



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2017 – 07:47 PM EDT

PDB ID : 5VY7  
Title : A self-assembling L-form DNA crystal lattice  
Authors : Simmons, C.R.; Yan, H.  
Deposited on : unknown  
Resolution : 3.00 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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

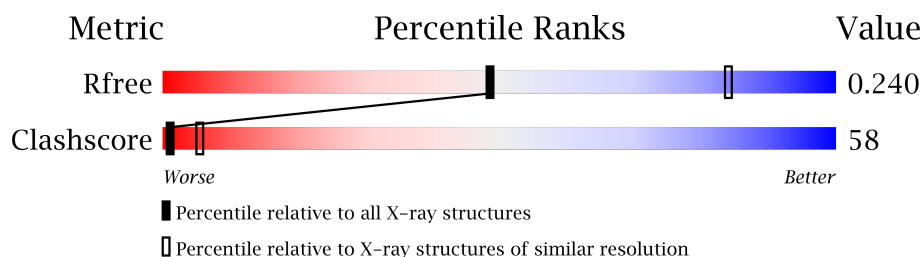
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)

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 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	21	
2	B	6	
3	C	8	
4	D	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	0DA	A	7	-	-	X	-
2	0DT	B	3	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0DC	B	4	-	-	X	-
3	0DT	C	1	-	-	X	-
3	0DC	C	2	-	-	X	-
3	0DG	C	4	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 851 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\*GP\*CP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*AP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			428	203	87	118	20			

- Molecule 2 is a DNA chain called DNA (5'-D(P\*CP\*CP\*GP\*TP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	P	0	0	0
			120	57	21	36	6			

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*GP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	P	0	0	0
			159	78	26	48	7			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*GP\*GP\*TP\*CP\*TP\*GP\*C)-3').

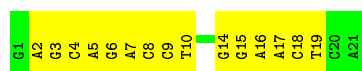
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	P	0	0	0
			144	68	25	44	7			

### 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 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.

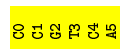
- Molecule 1: DNA (5'-D(\*GP\*AP\*GP\*CP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*AP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*CP\*A)-3')

Chain A: 

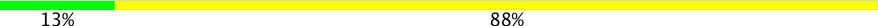


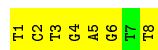
- Molecule 2: DNA (5'-D(P\*CP\*CP\*GP\*TP\*CP\*A)-3')

Chain B: 



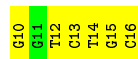
- Molecule 3: DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*GP\*TP\*T)-3')

Chain C: 



- Molecule 4: DNA (5'-D(P\*GP\*GP\*TP\*CP\*TP\*GP\*C)-3')

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.58 Å 68.58 Å 55.74 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.29 – 3.00 34.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	84.2 (34.29-3.00) 84.2 (34.29-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.00 Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.238 , 0.246 0.227 , 0.240	Depositor DCC
$R_{free}$ test set	258 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.4	Xtriage
Anisotropy	1.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.11 , 15.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.063 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 0DG, 0DT, 0DC, 0DA

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	428	0	231	36	0
2	B	120	0	68	18	1
3	C	159	0	90	19	3
4	D	144	0	80	11	3
All	All	851	0	469	71	4

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 58.

