



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 08:12 AM EDT

PDB ID : 7JL8
Title : Human PrimPol extending from the correct primer base C opposite the 8-oxoguanine lesion
Authors : Rechkoblit, O.; Aggarwal, A.K.
Deposited on : 2020-07-29
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

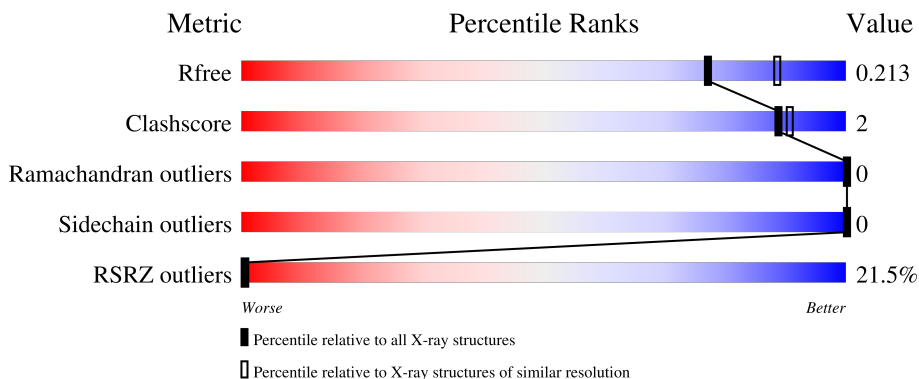
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	
1	B	354	
2	C	17	
2	G	17	
3	D	13	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	13	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '38%', a green segment in the middle labeled '69%', and a grey segment on the right labeled '31%'. The segments are stacked horizontally, with the red segment starting from the left, followed by the green segment, and the grey segment ending at the right. The total length of the bar represents 100%.</p>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9581 atoms, of which 4410 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	
			Total	C	H	N	O				S
1	A	270	4044	1354	1950	351	379	10	0	2	0
1	B	250	3913	1289	1922	330	362	10	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				P
2	C	12	376	115	134	44	71	12	0	0	0
2	G	10	286	86	101	31	58	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				P
3	D	9	292	89	102	37	55	9	0	0	0
3	H	9	292	89	102	37	55	9	0	0	0

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

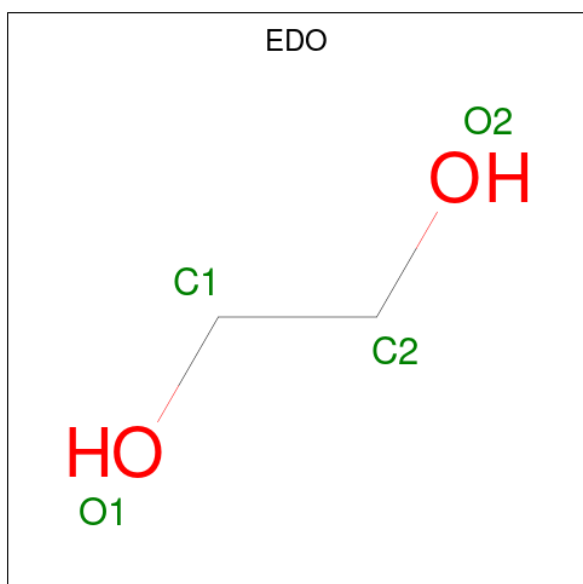
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0
5	B	2	2	2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



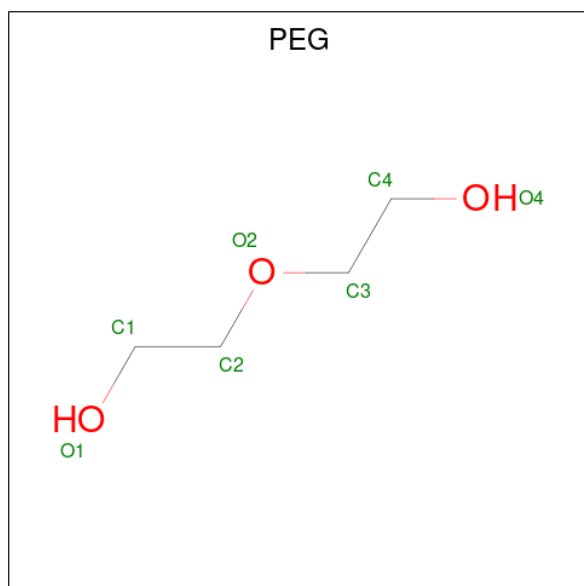
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			13	3	7	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	10	2	6	2	0	0

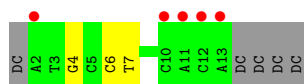
- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



