



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2023 – 10:14 AM EST

PDB ID : 7UID  
Title : Thyclotides peptide nucleic acid in complex with DNA  
Authors : Botos, I.; Appella, D.H.  
Deposited on : 2022-03-29  
Resolution : 2.00 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

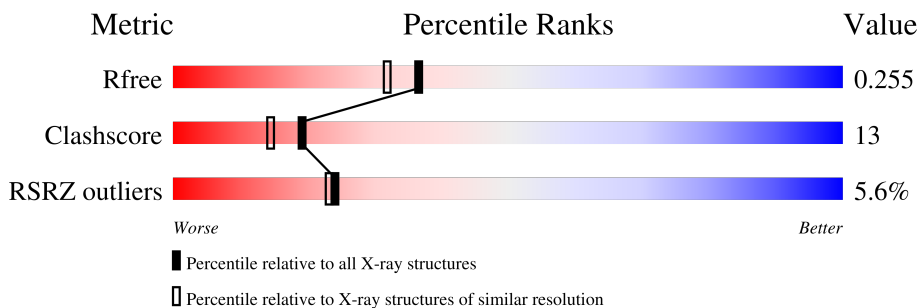
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	9	 11% 67% 33%
1	C	9	 44% 56%
2	B	10	 10% 30% 50% 10%
2	D	10	 10% 20% 50% 20%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 954 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 DNA (5'-D(\*GP\*AP\*TP\*GP\*TP\*GP\*AP\*TP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	9	Total 186	C 90	N 36	O 52	P 8	0	0	0
1	C	9	Total 186	C 90	N 36	O 52	P 8	0	0	0

- Molecule 2 is a protein called Thyclotide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	I	N				O
2	B	10	Total 209	C 119	I 1	N 50	O 39	0	0	0
2	D	10	Total 209	C 119	I 1	N 50	O 39	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Zn 3	0	0
3	C	3	Total 3	Zn 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	44	Total 44	O 44	0	0
5	C	35	Total 35	O 35	0	0
5	B	43	Total 43	O 43	0	0
5	D	34	Total 34	O 34	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 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: DNA (5'-D(\*GP\*AP\*TP\*GP\*TP\*GP\*AP\*TP\*A)-3')



- Molecule 1: DNA (5'-D(\*GP\*AP\*TP\*GP\*TP\*GP\*AP\*TP\*A)-3')



- Molecule 2: Thyclotide



- Molecule 2: Thyclotide



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.29Å 64.10Å 71.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.62 – 2.00 35.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.62-2.00) 97.5 (35.62-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.02 (at 2.00Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.232 , 0.265 0.230 , 0.255	Depositor DCC
$R_{free}$ test set	443 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: XDV, NSU, NRL, NR0, ZN, NSF, CL

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	0.92	0/209	0.98	0/322
1	C	0.78	0/209	0.96	0/322
All	All	0.85	0/418	0.97	0/644

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	8
2	D	0	5
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	NSF	Mainchain
2	B	2	NR0	Mainchain,Peptide
2	B	3	NSU	Mainchain,Peptide
2	B	5	NR0	Peptide
2	B	7	NR0	Peptide

## 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	A	186	0	104	7	0
1	C	186	0	104	9	0
2	B	209	0	0	1	0
2	D	209	0	0	4	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	44	0	0	0	0
5	B	43	0	0	0	0
5	C	35	0	0	0	0
5	D	34	0	0	0	0
All	All	954	0	208	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 13.

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:9:DA:H62	1:C:1:DG:H1'	1.38	0.88
1:C:1:DG:N2	2:D:9:NRL:N15	2.30	0.79
1:A:9:DA:N6	1:C:1:DG:H1'	1.97	0.78
1:A:9:DA:C2	1:C:2:DA:H1'	2.28	0.68
1:A:8:DT:H2'	1:A:9:DA:C8	2.38	0.58

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.



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

There are no protein residues with a non-rotameric sidechain to report 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](#)