All (71) 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:5:0DA:OP1	1:A:5:0DA:H8A	1.64	0.97
3:C:1:0DT:H2"	3:C:2:0DC:H6	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:0DT:H2"	2:B:4:0DC:H6	1.66	0.78
1:A:15:0DG:N2	2:B:0:0DC:O2	2.17	0.77
1:A:6:0DG:O6	4:D:13:0DC:N4	2.17	0.76
2:B:3:0DT:H2"	2:B:4:0DC:C6	2.16	0.76
1:A:16:0DA:H2"	1:A:17:0DA:H8A	1.68	0.75
1:A:4:0DC:H2"	1:A:5:0DA:C8A	2.17	0.74
3:C:4:0DG:H2'	3:C:4:0DG:OP1	1.87	0.74
3:C:1:0DT:C2'	3:C:2:0DC:H6	2.19	0.72
3:C:4:0DG:H1'	3:C:5:0DA:N7A	2.08	0.68
3:C:1:0DT:H2"	3:C:2:0DC:O5'	1.93	0.67
1:A:15:0DG:H2"	1:A:16:0DA:OP1	1.94	0.66
1:A:18:0DC:C2	3:C:6:0DG:H21	2.08	0.65
3:C:4:0DG:H2'	3:C:4:0DG:P	2.36	0.65
1:A:15:0DG:H21	2:B:0:0DC:C2	2.08	0.65
2:B:2:0DG:C8	2:B:3:0DT:H73	2.26	0.65
3:C:3:0DT:H1'	3:C:4:0DG:O5'	1.97	0.65
3:C:1:0DT:C2	3:C:2:0DC:C6	2.75	0.65
1:A:4:0DC:H2"	1:A:5:0DA:H8A	1.78	0.64
1:A:9:0DC:C5	1:A:10:0DT:H73	2.27	0.64
2:B:1:0DC:H2"	2:B:2:0DG:H5"	1.80	0.63
4:D:13:0DC:H1'	4:D:14:0DT:H5"	1.81	0.63
2:B:0:0DC:H2'	2:B:1:0DC:C6	2.28	0.63
1:A:16:0DA:H2"	1:A:17:0DA:C8A	2.29	0.63
4:D:12:0DT:H2"	4:D:13:0DC:H6	1.82	0.61
1:A:6:0DG:H2'	1:A:7:0DA:C8A	2.31	0.60
1:A:14:0DG:H2"	1:A:15:0DG:H8	1.84	0.59
1:A:16:0DA:H2"	1:A:17:0DA:OP1	2.06	0.55
2:B:3:0DT:H2'	2:B:4:0DC:H5	1.90	0.53
3:C:1:0DT:H2'	3:C:2:0DC:H5	1.90	0.53
1:A:5:0DA:H2"	1:A:6:0DG:O5'	2.08	0.53
1:A:6:0DG:C6	4:D:13:0DC:H41	2.17	0.52
1:A:18:0DC:H41	3:C:6:0DG:C6	2.23	0.50
1:A:2:0DA:H8A	1:A:2:0DA:O5'	2.10	0.50
1:A:9:0DC:C2	4:D:10:0DG:H21	2.23	0.50
3:C:1:0DT:C2	3:C:2:0DC:C5	2.90	0.49
1:A:9:0DC:C2'	1:A:10:0DT:H6	2.43	0.49
2:B:3:0DT:H2"	2:B:4:0DC:H5'	1.94	0.49
4:D:12:0DT:H2"	4:D:13:0DC:C6	2.42	0.49
1:A:5:0DA:H2'	1:A:5:0DA:OP1	2.13	0.48
3:C:4:0DG:H1'	3:C:5:0DA:C8A	2.42	0.48
2:B:4:0DC:H5"	2:B:4:0DC:H6	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:0DC:H2'	1:A:10:0DT:H6	1.95	0.48
2:B:1:0DC:C2'	2:B:2:0DG:H5''	2.44	0.47
1:A:17:0DA:C4A	1:A:18:0DC:C5	2.92	0.47
1:A:6:0DG:H2'	1:A:7:0DA:H8A	1.94	0.47
3:C:3:0DT:H2''	3:C:4:0DG:OP1	2.14	0.47
1:A:18:0DC:C4	3:C:6:0DG:H1	2.27	0.47
1:A:7:0DA:C5A	1:A:8:0DC:C4	2.92	0.47
3:C:4:0DG:H4'	3:C:5:0DA:OP2	2.15	0.46
1:A:3:0DG:H1	4:D:16:0DC:H41	1.64	0.46
2:B:2:0DG:N7	2:B:3:0DT:H73	2.30	0.46
2:B:3:0DT:C2'	2:B:4:0DC:C5	2.93	0.46
1:A:9:0DC:H2''	1:A:10:0DT:H5''	1.98	0.45
1:A:18:0DC:H2''	1:A:19:0DT:H5''	1.97	0.45
2:B:1:0DC:H2'	2:B:2:0DG:O4'	2.17	0.45
1:A:7:0DA:C6A	1:A:8:0DC:C4	2.96	0.44
1:A:5:0DA:C8A	1:A:5:0DA:OP1	2.53	0.44
1:A:6:0DG:C6	1:A:7:0DA:C6A	2.96	0.44
3:C:1:0DT:C2'	3:C:2:0DC:C6	2.95	0.43
2:B:5:0DA:H2''	4:D:10:0DG:O4'	2.18	0.43
2:B:3:0DT:C2'	2:B:4:0DC:C6	2.94	0.43
1:A:16:0DA:OP1	1:A:16:0DA:H8A	2.19	0.43
1:A:18:0DC:H41	3:C:6:0DG:H1	1.66	0.42
4:D:15:0DG:H2''	4:D:16:0DC:H6	2.01	0.42
2:B:0:0DC:H2''	2:B:1:0DC:O4'	2.20	0.42
1:A:7:0DA:C5A	1:A:8:0DC:C5	2.98	0.42
1:A:7:0DA:HN62	4:D:12:0DT:C4	2.30	0.41
4:D:12:0DT:H2''	4:D:13:0DC:H5''	2.02	0.41
2:B:0:0DC:H5''	3:C:8:0DT:H2''	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:0:0DC:OP2	2:B:5:0DA:O3'[3_654]	1.54	0.66
3:C:8:0DT:C3'	4:D:10:0DG:OP2[3_654]	1.83	0.37
3:C:8:0DT:C4'	4:D:10:0DG:OP2[3_654]	1.93	0.27
3:C:8:0DT:O3'	4:D:10:0DG:OP2[3_654]	1.94	0.26