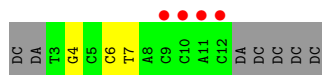
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	A	1	17	4	10	3	0	0
8	A	1	17	4	10	3	0	0
8	B	1	17	4	10	3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	55	55	55	0	0
9	C	2	2	2	0	0
9	B	98	98	98	0	0
9	G	5	5	5	0	0
9	H	1	1	1	0	0



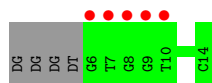
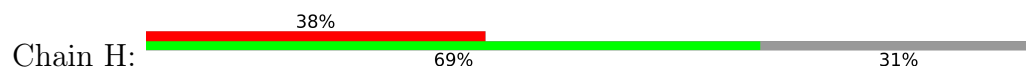
- Molecule 2: DNA (5'-D(P*AP*TP*(8OG)P*CP*CP*TP*AP*CP*CP*AP*CP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.69Å 65.33Å 72.00Å 68.47° 85.67° 86.92°	Depositor
Resolution (Å)	28.16 – 2.10 28.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (28.16-2.10) 97.2 (28.16-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.187 , 0.213 0.187 , 0.213	Depositor DCC
R_{free} test set	2308 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9581	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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: DTP, EDO, CA, GOL, PEG, 8OG

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	0.40	0/2143	0.55	0/2916
1	B	0.46	0/2038	0.61	1/2762 (0.0%)
2	C	0.81	0/243	0.97	0/368
2	G	0.80	0/178	1.03	0/269
3	D	0.88	0/213	0.95	0/328
3	H	0.76	0/213	0.93	0/328
All	All	0.52	0/5028	0.67	1/6971 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ARG	NE-CZ-NH2	-5.67	117.47	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	HIS	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	289	ASN	Sidechain

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	2094	1950	1947	8	0
1	B	1991	1922	1905	6	0
2	C	242	134	135	1	0
2	G	185	101	101	1	0
3	D	190	102	102	1	0
3	H	190	102	102	0	0
4	A	30	12	12	0	0
4	B	30	12	12	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	12	15	16	0	0
6	B	18	24	24	0	0
7	A	4	6	6	0	0
8	A	14	20	20	0	0
8	B	7	10	10	0	0
9	A	55	0	0	0	0
9	B	98	0	0	0	0
9	C	2	0	0	0	0
9	G	5	0	0	0	0
9	H	1	0	0	0	0
All	All	5171	4410	4392	17	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 2.

All (17) 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:315:ILE:O	1:B:325:GLN:NE2	2.31	0.64
1:B:340:THR:O	1:B:340:THR:HG23	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:O	1:A:325:GLN:NE2	2.37	0.58
1:A:70:LYS:HA	1:A:298:ILE:HD11	1.88	0.54
1:B:66:ALA:HB1	1:B:76:ARG:HG2	1.91	0.52
1:A:51:ALA:O	1:A:55:VAL:HG23	2.09	0.52
1:A:108:VAL:HG12	1:A:335:VAL:HG21	1.96	0.47
1:B:74:GLY:O	1:B:76:ARG:HD2	2.15	0.46
2:C:6:DC:H2''	2:C:7:DT:H71	1.97	0.46
2:G:6:DC:H2'	2:G:7:DT:H71	1.98	0.44
1:A:69:CYS:O	1:A:298:ILE:HD13	2.18	0.44
1:B:83:TYR:CE1	1:B:331:LEU:HD13	2.53	0.43
1:A:83:TYR:CE1	1:A:331:LEU:HD13	2.54	0.42
1:A:275:LYS:O	1:A:276:HIS:ND1	2.53	0.41
1:A:102:VAL:O	1:A:104:PRO:HD3	2.20	0.41
3:D:7:DT:H2''	3:D:8:DG:C8	2.56	0.41
1:B:100:TYR:HB3	1:B:289:ASN:HB3	2.03	0.41

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	266/354 (75%)	258 (97%)	8 (3%)	0	100	100
1	B	247/354 (70%)	237 (96%)	10 (4%)	0	100	100
All	All	513/708 (72%)	495 (96%)	18 (4%)	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	210/320 (66%)	210 (100%)	0	100	100
1	B	210/320 (66%)	210 (100%)	0	100	100
All	All	420/640 (66%)	420 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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	G	4	3,2	22,25,26	4.16	16 (72%)	30,37,40	2.09	9 (30%)
2	8OG	C	4	3,2	22,25,26	4.25	17 (77%)	30,37,40	2.10	9 (30%)

