



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:50 PM BST

PDB ID : 6L97
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

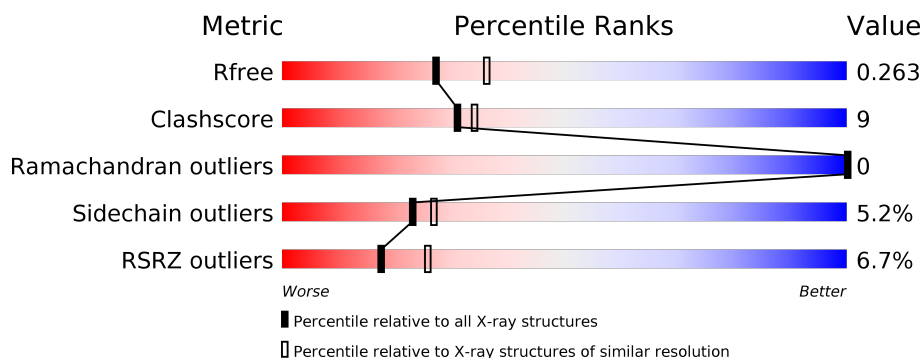
1 Overall quality at a glance

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 on 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	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>
1	B	360	<div> <div>8%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• 6%</div> </div> </div>
2	T	18	<div> <div></div> <div> <div>22%</div> <div>56%</div> <div>22%</div> </div> </div>
3	P	14	<div> <div></div> <div> <div>14%</div> <div>86%</div> </div> </div>

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	C	N	O	P	0	0	0
			292	138	60	81	13			

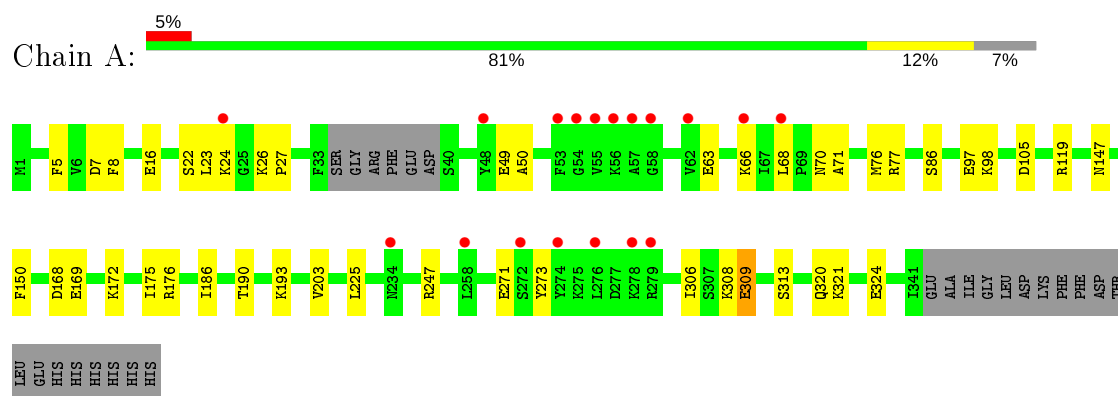
- Molecule 4 is water.

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

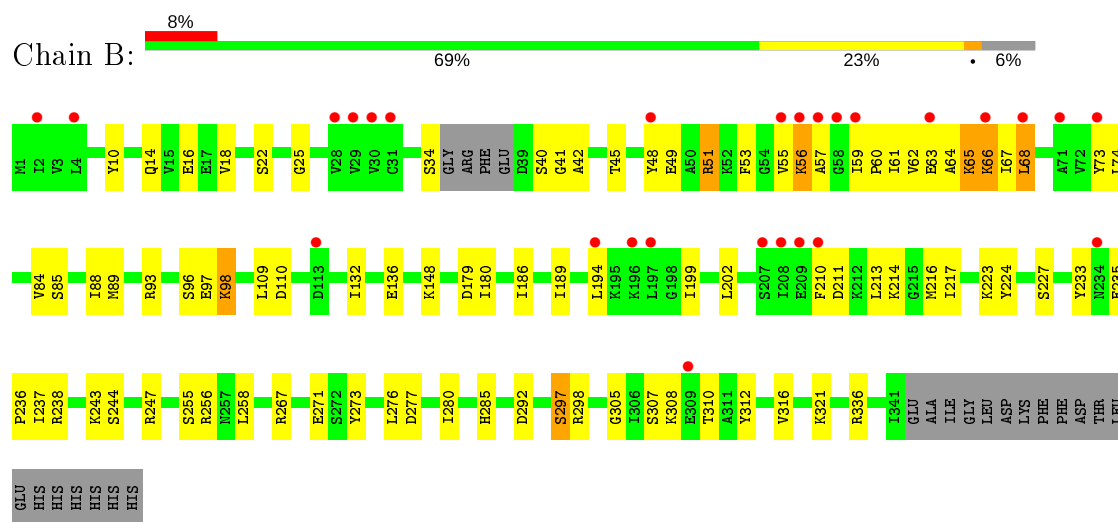
3 Residue-property plots [i](#)

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')

Chain P:  14% 86%

G1	G2	G3	G4	G5	A6	A7	G8	G9	A10	T11	T12	C13	C14
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.86 Å 54.97 Å 96.55 Å 90.00° 113.39° 90.00°	Depositor
Resolution (Å)	34.50 – 2.36 44.47 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.50-2.36) 97.7 (44.47-2.36)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.37 Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.230 , 0.266 0.230 , 0.263	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)	0.31 , 49.3	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

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/2731	0.45	0/3667
1	B	0.38	0/2745	0.49	0/3686
All	All	0.37	0/5476	0.47	0/7353

