



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 7JKL / pdb_00007jkl
Title : Human PrimPol misinserting dATP opposite the 8-oxoguanine lesion (3'-end base of the primer strand is 2',3'-dideoxy-terminated).
Authors : Rechkoblit, O.; Aggarwal, A.K.
Deposited on : 2020-07-28
Resolution : 2.38 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

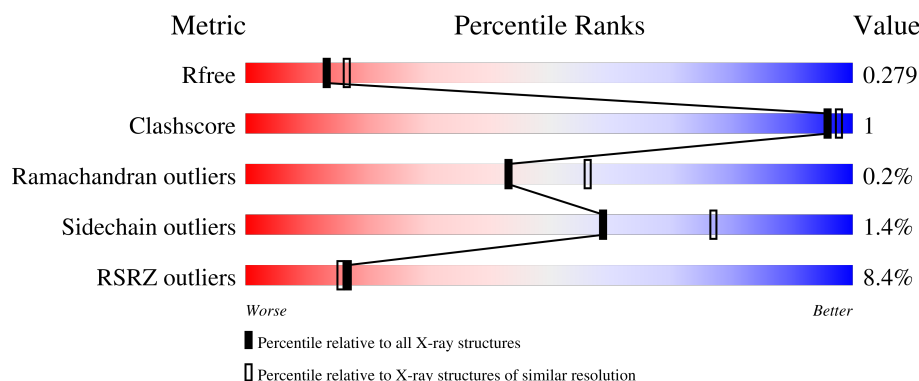
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	354	7% 73% 24%
1	B	354	6% 69% 29%
2	C	17	88% 6% 6%
2	G	17	71% 24% 6%
3	D	13	85% 15%

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Mol	Chain	Length	Quality of chain
3	H	13	77% 8% 15%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10125 atoms, of which 4643 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-directed primase/polymerase protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	H	N	O	S	0	0	0
			4160	1377	2028	356	389	10			
1	B	251	Total	C	H	N	O	S	0	0	0
			3995	1308	1968	341	369	9			

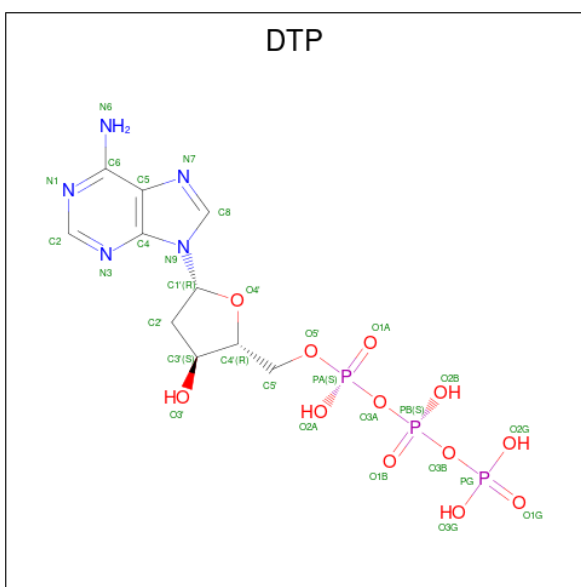
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*(8OG)P*CP*GP*CP*TP*AP*CP*CP*AP*CP*AP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	16	Total	C	H	N	O	P	0	0	0
			498	151	178	59	94	16			
2	G	16	Total	C	H	N	O	P	0	0	0
			476	151	156	59	94	16			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	13	Total	C	H	N	O	P	0	0	0
			420	129	148	54	77	12			
3	H	11	Total	C	H	N	O	P	0	0	0
			356	109	125	44	67	11			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 42	C 10	H 12	N 5	O 12	P 3	0	0
4	B	1	Total 42	C 10	H 12	N 5	O 12	P 3	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	2	Total Ca 2 2	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



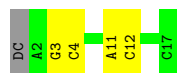
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total	O	0	0
			39	39		
7	C	3	Total	O	0	0
			3	3		
7	D	3	Total	O	0	0
			3	3		
7	B	54	Total	O	0	0
			54	54		
7	G	4	Total	O	0	0
			4	4		
7	H	2	Total	O	0	0
			2	2		

- Molecule 2: DNA (5'-D(P*AP*(8OG)P*CP*GP*CP*TP*AP*CP*CP*AP*CP*AP*CP*CP*CP*P*C)-3')

Chain G:  71% 24% 6%



- Molecule 3: DNA (5'-D(*GP*GP*GP*TP*GP*TP*GP*GP*TP*AP*GP*CP*(DDG))-3')

