



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:02 PM UTC

PDB ID : 6L97 / pdb_00006l97
Title : Complex of DNA polymerase IV and L-DNA duplex
Authors : Chung, H.S.; An, J.; Hwang, D.
Deposited on : 2019-11-08
Resolution : 2.36 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

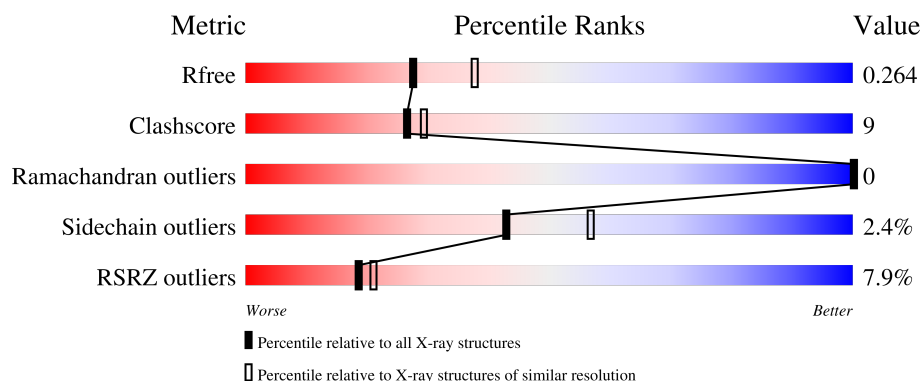
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

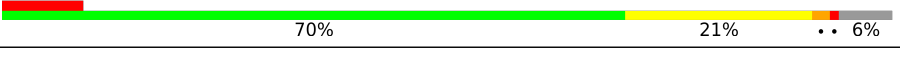
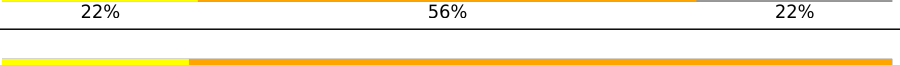
The reported resolution of this entry is 2.36 Å.

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	360	
1	B	360	
2	T	18	
3	P	14	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6088 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 protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2694	1731	463	493	7			
1	B	337	Total	C	N	O	S	0	0	0
			2708	1738	465	498	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	LEU	-	expression tag	UNP Q97W02
A	354	GLU	-	expression tag	UNP Q97W02
A	355	HIS	-	expression tag	UNP Q97W02
A	356	HIS	-	expression tag	UNP Q97W02
A	357	HIS	-	expression tag	UNP Q97W02
A	358	HIS	-	expression tag	UNP Q97W02
A	359	HIS	-	expression tag	UNP Q97W02
A	360	HIS	-	expression tag	UNP Q97W02
B	353	LEU	-	expression tag	UNP Q97W02
B	354	GLU	-	expression tag	UNP Q97W02
B	355	HIS	-	expression tag	UNP Q97W02
B	356	HIS	-	expression tag	UNP Q97W02
B	357	HIS	-	expression tag	UNP Q97W02
B	358	HIS	-	expression tag	UNP Q97W02
B	359	HIS	-	expression tag	UNP Q97W02
B	360	HIS	-	expression tag	UNP Q97W02

- Molecule 2 is a DNA chain called DNA (5'-D(P*(0DG)P*(0DG)P*(0DA)P*(0DA)P*(0DT)P*(0DC)P*(0DC)P*(0DT)P*(0DT)P*(0DC)P*(0DC)P*(0DC)P*(0DC)P*(0DC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	14	Total	C	N	O	P	0	0	0
			279	133	47	85	14			

- Molecule 3 is a DNA chain called DNA (5'-D(* (0DG)P*(0DG)P*(0DG)P*(0DG)P*(0DG)P*(0DA)P*(0DA)P*(0DG)P*(0DG)P*(0DA)P*(0DT)P*(0DT)P*(0DC)P*(0DC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	14	Total 292	C 138	N 60	O 81	P 13	0	0	0

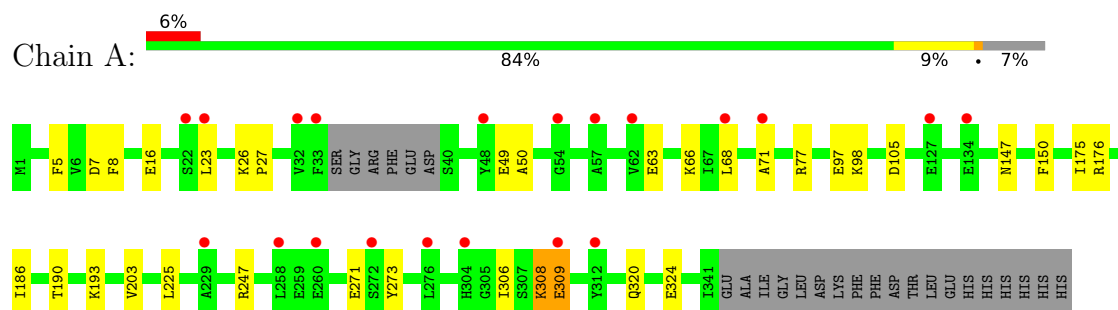
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total 64	O 64	0	0
4	B	37	Total 37	O 37	0	0
4	T	10	Total 10	O 10	0	0
4	P	4	Total 4	O 4	0	0

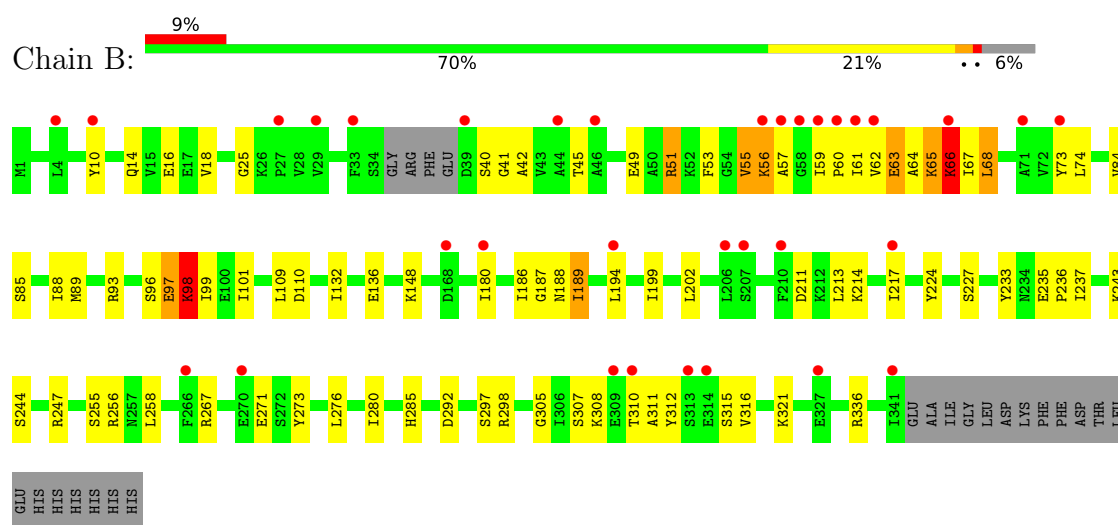
3 Residue-property plots [i](#)

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 polymerase IV



• Molecule 1: DNA polymerase IV



• Molecule 2: DNA (5'-D(P*(0DG)P*(0DG)P*(0DA)P*(0DA)P*(0DT)P*(0DC)P*(0DC)P*(0DT)P*(0DT)P*(0DC)P*(0DC)P*(0DC)P*(0DC)P*(0DC))-3')



• Molecule 3: DNA (5'-D(* (0DG)P*(0DG)P*(0DG)P*(0DG)P*(0DG)P*(0DA)P*(0DA)P*(0DG)P*(0DG)P*(0DA)P*(0DT)P*(0DT)P*(0DC)P*(0DC))-3')



G1	G2	G3	G4	G5	A6	A7	G8	G9	A10	T11	T12	C13	C14
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.86Å 54.97Å 96.55Å 90.00° 113.39° 90.00°	Depositor
Resolution (Å)	34.50 – 2.36 34.50 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.50-2.36) 97.7 (34.50-2.36)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.230 , 0.266 0.231 , 0.264	Depositor DCC
R_{free} test set	2015 reflections (6.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6088	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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.

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: 0DA, 0DG, 0DC, 0DT

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	0.35	1/2731 (0.0%)	0.39	0/3667
1	B	0.47	3/2745 (0.1%)	0.51	2/3686 (0.1%)
All	All	0.41	4/5476 (0.1%)	0.45	2/7353 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	ILE	C-O	-6.19	1.16	1.23
1	B	187	GLY	C-O	-5.98	1.19	1.24
1	B	98	LYS	C-O	-5.33	1.17	1.24
1	A	308	LYS	C-O	-5.04	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	LYS	N-CA-C	-5.96	107.24	114.75
1	B	63	GLU	N-CA-C	-5.89	104.81	112.23

There are no chirality outliers.

There are no planarity outliers.

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	2694	0	2848	18	0
1	B	2708	0	2857	71	0
2	T	279	0	137	13	0
3	P	292	0	121	19	0
4	A	64	0	0	1	0
4	B	37	0	0	3	0
4	P	4	0	0	0	0
4	T	10	0	0	0	0
All	All	6088	0	5963	108	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 9.

