



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:56 PM UTC

PDB ID : 5IM3 / pdb_00005im3
Title : Crystal structure of the class I ribonucleotide reductase from *Pseudomonas aeruginosa* in complex with dATP
Authors : Johansson, R.; Logan, D.T.
Deposited on : 2016-03-05
Resolution : 2.30 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

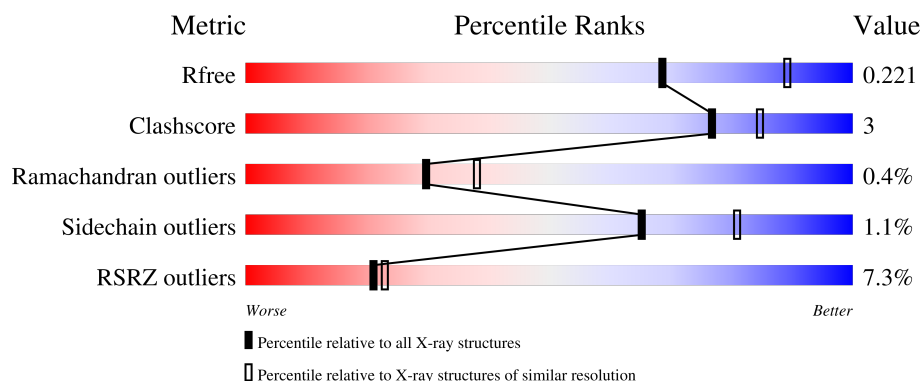
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	963	9% 84% 6% 9%
1	B	963	4% 84% 5% 11%

2 Entry composition [i](#)

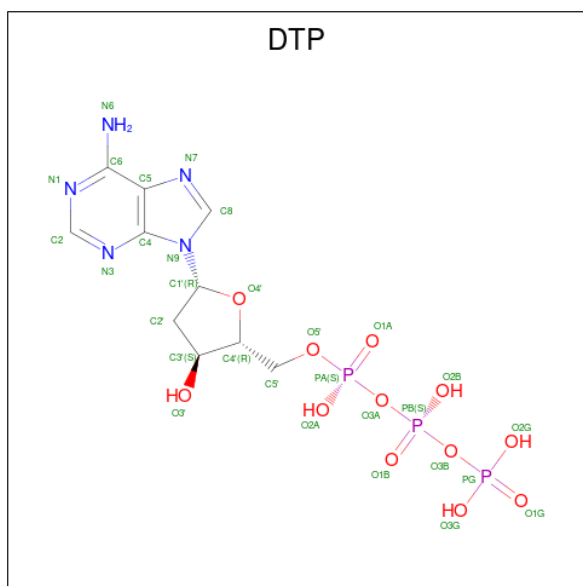
There are 4 unique types of molecules in this entry. The entry contains 14201 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	874	Total	C	N	O	S	0	1	0
			6925	4389	1193	1315	28			
1	B	860	Total	C	N	O	S	0	1	0
			6838	4337	1177	1296	28			

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$)



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

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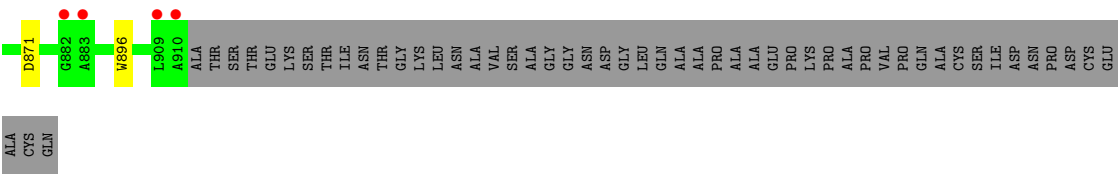
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	177	Total	O	0	0
			177	177		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	267.46Å 62.58Å 173.76Å 90.00° 127.81° 90.00°	Depositor
Resolution (Å)	46.09 – 2.30 46.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.09-2.30) 98.9 (46.09-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_2328: ???)	Depositor
R, R_{free}	0.186 , 0.217 0.193 , 0.221	Depositor DCC
R_{free} test set	5063 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14201	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, MG

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	0.14	0/7063	0.32	0/9573
1	B	0.16	0/6971	0.33	0/9441
All	All	0.15	0/14034	0.32	0/19014

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6925	0	6870	45	0
1	B	6838	0	6789	28	0
2	A	120	0	48	14	0
2	B	60	0	24	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	79	0	0	3	0
4	B	177	0	0	5	0
All	All	14201	0	13731	80	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 3.