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	G	4	3,2	-	0/7/21/22	0/3/3/3
2	8OG	C	4	3,2	-	1/7/21/22	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	8OG	C8-N7	7.61	1.52	1.38
2	C	4	8OG	C3'-C4'	-7.47	1.32	1.53
2	G	4	8OG	C8-N7	7.25	1.52	1.38
2	G	4	8OG	C3'-C4'	-7.04	1.33	1.53
2	G	4	8OG	O4'-C4'	6.82	1.60	1.45
2	C	4	8OG	O4'-C4'	6.20	1.58	1.45
2	C	4	8OG	C4-N3	5.97	1.48	1.34
2	G	4	8OG	C4-N3	5.80	1.48	1.34
2	C	4	8OG	C8-N9	5.77	1.50	1.40
2	C	4	8OG	C5-N7	5.22	1.46	1.37
2	G	4	8OG	C8-N9	5.06	1.49	1.40
2	G	4	8OG	C5-N7	5.02	1.45	1.37
2	C	4	8OG	O4'-C1'	-4.79	1.31	1.42
2	C	4	8OG	C2-N1	4.62	1.49	1.37
2	G	4	8OG	O4'-C1'	-4.59	1.32	1.42
2	G	4	8OG	C2-N1	4.50	1.48	1.37
2	C	4	8OG	C2-N3	4.28	1.43	1.33
2	G	4	8OG	O3'-C3'	4.24	1.52	1.43
2	G	4	8OG	C2-N2	4.13	1.44	1.34
2	C	4	8OG	C2-N2	3.99	1.43	1.34
2	G	4	8OG	C2-N3	3.87	1.42	1.33
2	C	4	8OG	C4-N9	3.69	1.45	1.39
2	G	4	8OG	C5-C6	3.63	1.51	1.42
2	C	4	8OG	C5-C6	3.62	1.51	1.42
2	C	4	8OG	C5-C4	3.48	1.42	1.37
2	G	4	8OG	C4-N9	3.27	1.45	1.39
2	C	4	8OG	O3'-C3'	3.06	1.49	1.43
2	G	4	8OG	C5-C4	2.98	1.41	1.37
2	C	4	8OG	O6-C6	-2.86	1.18	1.23
2	G	4	8OG	C6-N1	2.85	1.44	1.38
2	G	4	8OG	O6-C6	-2.69	1.18	1.23
2	C	4	8OG	C6-N1	2.68	1.43	1.38
2	C	4	8OG	O5'-C5'	-2.16	1.39	1.44

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	8OG	C5-C4-N3	-6.61	120.97	127.80
2	G	4	8OG	C5-C4-N3	-6.37	121.22	127.80
2	G	4	8OG	O4'-C1'-N9	-4.24	104.02	108.29
2	C	4	8OG	C2-N3-C4	4.01	119.44	112.30
2	G	4	8OG	C2-N3-C4	3.75	118.98	112.30
2	C	4	8OG	C2'-C1'-N9	-3.61	111.75	116.01
2	G	4	8OG	C2-N1-C6	-3.07	119.50	125.10
2	C	4	8OG	C2-N1-C6	-2.94	119.74	125.10
2	G	4	8OG	O6-C6-C5	-2.68	121.10	127.24
2	C	4	8OG	C2'-C3'-C4'	2.66	108.30	102.76
2	C	4	8OG	O6-C6-C5	-2.56	121.36	127.24
2	C	4	8OG	N9-C4-N3	2.49	128.66	125.81
2	C	4	8OG	C5-C6-N1	2.38	119.40	112.31
2	G	4	8OG	N9-C4-N3	2.29	128.43	125.81
2	G	4	8OG	O4'-C1'-C2'	-2.29	101.92	106.25
2	G	4	8OG	C5-C6-N1	2.18	118.80	112.31
2	C	4	8OG	C4'-O4'-C1'	-2.04	104.51	109.45
2	G	4	8OG	C4'-O4'-C1'	-2.04	104.53	109.45