All (108) 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:65:LYS:CE	1:B:73:TYR:CZ	2.24	1.19
1:B:65:LYS:HE2	1:B:73:TYR:CZ	1.79	1.17
3:P:13:0DC:H2''	3:P:14:0DC:H5'	1.18	1.16
1:B:65:LYS:HE3	1:B:73:TYR:CE2	1.83	1.11
1:B:56:LYS:CG	1:B:57:ALA:H	1.65	1.06
3:P:13:0DC:H2''	3:P:14:0DC:C5'	1.86	1.05
1:B:65:LYS:HE3	1:B:73:TYR:CZ	1.89	1.03
1:B:56:LYS:HG3	1:B:57:ALA:N	1.55	1.01
1:B:45:THR:HG21	4:B:426:HOH:O	1.64	0.97
3:P:13:0DC:C2'	3:P:14:0DC:H5'	1.98	0.93
1:B:56:LYS:HG3	1:B:57:ALA:H	0.77	0.91
1:B:65:LYS:HE2	1:B:73:TYR:OH	1.79	0.81
1:B:66:LYS:O	1:B:66:LYS:HD2	1.85	0.76
2:T:9:0DT:H3	3:P:10:0DA:H2A	1.49	0.76
1:B:65:LYS:CE	1:B:73:TYR:CE1	2.69	0.75
1:B:53:PHE:CB	1:B:68:LEU:HD11	2.18	0.74
2:T:13:0DT:H3	3:P:6:0DA:H2A	1.54	0.72
1:B:321:LYS:HE2	4:B:434:HOH:O	1.89	0.71
1:B:321:LYS:NZ	3:P:12:0DT:OP2	2.23	0.71
1:B:67:ILE:HG22	1:B:68:LEU:HD12	1.73	0.70
1:B:65:LYS:CE	1:B:73:TYR:CE2	2.61	0.69
1:B:53:PHE:HB2	1:B:68:LEU:HD11	1.73	0.69
1:B:273:TYR:HA	1:B:276:LEU:HD12	1.76	0.67
1:B:65:LYS:HE2	1:B:73:TYR:CE1	2.29	0.66
2:T:9:0DT:H3	3:P:10:0DA:C2A	2.09	0.65
2:T:16:0DC:C2	3:P:3:0DG:H21	2.09	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LYS:CG	1:B:57:ALA:N	2.28	0.63
1:B:211:ASP:HA	1:B:214:LYS:HB3	1.79	0.63
1:B:10:TYR:HB3	1:B:51:ARG:NH2	2.14	0.63
1:A:320:GLN:O	1:A:324:GLU:HG3	1.98	0.62
1:B:65:LYS:N	1:B:65:LYS:HD2	2.14	0.62
1:B:61:ILE:O	1:B:64:ALA:HB3	1.99	0.62
2:T:17:0DC:C2	3:P:2:0DG:H21	2.13	0.61
1:B:243:LYS:HG3	1:B:244:SER:N	2.16	0.60
1:B:280:ILE:HD11	1:B:305:GLY:HA3	1.83	0.60
1:B:97:GLU:HG2	1:B:98:LYS:HG2	1.83	0.60
1:B:42:ALA:HA	1:B:60:PRO:HA	1.83	0.59
1:B:65:LYS:HE3	1:B:73:TYR:CD2	2.35	0.59
1:B:97:GLU:OE1	1:B:97:GLU:N	2.35	0.59
1:B:62:VAL:HG22	1:B:62:VAL:O	2.03	0.58
1:B:194:LEU:HB3	1:B:199:ILE:HB	1.84	0.58
1:B:247:ARG:NH1	1:B:271:GLU:OE2	2.37	0.58
1:B:233:TYR:CZ	1:B:235:GLU:HG3	2.40	0.57
1:B:16:GLU:HG2	1:B:74:LEU:HD13	1.87	0.56
1:B:55:VAL:HG12	1:B:55:VAL:O	2.05	0.56
1:B:53:PHE:HB3	1:B:68:LEU:HD11	1.88	0.56
1:B:96:SER:HB3	1:B:109:LEU:HD23	1.87	0.56
2:T:13:0DT:H3	3:P:6:0DA:C2A	2.19	0.56
1:B:10:TYR:HB3	1:B:51:ARG:HH21	1.71	0.56
1:B:110:ASP:HB2	1:B:237:ILE:HG13	1.87	0.55
3:P:6:0DA:O5'	3:P:6:0DA:H8A	2.07	0.55
1:A:16:GLU:OE2	1:A:77:ARG:NH2	2.40	0.55
1:A:63:GLU:HA	1:A:66:LYS:HG3	1.90	0.54
2:T:15:0DC:O2	3:P:4:0DG:N2	2.28	0.54
3:P:13:0DC:C2'	3:P:14:0DC:C5'	2.73	0.53
1:B:89:MET:HE3	1:B:101:ILE:HG23	1.89	0.52
1:A:77:ARG:NH1	4:A:411:HOH:O	2.41	0.52
1:B:88:ILE:HG23	1:B:132:ILE:HD12	1.92	0.51
1:A:68:LEU:HD12	1:A:71:ALA:HB2	1.91	0.51
1:A:247:ARG:NH1	1:A:271:GLU:OE2	2.43	0.51
3:P:13:0DC:H2''	3:P:14:0DC:O5'	2.10	0.51
1:A:176:ARG:HG2	1:A:203:VAL:HG11	1.93	0.50
1:B:292:ASP:OD1	1:B:292:ASP:N	2.37	0.50
1:B:189:ILE:CD1	1:B:189:ILE:N	2.73	0.50
2:T:11:0DC:C2	3:P:8:0DG:H21	2.24	0.50
1:A:49:GLU:OE1	1:A:49:GLU:N	2.39	0.50
2:T:6:0DG:H21	3:P:13:0DC:C2	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLN:O	1:B:18:VAL:HG23	2.13	0.49
1:B:189:ILE:N	1:B:189:ILE:HD12	2.28	0.48
1:B:40:SER:OG	1:B:41:GLY:N	2.46	0.48
1:B:285:HIS:HB2	1:B:336:ARG:HG2	1.96	0.48
1:A:23:LEU:HD23	1:A:26:LYS:HE2	1.96	0.47
1:B:85:SER:O	1:B:89:MET:HG2	2.14	0.47
1:A:175:ILE:HG22	1:A:203:VAL:HG13	1.96	0.47
1:B:89:MET:O	1:B:93:ARG:HG3	2.16	0.46
1:B:224:TYR:O	1:B:227:SER:OG	2.27	0.46
1:B:267:ARG:NH1	4:B:404:HOH:O	2.41	0.46
1:B:25:GLY:O	1:B:49:GLU:HG2	2.15	0.46
1:B:59:ILE:HB	1:B:63:GLU:OE2	2.16	0.46
1:B:148:LYS:NZ	1:B:236:PRO:O	2.49	0.46
1:A:273:TYR:OH	1:A:306:ILE:O	2.23	0.45
2:T:14:0DC:C2	3:P:5:0DG:H21	2.29	0.45
1:A:147:ASN:HD21	1:A:150:PHE:HD2	1.65	0.45
1:B:67:ILE:CG2	1:B:68:LEU:HD12	2.44	0.45
1:B:180:ILE:O	1:B:186:ILE:HD11	2.17	0.45
1:A:8:PHE:CD2	1:A:105:ASP:HA	2.51	0.45
1:A:5:PHE:CE2	1:A:7:ASP:HB2	2.52	0.44
1:B:308:LYS:O	1:B:312:TYR:HD1	2.01	0.44
1:B:213:LEU:O	1:B:217:ILE:HG22	2.18	0.44
1:B:258:LEU:HD11	1:B:316:VAL:HG13	2.00	0.43
1:B:311:ALA:O	1:B:315:SER:OG	2.27	0.43
1:A:97:GLU:HG2	1:A:98:LYS:HG3	2.00	0.43
1:A:27:PRO:HB3	1:A:50:ALA:HB2	2.00	0.43
1:B:62:VAL:HA	1:B:65:LYS:HB2	2.01	0.43
2:T:11:0DC:H2"	2:T:12:0DT:H6	2.01	0.42
1:B:297:SER:O	1:B:298:ARG:NH1	2.46	0.42
1:B:148:LYS:NZ	1:B:237:ILE:HA	2.35	0.42
1:B:312:TYR:O	1:B:316:VAL:HG23	2.20	0.41
2:T:18:0DC:C2	3:P:1:0DG:H21	2.26	0.41
1:B:307:SER:HG	1:B:310:THR:H	1.65	0.41
1:A:186:ILE:HD12	1:A:225:LEU:HD21	2.02	0.41
1:B:255:SER:OG	1:B:256:ARG:N	2.52	0.41
2:T:12:0DT:H3	3:P:7:0DA:C2A	2.33	0.41
1:B:66:LYS:HD2	1:B:66:LYS:C	2.28	0.41
1:B:84:VAL:HG13	1:B:136:GLU:HG2	2.03	0.41
1:A:309:GLU:H	1:A:309:GLU:HG2	1.44	0.40
1:B:16:GLU:HG2	1:B:74:LEU:CD1	2.52	0.40
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/360 (92%)	320 (97%)	11 (3%)	0	100	100
1	B	333/360 (92%)	313 (94%)	20 (6%)	0	100	100
All	All	664/720 (92%)	633 (95%)	31 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/317 (93%)	291 (99%)	4 (1%)	59	73
1	B	297/317 (94%)	287 (97%)	10 (3%)	32	43
All	All	592/634 (93%)	578 (98%)	14 (2%)	43	57