Chain D:  85% 15%



- Molecule 3: DNA (5'-D(*GP*GP*GP*TP*GP*TP*GP*GP*TP*AP*GP*CP*(DDG))-3')

Chain H:  77% 8% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.52Å 65.64Å 74.31Å 69.44° 83.43° 87.74°	Depositor
Resolution (Å)	69.17 – 2.38 69.17 – 2.38	Depositor EDS
% Data completeness (in resolution range)	91.1 (69.17-2.38) 91.1 (69.17-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.220 , 0.277 0.223 , 0.279	Depositor DCC
R_{free} test set	1618 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10125	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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: DTP, DDG, CA, 8OG, GOL

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	0.09	0/2181	0.25	0/2958
1	B	0.09	0/2074	0.25	0/2808
2	C	0.20	0/330	0.41	0/501
2	G	0.19	0/330	0.39	0/501
3	D	0.17	0/282	0.36	0/436
3	H	0.17	0/235	0.39	0/362
All	All	0.12	0/5432	0.29	0/7566

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 [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	2132	2028	2031	3	0
1	B	2027	1968	1971	4	0
2	C	320	178	178	0	0
2	G	320	156	178	4	0
3	D	272	148	148	1	0
3	H	231	125	125	0	0
4	A	30	12	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	12	9	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	6	8	8	1	0
6	B	6	8	8	0	0
7	A	39	0	0	0	0
7	B	54	0	0	3	0
7	C	3	0	0	0	0
7	D	3	0	0	1	0
7	G	4	0	0	0	0
7	H	2	0	0	0	0
All	All	5482	4643	4666	11	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 1.

All (11) 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)
3:D:11:DA:N7	7:D:101:HOH:O	2.25	0.69
2:G:11:DA:H2''	2:G:12:DC:OP1	1.95	0.66
1:A:270:ASN:OD1	1:A:274:GLU:N	2.28	0.64
1:B:330:SER:OG	7:B:501:HOH:O	2.17	0.57
1:B:92:SER:OG	7:B:502:HOH:O	2.19	0.53
1:B:47:ARG:NH1	2:G:4:DC:OP2	2.45	0.49
1:B:316:GLN:NE2	7:B:507:HOH:O	2.48	0.45
2:G:11:DA:H2'	2:G:12:DC:C6	2.53	0.44
2:G:11:DA:H2'	2:G:12:DC:H6	1.82	0.43
1:A:159:ASP:HB2	1:A:307:THR:HG22	2.01	0.42
1:A:323:GLU:OE2	6:A:403:GOL:O1	2.38	0.41

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	263/354 (74%)	243 (92%)	20 (8%)	0	100	100
1	B	247/354 (70%)	233 (94%)	13 (5%)	1 (0%)	30	40
All	All	510/708 (72%)	476 (93%)	33 (6%)	1 (0%)	43	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	96	LEU

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	224/320 (70%)	220 (98%)	4 (2%)	51	71
1	B	220/320 (69%)	218 (99%)	2 (1%)	70	84
All	All	444/640 (69%)	438 (99%)	6 (1%)	59	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	97	LEU
1	A	276	HIS
1	A	295	SER
1	B	62	VAL
1	B	69	CYS

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	48	GLN

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	8OG	C	3	2	22,25,26	4.55	17 (77%)	26,37,40	1.67	7 (26%)
2	8OG	G	3	2	22,25,26	4.55	17 (77%)	26,37,40	1.73	7 (26%)
3	DDG	H	14	3,2	20,23,24	3.88	13 (65%)	27,33,36	2.42	13 (48%)
3	DDG	D	14	3,2	20,23,24	3.89	13 (65%)	27,33,36	2.75	14 (51%)

