



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2025 – 12:07 PM EDT

PDB ID : 7UID / pdb_00007uid
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 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

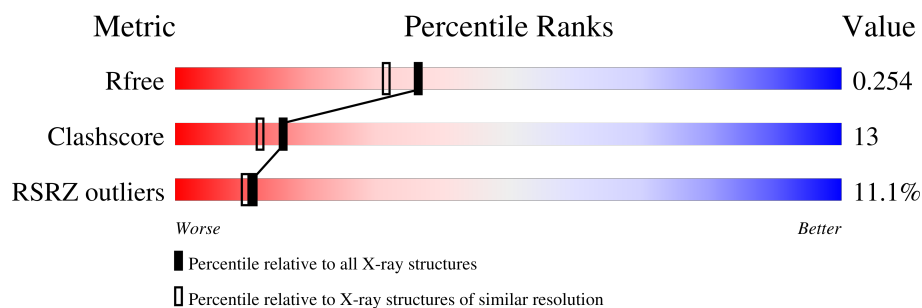
1 Overall quality at a glance

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
RSRZ outliers	164620	9409 (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 ≥ 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	<div> <div>11%</div> <div>67%</div> <div>33%</div> </div>
1	C	9	<div> <div>11%</div> <div>44%</div> <div>56%</div> </div>

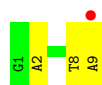
ENTRY-COMPOSITION INFOmissingINFO

2 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.

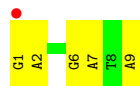
- Molecule 1: DNA (5'-D(*GP*AP*TP*GP*TP*GP*AP*TP*A)-3')

Chain A: 



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

Chain C: 



3 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	10.02 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.232 , 0.265 0.230 , 0.254	Depositor DCC
R_{free} test set	443 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	954	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NSU, NSF, NRL, NR0, ZN, CL, XDV

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	0.43	0/209	0.62	0/322
1	C	0.36	0/209	0.56	0/322
All	All	0.40	0/418	0.59	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.

All (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
2	B	8	NSU	Mainchain
2	D	2	NR0	Mainchain
2	D	3	NSU	Mainchain
2	D	5	NR0	Peptide

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Mol	Chain	Res	Type	Group
2	D	6	NRL	Mainchain
2	D	8	NSU	Mainchain

4.2 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	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.

All (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
1:C:6:DG:H2'	1:C:7:DA:C8	2.41	0.56
1:A:2:DA:N1	2:B:8:NSU:N15	2.59	0.50
1:A:9:DA:N3	1:C:2:DA:H1'	2.27	0.49
1:C:2:DA:N1	2:D:8:NSU:N15	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:DA:OP2	1:A:9:DA:H8	2.00	0.44
1:C:7:DA:N1	2:D:3:NSU:N15	2.66	0.44
1:C:9:DA:N1	2:D:1:NSF:N15	2.68	0.41

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](#)

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.