All (80) 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:B:1002:DTP:H5'1	2:B:1002:DTP:H8	1.49	0.93
2:A:1001:DTP:H8	2:A:1001:DTP:H5'2	1.54	0.88
1:B:749:ASP:O	4:B:1101:HOH:O	2.00	0.78
1:A:397:LYS:NZ	2:A:1004:DTP:O1A	2.18	0.73
1:B:840:ILE:O	1:B:845:LYS:NZ	2.23	0.70
1:B:334:GLU:HG2	1:B:340:ARG:HG3	1.74	0.69
1:B:528:GLU:OE2	4:B:1102:HOH:O	2.11	0.69
1:A:734:GLU:OE2	4:A:1101:HOH:O	2.12	0.68
2:A:1002:DTP:H8	2:A:1002:DTP:C5'	2.23	0.67
1:A:216:GLU:OE1	1:A:814:LYS:NZ	2.24	0.66
1:A:44:TYR:CE1	2:A:1001:DTP:H2	2.31	0.65
1:A:837:ILE:HD11	1:A:840:ILE:HD12	1.77	0.65
1:A:835:GLN:O	4:A:1102:HOH:O	2.14	0.65
1:B:334:GLU:OE2	1:B:632:ARG:NH2	2.29	0.63
1:A:150:ILE:N	1:A:158:SER:O	2.32	0.61
1:A:373[B]:CYS:HB3	1:A:602:CYS:SG	2.40	0.61
1:A:866:ARG:NH2	4:A:1104:HOH:O	2.26	0.61
1:A:801:GLU:N	1:A:801:GLU:OE2	2.34	0.60
1:B:861:GLU:OE2	4:B:1103:HOH:O	2.16	0.59
2:A:1002:DTP:H8	2:A:1002:DTP:H5'2	1.84	0.59
1:A:840:ILE:O	1:A:845:LYS:NZ	2.38	0.57
1:A:102:GLN:OE1	2:A:1001:DTP:O3'	2.21	0.57
1:B:132:ARG:NH2	4:B:1109:HOH:O	2.36	0.57
1:B:216:GLU:OE1	1:B:814:LYS:NZ	2.37	0.57
1:B:797:ASN:OD1	1:B:798:LEU:N	2.36	0.56
1:A:101:ILE:HD13	2:A:1001:DTP:N3	2.22	0.55
1:B:166:ASN:ND2	1:B:185:GLU:OE2	2.40	0.55
1:B:49:ILE:HG12	2:B:1001:DTP:H2'1	1.88	0.55
1:A:837:ILE:HD11	1:A:840:ILE:CD1	2.40	0.52
1:A:236:LEU:HD11	1:A:250:MET:HE1	1.91	0.51
1:B:571:LEU:HD22	1:B:734:GLU:OE1	2.11	0.51
1:A:794:VAL:HG12	1:A:803:THR:HG22	1.94	0.50
1:A:44:TYR:CD1	2:A:1001:DTP:H2	2.46	0.50
1:A:816:ARG:NH2	1:A:843:ASP:OD2	2.45	0.50
1:B:730:LYS:HE2	1:B:734:GLU:OE2	2.12	0.49
1:A:143:GLN:H	1:A:144:PRO:CD	2.25	0.49
1:B:814:LYS:HE2	1:B:819:TRP:CD1	2.48	0.49
1:A:367:ARG:NH1	1:A:642:TYR:OH	2.46	0.48
2:A:1002:DTP:H8	2:A:1002:DTP:H5'1	1.95	0.48
1:B:622:LYS:NZ	4:B:1107:HOH:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:DTP:H8	2:B:1002:DTP:C5'	2.34	0.47
1:A:38:ASN:OD1	1:A:38:ASN:N	2.48	0.46
1:A:37:ARG:HG2	1:A:98:ILE:HG21	1.98	0.46
1:A:838:GLU:H	1:A:838:GLU:CD	2.23	0.46
1:B:735:ARG:NH2	1:B:896:TRP:O	2.49	0.46
1:A:381:ASP:HB2	2:A:1005:DTP:O1A	2.15	0.45
1:A:453:TYR:CG	1:A:583:SER:HB2	2.51	0.45
1:A:381:ASP:CB	2:A:1005:DTP:O1A	2.65	0.45
1:A:143:GLN:N	1:A:144:PRO:CD	2.79	0.45
1:A:189:LEU:HA	1:A:192:LEU:HD13	1.97	0.45
1:A:763:ASN:HB2	1:A:766:ILE:HD13	1.99	0.45
1:A:850:THR:H	1:A:853:GLU:HG3	1.82	0.45
1:B:150:ILE:HD11	1:B:160:LEU:HG	1.99	0.45
1:B:261:TYR:OH	1:B:317:GLU:OE2	2.32	0.45
2:A:1002:DTP:C5'	2:A:1002:DTP:C8	2.94	0.45
1:A:850:THR:CG2	1:A:851:ALA:N	2.79	0.44
2:A:1002:DTP:H5'1	2:A:1002:DTP:C8	2.48	0.44
1:B:373[B]:CYS:HB3	1:B:602:CYS:SG	2.58	0.44
1:A:663:MET:HA	1:A:784:SER:HA	2.00	0.44
1:B:453:TYR:CG	1:B:583:SER:HB2	2.54	0.43
1:B:537:LYS:HG3	1:B:538:LEU:N	2.34	0.43
1:A:144:PRO:O	1:A:145:HIS:CG	2.71	0.43
1:A:72:HIS:CE1	1:A:76:ARG:HH11	2.36	0.43
1:A:143:GLN:H	1:A:144:PRO:HD3	1.85	0.42
1:A:145:HIS:HB3	1:A:146:PRO:HA	2.00	0.42
1:A:193:TYR:O	1:A:196:VAL:HG23	2.19	0.42
1:B:537:LYS:HG3	1:B:538:LEU:H	1.83	0.42
1:A:723:LEU:HD21	1:A:757:VAL:HG11	2.00	0.42
1:A:718:TRP:CD1	1:A:761:ILE:HD11	2.55	0.42
1:B:871:ASP:OD1	1:B:871:ASP:N	2.48	0.42
1:B:571:LEU:O	1:B:576:GLN:NE2	2.52	0.41
1:A:382:LEU:HG	1:B:394:MET:HE1	2.02	0.41
1:A:701:CYS:SG	1:A:761:ILE:HG22	2.61	0.41
1:A:739:TYR:HB3	1:A:896:TRP:CH2	2.55	0.41
1:A:381:ASP:HA	2:A:1005:DTP:O1A	2.21	0.41
1:A:696:ALA:HB1	1:A:766:ILE:HG21	2.03	0.40
1:B:624:GLU:O	1:B:628:LYS:HG2	2.21	0.40
1:B:127:ALA:O	1:B:131:GLU:HG2	2.21	0.40
1:B:258:LEU:HB3	1:B:259:PRO:HD3	2.04	0.40
1:A:379:PRO:HG2	1:A:384:GLY:HA3	2.03	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	871/963 (90%)	839 (96%)	25 (3%)	7 (1%)	16	20
1	B	853/963 (89%)	830 (97%)	23 (3%)	0	100	100
All	All	1724/1926 (90%)	1669 (97%)	48 (3%)	7 (0%)	30	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	146	PRO
1	A	614	VAL
1	A	883	ALA
1	A	784	SER
1	A	144	PRO
1	A	143	GLN

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	736/800 (92%)	727 (99%)	9 (1%)	63	79
1	B	728/800 (91%)	721 (99%)	7 (1%)	68	82
All	All	1464/1600 (92%)	1448 (99%)	16 (1%)	65	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LEU
1	A	254	TYR
1	A	357	THR
1	A	530	LEU
1	A	602	CYS
1	A	638	ILE
1	A	689	MET
1	A	810	VAL
1	A	850	THR
1	B	32	LEU
1	B	252	GLU
1	B	254	TYR
1	B	334	GLU
1	B	602	CYS
1	B	733	GLU
1	B	783	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	247	HIS
1	A	289	HIS
1	A	301	GLN
1	A	424	GLN
1	A	482	ASN
1	A	576	GLN
1	A	673	HIS
1	B	289	HIS
1	B	392	ASN
1	B	404	ASN
1	B	560	HIS
1	B	673	HIS
1	B	825	ASN
1	B	835	GLN
1	B	874	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
2	DTP	B	1001	3	31,32,32	0.47	0	46,50,50	0.50	0
2	DTP	A	1004	-	31,32,32	0.24	0	46,50,50	0.38	0
2	DTP	A	1005	-	31,32,32	0.39	0	46,50,50	0.49	1 (2%)
2	DTP	A	1002	3	31,32,32	0.52	0	46,50,50	0.53	0
2	DTP	B	1002	3	31,32,32	0.48	0	46,50,50	0.58	2 (4%)
2	DTP	A	1001	3	31,32,32	0.38	0	46,50,50	0.57	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
2	DTP	B	1001	3	-	5/22/34/34	0/3/3/3
2	DTP	A	1004	-	-	2/22/34/34	0/3/3/3
2	DTP	A	1005	-	-	6/22/34/34	0/3/3/3
2	DTP	A	1002	3	-	4/22/34/34	0/3/3/3
2	DTP	B	1002	3	-	5/22/34/34	0/3/3/3
2	DTP	A	1001	3	-	8/22/34/34	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	DTP	O3A-PA-O1A	-2.28	103.85	110.70
2	B	1002	DTP	O5'-PA-O1A	2.16	117.48	108.94
2	B	1002	DTP	O2B-PB-O3B	2.08	112.89	107.27

There are no chirality outliers.