## 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](#)

42 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	ODG	A	1	1	15,19,25	1.37	2 (13%)	16,28,38	2.72	4 (25%)
1	ODT	A	10	1	13,21,22	1.49	3 (23%)	17,30,33	4.01	2 (11%)
1	ODG	A	11	1,2	17,24,25	1.12	1 (5%)	20,35,38	2.53	4 (20%)
1	ODA	A	12	1	17,23,24	0.80	1 (5%)	18,33,36	0.54	0
1	ODC	A	13	1,2	14,20,21	1.06	1 (7%)	17,28,31	0.44	0
1	ODG	A	14	1,2	17,24,25	1.32	3 (17%)	20,35,38	2.49	4 (20%)
1	ODG	A	15	1,2	17,24,25	1.25	2 (11%)	20,35,38	2.56	4 (20%)
1	ODA	A	16	1	17,23,24	0.75	0	18,33,36	0.62	0
1	ODA	A	17	1	17,23,24	0.86	1 (5%)	18,33,36	0.59	0
1	ODC	A	18	1,3	14,20,21	1.52	1 (7%)	17,28,31	0.81	0
1	ODT	A	19	1	13,21,22	1.48	3 (23%)	17,30,33	4.03	2 (11%)
1	ODA	A	2	1	17,23,24	0.60	0	18,33,36	0.62	0
1	ODC	A	20	1,3	14,20,21	1.21	1 (7%)	17,28,31	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	0DA	A	21	1	17,23,24	0.56	0	18,33,36	0.64	0
1	0DG	A	3	1,4	17,24,25	1.39	3 (17%)	20,35,38	2.56	4 (20%)
1	0DC	A	4	1,4	14,20,21	1.07	1 (7%)	17,28,31	0.53	0
1	0DA	A	5	1	17,23,24	0.65	0	18,33,36	0.60	0
1	0DG	A	6	1,4	17,24,25	1.32	1 (5%)	20,35,38	2.57	4 (20%)
1	0DA	A	7	1	17,23,24	0.75	0	18,33,36	0.60	0
1	0DC	A	8	1,4	14,20,21	1.16	1 (7%)	17,28,31	0.50	0
1	0DC	A	9	1,4	14,20,21	0.92	1 (7%)	17,28,31	0.42	0
2	0DC	B	0	1,2	14,20,21	1.56	1 (7%)	17,28,31	1.03	2 (11%)
2	0DC	B	1	1,2	14,20,21	1.36	2 (14%)	17,28,31	0.71	0
2	0DG	B	2	1,2	17,24,25	4.27	3 (17%)	20,35,38	2.59	4 (20%)
2	0DT	B	3	2	13,21,22	2.23	3 (23%)	17,30,33	4.03	2 (11%)
2	0DC	B	4	1,2	14,20,21	2.07	1 (7%)	17,28,31	0.44	0
2	0DA	B	5	2	17,23,24	0.80	0	18,33,36	0.71	0
3	0DT	C	1	3	11,16,22	1.31	2 (18%)	13,23,33	4.55	3 (23%)
3	0DC	C	2	3	14,20,21	1.04	2 (14%)	17,28,31	0.54	0
3	0DT	C	3	3	13,21,22	1.35	3 (23%)	17,30,33	4.00	2 (11%)
3	0DG	C	4	1,3	17,24,25	1.92	3 (17%)	20,35,38	2.58	6 (30%)
3	0DA	C	5	3	17,23,24	2.23	1 (5%)	18,33,36	0.69	0
3	0DG	C	6	1,3	17,24,25	1.66	3 (17%)	20,35,38	2.56	4 (20%)
3	0DT	C	7	3	13,21,22	3.01	2 (15%)	17,30,33	4.10	2 (11%)
3	0DT	C	8	3	13,21,22	2.39	3 (23%)	17,30,33	3.94	2 (11%)
4	0DG	D	10	1,4	17,24,25	1.19	2 (11%)	20,35,38	2.51	4 (20%)
4	0DG	D	11	1,4	17,24,25	1.19	1 (5%)	20,35,38	2.58	4 (20%)
4	0DT	D	12	4	13,21,22	1.23	2 (15%)	17,30,33	4.02	2 (11%)
4	0DC	D	13	1,4	14,20,21	2.26	1 (7%)	17,28,31	0.38	0
4	0DT	D	14	4	13,21,22	1.21	2 (15%)	17,30,33	4.02	2 (11%)
4	0DG	D	15	1,4	17,24,25	2.29	2 (11%)	20,35,38	2.57	4 (20%)
4	0DC	D	16	1,4	14,20,21	1.16	1 (7%)	17,28,31	0.41	0