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	THR
1	A	193	LYS
1	A	308	LYS
1	A	309	GLU
1	B	51	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	55	VAL
1	B	56	LYS
1	B	65	LYS
1	B	66	LYS
1	B	68	LEU
1	B	97	GLU
1	B	98	LYS
1	B	188	ASN
1	B	189	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	B	82	GLN
1	B	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

28 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	0DT	T	12	2	18,21,22	5.34	14 (77%)	25,30,33	2.35	12 (48%)
2	0DC	T	14	3,2	17,20,21	4.50	12 (70%)	23,28,31	0.93	1 (4%)
2	0DC	T	17	3,2	17,20,21	4.54	12 (70%)	23,28,31	1.03	1 (4%)
3	0DT	P	11	3	18,21,22	5.38	14 (77%)	25,30,33	2.32	7 (28%)
3	0DG	P	5	3,2	21,24,25	4.52	16 (76%)	30,35,38	2.73	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0DC	T	10	3,2	17,20,21	4.52	12 (70%)	23,28,31	1.01	1 (4%)
3	0DC	P	14	3,2	17,20,21	0.85	0	23,28,31	1.01	0
2	0DC	T	11	3,2	17,20,21	4.53	12 (70%)	23,28,31	1.22	2 (8%)
2	0DA	T	7	2	20,23,24	3.73	8 (40%)	28,33,36	2.77	13 (46%)
3	0DG	P	9	3,2	21,24,25	4.53	16 (76%)	30,35,38	2.99	12 (40%)
3	0DG	P	8	3,2	21,24,25	4.54	16 (76%)	30,35,38	3.02	13 (43%)
2	0DT	T	13	2	18,21,22	5.34	14 (77%)	25,30,33	2.35	9 (36%)
2	0DC	T	15	3,2	17,20,21	4.50	12 (70%)	23,28,31	0.95	0
3	0DG	P	2	3,2	21,24,25	4.45	15 (71%)	30,35,38	3.00	14 (46%)
3	0DG	P	3	3,2	21,24,25	4.44	15 (71%)	30,35,38	2.98	11 (36%)
2	0DA	T	8	2	20,23,24	3.71	9 (45%)	28,33,36	2.85	13 (46%)
2	0DG	T	5	3,2	21,24,25	4.45	15 (71%)	30,35,38	2.85	13 (43%)
3	0DA	P	6	3	20,23,24	3.73	8 (40%)	28,33,36	2.67	13 (46%)
2	0DC	T	18	3,2	17,20,21	4.51	12 (70%)	23,28,31	1.02	1 (4%)
3	0DA	P	7	3	20,23,24	3.69	9 (45%)	28,33,36	2.77	11 (39%)
3	0DA	P	10	3	20,23,24	3.70	9 (45%)	28,33,36	2.72	15 (53%)
2	0DG	T	6	3,2	21,24,25	4.49	15 (71%)	30,35,38	2.91	13 (43%)
2	0DC	T	16	3,2	17,20,21	4.53	12 (70%)	23,28,31	0.94	1 (4%)
3	0DT	P	12	3	18,21,22	5.37	14 (77%)	25,30,33	2.22	9 (36%)
2	0DT	T	9	2	18,21,22	5.35	15 (83%)	25,30,33	2.21	9 (36%)
3	0DG	P	4	3,2	21,24,25	4.49	15 (71%)	30,35,38	3.03	12 (40%)
3	0DG	P	1	3,2	21,21,25	4.49	15 (71%)	31,31,38	2.98	13 (41%)
3	0DC	P	13	3,2	17,20,21	4.56	12 (70%)	23,28,31	0.88	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
2	0DT	T	12	2	-	0/7/21/22	0/2/2/2
2	0DC	T	14	3,2	-	0/7/21/22	0/2/2/2
2	0DC	T	17	3,2	-	0/7/21/22	0/2/2/2
3	0DT	P	11	3	-	2/7/21/22	0/2/2/2
3	0DG	P	5	3,2	-	2/7/21/22	0/3/3/3
2	0DC	T	10	3,2	-	2/7/21/22	0/2/2/2
3	0DC	P	14	3,2	-	2/7/21/22	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0DC	T	11	3,2	-	2/7/21/22	0/2/2/2
2	0DA	T	7	2	-	4/7/21/22	0/3/3/3
3	0DG	P	9	3,2	-	3/7/21/22	0/3/3/3
3	0DG	P	8	3,2	-	0/7/21/22	0/3/3/3
2	0DT	T	13	2	-	2/7/21/22	0/2/2/2
2	0DC	T	15	3,2	-	0/7/21/22	0/2/2/2
3	0DG	P	2	3,2	-	0/7/21/22	0/3/3/3
3	0DG	P	3	3,2	-	0/7/21/22	0/3/3/3
2	0DA	T	8	2	-	0/7/21/22	0/3/3/3
2	0DG	T	5	3,2	-	2/7/21/22	0/3/3/3
3	0DA	P	6	3	-	2/7/21/22	0/3/3/3
2	0DC	T	18	3,2	-	0/7/21/22	0/2/2/2
3	0DA	P	7	3	-	2/7/21/22	0/3/3/3
3	0DA	P	10	3	-	2/7/21/22	0/3/3/3
2	0DG	T	6	3,2	-	0/7/21/22	0/3/3/3
2	0DC	T	16	3,2	-	2/7/21/22	0/2/2/2
3	0DT	P	12	3	-	0/7/21/22	0/2/2/2
2	0DT	T	9	2	-	2/7/21/22	0/2/2/2
3	0DG	P	4	3,2	-	0/7/21/22	0/3/3/3
3	0DG	P	1	3,2	-	0/6/18/22	0/3/3/3
3	0DC	P	13	3,2	-	2/7/21/22	0/2/2/2

