



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:11 pm BST

PDB ID : 5OMQ  
Title : Ternary complex of 9N DNA polymerase in the replicative state with three metal ions in the active site  
Authors : Betz, K.; Marx, A.; Diederichs, K.  
Deposited on : 2017-08-01  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

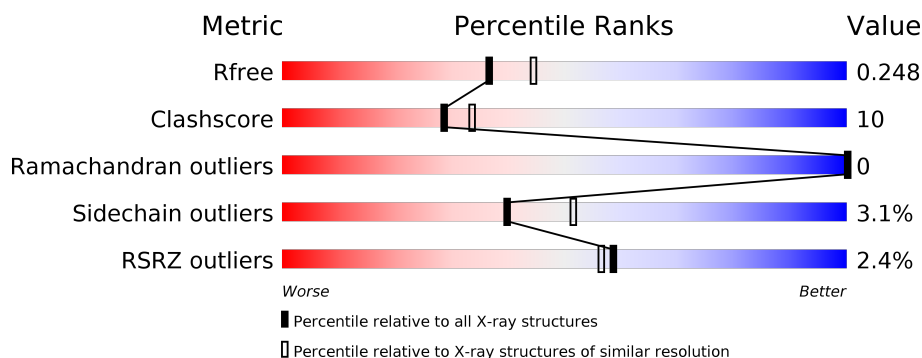
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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  $\geq 3$ , 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	775	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
2	T	16	<div> <div>56%</div> <div>31%</div> <div>13%</div> </div>
3	P	12	<div> <div>67%</div> <div>33%</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6922 atoms, of which 12 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	4	0
			6244	4021	1069	1139	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q56366
A	143	ALA	GLU	engineered mutation	UNP Q56366

- Molecule 2 is a DNA chain called DNA Template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	14	Total	C	N	O	P	0	0	0
			288	136	50	88	14			

- Molecule 3 is a DNA chain called DNA Primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	12	Total	C	N	O	P	0	0	0
			239	114	48	66	11			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

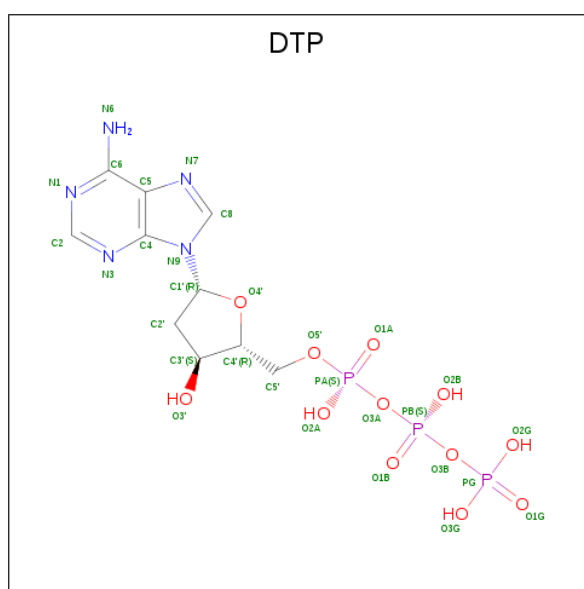
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mn	0	1
			1	1		