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	8OG	O4'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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$
6	GOL	B	405	-	5,5,5	1.05	0	5,5,5	1.01	0
8	PEG	B	407	-	6,6,6	0.45	0	5,5,5	0.16	0
4	DTP	A	401	5	26,32,32	0.81	1 (3%)	30,50,50	1.47	5 (16%)
7	EDO	A	404	-	3,3,3	0.51	0	2,2,2	0.43	0
8	PEG	A	407	-	6,6,6	0.56	0	5,5,5	0.36	0
6	GOL	A	406	-	5,5,5	0.91	0	5,5,5	1.18	0
4	DTP	B	401	5	26,32,32	0.91	1 (3%)	30,50,50	1.42	4 (13%)
6	GOL	B	406	-	5,5,5	0.87	0	5,5,5	1.00	0
8	PEG	A	405	-	6,6,6	0.50	0	5,5,5	0.30	0
6	GOL	A	403	-	5,5,5	0.94	0	5,5,5	1.15	0
6	GOL	B	404	-	5,5,5	0.80	0	5,5,5	0.90	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
6	GOL	B	405	-	-	2/4/4/4	-
8	PEG	B	407	-	-	1/4/4/4	-
4	DTP	A	401	5	-	6/18/34/34	0/3/3/3
7	EDO	A	404	-	-	0/1/1/1	-
8	PEG	A	407	-	-	1/4/4/4	-
6	GOL	A	406	-	-	0/4/4/4	-
4	DTP	B	401	5	-	6/18/34/34	0/3/3/3
6	GOL	B	406	-	-	2/4/4/4	-
8	PEG	A	405	-	-	1/4/4/4	-
6	GOL	A	403	-	-	2/4/4/4	-
6	GOL	B	404	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	DTP	C5-C4	2.40	1.47	1.40
4	A	401	DTP	C5-C4	2.02	1.46	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	DTP	N3-C2-N1	-3.99	122.44	128.68
4	B	401	DTP	N3-C2-N1	-3.49	123.22	128.68
4	A	401	DTP	C2'-C1'-N9	-3.42	106.39	114.27
4	B	401	DTP	C2'-C1'-N9	-3.12	107.07	114.27
4	B	401	DTP	C4-C5-N7	-2.41	106.88	109.40
4	B	401	DTP	PB-O3B-PG	-2.30	124.94	132.83
4	A	401	DTP	O2B-PB-O1B	2.23	123.25	112.24
4	A	401	DTP	N6-C6-N1	2.16	123.07	118.57
4	A	401	DTP	O2G-PG-O3B	2.07	111.56	104.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

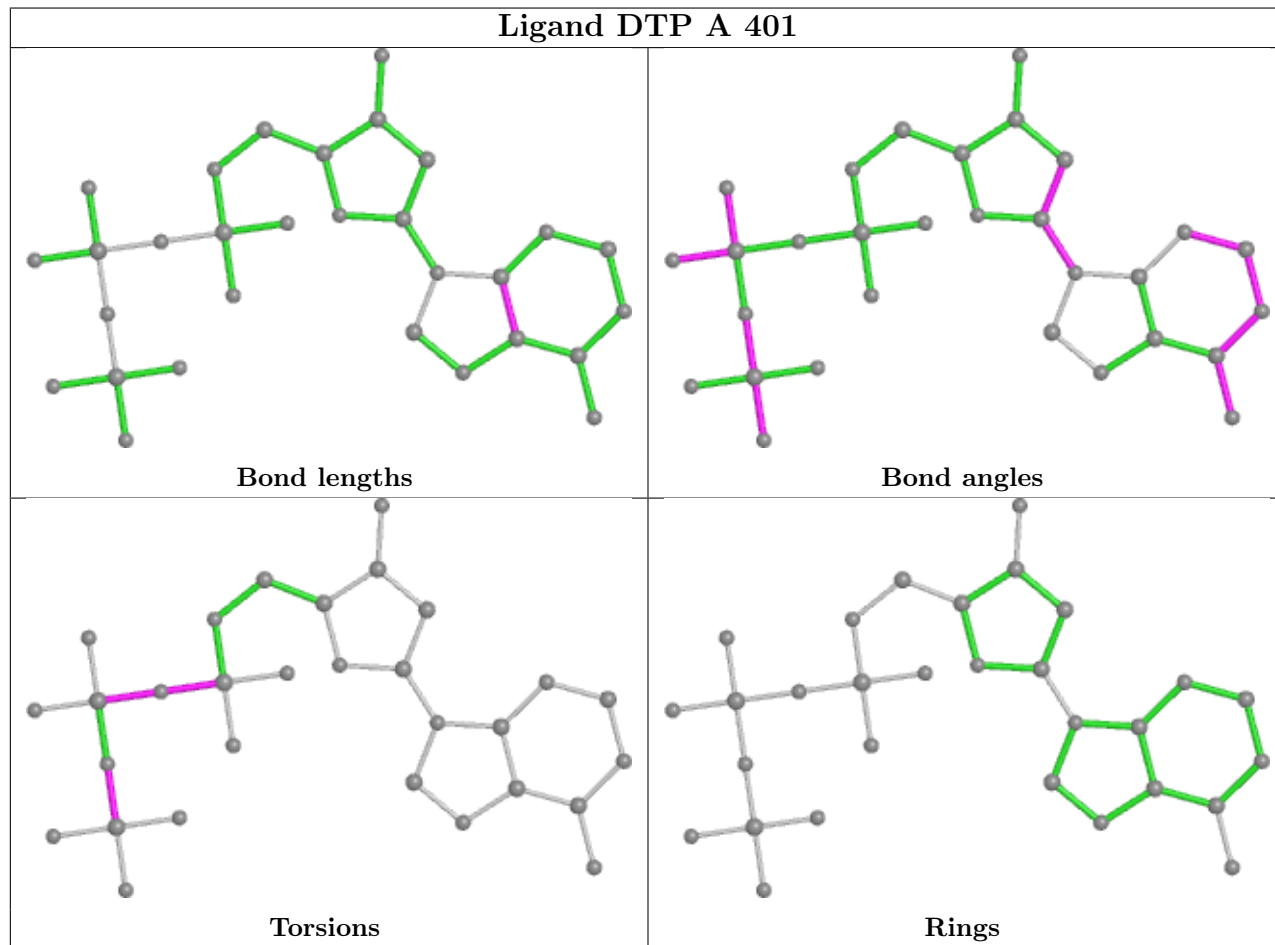
Mol	Chain	Res	Type	Atoms
4	A	401	DTP	PB-O3B-PG-O2G
4	B	401	DTP	PB-O3B-PG-O2G
6	A	403	GOL	C1-C2-C3-O3
6	B	406	GOL	C1-C2-C3-O3
6	B	406	GOL	O2-C2-C3-O3
6	B	404	GOL	C1-C2-C3-O3
8	A	407	PEG	O1-C1-C2-O2
6	A	403	GOL	O2-C2-C3-O3
8	B	407	PEG	O2-C3-C4-O4
4	A	401	DTP	PA-O3A-PB-O1B
6	B	404	GOL	O2-C2-C3-O3
6	B	405	GOL	O2-C2-C3-O3
4	A	401	DTP	PB-O3A-PA-O1A
4	B	401	DTP	PA-O3A-PB-O1B
4	A	401	DTP	PA-O3A-PB-O2B
4	A	401	DTP	PB-O3A-PA-O2A
6	B	405	GOL	C1-C2-C3-O3
4	B	401	DTP	PB-O3B-PG-O1G
8	A	405	PEG	O2-C3-C4-O4
4	A	401	DTP	PB-O3B-PG-O3G
4	B	401	DTP	PB-O3B-PG-O3G
4	B	401	DTP	PA-O3A-PB-O2B
4	B	401	DTP	PB-O3A-PA-O2A

