



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XJ9  
Title : Crystal structure of a partly self-complementary peptide nucleic acid (PNA) oligomer showing a duplex-triplex network  
Authors : Petersson, B.; Nielsen, B.B.; Rasmussen, H.; Larsen, I.K.; Gajhede, M.; Nielsen, P.E.; Kastrup, J.S.  
Deposited on : 2004-09-23  
Resolution : 2.60 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

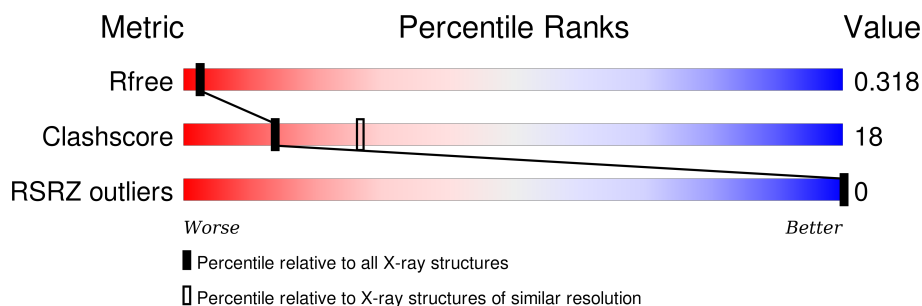
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	11	<div> <div></div> <div>45%</div> <div>36%</div> <div>18%</div> </div>
1	B	11	<div> <div>27%</div> <div>55%</div> <div>18%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 413 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(\*GPN\*TPN\*APN\*GPN\*APN\*TPN\*CPN\*APN\*CPN\*TPN)-LYS-NH<sub>2</sub>).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	9	Total	C	N	O	0	5	1
			190	106	57	27			
1	B	9	Total	C	N	O	0	5	1
			190	106	57	27			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	14	Total	O	0	0
			14	14		

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

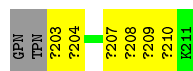
- Molecule 1: peptide nucleic acid, (H-P(\*GPN\*TPN\*APN\*GPN\*APN\*TPN\*CPN\*APN\*CPN\*TPN)-LYS-NH<sub>2</sub>)

Chain A: 



- Molecule 1: peptide nucleic acid, (H-P(\*GPN\*TPN\*APN\*GPN\*APN\*TPN\*CPN\*APN\*CPN\*TPN)-LYS-NH<sub>2</sub>)

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.60Å 41.90Å 30.10Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	27.00 – 2.60 26.65 – 2.63	Depositor EDS
% Data completeness (in resolution range)	78.2 (27.00-2.60) 98.2 (26.65-2.63)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.37 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.255 , 0.277 0.280 , 0.318	Depositor DCC
$R_{free}$ test set	172 reflections (10.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.64$ , $\langle L^2 \rangle = 0.51$	Xtriage
Outliers	3 of 1839 reflections (0.163%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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

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 ⓘ

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	190	0	104	5	0
1	B	190	0	103	7	0
2	A	19	0	0	1	0
2	B	14	0	0	1	0
All	All	413	0	207	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 18.

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:B:204[A]:GPN:H2'1	2:B:19:HOH:O	1.87	0.74
2:A:11:HOH:O	1:B:203[A]:APN:H2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:TPN:O7'	1:B:210:TPN:C'	2.56	0.54
1:A:107[B]:CPN:O1'	1:A:108[B]:APN:H3'2	2.09	0.53
1:B:207[B]:CPN:O1'	1:B:208[B]:APN:H3'1	2.09	0.52

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](#)

