



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:57 AM UTC

PDB ID : 6PWY / pdb_00006pwy
Title : Structure of *C. elegans* ZK177.8, SAMHD1 ortholog
Authors : Lim, C.S.; Maehigashi, T.; Wade, L.R.; Bowen, N.; Knecht, K.; Xiong, Y.;
Kim, B.
Deposited on : 2019-07-24
Resolution : 1.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

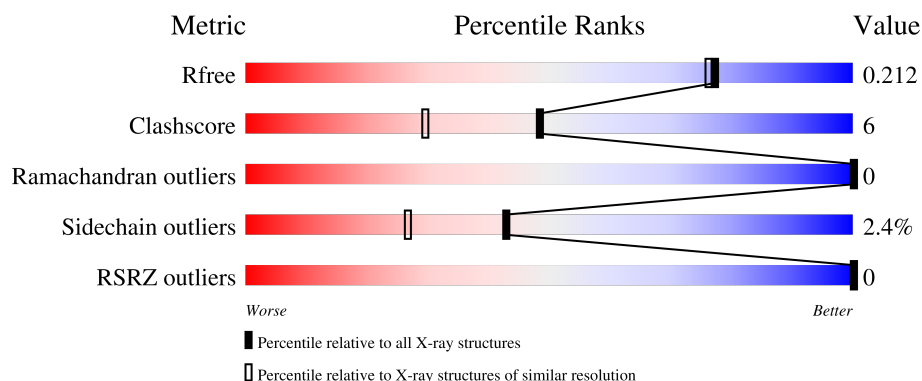
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	526	 86% 9% . .
1	B	526	 87% 10% . .
1	C	526	 85% 11% . .
1	D	526	 86% 9% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SIN	B	605	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18205 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 ZK177.8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	4	0
			4040	2566	684	768	22			
1	B	513	Total	C	N	O	S	0	4	0
			4119	2615	703	779	22			
1	D	503	Total	C	N	O	S	0	4	0
			4033	2562	683	766	22			
1	C	513	Total	C	N	O	S	0	3	0
			4111	2609	702	778	22			

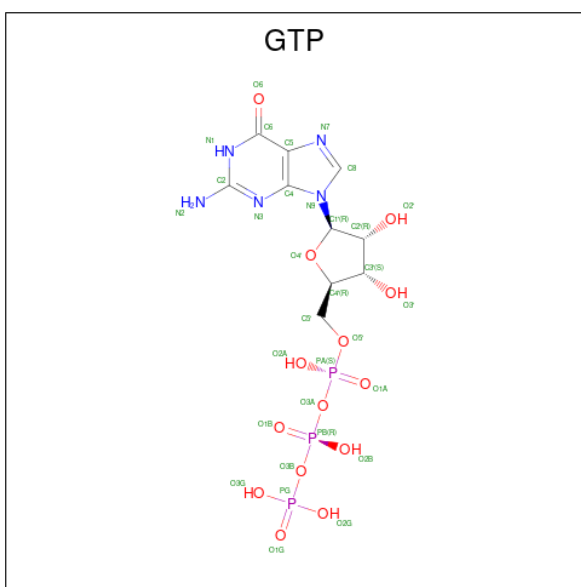
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	expression tag	UNP Q09374
A	134	ARG	HIS	engineered mutation	UNP Q09374
A	135	ASN	ASP	engineered mutation	UNP Q09374
B	40	MET	-	expression tag	UNP Q09374
B	134	ARG	HIS	engineered mutation	UNP Q09374
B	135	ASN	ASP	engineered mutation	UNP Q09374
D	40	MET	-	expression tag	UNP Q09374
D	134	ARG	HIS	engineered mutation	UNP Q09374
D	135	ASN	ASP	engineered mutation	UNP Q09374
C	40	MET	-	expression tag	UNP Q09374
C	134	ARG	HIS	engineered mutation	UNP Q09374
C	135	ASN	ASP	engineered mutation	UNP Q09374

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

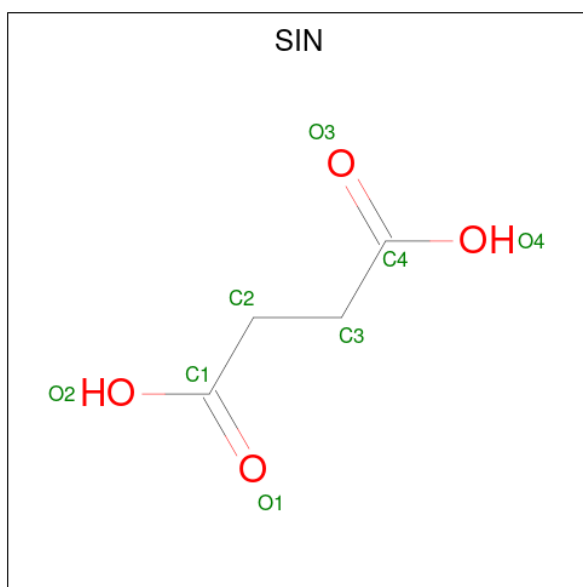


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		
5	C	1	Total	C	O	0	0
			8	4	4		
5	C	1	Total	C	O	0	0
			8	4	4		