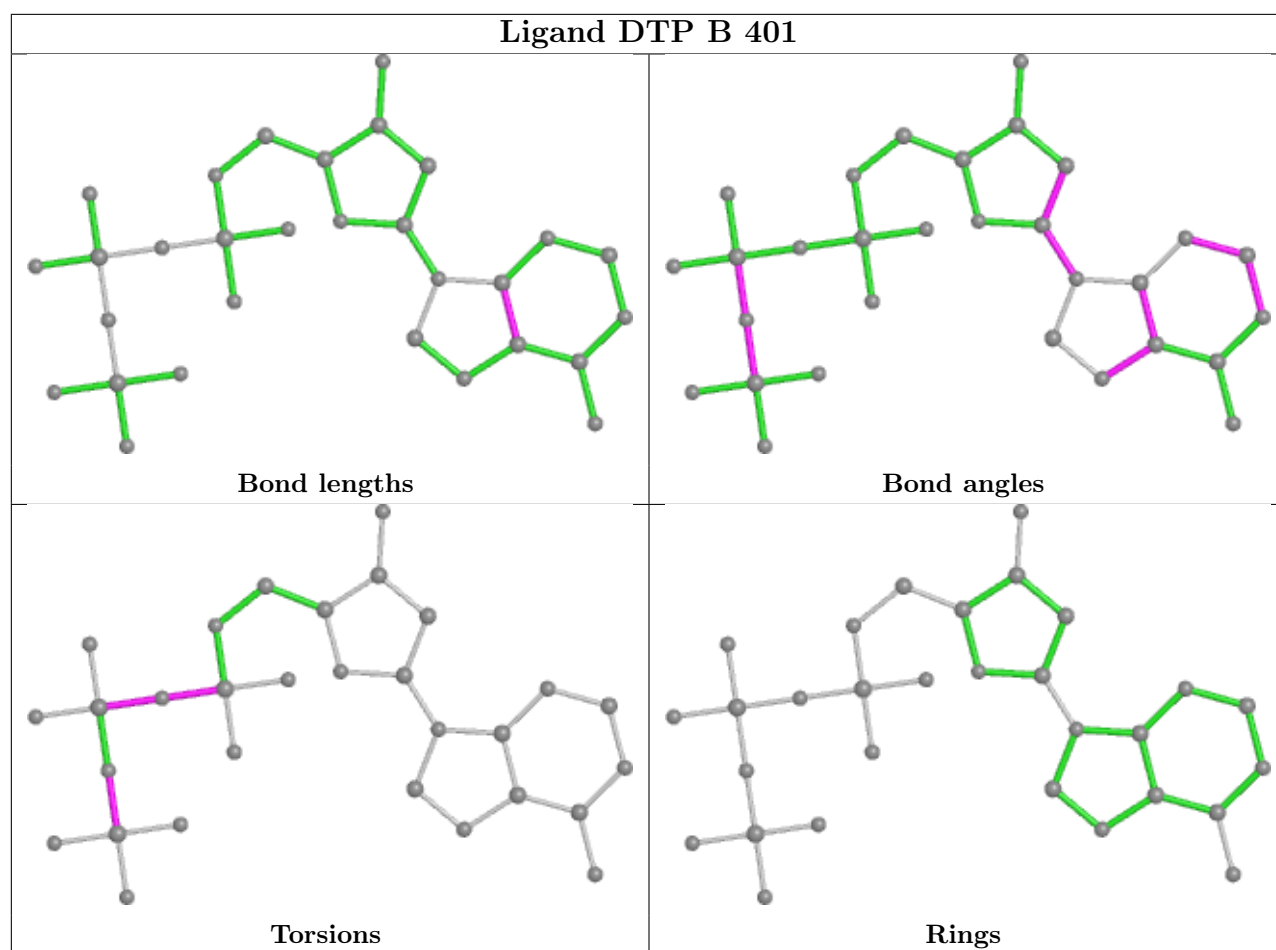
There are no ring outliers.