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	2694	0	2848	18	0
1	B	2708	0	2857	68	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	105	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 (105) 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:56:LYS:HG3	1:B:57:ALA:N	1.55	1.14
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: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
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:HD2	1:B:65:LYS:N	2.14	0.62
1:B:61:ILE:O	1:B:64:ALA:HB3	1.99	0.62
1:B:243:LYS:HG3	1:B:244:SER:N	2.16	0.61
2:T:17:0DC:C2	3:P:2:0DG:H21	2.13	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H8A	3:P:6:0DA:O5'	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: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:247:ARG:NH1	1:A:271:GLU:OE2	2.43	0.51
1:A:68:LEU:HD12	1:A:71:ALA:HB2	1.91	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:N	1:B:189:ILE:CD1	2.73	0.50
2:T:11:0DC:C2	3:P:8:0DG:H21	2.24	0.50
1:A:49:GLU:N	1:A:49:GLU:OE1	2.39	0.50
2:T:6:0DG:H21	3:P:13:0DC:C2	2.26	0.49
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:224:TYR:O	1:B:227:SER:OG	2.27	0.46
1:B:89:MET:O	1:B:93:ARG:HG3	2.16	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:148:LYS:NZ	1:B:236:PRO:O	2.49	0.46
1:B:59:ILE:HB	1:B:63:GLU:OE2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:HD21	1:A:150:PHE:HD2	1.65	0.45
1:B:180:ILE:O	1:B:186:ILE:HD11	2.17	0.45
1:B:67:ILE:CG2	1:B:68:LEU:HD12	2.44	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: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
1:B:307:SER:HG	1:B:310:THR:H	1.64	0.42
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: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:84:VAL:HG13	1:B:136:GLU:HG2	2.03	0.41
1:A:309:GLU:HG2	1:A:309:GLU:H	1.44	0.40
1:B:16:GLU:HG2	1:B:74:LEU:CD1	2.52	0.40
1:B:202:LEU:HA	1:B:202:LEU:HD12	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	280 (95%)	15 (5%)	24	27
1	B	297/317 (94%)	281 (95%)	16 (5%)	22	25
All	All	592/634 (93%)	561 (95%)	31 (5%)	23	27

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	24	LYS
1	A	70	ASN
1	A	76	MET
1	A	86	SER
1	A	119	ARG
1	A	168	ASP
1	A	169	GLU
1	A	172	LYS
1	A	190	THR
1	A	193	LYS
1	A	308	LYS
1	A	309	GLU
1	A	313	SER
1	A	321	LYS
1	B	22	SER
1	B	34	SER
1	B	48	TYR

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Mol	Chain	Res	Type
1	B	51	ARG
1	B	56	LYS
1	B	65	LYS
1	B	66	LYS
1	B	68	LEU
1	B	98	LYS
1	B	179	ASP
1	B	210	PHE
1	B	216	MET
1	B	223	LYS
1	B	238	ARG
1	B	277	ASP
1	B	297	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\# Z > 2$
3	0DG	P	1	3,2	18,21,25	5.32	13 (72%)	19,31,38	2.10	6 (31%)
2	0DA	T	7	2	18,23,24	3.83	9 (50%)	17,33,36	3.00	3 (17%)
2	0DT	T	9	2	15,21,22	5.06	11 (73%)	16,30,33	2.01	3 (18%)
3	0DA	P	10	3	18,23,24	3.79	9 (50%)	17,33,36	3.02	4 (23%)
2	0DG	T	5	3,2	18,24,25	5.30	13 (72%)	19,35,38	2.15	7 (36%)
2	0DT	T	12	2	15,21,22	5.04	12 (80%)	16,30,33	1.86	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ODG	P	5	3,2	18,24,25	5.36	14 (77%)	19,35,38	1.96	5 (26%)
2	ODC	T	11	3,2	15,20,21	4.82	10 (66%)	17,28,31	1.50	2 (11%)
3	ODG	P	9	3,2	18,24,25	5.36	14 (77%)	19,35,38	2.07	6 (31%)
2	ODC	T	16	3,2	15,20,21	4.83	11 (73%)	17,28,31	1.52	3 (17%)
3	ODA	P	7	3	18,23,24	3.79	9 (50%)	17,33,36	2.93	3 (17%)
3	ODC	P	14	3,2	15,20,21	0.68	0	17,28,31	1.45	3 (17%)
2	ODC	T	17	3,2	15,20,21	4.84	11 (73%)	17,28,31	1.39	2 (11%)
3	ODG	P	2	3,2	18,24,25	5.33	13 (72%)	19,35,38	2.26	8 (42%)
3	ODG	P	4	3,2	18,24,25	5.36	14 (77%)	19,35,38	2.12	6 (31%)
3	ODG	P	3	3,2	18,24,25	5.31	14 (77%)	19,35,38	2.05	7 (36%)
3	ODC	P	13	3,2	15,20,21	4.87	10 (66%)	17,28,31	1.43	2 (11%)
2	ODC	T	15	3,2	15,20,21	4.79	10 (66%)	17,28,31	1.48	2 (11%)
2	ODT	T	13	2	15,21,22	5.08	12 (80%)	16,30,33	1.79	2 (12%)
2	ODC	T	10	3,2	15,20,21	4.82	10 (66%)	17,28,31	1.46	1 (5%)
3	ODT	P	11	3	15,21,22	5.10	12 (80%)	16,30,33	1.85	2 (12%)
2	ODC	T	14	3,2	15,20,21	4.78	10 (66%)	17,28,31	1.30	1 (5%)
2	ODG	T	6	3,2	18,24,25	5.38	14 (77%)	19,35,38	2.13	7 (36%)
2	ODA	T	8	2	18,23,24	3.82	9 (50%)	17,33,36	3.06	3 (17%)
3	ODG	P	8	3,2	18,24,25	5.38	14 (77%)	19,35,38	1.99	6 (31%)
3	ODA	P	6	3	18,23,24	3.82	9 (50%)	17,33,36	2.91	3 (17%)
2	ODC	T	18	3,2	15,20,21	4.76	10 (66%)	17,28,31	1.50	2 (11%)
3	ODT	P	12	3	15,21,22	5.08	11 (73%)	16,30,33	1.91	2 (12%)