18 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$
2	NSF	D	1	2	23,23,24	2.30	6 (26%)	24,32,34	1.80	7 (29%)
2	NRL	D	6	2	22,22,23	1.66	6 (27%)	21,30,32	2.39	8 (38%)
2	NR0	D	7	2	22,25,26	2.08	7 (31%)	16,35,37	1.82	2 (12%)
2	NR0	B	5	2	22,25,26	1.57	5 (22%)	16,35,37	1.30	3 (18%)
2	NSU	D	3	2	23,23,24	1.67	2 (8%)	24,32,34	1.85	7 (29%)
2	NSU	D	8	2	23,23,24	1.56	6 (26%)	24,32,34	2.08	9 (37%)
2	NSU	B	3	2	23,23,24	1.33	3 (13%)	24,32,34	2.11	9 (37%)
2	NSF	B	1	2	23,23,24	2.57	9 (39%)	24,32,34	1.47	5 (20%)
2	NR0	D	5	2	22,25,26	1.79	6 (27%)	16,35,37	1.18	2 (12%)
2	NRL	B	6	2	22,22,23	1.74	5 (22%)	21,30,32	1.89	7 (33%)
2	NSU	B	8	2	23,23,24	1.32	3 (13%)	24,32,34	1.82	5 (20%)
2	NR0	D	2	2	22,25,26	1.62	6 (27%)	16,35,37	1.47	3 (18%)
2	NRL	D	4	2	22,22,23	1.63	4 (18%)	21,30,32	2.19	7 (33%)
2	NRL	B	9	2	22,22,23	1.71	4 (18%)	21,30,32	2.22	9 (42%)
2	NR0	B	7	2	22,25,26	1.41	6 (27%)	16,35,37	1.55	4 (25%)
2	NR0	B	2	2	22,25,26	1.73	6 (27%)	16,35,37	1.15	1 (6%)
2	NRL	B	4	2	22,22,23	1.64	5 (22%)	21,30,32	2.20	7 (33%)
2	NRL	D	9	2	22,22,23	2.26	7 (31%)	21,30,32	2.75	5 (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
2	NSF	D	1	2	-	0/14/25/26	0/2/2/2
2	NRL	D	6	2	-	0/14/25/26	0/2/2/2
2	NR0	D	7	2	-	0/14/25/26	0/3/3/3
2	NR0	B	5	2	-	0/14/25/26	0/3/3/3
2	NSU	D	3	2	-	2/14/25/26	0/2/2/2
2	NSU	D	8	2	-	2/14/25/26	0/2/2/2
2	NSU	B	3	2	-	2/14/25/26	0/2/2/2
2	NSF	B	1	2	-	0/14/25/26	0/2/2/2
2	NR0	D	5	2	-	0/14/25/26	0/3/3/3
2	NRL	B	6	2	-	2/14/25/26	0/2/2/2
2	NSU	B	8	2	-	0/14/25/26	0/2/2/2
2	NR0	D	2	2	-	0/14/25/26	0/3/3/3
2	NRL	D	4	2	-	0/14/25/26	0/2/2/2
2	NRL	B	9	2	-	2/14/25/26	0/2/2/2
2	NR0	B	7	2	-	0/14/25/26	0/3/3/3
2	NR0	B	2	2	-	0/14/25/26	0/3/3/3
2	NRL	B	4	2	-	2/14/25/26	0/2/2/2
2	NRL	D	9	2	-	0/14/25/26	0/2/2/2

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NSF	C14-N13	8.15	1.49	1.37
2	D	1	NSF	C14-N13	6.79	1.47	1.37
2	D	4	NRL	C14-N13	5.07	1.46	1.40
2	D	3	NSU	C05-N04	5.01	1.55	1.47
2	D	9	NRL	C12-C11	4.87	1.59	1.53

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	NRL	C11-C12-N13	7.56	117.67	110.99
2	D	9	NRL	C18-N13-C14	-5.80	116.32	120.23
2	D	7	NR0	O-C-C03	-5.77	108.98	126.39
2	D	9	NRL	C12-C11-N04	5.63	124.61	117.11
2	D	6	NRL	C12-C11-N04	5.38	124.28	117.11

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	8	NSU	C-C03-N04-C11
2	B	3	NSU	C-C03-N04-C05
2	B	4	NRL	C-C03-N04-C05
2	B	6	NRL	C-C03-N04-C05
2	D	8	NSU	C-C03-N04-C05

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NSF	1	0
2	D	3	NSU	1	0
2	D	8	NSU	1	0
2	B	8	NSU	1	0
2	D	9	NRL	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	9/9 (100%)	0.27	1 (11%) 5 4	13, 19, 30, 52	0
1	C	9/9 (100%)	0.18	0 100 100	13, 25, 34, 40	0
2	B	0/10	-	-	-	-
2	D	0/10	-	-	-	-
All	All	18/38 (47%)	0.22	1 (5%) 24 23	13, 23, 40, 52	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	DA	3.0

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

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	NR0	D	7	23/24	0.89	0.18	22,27,33,34	0
2	NSU	D	8	22/23	0.89	0.22	28,30,34,34	0
2	NRL	D	9	21/22	0.89	0.16	23,25,29,29	0
2	NRL	D	6	21/22	0.90	0.16	19,26,30,31	0
2	NSF	B	1	22/23	0.93	0.16	22,26,26,26	1
2	NRL	D	4	21/22	0.94	0.14	11,12,15,17	0
2	NR0	D	5	23/24	0.94	0.12	12,16,23,27	0
2	NRL	B	9	21/22	0.94	0.12	14,17,22,23	0
2	NSF	D	1	22/23	0.94	0.16	14,19,25,25	1
2	NRL	B	4	21/22	0.95	0.13	9,12,14,16	0
2	NR0	B	2	23/24	0.95	0.14	14,16,19,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NSU	B	8	22/23	0.95	0.12	15,16,19,20	0
2	NR0	B	5	23/24	0.95	0.13	10,13,18,19	0
2	NSU	B	3	22/23	0.95	0.13	11,12,14,15	0
2	NRL	B	6	21/22	0.95	0.15	12,13,15,16	0
2	NSU	D	3	22/23	0.96	0.15	11,13,14,15	0
2	NR0	D	2	23/24	0.96	0.13	9,13,20,21	0
2	NR0	B	7	23/24	0.97	0.12	13,14,15,16	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	D	101	1/1	0.82	0.11	37,37,37,37	0
4	CL	B	101	1/1	0.86	0.10	46,46,46,46	0
3	ZN	C	103	1/1	0.86	0.12	66,66,66,66	1
3	ZN	A	103	1/1	0.93	0.07	47,47,47,47	1
3	ZN	C	102	1/1	0.99	0.10	27,27,27,27	1
3	ZN	C	101	1/1	0.99	0.10	29,29,29,29	1
3	ZN	A	101	1/1	1.00	0.11	18,18,18,18	0
3	ZN	A	102	1/1	1.00	0.10	21,21,21,21	0

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

There are no such residues in this entry.