4.7 Other polymers ⓘ

20 such 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	NR0	B	2	2	21,25,26	1.84	6 (28%)	17,35,37	1.08	1 (5%)
2	XDV	B	10	2	10,10,10	1.57	1 (10%)	10,10,10	0.92	0
2	NSF	D	1	2	23,23,24	2.40	6 (26%)	24,32,34	1.78	7 (29%)
2	NRL	D	4	2	22,22,23	1.59	5 (22%)	22,30,32	2.02	5 (22%)
2	NR0	D	7	2	21,25,26	2.21	7 (33%)	17,35,37	1.50	2 (11%)
2	NRL	D	6	2	22,22,23	1.67	7 (31%)	22,30,32	2.14	7 (31%)
2	NRL	B	6	2	22,22,23	1.76	5 (22%)	22,30,32	1.66	5 (22%)
2	NR0	D	2	2	21,25,26	1.71	6 (28%)	17,35,37	1.42	4 (23%)
2	NR0	D	5	2	21,25,26	1.90	6 (28%)	17,35,37	1.11	3 (17%)
2	NR0	B	5	2	21,25,26	1.66	5 (23%)	17,35,37	1.29	5 (29%)
2	XDV	D	10	2	10,10,10	1.49	1 (10%)	10,10,10	0.85	0
2	NSU	D	8	2	23,23,24	1.62	6 (26%)	25,32,34	2.04	8 (32%)
2	NSF	B	1	2	23,23,24	2.66	8 (34%)	24,32,34	1.37	4 (16%)
2	NSU	B	8	2	23,23,24	1.38	3 (13%)	25,32,34	1.72	7 (28%)
2	NSU	D	3	2	23,23,24	1.76	2 (8%)	25,32,34	1.68	7 (28%)
2	NSU	B	3	2	23,23,24	1.39	4 (17%)	25,32,34	2.06	8 (32%)
2	NRL	D	9	2	22,22,23	2.23	7 (31%)	22,30,32	2.20	4 (18%)
2	NRL	B	9	2	22,22,23	1.68	5 (22%)	22,30,32	2.07	7 (31%)
2	NRL	B	4	2	22,22,23	1.61	5 (22%)	22,30,32	2.04	5 (22%)
2	NR0	B	7	2	21,25,26	1.48	6 (28%)	17,35,37	1.54	5 (29%)

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	NR0	B	2	2	-	0/14/25/26	0/3/3/3
2	XDV	B	10	2	-	6/8/8/8	-
2	NSF	D	1	2	-	0/14/25/26	0/2/2/2
2	NRL	D	4	2	-	0/14/25/26	0/2/2/2
2	NR0	D	7	2	-	0/14/25/26	0/3/3/3
2	NRL	D	6	2	-	0/14/25/26	0/2/2/2
2	NRL	B	6	2	-	2/14/25/26	0/2/2/2
2	NR0	D	2	2	-	0/14/25/26	0/3/3/3
2	NR0	D	5	2	-	0/14/25/26	0/3/3/3
2	NR0	B	5	2	-	0/14/25/26	0/3/3/3
2	XDV	D	10	2	-	5/8/8/8	-
2	NSU	D	8	2	-	2/14/25/26	0/2/2/2
2	NSF	B	1	2	-	0/14/25/26	0/2/2/2
2	NSU	B	8	2	-	0/14/25/26	0/2/2/2
2	NSU	D	3	2	-	1/14/25/26	0/2/2/2
2	NSU	B	3	2	-	2/14/25/26	0/2/2/2
2	NRL	D	9	2	-	0/14/25/26	0/2/2/2
2	NRL	B	9	2	-	2/14/25/26	0/2/2/2
2	NRL	B	4	2	-	2/14/25/26	0/2/2/2
2	NR0	B	7	2	-	0/14/25/26	0/3/3/3