All (30) torsion outliers are listed below:

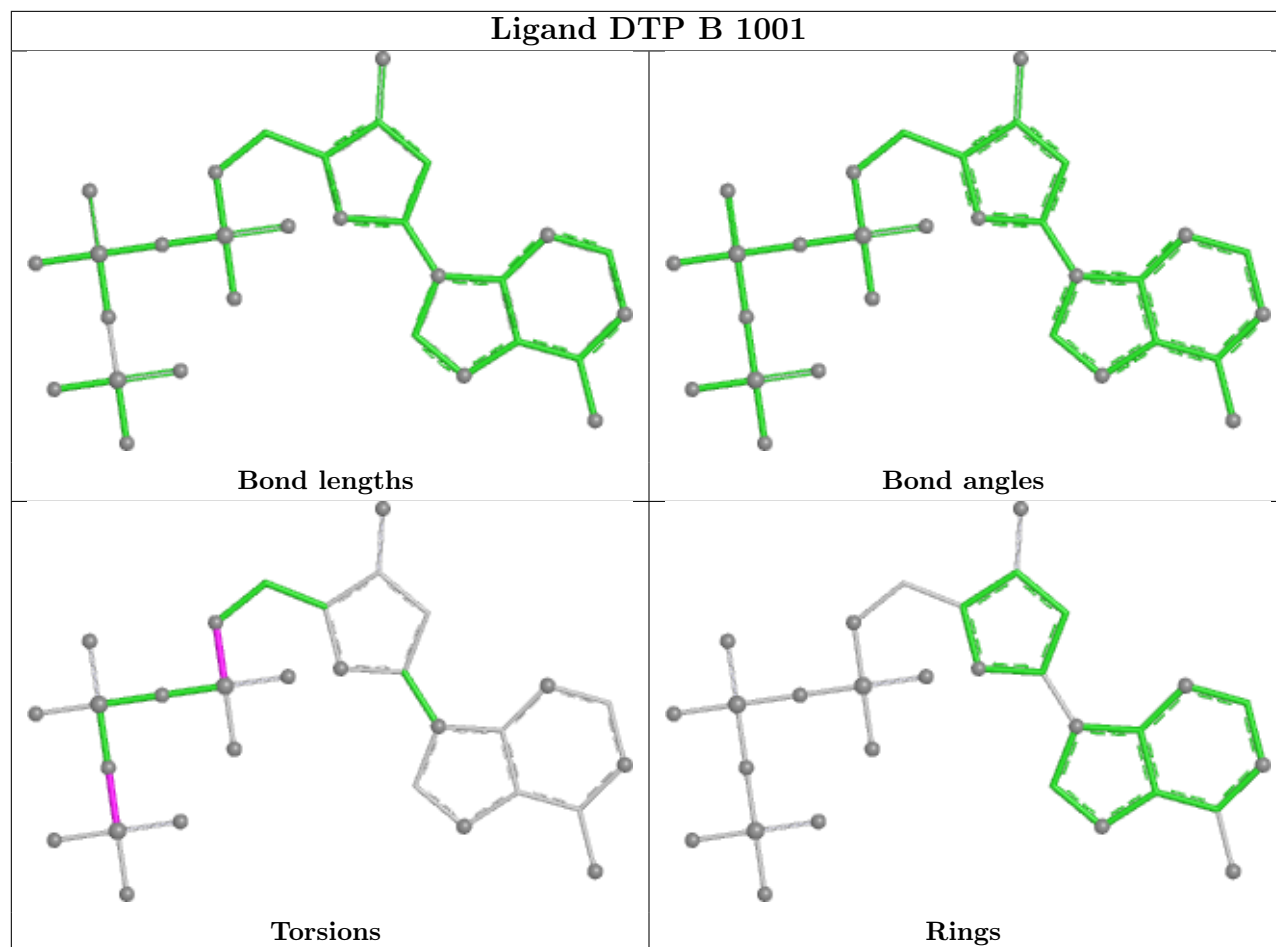
Mol	Chain	Res	Type	Atoms
2	A	1001	DTP	PB-O3B-PG-O2G
2	A	1001	DTP	O4'-C4'-C5'-O5'
2	A	1002	DTP	PB-O3B-PG-O3G
2	A	1004	DTP	PB-O3B-PG-O2G
2	A	1005	DTP	PB-O3B-PG-O3G
2	B	1001	DTP	PB-O3B-PG-O2G
2	B	1001	DTP	C5'-O5'-PA-O1A
2	B	1001	DTP	C5'-O5'-PA-O2A
2	B	1001	DTP	C5'-O5'-PA-O3A
2	B	1002	DTP	C5'-O5'-PA-O1A
2	B	1002	DTP	C5'-O5'-PA-O3A
2	A	1001	DTP	C3'-C4'-C5'-O5'
2	A	1002	DTP	O4'-C4'-C5'-O5'
2	A	1002	DTP	C3'-C4'-C5'-O5'
2	A	1001	DTP	O4'-C1'-N9-C4
2	A	1005	DTP	O4'-C1'-N9-C4
2	B	1002	DTP	PB-O3B-PG-O2G
2	A	1005	DTP	PB-O3A-PA-O1A
2	B	1002	DTP	C5'-O5'-PA-O2A
2	A	1005	DTP	C2'-C1'-N9-C4
2	A	1002	DTP	PB-O3A-PA-O1A
2	A	1001	DTP	PB-O3B-PG-O1G
2	A	1004	DTP	PB-O3B-PG-O1G
2	A	1005	DTP	PB-O3B-PG-O1G
2	B	1001	DTP	PB-O3B-PG-O1G
2	A	1001	DTP	PB-O3B-PG-O3G
2	A	1005	DTP	PB-O3B-PG-O2G
2	B	1002	DTP	PA-O3A-PB-O2B
2	A	1001	DTP	C2'-C1'-N9-C4
2	A	1001	DTP	PA-O3A-PB-O2B

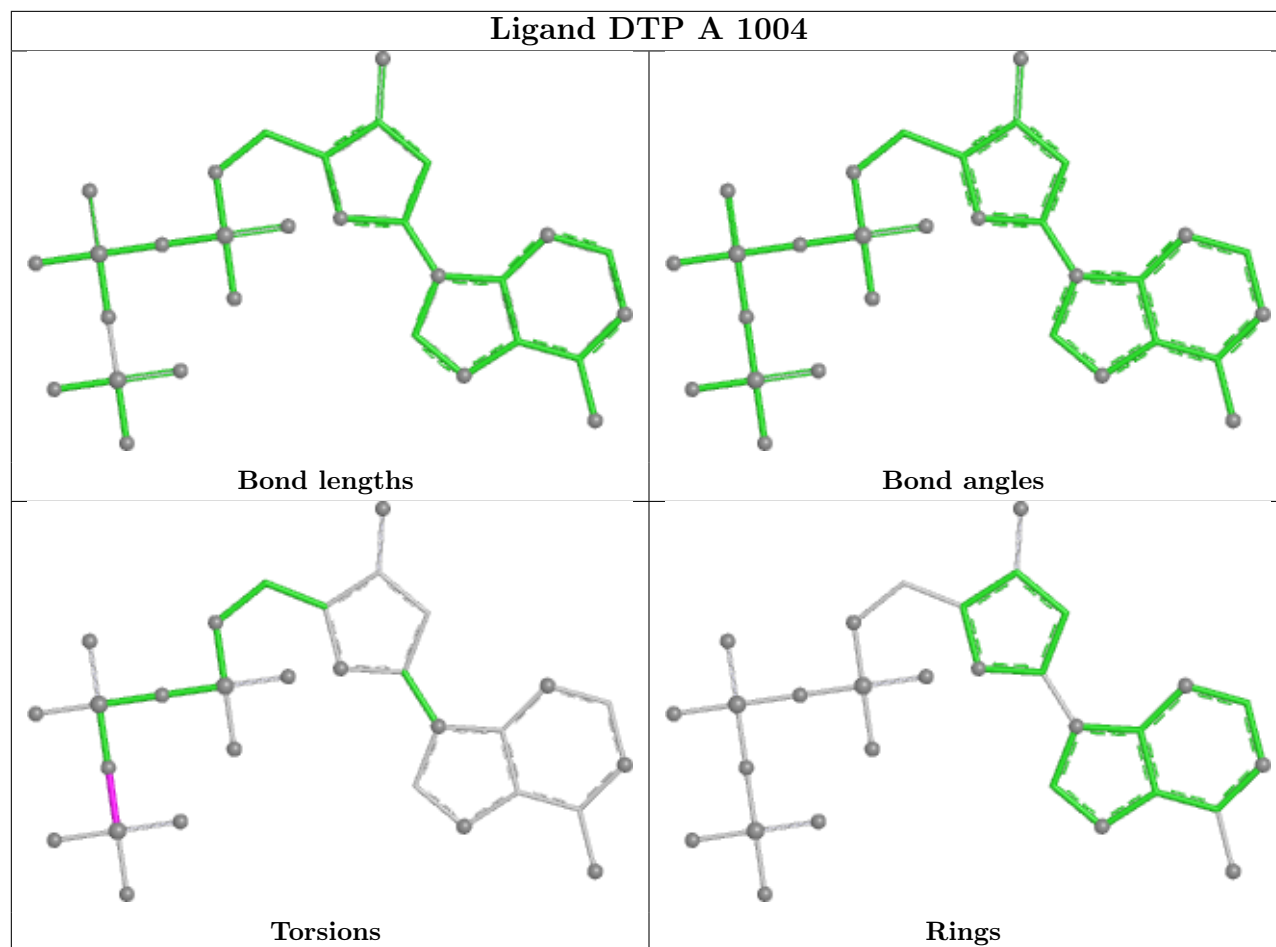
There are no ring outliers.

