



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:12 PM UTC

PDB ID : 1N4E / pdb_00001n4e
Title : Crystal Structure of a DNA Decamer Containing a Thymine-dimer
Authors : Park, H.; Zhang, K.; Ren, Y.; Nadji, S.; Sinha, N.; Taylor, J.-S.; Kang, C.
Deposited on : 2002-10-30
Resolution : 2.50 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
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

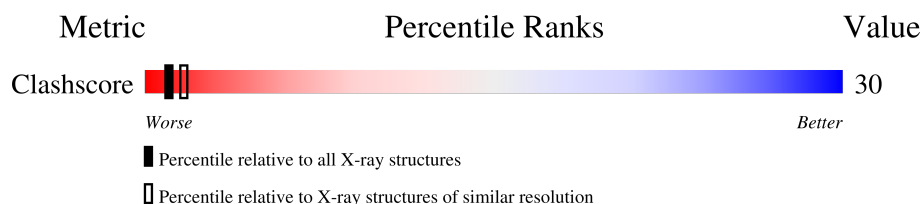
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	10	
1	C	10	
2	B	10	
2	D	10	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 864 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 5'-D(*GP*CP*TP*TP*AP*AP*TP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	P	0	0	0
			201	98	34	60	9			
1	C	10	Total	C	N	O	P	0	0	0
			201	98	34	60	9			

- Molecule 2 is a DNA chain called 5'-D(*CP*GP*AP*AP*TP*TP*AP*AP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	0	0
			203	98	40	56	9			
2	D	10	Total	C	N	O	P	0	0	0
			203	98	40	56	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	10	Total	O	0	0
			10	10		
3	C	12	Total	O	0	0
			12	12		
3	D	16	Total	O	0	0
			16	16		

3 Residue-property plots [i](#)

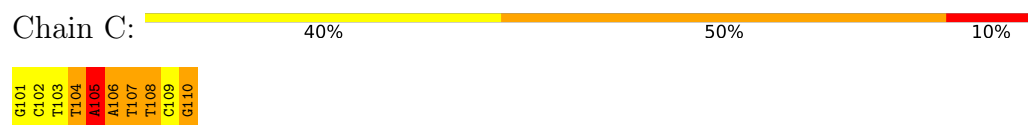
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 5'-D(*GP*CP*TP*TP*AP*AP*TP*TP*CP*G)-3'



- Molecule 1: 5'-D(*GP*CP*TP*TP*AP*AP*TP*TP*CP*G)-3'



- Molecule 2: 5'-D(*CP*GP*AP*AP*TP*TP*AP*AP*GP*C)-3'



- Molecule 2: 5'-D(*CP*GP*AP*AP*TP*TP*AP*AP*GP*C)-3'



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	21.11Å 54.01Å 74.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	864	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.78	3/224 (1.3%)	2.57	23/344 (6.7%)
1	C	1.47	1/224 (0.4%)	2.45	24/344 (7.0%)
2	B	1.86	5/228 (2.2%)	3.03	37/350 (10.6%)
2	D	1.88	4/228 (1.8%)	2.79	32/350 (9.1%)
All	All	1.75	13/904 (1.4%)	2.72	116/1388 (8.4%)

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
1	A	0	2
1	C	0	1
2	B	0	1
2	D	0	2
All	All	0	6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	113	DA	O3'-P	-8.07	1.49	1.61
2	B	11	DC	O3'-P	-7.49	1.50	1.61
2	D	112	DG	P-O5'	-7.10	1.46	1.60
1	A	5	DA	O3'-P	-6.75	1.51	1.61
1	A	2	DC	C2'-C1'	-6.57	1.39	1.52
2	D	112	DG	O3'-P	-6.49	1.51	1.61
2	B	12	DG	O3'-P	-5.75	1.52	1.61
2	B	15	DT	C5-C7	5.67	1.61	1.50
1	C	102	DC	O3'-P	-5.27	1.53	1.61
2	D	114	DA	O3'-P	-5.20	1.53	1.61
2	B	11	DC	N1-C2	-5.04	1.30	1.40
1	A	7	DT	C5'-C4'	-5.03	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	19	DG	O3'-P	-5.01	1.53	1.61