No monomer is involved in short contacts.

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	270/354 (76%)	1.09	57 (21%) 1 0	34, 54, 118, 138	0
1	B	250/354 (70%)	0.93	43 (17%) 1 1	29, 42, 70, 100	0
2	C	11/17 (64%)	2.81	5 (45%) 0 0	63, 110, 151, 153	0
2	G	9/17 (52%)	2.14	4 (44%) 0 0	49, 82, 157, 174	0
3	D	9/13 (69%)	2.99	6 (66%) 0 0	73, 124, 170, 171	0
3	H	9/13 (69%)	3.03	5 (55%) 0 0	65, 109, 171, 178	0
All	All	558/768 (72%)	1.13	120 (21%) 0 0	29, 48, 122, 178	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	SER	8.3
3	H	6	DG	8.1
3	D	6	DG	7.0
1	A	16	ALA	6.8
1	B	112	TYR	6.2
1	A	72	GLY	6.0
2	C	2	DA	6.0
3	H	7	DT	6.0
2	C	12	DC	5.8
1	A	3	ARG	5.7
2	C	11	DA	5.6
2	C	13	DA	5.4
1	B	70	LYS	5.2
2	G	12	DC	5.1
1	B	113	PHE	5.1
3	D	7	DT	5.0
1	B	290	PHE	4.8
1	B	111	LEU	4.7
1	B	72	GLY	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	112	TYR	4.6
2	G	11	DA	4.6
1	A	73	ASP	4.5
1	A	290	PHE	4.5
1	B	172	PHE	4.5
1	A	2	ASN	4.4
3	H	8	DG	4.4
1	A	71	VAL	4.4
1	A	113	PHE	4.4
1	B	170	LEU	4.3
1	A	272	MET	4.3
1	B	39	PRO	4.2
1	B	331	LEU	4.2
1	A	261	PRO	4.1
1	B	279	VAL	4.1
1	A	331	LEU	3.9
1	B	348	PRO	3.9
3	D	8	DG	3.9
3	D	12	DG	3.9
2	C	10	DC	3.9
1	B	71	VAL	3.9
1	A	103	ILE	3.8
1	A	111	LEU	3.8
2	G	9	DC	3.7
1	A	198	ASP	3.6
1	B	38	PRO	3.6
1	A	292	LEU	3.6
1	A	99	CYS	3.5
1	B	171	ILE	3.5
1	A	271	ASN	3.5
1	A	70	LYS	3.5
1	A	262	ASP	3.4
1	A	170	LEU	3.4
1	B	94	LYS	3.4
1	A	15	ARG	3.4
1	B	115	LEU	3.3
1	A	283	VAL	3.3
1	A	284	TYR	3.2
1	A	338	SER	3.2
1	A	163	ASP	3.2
2	G	10	DC	3.2
1	B	97	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	171	ILE	3.1
1	B	169	HIS	3.0
1	A	348	PRO	3.0
1	A	172	PHE	2.9
1	B	95	ASN	2.9
1	B	103	ILE	2.9
1	B	278	PHE	2.9
3	D	9	DG	2.9
1	A	332	VAL	2.8
1	A	6	GLU	2.8
1	B	262	ASP	2.8
1	A	120	PRO	2.7
1	A	102	VAL	2.7
1	B	134	LEU	2.7
1	B	200	LEU	2.7
1	A	65	PHE	2.7
1	A	337	PHE	2.7
1	A	66	ALA	2.7
1	A	100	TYR	2.6
1	B	66	ALA	2.6
1	A	36	GLU	2.6
3	D	11	DA	2.5
1	B	332	VAL	2.5
3	H	9	DG	2.4
1	B	138	VAL	2.4
1	B	175	HIS	2.4
1	B	330	SER	2.4
1	B	327	PHE	2.4
3	H	10	DT	2.4
1	A	5	TRP	2.4
1	B	292	LEU	2.4
1	B	299	GLY	2.4
1	A	199	LEU	2.4
1	A	327	PHE	2.3
1	B	316	GLN	2.3
1	A	274	GLU	2.3
1	A	46	HIS	2.3
1	A	330	SER	2.3
1	A	169	HIS	2.3
1	A	1	MET	2.2
1	B	189	LEU	2.2
1	A	339	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	200	LEU	2.2
1	B	101	GLU	2.2
1	A	194	GLN	2.2
1	A	158	LEU	2.1
1	A	189	LEU	2.1
1	B	284	TYR	2.1
1	B	283	VAL	2.1
1	A	156	LEU	2.1
1	B	96	LEU	2.1
1	B	102	VAL	2.1
1	A	101	GLU	2.1
1	B	93	ARG	2.1
1	A	47	ARG	2.1
1	A	162	THR	2.1
1	B	109	CYS	2.1
1	A	293	TYR	2.0
1	B	99	CYS	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
2	8OG	C	4	23/24	0.94	0.14	55,69,82,83	0
2	8OG	G	4	23/24	0.95	0.14	41,46,55,56	0