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NSF	C14-N13	8.58	1.49	1.37
2	D	1	NSF	C14-N13	7.15	1.47	1.37
2	D	3	NSU	C05-N04	5.43	1.55	1.47
2	D	9	NRL	C12-C11	4.78	1.59	1.53
2	D	3	NSU	C14-N13	4.66	1.44	1.37
2	B	6	NRL	C05-N04	4.62	1.54	1.47
2	D	4	NRL	C14-N13	4.51	1.46	1.40
2	D	7	NR0	C11-N04	4.47	1.48	1.35
2	B	10	XDV	C09-N10	4.16	1.46	1.32
2	B	9	NRL	C14-N13	4.13	1.45	1.40
2	D	7	NR0	O09-C08	4.05	1.53	1.42
2	D	9	NRL	C16-N19	4.05	1.43	1.33
2	D	10	XDV	C09-N10	4.03	1.45	1.32
2	B	4	NRL	C14-N13	3.91	1.45	1.40
2	D	1	NSF	C16-C17	3.91	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NR0	C05-N04	3.88	1.53	1.47
2	D	1	NSF	C05-N04	3.87	1.53	1.47
2	D	1	NSF	C11-N04	3.84	1.46	1.35
2	D	8	NSU	C05-N04	3.83	1.53	1.47
2	B	6	NRL	C14-N13	3.81	1.45	1.40
2	D	9	NRL	C14-N13	3.79	1.45	1.40
2	D	5	NR0	O09-C10	3.74	1.52	1.42
2	B	5	NR0	O09-C08	3.71	1.52	1.42
2	D	7	NR0	C05-N04	3.68	1.53	1.47
2	B	1	NSF	C16-N15	3.56	1.45	1.38
2	B	2	NR0	O09-C08	3.55	1.51	1.42
2	B	1	NSF	C16-C17	3.54	1.53	1.45
2	D	9	NRL	C12-N13	3.50	1.50	1.46
2	D	7	NR0	C21-N22	3.47	1.37	1.32
2	D	5	NR0	C21-N22	3.44	1.37	1.32
2	B	1	NSF	C11-N04	3.42	1.45	1.35
2	D	2	NR0	C21-N22	3.40	1.37	1.32
2	B	8	NSU	C14-N13	3.36	1.42	1.37
2	D	9	NRL	C11-N04	3.34	1.44	1.35
2	D	7	NR0	O09-C10	3.33	1.51	1.42
2	D	7	NR0	C21-N20	3.25	1.39	1.33
2	D	5	NR0	O09-C08	3.24	1.51	1.42
2	D	6	NRL	C05-N04	3.22	1.52	1.47
2	B	3	NSU	C05-N04	3.19	1.52	1.47
2	B	8	NSU	C05-N04	3.17	1.52	1.47
2	B	2	NR0	O09-C10	3.16	1.50	1.42
2	B	9	NRL	C14-N15	3.07	1.42	1.36
2	B	6	NRL	C11-N04	3.05	1.44	1.35
2	B	1	NSF	C05-N04	3.00	1.52	1.47
2	D	2	NR0	O09-C08	2.99	1.50	1.42
2	B	5	NR0	C03-N04	2.98	1.51	1.46
2	B	9	NRL	C11-N04	2.96	1.43	1.35
2	D	2	NR0	C11-N04	2.95	1.43	1.35
2	D	9	NRL	C14-N15	2.94	1.42	1.36
2	D	8	NSU	C14-N13	2.93	1.41	1.37
2	B	7	NR0	O09-C08	2.92	1.50	1.42
2	D	4	NRL	C05-N04	2.91	1.51	1.47
2	D	8	NSU	C11-N04	2.91	1.43	1.35
2	D	8	NSU	C05-CA	2.89	1.59	1.52
2	D	5	NR0	C11-N04	2.89	1.43	1.35
2	B	5	NR0	C21-N22	2.87	1.36	1.32
2	D	1	NSF	C17-I1	-2.79	2.00	2.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	NRL	C11-N04	2.77	1.43	1.35
2	B	4	NRL	C11-N04	2.77	1.43	1.35
2	B	1	NSF	C18-N13	2.76	1.42	1.37
2	D	6	NRL	C12-C11	2.73	1.57	1.53
2	B	2	NR0	C11-N04	2.73	1.43	1.35
2	B	6	NRL	C14-N15	2.71	1.41	1.36
2	B	1	NSF	C14-N15	2.66	1.42	1.38
2	B	5	NR0	C12-N13	-2.62	1.42	1.48
2	B	6	NRL	C10-C05	2.61	1.57	1.53
2	B	4	NRL	C14-N15	2.55	1.41	1.36
2	B	5	NR0	C11-N04	2.53	1.42	1.35
2	D	7	NR0	C18-N19	2.49	1.43	1.34
2	D	5	NR0	C21-N20	2.47	1.38	1.33
2	D	1	NSF	C03-C	2.47	1.58	1.49
2	D	2	NR0	C05-CA	2.45	1.58	1.52
2	B	7	NR0	C11-N04	2.42	1.42	1.35
2	D	6	NRL	C16-N19	2.42	1.39	1.33
2	D	9	NRL	C05-CA	2.38	1.57	1.52
2	B	7	NR0	C21-N20	2.37	1.38	1.33
2	D	4	NRL	C14-N15	2.36	1.41	1.36
2	D	2	NR0	C18-N19	2.36	1.42	1.34
2	B	2	NR0	C18-N19	2.33	1.42	1.34
2	D	6	NRL	C14-N15	2.33	1.41	1.36
2	B	1	NSF	C08-CA	2.28	1.57	1.53
2	B	9	NRL	C16-N19	2.28	1.39	1.33
2	B	2	NR0	C21-N22	2.27	1.35	1.32
2	D	5	NR0	C17-N15	2.26	1.48	1.39
2	B	7	NR0	C12-N13	-2.24	1.43	1.48
2	B	4	NRL	C16-N19	2.23	1.39	1.33
2	B	8	NSU	C11-N04	2.23	1.41	1.35
2	D	2	NR0	C03-N04	2.18	1.50	1.46
2	B	3	NSU	C11-N04	2.16	1.41	1.35
2	D	4	NRL	O09-C10	-2.16	1.37	1.42
2	D	8	NSU	C12-N13	2.15	1.49	1.46
2	B	3	NSU	C05-CA	2.15	1.57	1.52
2	D	8	NSU	C03-N04	2.14	1.50	1.46
2	B	4	NRL	O09-C08	-2.13	1.37	1.42
2	D	6	NRL	C14-N13	2.12	1.42	1.40
2	B	7	NR0	C21-N22	2.08	1.35	1.32
2	B	3	NSU	C12-N13	2.08	1.49	1.46
2	B	7	NR0	C18-N19	2.04	1.41	1.34
2	D	4	NRL	C05-CA	2.03	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	NRL	C05-CA	2.02	1.57	1.52
2	D	6	NRL	C08-CA	2.01	1.56	1.53