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
3	ODG	P	1	3,2	-	0/2/18/22	0/3/3/3
2	ODA	T	7	2	-	2/3/21/22	0/3/3/3
2	ODT	T	9	2	-	2/4/21/22	0/2/2/2
3	ODA	P	10	3	-	2/3/21/22	0/3/3/3
2	ODG	T	5	3,2	-	2/3/21/22	0/3/3/3
2	ODT	T	12	2	-	0/4/21/22	0/2/2/2
3	ODG	P	5	3,2	-	2/3/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0DC	T	11	3,2	-	2/4/21/22	0/2/2/2
3	0DG	P	9	3,2	-	3/3/21/22	0/3/3/3
2	0DC	T	16	3,2	-	2/4/21/22	0/2/2/2
3	0DA	P	7	3	-	0/3/21/22	0/3/3/3
3	0DC	P	14	3,2	-	2/4/21/22	0/2/2/2
2	0DC	T	17	3,2	-	0/4/21/22	0/2/2/2
3	0DG	P	2	3,2	-	0/3/21/22	0/3/3/3
3	0DG	P	4	3,2	-	0/3/21/22	0/3/3/3
3	0DG	P	3	3,2	-	0/3/21/22	0/3/3/3
3	0DC	P	13	3,2	-	2/4/21/22	0/2/2/2
2	0DC	T	15	3,2	-	0/4/21/22	0/2/2/2
2	0DT	T	13	2	-	2/4/21/22	0/2/2/2
2	0DC	T	10	3,2	-	2/4/21/22	0/2/2/2
3	0DT	P	11	3	-	2/4/21/22	0/2/2/2
2	0DC	T	14	3,2	-	1/4/21/22	0/2/2/2
2	0DG	T	6	3,2	-	0/3/21/22	0/3/3/3
2	0DA	T	8	2	-	0/3/21/22	0/3/3/3
3	0DG	P	8	3,2	-	0/3/21/22	0/3/3/3
3	0DA	P	6	3	-	2/3/21/22	0/3/3/3
2	0DC	T	18	3,2	-	1/4/21/22	0/2/2/2
3	0DT	P	12	3	-	0/4/21/22	0/2/2/2