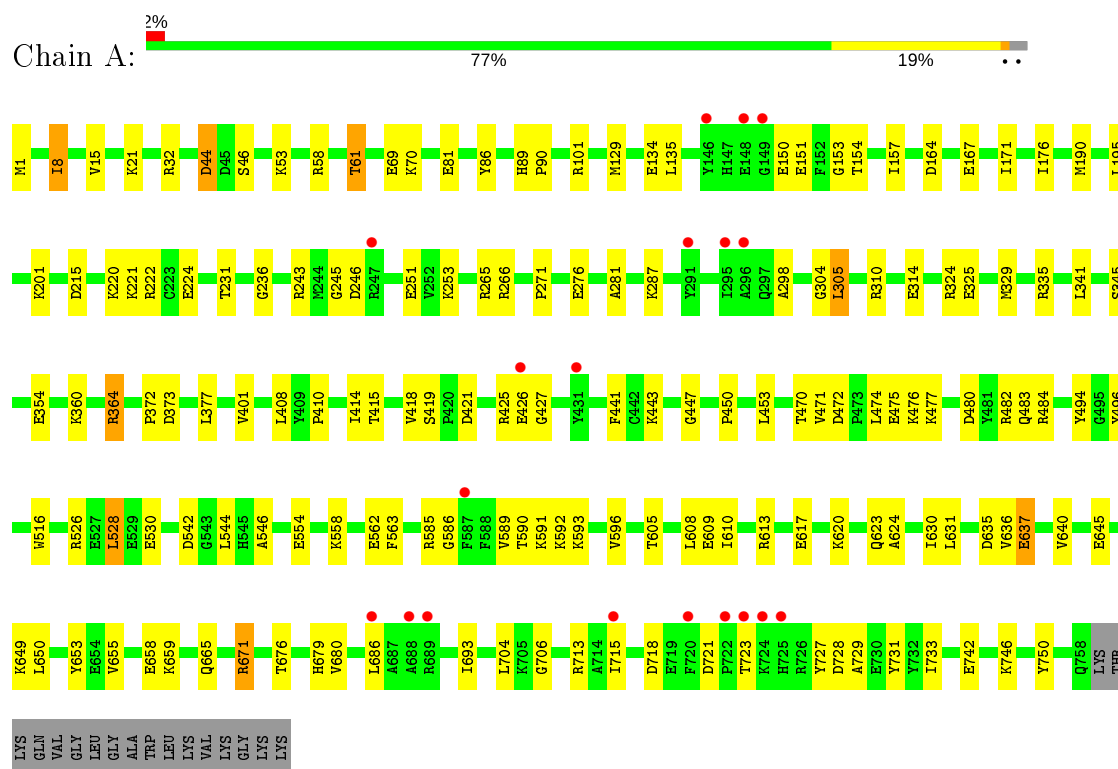
- Molecule 8 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ) (labeled as "Ligand of Interest" by author).



### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

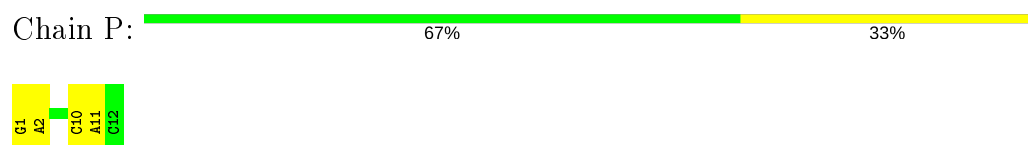
#### • Molecule 1: DNA polymerase



#### • Molecule 2: DNA Template



#### • Molecule 3: DNA Primer



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.79 Å 93.68 Å 158.21 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.84 – 2.20 46.84 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.84-2.20) 99.6 (46.84-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (1.12rc0_2787: ???)	Depositor
R, $R_{free}$	0.193 , 0.248 0.193 , 0.248	Depositor DCC
$R_{free}$ test set	2611 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, PGE, DTP, MN

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	0.41	0/6386	0.55	0/8613
2	T	1.08	1/321 (0.3%)	1.12	0/494
3	P	1.03	0/268	0.93	0/410
All	All	0.50	1/6975 (0.0%)	0.61	0/9517

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	6	DT	C5-C7	5.26	1.53	1.50

There are no bond angle outliers.

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	6244	0	6294	121	0
2	T	288	0	159	8	0
3	P	239	0	132	3	0
4	A	6	0	8	0	0
5	A	10	0	14	1	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	30	12	12	0	0
9	A	73	0	0	2	0
9	P	7	0	0	0	0
9	T	10	0	0	0	0
All	All	6910	12	6619	131	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 10.