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	0DG	A	1	1	-	0/0/13/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	0DT	A	10	1	-	0/3/21/22	0/2/2/2
1	0DG	A	11	1,2	-	0/3/21/22	0/3/3/3
1	0DA	A	12	1	-	0/3/21/22	0/3/3/3
1	0DC	A	13	1,2	-	0/3/21/22	0/2/2/2
1	0DG	A	14	1,2	-	0/3/21/22	0/3/3/3
1	0DG	A	15	1,2	-	0/3/21/22	0/3/3/3
1	0DA	A	16	1	-	0/3/21/22	0/3/3/3
1	0DA	A	17	1	-	0/3/21/22	0/3/3/3
1	0DC	A	18	1,3	-	0/3/21/22	0/2/2/2
1	0DT	A	19	1	-	0/3/21/22	0/2/2/2
1	0DA	A	2	1	-	0/3/21/22	0/3/3/3
1	0DC	A	20	1,3	-	0/3/21/22	0/2/2/2
1	0DA	A	21	1	-	0/3/21/22	0/3/3/3
1	0DG	A	3	1,4	-	0/3/21/22	0/3/3/3
1	0DC	A	4	1,4	-	0/3/21/22	0/2/2/2
1	0DA	A	5	1	-	0/3/21/22	0/3/3/3
1	0DG	A	6	1,4	-	0/3/21/22	0/3/3/3
1	0DA	A	7	1	-	0/3/21/22	0/3/3/3
1	0DC	A	8	1,4	-	0/3/21/22	0/2/2/2
1	0DC	A	9	1,4	-	0/3/21/22	0/2/2/2
2	0DC	B	0	1,2	-	0/3/21/22	0/2/2/2
2	0DC	B	1	1,2	-	0/3/21/22	0/2/2/2
2	0DG	B	2	1,2	-	0/3/21/22	0/3/3/3
2	0DT	B	3	2	-	0/3/21/22	0/2/2/2
2	0DC	B	4	1,2	-	0/3/21/22	0/2/2/2
2	0DA	B	5	2	-	0/3/21/22	0/3/3/3
3	0DT	C	1	3	-	0/0/13/22	0/2/2/2
3	0DC	C	2	3	-	0/3/21/22	0/2/2/2
3	0DT	C	3	3	-	0/3/21/22	0/2/2/2
3	0DG	C	4	1,3	-	0/3/21/22	0/3/3/3
3	0DA	C	5	3	-	0/3/21/22	0/3/3/3
3	0DG	C	6	1,3	-	0/3/21/22	0/3/3/3
3	0DT	C	7	3	-	0/3/21/22	0/2/2/2
3	0DT	C	8	3	-	0/3/21/22	0/2/2/2
4	0DG	D	10	1,4	-	0/3/21/22	0/3/3/3
4	0DG	D	11	1,4	-	0/3/21/22	0/3/3/3
4	0DT	D	12	4	-	0/3/21/22	0/2/2/2
4	0DC	D	13	1,4	-	0/3/21/22	0/2/2/2
4	0DT	D	14	4	-	0/3/21/22	0/2/2/2
4	0DG	D	15	1,4	-	0/3/21/22	0/3/3/3
4	0DC	D	16	1,4	-	0/3/21/22	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	0DG	O5'-C5'	-16.82	1.21	1.44
3	C	7	0DT	O5'-C5'	-10.22	1.30	1.44
4	D	13	0DC	O5'-C5'	-7.89	1.33	1.44
3	C	8	0DT	O5'-C5'	-7.45	1.34	1.44
2	B	3	0DT	O5'-C5'	-7.12	1.34	1.44
2	B	4	0DC	O5'-C5'	-7.11	1.34	1.44
1	A	18	0DC	O5'-C5'	-4.82	1.38	1.44
2	B	0	0DC	O5'-C5'	-4.78	1.38	1.44
3	C	6	0DG	O5'-C5'	-4.31	1.38	1.44
1	A	19	0DT	O5'-C5'	-3.50	1.39	1.44