All (308) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	7	0DA	C2'-C3'	-12.21	1.20	1.52
3	P	6	0DA	C2'-C3'	-12.18	1.20	1.52
3	P	7	0DA	C2'-C3'	-12.14	1.20	1.52
3	P	10	0DA	C2'-C3'	-12.14	1.20	1.52
2	T	8	0DA	C2'-C3'	-12.13	1.20	1.52
3	P	5	0DG	C2'-C3'	-11.70	1.21	1.52
3	P	9	0DG	C2'-C3'	-11.67	1.22	1.52
3	P	1	0DG	C2'-C3'	-11.64	1.22	1.52
2	T	6	0DG	C2'-C3'	-11.60	1.22	1.52
3	P	2	0DG	C2'-C3'	-11.58	1.22	1.52
3	P	4	0DG	C2'-C3'	-11.50	1.22	1.52
2	T	5	0DG	C2'-C3'	-11.49	1.22	1.52
3	P	8	0DG	C2'-C3'	-11.49	1.22	1.52
3	P	3	0DG	C2'-C3'	-11.44	1.22	1.52
3	P	11	0DT	C2'-C3'	-11.40	1.22	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	12	0DT	C2'-C3'	-11.30	1.23	1.52
2	T	13	0DT	C2'-C3'	-11.30	1.23	1.52
2	T	9	0DT	C2'-C3'	-11.15	1.23	1.52
2	T	12	0DT	C2'-C3'	-11.09	1.23	1.52
2	T	5	0DG	O4'-C4'	-8.49	1.26	1.45
2	T	17	0DC	C3'-C4'	-8.41	1.29	1.53
3	P	4	0DG	C4-N3	8.37	1.48	1.35
3	P	9	0DG	C4-N3	8.37	1.48	1.35
3	P	1	0DG	C4-N3	8.33	1.48	1.35
3	P	8	0DG	C4-N3	8.31	1.48	1.35
3	P	13	0DC	C3'-C4'	-8.24	1.30	1.53
2	T	6	0DG	C4-N3	8.22	1.48	1.35
2	T	10	0DC	C6-N1	8.22	1.46	1.35
2	T	17	0DC	O4'-C4'	8.21	1.63	1.45
3	P	13	0DC	O4'-C4'	8.18	1.63	1.45
2	T	16	0DC	C3'-C4'	-8.18	1.30	1.53
2	T	11	0DC	O4'-C4'	8.17	1.63	1.45
3	P	3	0DG	C4-N3	8.17	1.48	1.35
2	T	14	0DC	O4'-C4'	8.17	1.63	1.45
2	T	10	0DC	C3'-C4'	-8.14	1.30	1.53
3	P	8	0DG	O4'-C4'	-8.13	1.26	1.45
2	T	10	0DC	O4'-C4'	8.12	1.63	1.45
3	P	13	0DC	C6-N1	8.11	1.45	1.35
3	P	5	0DG	O4'-C4'	-8.08	1.26	1.45
2	T	11	0DC	C6-N1	8.07	1.45	1.35
2	T	6	0DG	O4'-C4'	-8.07	1.27	1.45
2	T	16	0DC	O4'-C4'	8.05	1.63	1.45
2	T	15	0DC	O4'-C4'	8.05	1.63	1.45
3	P	9	0DG	O4'-C4'	-8.04	1.27	1.45
3	P	1	0DG	O4'-C4'	-8.02	1.27	1.45
2	T	14	0DC	C6-N1	8.00	1.45	1.35
2	T	14	0DC	C3'-C4'	-7.98	1.31	1.53
3	P	4	0DG	O4'-C4'	-7.98	1.27	1.45
2	T	17	0DC	C6-N1	7.97	1.45	1.35
2	T	16	0DC	C6-N1	7.97	1.45	1.35
2	T	18	0DC	C3'-C4'	-7.96	1.31	1.53
3	P	2	0DG	O4'-C4'	-7.93	1.27	1.45
2	T	15	0DC	C3'-C4'	-7.90	1.31	1.53
3	P	12	0DT	O4'-C4'	-7.89	1.27	1.45
2	T	18	0DC	O4'-C4'	7.89	1.62	1.45
3	P	2	0DG	C4-N3	7.89	1.48	1.35
2	T	9	0DT	O4'-C4'	-7.88	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	11	0DC	C3'-C4'	-7.86	1.31	1.53
2	T	15	0DC	C6-N1	7.85	1.45	1.35
3	P	3	0DG	O4'-C4'	-7.84	1.27	1.45
3	P	11	0DT	O4'-C4'	-7.84	1.27	1.45
3	P	5	0DG	C4-N3	7.83	1.47	1.35
3	P	2	0DG	C6-C5	7.79	1.54	1.41
2	T	13	0DT	O4'-C4'	-7.78	1.27	1.45
2	T	5	0DG	C4-N3	7.77	1.47	1.35
2	T	12	0DT	O4'-C4'	-7.72	1.27	1.45
3	P	11	0DT	C4-N3	7.70	1.46	1.33
3	P	3	0DG	C6-C5	7.62	1.54	1.41
2	T	6	0DG	C6-C5	7.61	1.54	1.41
2	T	13	0DT	C4-N3	7.60	1.46	1.33
2	T	12	0DT	C4-N3	7.55	1.46	1.33
2	T	9	0DT	C4-N3	7.49	1.46	1.33
3	P	12	0DT	C4-N3	7.46	1.46	1.33
3	P	4	0DG	C6-C5	7.45	1.54	1.41
2	T	5	0DG	C6-C5	7.43	1.54	1.41
2	T	18	0DC	C6-N1	7.40	1.45	1.35
3	P	1	0DG	C6-C5	7.32	1.54	1.41
3	P	5	0DG	C6-C5	7.27	1.53	1.41
3	P	8	0DG	C6-C5	7.10	1.53	1.41
3	P	9	0DG	C6-C5	7.07	1.53	1.41
2	T	18	0DC	C4-N3	6.23	1.45	1.35
3	P	13	0DC	C4-N3	6.16	1.45	1.35
2	T	12	0DT	C2-N3	6.12	1.50	1.38
3	P	5	0DG	C2-N1	6.10	1.46	1.35
3	P	11	0DT	C2-N3	6.10	1.50	1.38
3	P	8	0DG	C2-N1	6.10	1.46	1.35
3	P	12	0DT	C2-N3	6.08	1.50	1.38
2	T	13	0DT	C2-N3	6.02	1.50	1.38
2	T	9	0DT	C2-N3	5.99	1.50	1.38
2	T	6	0DG	C2-N1	5.95	1.46	1.35
3	P	9	0DG	C2-N1	5.94	1.46	1.35
2	T	15	0DC	C4-N3	5.90	1.45	1.35
3	P	4	0DG	C2-N1	5.88	1.45	1.35
2	T	16	0DC	C4-N3	5.88	1.45	1.35
2	T	5	0DG	C6-N1	5.86	1.43	1.33
3	P	2	0DG	C2-N1	5.84	1.45	1.35
2	T	17	0DC	C4-N3	5.83	1.45	1.35
3	P	1	0DG	C2-N1	5.82	1.45	1.35
3	P	2	0DG	C6-N1	5.82	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	6	0DG	C6-N1	5.82	1.43	1.33