All (348) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	7	0DA	C2'-C3'	-12.71	1.20	1.52
3	P	6	0DA	C2'-C3'	-12.68	1.20	1.52
3	P	7	0DA	C2'-C3'	-12.64	1.20	1.52
3	P	10	0DA	C2'-C3'	-12.63	1.20	1.52
2	T	8	0DA	C2'-C3'	-12.63	1.20	1.52
3	P	5	0DG	C2'-C3'	-12.17	1.21	1.52
3	P	9	0DG	C2'-C3'	-12.15	1.22	1.52
3	P	1	0DG	C2'-C3'	-12.11	1.22	1.52
2	T	6	0DG	C2'-C3'	-12.08	1.22	1.52
3	P	2	0DG	C2'-C3'	-12.05	1.22	1.52
3	P	4	0DG	C2'-C3'	-11.97	1.22	1.52
2	T	5	0DG	C2'-C3'	-11.96	1.22	1.52
3	P	8	0DG	C2'-C3'	-11.96	1.22	1.52
3	P	3	0DG	C2'-C3'	-11.90	1.22	1.52
3	P	11	0DT	C2'-C3'	-11.87	1.22	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	12	0DT	C2'-C3'	-11.76	1.23	1.52
2	T	13	0DT	C2'-C3'	-11.76	1.23	1.52
2	T	9	0DT	C2'-C3'	-11.60	1.23	1.52
2	T	12	0DT	C2'-C3'	-11.54	1.23	1.52
2	T	9	0DT	C6-C5	9.38	1.49	1.34
3	P	11	0DT	C6-C5	9.25	1.49	1.34
3	P	12	0DT	C6-C5	9.20	1.49	1.34
2	T	13	0DT	C6-C5	9.11	1.49	1.34
2	T	12	0DT	C6-C5	9.06	1.49	1.34
2	T	17	0DC	C3'-C4'	-8.79	1.29	1.53
3	P	13	0DC	C3'-C4'	-8.61	1.30	1.53
2	T	16	0DC	C3'-C4'	-8.55	1.30	1.53
2	T	5	0DG	O4'-C4'	-8.53	1.26	1.45
2	T	10	0DC	C3'-C4'	-8.51	1.30	1.53
2	T	14	0DC	C3'-C4'	-8.34	1.31	1.53
2	T	18	0DC	C3'-C4'	-8.32	1.31	1.53
2	T	15	0DC	C3'-C4'	-8.26	1.31	1.53
2	T	17	0DC	O4'-C4'	8.26	1.63	1.45
3	P	13	0DC	O4'-C4'	8.23	1.63	1.45
2	T	11	0DC	C3'-C4'	-8.22	1.31	1.53
2	T	11	0DC	O4'-C4'	8.22	1.63	1.45
2	T	14	0DC	O4'-C4'	8.21	1.63	1.45
3	P	8	0DG	O4'-C4'	-8.17	1.26	1.45
2	T	10	0DC	O4'-C4'	8.17	1.63	1.45
3	P	5	0DG	O4'-C4'	-8.12	1.26	1.45
2	T	6	0DG	O4'-C4'	-8.11	1.27	1.45
2	T	16	0DC	O4'-C4'	8.10	1.63	1.45
2	T	15	0DC	O4'-C4'	8.10	1.63	1.45
3	P	9	0DG	O4'-C4'	-8.08	1.27	1.45
3	P	1	0DG	O4'-C4'	-8.06	1.27	1.45
3	P	4	0DG	O4'-C4'	-8.02	1.27	1.45
3	P	2	0DG	O4'-C4'	-7.97	1.27	1.45
2	T	18	0DC	O4'-C4'	7.93	1.62	1.45
3	P	12	0DT	O4'-C4'	-7.93	1.27	1.45
2	T	9	0DT	O4'-C4'	-7.92	1.27	1.45
3	P	3	0DG	O4'-C4'	-7.88	1.27	1.45
3	P	11	0DT	O4'-C4'	-7.88	1.27	1.45
2	T	13	0DT	O4'-C4'	-7.82	1.27	1.45
2	T	12	0DT	O4'-C4'	-7.76	1.27	1.45
2	T	12	0DT	C2-N1	7.31	1.49	1.38
2	T	12	0DT	C2-N3	7.08	1.50	1.38
3	P	11	0DT	C2-N3	7.06	1.50	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	12	0DT	C2-N3	7.04	1.50	1.38
3	P	12	0DT	C2-N1	7.01	1.49	1.38
3	P	11	0DT	C2-N1	6.98	1.49	1.38
2	T	13	0DT	C2-N3	6.97	1.50	1.38
2	T	9	0DT	C2-N3	6.93	1.50	1.38
2	T	13	0DT	C2-N1	6.87	1.49	1.38
2	T	9	0DT	C2-N1	6.86	1.49	1.38
3	P	13	0DC	C2-N3	6.56	1.49	1.36
2	T	16	0DC	C2-N3	6.53	1.49	1.36
2	T	18	0DC	C2-N3	6.53	1.49	1.36
2	T	17	0DC	C6-C5	6.45	1.50	1.35
2	T	10	0DC	C6-C5	6.39	1.49	1.35
3	P	4	0DG	C4-N3	6.35	1.48	1.34
3	P	9	0DG	C4-N3	6.35	1.48	1.34
3	P	1	0DG	C4-N3	6.33	1.48	1.34
3	P	8	0DG	C4-N3	6.31	1.48	1.34
2	T	14	0DC	C6-C5	6.28	1.49	1.35
2	T	16	0DC	C6-C5	6.27	1.49	1.35
2	T	11	0DC	C6-C5	6.27	1.49	1.35
3	P	13	0DC	C6-C5	6.25	1.49	1.35
2	T	6	0DG	C4-N3	6.25	1.48	1.34
2	T	11	0DC	C2-N3	6.24	1.48	1.36
2	T	15	0DC	C6-C5	6.24	1.49	1.35
2	T	15	0DC	C2-N3	6.24	1.48	1.36
2	T	14	0DC	C2-N3	6.23	1.48	1.36
3	P	3	0DG	C4-N3	6.21	1.48	1.34
2	T	17	0DC	C2-N3	6.16	1.48	1.36
2	T	10	0DC	C2-N3	6.11	1.48	1.36
2	T	18	0DC	C6-C5	6.08	1.49	1.35
3	P	2	0DG	C4-N3	6.02	1.48	1.34
3	P	5	0DG	C4-N3	5.98	1.47	1.34
2	T	5	0DG	C4-N3	5.94	1.47	1.34
2	T	18	0DC	C4-N3	5.61	1.45	1.34
3	P	13	0DC	C4-N3	5.55	1.45	1.34
3	P	2	0DG	C1'-N9	-5.42	1.34	1.48
3	P	1	0DG	C1'-N9	-5.36	1.34	1.48
3	P	9	0DG	C1'-N9	-5.34	1.34	1.48
2	T	15	0DC	C4-N3	5.34	1.45	1.34
2	T	5	0DG	C1'-N9	-5.34	1.34	1.48
2	T	16	0DC	C4-N3	5.32	1.45	1.34
3	P	8	0DG	C1'-N9	-5.30	1.34	1.48
3	P	8	0DG	C2-N3	5.29	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	17	0DC	C4-N3	5.28	1.45	1.34
3	P	5	0DG	C1'-N9	-5.27	1.34	1.48
3	P	9	0DG	C2-N3	5.26	1.45	1.33
2	T	6	0DG	C1'-N9	-5.23	1.34	1.48
2	T	18	0DC	O4'-C1'	-5.22	1.30	1.42
3	P	3	0DG	C1'-N9	-5.20	1.35	1.48
2	T	11	0DC	C4-N3	5.20	1.44	1.34
3	P	1	0DG	C2-N3	5.20	1.45	1.33
3	P	4	0DG	C2-N3	5.17	1.45	1.33
3	P	4	0DG	C1'-N9	-5.16	1.35	1.48
2	T	10	0DC	C4-N3	5.16	1.44	1.34
2	T	14	0DC	C4-N3	5.14	1.44	1.34
3	P	7	0DA	O4'-C1'	-5.11	1.31	1.42
2	T	8	0DA	O4'-C1'	-5.09	1.31	1.42
3	P	10	0DA	O4'-C1'	-5.04	1.31	1.42
3	P	5	0DG	C2-N3	5.03	1.45	1.33
3	P	3	0DG	C2-N3	5.03	1.45	1.33
3	P	6	0DA	O4'-C1'	-5.00	1.31	1.42
2	T	6	0DG	C2-N3	4.96	1.45	1.33
3	P	11	0DT	C1'-N1	-4.94	1.35	1.48
2	T	7	0DA	O4'-C1'	-4.94	1.31	1.42
2	T	15	0DC	O4'-C1'	-4.92	1.31	1.42
3	P	1	0DG	C3'-C4'	4.91	1.65	1.53
2	T	11	0DC	C4-N4	4.90	1.45	1.33
2	T	13	0DT	C1'-N1	-4.89	1.35	1.48
3	P	2	0DG	C2-N3	4.88	1.45	1.33
2	T	16	0DC	O4'-C1'	-4.88	1.31	1.42
2	T	16	0DC	C4-N4	4.85	1.45	1.33
2	T	18	0DC	C4-N4	4.85	1.45	1.33
2	T	6	0DG	C3'-C4'	4.84	1.65	1.53
2	T	17	0DC	C4-N4	4.84	1.45	1.33
2	T	10	0DC	O4'-C1'	-4.84	1.31	1.42
3	P	10	0DA	C2'-C1'	4.83	1.65	1.52
2	T	15	0DC	C4-N4	4.81	1.45	1.33
2	T	5	0DG	C2-N3	4.80	1.44	1.33
3	P	12	0DT	C1'-N1	-4.80	1.36	1.48
2	T	12	0DT	C1'-N1	-4.79	1.36	1.48
2	T	8	0DA	C2'-C1'	4.79	1.65	1.52
3	P	8	0DG	C3'-C4'	4.79	1.65	1.53
2	T	11	0DC	O4'-C1'	-4.78	1.31	1.42
3	P	4	0DG	C3'-C4'	4.78	1.65	1.53
2	T	9	0DT	C1'-N1	-4.77	1.36	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	14	0DC	C4-N4	4.77	1.45	1.33
3	P	9	0DG	C3'-C4'	4.76	1.65	1.53
2	T	14	0DC	O4'-C1'	-4.75	1.31	1.42
2	T	9	0DT	C3'-C4'	4.75	1.65	1.53
3	P	2	0DG	C3'-C4'	4.75	1.65	1.53
3	P	13	0DC	C4-N4	4.75	1.45	1.33
3	P	13	0DC	O4'-C1'	-4.75	1.31	1.42
2	T	10	0DC	C4-N4	4.75	1.45	1.33
2	T	13	0DT	C3'-C4'	4.74	1.65	1.53
2	T	12	0DT	C3'-C4'	4.74	1.65	1.53
3	P	8	0DG	O3'-C3'	4.73	1.53	1.43
3	P	6	0DA	C2'-C1'	4.73	1.65	1.52
2	T	7	0DA	C2'-C1'	4.70	1.65	1.52
3	P	7	0DA	C2'-C1'	4.69	1.65	1.52
3	P	3	0DG	C3'-C4'	4.68	1.65	1.53
2	T	17	0DC	O4'-C1'	-4.65	1.32	1.42
3	P	9	0DG	C2-N2	4.65	1.45	1.34
2	T	5	0DG	C3'-C4'	4.64	1.65	1.53
3	P	12	0DT	C3'-C4'	4.63	1.65	1.53
3	P	5	0DG	C3'-C4'	4.63	1.65	1.53
3	P	4	0DG	C2-N2	4.59	1.44	1.34
2	T	7	0DA	O3'-C3'	4.58	1.52	1.43
3	P	12	0DT	C6-N1	4.57	1.45	1.38
3	P	5	0DG	C2-N2	4.57	1.44	1.34
3	P	11	0DT	C6-N1	4.56	1.45	1.38
3	P	6	0DA	O3'-C3'	4.54	1.52	1.43
3	P	8	0DG	C2-N2	4.54	1.44	1.34
2	T	13	0DT	C6-N1	4.53	1.45	1.38
3	P	11	0DT	C3'-C4'	4.47	1.64	1.53
2	T	9	0DT	C6-N1	4.46	1.45	1.38