All (131) 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:16:DC:H6	2:T:16:DC:H5"	1.34	0.92
1:A:44[B]:ASP:OD2	1:A:46:SER:OG	1.88	0.91
1:A:1:MET:CE	1:A:135:LEU:HD11	2.03	0.88
1:A:1:MET:HE1	1:A:135:LEU:HD11	1.56	0.87
1:A:310:ARG:NH1	1:A:314:GLU:OE2	2.10	0.84
1:A:704:LEU:HD11	1:A:715:ILE:HD13	1.60	0.84
1:A:176:ILE:HD12	1:A:305:LEU:HB3	1.63	0.81
1:A:150:GLU:HB3	1:A:154:THR:HG21	1.61	0.81
1:A:721:ASP:OD1	1:A:723:THR:HG22	1.81	0.80
2:T:16:DC:C6	2:T:16:DC:H5"	2.21	0.76
1:A:231:THR:HG23	1:A:236:GLY:O	1.90	0.72
1:A:704:LEU:O	1:A:713:ARG:HD2	1.91	0.71
1:A:650:LEU:HD23	1:A:655:VAL:HG11	1.71	0.71
1:A:329:MET:HG3	1:A:482:ARG:HG2	1.72	0.70
1:A:271:PRO:HA	1:A:613:ARG:HB3	1.73	0.70
1:A:325:GLU:OE1	1:A:474:LEU:HD11	1.93	0.68
1:A:176:ILE:CD1	1:A:305:LEU:HB3	2.22	0.68
1:A:713:ARG:NH1	1:A:728:ASP:OD2	2.26	0.68
1:A:610:ILE:HG12	1:A:623:GLN:OE1	1.93	0.67
1:A:653:TYR:HA	1:A:727:TYR:OH	1.94	0.67
1:A:415:THR:O	1:A:443:LYS:NZ	2.26	0.67
1:A:157:ILE:HG13	1:A:222:ARG:HG3	1.79	0.65
1:A:544:LEU:HD12	1:A:544:LEU:O	1.98	0.64
1:A:151:GLU:O	1:A:154:THR:HG22	1.98	0.64
1:A:610:ILE:HD11	1:A:623:GLN:HB3	1.81	0.63
1:A:470:THR:O	1:A:476:LYS:HE2	1.98	0.63
1:A:526:ARG:HG3	1:A:530:GLU:OE2	2.00	0.62
1:A:425:ARG:HG3	1:A:426:GLU:HG2	1.81	0.62
1:A:8:ILE:CD1	1:A:15:VAL:HB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE2	1:A:135:LEU:HD11	1.79	0.60
1:A:721:ASP:CG	1:A:723:THR:HG22	2.22	0.60
1:A:640:VAL:HG21	1:A:750:TYR:CE1	2.36	0.60
1:A:70:LYS:HZ2	1:A:81:GLU:HB3	1.66	0.60
1:A:265:ARG:HH21	1:A:665:GLN:HE22	1.50	0.59
1:A:53:LYS:NZ	9:A:903:HOH:O	2.37	0.58
2:T:15:DT:H6	2:T:15:DT:H5"	1.68	0.58
1:A:480:ASP:O	1:A:484:ARG:HG3	2.02	0.57
1:A:610:ILE:HD13	1:A:620:LYS:O	2.05	0.57
1:A:613:ARG:HG3	3:P:10:DC:OP1	2.05	0.57
1:A:164:ASP:OD2	1:A:201:LYS:HE2	2.06	0.56
1:A:609:GLU:N	1:A:609:GLU:OE1	2.30	0.56
1:A:401:VAL:HG12	1:A:546:ALA:O	2.06	0.55
1:A:304:GLY:N	9:A:904:HOH:O	2.37	0.55
1:A:8:ILE:HD11	1:A:15:VAL:HB	1.88	0.54
1:A:408:LEU:HD22	1:A:542:ASP:HB3	1.89	0.54
1:A:650:LEU:CD2	1:A:655:VAL:HG11	2.35	0.54