1	A	20	0DC	O5'-C5'	-3.31	1.40	1.44
2	B	1	0DC	O5'-C5'	-3.22	1.40	1.44
1	A	8	0DC	O5'-C5'	-3.20	1.40	1.44
1	A	10	0DT	O5'-C5'	-3.17	1.40	1.44
1	A	3	0DG	O5'-C5'	-3.05	1.40	1.44
1	A	4	0DC	O5'-C5'	-2.95	1.40	1.44
3	C	3	0DT	O5'-C5'	-2.95	1.40	1.44
3	C	2	0DC	O5'-C5'	-2.81	1.40	1.44
1	A	13	0DC	O5'-C5'	-2.69	1.41	1.44
1	A	17	0DA	O5'-C5'	-2.66	1.41	1.44
4	D	10	0DG	O5'-C5'	-2.54	1.41	1.44
1	A	14	0DG	O5'-C5'	-2.35	1.41	1.44
3	C	8	0DT	C6-C5	-2.27	1.34	1.40
2	B	1	0DC	O3'-C3'	-2.26	1.38	1.43
3	C	3	0DT	C6-C5	-2.21	1.34	1.40
1	A	1	0DG	C8-N7	-2.16	1.30	1.34
1	A	9	0DC	O5'-C5'	-2.15	1.41	1.44
4	D	14	0DT	C6-C5	-2.13	1.34	1.40
3	C	2	0DC	C6-C5	-2.12	1.33	1.38
1	A	12	0DA	O5'-C5'	-2.11	1.41	1.44
3	C	4	0DG	C8-N7	-2.09	1.30	1.34
1	A	14	0DG	C8-N7	-2.07	1.30	1.34
4	D	12	0DT	C6-C5	-2.06	1.34	1.40
1	A	3	0DG	C8-N7	-2.03	1.30	1.34
1	A	10	0DT	C6-C5	-2.03	1.34	1.40
3	C	1	0DT	C6-C5	-2.02	1.34	1.40
2	B	3	0DT	C6-C5	-2.02	1.34	1.40
1	A	19	0DT	C6-C5	-2.01	1.34	1.40
1	A	15	0DG	C2-N1	2.03	1.39	1.35
2	B	2	0DG	C2-N1	2.14	1.39	1.35
3	C	6	0DG	C2-N1	2.15	1.39	1.35
3	C	3	0DT	C4-N3	2.72	1.38	1.33
2	B	3	0DT	C4-N3	2.81	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	8	0DT	C4-N3	2.91	1.38	1.33
3	C	7	0DT	C4-N3	2.96	1.38	1.33
1	A	19	0DT	C4-N3	3.07	1.38	1.33
4	D	12	0DT	C4-N3	3.15	1.38	1.33
4	D	10	0DG	C6-N1	3.16	1.38	1.33
1	A	10	0DT	C4-N3	3.23	1.38	1.33
3	C	4	0DG	C6-N1	3.29	1.39	1.33
4	D	14	0DT	C4-N3	3.42	1.39	1.33
3	C	1	0DT	C4-N3	3.43	1.39	1.33
1	A	11	0DG	C6-N1	3.55	1.39	1.33
4	D	16	0DC	O5'-C5'	3.67	1.49	1.44
4	D	11	0DG	C6-N1	3.76	1.39	1.33
1	A	3	0DG	C6-N1	3.80	1.39	1.33
1	A	14	0DG	C6-N1	3.89	1.40	1.33
2	B	2	0DG	C6-N1	3.92	1.40	1.33
1	A	6	0DG	C6-N1	3.92	1.40	1.33
4	D	15	0DG	C6-N1	3.94	1.40	1.33
1	A	15	0DG	C6-N1	3.99	1.40	1.33
1	A	1	0DG	C6-N1	4.13	1.40	1.33
3	C	6	0DG	C6-N1	4.20	1.40	1.33
3	C	4	0DG	O5'-C5'	6.41	1.53	1.44
4	D	15	0DG	O5'-C5'	7.77	1.55	1.44
3	C	5	0DA	O5'-C5'	8.93	1.57	1.44