3	P	3	0DG	C2-N1	5.77	1.45	1.35
3	P	8	0DG	C6-N1	5.76	1.43	1.33
2	T	5	0DG	C2-N1	5.76	1.45	1.35
3	P	5	0DG	C6-N1	5.75	1.43	1.33
2	T	11	0DC	C4-N3	5.73	1.44	1.35
2	T	10	0DC	C4-N3	5.69	1.44	1.35
3	P	4	0DG	C6-N1	5.68	1.42	1.33
2	T	14	0DC	C4-N3	5.66	1.44	1.35
3	P	1	0DG	C6-N1	5.66	1.42	1.33
3	P	13	0DC	C2-N3	5.65	1.49	1.38
2	T	16	0DC	C2-N3	5.62	1.49	1.38
2	T	18	0DC	C2-N3	5.62	1.49	1.38
3	P	9	0DG	C6-N1	5.62	1.42	1.33
3	P	3	0DG	C6-N1	5.62	1.42	1.33
3	P	9	0DG	C2-N2	5.58	1.45	1.33
3	P	4	0DG	C2-N2	5.50	1.44	1.33
3	P	5	0DG	C2-N2	5.49	1.44	1.33
3	P	8	0DG	C2-N2	5.45	1.44	1.33
2	T	17	0DC	C6-C5	5.41	1.50	1.38
2	T	10	0DC	C6-C5	5.36	1.49	1.38
2	T	6	0DG	C2-N2	5.35	1.44	1.33
2	T	11	0DC	C2-N3	5.33	1.48	1.38
2	T	15	0DC	C2-N3	5.33	1.48	1.38
2	T	14	0DC	C2-N3	5.32	1.48	1.38
3	P	1	0DG	C2-N2	5.28	1.44	1.33
2	T	17	0DC	C2-N3	5.25	1.48	1.38
2	T	14	0DC	C6-C5	5.24	1.49	1.38
2	T	16	0DC	C6-C5	5.23	1.49	1.38
2	T	11	0DC	C6-C5	5.22	1.49	1.38
3	P	2	0DG	C2-N2	5.21	1.44	1.33
3	P	13	0DC	C6-C5	5.21	1.49	1.38
2	T	10	0DC	C2-N3	5.20	1.48	1.38
2	T	15	0DC	C6-C5	5.20	1.49	1.38
2	T	18	0DC	O4'-C1'	-5.17	1.30	1.42
3	P	3	0DG	C2-N2	5.17	1.44	1.33
3	P	7	0DA	O4'-C1'	-5.06	1.31	1.42
2	T	8	0DA	O4'-C1'	-5.05	1.31	1.42
3	P	2	0DG	C1'-N9	-5.04	1.34	1.49
2	T	5	0DG	C2-N2	5.03	1.44	1.33
2	T	18	0DC	C6-C5	5.03	1.49	1.38
3	P	10	0DA	O4'-C1'	-5.00	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	0DG	C1'-N9	-4.99	1.34	1.49
3	P	9	0DG	C1'-N9	-4.97	1.34	1.49
2	T	5	0DG	C1'-N9	-4.97	1.34	1.49
3	P	6	0DA	O4'-C1'	-4.96	1.31	1.42
3	P	8	0DG	C1'-N9	-4.94	1.34	1.49
3	P	5	0DG	C1'-N9	-4.91	1.34	1.49
2	T	7	0DA	O4'-C1'	-4.89	1.31	1.42
2	T	6	0DG	C1'-N9	-4.87	1.34	1.49
2	T	15	0DC	O4'-C1'	-4.87	1.31	1.42
3	P	3	0DG	C1'-N9	-4.85	1.35	1.49
2	T	16	0DC	O4'-C1'	-4.83	1.31	1.42
3	P	4	0DG	C1'-N9	-4.82	1.35	1.49
2	T	10	0DC	O4'-C1'	-4.80	1.31	1.42
2	T	11	0DC	O4'-C1'	-4.74	1.31	1.42
2	T	14	0DC	O4'-C1'	-4.71	1.31	1.42
3	P	13	0DC	O4'-C1'	-4.70	1.31	1.42
3	P	1	0DG	C3'-C4'	4.70	1.65	1.53
3	P	10	0DA	C2'-C1'	4.69	1.65	1.52
3	P	8	0DG	O3'-C3'	4.68	1.53	1.43
2	T	8	0DA	C2'-C1'	4.65	1.65	1.52
2	T	6	0DG	C3'-C4'	4.64	1.65	1.53
3	P	11	0DT	C1'-N1	-4.63	1.35	1.49
2	T	17	0DC	O4'-C1'	-4.61	1.32	1.42
3	P	6	0DA	C2'-C1'	4.60	1.65	1.52
2	T	13	0DT	C1'-N1	-4.59	1.35	1.49
3	P	8	0DG	C3'-C4'	4.58	1.65	1.53
2	T	7	0DA	C2'-C1'	4.57	1.65	1.52
3	P	4	0DG	C3'-C4'	4.57	1.65	1.53
3	P	9	0DG	C3'-C4'	4.56	1.65	1.53
3	P	7	0DA	C2'-C1'	4.55	1.65	1.52
2	T	9	0DT	C3'-C4'	4.55	1.65	1.53
3	P	2	0DG	C3'-C4'	4.55	1.65	1.53
2	T	13	0DT	C3'-C4'	4.54	1.65	1.53
2	T	12	0DT	C3'-C4'	4.54	1.65	1.53
2	T	7	0DA	O3'-C3'	4.52	1.52	1.43
3	P	12	0DT	C1'-N1	-4.51	1.36	1.49
2	T	12	0DT	C1'-N1	-4.50	1.36	1.49
2	T	9	0DT	C1'-N1	-4.49	1.36	1.49
3	P	6	0DA	O3'-C3'	4.49	1.52	1.43
3	P	3	0DG	C3'-C4'	4.48	1.65	1.53
2	T	5	0DG	C3'-C4'	4.44	1.65	1.53
3	P	12	0DT	C3'-C4'	4.43	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	5	0DG	C3'-C4'	4.43	1.65	1.53
3	P	5	0DG	O3'-C3'	4.32	1.52	1.43
3	P	11	0DT	C3'-C4'	4.28	1.64	1.53
2	T	8	0DA	O3'-C3'	4.26	1.52	1.43
3	P	1	0DG	O3'-C3'	4.22	1.52	1.43
2	T	8	0DA	C2A-N3A	4.21	1.38	1.32
2	T	6	0DG	O3'-C3'	4.19	1.52	1.43
3	P	9	0DG	O3'-C3'	4.17	1.52	1.43
3	P	10	0DA	O3'-C3'	4.13	1.52	1.43
2	T	7	0DA	C2A-N3A	4.12	1.38	1.32
3	P	4	0DG	O3'-C3'	4.10	1.52	1.43
3	P	7	0DA	C2A-N3A	4.07	1.38	1.32
2	T	5	0DG	O3'-C3'	4.04	1.51	1.43
3	P	3	0DG	O3'-C3'	4.02	1.51	1.43
3	P	2	0DG	O3'-C3'	4.01	1.51	1.43
3	P	7	0DA	O3'-C3'	3.95	1.51	1.43
3	P	6	0DA	C2A-N3A	3.94	1.38	1.32
3	P	11	0DT	O4'-C1'	3.93	1.51	1.42
2	T	9	0DT	C4-C5	3.92	1.49	1.41
2	T	13	0DT	C4-C5	3.91	1.49	1.41
3	P	10	0DA	C2A-N3A	3.83	1.38	1.32