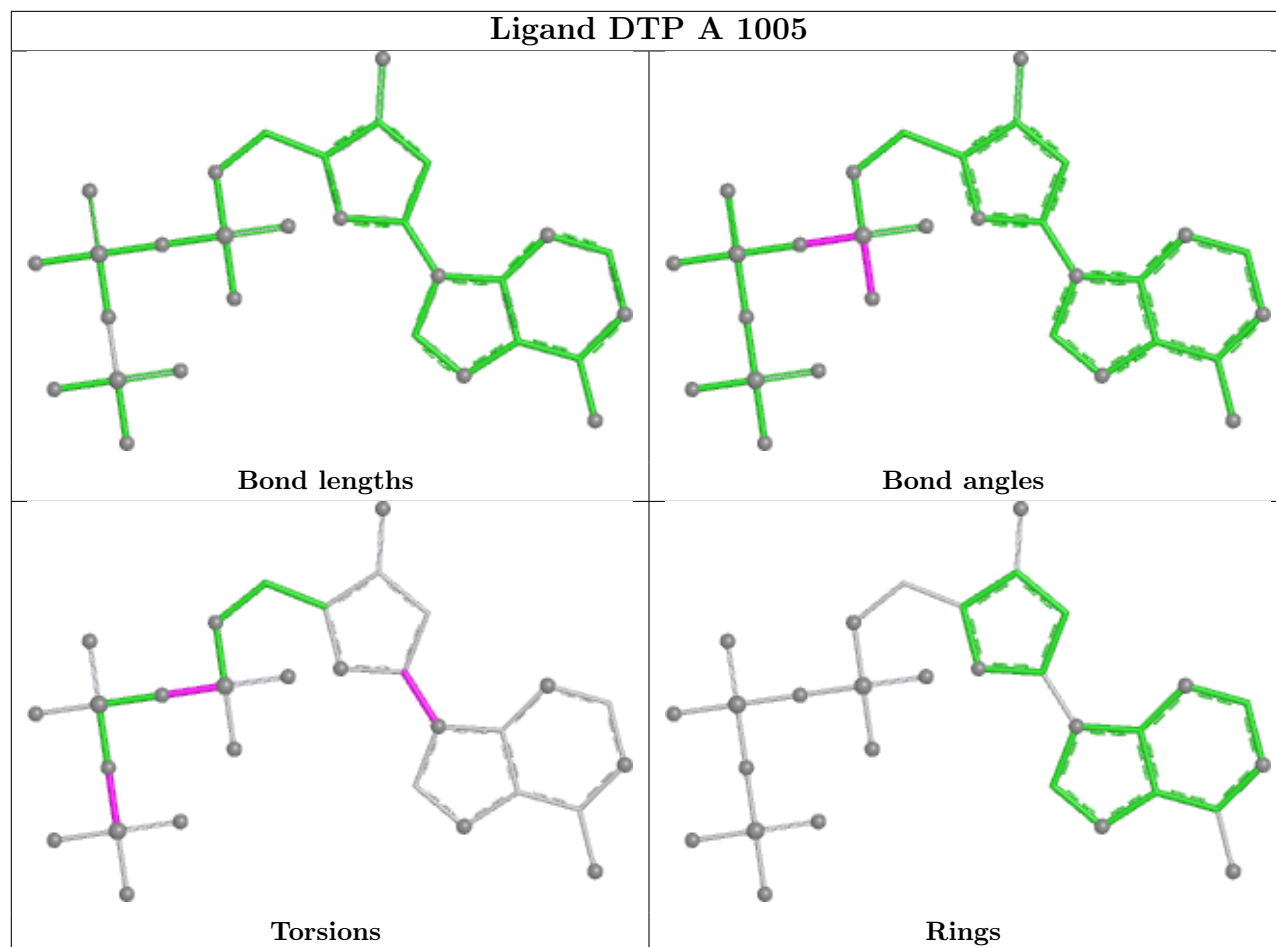
6 monomers are involved in 17 short contacts:

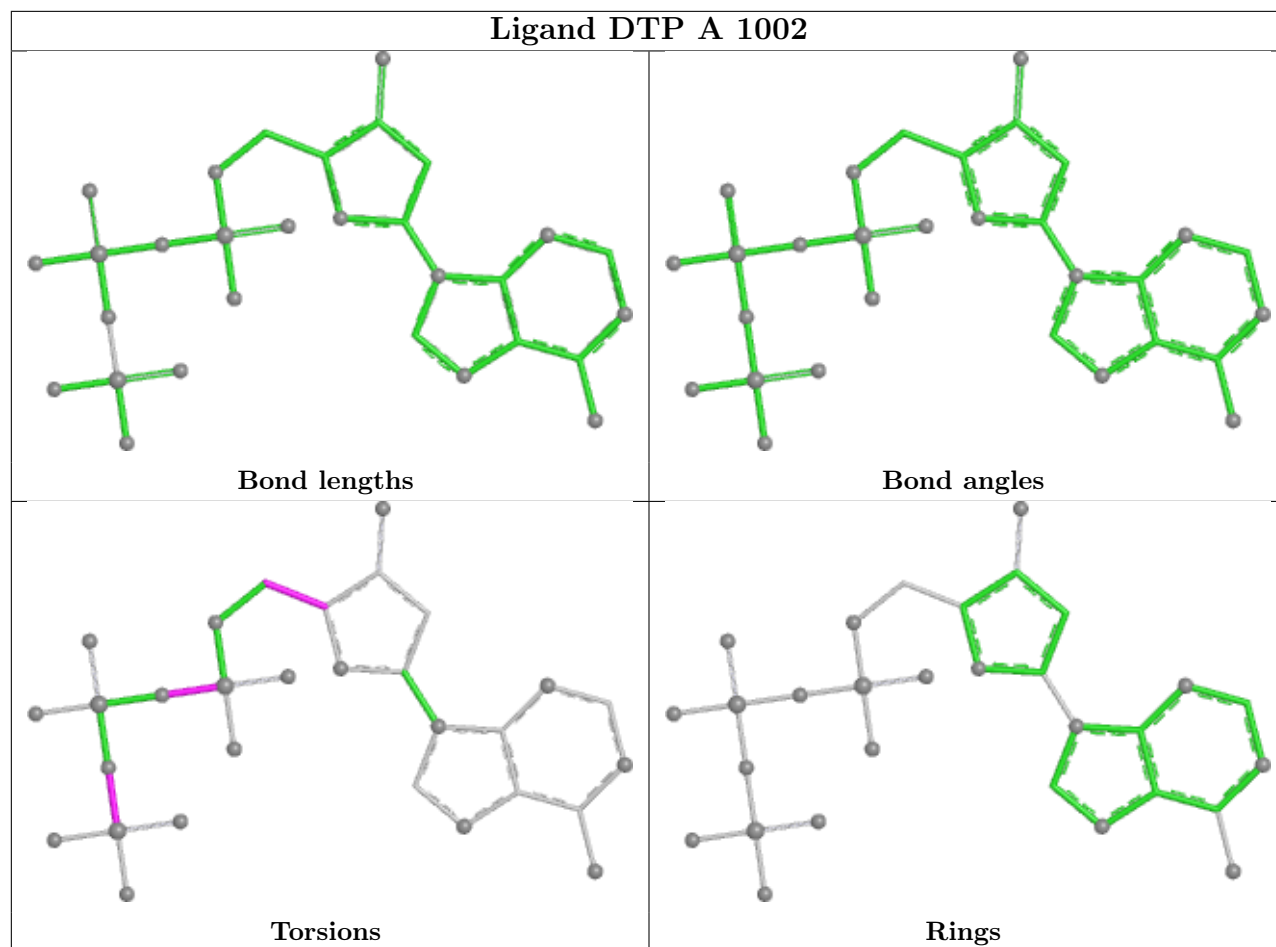
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	DTP	1	0
2	A	1004	DTP	1	0
2	A	1005	DTP	3	0
2	A	1002	DTP	5	0
2	B	1002	DTP	2	0
2	A	1001	DTP	5	0

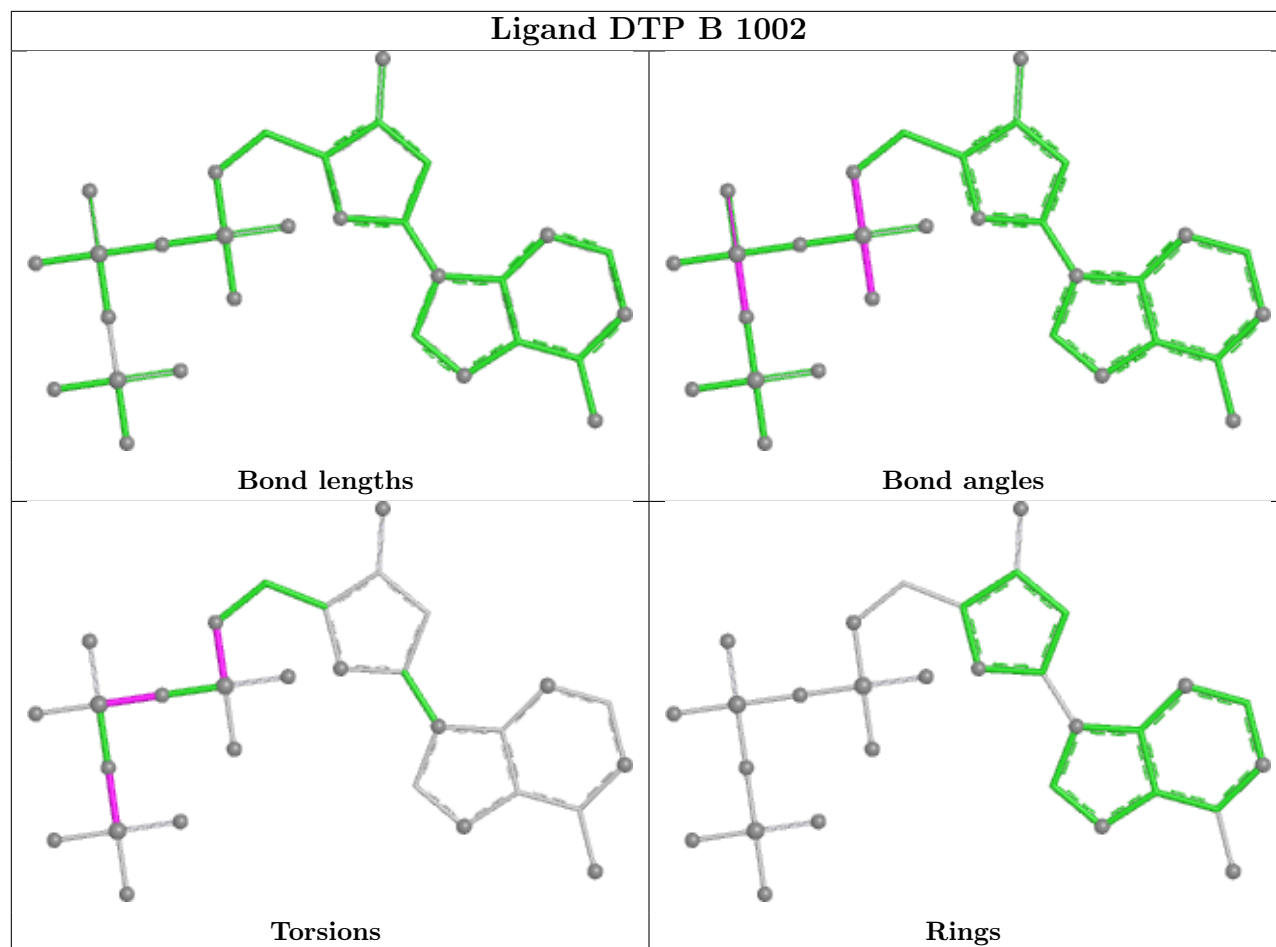
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