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	12	0DT	C5-C4-N3	-9.22	115.07	125.24
1	A	10	0DT	C5-C4-N3	-9.20	115.10	125.24
3	C	8	0DT	C5-C4-N3	-9.17	115.13	125.24
2	B	3	0DT	C5-C4-N3	-9.13	115.17	125.24
3	C	7	0DT	C5-C4-N3	-9.05	115.26	125.24
4	D	14	0DT	C5-C4-N3	-9.04	115.27	125.24
3	C	3	0DT	C5-C4-N3	-9.00	115.31	125.24
3	C	1	0DT	C5-C4-N3	-8.93	115.39	125.24
1	A	15	0DG	C5-C6-N1	-8.81	110.93	123.48
1	A	19	0DT	C5-C4-N3	-8.78	115.56	125.24
3	C	6	0DG	C5-C6-N1	-8.55	111.30	123.48
4	D	11	0DG	C5-C6-N1	-8.48	111.41	123.48
1	A	3	0DG	C5-C6-N1	-8.43	111.48	123.48
4	D	15	0DG	C5-C6-N1	-8.41	111.50	123.48
2	B	2	0DG	C5-C6-N1	-8.37	111.56	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	0DG	C5-C6-N1	-8.35	111.59	123.48
1	A	6	0DG	C5-C6-N1	-8.35	111.60	123.48
4	D	10	0DG	C5-C6-N1	-8.20	111.80	123.48
1	A	11	0DG	C5-C6-N1	-8.20	111.81	123.48
1	A	1	0DG	C5-C6-N1	-8.06	112.00	123.48
3	C	4	0DG	C5-C6-N1	-8.06	112.01	123.48
4	D	11	0DG	C2-N3-C4	-3.34	111.25	115.16
1	A	6	0DG	C2-N3-C4	-3.17	111.45	115.16
3	C	6	0DG	C2-N3-C4	-3.13	111.50	115.16
3	C	4	0DG	C2-N3-C4	-3.12	111.51	115.16
4	D	10	0DG	C2-N3-C4	-3.09	111.55	115.16
1	A	11	0DG	C2-N3-C4	-3.08	111.56	115.16
2	B	2	0DG	C2-N3-C4	-3.07	111.57	115.16
1	A	15	0DG	C2-N3-C4	-3.04	111.61	115.16
1	A	3	0DG	C2-N3-C4	-3.03	111.63	115.16
1	A	14	0DG	C2-N3-C4	-2.96	111.70	115.16
4	D	15	0DG	C2-N3-C4	-2.94	111.72	115.16
1	A	1	0DG	C2-N3-C4	-2.92	111.75	115.16
2	B	0	0DC	C4'-O4'-C1'	-2.49	103.33	109.42
3	C	4	0DG	N3-C2-N1	-2.47	123.86	127.46
2	B	2	0DG	N3-C2-N1	-2.46	123.86	127.46
3	C	6	0DG	N3-C2-N1	-2.36	124.01	127.46
1	A	6	0DG	N3-C2-N1	-2.34	124.04	127.46
1	A	11	0DG	N3-C2-N1	-2.33	124.06	127.46
4	D	15	0DG	N3-C2-N1	-2.29	124.11	127.46
1	A	1	0DG	N3-C2-N1	-2.29	124.11	127.46
4	D	10	0DG	N3-C2-N1	-2.24	124.19	127.46
1	A	3	0DG	N3-C2-N1	-2.21	124.23	127.46
3	C	4	0DG	C6-C5-C4	-2.20	118.66	120.84