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	DT	O3'-P-O5'	-13.71	83.44	104.00
2	D	115	DT	C4-C5-C7	-13.36	102.36	122.40
2	B	15	DT	C4-C5-C7	-12.29	103.97	122.40
2	B	19	DG	O4'-C1'-C2'	-12.19	88.12	106.40
2	B	16	DT	O3'-P-O5'	-10.88	87.68	104.00
2	B	12	DG	O3'-P-O5'	-10.59	88.12	104.00
2	B	17	DA	O3'-P-O5'	-9.69	89.47	104.00
1	C	102	DC	O3'-P-O5'	-9.40	89.90	104.00
1	C	106	DA	P-O3'-C3'	9.38	134.27	120.20
1	C	102	DC	C5'-C4'-C3'	-9.23	101.06	114.90
2	D	116	DT	C4-C5-C7	-9.06	108.82	122.40
2	B	16	DT	C4-C5-C7	-9.04	108.83	122.40
2	B	19	DG	O3'-P-O5'	-8.91	90.64	104.00
2	B	16	DT	O4'-C1'-N1	8.83	121.65	108.40
1	A	8	DT	O4'-C1'-C2'	-8.75	93.28	106.40
2	D	116	DT	P-O3'-C3'	-8.53	107.40	120.20
2	D	115	DT	O4'-C1'-N1	-8.41	95.79	108.40
1	A	8	DT	C4'-C3'-O3'	-8.38	97.43	110.00
2	B	16	DT	P-O3'-C3'	-8.36	107.66	120.20
2	B	11	DC	P-O3'-C3'	8.30	132.65	120.20
2	D	112	DG	O5'-C5'-C4'	-8.04	98.74	110.80
2	B	16	DT	C1'-O4'-C4'	-7.99	97.72	109.70
2	D	112	DG	C4'-C3'-O3'	-7.91	98.14	110.00
2	D	113	DA	C4'-C3'-O3'	-7.87	98.19	110.00
2	D	116	DT	C6-N1-C1'	7.84	131.10	119.35
2	B	12	DG	C4-N9-C1'	-7.78	115.34	127.00
2	D	116	DT	C1'-O4'-C4'	-7.72	98.12	109.70
2	D	112	DG	O3'-P-O5'	-7.66	92.51	104.00
1	C	103	DT	O3'-P-O5'	-7.57	92.65	104.00
1	C	107	DT	C5'-C4'-C3'	-7.50	103.64	114.90
2	B	15	DT	C6-C5-C7	-7.45	112.83	124.00
2	D	113	DA	O3'-P-O5'	-7.45	92.83	104.00
1	A	3	DT	O3'-P-O5'	-7.44	92.83	104.00
2	B	13	DA	P-O3'-C3'	7.34	131.22	120.20
2	B	18	DA	P-O3'-C3'	-7.31	109.23	120.20
2	D	116	DT	C2-N1-C1'	-7.18	108.57	119.35
2	D	115	DT	C2-N1-C1'	-7.16	108.60	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	DT	C3'-C2'-C1'	7.12	112.28	101.60
2	B	15	DT	C2-N1-C1'	-6.92	108.96	119.35
1	A	4	DT	C4'-C3'-O3'	-6.92	99.62	110.00
1	C	108	DT	O3'-P-O5'	-6.91	93.64	104.00
2	D	111	DC	O3'-P-O5'	-6.89	93.67	104.00
1	A	8	DT	C4-C5-C7	-6.87	112.10	122.40
2	D	119	DG	P-O5'-C5'	-6.79	109.81	120.00
2	D	116	DT	O3'-P-O5'	-6.76	93.86	104.00
2	D	120	DC	O4'-C4'-C3'	-6.75	95.28	105.40
2	B	16	DT	C6-N1-C1'	6.73	129.45	119.35
1	C	107	DT	C4'-C3'-O3'	-6.62	100.07	110.00
2	B	12	DG	C8-N9-C1'	6.50	136.75	127.00
1	A	8	DT	P-O5'-C5'	6.48	129.72	120.00
1	C	106	DA	O3'-P-O5'	-6.47	94.29	104.00
2	D	116	DT	O4'-C1'-N1	6.46	118.08	108.40
1	A	2	DC	O3'-P-O5'	-6.45	94.33	104.00
1	A	5	DA	P-O3'-C3'	6.44	129.86	120.20
2	B	12	DG	C1'-O4'-C4'	-6.40	100.10	109.70
1	A	4	DT	C5'-C4'-C3'	-6.33	105.40	114.90
1	C	110	DG	C3'-C2'-C1'	6.32	111.08	101.60
1	C	106	DA	O5'-C5'-C4'	-6.28	101.38	110.80
2	B	14	DA	N9-C1'-C2'	-6.28	104.09	113.50
2	B	14	DA	O4'-C1'-N9	6.27	117.81	108.40