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	8OG	C	3	2	-	0/7/21/22	0/3/3/3
2	8OG	G	3	2	-	0/7/21/22	0/3/3/3
3	DDG	H	14	3,2	-	2/7/18/19	0/3/3/3
3	DDG	D	14	3,2	-	0/7/18/19	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	14	DDG	C2'-C1'	-8.79	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	14	DDG	C2'-C1'	-8.63	1.33	1.52
2	C	3	8OG	C3'-C4'	-8.37	1.31	1.53
2	G	3	8OG	C3'-C4'	-8.27	1.31	1.53
2	C	3	8OG	O4'-C4'	8.20	1.63	1.45
2	G	3	8OG	O4'-C4'	8.13	1.63	1.45
2	G	3	8OG	C8-N7	7.30	1.51	1.38
2	C	3	8OG	C8-N7	7.20	1.51	1.38
3	H	14	DDG	C4-N3	6.61	1.49	1.34
3	D	14	DDG	C4-N3	6.59	1.49	1.34
3	H	14	DDG	O4'-C4'	6.36	1.56	1.44
3	D	14	DDG	O4'-C4'	6.35	1.56	1.44
2	C	3	8OG	C8-N9	6.25	1.51	1.40
2	G	3	8OG	C8-N9	6.13	1.51	1.40
2	C	3	8OG	C2-N3	6.07	1.47	1.33
2	G	3	8OG	C2-N3	6.06	1.47	1.33
2	C	3	8OG	C4-N3	5.74	1.47	1.34
2	G	3	8OG	C4-N3	5.71	1.47	1.34
3	H	14	DDG	C2-N3	5.50	1.46	1.33
3	D	14	DDG	C2-N3	5.48	1.46	1.33
2	G	3	8OG	O4'-C1'	-4.90	1.31	1.42
2	G	3	8OG	C2-N2	4.87	1.45	1.34
2	C	3	8OG	C2-N2	4.84	1.45	1.34
3	D	14	DDG	C2-N2	4.82	1.45	1.34
3	H	14	DDG	C2-N2	4.81	1.45	1.34
2	C	3	8OG	O4'-C1'	-4.79	1.31	1.42
3	H	14	DDG	C3'-C4'	-4.61	1.28	1.52
2	G	3	8OG	C5-C4	4.55	1.43	1.37
3	D	14	DDG	C3'-C4'	-4.50	1.29	1.52
2	C	3	8OG	C5-C4	4.48	1.43	1.37
2	G	3	8OG	C5-N7	4.22	1.44	1.37
2	C	3	8OG	C2-N1	4.17	1.47	1.37
2	G	3	8OG	C2-N1	4.15	1.47	1.37
2	C	3	8OG	C5-N7	4.07	1.44	1.37
3	H	14	DDG	O4'-C1'	4.04	1.51	1.42
3	D	14	DDG	O4'-C1'	3.81	1.50	1.42
2	C	3	8OG	C5-C6	3.48	1.52	1.41
2	G	3	8OG	C6-N1	3.47	1.45	1.38
2	G	3	8OG	C5-C6	3.45	1.52	1.41
2	C	3	8OG	C6-N1	3.45	1.45	1.38
2	G	3	8OG	C4-N9	2.96	1.44	1.39
2	C	3	8OG	O3'-C3'	2.93	1.49	1.43
2	G	3	8OG	O3'-C3'	2.91	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	14	DDG	C2-N1	2.89	1.44	1.37
2	C	3	8OG	C4-N9	2.88	1.44	1.39
3	D	14	DDG	C2-N1	2.87	1.44	1.37
3	D	14	DDG	C5-N7	-2.82	1.33	1.39
3	H	14	DDG	C5-N7	-2.81	1.33	1.39
3	D	14	DDG	C6-N1	2.60	1.43	1.38
3	H	14	DDG	C5-C6	2.56	1.54	1.44
3	D	14	DDG	C5-C6	2.56	1.54	1.44
3	H	14	DDG	C6-N1	2.51	1.43	1.38
3	D	14	DDG	C2'-C3'	2.51	1.60	1.54
2	G	3	8OG	O6-C6	-2.45	1.18	1.23
3	H	14	DDG	O6-C6	-2.41	1.19	1.23
2	C	3	8OG	O8-C8	-2.41	1.18	1.23
3	H	14	DDG	C2'-C3'	2.41	1.60	1.54
3	D	14	DDG	O6-C6	-2.40	1.19	1.23
2	C	3	8OG	O6-C6	-2.40	1.19	1.23
2	G	3	8OG	O8-C8	-2.35	1.18	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	14	DDG	C4'-O4'-C1'	-7.56	102.67	109.81
3	H	14	DDG	C4'-O4'-C1'	-5.42	104.69	109.81
3	H	14	DDG	C5-C4-N3	-5.10	120.27	128.39
3	D	14	DDG	C5-C4-N3	-5.08	120.30	128.39
2	G	3	8OG	C2-N3-C4	4.59	120.21	112.30
3	D	14	DDG	C2-N3-C4	4.58	120.19	112.30
2	C	3	8OG	C2-N3-C4	4.49	120.03	112.30
3	H	14	DDG	C2-N3-C4	4.48	120.01	112.30
3	D	14	DDG	O4'-C1'-C2'	-3.62	102.13	106.41
3	D	14	DDG	C1'-N9-C8	-3.26	120.59	127.91
3	H	14	DDG	C2-N1-C6	-3.09	119.51	125.11
3	D	14	DDG	C2-N1-C6	-3.07	119.54	125.11
2	C	3	8OG	O6-C6-C5	-3.02	119.98	127.26
2	G	3	8OG	C2-N1-C6	-3.01	119.66	125.11
3	H	14	DDG	C1'-N9-C8	-3.00	121.18	127.91
2	C	3	8OG	C2-N1-C6	-2.99	119.68	125.11
2	G	3	8OG	O6-C6-C5	-2.95	120.14	127.26
3	D	14	DDG	N9-C8-N7	-2.94	107.95	113.40
3	H	14	DDG	N9-C8-N7	-2.91	108.01	113.40
2	G	3	8OG	N9-C4-N3	2.86	129.71	126.13
3	H	14	DDG	N9-C4-N3	2.74	131.44	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	8OG	N9-C4-N3	2.74	129.56	126.13
3	D	14	DDG	N9-C4-N3	2.74	131.44	125.95
2	G	3	8OG	C5-C6-N1	2.74	119.65	112.13
2	C	3	8OG	C5-C6-N1	2.69	119.53	112.13
