



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 03:07 pm BST

PDB ID : 1T7P
Title : T7 DNA POLYMERASE COMPLEXED TO DNA PRIMER/TEMPLATE, A NUCLEOSIDE TRIPHOSPHATE, AND ITS PROCESSIVITY FACTOR THIOREDOXIN
Authors : Doublié, S.; Tabor, S.; Long, A.M.; Richardson, C.C.; Ellenberger, T.
Deposited on : 1997-09-24
Resolution : 2.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

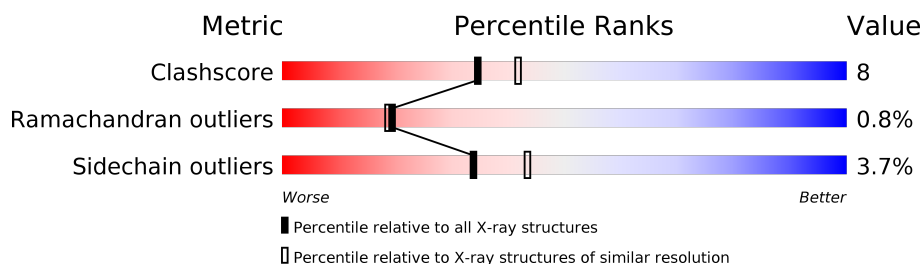
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	P	11	
2	T	13	
3	A	698	
4	B	108	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7092 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(P*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*2DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	11	Total	C	N	O	P	0	0	0
			224	106	44	63	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	13	Total	C	N	O	P	0	0	0
			264	125	46	80	13			

- Molecule 3 is a protein called DNA-directed DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	662	Total	C	N	O	S	0	0	0
			5266	3356	912	975	23			

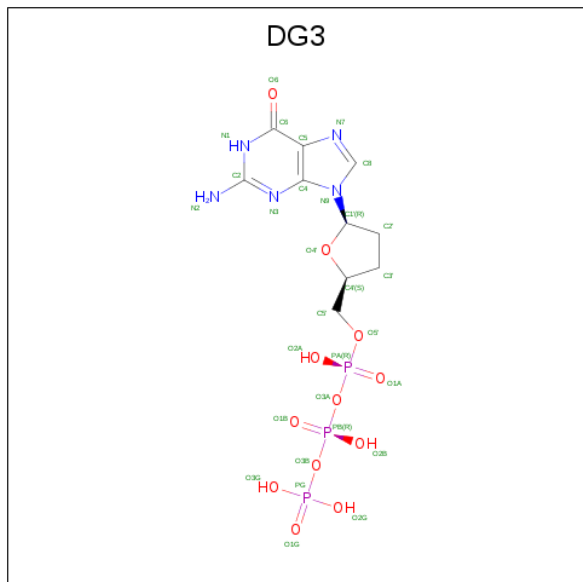
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P00581
A	?	-	ARG	deletion	UNP P00581
A	?	-	PHE	deletion	UNP P00581
A	?	-	GLY	deletion	UNP P00581
A	?	-	SER	deletion	UNP P00581
A	?	-	HIS	deletion	UNP P00581

- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			

- Molecule 5 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	P	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Mg	0	0
			3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	16	Total	O	0	0
			16	16		
7	T	29	Total	O	0	0
			29	29		
7	A	419	Total	O	0	0
			419	419		
7	B	39	Total	O	0	0
			39	39		

Note EDS was not executed.

- | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| G12 | C13 | C14 | A15 | G16 | T17 | G18 | C19 | C20 | A21 | A22 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

-

- | | | | |
|------|------|------|------|
| GLN | V368 | T239 | M1 |
| TRP | V372 | T279 | H19 |
| ALA | E388 | P282 | R35 |
| GLY | K391 | L283 | P36 |
| GLN | L392 | P294 | E49 |
| VAL | Q393 | P293 | R52 |
| K587 | K394 | GLY | H62 |
| K588 | K395 | GLY | V66 |
| K589 | R396 | ILE | P67 |
| R590 | A400 | PHE | R79 |
| R591 | A404 | LYS | R85 |
| D597 | K404 | LYS | L94 |
| G598 | L407 | PRO | W128 |
| R599 | L408 | ARG | M135 |
| L620 | Y409 | GLU | K140 |
| L624 | V410 | GLU | D141 |
| L633 | M421 | PRO | D142 |
| L638 | T431 | CYS | R145 |
| D645 | H432 | GLU | E149 |
| H653 | T440 | ASP | Y154 |
| D654 | R452 | THR | V155 |
| E655 | G456 | ARG | D156 |
| E664 | D475 | E319 | M171 |
| I665 | E480 | P320 | V172 |
| E671 | L479 | V321 | Q173 |
| Q674 | E484 | A322 | D174 |
| E675 | L484 | G323 | V175 |
| A676 | K484 | A324 | V176 |
| P677 | M489 | P325 | L181 |
| R678 | L501 | P326 | L185 |
| W679 | V332 | V332 | P193 |
| V680 | A532 | S338 | P194 |
| F686 | G533 | R339 | W222 |
| W700 | D534 | D340 | P232 |
| H704 | K549 | R341 | F233 |
| | E550 | T342 | F234 |
| | L551 | Q343 | |
| | K552 | P353 | |
| | K553 | Y356 | |
| | E557 | K359 | |
| | E575 | G360 | |
| | SR | | |

- [illegible]

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.60 Å 216.30 Å 52.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.240 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7092	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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: DG3, MG, 2DA

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	P	0.48	0/228	0.81	0/349
2	T	0.46	0/294	0.84	0/451
3	A	0.38	0/5396	0.63	0/7306
4	B	0.36	0/817	0.65	0/1108
All	All	0.39	0/6735	0.65	0/9214