6.3 Carbohydrates [i](#)

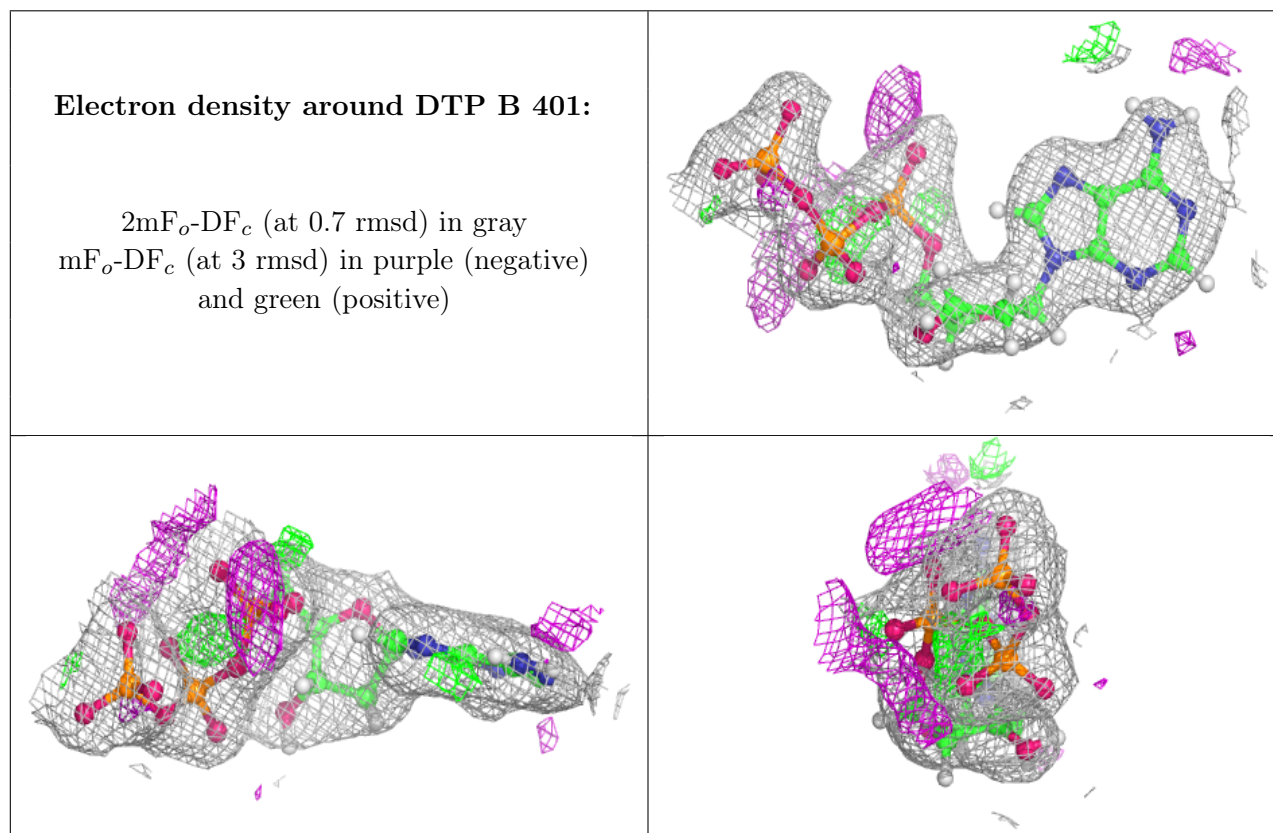
There are no monosaccharides in this entry.