1	A	14	0DG	N3-C2-N1	-2.17	124.28	127.46
4	D	11	0DG	N3-C2-N1	-2.17	124.30	127.46
1	A	15	0DG	N3-C2-N1	-2.08	124.42	127.46
2	B	0	0DC	O4'-C1'-N1	2.28	111.62	107.78
3	C	1	0DT	C2'-C3'-C4'	2.39	105.30	102.11
3	C	4	0DG	O5'-C5'-C4'	2.43	117.56	109.01
1	A	1	0DG	C6-N1-C2	5.65	124.18	116.06
1	A	14	0DG	C6-N1-C2	5.81	124.42	116.06
1	A	15	0DG	C6-N1-C2	5.89	124.54	116.06
3	C	4	0DG	C6-N1-C2	5.92	124.58	116.06
3	C	6	0DG	C6-N1-C2	5.98	124.66	116.06
4	D	10	0DG	C6-N1-C2	6.01	124.70	116.06
1	A	11	0DG	C6-N1-C2	6.06	124.77	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	15	0DG	C6-N1-C2	6.06	124.78	116.06
1	A	3	0DG	C6-N1-C2	6.10	124.83	116.06
4	D	11	0DG	C6-N1-C2	6.11	124.86	116.06
2	B	2	0DG	C6-N1-C2	6.12	124.86	116.06
1	A	6	0DG	C6-N1-C2	6.18	124.94	116.06
3	C	8	0DT	C4-N3-C2	13.21	126.72	115.16
3	C	1	0DT	C4-N3-C2	13.28	126.78	115.16
4	D	12	0DT	C4-N3-C2	13.42	126.90	115.16
1	A	10	0DT	C4-N3-C2	13.49	126.96	115.16
3	C	3	0DT	C4-N3-C2	13.60	127.06	115.16
2	B	3	0DT	C4-N3-C2	13.63	127.08	115.16
4	D	14	0DT	C4-N3-C2	13.73	127.17	115.16
1	A	19	0DT	C4-N3-C2	13.84	127.26	115.16
3	C	7	0DT	C4-N3-C2	13.87	127.29	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	10	0DT	4	0
1	A	14	0DG	1	0
1	A	15	0DG	4	0
1	A	16	0DA	5	0
1	A	17	0DA	4	0
1	A	18	0DC	6	0
1	A	19	0DT	1	0
1	A	2	0DA	1	0
1	A	3	0DG	1	0
1	A	4	0DC	2	0
1	A	5	0DA	6	0
1	A	6	0DG	6	0
1	A	7	0DA	7	0
1	A	8	0DC	3	0
1	A	9	0DC	5	0
2	B	0	0DC	5	1
2	B	1	0DC	5	0
2	B	2	0DG	5	0
2	B	3	0DT	8	0
2	B	4	0DC	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5	0DA	1	1
3	C	1	0DT	7	0
3	C	2	0DC	7	0
3	C	3	0DT	2	0
3	C	4	0DG	7	0
3	C	5	0DA	3	0
3	C	6	0DG	4	0
3	C	8	0DT	1	3
4	D	10	0DG	2	3
4	D	12	0DT	4	0
4	D	13	0DC	6	0
4	D	14	0DT	1	0
4	D	15	0DG	1	0
4	D	16	0DC	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	0/21	-	-	-	-
2	B	0/6	-	-	-	-
3	C	0/8	-	-	-	-
4	D	0/7	-	-	-	-
All	All	0/42	-	-	-	-