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
2	T	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	20	DC	Sidechain
2	T	7	DG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	224	0	123	24	0
2	T	264	0	147	14	0
3	A	5266	0	5140	66	0
4	B	802	0	816	14	0
5	P	30	0	12	1	0
6	A	3	0	0	0	0
7	A	419	0	0	9	0
7	B	39	0	0	2	0
7	P	16	0	0	0	0
7	T	29	0	0	1	0
All	All	7092	0	6238	106	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 8.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:6:DT:H2''	2:T:7:DG:C5'	1.80	1.11
2:T:6:DT:H2''	2:T:7:DG:H5''	1.07	1.03
2:T:6:DT:C2'	2:T:7:DG:H5''	2.00	0.91
1:P:20:DC:H5'	3:A:394:LYS:HZ2	1.35	0.90
1:P:17:DT:H2''	1:P:18:DG:H5'	1.56	0.85
1:P:17:DT:H2''	1:P:18:DG:C5'	2.09	0.83
2:T:4:DC:H5''	3:A:532:ALA:HA	1.64	0.78
1:P:16:DG:H2''	1:P:17:DT:H5'	1.69	0.74
1:P:20:DC:H5'	3:A:394:LYS:NZ	2.03	0.73
1:P:19:DC:H1'	3:A:394:LYS:HZ3	1.55	0.72
2:T:4:DC:H2'	2:T:5:DT:H72	1.71	0.70
1:P:19:DC:H1'	3:A:394:LYS:NZ	2.06	0.70
1:P:16:DG:H2''	1:P:17:DT:C5'	2.22	0.70
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.75	0.68
3:A:391:MET:HE1	3:A:392:ILE:HD13	1.77	0.67
1:P:22:2DA:H5''	7:A:3195:HOH:O	1.95	0.66
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:4:DC:H2'	2:T:5:DT:C7	2.25	0.66
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.77	0.66
3:A:368:VAL:O	3:A:372:VAL:HG23	1.97	0.64
3:A:282:PRO:O	3:A:284:PRO:HD3	1.98	0.64
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.33	0.63
2:T:8:DG:H4'	3:A:432:HIS:O	1.99	0.63
1:P:21:DA:H5''	3:A:440:ILE:O	1.99	0.62
5:P:23:DG3:H2'1	3:A:480:GLU:CD	2.20	0.61
3:A:321:VAL:HG23	4:B:90:LYS:HD2	1.81	0.61
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.41	0.61
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.83	0.59
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.85	0.57
3:A:404:LYS:HA	3:A:409:TYR:HE2	1.69	0.57
3:A:553:LYS:O	3:A:557:GLU:HB2	2.04	0.56
3:A:66:VAL:HB	3:A:67:PRO:HD3	1.87	0.56
3:A:79:ARG:HD3	7:A:3099:HOH:O	2.06	0.56
3:A:676:ALA:O	3:A:680:VAL:HG23	2.07	0.54
3:A:341:HIS:N	7:A:3435:HOH:O	2.40	0.54
3:A:575:GLU:HB3	3:A:589:LYS:HE2	1.90	0.53
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.89	0.53
1:P:17:DT:C2'	1:P:18:DG:H5''	2.38	0.53
2:T:12:DT:H4'	3:A:338:SER:HA	1.91	0.53
3:A:391:MET:HE1	3:A:392:ILE:HA	1.91	0.53
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.08	0.52
3:A:85:ARG:HD3	7:A:3336:HOH:O	2.08	0.52
1:P:17:DT:C2'	1:P:18:DG:C5'	2.86	0.52
1:P:16:DG:H4'	3:A:359:LYS:NZ	2.26	0.51
1:P:17:DT:H2''	1:P:18:DG:H5''	1.89	0.51
3:A:400:ALA:HB2	3:A:407:LEU:HD12	1.94	0.50
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.12	0.50
2:T:5:DT:H2'	2:T:6:DT:H72	1.93	0.50
2:T:4:DC:C2'	2:T:5:DT:C7	2.90	0.49
3:A:674:GLN:O	3:A:678:ARG:HG2	2.13	0.48