2	T	12	0DT	O4'-C1'	3.80	1.50	1.42
3	P	12	0DT	O4'-C1'	3.78	1.50	1.42
3	P	12	0DT	C4-C5	3.78	1.49	1.41
2	T	12	0DT	C4-C5	3.76	1.49	1.41
2	T	13	0DT	O4'-C1'	3.69	1.50	1.42
3	P	11	0DT	C4-C5	3.67	1.49	1.41
2	T	11	0DC	O3'-C3'	3.64	1.51	1.43
2	T	11	0DC	C4-N4	3.59	1.45	1.35
2	T	9	0DT	O4'-C1'	3.58	1.50	1.42
2	T	16	0DC	C4-N4	3.55	1.45	1.35
2	T	18	0DC	C4-N4	3.55	1.45	1.35
2	T	17	0DC	C4-N4	3.55	1.45	1.35
2	T	9	0DT	C6-C5	3.54	1.49	1.40
3	P	3	0DG	O4'-C1'	3.53	1.50	1.42
3	P	5	0DG	O4'-C1'	3.52	1.50	1.42
2	T	15	0DC	C4-N4	3.52	1.45	1.35
2	T	11	0DC	C5-C4	3.52	1.49	1.41
2	T	14	0DC	C5-C4	3.51	1.49	1.41
2	T	14	0DC	C4-N4	3.48	1.45	1.35
3	P	4	0DG	O4'-C1'	3.48	1.50	1.42
3	P	13	0DC	C4-N4	3.47	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	10	0DC	C4-N4	3.47	1.45	1.35
3	P	11	0DT	C6-C5	3.46	1.49	1.40
2	T	15	0DC	C5-C4	3.45	1.49	1.41
2	T	17	0DC	C5-C4	3.43	1.49	1.41
3	P	12	0DT	C6-C5	3.43	1.49	1.40
2	T	10	0DC	C5-C4	3.40	1.49	1.41
2	T	16	0DC	C5-C4	3.39	1.49	1.41
2	T	13	0DT	C6-C5	3.38	1.49	1.40
2	T	12	0DT	C6-C5	3.35	1.49	1.40
3	P	8	0DG	O4'-C1'	3.35	1.49	1.42
3	P	12	0DT	O3'-C3'	3.32	1.50	1.43
2	T	6	0DG	O4'-C1'	3.31	1.49	1.42
3	P	1	0DG	O4'-C1'	3.30	1.49	1.42
2	T	15	0DC	O3'-C3'	3.29	1.50	1.43
3	P	6	0DA	C3'-C4'	3.27	1.62	1.53
3	P	13	0DC	C5-C4	3.26	1.49	1.41
3	P	9	0DG	O4'-C1'	3.25	1.49	1.42
2	T	9	0DT	O3'-C3'	3.22	1.50	1.43
2	T	8	0DA	C3'-C4'	3.22	1.61	1.53
3	P	2	0DG	O4'-C1'	3.18	1.49	1.42
2	T	13	0DT	O3'-C3'	3.18	1.50	1.43
2	T	18	0DC	C5-C4	3.17	1.48	1.41
2	T	12	0DT	O3'-C3'	3.17	1.50	1.43
2	T	7	0DA	C3'-C4'	3.14	1.61	1.53
3	P	7	0DA	C3'-C4'	3.13	1.61	1.53
2	T	5	0DG	O4'-C1'	3.08	1.49	1.42
3	P	10	0DA	C3'-C4'	3.00	1.61	1.53
3	P	2	0DG	O5'-C5'	-2.99	1.37	1.44
3	P	5	0DG	O5'-C5'	-2.98	1.37	1.44
3	P	3	0DG	O5'-C5'	-2.95	1.37	1.44
3	P	11	0DT	O3'-C3'	2.95	1.49	1.43
2	T	10	0DC	O3'-C3'	2.95	1.49	1.43
2	T	6	0DG	O5'-C5'	-2.95	1.37	1.44
3	P	4	0DG	O5'-C5'	-2.94	1.37	1.44
3	P	9	0DG	O5'-C5'	-2.93	1.37	1.44
2	T	18	0DC	O3'-C3'	2.92	1.49	1.43
2	T	14	0DC	O3'-C3'	2.89	1.49	1.43
2	T	5	0DG	O5'-C5'	-2.83	1.37	1.44
3	P	8	0DG	O5'-C5'	-2.82	1.37	1.44
2	T	16	0DC	O3'-C3'	2.71	1.49	1.43
3	P	13	0DC	O3'-C3'	2.71	1.49	1.43
3	P	10	0DA	C5'-C4'	-2.61	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	7	0DA	C5'-C4'	-2.60	1.43	1.51
3	P	6	0DA	C5'-C4'	-2.60	1.43	1.51
2	T	8	0DA	C5'-C4'	-2.49	1.43	1.51
2	T	7	0DA	C6A-N6A	2.48	1.43	1.34
3	P	7	0DA	C5'-C4'	-2.48	1.43	1.51
2	T	17	0DC	O3'-C3'	2.42	1.48	1.43
3	P	8	0DG	C2-N3	2.41	1.46	1.34
3	P	9	0DG	C2-N3	2.40	1.45	1.34
3	P	7	0DA	C6A-N6A	2.39	1.42	1.34
3	P	1	0DG	C2-N3	2.37	1.45	1.34
3	P	4	0DG	C2-N3	2.35	1.45	1.34
2	T	8	0DA	C6A-N6A	2.34	1.42	1.34
3	P	6	0DA	C6A-N6A	2.33	1.42	1.34
3	P	10	0DA	C6A-N6A	2.32	1.42	1.34
2	T	9	0DT	C5M-C5	2.29	1.55	1.51
2	T	17	0DC	O5'-C5'	-2.28	1.39	1.44
3	P	5	0DG	C2-N3	2.28	1.45	1.34
3	P	3	0DG	C2-N3	2.28	1.45	1.34
2	T	6	0DG	C2-N3	2.24	1.45	1.34
2	T	12	0DT	C5M-C5	2.24	1.55	1.51
3	P	2	0DG	C2-N3	2.20	1.45	1.34
3	P	3	0DG	O6-C6	-2.17	1.19	1.24
2	T	5	0DG	C2-N3	2.16	1.44	1.34
3	P	8	0DG	O6-C6	-2.15	1.19	1.24
3	P	12	0DT	C5M-C5	2.15	1.55	1.51
3	P	4	0DG	O6-C6	-2.15	1.19	1.24
3	P	9	0DG	O6-C6	-2.14	1.19	1.24
3	P	7	0DA	C5A-C4A	-2.11	1.35	1.40
3	P	5	0DG	O6-C6	-2.08	1.19	1.24
2	T	13	0DT	C5M-C5	2.07	1.54	1.51
3	P	1	0DG	O6-C6	-2.07	1.19	1.24
3	P	11	0DT	C5M-C5	2.07	1.54	1.51
3	P	10	0DA	C5A-C4A	-2.07	1.35	1.40
2	T	6	0DG	O6-C6	-2.06	1.19	1.24
2	T	16	0DC	O5'-C5'	-2.06	1.39	1.44
2	T	8	0DA	C5A-C4A	-2.05	1.35	1.40
2	T	12	0DT	O4-C4	-2.04	1.19	1.24
2	T	13	0DT	O4-C4	-2.03	1.19	1.24
3	P	6	0DA	C5A-C4A	-2.03	1.35	1.40
3	P	11	0DT	O4-C4	-2.01	1.19	1.24
2	T	7	0DA	C5A-C4A	-2.01	1.35	1.40