1:A:635:ASP:OD1	1:A:637:GLU:HG3	2.08	0.54
1:A:58:ARG:O	1:A:61:THR:HG23	2.08	0.54
1:A:610:ILE:HD11	1:A:624:ALA:N	2.23	0.53
1:A:266:ARG:NH2	1:A:345:SER:O	2.41	0.53
1:A:686:LEU:HB2	1:A:693:ILE:HD11	1.90	0.53
1:A:70:LYS:NZ	1:A:81:GLU:HB3	2.23	0.53
1:A:640:VAL:HG21	1:A:750:TYR:CZ	2.44	0.53
1:A:630:ILE:HG12	1:A:636:VAL:HG22	1.90	0.52
1:A:354:GLU:OE1	1:A:496:TYR:OH	2.22	0.52
1:A:706:GLY:CA	1:A:713:ARG:HD3	2.40	0.51
2:T:15:DT:C6	2:T:15:DT:H5"	2.44	0.51
1:A:610:ILE:CD1	1:A:623:GLN:HB3	2.41	0.51
1:A:251:GLU:OE1	1:A:253:LYS:HE2	2.11	0.51
1:A:528:LEU:HD13	1:A:563:PHE:CE2	2.46	0.51
1:A:728:ASP:HB3	1:A:731:TYR:HB3	1.92	0.51
1:A:585:ARG:NH1	1:A:631:LEU:O	2.44	0.50
1:A:243:ARG:NH1	1:A:245:GLY:O	2.43	0.50
1:A:101:ARG:HG2	1:A:101:ARG:O	2.11	0.49
1:A:372:PRO:HB2	1:A:377:LEU:HD22	1.94	0.49
1:A:373:ASP:O	1:A:377:LEU:HD23	2.12	0.49
1:A:150:GLU:CB	1:A:154:THR:HG21	2.38	0.49
1:A:605:THR:HG23	1:A:608:LEU:HD12	1.95	0.48
1:A:364:ARG:HH11	1:A:364:ARG:HG2	1.78	0.48
1:A:276:GLU:HG3	1:A:287:LYS:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:NH2	1:A:613:ARG:HH12	2.11	0.48
1:A:8:ILE:HD13	1:A:15:VAL:HB	1.95	0.48
1:A:591:LYS:HD3	2:T:8:DG:H5''	1.96	0.48
1:A:591:LYS:O	1:A:592:LYS:HB2	2.14	0.47
1:A:220:LYS:O	1:A:224:GLU:HG3	2.14	0.47
1:A:281:ALA:O	1:A:477:LYS:NZ	2.47	0.47
1:A:718:ASP:OD1	1:A:718:ASP:N	2.47	0.47
1:A:372:PRO:HG2	1:A:377:LEU:CD2	2.45	0.47
1:A:408:LEU:HD22	1:A:542:ASP:CB	2.44	0.47
1:A:586:GLY:HA3	1:A:596:VAL:HG12	1.98	0.46
1:A:590:THR:HG22	1:A:593:LYS:HB2	1.96	0.46
1:A:341:LEU:HD23	1:A:341:LEU:O	2.16	0.46
1:A:447:GLY:C	1:A:450:PRO:HD2	2.36	0.46
1:A:650:LEU:HD23	1:A:655:VAL:CG1	2.42	0.46
1:A:167:GLU:OE2	1:A:201:LYS:NZ	2.47	0.46
1:A:528:LEU:HD13	1:A:563:PHE:CZ	2.50	0.46
5:A:802:PGE:H3	5:A:802:PGE:H5	1.31	0.46
1:A:1:MET:HE2	1:A:135:LEU:HD21	1.97	0.46
1:A:266:ARG:HH22	1:A:345:SER:HA	1.81	0.46
1:A:298:ALA:O	1:A:305:LEU:HD21	2.17	0.45
1:A:15:VAL:HG22	1:A:32:ARG:HG2	1.98	0.45
3:P:10:DC:H2''	3:P:11:DA:O5'	2.16	0.45
1:A:8:ILE:HD13	1:A:8:ILE:H	1.82	0.45
1:A:410:PRO:O	1:A:414:ILE:HG13	2.16	0.45
1:A:421:ASP:OD1	1:A:421:ASP:N	2.47	0.44