1:P:13:DC:H1'	1:P:14:DC:H5'	1.95	0.48
4:B:97:GLY:HA2	4:B:100:LYS:NZ	2.29	0.48
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.96	0.48
1:P:20:DC:H2''	1:P:21:DA:OP2	2.14	0.48
3:A:479:LEU:HD22	3:A:654:ASP:HB3	1.95	0.47
3:A:671:GLU:HA	7:A:3527:HOH:O	2.15	0.47
3:A:484:LEU:O	3:A:488:MET:HG2	2.14	0.47
3:A:173:GLN:O	3:A:176:VAL:HG22	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:452:ARG:NH2	7:A:3402:HOH:O	2.46	0.46
3:A:452:ARG:HG3	3:A:700:TRP:HB3	1.96	0.46
4:B:73:ARG:O	4:B:73:ARG:HD2	2.16	0.46
2:T:4:DC:C2'	2:T:5:DT:H72	2.41	0.46
3:A:135:MET:HG3	3:A:174:ASP:OD1	2.15	0.46
3:A:388:GLU:O	3:A:392:ILE:HG12	2.16	0.46
3:A:591:ARG:CZ	7:A:3106:HOH:O	2.64	0.46
2:T:4:DC:C6	2:T:5:DT:H72	2.51	0.46
3:A:338:SER:C	7:A:3435:HOH:O	2.54	0.46
3:A:128:TRP:HB2	3:A:181:LEU:HG	1.97	0.45
1:P:17:DT:H1'	1:P:18:DG:H5''	1.97	0.45
3:A:145:ARG:O	3:A:149:GLU:HG3	2.16	0.45
3:A:19:HIS:O	3:A:36:PRO:HD3	2.16	0.45
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.51	0.45
3:A:588:TRP:HB2	7:A:3464:HOH:O	2.15	0.45
3:A:553:LYS:NZ	3:A:553:LYS:HB2	2.30	0.45
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.84	0.45
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.99	0.45
4:B:94:LEU:HB3	4:B:98:GLN:HB2	1.99	0.45
3:A:233:PRO:HB2	3:A:456:GLY:O	2.17	0.44
1:P:16:DG:H1'	1:P:17:DT:H5''	1.99	0.44
2:T:5:DT:C6	2:T:6:DT:H72	2.52	0.44
3:A:404:LYS:HA	3:A:409:TYR:CE2	2.51	0.43
1:P:19:DC:C2	1:P:20:DC:C5	3.06	0.43
4:B:4:ILE:HG12	7:B:3499:HOH:O	2.18	0.43
1:P:16:DG:C2'	1:P:17:DT:H5''	2.48	0.43
3:A:353:PRO:HB2	3:A:356:TYR:CZ	2.53	0.43
3:A:534:ASP:CG	3:A:549:LYS:HG2	2.39	0.43
3:A:475:ASP:OD2	3:A:655:GLU:HB3	2.19	0.42
4:B:46:ALA:HB2	7:B:3499:HOH:O	2.18	0.42
1:P:20:DC:C2'	1:P:21:DA:OP2	2.65	0.42
3:A:363:VAL:O	3:A:368:VAL:HG21	2.20	0.42
4:B:53:LEU:HG	4:B:54:THR:N	2.35	0.42
3:A:400:ALA:CB	3:A:407:LEU:HD12	2.50	0.42
3:A:234:PHE:CD2	3:A:410:VAL:HG11	2.55	0.42
3:A:49:GLU:OE1	3:A:52:ARG:NH1	2.53	0.42
3:A:633:LEU:HD22	3:A:638:LEU:HD23	2.02	0.42
1:P:16:DG:H4'	3:A:359:LYS:HZ3	1.83	0.42
2:T:11:DC:H2'	7:T:3213:HOH:O	2.20	0.41
1:P:16:DG:C2'	1:P:17:DT:C5'	2.97	0.41
3:A:172:VAL:O	3:A:176:VAL:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:323:GLY:O	3:A:325:PRO:HD3	2.20	0.41
3:A:392:ILE:O	3:A:396:ILE:HG13	2.21	0.41
3:A:549:LYS:HB3	3:A:549:LYS:HE2	1.94	0.41
3:A:140:LYS:HE3	3:A:154:TYR:OH	2.21	0.41
4:B:23:ILE:HD13	4:B:54:THR:HB	2.03	0.41
1:P:21:DA:H2"	1:P:22:2DA:H8	2.03	0.41
4:B:7:LEU:HD13	4:B:12:PHE:CD2	2.56	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	
3	A	656/698 (94%)	633 (96%)	17 (3%)	6 (1%)	17	16
4	B	103/108 (95%)	100 (97%)	3 (3%)	0	100	100
All	All	759/806 (94%)	733 (97%)	20 (3%)	6 (1%)	19	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	359	LYS
3	A	279	THR
3	A	479	LEU
3	A	360	GLY
3	A	653	HIS