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	8	0DA	C5A-C6A-N6A	9.13	134.22	120.35
3	P	10	0DA	C5A-C6A-N6A	8.79	133.70	120.35
3	P	6	0DA	C5A-C6A-N6A	8.75	133.65	120.35
2	T	7	0DA	C5A-C6A-N6A	8.69	133.56	120.35
3	P	7	0DA	C5A-C6A-N6A	8.38	133.09	120.35
2	T	9	0DT	C4-N3-C2	6.57	120.69	115.14
3	P	12	0DT	C4-N3-C2	6.33	120.48	115.14
2	T	8	0DA	N6A-C6A-N1A	-6.16	105.79	118.57
3	P	11	0DT	C4-N3-C2	5.83	120.06	115.14
2	T	12	0DT	C4-N3-C2	5.79	120.03	115.14
2	T	7	0DA	N3A-C2A-N1A	-5.70	119.77	128.68
2	T	13	0DT	C4-N3-C2	5.63	119.89	115.14
3	P	10	0DA	N6A-C6A-N1A	-5.62	106.90	118.57
3	P	6	0DA	N6A-C6A-N1A	-5.62	106.91	118.57
2	T	7	0DA	N6A-C6A-N1A	-5.55	107.06	118.57
3	P	7	0DA	N6A-C6A-N1A	-5.49	107.19	118.57
3	P	7	0DA	N3A-C2A-N1A	-5.44	120.17	128.68
2	T	8	0DA	N3A-C2A-N1A	-5.42	120.21	128.68
3	P	9	0DG	N3-C2-N1	-5.41	120.01	127.22
2	T	6	0DG	N3-C2-N1	-5.27	120.19	127.22
3	P	4	0DG	N3-C2-N1	-5.24	120.23	127.22
3	P	6	0DA	N3A-C2A-N1A	-5.19	120.56	128.68
3	P	5	0DG	N3-C2-N1	-5.19	120.30	127.22
3	P	1	0DG	N3-C2-N1	-5.18	120.32	127.22
3	P	3	0DG	N3-C2-N1	-5.11	120.40	127.22
3	P	10	0DA	N3A-C2A-N1A	-5.11	120.69	128.68
3	P	2	0DG	N3-C2-N1	-5.05	120.48	127.22
2	T	5	0DG	N3-C2-N1	-4.97	120.59	127.22
3	P	8	0DG	N3-C2-N1	-4.97	120.60	127.22
2	T	10	0DC	C2-N3-C4	4.51	120.91	116.34
2	T	16	0DC	C2-N3-C4	4.26	120.66	116.34
2	T	15	0DC	C2-N3-C4	4.23	120.63	116.34
3	P	13	0DC	C2-N3-C4	4.22	120.62	116.34
3	P	3	0DG	C2-N3-C4	4.20	120.16	115.36
3	P	4	0DG	C2-N3-C4	4.10	120.04	115.36
3	P	14	0DC	C2-N3-C4	3.94	120.34	116.34
2	T	6	0DG	C2-N3-C4	3.89	119.81	115.36
2	T	14	0DC	C2-N3-C4	3.86	120.25	116.34
2	T	11	0DC	C2-N3-C4	3.83	120.22	116.34
3	P	2	0DG	C2-N3-C4	3.81	119.70	115.36
2	T	17	0DC	C2-N3-C4	3.76	120.15	116.34
3	P	5	0DG	C2-N3-C4	3.73	119.61	115.36
3	P	1	0DG	C2-N3-C4	3.63	119.50	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	9	0DG	C2-N3-C4	3.62	119.50	115.36
2	T	18	0DC	C2-N3-C4	3.62	120.01	116.34
3	P	8	0DG	C2-N3-C4	3.58	119.45	115.36
2	T	5	0DG	C5-C6-N1	-3.43	118.74	123.43
2	T	5	0DG	C2-N3-C4	3.31	119.13	115.36
2	T	18	0DC	N4-C4-N3	3.28	121.68	116.49
3	P	2	0DG	C4'-O4'-C1'	-3.25	101.61	109.45
2	T	5	0DG	C4'-O4'-C1'	-3.15	101.85	109.45
3	P	2	0DG	C5-C6-N1	-3.12	119.17	123.43
3	P	9	0DG	C5-C6-N1	-2.98	119.36	123.43
3	P	1	0DG	C5-C6-N1	-2.94	119.42	123.43
3	P	2	0DG	N2-C2-N1	2.93	121.81	117.25
3	P	5	0DG	C5-C6-N1	-2.92	119.43	123.43
2	T	9	0DT	C4'-O4'-C1'	-2.85	102.58	109.45
3	P	9	0DG	C6-N1-C2	2.82	120.42	115.93
2	T	5	0DG	C6-N1-C2	2.81	120.40	115.93
2	T	13	0DT	C2'-C3'-C4'	2.81	108.62	102.76
2	T	6	0DG	C5-C6-N1	-2.77	119.65	123.43
3	P	8	0DG	C2'-C3'-C4'	2.76	108.51	102.76
3	P	10	0DA	C4'-O4'-C1'	-2.72	102.89	109.45
3	P	13	0DC	N4-C4-N3	2.69	120.74	116.49
3	P	4	0DG	C5-C6-N1	-2.66	119.79	123.43
3	P	1	0DG	C6-N1-C2	2.65	120.14	115.93
3	P	5	0DG	N2-C2-N1	2.63	121.34	117.25
3	P	3	0DG	C5-C6-N1	-2.62	119.85	123.43
3	P	8	0DG	C5-C6-N1	-2.61	119.86	123.43
2	T	5	0DG	N2-C2-N1	2.61	121.32	117.25
2	T	6	0DG	C6-N1-C2	2.58	120.02	115.93
3	P	2	0DG	C4-C5-N7	-2.56	106.73	109.40
3	P	2	0DG	C6-N1-C2	2.55	119.99	115.93
2	T	6	0DG	N2-C2-N1	2.55	121.22	117.25
3	P	2	0DG	O4'-C1'-C2'	-2.55	101.43	106.25
3	P	4	0DG	C4'-O4'-C1'	-2.52	103.36	109.45
3	P	5	0DG	C6-N1-C2	2.46	119.83	115.93
2	T	5	0DG	C2'-C3'-C4'	2.42	107.81	102.76
2	T	16	0DC	N4-C4-N3	2.41	120.31	116.49
3	P	4	0DG	C6-N1-C2	2.41	119.76	115.93
2	T	6	0DG	C4'-O4'-C1'	-2.37	103.73	109.45
2	T	12	0DT	C2'-C3'-C4'	2.37	107.69	102.76
2	T	11	0DC	C2'-C1'-N1	-2.36	108.82	114.27
3	P	1	0DG	C4'-O4'-C1'	-2.36	103.75	109.45
3	P	8	0DG	C4'-O4'-C1'	-2.34	103.80	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	3	0DG	C6-N1-C2	2.31	119.59	115.93
3	P	3	0DG	C2'-C3'-C4'	2.30	107.56	102.76
3	P	4	0DG	O4'-C1'-C2'	-2.28	101.95	106.25
2	T	12	0DT	C4'-O4'-C1'	-2.25	104.02	109.45
2	T	9	0DT	C2'-C3'-C4'	2.23	107.40	102.76
3	P	8	0DG	C6-N1-C2	2.22	119.45	115.93
3	P	14	0DC	N4-C4-N3	2.22	119.99	116.49
3	P	1	0DG	C2'-C3'-C4'	2.21	107.37	102.76
3	P	11	0DT	C4'-O4'-C1'	-2.19	104.16	109.45
3	P	3	0DG	C4-C5-N7	-2.17	107.14	109.40
3	P	9	0DG	C4'-O4'-C1'	-2.16	104.23	109.45
3	P	3	0DG	N2-C2-N1	2.15	120.60	117.25
2	T	12	0DT	O4'-C1'-C2'	-2.14	102.21	106.25
3	P	12	0DT	C4'-O4'-C1'	-2.10	104.37	109.45
2	T	6	0DG	C4-C5-N7	-2.09	107.22	109.40
2	T	17	0DC	N4-C4-N3	2.05	119.73	116.49
2	T	16	0DC	C2'-C3'-C4'	2.03	106.98	102.76
2	T	15	0DC	N4-C4-N3	2.02	119.68	116.49
3	P	14	0DC	C2'-C1'-N1	-2.02	109.62	114.27
3	P	9	0DG	C2'-C3'-C4'	2.01	106.96	102.76