2	T	10	0DC	C2-N1	4.46	1.49	1.40
2	T	6	0DG	C2-N2	4.45	1.44	1.34
2	T	14	0DC	C2-N1	4.45	1.49	1.40
3	P	13	0DC	C2-N1	4.42	1.49	1.40
2	T	12	0DT	C6-N1	4.41	1.45	1.38
3	P	1	0DG	C2-N2	4.39	1.44	1.34
3	P	5	0DG	O3'-C3'	4.37	1.52	1.43
3	P	2	0DG	C2-N2	4.34	1.44	1.34
2	T	11	0DC	C2-N1	4.32	1.49	1.40
2	T	8	0DA	O3'-C3'	4.31	1.52	1.43
3	P	3	0DG	C2-N2	4.30	1.44	1.34
3	P	1	0DG	O3'-C3'	4.27	1.52	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	6	0DG	O3'-C3'	4.24	1.52	1.43
3	P	9	0DG	O3'-C3'	4.22	1.52	1.43
2	T	16	0DC	C2-N1	4.19	1.48	1.40
2	T	5	0DG	C2-N2	4.19	1.44	1.34
3	P	10	0DA	O3'-C3'	4.18	1.52	1.43
2	T	17	0DC	C2-N1	4.16	1.48	1.40
2	T	18	0DC	C2-N1	4.15	1.48	1.40
2	T	15	0DC	C2-N1	4.15	1.48	1.40
3	P	4	0DG	O3'-C3'	4.15	1.52	1.43
2	T	5	0DG	O3'-C3'	4.09	1.51	1.43
3	P	3	0DG	O3'-C3'	4.07	1.51	1.43
3	P	2	0DG	O3'-C3'	4.06	1.51	1.43
3	P	11	0DT	C4-N3	4.06	1.46	1.38
3	P	7	0DA	O3'-C3'	3.99	1.51	1.43
2	T	13	0DT	C4-N3	3.96	1.46	1.38
3	P	11	0DT	O4'-C1'	3.94	1.51	1.42
2	T	12	0DT	C4-N3	3.92	1.46	1.38
2	T	9	0DT	C4-N3	3.86	1.46	1.38
3	P	12	0DT	C4-N3	3.84	1.46	1.38
2	T	12	0DT	O4'-C1'	3.82	1.50	1.42
3	P	12	0DT	O4'-C1'	3.79	1.50	1.42
2	T	13	0DT	O4'-C1'	3.71	1.50	1.42
2	T	11	0DC	O3'-C3'	3.69	1.51	1.43
2	T	9	0DT	O4'-C1'	3.59	1.50	1.42
3	P	5	0DG	C2-N1	3.55	1.46	1.37
3	P	3	0DG	O4'-C1'	3.54	1.50	1.42
3	P	8	0DG	C2-N1	3.54	1.46	1.37
3	P	5	0DG	O4'-C1'	3.54	1.50	1.42
3	P	4	0DG	O4'-C1'	3.49	1.50	1.42
2	T	7	0DA	C6A-N6A	3.47	1.43	1.34
2	T	6	0DG	C2-N1	3.43	1.46	1.37
3	P	9	0DG	C2-N1	3.43	1.46	1.37
3	P	6	0DA	C3'-C4'	3.42	1.62	1.53
3	P	4	0DG	C2-N1	3.39	1.45	1.37
3	P	12	0DT	O3'-C3'	3.37	1.50	1.43
2	T	8	0DA	C3'-C4'	3.36	1.61	1.53
3	P	2	0DG	C2-N1	3.36	1.45	1.37
3	P	8	0DG	O4'-C1'	3.35	1.49	1.42
3	P	1	0DG	C2-N1	3.34	1.45	1.37
3	P	7	0DA	C6A-N6A	3.34	1.42	1.34
2	T	15	0DC	O3'-C3'	3.33	1.50	1.43
2	T	6	0DG	O4'-C1'	3.32	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	0DG	O4'-C1'	3.31	1.49	1.42
2	T	10	0DC	C6-N1	3.31	1.46	1.38
3	P	3	0DG	C2-N1	3.30	1.45	1.37
2	T	5	0DG	C2-N1	3.30	1.45	1.37
2	T	7	0DA	C3'-C4'	3.28	1.61	1.53
2	T	8	0DA	C6A-N6A	3.27	1.42	1.34
3	P	7	0DA	C3'-C4'	3.27	1.61	1.53
2	T	9	0DT	O3'-C3'	3.26	1.50	1.43
3	P	9	0DG	O4'-C1'	3.26	1.49	1.42
3	P	13	0DC	C6-N1	3.25	1.45	1.38
3	P	6	0DA	C6A-N6A	3.25	1.42	1.34
3	P	10	0DA	C6A-N6A	3.25	1.42	1.34
2	T	11	0DC	C6-N1	3.23	1.45	1.38
2	T	13	0DT	O3'-C3'	3.22	1.50	1.43
2	T	12	0DT	O3'-C3'	3.21	1.50	1.43
2	T	14	0DC	C6-N1	3.20	1.45	1.38
3	P	2	0DG	O4'-C1'	3.19	1.49	1.42
2	T	17	0DC	C6-N1	3.18	1.45	1.38
2	T	16	0DC	C6-N1	3.18	1.45	1.38
3	P	10	0DA	C3'-C4'	3.13	1.61	1.53
2	T	15	0DC	C6-N1	3.12	1.45	1.38
2	T	9	0DT	C4-C5	3.09	1.49	1.44
2	T	5	0DG	O4'-C1'	3.09	1.49	1.42
2	T	13	0DT	C4-C5	3.08	1.49	1.44
3	P	11	0DT	O3'-C3'	2.99	1.49	1.43
2	T	10	0DC	O3'-C3'	2.99	1.49	1.43
2	T	18	0DC	O3'-C3'	2.96	1.49	1.43
2	T	14	0DC	O3'-C3'	2.93	1.49	1.43
3	P	12	0DT	C4-C5	2.91	1.49	1.44
2	T	11	0DC	C5-C4	2.91	1.49	1.42
2	T	14	0DC	C5-C4	2.90	1.49	1.42
2	T	12	0DT	C4-C5	2.89	1.49	1.44
2	T	18	0DC	C6-N1	2.89	1.45	1.38
2	T	9	0DT	O2-C2	-2.87	1.18	1.23
2	T	13	0DT	O2-C2	-2.85	1.18	1.23
2	T	15	0DC	C5-C4	2.84	1.49	1.42
2	T	17	0DC	C5-C4	2.82	1.49	1.42
2	T	12	0DT	O2-C2	-2.80	1.18	1.23
2	T	10	0DC	C5-C4	2.79	1.49	1.42
2	T	8	0DA	C2A-N3A	2.78	1.38	1.33
3	P	2	0DG	C5-C6	2.78	1.54	1.44
2	T	16	0DC	C5-C4	2.77	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	12	0DT	O2-C2	-2.77	1.18	1.23
3	P	11	0DT	C4-C5	2.76	1.49	1.44
2	T	16	0DC	O3'-C3'	2.75	1.49	1.43
3	P	13	0DC	O3'-C3'	2.74	1.49	1.43
3	P	11	0DT	O2-C2	-2.73	1.18	1.23
2	T	7	0DA	C2A-N3A	2.71	1.38	1.33
3	P	3	0DG	C5-C6	2.70	1.54	1.44
2	T	6	0DG	C5-C6	2.70	1.54	1.44
3	P	10	0DA	C5'-C4'	-2.70	1.43	1.51
2	T	7	0DA	C5'-C4'	-2.69	1.43	1.51
3	P	6	0DA	C5'-C4'	-2.68	1.43	1.51
3	P	7	0DA	C2A-N3A	2.66	1.38	1.33
2	T	14	0DC	O2-C2	-2.65	1.18	1.23
3	P	13	0DC	C5-C4	2.65	1.49	1.42
2	T	17	0DC	O2-C2	-2.63	1.18	1.23
3	P	4	0DG	C5-C6	2.62	1.54	1.44
2	T	11	0DC	O2-C2	-2.61	1.18	1.23
2	T	5	0DG	C5-C6	2.61	1.54	1.44
2	T	15	0DC	O2-C2	-2.58	1.18	1.23
2	T	8	0DA	C5'-C4'	-2.57	1.43	1.51
2	T	18	0DC	O2-C2	-2.57	1.18	1.23
3	P	1	0DG	C5-C6	2.56	1.54	1.44
3	P	7	0DA	C5'-C4'	-2.56	1.43	1.51
2	T	18	0DC	C5-C4	2.55	1.48	1.42
3	P	5	0DG	C5-C6	2.54	1.53	1.44
3	P	6	0DA	C2A-N3A	2.54	1.38	1.33
2	T	10	0DC	O2-C2	-2.51	1.19	1.23
3	P	13	0DC	O2-C2	-2.46	1.19	1.23
3	P	8	0DG	C5-C6	2.46	1.53	1.44
2	T	17	0DC	O3'-C3'	2.45	1.48	1.43
3	P	9	0DG	C5-C6	2.45	1.53	1.44
3	P	10	0DA	C2A-N3A	2.44	1.38	1.33
2	T	16	0DC	O2-C2	-2.38	1.19	1.23
3	P	3	0DG	O6-C6	-2.36	1.19	1.23
2	T	5	0DG	C6-N1	2.34	1.43	1.38
3	P	8	0DG	O6-C6	-2.33	1.19	1.23
3	P	4	0DG	O6-C6	-2.33	1.19	1.23
3	P	9	0DG	O6-C6	-2.32	1.19	1.23
2	T	5	0DG	C4-N9	-2.31	1.32	1.38
3	P	2	0DG	C6-N1	2.31	1.43	1.38
2	T	6	0DG	C6-N1	2.30	1.43	1.38
3	P	2	0DG	O5'-C5'	-2.30	1.37	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	5	0DG	O5'-C5'	-2.29	1.37	1.44
3	P	5	0DG	C4-N9	-2.29	1.32	1.38
3	P	3	0DG	O5'-C5'	-2.27	1.37	1.44
2	T	6	0DG	O5'-C5'	-2.26	1.37	1.44
3	P	8	0DG	C6-N1	2.25	1.43	1.38
3	P	4	0DG	O5'-C5'	-2.25	1.37	1.44
3	P	9	0DG	O5'-C5'	-2.25	1.37	1.44
3	P	5	0DG	C6-N1	2.24	1.43	1.38
3	P	5	0DG	O6-C6	-2.23	1.19	1.23
3	P	1	0DG	O6-C6	-2.23	1.19	1.23
3	P	2	0DG	C4-N9	-2.23	1.32	1.38
2	T	6	0DG	O6-C6	-2.22	1.19	1.23
3	P	5	0DG	C5-N7	-2.19	1.34	1.39
3	P	4	0DG	C5-N7	-2.18	1.34	1.39
3	P	3	0DG	C5-N7	-2.18	1.34	1.39
3	P	9	0DG	C5-N7	-2.18	1.34	1.39
3	P	4	0DG	C6-N1	2.18	1.42	1.38
2	T	12	0DT	O4-C4	-2.18	1.19	1.23
2	T	13	0DT	O4-C4	-2.18	1.19	1.23
2	T	5	0DG	O5'-C5'	-2.16	1.37	1.44
3	P	1	0DG	C6-N1	2.16	1.42	1.38
3	P	8	0DG	O5'-C5'	-2.15	1.37	1.44
3	P	11	0DT	O4-C4	-2.15	1.19	1.23
3	P	8	0DG	C5-N7	-2.14	1.34	1.39
3	P	1	0DG	C5-N7	-2.14	1.34	1.39
3	P	12	0DT	O4-C4	-2.12	1.19	1.23
3	P	1	0DG	C4-N9	-2.12	1.32	1.38
3	P	9	0DG	C6-N1	2.12	1.42	1.38
3	P	3	0DG	C6-N1	2.12	1.42	1.38
3	P	7	0DA	C5A-C4A	-2.09	1.35	1.39
2	T	6	0DG	C4-N9	-2.08	1.32	1.38
3	P	9	0DG	C4-N9	-2.08	1.32	1.38
3	P	2	0DG	C5-N7	-2.08	1.34	1.39
3	P	8	0DG	C4-N9	-2.07	1.32	1.38
2	T	9	0DT	C2'-C1'	2.05	1.57	1.52
3	P	10	0DA	C5A-C4A	-2.04	1.35	1.39
2	T	5	0DG	C5-N7	-2.03	1.35	1.39
2	T	9	0DT	O4-C4	-2.03	1.19	1.23
2	T	8	0DA	C5A-C4A	-2.01	1.35	1.39

