

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1PUP
Title	:	CRYSTAL STRUCTURE OF A PEPTIDE NUCLEIC ACID (PNA) DU-
		PLEX AT 1.7 ANGSTROMS RESOLUTION
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Deposited on		
Resolution	:	1.70 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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)
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.70 Å.

141614

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	Percent	ile Ranks Value
Clashscore		8
Worse	2	Better
Perc	entile relative to all X-ray structures	
Pero	entile relative to X-ray structures of sir	nilar resolution
Materia	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# \text{Entries}, \text{resolution range}(\text{\AA}))$

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

4695 (1.70-1.70)

Note EDS was not executed.

Clashscore

Mol	Chain	Length		Quality of a	chain	
1	А	7	14%	71%		14%
1	В	7	14%	43%	43%	



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 338 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 PNA (H-P(*CPN*GPN*TPN*APN*CPN*GPN)-NH2).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	А	7	Total 128				0	2	1
1	В	7	Total 128		N 38	O 20	0	2	1

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	33	Total O 33 33	0	0
2	В	49	Total O 49 49	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PNA (H-P(*CPN*GPN*TPN*APN*CPN*GPN)-NH2)

Chain A:	14%	71%	14%	-
CPN1 CPN2 TPN3 APN4 CPN5 CPN5 GPN6 MH27				
• Molecule	1: PNA	(H-P(*CPN*GPN*TPN*A	PN*CPN*GPN)-NH2)	
Chain B:	14%	43%	43%	
CPN8 GPN9 TPN10 APN11 CPN12 GPN13 MH214				



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P -1	Depositor
Cell constants	17.97Å 26.92Å 33.78Å	Depositor
a, b, c, α , β , γ	88.20° 79.40° 82.50°	Depositor
Resolution (Å)	6.00 - 1.70	Depositor
% Data completeness	77.0 (6.00-1.70)	Depositor
(in resolution range)	11.0 (0.00-1.10)	Depositor
R_{merge}	0.03	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.205 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	338	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, TPN, GPN, APN, CPN

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 (i)

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	А	128	0	40	1	0
1	В	128	0	40	2	0
2	А	33	0	0	1	0
2	В	49	0	0	1	0
All	All	338	0	80	3	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 8.

All (3) 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:3[B]:TPN:O	2:A:65:HOH:O	1.92	0.87
1:B:10[A]:TPN:O	2:B:33:HOH:O	2.15	0.63
1:B:8:CPN:O7'	1:B:9:GPN:H8'1	2.17	0.45



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).

Mal	Trung	Chain	Dec	Link	Bo	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	TPN	А	3[B]	1	19,19,20	0.93	1 (5%)	$23,\!25,\!27$	1.87	6 (26%)
1	GPN	А	6	1	18,22,23	1.23	2 (11%)	17,30,32	1.20	2 (11%)
1	CPN	А	5	1	18,18,19	0.90	1 (5%)	20,23,25	1.34	2 (10%)
1	APN	В	11[A]	1	18,21,22	0.92	0	15,28,30	1.27	0
1	APN	А	4[A]	1	18,21,22	0.95	1 (5%)	15,28,30	1.80	3 (20%)
1	TPN	А	3[A]	1	19,19,20	0.93	1 (5%)	23,25,27	1.60	5 (21%)
1	CPN	В	8	1	18,18,19	0.72	0	20,23,25	1.59	5 (25%)
1	GPN	В	13	1	18,22,23	1.39	3 (16%)	17,30,32	1.83	3 (17%)
1	TPN	В	10[B]	1	19,19,20	1.13	1 (5%)	23,25,27	1.83	5 (21%)
1	APN	В	11[B]	1	18,21,22	0.92	0	15,28,30	1.38	2 (13%)
1	GPN	А	2	1	18,22,23	1.16	2 (11%)	17,30,32	1.60	5 (29%)



Mol	Tuno	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CPN	В	12	1	18,18,19	1.18	1 (5%)	20,23,25	1.25	2 (10%)
1	TPN	В	10[A]	1	19,19,20	1.11	1 (5%)	$23,\!25,\!27$	1.76	5 (21%)
1	CPN	А	1	1	18,18,19	0.71	0	20,23,25	1.41	4 (20%)
1	APN	А	4[B]	1	18,21,22	0.97	1 (5%)	15,28,30	1.94	4 (26%)
1	GPN	В	9	1	18,22,23	1.03	2 (11%)	$17,\!30,\!32$	1.43	4 (23%)

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	TPN	А	3[B]	1	-	0/13/14/15	0/1/1/1
1	GPN	А	6	1	-	0/13/14/15	0/2/2/2
1	CPN	А	5	1	-	0/13/14/15	0/1/1/1
1	APN	В	11[A]	1	-	0/13/14/15	0/2/2/2
1	APN	А	4[A]	1	-	0/13/14/15	0/2/2/2
1	TPN	А	3[A]	1	-	1/13/14/15	0/1/1/1
1	CPN	В	8	1	-	1/13/14/15	0/1/1/1
1	GPN	В	13	1	-	1/13/14/15	0/2/2/2
1	TPN	В	10[B]	1	-	1/13/14/15	0/1/1/1
1	APN	В	11[B]	1	-	0/13/14/15	0/2/2/2
1	GPN	А	2	1	-	0/13/14/15	0/2/2/2
1	CPN	В	12	1	-	0/13/14/15	0/1/1/1
1	TPN	В	10[A]	1	-	0/13/14/15	0/1/1/1
1	CPN	А	1	1	-	2/13/14/15	0/1/1/1
1	APN	А	4[B]	1	-	0/13/14/15	0/2/2/2
1	GPN	В	9	1	-	0/13/14/15	0/2/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	В	12	CPN	C8'-N1	3.69	1.50	1.46
1	В	10[A]	TPN	C2-N1	2.84	1.41	1.37
1	В	10[B]	TPN	C2-N1	2.84	1.41	1.37
1	А	6	GPN	C8-N7	-2.69	1.30	1.35
1	А	2	GPN	C5-C4	-2.61	1.36	1.43

The worst 5 of 57 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	13	GPN	O-C-C5'	-5.30	110.40	126.39
1	А	3[B]	TPN	C2'-C3'-N4'	-4.33	104.92	113.11
1	А	4[A]	APN	C8'-N9-C8	4.14	130.54	125.66
1	А	4[B]	APN	C8'-N9-C8	4.14	130.54	125.66
1	В	10[A]	TPN	C8'-N1-C6	4.08	124.88	120.08

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	В	10[B]	TPN	O7'-C7'-N4'-C5'
1	А	1	CPN	C8'-C7'-N4'-C3'
1	А	3[A]	TPN	C-C5'-N4'-C7'
1	В	13	GPN	C-C5'-N4'-C7'
1	А	1	CPN	C-C5'-N4'-C3'

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	3[B]	TPN	1	0
1	В	8	CPN	1	0
1	В	10[A]	TPN	1	0
1	В	9	GPN	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