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	7	0DA	C3'-C4'-C5'-O5'
2	T	9	0DT	C3'-C4'-C5'-O5'
3	P	10	0DA	O4'-C4'-C5'-O5'
3	P	9	0DG	C3'-C4'-C5'-O5'
2	T	16	0DC	O4'-C4'-C5'-O5'
2	T	16	0DC	C3'-C4'-C5'-O5'
3	P	14	0DC	C3'-C4'-C5'-O5'
3	P	13	0DC	O4'-C4'-C5'-O5'
3	P	13	0DC	C3'-C4'-C5'-O5'
2	T	13	0DT	C3'-C4'-C5'-O5'
2	T	10	0DC	C3'-C4'-C5'-O5'
2	T	14	0DC	O4'-C1'-N1-C6
3	P	6	0DA	O4'-C4'-C5'-O5'
3	P	6	0DA	C3'-C4'-C5'-O5'
2	T	18	0DC	O4'-C1'-N1-C6
3	P	10	0DA	C3'-C4'-C5'-O5'
2	T	5	0DG	O4'-C4'-C5'-O5'

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

There are no ring outliers.

22 monomers are involved in 20 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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%)	0.35	18 (5%) 25 37	31, 57, 91, 109	1 (0%)
1	B	337/360 (93%)	0.59	27 (8%) 12 18	37, 67, 114, 127	0
2	T	0/18	-	-	-	-
3	P	0/14	-	-	-	-
All	All	672/752 (89%)	0.47	45 (6%) 17 26	31, 62, 104, 127	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	GLY	7.6
1	A	54	GLY	7.4
1	A	57	ALA	4.8
1	B	59	ILE	4.5
1	B	73	TYR	4.4
1	B	210	PHE	4.3
1	B	66	LYS	4.0
1	B	309	GLU	3.6
1	A	58	GLY	3.5
1	B	194	LEU	3.5
1	B	56	LYS	3.5
1	B	234	ASN	3.4
1	B	209	GLU	3.3
1	A	24	LYS	3.3
1	A	276	LEU	3.1
1	B	57	ALA	3.1
1	B	197	LEU	3.1
1	A	66	LYS	3.0
1	B	196	LYS	3.0
1	B	4	LEU	2.9
1	B	29	VAL	2.9
1	A	55	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	28	VAL	2.8
1	A	68	LEU	2.8
1	A	56	LYS	2.8
1	A	62	VAL	2.7
1	A	48	TYR	2.7
1	A	53	PHE	2.7
1	B	31	CYS	2.6
1	B	48	TYR	2.6
1	B	63	GLU	2.3
1	A	278	LYS	2.3
1	A	272	SER	2.3
1	B	113	ASP	2.3
1	B	68	LEU	2.3
1	B	30	VAL	2.2
1	A	274	TYR	2.2
1	B	55	VAL	2.2
1	A	258	LEU	2.2
1	A	279	ARG	2.2
1	B	207	SER	2.2
1	B	2	ILE	2.2
1	B	71	ALA	2.2
1	A	234	ASN	2.1
1	B	208	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	0.77	0.17	56,91,110,115	0
3	ODG	P	8	22/23	0.78	0.16	56,74,111,127	0
3	ODA	P	10	21/22	0.80	0.19	52,78,101,105	0
3	ODA	P	7	21/22	0.83	0.18	61,85,120,137	0
2	ODT	T	13	20/21	0.83	0.24	59,88,108,112	0
2	ODT	T	9	20/21	0.83	0.15	51,76,92,96	0
3	ODA	P	6	21/22	0.83	0.14	49,89,107,125	0
2	ODC	T	14	19/20	0.85	0.13	50,80,108,111	0
3	ODG	P	2	22/23	0.85	0.13	43,68,93,105	0
3	ODG	P	5	22/23	0.85	0.15	50,78,97,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	0DC	T	10	19/20	0.86	0.14	45,69,102,114	0
2	0DA	T	7	21/22	0.87	0.11	41,63,98,112	0
2	0DG	T	6	22/23	0.88	0.12	45,65,92,102	0
3	0DG	P	9	22/23	0.89	0.17	55,74,105,123	0
2	0DC	T	11	19/20	0.90	0.12	49,71,83,88	0
2	0DG	T	5	22/23	0.90	0.17	43,58,124,141	0
2	0DC	T	15	19/20	0.90	0.11	49,71,89,90	0
3	0DC	P	14	19/20	0.91	0.14	51,67,91,96	0
3	0DT	P	11	20/21	0.91	0.18	58,70,93,96	0
2	0DT	T	12	20/21	0.91	0.12	52,72,101,101	0
3	0DC	P	13	19/20	0.92	0.13	49,66,98,107	0
2	0DA	T	8	21/22	0.92	0.11	48,63,99,102	0
3	0DG	P	4	22/23	0.92	0.14	45,64,86,91	0
3	0DG	P	3	22/23	0.92	0.13	47,56,70,81	0
2	0DC	T	17	19/20	0.93	0.15	33,57,85,89	0
2	0DC	T	16	19/20	0.93	0.14	49,62,89,126	0
2	0DC	T	18	19/20	0.93	0.16	35,51,78,87	0
3	0DT	P	12	20/21	0.94	0.12	55,68,88,88	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.