3	D	14	DDG	C5-C6-N1	2.64	119.97	113.25
3	H	14	DDG	C5-C6-N1	2.61	119.89	113.25
3	H	14	DDG	O4'-C1'-C2'	-2.46	103.50	106.41
3	D	14	DDG	O6-C6-C5	-2.43	120.12	126.53
3	H	14	DDG	O6-C6-C5	-2.40	120.20	126.53
3	D	14	DDG	O4'-C1'-N9	2.30	111.95	107.86
3	H	14	DDG	C8-N7-C5	2.24	108.25	104.26
3	D	14	DDG	C1'-N9-C4	2.22	131.50	125.50
2	C	3	8OG	C4-C5-N7	2.20	110.10	106.06
2	G	3	8OG	C4-C5-N7	2.20	110.09	106.06
3	D	14	DDG	C8-N7-C5	2.15	108.09	104.26
3	H	14	DDG	C2'-C1'-N9	2.09	116.36	112.40
2	G	3	8OG	C5-N7-C8	-2.06	106.63	109.47
3	H	14	DDG	C1'-N9-C4	2.06	131.05	125.50
3	D	14	DDG	C2'-C3'-C4'	2.06	106.56	102.75
2	C	3	8OG	C5-N7-C8	-2.01	106.70	109.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	14	DDG	O4'-C4'-C5'-O5'
3	H	14	DDG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	DTP	A	401	5	31,32,32	4.20	15 (48%)	46,50,50	1.89	12 (26%)
4	DTP	B	403	5	31,32,32	4.21	15 (48%)	46,50,50	1.92	12 (26%)
6	GOL	B	404	-	5,5,5	0.37	0	5,5,5	0.21	0
6	GOL	A	403	-	5,5,5	0.36	0	5,5,5	0.26	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	DTP	A	401	5	-	8/22/34/34	0/3/3/3
4	DTP	B	403	5	-	4/22/34/34	0/3/3/3
6	GOL	B	404	-	-	2/4/4/4	-
6	GOL	A	403	-	-	1/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	DTP	C2'-C3'	-11.92	1.22	1.52
4	A	401	DTP	C2'-C3'	-11.85	1.22	1.52
4	B	403	DTP	PA-O3A	8.55	1.68	1.59
4	A	401	DTP	PA-O3A	8.52	1.68	1.59
4	A	401	DTP	O4'-C4'	-8.24	1.26	1.45
4	B	403	DTP	O4'-C4'	-8.19	1.26	1.45
4	B	403	DTP	PB-O3A	7.59	1.67	1.59
4	A	401	DTP	PB-O3A	7.54	1.67	1.59
4	A	401	DTP	C1'-N9	-7.52	1.32	1.46
4	B	403	DTP	C1'-N9	-7.49	1.32	1.46
4	B	403	DTP	C6-N6	5.94	1.49	1.34
4	A	401	DTP	C6-N6	5.89	1.49	1.34
4	B	403	DTP	C3'-C4'	5.59	1.67	1.53
4	A	401	DTP	C3'-C4'	5.58	1.67	1.53
4	A	401	DTP	O4'-C1'	4.72	1.52	1.42
4	B	403	DTP	O4'-C1'	4.71	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	DTP	PB-O3B	3.21	1.63	1.59
4	B	403	DTP	C5-N7	-3.19	1.33	1.39
4	A	401	DTP	C5-N7	-3.10	1.33	1.39
4	B	403	DTP	PB-O3B	2.95	1.62	1.59
4	A	401	DTP	O3'-C3'	2.88	1.49	1.43
4	B	403	DTP	O3'-C3'	2.85	1.49	1.43
4	A	401	DTP	C4-N9	-2.44	1.32	1.37
4	B	403	DTP	PB-O2B	-2.41	1.44	1.55
4	B	403	DTP	C4-N9	-2.40	1.32	1.37
4	A	401	DTP	PB-O2B	-2.36	1.44	1.55
4	A	401	DTP	C5-C4	-2.30	1.35	1.39
4	B	403	DTP	C5-C4	-2.29	1.35	1.39
4	B	403	DTP	C2'-C1'	2.27	1.58	1.52
4	A	401	DTP	C2'-C1'	2.19	1.58	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	DTP	N3-C2-N1	-5.79	119.81	128.58
4	B	403	DTP	N3-C2-N1	-5.71	119.94	128.58
4	B	403	DTP	C5-C4-N3	-5.12	119.66	126.72
4	A	401	DTP	C5-C4-N3	-5.03	119.80	126.72
4	B	403	DTP	N9-C8-N7	-4.07	108.16	113.94
4	A	401	DTP	N9-C8-N7	-3.99	108.27	113.94
4	B	403	DTP	C2-N3-C4	3.45	120.25	111.83
4	A	401	DTP	C2-N3-C4	3.43	120.21	111.83
4	B	403	DTP	N6-C6-N1	-3.41	110.79	118.38
4	A	401	DTP	N6-C6-N1	-3.34	110.94	118.38
4	B	403	DTP	N3-C4-N9	3.13	132.50	127.17
4	A	401	DTP	N3-C4-N9	3.10	132.43	127.17
4	B	403	DTP	C5-N7-C8	2.93	108.06	103.45
4	A	401	DTP	C5-N7-C8	2.81	107.86	103.45
4	A	401	DTP	C5-C6-N6	2.39	129.19	123.29
4	B	403	DTP	C5-C6-N6	2.38	129.17	123.29
4	B	403	DTP	C2'-C1'-N9	-2.31	109.19	114.63
4	A	401	DTP	C2'-C1'-N9	-2.26	109.31	114.63
4	B	403	DTP	C4-C5-N7	-2.19	108.07	110.58
4	A	401	DTP	C4-C5-N7	-2.08	108.21	110.58
4	B	403	DTP	C6-C5-C4	2.07	120.01	117.18
4	A	401	DTP	C6-C5-C4	2.06	119.99	117.18
4	A	401	DTP	C4-N9-C8	2.04	107.89	105.74
4	B	403	DTP	C4-N9-C8	2.02	107.86	105.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