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	9	0DG	C1'-N9-C8	-10.12	105.22	127.91
3	P	1	0DG	C1'-N9-C8	-10.03	105.41	127.91
3	P	4	0DG	C1'-N9-C8	-9.84	105.83	127.91
3	P	8	0DG	C1'-N9-C8	-9.84	105.85	127.91
3	P	3	0DG	C1'-N9-C8	-9.61	106.37	127.91
3	P	2	0DG	C1'-N9-C8	-9.33	106.99	127.91
2	T	6	0DG	C1'-N9-C8	-9.31	107.03	127.91
2	T	5	0DG	C1'-N9-C8	-9.28	107.09	127.91
3	P	5	0DG	C1'-N9-C8	-8.83	108.10	127.91
3	P	9	0DG	C1'-N9-C4	7.54	145.84	125.50
3	P	1	0DG	C1'-N9-C4	7.43	145.55	125.50
3	P	8	0DG	C1'-N9-C4	7.31	145.22	125.50
3	P	4	0DG	C1'-N9-C4	7.31	145.21	125.50
3	P	3	0DG	C1'-N9-C4	7.29	145.15	125.50
2	T	5	0DG	C1'-N9-C4	7.05	144.52	125.50
3	P	2	0DG	C1'-N9-C4	6.92	144.16	125.50
2	T	6	0DG	C1'-N9-C4	6.84	143.95	125.50
3	P	5	0DG	C1'-N9-C4	6.58	143.26	125.50
2	T	7	0DA	N1A-C2A-N3A	-5.82	119.77	128.58
2	T	13	0DT	C4-N3-C2	-5.68	119.89	127.34
2	T	8	0DA	N6A-C6A-N1A	-5.65	105.79	118.38
2	T	12	0DT	C4-N3-C2	-5.58	120.03	127.34
3	P	7	0DA	N1A-C2A-N3A	-5.56	120.17	128.58
3	P	11	0DT	C4-N3-C2	-5.55	120.06	127.34
2	T	8	0DA	N1A-C2A-N3A	-5.53	120.21	128.58
2	T	8	0DA	C1'-N9A-C8A	-5.37	108.17	126.95
3	P	6	0DA	N1A-C2A-N3A	-5.30	120.56	128.58
3	P	12	0DT	C4-N3-C2	-5.23	120.48	127.34
3	P	7	0DA	C1'-N9A-C8A	-5.22	108.69	126.95
3	P	10	0DA	N1A-C2A-N3A	-5.21	120.69	128.58
3	P	10	0DA	N6A-C6A-N1A	-5.15	106.90	118.38
3	P	6	0DA	N6A-C6A-N1A	-5.15	106.91	118.38
2	T	13	0DT	C5-C4-N3	5.10	119.75	115.32
2	T	7	0DA	N6A-C6A-N1A	-5.08	107.06	118.38
2	T	9	0DT	C4-N3-C2	-5.07	120.69	127.34
3	P	7	0DA	N6A-C6A-N1A	-5.02	107.19	118.38
3	P	11	0DT	C5-C4-N3	5.00	119.67	115.32
2	T	12	0DT	C5-C4-N3	4.99	119.66	115.32
3	P	3	0DG	C5-C4-N3	-4.96	120.49	128.39
2	T	7	0DA	C1'-N9A-C8A	-4.96	109.61	126.95
3	P	4	0DG	C5-C4-N3	-4.94	120.52	128.39
2	T	8	0DA	C5A-C4A-N3A	-4.92	119.94	126.72
3	P	10	0DA	C1'-N9A-C8A	-4.82	110.08	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	8	0DG	C5-C4-N3	-4.73	120.85	128.39
3	P	6	0DA	C1'-N9A-C8A	-4.73	110.42	126.95
3	P	1	0DG	C5-C4-N3	-4.65	120.98	128.39
3	P	9	0DG	C5-C4-N3	-4.62	121.03	128.39
3	P	12	0DT	C5-C4-N3	4.62	119.34	115.32
2	T	7	0DA	C5A-C4A-N3A	-4.58	120.41	126.72
3	P	3	0DG	C2-N3-C4	4.56	120.16	112.30
3	P	11	0DT	O4-C4-C5	-4.56	119.70	124.92
3	P	7	0DA	C5A-C4A-N3A	-4.55	120.45	126.72
3	P	6	0DA	C5A-C4A-N3A	-4.54	120.47	126.72
3	P	4	0DG	C2-N3-C4	4.49	120.04	112.30
3	P	5	0DG	C5-C4-N3	-4.48	121.26	128.39
3	P	2	0DG	C5-C4-N3	-4.47	121.27	128.39
2	T	6	0DG	C5-C4-N3	-4.45	121.31	128.39
2	T	8	0DA	C5A-C6A-N6A	4.42	134.22	123.29
3	P	7	0DA	N9A-C8A-N7A	-4.37	107.73	113.94
2	T	6	0DG	C2-N3-C4	4.36	119.81	112.30
2	T	9	0DT	C5-C4-N3	4.35	119.11	115.32
3	P	2	0DG	C2-N3-C4	4.30	119.70	112.30
2	T	8	0DA	C4A-N9A-C1'	4.29	143.69	126.50
3	P	5	0DG	C2-N3-C4	4.25	119.61	112.30
2	T	8	0DA	N9A-C8A-N7A	-4.24	107.92	113.94
3	P	10	0DA	C5A-C4A-N3A	-4.22	120.90	126.72
3	P	10	0DA	C5A-C6A-N6A	4.21	133.70	123.29
3	P	6	0DA	C5A-C6A-N6A	4.19	133.65	123.29
3	P	1	0DG	C2-N3-C4	4.18	119.50	112.30
3	P	9	0DG	C2-N3-C4	4.18	119.50	112.30
2	T	5	0DG	C5-C4-N3	-4.17	121.76	128.39
3	P	10	0DA	N9A-C8A-N7A	-4.16	108.03	113.94
3	P	8	0DG	C2-N3-C4	4.15	119.45	112.30
2	T	7	0DA	C5A-C6A-N6A	4.15	133.56	123.29
2	T	7	0DA	N9A-C8A-N7A	-4.12	108.09	113.94
2	T	12	0DT	N3-C2-N1	4.10	120.23	114.89
2	T	13	0DT	N3-C2-N1	4.09	120.22	114.89
3	P	7	0DA	C4A-N9A-C1'	4.08	142.86	126.50
2	T	5	0DG	C2-N3-C4	3.97	119.13	112.30
2	T	7	0DA	C4A-N9A-C1'	3.96	142.40	126.50
3	P	7	0DA	C5A-C6A-N6A	3.96	133.09	123.29
2	T	9	0DT	N3-C2-N1	3.96	120.04	114.89
3	P	6	0DA	N9A-C8A-N7A	-3.94	108.35	113.94
3	P	12	0DT	N3-C2-N1	3.92	120.00	114.89
3	P	11	0DT	N3-C2-N1	3.91	119.98	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	12	0DT	O4-C4-C5	-3.85	120.51	124.92
3	P	6	0DA	C4A-N9A-C1'	3.84	141.88	126.50
3	P	10	0DA	C4A-N9A-C1'	3.84	141.88	126.50
2	T	13	0DT	O4-C4-C5	-3.79	120.58	124.92
3	P	2	0DG	N9-C8-N7	-3.52	106.87	113.40
2	T	8	0DA	C2A-N3A-C4A	3.44	120.24	111.83
2	T	6	0DG	N9-C8-N7	-3.42	107.06	113.40
3	P	12	0DT	O4-C4-C5	-3.35	121.08	124.92
2	T	7	0DA	C2A-N3A-C4A	3.33	119.97	111.83
3	P	2	0DG	C4'-O4'-C1'	-3.33	101.61	109.51
3	P	4	0DG	N9-C8-N7	-3.31	107.27	113.40
3	P	5	0DG	N9-C8-N7	-3.26	107.36	113.40
3	P	3	0DG	N9-C8-N7	-3.25	107.38	113.40
3	P	1	0DG	N9-C8-N7	-3.24	107.40	113.40
3	P	7	0DA	C2A-N3A-C4A	3.23	119.73	111.83
2	T	5	0DG	C4'-O4'-C1'	-3.23	101.85	109.51
3	P	8	0DG	N9-C8-N7	-3.22	107.44	113.40
3	P	6	0DA	C2A-N3A-C4A	3.17	119.56	111.83
2	T	5	0DG	N9-C8-N7	-3.13	107.59	113.40
3	P	8	0DG	C2-N1-C6	-3.12	119.45	125.11
3	P	9	0DG	N9-C8-N7	-3.11	107.64	113.40
2	T	9	0DT	O4-C4-C5	-3.10	121.37	124.92
3	P	3	0DG	C2-N1-C6	-3.04	119.59	125.11
3	P	10	0DA	C2A-N3A-C4A	3.01	119.17	111.83
3	P	4	0DG	C2-N1-C6	-2.95	119.76	125.11
2	T	9	0DT	C4'-O4'-C1'	-2.92	102.58	109.51
3	P	5	0DG	C2-N1-C6	-2.91	119.83	125.11
2	T	8	0DA	C5A-N7A-C8A	2.89	107.99	103.45
2	T	13	0DT	C2'-C3'-C4'	2.87	108.62	102.80
2	T	8	0DA	N3A-C4A-N9A	2.84	132.00	127.17
3	P	2	0DG	C2-N1-C6	-2.82	119.99	125.11
3	P	4	0DG	N9-C4-N3	2.82	131.59	125.95
2	T	11	0DC	O4'-C1'-N1	2.82	112.87	107.86
3	P	8	0DG	C2'-C3'-C4'	2.81	108.51	102.80
2	T	6	0DG	C2-N1-C6	-2.80	120.02	125.11
3	P	9	0DG	N9-C4-N3	2.80	131.55	125.95
3	P	10	0DA	C4'-O4'-C1'	-2.79	102.89	109.51
3	P	1	0DG	C2-N1-C6	-2.74	120.14	125.11
3	P	2	0DG	O4'-C1'-N9	2.74	112.72	107.86
3	P	11	0DT	C5-C6-N1	-2.74	120.34	123.31
3	P	8	0DG	N9-C4-N3	2.74	131.43	125.95
3	P	1	0DG	N9-C4-N3	2.73	131.41	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	7	0DA	C5A-N7A-C8A	2.72	107.73	103.45
3	P	7	0DA	N3A-C4A-N9A	2.72	131.79	127.17
2	T	7	0DA	C5A-N7A-C8A	2.70	107.69	103.45
2	T	13	0DT	C5-C6-N1	-2.66	120.42	123.31
3	P	10	0DA	C5A-N7A-C8A	2.63	107.58	103.45
2	T	7	0DA	N3A-C4A-N9A	2.61	131.60	127.17
2	T	5	0DG	C2-N1-C6	-2.60	120.40	125.11
3	P	8	0DG	C5-C6-N1	2.59	119.86	113.25
3	P	3	0DG	C5-C6-N1	2.59	119.85	113.25
3	P	4	0DG	C4'-O4'-C1'	-2.59	103.36	109.51
3	P	9	0DG	C2-N1-C6	-2.59	120.42	125.11
3	P	6	0DA	C5A-N7A-C8A	2.59	107.51	103.45
3	P	7	0DA	C4A-N9A-C8A	2.58	108.44	105.74
3	P	2	0DG	O4'-C1'-C2'	-2.58	101.43	106.25
3	P	4	0DG	C5-C6-N1	2.57	119.79	113.25
3	P	11	0DT	C6-C5-C4	2.56	120.13	118.02
3	P	2	0DG	C8-N7-C5	2.56	108.82	104.26
3	P	8	0DG	O4'-C1'-N9	2.54	112.37	107.86
2	T	6	0DG	C5-C6-N1	2.51	119.65	113.25
3	P	3	0DG	N9-C4-N3	2.51	130.97	125.95
2	T	13	0DT	C5M-C5-C6	-2.50	119.46	122.85
3	P	12	0DT	C6-C5-C4	2.50	120.08	118.02
3	P	2	0DG	C4-C5-N7	-2.49	106.73	110.67
2	T	5	0DG	C2'-C3'-C4'	2.47	107.81	102.80
3	P	8	0DG	O6-C6-C5	-2.45	120.06	126.53
3	P	1	0DG	O4'-C1'-N9	2.44	112.20	107.86
2	T	6	0DG	C4'-O4'-C1'	-2.43	103.73	109.51
3	P	5	0DG	C5-C6-N1	2.43	119.43	113.25
3	P	1	0DG	C4'-O4'-C1'	-2.42	103.75	109.51
3	P	1	0DG	C5-C6-N1	2.42	119.42	113.25
3	P	6	0DA	N3A-C4A-N9A	2.42	131.28	127.17
2	T	9	0DT	C5M-C5-C6	-2.42	119.58	122.85
2	T	12	0DT	C2'-C3'-C4'	2.41	107.69	102.80
3	P	8	0DG	C4'-O4'-C1'	-2.40	103.80	109.51
3	P	6	0DA	O4'-C1'-N9A	2.40	112.28	107.96
3	P	9	0DG	C5-C6-N1	2.40	119.36	113.25
3	P	12	0DT	C5-C6-N1	-2.39	120.72	123.31
3	P	2	0DG	N2-C2-N1	2.39	121.81	116.76
3	P	3	0DG	C8-N7-C5	2.39	108.51	104.26
2	T	12	0DT	C6-C5-C4	2.37	119.97	118.02
2	T	9	0DT	C6-C5-C4	2.36	119.97	118.02
2	T	13	0DT	C6-C5-C4	2.36	119.96	118.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	3	0DG	C2'-C3'-C4'	2.35	107.56	102.80
2	T	8	0DA	C4A-C5A-N7A	-2.35	107.90	110.58
2	T	6	0DG	C8-N7-C5	2.33	108.42	104.26
3	P	9	0DG	O6-C6-C5	-2.33	120.39	126.53
3	P	2	0DG	C5-C6-N1	2.32	119.17	113.25
3	P	12	0DT	C5M-C5-C6	-2.32	119.71	122.85
2	T	17	0DC	O4'-C1'-N1	2.32	111.98	107.86
2	T	9	0DT	C5-C6-N1	-2.32	120.80	123.31
2	T	12	0DT	C4'-O4'-C1'	-2.31	104.02	109.51
3	P	4	0DG	O4'-C1'-C2'	-2.30	101.95	106.25
3	P	4	0DG	C8-N7-C5	2.29	108.33	104.26
2	T	8	0DA	C4A-N9A-C8A	2.28	108.13	105.74
3	P	10	0DA	C5A-C4A-N9A	2.27	108.29	105.81
2	T	9	0DT	C2'-C3'-C4'	2.27	107.40	102.80
3	P	1	0DG	C2'-C3'-C4'	2.25	107.37	102.80
3	P	11	0DT	C4'-O4'-C1'	-2.25	104.16	109.51
3	P	6	0DA	C5A-C4A-N9A	2.24	108.25	105.81
3	P	1	0DG	O6-C6-C5	-2.23	120.64	126.53
3	P	5	0DG	O6-C6-C5	-2.23	120.65	126.53
3	P	3	0DG	C4-C5-N7	-2.23	107.14	110.67
3	P	9	0DG	C4'-O4'-C1'	-2.22	104.23	109.51
2	T	6	0DG	N9-C4-N3	2.22	130.39	125.95
3	P	10	0DA	C4A-C5A-N7A	-2.21	108.06	110.58
3	P	5	0DG	N9-C4-N3	2.20	130.35	125.95
3	P	10	0DA	C4A-N9A-C8A	2.20	108.04	105.74
2	T	10	0DC	O2-C2-N3	-2.18	118.89	122.33
2	T	6	0DG	C4-C5-N7	-2.18	107.22	110.67
3	P	4	0DG	O6-C6-C5	-2.18	120.79	126.53
2	T	12	0DT	C5-C6-N1	-2.17	120.95	123.31
2	T	6	0DG	O4'-C1'-N9	2.17	111.72	107.86
3	P	5	0DG	N2-C2-N1	2.17	121.34	116.76
3	P	12	0DT	C4'-O4'-C1'	-2.16	104.37	109.51
2	T	12	0DT	O4'-C1'-C2'	-2.16	102.21	106.25
2	T	5	0DG	N2-C2-N1	2.16	121.32	116.76
3	P	12	0DT	O4'-C1'-N1	2.16	111.69	107.86
2	T	5	0DG	C5-C6-N1	2.16	118.74	113.25
2	T	12	0DT	C6-N1-C2	-2.15	119.16	121.30
2	T	7	0DA	C4A-N9A-C8A	2.15	107.99	105.74
3	P	5	0DG	C8-N7-C5	2.14	108.08	104.26
2	T	5	0DG	O6-C6-C5	-2.14	120.88	126.53
3	P	10	0DA	N3A-C4A-N9A	2.14	130.81	127.17
2	T	13	0DT	O2-C2-N1	-2.12	120.04	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	12	0DT	C5M-C5-C6	-2.12	119.98	122.85
2	T	6	0DG	N2-C2-N1	2.11	121.22	116.76
2	T	18	0DC	N4-C4-N3	2.11	121.68	117.91
3	P	9	0DG	O4'-C1'-N9	2.11	111.61	107.86
2	T	5	0DG	C4-C5-N7	-2.11	107.33	110.67
3	P	6	0DA	C4A-C5A-N7A	-2.09	108.19	110.58
3	P	1	0DG	C8-N7-C5	2.09	107.98	104.26
2	T	5	0DG	C8-N7-C5	2.08	107.96	104.26
3	P	10	0DA	O4'-C1'-N9A	2.07	111.67	107.96
2	T	8	0DA	C5A-C4A-N9A	2.06	108.06	105.81
2	T	16	0DC	C2'-C3'-C4'	2.06	106.98	102.80
3	P	8	0DG	C8-N7-C5	2.05	107.92	104.26
3	P	9	0DG	C2'-C3'-C4'	2.05	106.96	102.80
2	T	7	0DA	C4A-C5A-N7A	-2.05	108.24	110.58
2	T	11	0DC	C4'-O4'-C1'	-2.05	104.65	109.51
2	T	14	0DC	O2-C2-N3	-2.04	119.11	122.33
2	T	7	0DA	O4'-C1'-N9A	2.04	111.63	107.96
3	P	2	0DG	N9-C4-N3	2.02	129.99	125.95
2	T	12	0DT	C1'-N1-C2	2.02	121.60	117.66