2	B	11	DC	O4'-C4'-C3'	-6.24	96.04	105.40
2	B	15	DT	C6-N1-C1'	6.23	128.70	119.35
1	A	5	DA	O3'-P-O5'	-6.23	94.66	104.00
1	A	5	DA	O5'-C5'-C4'	-6.20	101.50	110.80
1	A	8	DT	C2'-C3'-O3'	6.17	120.75	111.50
2	B	13	DA	C3'-C2'-C1'	6.17	110.85	101.60
2	B	16	DT	C5'-C4'-C3'	-6.17	105.65	114.90
2	D	115	DT	C6-N1-C1'	6.16	128.59	119.35
1	A	10	DG	C1'-O4'-C4'	-6.13	100.51	109.70
2	B	16	DT	C2-N1-C1'	-6.13	110.16	119.35
2	D	111	DC	O4'-C1'-C2'	-6.11	97.23	106.40
1	A	7	DT	C5'-C4'-C3'	-6.06	105.81	114.90
1	C	107	DT	C6-N1-C1'	6.06	128.44	119.35
1	C	104	DT	O3'-P-O5'	-6.00	95.00	104.00
2	B	15	DT	O4'-C1'-N1	-5.94	99.49	108.40
2	B	17	DA	N9-C1'-C2'	-5.92	104.62	113.50
1	C	105	DA	C5'-C4'-O4'	-5.83	100.65	109.40
2	D	115	DT	C6-C5-C7	-5.81	115.28	124.00
2	D	112	DG	C5'-C4'-C3'	-5.79	106.22	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	DA	P-O5'-C5'	5.77	128.65	120.00
2	B	11	DC	C3'-C2'-C1'	-5.76	92.95	101.60
1	C	104	DT	C3'-C2'-C1'	-5.75	92.97	101.60
1	C	101	DG	O5'-C5'-C4'	5.71	119.37	110.80
2	D	111	DC	C1'-O4'-C4'	-5.71	101.14	109.70
2	B	20	DC	P-O5'-C5'	5.69	128.54	120.00
2	B	13	DA	O5'-C5'-C4'	-5.69	102.27	110.80
1	C	106	DA	C4'-C3'-O3'	-5.65	101.52	110.00
2	B	20	DC	O4'-C1'-C2'	-5.58	98.04	106.40
2	D	111	DC	C5'-C4'-C3'	-5.53	106.60	114.90
2	D	117	DA	N9-C1'-C2'	-5.50	105.25	113.50
2	B	13	DA	C4'-C3'-O3'	5.48	118.22	110.00
2	D	114	DA	N9-C1'-C2'	-5.48	105.28	113.50
1	C	105	DA	C4-N9-C1'	-5.45	118.88	127.05
1	C	105	DA	P-O5'-C5'	-5.39	111.92	120.00
2	D	116	DT	C5'-C4'-C3'	-5.38	106.83	114.90
2	B	11	DC	C5-C4-N4	-5.38	112.23	120.30
1	A	10	DG	P-O5'-C5'	-5.37	111.94	120.00
1	C	102	DC	C3'-C2'-C1'	5.36	109.64	101.60
1	C	101	DG	O3'-P-O5'	-5.35	95.98	104.00
1	A	8	DT	P-O3'-C3'	5.33	128.19	120.20
2	D	113	DA	C5'-C4'-C3'	-5.32	106.92	114.90
2	D	119	DG	O4'-C1'-N9	5.24	116.26	108.40
2	D	114	DA	C4'-C3'-C2'	5.24	110.26	102.40
1	C	101	DG	C4'-C3'-O3'	-5.22	102.18	110.00
1	A	6	DA	C5'-C4'-C3'	-5.18	107.13	114.90
2	B	20	DC	O4'-C4'-C3'	-5.17	97.65	105.40
1	A	5	DA	C2'-C3'-O3'	5.15	119.22	111.50
1	C	103	DT	C6-C5-C7	-5.12	116.32	124.00
1	C	102	DC	C5'-C4'-O4'	5.12	117.08	109.40
1	C	108	DT	O4'-C1'-C2'	-5.12	98.72	106.40
2	B	12	DG	C3'-C2'-C1'	-5.09	93.97	101.60
1	A	8	DT	C5'-C4'-C3'	-5.06	107.31	114.90
2	B	14	DA	C4'-C3'-O3'	-5.04	102.44	110.00
2	D	120	DC	P-O5'-C5'	5.01	127.51	120.00
1	A	4	DT	C2'-C3'-O3'	5.00	119.00	111.50
2	D	112	DG	C4-N9-C1'	-5.00	119.50	127.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	DG	Sidechain
1	A	2	DC	Sidechain
2	B	11	DC	Sidechain
1	C	105	DA	Sidechain
2	D	112	DG	Sidechain
2	D	119	DG	Sidechain