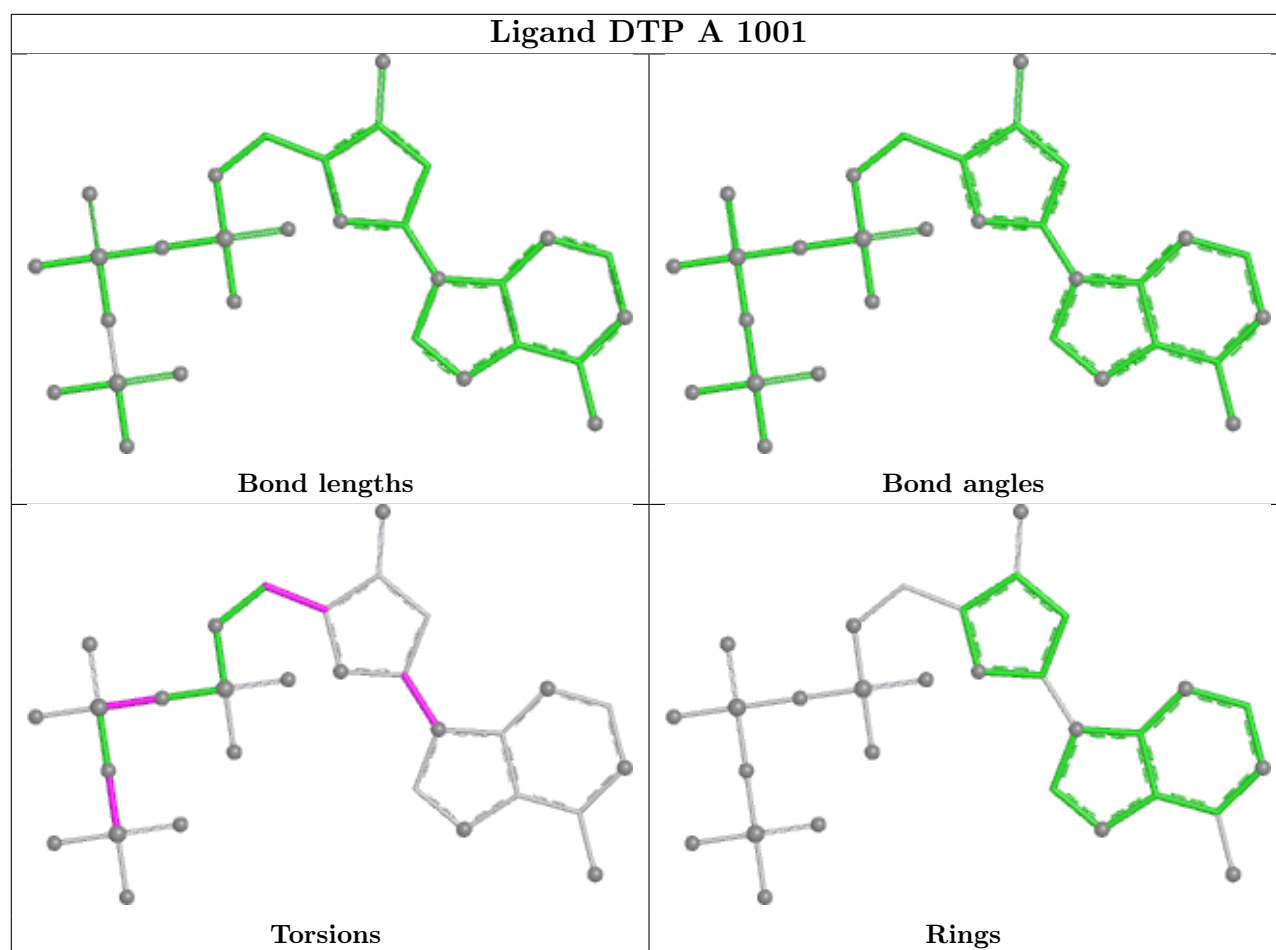












5.7 Other polymers [i](#)

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	874/963 (90%)	0.65	90 (10%) 12 13	25, 62, 112, 154	1 (0%)
1	B	860/963 (89%)	0.22	37 (4%) 40 41	20, 46, 86, 130	1 (0%)
All	All	1734/1926 (90%)	0.43	127 (7%) 21 23	20, 54, 103, 154	2 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	ALA	4.8
1	A	189	LEU	4.7
1	B	910	ALA	4.7
1	B	66	ALA	4.6
1	A	32	LEU	4.4
1	B	734	GLU	4.4
1	B	537	LYS	4.3
1	A	169	ILE	4.3
1	B	399	ALA	4.2
1	A	798	LEU	4.0
1	B	67	ALA	4.0
1	A	67	ALA	3.8
1	B	65	ALA	3.8
1	A	41	VAL	3.8
1	B	418	GLY	3.8
1	A	912	THR	3.8
1	A	90	MET	3.7
1	A	91	PRO	3.7
1	A	43	PRO	3.6
1	A	142	ALA	3.6
1	A	795	LYS	3.6
1	A	419	THR	3.5
1	A	418	GLY	3.5
1	A	95	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	883	ALA	3.4
1	B	361	PHE	3.4
1	A	153	ALA	3.4
1	B	61	GLU	3.3
1	A	614	VAL	3.2
1	A	208	THR	3.2
1	A	193	TYR	3.1
1	A	146	PRO	3.1
1	A	86	PHE	3.1
1	A	184	ILE	3.0
1	A	883	ALA	3.0
1	A	44	TYR	3.0
1	A	803	THR	3.0
1	B	147	SER	3.0
1	B	419	THR	3.0
1	A	38	ASN	3.0
1	A	62	GLY	3.0
1	A	94	GLY	3.0
1	B	882	GLY	2.9
1	A	198	GLU	2.9
1	A	42	VAL	2.9
1	B	533	TYR	2.8
1	A	911	ALA	2.8
1	A	68	SER	2.7
1	A	157	LEU	2.7
1	A	188	THR	2.7
1	A	148	ILE	2.7
1	A	252	GLU	2.7
1	A	793	TYR	2.7
1	A	37	ARG	2.7
1	B	40	THR	2.6
1	A	34	VAL	2.6
1	B	441	ASN	2.6
1	B	797	ASN	2.6
1	B	421	GLY	2.6
1	A	620	THR	2.6
1	A	60	VAL	2.5
1	A	69	SER	2.5
1	B	909	LEU	2.5
1	A	757	VAL	2.5
1	A	794	VAL	2.5
1	A	96	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	415	TYR	2.5
1	B	153	ALA	2.5
1	B	69	SER	2.5
1	B	243	GLU	2.4
1	A	800	GLY	2.4
1	A	87	LYS	2.4
1	A	196	VAL	2.4
1	A	644	SER	2.4
1	A	201	VAL	2.4
1	A	192	LEU	2.4
1	B	536	LEU	2.4
1	B	32	LEU	2.3
1	A	214	GLU	2.3
1	A	441	ASN	2.3
1	A	93	GLY	2.3
1	A	151	THR	2.3
1	B	89	ARG	2.3
1	A	35	ILE	2.3
1	A	173	CYS	2.3
1	A	168	ILE	2.3
1	A	332	ILE	2.3
1	A	213	VAL	2.3
1	A	176	LEU	2.3
1	A	190	LYS	2.3
1	B	798	LEU	2.3
1	A	470	ASN	2.3
1	B	30	GLY	2.3
1	A	416	ILE	2.2
1	A	837	ILE	2.2
1	A	398	PHE	2.2
1	A	797	ASN	2.2
1	A	882	GLY	2.2
1	A	417	LYS	2.2
1	B	369	GLN	2.2
1	A	45	THR	2.2
1	A	197	ALA	2.2
1	B	803	THR	2.2
1	A	120	ASP	2.2
1	A	178	GLU	2.2
1	A	449	ALA	2.2
1	B	777	ASN	2.2
1	A	159	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	39	GLY	2.2
1	A	64	THR	2.2
1	A	97	HIS	2.1
1	A	150	ILE	2.1
1	B	207	MET	2.1
1	B	538	LEU	2.1
1	A	200	ASP	2.1
1	A	147	SER	2.1
1	A	533	TYR	2.1
1	A	162	MET	2.1
1	A	714	GLN	2.1
1	A	421	GLY	2.1
1	A	215	ARG	2.1
1	A	40	THR	2.0
1	B	372	SER	2.0
1	B	799	SER	2.0
1	A	792	LEU	2.0
1	A	203	THR	2.0
1	B	470	ASN	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 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
2	DTP	A	1001	30/30	0.88	0.14	85,94,104,105	0
2	DTP	A	1002	30/30	0.88	0.12	61,70,79,82	0
2	DTP	A	1005	30/30	0.93	0.10	41,44,74,79	0
2	DTP	B	1001	30/30	0.93	0.10	53,62,70,71	0