26 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	APN	A	103[A]	1	18,21,22	0.79	0	14,28,30	1.40	2 (14%)
1	APN	A	103[B]	1	18,21,22	0.78	0	14,28,30	1.51	2 (14%)
1	GPN	A	104[A]	1	19,22,23	1.15	2 (10%)	17,30,32	3.10	5 (29%)
1	GPN	A	104[B]	1	19,22,23	1.16	2 (10%)	17,30,32	3.10	5 (29%)
1	APN	A	105	1	18,21,22	0.96	0	14,28,30	1.44	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPN	A	106	1	15,19,20	1.50	3 (20%)	15,25,27	4.37	3 (20%)
1	CPN	A	107[A]	1	15,18,19	0.96	0	17,23,25	1.43	4 (23%)
1	CPN	A	107[B]	1	15,18,19	0.85	0	17,23,25	1.67	5 (29%)
1	APN	A	108[A]	1	18,21,22	1.13	1 (5%)	14,28,30	1.36	2 (14%)
1	APN	A	108[B]	1	18,21,22	1.29	2 (11%)	14,28,30	1.90	4 (28%)
1	CPN	A	109[A]	1	15,18,19	1.01	1 (6%)	17,23,25	1.39	3 (17%)
1	CPN	A	109[B]	1	15,18,19	1.03	1 (6%)	17,23,25	1.39	3 (17%)
1	TPN	A	110	1	15,19,20	1.19	2 (13%)	15,25,27	4.42	4 (26%)
1	APN	B	203[A]	1	18,21,22	0.82	0	14,28,30	1.43	2 (14%)
1	APN	B	203[B]	1	18,21,22	0.77	0	14,28,30	1.46	2 (14%)
1	GPN	B	204[A]	1	19,22,23	1.20	1 (5%)	17,30,32	3.08	5 (29%)
1	GPN	B	204[B]	1	19,22,23	1.20	1 (5%)	17,30,32	3.08	5 (29%)
1	APN	B	205	1	18,21,22	0.89	0	14,28,30	1.36	2 (14%)
1	TPN	B	206	1	15,19,20	1.33	1 (6%)	15,25,27	4.43	5 (33%)
1	CPN	B	207[A]	1	15,18,19	0.94	0	17,23,25	1.50	4 (23%)
1	CPN	B	207[B]	1	15,18,19	0.82	0	17,23,25	1.88	5 (29%)
1	APN	B	208[A]	1	18,21,22	0.75	0	14,28,30	1.43	2 (14%)
1	APN	B	208[B]	1	18,21,22	0.86	0	14,28,30	1.79	4 (28%)
1	CPN	B	209[A]	1	15,18,19	0.98	1 (6%)	17,23,25	1.34	2 (11%)
1	CPN	B	209[B]	1	15,18,19	1.03	1 (6%)	17,23,25	1.32	2 (11%)
1	TPN	B	210	1	15,19,20	1.32	2 (13%)	15,25,27	4.42	4 (26%)

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	APN	A	103[A]	1	-	0/13/14/15	0/2/2/2
1	APN	A	103[B]	1	-	0/13/14/15	0/2/2/2
1	GPN	A	104[A]	1	-	0/13/14/15	0/2/2/2
1	GPN	A	104[B]	1	-	0/13/14/15	0/2/2/2
1	APN	A	105	1	-	0/13/14/15	0/2/2/2
1	TPN	A	106	1	-	0/13/14/15	0/1/1/1
1	CPN	A	107[A]	1	-	0/13/14/15	0/1/1/1
1	CPN	A	107[B]	1	-	0/13/14/15	0/1/1/1
1	APN	A	108[A]	1	-	0/13/14/15	0/2/2/2
1	APN	A	108[B]	1	-	0/13/14/15	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CPN	A	109[A]	1	-	0/13/14/15	0/1/1/1
1	CPN	A	109[B]	1	-	0/13/14/15	0/1/1/1
1	TPN	A	110	1	-	0/13/14/15	0/1/1/1
1	APN	B	203[A]	1	-	0/13/14/15	0/2/2/2
1	APN	B	203[B]	1	-	0/13/14/15	0/2/2/2
1	GPN	B	204[A]	1	-	0/13/14/15	0/2/2/2
1	GPN	B	204[B]	1	-	0/13/14/15	0/2/2/2
1	APN	B	205	1	-	0/13/14/15	0/2/2/2
1	TPN	B	206	1	-	0/13/14/15	0/1/1/1
1	CPN	B	207[A]	1	-	0/13/14/15	0/1/1/1
1	CPN	B	207[B]	1	-	0/13/14/15	0/1/1/1
1	APN	B	208[A]	1	-	0/13/14/15	0/2/2/2
1	APN	B	208[B]	1	-	0/13/14/15	0/2/2/2
1	CPN	B	209[A]	1	-	0/13/14/15	0/1/1/1
1	CPN	B	209[B]	1	-	0/13/14/15	0/1/1/1
1	TPN	B	210	1	-	0/13/14/15	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	TPN	C8'-N1	-3.59	1.43	1.47
1	A	106	TPN	C6-C5	-2.27	1.33	1.40
1	B	209[B]	CPN	C8'-N1	-2.19	1.45	1.47
1	B	209[A]	CPN	C8'-N1	-2.19	1.45	1.47
1	A	109[A]	CPN	C8'-N1	-2.13	1.45	1.47