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	NRL	C12-C11-N04	5.99	124.61	116.98
2	D	6	NRL	C12-C11-N04	5.72	124.28	116.98
2	D	9	NRL	C11-C12-N13	5.13	117.67	110.73
2	B	4	NRL	C-C03-N04	5.05	121.03	112.62
2	B	9	NRL	C12-C11-N04	5.00	123.35	116.98
2	D	4	NRL	C12-C11-N04	4.89	123.22	116.98
2	B	4	NRL	C12-C11-N04	4.56	122.80	116.98
2	D	4	NRL	C-C03-N04	4.43	119.99	112.62
2	D	8	NSU	C12-C11-N04	4.26	122.41	116.98
2	B	3	NSU	C12-C11-N04	3.95	122.01	116.98
2	B	9	NRL	O21-C14-N13	-3.80	115.58	119.17
2	B	3	NSU	O21-C14-N13	-3.79	119.66	122.87
2	D	8	NSU	C18-C17-C16	3.70	121.07	118.02
2	D	7	NR0	O-C-C03	-3.66	108.98	125.47
2	D	9	NRL	C18-N13-C14	-3.66	116.32	120.06
2	D	1	NSF	O21-C14-N13	-3.65	119.77	122.87
2	B	8	NSU	C12-C11-N04	3.64	121.62	116.98
2	B	3	NSU	C16-N15-C14	-3.61	122.61	127.34
2	B	6	NRL	C12-C11-N04	3.55	121.51	116.98
2	D	1	NSF	C12-N13-C18	3.49	124.65	120.20
2	D	8	NSU	N15-C14-N13	3.47	117.84	114.86
2	D	7	NR0	C12-C11-N04	3.46	121.80	116.92
2	B	3	NSU	C19-C17-C16	-3.45	115.10	118.78
2	D	8	NSU	C19-C17-C16	-3.44	115.11	118.78
2	D	6	NRL	C11-C12-N13	3.44	115.38	110.73
2	B	8	NSU	C19-C17-C16	-3.24	115.33	118.78
2	B	1	NSF	O21-C14-N13	-3.19	120.16	122.87
2	D	1	NSF	C10-C05-CA	3.14	106.41	102.01
2	D	6	NRL	O21-C14-N13	-3.14	116.20	119.17
2	B	9	NRL	N13-C14-N15	3.14	121.45	118.48
2	D	1	NSF	N15-C14-N13	3.08	117.50	114.86
2	D	8	NSU	C16-N15-C14	-3.06	123.33	127.34
2	D	3	NSU	C18-C17-C16	3.05	120.54	118.02
2	B	4	NRL	O22-C11-C12	-3.05	116.05	120.56
2	B	7	NR0	C12-C11-N04	3.04	121.20	116.92
2	B	6	NRL	C-C03-N04	3.02	117.65	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	NRL	C-C03-N04	2.96	117.55	112.62
2	D	2	NR0	C10-C05-CA	2.95	106.14	102.01
2	B	1	NSF	C18-N13-C14	-2.93	118.39	121.29
2	B	6	NRL	C11-C12-N13	2.90	114.65	110.73
2	D	9	NRL	N13-C14-N15	2.88	121.20	118.48
2	D	3	NSU	C19-C17-C16	-2.85	115.74	118.78
2	D	3	NSU	C12-C11-N04	2.84	120.60	116.98
2	B	9	NRL	O22-C11-C12	-2.83	116.37	120.56
2	D	4	NRL	O22-C11-C12	-2.80	116.42	120.56
2	D	3	NSU	C16-N15-C14	-2.75	123.73	127.34
