



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1PUP / pdb_00001pup
Title : CRYSTAL STRUCTURE OF A PEPTIDE NUCLEIC ACID (PNA) DUPLEX AT 1.7 ANGSTROMS RESOLUTION
Authors : Rasmussen, H.; Kastrup, J.S.
Deposited on : 1996-11-01
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

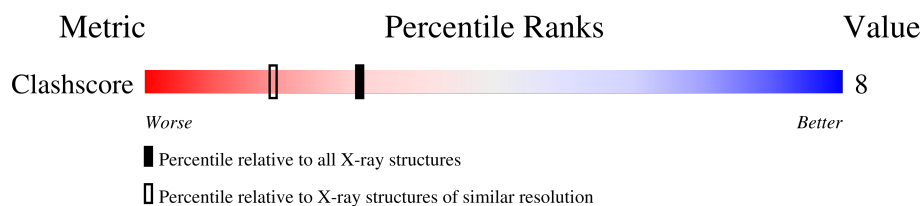
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	190562	5924 (1.70-1.70)

ENTRY-COMPOSITION INFOmissingINFO

2 Residue-property plots

There is no protein, DNA or RNA chain in this entry to show sequence plots.

3 Data and refinement statistics

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

Property	Value	Source
Space group	P -1	Depositor
Cell constants a, b, c, α , β , γ	17.97Å 26.92Å 33.78Å 88.20° 79.40° 82.50°	Depositor
Resolution (Å)	6.00 – 1.70	Depositor
% Data completeness (in resolution range)	77.0 (6.00-1.70)	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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

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.

4.2 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	A	128	0	40	1	0
1	B	128	0	40	2	0
2	A	33	0	0	1	0
2	B	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.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

4.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

Of 18 such residues modelled in this entry, 2 are modelled with single atom - leaving 16 for Mogul analysis.