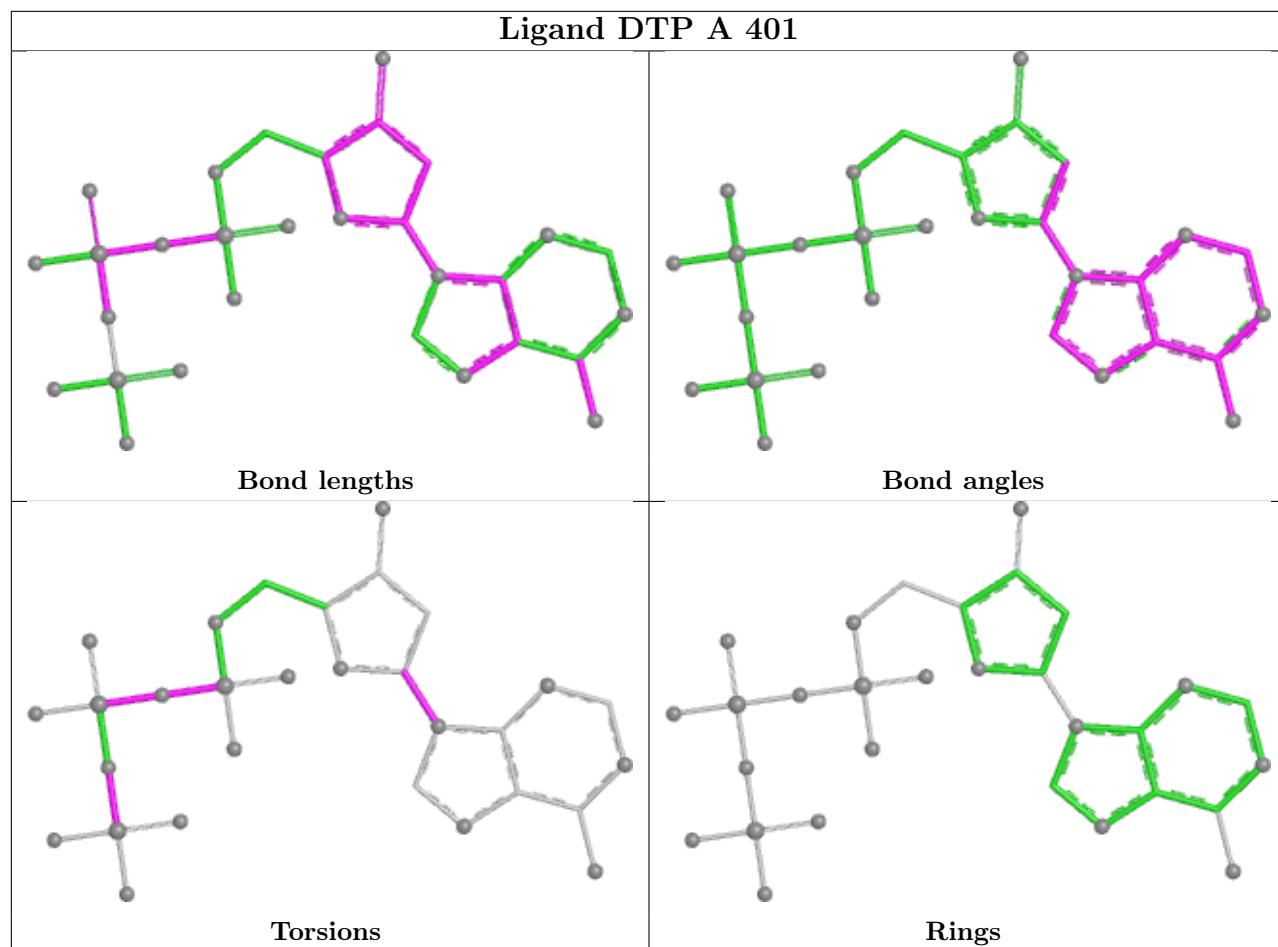
Mol	Chain	Res	Type	Atoms
4	A	401	DTP	PB-O3B-PG-O2G
6	B	404	GOL	O1-C1-C2-O2
6	B	404	GOL	O1-C1-C2-C3
4	A	401	DTP	PA-O3A-PB-O1B
4	B	403	DTP	PB-O3A-PA-O1A
6	A	403	GOL	O1-C1-C2-O2
4	B	403	DTP	PA-O3A-PB-O2B
4	A	401	DTP	PB-O3A-PA-O2A
4	A	401	DTP	PB-O3B-PG-O1G
4	A	401	DTP	PB-O3B-PG-O3G
4	B	403	DTP	PB-O3B-PG-O3G
4	A	401	DTP	PA-O3A-PB-O2B
4	A	401	DTP	PB-O3A-PA-O1A
4	B	403	DTP	PA-O3A-PB-O1B
4	A	401	DTP	O4'-C1'-N9-C4