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	16	0DC	O4'-C4'-C5'-O5'
3	P	6	0DA	O4'-C4'-C5'-O5'
3	P	6	0DA	C3'-C4'-C5'-O5'
3	P	10	0DA	O4'-C4'-C5'-O5'
3	P	13	0DC	O4'-C4'-C5'-O5'
2	T	5	0DG	O4'-C4'-C5'-O5'
2	T	7	0DA	C3'-C4'-C5'-O5'
2	T	9	0DT	C3'-C4'-C5'-O5'
2	T	10	0DC	C3'-C4'-C5'-O5'
2	T	11	0DC	O4'-C4'-C5'-O5'
2	T	13	0DT	C3'-C4'-C5'-O5'
2	T	16	0DC	C3'-C4'-C5'-O5'
3	P	9	0DG	C3'-C4'-C5'-O5'
3	P	13	0DC	C3'-C4'-C5'-O5'
3	P	14	0DC	C3'-C4'-C5'-O5'
2	T	5	0DG	C3'-C4'-C5'-O5'
2	T	9	0DT	O4'-C4'-C5'-O5'
2	T	10	0DC	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	P	9	0DG	O4'-C4'-C5'-O5'
3	P	5	0DG	O4'-C4'-C5'-O5'
3	P	10	0DA	C3'-C4'-C5'-O5'
3	P	11	0DT	C3'-C4'-C5'-O5'
2	T	7	0DA	O4'-C4'-C5'-O5'
2	T	13	0DT	O4'-C4'-C5'-O5'
3	P	14	0DC	O4'-C4'-C5'-O5'
3	P	9	0DG	C4'-C5'-O5'-P
2	T	11	0DC	C3'-C4'-C5'-O5'
3	P	5	0DG	C3'-C4'-C5'-O5'
3	P	11	0DT	O4'-C4'-C5'-O5'
3	P	7	0DA	C2'-C1'-N9A-C4A
2	T	7	0DA	O4'-C1'-N9A-C8A
2	T	7	0DA	O4'-C1'-N9A-C4A
3	P	7	0DA	O4'-C1'-N9A-C4A