1:A:472:ASP:OD2	1:A:475:GLU:HB2	2.17	0.44
1:A:372:PRO:HG2	1:A:377:LEU:HD21	1.99	0.44
1:A:426:GLU:HG3	1:A:427:GLY:N	2.33	0.44
1:A:276:GLU:CD	1:A:276:GLU:H	2.20	0.44
1:A:69:GLU:HG2	1:A:86:TYR:HE1	1.82	0.44
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.70	0.44
1:A:89:HIS:ND1	1:A:90:PRO:HD2	2.32	0.44
1:A:1:MET:HE3	1:A:129:MET:SD	2.59	0.43
1:A:171:ILE:HG22	1:A:190:MET:HG3	1.99	0.43
1:A:704:LEU:O	1:A:728:ASP:HB2	2.19	0.43
1:A:679:HIS:CE1	1:A:680:VAL:HG23	2.54	0.43
1:A:305:LEU:HD13	1:A:305:LEU:HA	1.91	0.43
3:P:1:DG:H2''	3:P:2:DA:H5'	2.01	0.43
1:A:742:GLU:OE2	1:A:746:LYS:HB2	2.18	0.43
2:T:14:DG:H2''	2:T:15:DT:O5'	2.18	0.43
1:A:418:VAL:HG13	1:A:441:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:ALA:O	1:A:733:ILE:HG13	2.19	0.42
1:A:360:LYS:O	1:A:364:ARG:HD2	2.19	0.42
1:A:704:LEU:HD11	1:A:715:ILE:CD1	2.40	0.42
1:A:721:ASP:OD2	1:A:723:THR:HG22	2.20	0.42
1:A:153:GLY:HA3	1:A:221:LYS:HG2	2.02	0.42
1:A:671:ARG:HB2	1:A:671:ARG:HE	1.41	0.41
2:T:14:DG:H2'	2:T:15:DT:C7	2.50	0.41
1:A:650:LEU:HA	1:A:655:VAL:CG1	2.51	0.41
1:A:617:GLU:HB3	1:A:659:LYS:HA	2.03	0.41
1:A:129:MET:O	1:A:335:ARG:HD3	2.21	0.41
1:A:419:SER:HB2	1:A:450:PRO:CD	2.50	0.41
1:A:480:ASP:O	1:A:483:GLN:HG3	2.21	0.41
1:A:706:GLY:C	1:A:713:ARG:HD3	2.42	0.40
1:A:364:ARG:HG2	1:A:364:ARG:NH1	2.36	0.40
1:A:558:LYS:O	1:A:562:GLU:HG3	2.21	0.40
2:T:15:DT:H6	2:T:15:DT:C5'	2.32	0.40
1:A:610:ILE:HD12	1:A:624:ALA:HB2	2.02	0.40
1:A:589:VAL:HG21	1:A:608:LEU:HD21	2.02	0.40
1:A:414:ILE:HD11	1:A:453:LEU:CB	2.52	0.40
1:A:676:THR:O	1:A:676:THR:OG1	2.38	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	760/775 (98%)	740 (97%)	20 (3%)	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	657/666 (99%)	636 (97%)	21 (3%)	39 50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	21	LYS
1	A	44[A]	ASP
1	A	44[B]	ASP
1	A	61	THR
1	A	134	GLU
1	A	215	ASP
1	A	246	ASP
1	A	305	LEU
1	A	324	ARG
1	A	364	ARG
1	A	471	VAL
1	A	494	TYR
1	A	516	TRP
1	A	528	LEU
1	A	554	GLU
1	A	637	GLU
1	A	645	GLU
1	A	649	LYS
1	A	658	GLU
1	A	671	ARG