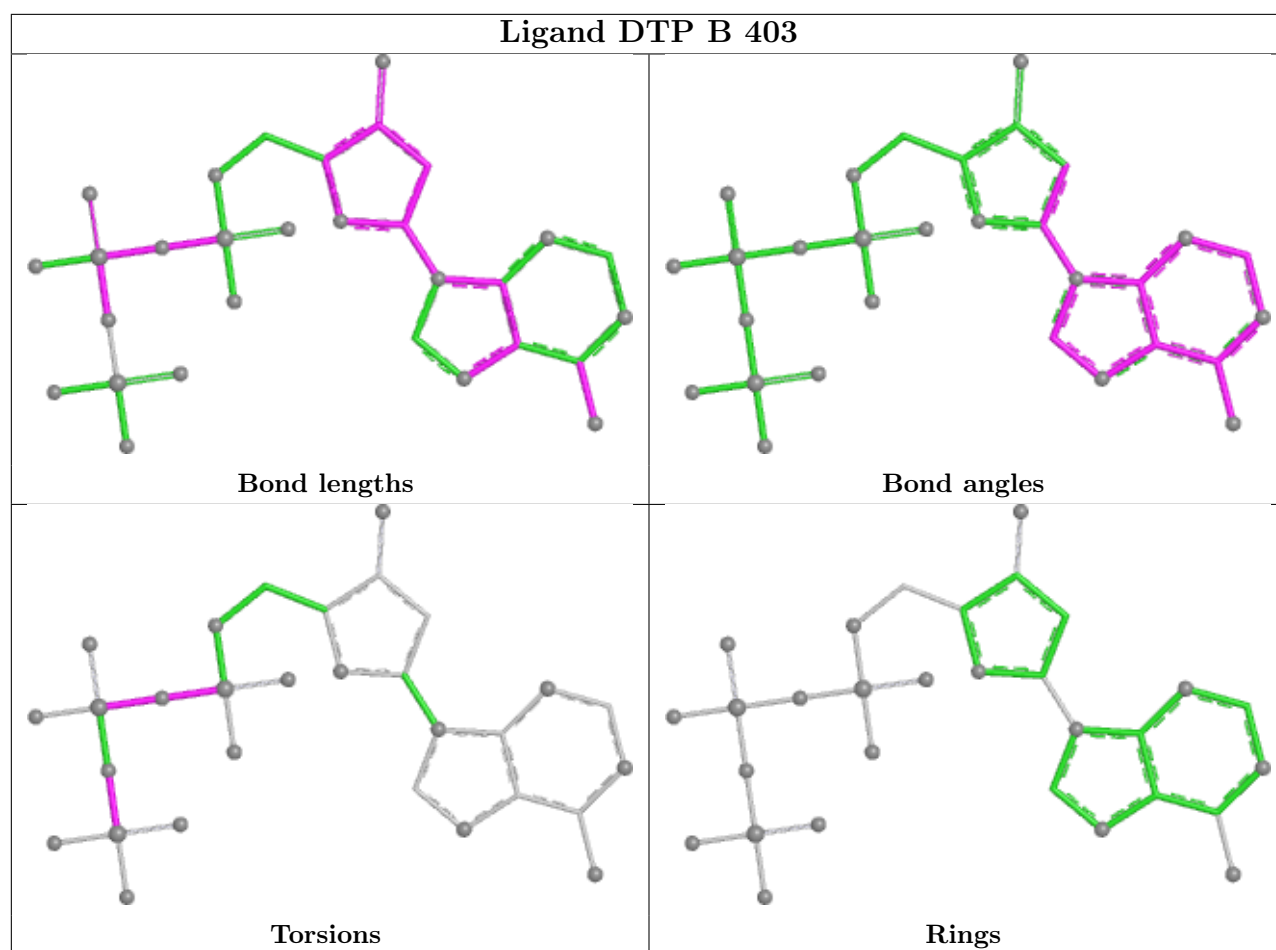
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	403	GOL	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, 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	269/354 (75%)	0.95	25 (9%)	14 13	47, 76, 114, 128	0
1	B	251/354 (70%)	0.75	23 (9%)	14 13	46, 65, 101, 126	0
2	C	15/17 (88%)	0.44	0	100 100	69, 113, 192, 193	0
2	G	15/17 (88%)	0.61	0	100 100	72, 124, 184, 192	0
3	D	12/13 (92%)	0.50	0	100 100	90, 129, 191, 195	0
3	H	10/13 (76%)	0.53	0	100 100	112, 123, 172, 176	0
All	All	572/768 (74%)	0.82	48 (8%)	17 15	46, 73, 126, 195	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	CYS	6.1
1	B	39	PRO	4.4
1	B	38	PRO	4.2
1	A	200	LEU	3.7
1	A	337	PHE	3.7
1	B	96	LEU	3.6
1	B	262	ASP	3.4
1	B	278	PHE	3.3
1	A	16	ALA	3.2
1	A	117	PHE	3.1
1	A	277	LEU	3.0
1	A	15	ARG	2.9
1	B	95	ASN	2.9
1	B	70	LYS	2.9
1	B	273	GLY	2.8
1	B	37	GLU	2.8
1	B	277	LEU	2.8
1	B	337	PHE	2.7
1	A	71	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	2.7
1	A	166	PHE	2.7
1	A	265	PHE	2.6
1	A	97	LEU	2.6
1	A	298	ILE	2.6
1	A	267	VAL	2.5
1	A	271	ASN	2.5
1	A	70	LYS	2.5
1	A	261	PRO	2.5
1	A	5	TRP	2.4
1	B	299	GLY	2.4
1	A	72	GLY	2.3
1	A	307	THR	2.3
1	B	50	GLN	2.3
1	A	283	VAL	2.3
1	B	133	LEU	2.2
1	A	278	PHE	2.2
1	A	127	GLY	2.2
1	B	72	GLY	2.2
1	A	199	LEU	2.2
1	B	79	LEU	2.2
1	A	131	VAL	2.2
1	B	40	SER	2.2
1	A	69	CYS	2.1
1	B	69	CYS	2.1
1	B	125	ALA	2.1
1	A	11	GLN	2.1
1	B	165	LYS	2.1
1	B	41	ILE	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	DDG	H	14	21/22	0.74	0.15	62,85,127,127	0
3	DDG	D	14	21/22	0.88	0.10	54,74,100,112	0
2	8OG	C	3	23/24	0.89	0.10	60,82,106,106	0
2	8OG	G	3	23/24	0.92	0.10	61,81,108,111	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