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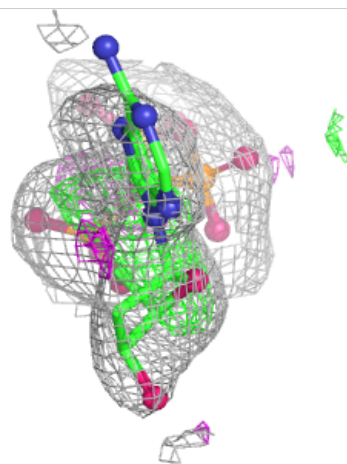
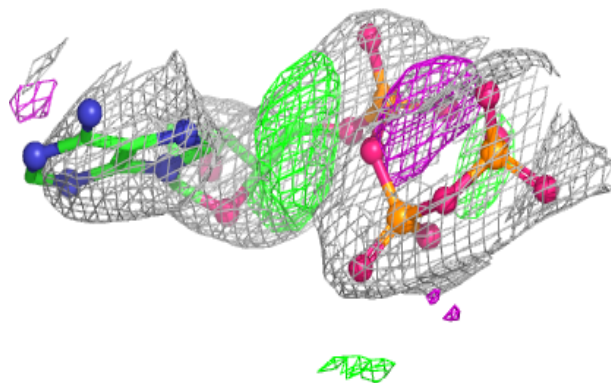
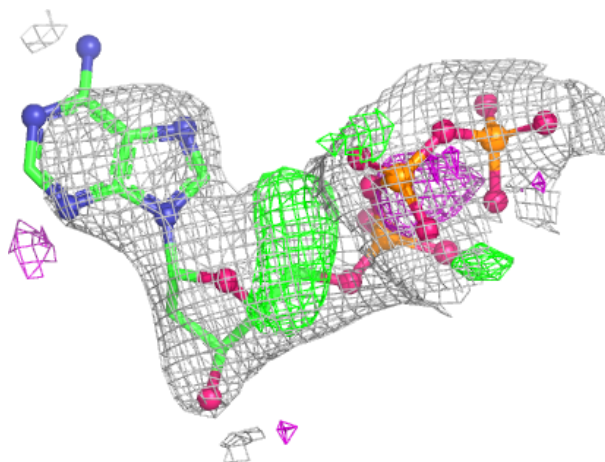
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DTP	A	1004	30/30	0.94	0.09	39,49,83,85	0
2	DTP	B	1002	30/30	0.95	0.09	53,58,65,66	0
3	MG	A	1003	1/1	0.95	0.10	81,81,81,81	1
3	MG	B	1003	1/1	0.98	0.12	63,63,63,63	0

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.

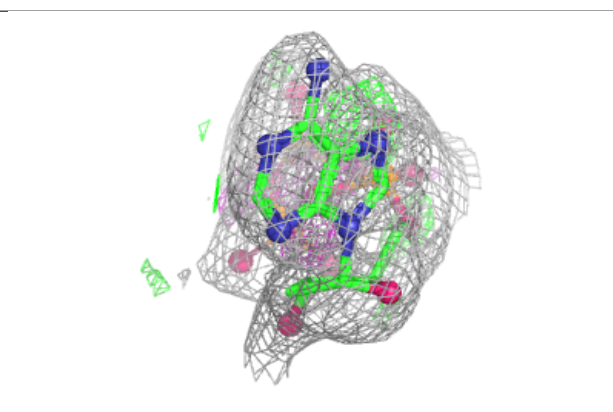
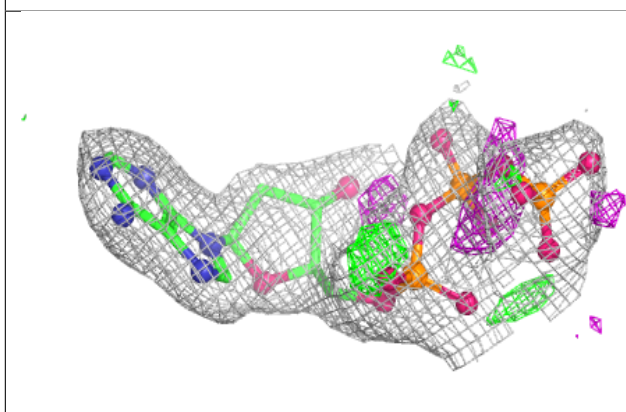
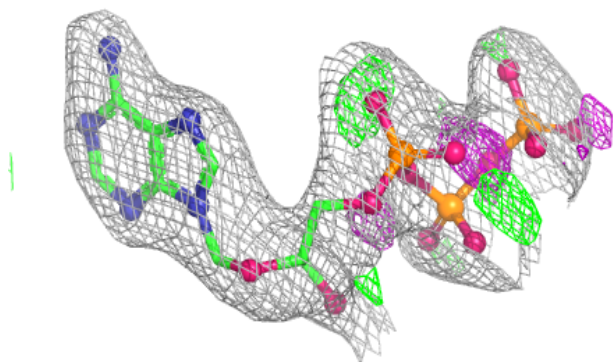
Electron density around DTP A 1001:

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



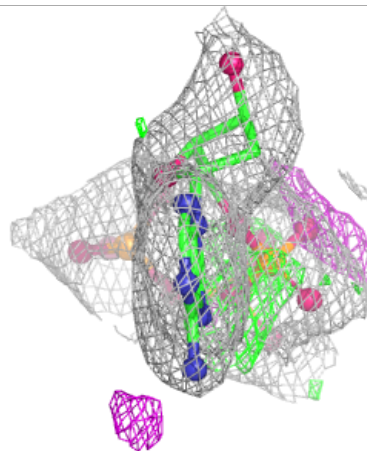
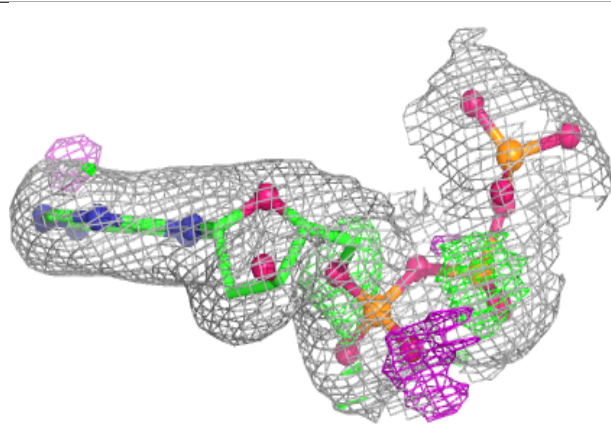
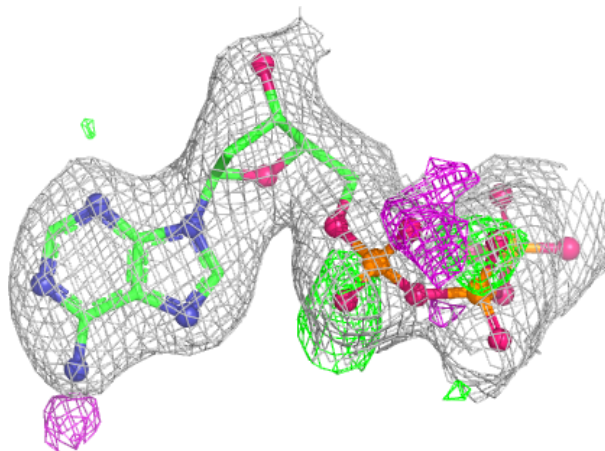
Electron density around DTP A 1002:

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



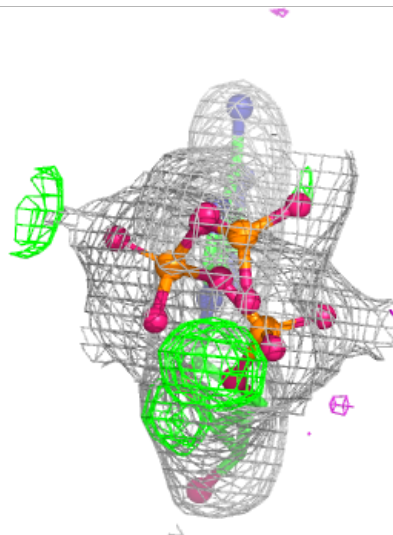
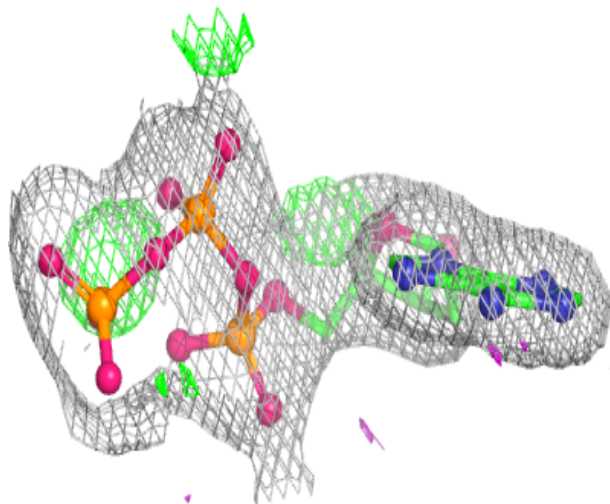
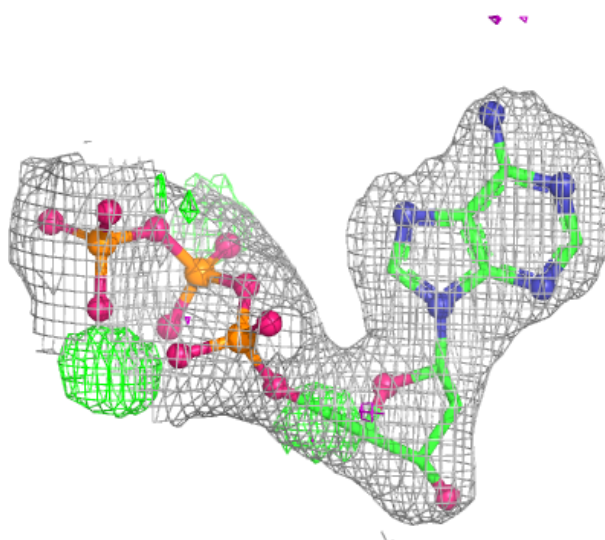
Electron density around DTP A 1005:

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



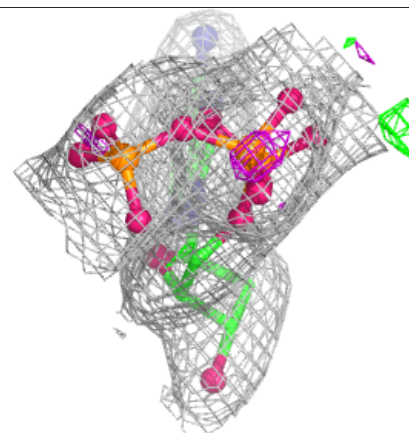
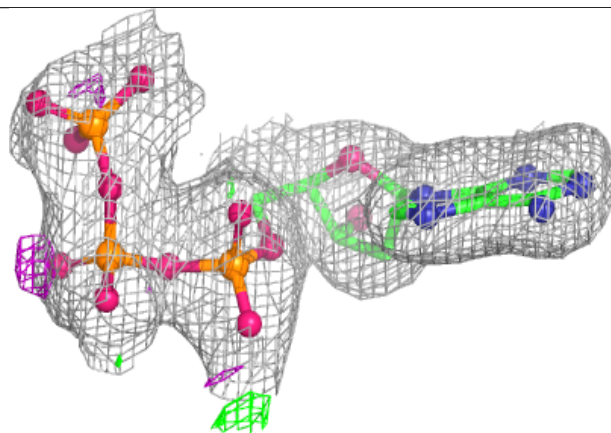
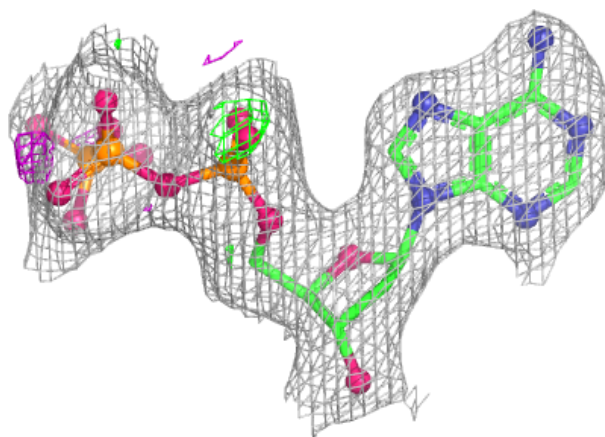
Electron density around DTP B 1001:

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

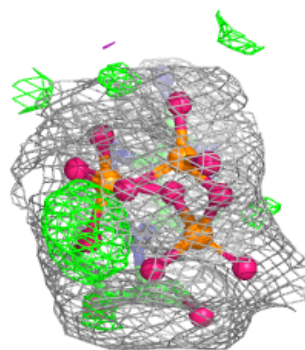
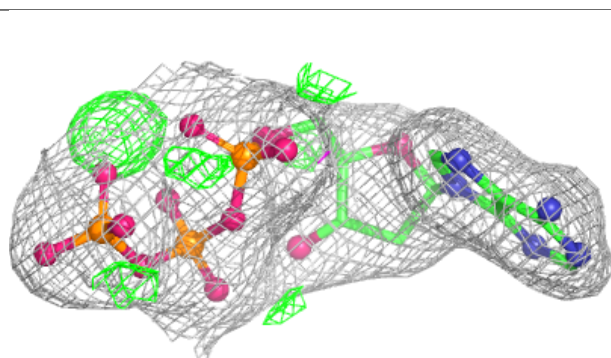
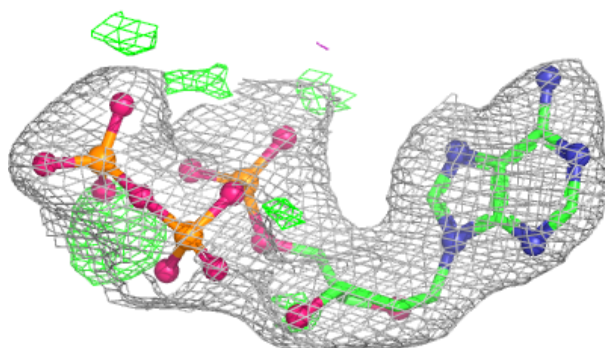


Electron density around DTP A 1004:

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

**Electron density around DTP B 1002:**

$2mF_o-DF_c$ (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.