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	
3	A	544/579 (94%)	524 (96%)	20 (4%)	34	43
4	B	85/87 (98%)	82 (96%)	3 (4%)	36	46
All	All	629/666 (94%)	606 (96%)	23 (4%)	34	43

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	62	HIS
3	A	142	ASP
3	A	171	ASN
3	A	181	LEU
3	A	232	PHE
3	A	237	LYS
3	A	332	VAL
3	A	340	ASP
3	A	343	GLN
3	A	391	MET
3	A	394	LYS
3	A	501	LEU
3	A	551	LEU
3	A	553	LYS
3	A	557	GLU
3	A	599	ARG
3	A	624	LEU
3	A	638	LEU
3	A	664	GLU
3	A	686	PHE
4	B	53	LEU
4	B	89	THR
4	B	99	LEU

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

Mol	Chain	Res	Type
3	A	343	GLN
3	A	347	GLN
3	A	667	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	2DA	P	22	1,2	17,22,23	0.62	0	13,31,34	1.01	1 (7%)

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	2DA	P	22	1,2	-	0/3/18/19	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	22	2DA	C5-C6-N6	2.55	124.23	120.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	22	2DA	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	DG3	P	23	6	25,32,32	1.16	1 (4%)	28,50,50	2.34	6 (21%)

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
5	DG3	P	23	6	-	3/18/31/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	23	DG3	C6-N1	3.76	1.39	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	23	DG3	C5-C6-N1	-8.83	111.35	123.43
5	P	23	DG3	C6-N1-C2	5.78	125.12	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	23	DG3	C2-N3-C4	-2.92	112.02	115.36
5	P	23	DG3	N3-C2-N1	-2.32	124.12	127.22
5	P	23	DG3	O2G-PG-O1G	2.26	119.52	110.68
5	P	23	DG3	C6-C5-C4	-2.17	118.73	120.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

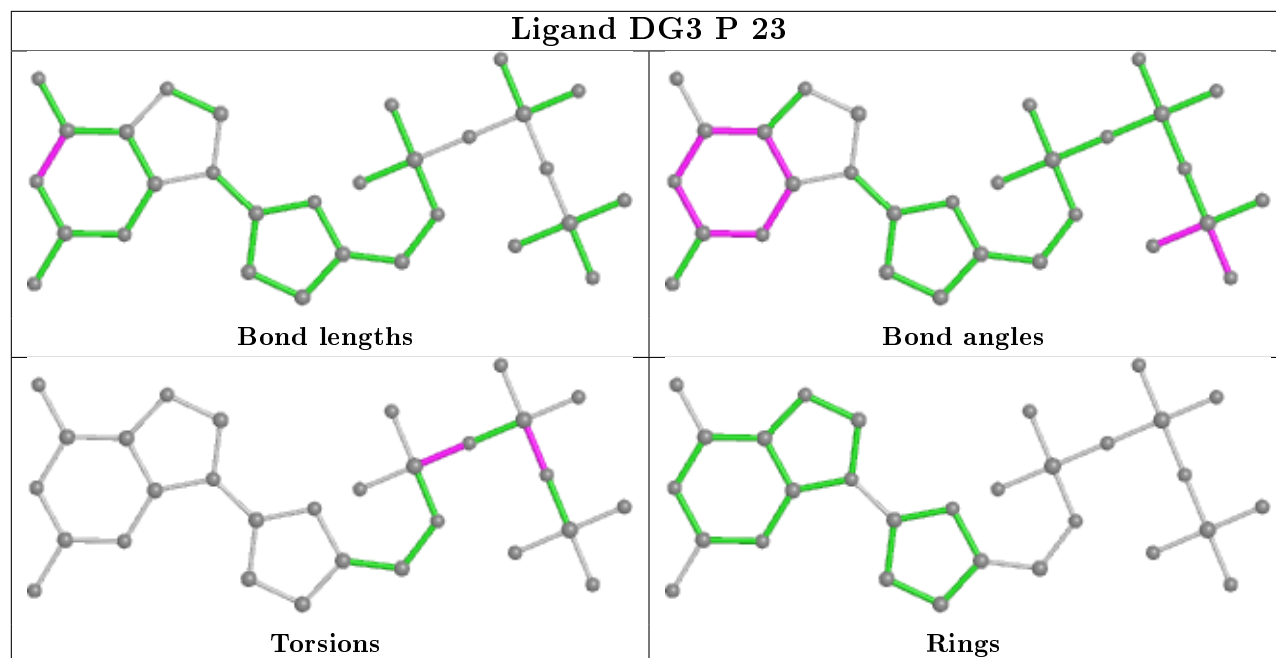
Mol	Chain	Res	Type	Atoms
5	P	23	DG3	PG-O3B-PB-O1B
5	P	23	DG3	PG-O3B-PB-O2B
5	P	23	DG3	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	23	DG3	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.