2	D	6	NRL	N13-C14-N15	2.75	121.08	118.48
2	B	3	NSU	C18-C17-C16	2.69	120.24	118.02
2	D	8	NSU	O22-C11-C12	-2.68	116.60	120.56
2	D	3	NSU	C11-C12-N13	2.65	114.31	110.73
2	B	7	NR0	C18-C17-C16	-2.63	112.79	117.90
2	B	4	NRL	O21-C14-N13	-2.59	116.72	119.17
2	B	8	NSU	C18-C17-C16	2.58	120.15	118.02
2	B	5	NR0	C18-C17-C16	-2.56	112.92	117.90
2	D	1	NSF	C-C03-N04	-2.56	108.36	112.62
2	B	8	NSU	C16-N15-C14	-2.55	124.00	127.34
2	B	3	NSU	O22-C11-C12	-2.50	116.87	120.56
2	B	3	NSU	N15-C14-N13	2.50	117.00	114.86
2	D	2	NR0	C08-CA-C05	2.47	105.47	102.01
2	B	1	NSF	N15-C14-N13	2.43	116.94	114.86
2	D	4	NRL	O-C-C03	-2.39	114.72	125.47
2	D	6	NRL	C18-N13-C14	-2.37	117.64	120.06
2	D	5	NR0	C12-C11-N04	2.37	120.26	116.92
2	D	2	NR0	C18-C17-C16	-2.37	113.30	117.90
2	D	6	NRL	C12-N13-C18	2.35	123.12	119.72
2	B	6	NRL	C10-C05-CA	-2.34	98.74	102.01
2	B	9	NRL	C18-N13-C14	-2.31	117.70	120.06
2	D	1	NSF	C18-N13-C14	-2.31	119.00	121.29
2	D	4	NRL	C17-C16-N19	-2.31	116.59	120.63
2	D	5	NR0	C18-C17-C16	-2.28	113.46	117.90
2	B	8	NSU	O-C-C03	-2.26	115.30	125.47
2	D	8	NSU	O20-C16-C17	2.26	127.50	124.92
2	D	1	NSF	C08-CA-C05	2.24	105.15	102.01
2	B	7	NR0	O-C-C03	-2.23	115.44	125.47
2	B	9	NRL	C17-C16-N19	-2.22	116.75	120.63
2	B	4	NRL	O-C-C03	-2.21	115.55	125.47
2	B	6	NRL	O21-C14-N13	-2.20	117.10	119.17
2	D	3	NSU	O22-C11-C12	-2.19	117.32	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NSF	C11-C12-N13	2.17	113.66	110.73
2	B	2	NR0	C18-C17-C16	-2.17	113.69	117.90
2	B	5	NR0	C12-C11-N04	2.14	119.93	116.92
2	B	5	NR0	C08-CA-C05	2.11	104.97	102.01
2	D	3	NSU	O-C-C03	-2.11	115.97	125.47
2	B	5	NR0	C10-C05-CA	2.08	104.93	102.01
2	D	5	NR0	O-C-C03	-2.07	116.16	125.47
2	B	9	NRL	C12-N13-C18	2.06	122.71	119.72
2	B	5	NR0	O-C-C03	-2.05	116.25	125.47
2	B	8	NSU	C-C03-N04	2.05	116.03	112.62
2	B	7	NR0	C08-CA-C05	2.04	104.87	102.01
2	B	7	NR0	C10-C05-CA	2.04	104.87	102.01
2	D	2	NR0	C12-C11-N04	2.03	119.78	116.92
2	D	8	NSU	O21-C14-N13	-2.02	121.16	122.87
2	B	3	NSU	C-C03-N04	2.01	115.97	112.62
2	B	8	NSU	O20-C16-N15	-2.01	116.33	120.11