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
2	0DC	B	4	19/20	0.92	0.11	-	17,22,51,53	0
4	0DC	D	16	19/20	0.95	0.11	-	34,49,70,72	0
3	0DG	C	4	22/23	0.91	0.09	-	15,28,42,52	0
1	0DT	A	19	20/21	0.96	0.11	-	9,20,35,37	0
1	0DG	A	3	22/23	0.91	0.08	-	27,33,54,57	0
1	0DG	A	15	22/23	0.93	0.08	-	16,26,44,53	0
1	0DC	A	18	19/20	0.96	0.10	-	11,15,40,43	0
1	0DA	A	21	21/22	0.95	0.09	-	20,30,45,47	0
1	0DG	A	6	22/23	0.93	0.07	-	32,41,62,70	0
4	0DT	D	12	20/21	0.91	0.12	-	27,35,51,55	0
3	0DC	C	2	19/20	0.88	0.11	-	24,37,56,57	0
2	0DC	B	0	19/20	0.86	0.14	-	18,27,38,49	0
1	0DC	A	20	19/20	0.93	0.12	-	16,30,37,43	0
4	0DT	D	14	20/21	0.92	0.07	-	38,53,69,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	0DA	A	16	21/22	0.96	0.06	-	18,25,42,53	0
4	0DG	D	11	22/23	0.93	0.10	-	19,26,34,36	0
1	0DA	A	2	21/22	0.94	0.08	-	27,35,49,54	0
2	0DC	B	1	19/20	0.94	0.12	-	24,31,38,39	0
1	0DA	A	7	21/22	0.94	0.08	-	36,43,68,72	0
1	0DA	A	12	21/22	0.95	0.08	-	23,33,45,48	0
3	0DG	C	6	22/23	0.96	0.07	-	15,20,37,49	0
1	0DA	A	5	21/22	0.93	0.09	-	30,37,51,55	0
1	0DT	A	10	20/21	0.94	0.10	-	25,37,64,72	0
3	0DT	C	1	15/21	0.93	0.10	-	24,31,41,45	0
2	0DG	B	2	22/23	0.94	0.07	-	22,29,43,45	0
4	0DC	D	13	19/20	0.91	0.09	-	36,43,59,67	0
1	0DG	A	11	22/23	0.93	0.09	-	21,30,57,66	0
3	0DT	C	7	20/21	0.95	0.11	-	14,21,33,35	0
2	0DT	B	3	20/21	0.93	0.12	-	23,31,47,55	0
1	0DC	A	8	19/20	0.95	0.06	-	33,47,71,77	0
1	0DG	A	14	22/23	0.93	0.10	-	22,27,44,55	0
3	0DT	C	8	20/21	0.94	0.16	-	13,19,31,34	0
3	0DT	C	3	20/21	0.91	0.09	-	20,32,53,54	0
1	0DC	A	9	19/20	0.91	0.10	-	24,42,61,66	0
2	0DA	B	5	21/22	0.94	0.14	-	11,19,29,35	0
3	0DA	C	5	21/22	0.97	0.06	-	19,32,45,52	0
1	0DA	A	17	21/22	0.94	0.08	-	15,24,42,52	0
1	0DC	A	4	19/20	0.88	0.11	-	28,38,51,65	0
4	0DG	D	15	22/23	0.93	0.06	-	34,50,69,76	0
4	0DG	D	10	22/23	0.94	0.11	-	16,22,35,49	0
1	0DG	A	1	17/23	0.92	0.07	-	21,26,39,48	0
1	0DC	A	13	19/20	0.95	0.09	-	21,28,50,53	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.