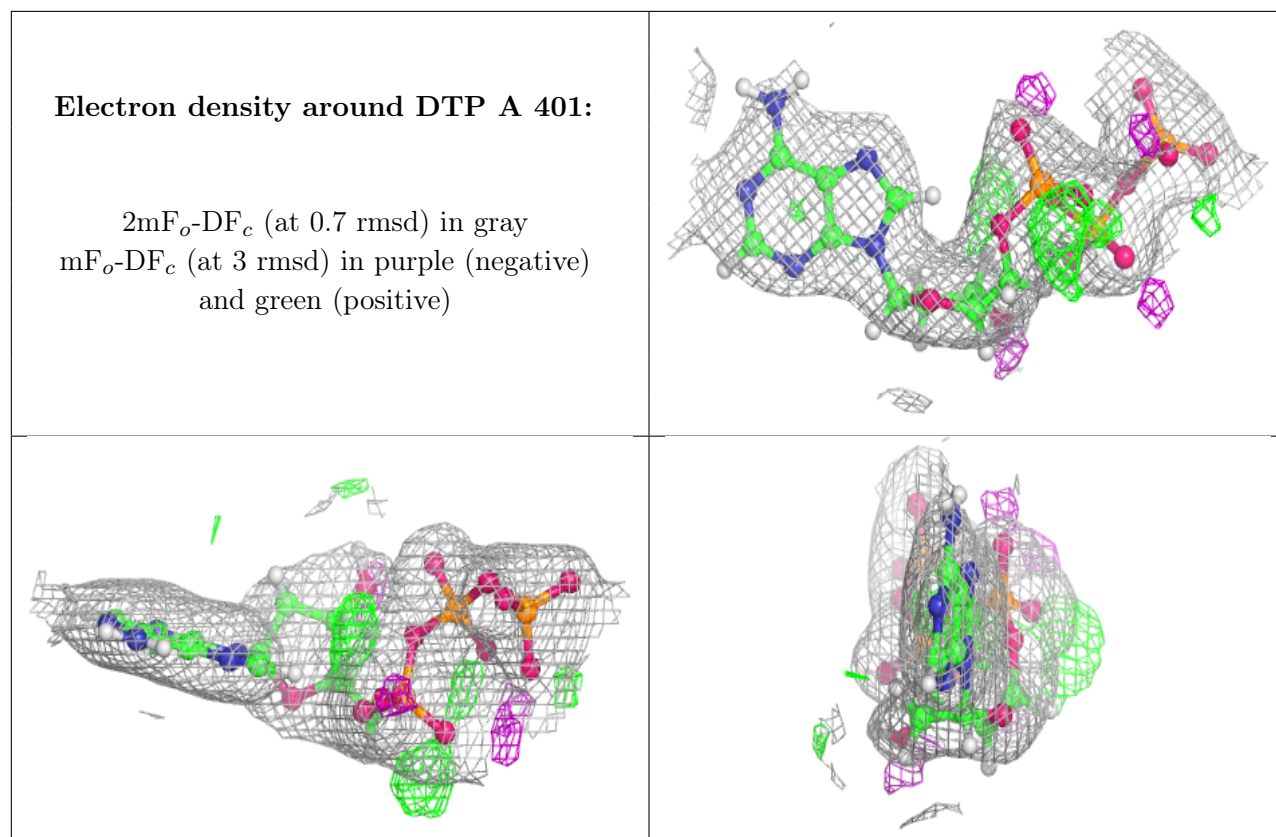
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
5	CA	B	403	1/1	0.76	0.36	75,75,75,75	0
6	GOL	B	404	6/6	0.77	0.18	74,91,109,109	0
8	PEG	A	407	7/7	0.80	0.20	50,64,74,74	0
8	PEG	A	405	7/7	0.81	0.34	66,87,96,112	0
6	GOL	B	406	6/6	0.81	0.38	69,88,103,106	0
6	GOL	A	403	6/6	0.82	0.21	73,88,99,104	0
8	PEG	B	407	7/7	0.82	0.25	32,71,86,86	0
6	GOL	A	406	6/6	0.86	0.20	53,66,79,89	0
7	EDO	A	404	4/4	0.88	0.17	45,54,61,61	0
6	GOL	B	405	6/6	0.89	0.14	71,85,101,101	0
5	CA	A	402	1/1	0.91	0.12	47,47,47,47	0
4	DTP	B	401	30/30	0.95	0.18	30,39,49,53	0
4	DTP	A	401	30/30	0.95	0.16	36,49,63,77	0
5	CA	B	402	1/1	0.98	0.08	33,33,33,33	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.