)
1	CPN	B	13	1	15,18,19	1.21	2 (13%)	16,23,25	2.16	5 (31%)
1	TPN	A	3[B]	1	16,19,20	1.14	2 (12%)	15,25,27	3.34	4 (26%)
1	GPN	B	10	1	18,22,23	1.36	3 (16%)	17,30,32	4.27	9 (52%)
1	TPN	A	3[A]	1	16,19,20	1.15	2 (12%)	15,25,27	3.34	3 (20%)
1	GPN	A	2	1	18,22,23	1.49	3 (16%)	17,30,32	3.09	6 (35%)
1	GPN	B	14	1	18,22,23	1.61	4 (22%)	17,30,32	3.12	10 (58%)
1	GPN	A	6	1	18,22,23	1.72	3 (16%)	17,30,32	2.62	4 (23%)
1	APN	B	12[B]	1	18,21,22	1.73	3 (16%)	15,28,30	2.66	6 (40%)

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
1	CPN	A	1	1	-	1/13/14/15	0/1/1/1
1	APN	A	4[A]	1	-	0/13/14/15	0/2/2/2
1	TPN	B	11[B]	1	-	1/13/14/15	0/1/1/1
1	APN	B	12[A]	1	-	0/13/14/15	0/2/2/2
1	TPN	B	11[A]	1	-	1/13/14/15	0/1/1/1
1	CPN	A	5	1	-	0/13/14/15	0/1/1/1
1	CPN	B	9	1	-	0/13/14/15	0/1/1/1
1	APN	A	4[B]	1	-	1/13/14/15	0/2/2/2
1	CPN	B	13	1	-	1/13/14/15	0/1/1/1
1	TPN	A	3[B]	1	-	3/13/14/15	0/1/1/1
1	GPN	B	10	1	-	0/13/14/15	0/2/2/2
1	TPN	A	3[A]	1	-	1/13/14/15	0/1/1/1
1	GPN	A	2	1	-	0/13/14/15	0/2/2/2
1	GPN	B	14	1	-	0/13/14/15	0/2/2/2
1	GPN	A	6	1	-	0/13/14/15	0/2/2/2
1	APN	B	12[B]	1	-	1/13/14/15	0/2/2/2

The worst 5 of 45 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12[A]	APN	C4-N3	-5.44	1.28	1.35
1	B	12[B]	APN	C4-N3	-5.44	1.28	1.35
1	B	9	CPN	C8'-N1	-4.94	1.42	1.47
1	A	6	GPN	C6-N1	4.62	1.41	1.33
1	A	6	GPN	C3'-C2'	3.65	1.64	1.50

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3[B]	TPN	C4-N3-C2	11.85	125.15	115.14
1	A	3[A]	TPN	C4-N3-C2	11.85	125.15	115.14
1	B	11[B]	TPN	C4-N3-C2	10.23	123.78	115.14
1	B	11[A]	TPN	C4-N3-C2	10.23	123.78	115.14
1	B	10	GPN	C5-C6-N1	-9.86	109.95	123.43

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CPN	N1'-C2'-C3'-N4'
1	B	11[B]	TPN	C7'-C8'-N1-C2
1	B	11[A]	TPN	C7'-C8'-N1-C2
1	A	4[B]	APN	N1'-C2'-C3'-N4'
1	B	13	CPN	C7'-C8'-N1-C2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	CPN	1	0
1	A	4[A]	APN	2	0
1	B	12[A]	APN	1	0
1	A	5	CPN	2	0
1	A	4[B]	APN	1	0
1	A	6	GPN	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.