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	9	NRL	C-C03-N04-C05
2	B	10	XDV	N01-C02-C03-O04
2	D	8	NSU	C-C03-N04-C05
2	D	8	NSU	C-C03-N04-C11
2	D	10	XDV	N01-C02-C03-O04
2	D	10	XDV	O07-C08-C09-N10
2	B	10	XDV	C05-C06-O07-C08
2	D	10	XDV	C02-C03-O04-C05
2	D	10	XDV	C06-C05-O04-C03
2	B	10	XDV	C02-C03-O04-C05
2	B	3	NSU	C-C03-N04-C11
2	B	4	NRL	C-C03-N04-C11
2	B	6	NRL	C-C03-N04-C11
2	B	9	NRL	C-C03-N04-C11
2	D	3	NSU	C-C03-N04-C11
2	B	10	XDV	O07-C08-C09-O11
2	B	10	XDV	O04-C05-C06-O07
2	B	10	XDV	C09-C08-O07-C06

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Mol	Chain	Res	Type	Atoms
2	D	10	XDV	C09-C08-O07-C06

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	8	NSU	1	0
2	B	8	NSU	1	0
2	D	3	NSU	1	0
2	D	9	NRL	1	0

4.8 Polymer linkage issues

There are no chain breaks in this entry.

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

5.1 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, 95th 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 ²)	Q<0.9
1	A	9/9 (100%)	0.27	1 (11%) 12 10	13, 19, 30, 52	0
1	C	9/9 (100%)	0.36	1 (11%) 12 10	13, 25, 34, 40	0
All	All	18/18 (100%)	0.31	2 (11%) 12 10	13, 23, 40, 52	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	DA	4.0
1	C	1	DG	2.4

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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, 95th 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 ²)	Q<0.9
4	CL	D	101	1/1	0.84	0.12	37,37,37,37	0
4	CL	B	101	1/1	0.87	0.11	46,46,46,46	0
3	ZN	C	103	1/1	0.89	0.15	66,66,66,66	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	A	103	1/1	0.93	0.11	47,47,47,47	1
3	ZN	C	101	1/1	0.98	0.06	29,29,29,29	1
3	ZN	C	102	1/1	0.99	0.06	27,27,27,27	1
3	ZN	A	102	1/1	0.99	0.07	21,21,21,21	0
3	ZN	A	101	1/1	1.00	0.07	18,18,18,18	0

5.5 Other polymers [i](#)

There are no such residues in this entry.