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z  > 2$
4	GOL	A	801	-	5,5,5	0.91	0	5,5,5	1.07	0
8	DTP	A	806	7,6	26,32,32	0.77	0	30,50,50	0.86	1 (3%)
5	PGE	A	802	-	9,9,9	0.31	0	8,8,8	0.39	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
4	GOL	A	801	-	-	4/4/4/4	-
8	DTP	A	806	7,6	-	4/18/34/34	0/3/3/3
5	PGE	A	802	-	-	4/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	806	DTP	C5-C6-N6	2.37	123.96	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

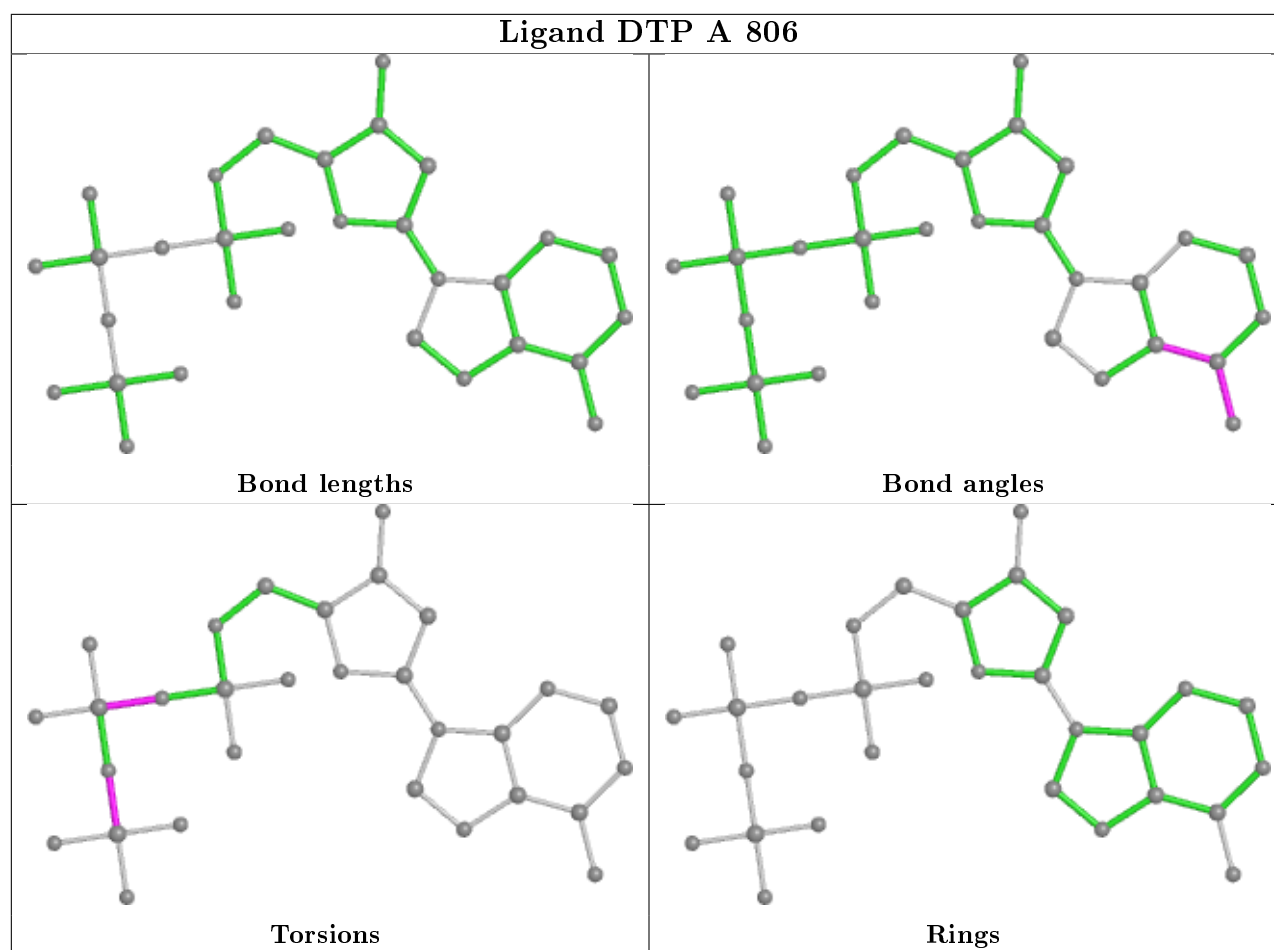
Mol	Chain	Res	Type	Atoms
4	A	801	GOL	O1-C1-C2-C3
8	A	806	DTP	PB-O3B-PG-O2G
5	A	802	PGE	C3-C4-O3-C5
5	A	802	PGE	O2-C3-C4-O3
4	A	801	GOL	C1-C2-C3-O3
4	A	801	GOL	O1-C1-C2-O2
4	A	801	GOL	O2-C2-C3-O3
8	A	806	DTP	PA-O3A-PB-O1B
8	A	806	DTP	PB-O3B-PG-O3G
5	A	802	PGE	C1-C2-O2-C3
5	A	802	PGE	O1-C1-C2-O2
8	A	806	DTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	802	PGE	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	758/775 (97%)	0.22	19 (2%) 57 55	37, 59, 89, 126	0
2	T	14/16 (87%)	0.19	0 100 100	42, 52, 72, 107	0
3	P	12/12 (100%)	-0.07	0 100 100	44, 54, 62, 66	0
All	All	784/803 (97%)	0.22	19 (2%) 59 56	37, 59, 89, 126	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	688	ALA	4.9
1	A	725	HIS	4.5
1	A	426	GLU	3.7
1	A	296	ALA	3.6
1	A	149	GLY	3.2
1	A	146	TYR	3.2
1	A	148	GLU	2.8
1	A	291	TYR	2.7
1	A	431	TYR	2.7
1	A	247	ARG	2.6
1	A	715	ILE	2.6
1	A	720	PHE	2.6
1	A	724	LYS	2.5
1	A	689	ARG	2.3
1	A	587[A]	PHE	2.3
1	A	295	ILE	2.3
1	A	686	LEU	2.1
1	A	722	PRO	2.0
1	A	723	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