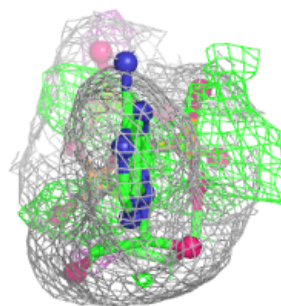
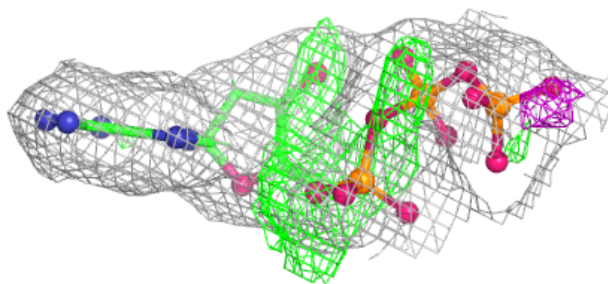
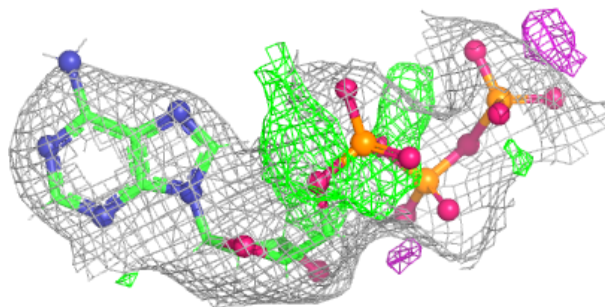
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	403	6/6	0.89	0.12	71,86,91,92	0
5	CA	B	402	1/1	0.90	0.08	65,65,65,65	1
6	GOL	B	404	6/6	0.90	0.19	49,59,68,68	14
5	CA	A	402	1/1	0.94	0.10	71,71,71,71	0
4	DTP	B	403	30/30	0.94	0.11	40,59,70,85	0
4	DTP	A	401	30/30	0.95	0.09	45,59,72,79	0
5	CA	B	401	1/1	0.98	0.04	53,53,53,53	0