There are no ring outliers.

22 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	12	0DT	2	0
2	T	14	0DC	1	0
2	T	17	0DC	1	0
3	P	5	0DG	1	0
3	P	14	0DC	5	0
2	T	11	0DC	2	0
3	P	8	0DG	1	0
2	T	13	0DT	2	0
2	T	15	0DC	1	0
3	P	2	0DG	1	0
3	P	3	0DG	1	0
3	P	6	0DA	3	0
2	T	18	0DC	1	0
3	P	7	0DA	1	0
3	P	10	0DA	2	0
2	T	6	0DG	1	0
2	T	16	0DC	1	0
3	P	12	0DT	1	0
2	T	9	0DT	2	0
3	P	4	0DG	1	0
3	P	1	0DG	1	0
3	P	13	0DC	6	0

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 ⓘ

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	335/360 (93%)	0.56	20 (5%) 27 31	31, 57, 91, 109	1 (0%)
1	B	337/360 (93%)	0.84	33 (9%) 13 15	37, 67, 114, 127	0
2	T	0/18	-	-	-	-
3	P	0/14	-	-	-	-
All	All	672/752 (89%)	0.70	53 (7%) 18 21	31, 62, 104, 127	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	GLY	5.5
1	A	57	ALA	5.2
1	B	270	GLU	4.3
1	B	56	LYS	4.3
1	B	194	LEU	4.2
1	A	309	GLU	4.2
1	A	276	LEU	4.1
1	A	62	VAL	3.9
1	B	57	ALA	3.9
1	A	54	GLY	3.6
1	B	309	GLU	3.6
1	B	217	ILE	3.2
1	B	4	LEU	3.1
1	B	59	ILE	3.1
1	B	314	GLU	3.0
1	B	61	ILE	3.0
1	B	73	TYR	3.0
1	A	272	SER	2.9
1	A	127	GLU	2.9
1	B	310	THR	2.9
1	B	71	ALA	2.8
1	B	210	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	168	ASP	2.7
1	B	327	GLU	2.7
1	B	313	SER	2.7
1	B	39	ASP	2.5
1	A	22	SER	2.5
1	B	62	VAL	2.5
1	A	32	VAL	2.5
1	B	29	VAL	2.4
1	A	23	LEU	2.4
1	B	60	PRO	2.3
1	B	66	LYS	2.3
1	A	260	GLU	2.3
1	B	341	ILE	2.3
1	A	71	ALA	2.3
1	B	207	SER	2.3
1	A	33	PHE	2.3
1	A	229	ALA	2.2
1	A	48	TYR	2.2
1	A	312	TYR	2.2
1	B	206	LEU	2.2
1	B	27	PRO	2.2
1	B	10	TYR	2.1
1	A	134	GLU	2.1
1	B	266	PHE	2.1
1	A	258	LEU	2.1
1	A	304	HIS	2.1
1	B	33	PHE	2.0
1	B	44	ALA	2.0
1	B	46	ALA	2.0
1	A	68	LEU	2.0
1	B	180	ILE	2.0

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, 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
3	ODG	P	1	19/23	0.62	0.18	56,91,110,115	0
3	ODG	P	8	22/23	0.72	0.13	56,74,111,127	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ODA	T	7	21/22	0.73	0.16	41,63,98,112	0
3	ODA	P	7	21/22	0.75	0.13	61,85,120,137	0
3	ODG	P	2	22/23	0.75	0.15	43,68,93,105	0
2	ODC	T	14	19/20	0.77	0.12	50,80,108,111	0
3	ODA	P	6	21/22	0.77	0.14	49,89,107,125	0
2	ODT	T	13	20/21	0.78	0.17	59,88,108,112	0
3	ODG	P	9	22/23	0.79	0.13	55,74,105,123	0
2	ODG	T	6	22/23	0.80	0.14	45,65,92,102	0
2	ODT	T	12	20/21	0.81	0.12	52,72,101,101	0
2	ODC	T	11	19/20	0.82	0.12	49,71,83,88	0
3	ODG	P	5	22/23	0.82	0.13	50,78,97,100	0
3	ODA	P	10	21/22	0.82	0.14	52,78,101,105	0
2	ODT	T	9	20/21	0.83	0.15	51,76,92,96	0
2	ODA	T	8	21/22	0.85	0.12	48,63,99,102	0
2	ODG	T	5	22/23	0.85	0.14	43,58,124,141	0
2	ODC	T	10	19/20	0.86	0.14	45,69,102,114	0
3	ODC	P	13	19/20	0.86	0.11	49,66,98,107	0
2	ODC	T	16	19/20	0.87	0.13	49,62,89,126	0
3	ODT	P	11	20/21	0.87	0.13	58,70,93,96	0
2	ODC	T	15	19/20	0.87	0.12	49,71,89,90	0
3	ODT	P	12	20/21	0.88	0.11	55,68,88,88	0
2	ODC	T	17	19/20	0.88	0.11	33,57,85,89	0
3	ODG	P	3	22/23	0.89	0.11	47,56,70,81	0
2	ODC	T	18	19/20	0.89	0.12	35,51,78,87	0
3	ODG	P	4	22/23	0.90	0.12	45,64,86,91	0
3	ODC	P	14	19/20	0.90	0.10	51,67,91,96	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.