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	201	0	116	11	0
1	C	201	0	116	9	0
2	B	203	0	113	7	0
2	D	203	0	113	10	0
3	A	18	0	0	1	0
3	B	10	0	0	0	0
3	C	12	0	0	0	0
3	D	16	0	0	0	0
All	All	864	0	458	30	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 30.

All (30) 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)
2:D:112:DG:H2'	2:D:113:DA:C8	2.16	0.81
2:D:115:DT:H1'	2:D:116:DT:O4'	1.89	0.72
2:B:15:DT:H1'	2:B:16:DT:O4'	1.90	0.71
2:D:111:DC:H2''	2:D:112:DG:C8	2.32	0.63
1:C:107:DT:H2'	1:C:108:DT:C6	2.33	0.63
2:B:19:DG:H2'	2:B:19:DG:OP2	1.99	0.62
1:A:5:DA:H2''	1:A:6:DA:C8	2.36	0.60
1:A:2:DC:H2''	1:A:3:DT:H5'	1.84	0.60
1:A:2:DC:H2'	1:A:3:DT:C6	2.38	0.59
1:C:106:DA:H2''	1:C:107:DT:O4'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:DT:H71	2:B:13:DA:N6	2.26	0.51
1:C:110:DG:H1	2:D:111:DC:H42	1.57	0.50
2:D:115:DT:C1'	2:D:116:DT:O4'	2.60	0.49
1:C:108:DT:H2''	1:C:109:DC:C6	2.49	0.48
1:C:106:DA:N1	2:D:115:DT:C4	2.82	0.47
2:D:114:DA:H2''	2:D:115:DT:O5'	2.14	0.47
1:A:8:DT:H2'	1:A:9:DC:C4	2.51	0.46
2:B:17:DA:H8	2:B:17:DA:O5'	1.99	0.46
2:D:112:DG:H2''	2:D:113:DA:O4'	2.16	0.45
1:A:8:DT:C7	2:B:13:DA:H61	2.29	0.45
1:A:8:DT:H6	2:B:13:DA:H61	1.63	0.45
1:A:5:DA:H1'	3:A:245:HOH:O	2.17	0.45
1:C:104:DT:O5'	1:C:104:DT:H2'	2.17	0.44
1:C:110:DG:H1	2:D:111:DC:N4	2.15	0.43
1:A:7:DT:O5'	1:A:7:DT:H2'	2.18	0.42
1:C:110:DG:C2	2:D:112:DG:N2	2.87	0.42
1:C:105:DA:H2''	1:C:106:DA:OP2	2.20	0.41
2:B:17:DA:H2''	2:B:18:DA:C8	2.56	0.41
1:A:2:DC:H2''	1:A:3:DT:C5'	2.49	0.41
1:A:5:DA:H2''	1:A:6:DA:H8	1.82	0.41

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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.