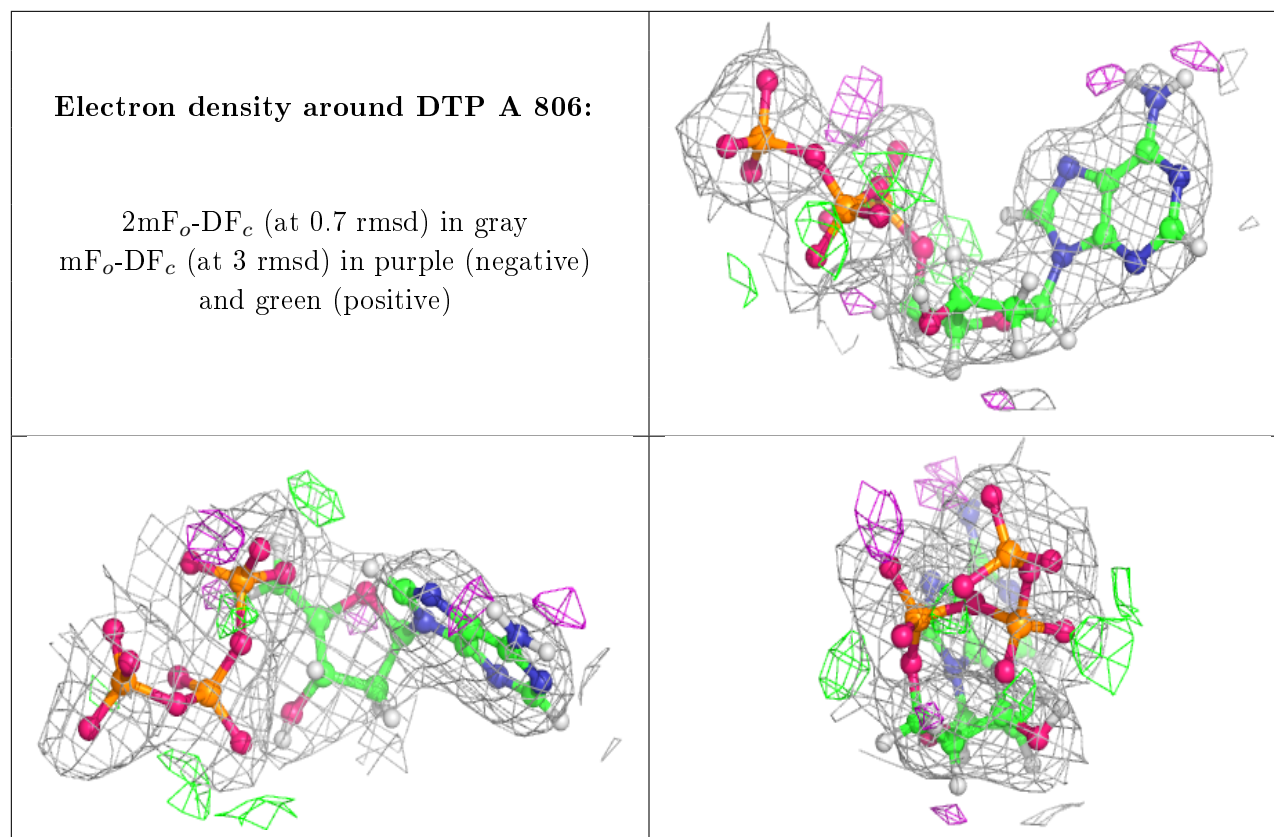
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PGE	A	802	10/10	0.89	0.13	65,74,83,83	0
4	GOL	A	801	6/6	0.90	0.15	57,62,65,70	0
6	MG	A	803	1/1	0.95	0.08	44,44,44,44	0
6	MG	A	804	1/1	0.97	0.06	43,43,43,43	0
8	DTP	A	806	30/30	0.98	0.14	30,42,49,58	0
7	MN	A	805[A]	1/1	0.99	0.13	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.