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	B	8	1	18,18,19	0.69	0	21,23,25	1.41	2 (9%)
1	CPN	B	12	1	18,18,19	1.13	1 (5%)	21,23,25	1.11	1 (4%)
1	TPN	A	3[B]	1	19,19,20	0.94	1 (5%)	24,25,27	1.69	6 (25%)
1	CPN	A	1	1	18,18,19	0.68	0	21,23,25	1.24	2 (9%)
1	GPN	B	9	1	22,22,23	0.75	0	29,30,32	0.86	1 (3%)
1	TPN	B	10[A]	1	19,19,20	1.13	1 (5%)	24,25,27	1.61	5 (20%)
1	TPN	B	10[B]	1	19,19,20	1.15	1 (5%)	24,25,27	1.70	6 (25%)
1	APN	B	11[B]	1	21,21,22	0.73	0	27,28,30	0.85	0
1	APN	A	4[B]	1	21,21,22	0.74	0	27,28,30	1.35	3 (11%)
1	GPN	A	6	1	22,22,23	0.92	1 (4%)	29,30,32	0.78	0
1	APN	B	11[A]	1	21,21,22	0.73	0	27,28,30	0.80	0
1	APN	A	4[A]	1	21,21,22	0.72	0	27,28,30	1.27	2 (7%)
1	TPN	A	3[A]	1	19,19,20	0.94	1 (5%)	24,25,27	1.49	5 (20%)
1	CPN	A	5	1	18,18,19	0.84	1 (5%)	21,23,25	1.23	2 (9%)
1	GPN	B	13	1	22,22,23	1.00	1 (4%)	29,30,32	1.13	3 (10%)
1	GPN	A	2	1	22,22,23	0.79	0	29,30,32	0.96	2 (6%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	CPN	C8'-N1	3.55	1.50	1.46
1	B	10[A]	TPN	C2-N1	2.98	1.41	1.37
1	B	10[B]	TPN	C2-N1	2.98	1.41	1.37
1	B	13	GPN	O-C	2.45	1.33	1.20
1	A	3[A]	TPN	C2-N1	2.30	1.41	1.37
1	A	3[B]	TPN	C2-N1	2.30	1.41	1.37
1	A	5	CPN	C2-N1	2.14	1.42	1.40
1	A	6	GPN	C8'-N9	2.05	1.49	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4[A]	APN	C8'-C7'-N4'	4.00	121.89	117.04
1	A	4[B]	APN	C8'-C7'-N4'	4.00	121.89	117.04
1	B	12	CPN	C8'-N1-C6	3.67	125.03	119.72
1	B	10[A]	TPN	C8'-N1-C6	3.67	124.88	120.20
1	B	10[B]	TPN	C8'-N1-C6	3.67	124.88	120.20
1	A	5	CPN	C8'-N1-C6	3.58	124.91	119.72
1	A	3[B]	TPN	C2'-C3'-N4'	-3.56	104.92	112.91
1	B	10[A]	TPN	C6-C5-C4	3.51	120.92	118.02
1	B	10[B]	TPN	C6-C5-C4	3.51	120.92	118.02
1	B	8	CPN	O2-C2-N1	3.44	122.42	119.17
1	A	3[A]	TPN	C6-C5-C4	3.37	120.80	118.02
1	A	3[B]	TPN	C6-C5-C4	3.37	120.80	118.02
1	B	13	GPN	O-C-C5'	-3.35	110.40	125.47
1	B	10[A]	TPN	C8'-N1-C2	-3.35	113.53	117.73
1	B	10[B]	TPN	C8'-N1-C2	-3.35	113.53	117.73
1	A	4[A]	APN	C8'-N9-C8	3.30	130.54	127.27
1	A	4[B]	APN	C8'-N9-C8	3.30	130.54	127.27
1	B	13	GPN	C5'-N4'-C3'	-3.25	112.44	117.06
1	B	10[B]	TPN	C5'-N4'-C3'	-3.11	112.64	117.06
1	A	3[A]	TPN	C8'-N1-C6	3.03	124.06	120.20
1	A	3[B]	TPN	C8'-N1-C6	3.03	124.06	120.20
1	A	1	CPN	C8'-N1-C6	2.82	123.81	119.72
1	A	3[B]	TPN	C5'-N4'-C3'	-2.73	113.18	117.06
1	A	2	GPN	C5'-N4'-C3'	-2.66	113.28	117.06
1	A	1	CPN	C5'-N4'-C3'	-2.65	113.30	117.06
1	A	3[A]	TPN	C5M-C5-C6	-2.62	119.31	122.85
1	A	3[B]	TPN	C5M-C5-C6	-2.62	119.31	122.85
1	A	4[B]	APN	C2'-C3'-N4'	-2.50	107.30	112.91
1	B	10[A]	TPN	C5M-C5-C6	-2.42	119.58	122.85
1	B	10[B]	TPN	C5M-C5-C6	-2.42	119.58	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3[A]	TPN	C8'-N1-C2	-2.38	114.74	117.73
1	A	3[B]	TPN	C8'-N1-C2	-2.38	114.74	117.73
1	B	9	GPB	C8'-C7'-N4'	2.37	119.91	117.04
1	A	2	GPB	C7'-C8'-N9	-2.22	107.74	110.73
1	A	3[A]	TPN	C5'-N4'-C3'	-2.19	113.95	117.06
1	B	13	GPB	C7'-C8'-N9	-2.14	107.83	110.73
1	B	8	CPN	C8'-N1-C6	2.09	122.75	119.72
1	A	5	CPN	O2-C2-N1	2.02	121.08	119.17
1	B	10[A]	TPN	C5-C6-N1	-2.01	121.31	123.54
1	B	10[B]	TPN	C5-C6-N1	-2.01	121.31	123.54

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	3[A]	TPN	C-C5'-N4'-C7'
1	B	13	GPB	C-C5'-N4'-C7'
1	B	10[B]	TPN	O7'-C7'-N4'-C5'
1	A	1	CPN	C8'-C7'-N4'-C3'
1	A	1	CPN	C-C5'-N4'-C3'
1	B	8	CPN	C-C5'-N4'-C3'
1	B	8	CPN	C2'-C3'-N4'-C7'

There are no ring outliers.

4 monomers are involved in 3 short contacts:

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

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.