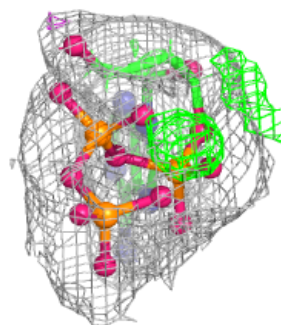
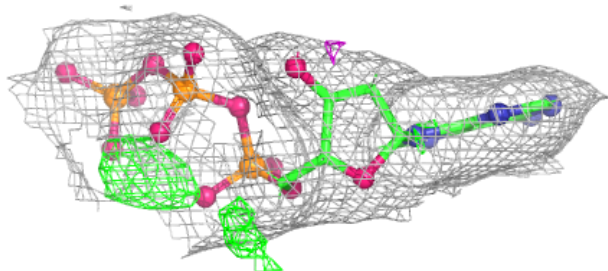
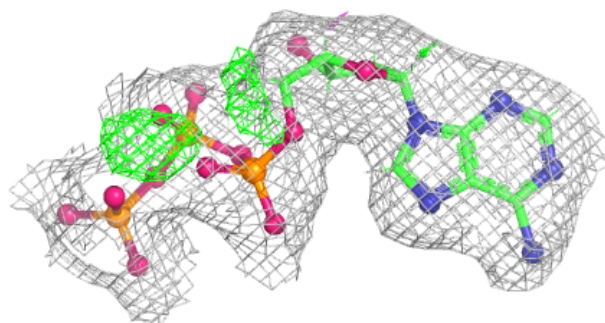
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP B 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DTP A 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.