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	TPN	C5-C4-N3	-9.09	115.02	125.14
1	A	106	TPN	C5-C4-N3	-9.07	115.03	125.14
1	A	110	TPN	C5-C4-N3	-8.91	115.21	125.14
1	B	206	TPN	C5-C4-N3	-8.87	115.26	125.14
1	A	104[B]	GPN	C5-C6-N1	-8.75	111.63	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	104[A]	GPN	1	0
1	A	107[B]	CPN	2	0
1	A	108[A]	APN	1	0
1	A	108[B]	APN	1	0
1	A	109[B]	CPN	1	0
1	B	203[A]	APN	1	0
1	B	204[A]	GPN	1	0
1	B	207[B]	CPN	1	0
1	B	208[B]	APN	1	0
1	B	209[B]	CPN	2	0
1	B	210	TPN	2	0

## 5.5 Carbohydrates [i](#)

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1/11 (9%)	1.74	0 100 100	59, 59, 59, 59	0
1	B	1/11 (9%)	0.88	0 100 100	58, 58, 58, 58	0
All	All	2/22 (9%)	1.31	0 100 100	58, 58, 58, 59	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	GPN	A	104[B]	21/22	0.94	0.20	-	40,42,44,47	2
1	GPN	B	204[B]	21/22	0.92	0.24	-	41,43,45,46	2
1	CPN	B	209[B]	18/19	0.91	0.26	-	35,42,50,52	3
1	APN	B	208[B]	20/21	0.91	0.22	-	40,46,47,48	6
1	APN	A	103[A]	20/21	0.84	0.27	-	37,39,44,45	20
1	APN	B	203[B]	20/21	0.80	0.29	-	39,41,43,44	20
1	APN	A	108[B]	20/21	0.89	0.24	-	41,44,47,49	6
1	APN	A	108[A]	20/21	0.89	0.24	-	38,44,46,46	6
1	CPN	A	107[B]	18/19	0.92	0.20	-	31,40,42,42	3
1	CPN	A	109[A]	18/19	0.91	0.23	-	45,49,52,52	3
1	CPN	A	107[A]	18/19	0.92	0.20	-	31,36,42,42	3
1	TPN	A	110	19/20	0.90	0.28	-	42,48,58,60	0
1	CPN	A	109[B]	18/19	0.91	0.23	-	45,49,52,52	3
1	APN	B	208[A]	20/21	0.91	0.22	-	37,44,47,48	6
1	APN	B	203[A]	20/21	0.80	0.29	-	39,44,45,47	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CPN	B	207[B]	18/19	0.93	0.19	-	30,38,40,41	3
1	CPN	B	209[A]	18/19	0.91	0.26	-	35,42,50,52	3
1	APN	B	205	20/21	0.97	0.19	-	30,35,43,44	0
1	CPN	B	207[A]	18/19	0.93	0.19	-	30,34,40,41	3
1	TPN	A	106	19/20	0.94	0.20	-	31,33,35,35	0
1	GPN	B	204[A]	21/22	0.92	0.24	-	41,43,45,46	2
1	APN	A	103[B]	20/21	0.84	0.27	-	37,40,43,43	20
1	TPN	B	206	19/20	0.93	0.18	-	30,33,36,37	0
1	GPN	A	104[A]	21/22	0.94	0.20	-	38,42,44,47	2
1	TPN	B	210	19/20	0.87	0.23	-	39,46,56,57	0
1	APN	A	105	20/21	0.97	0.19	-	28,37,40,42	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.