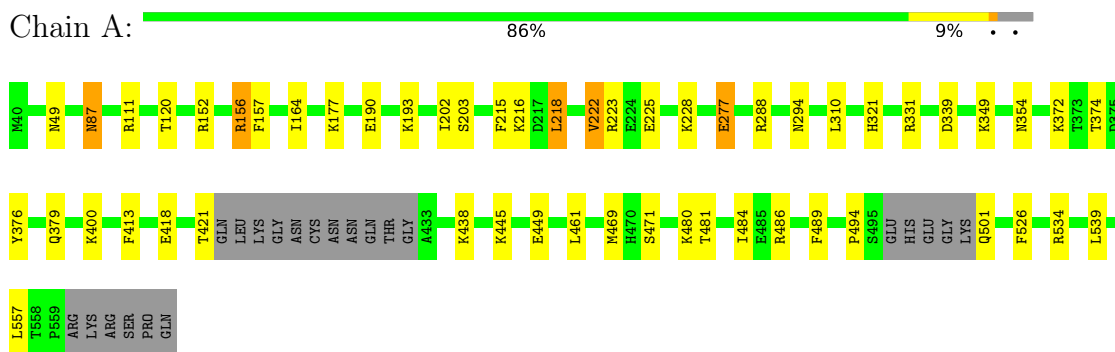
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	362	Total	O	0	0
			362	362		
6	B	385	Total	O	0	0
			385	385		
6	D	354	Total	O	0	0
			354	354		
6	C	381	Total	O	0	0
			381	381		

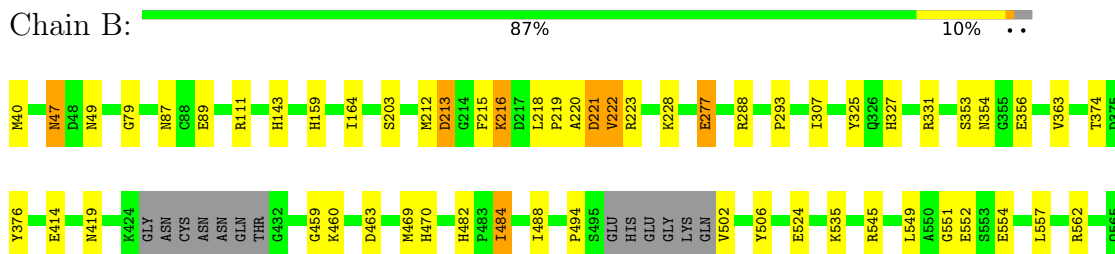
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

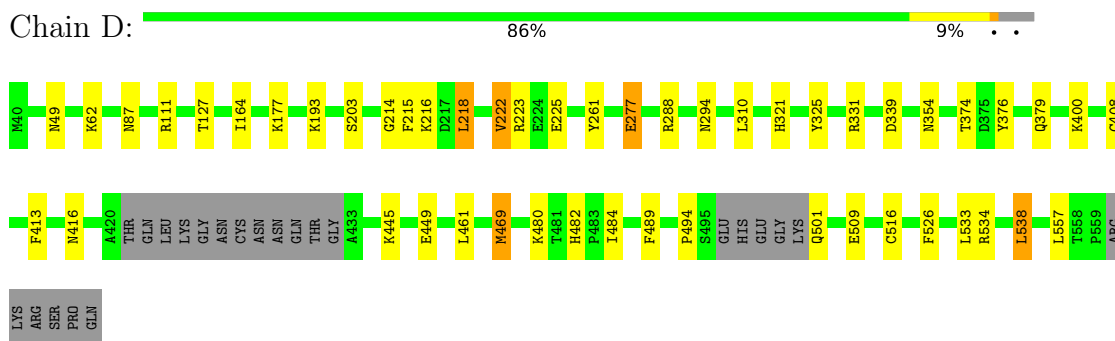
- Molecule 1: ZK177.8



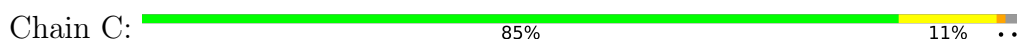
- Molecule 1: ZK177.8



- Molecule 1: ZK177.8



- Molecule 1: ZK177.8



M40	S353	L549	E41	N354	A550	E552	P42	G355	E356	V363	K372	T373	T374	D375	Y376	E414	N419	K424	GLY	ASN	CYS	ASN	ASN	GLN	THR	G432	G459	K460	D463	I464	Q465	M469	H470	I484	I488	P494	S495	GLU	HIS	GLU	GLY	LYS	GLN	V502	Y506	E524	M528	K535	R545	G565
I45	I46	N47	D48	N49	R111	H143	K151	I164	K168	S203	M212	D213	G214	F215	K216	D217	L218	P219	A220	D221	V222	R223	E224	E225	K228	Y261	E277	E281	R288	R299	I300	A301	I307	Y325	Q326	H327	R331	G352												

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.68Å 90.56Å 93.36Å 65.58° 65.49° 86.22°	Depositor
Resolution (Å)	46.03 – 1.81 46.03 – 1.81	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.03-1.81) 93.6 (46.03-1.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.182 , 0.209 0.188 , 0.212	Depositor DCC
R_{free} test set	10556 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.449 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18205	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: MG, SIN, GTP, DTP

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	1.18	5/4127 (0.1%)	1.31	1/5559 (0.0%)
1	B	1.21	6/4204 (0.1%)	1.32	4/5660 (0.1%)
1	C	1.23	6/4196 (0.1%)	1.33	5/5649 (0.1%)
1	D	1.17	1/4120 (0.0%)	1.30	3/5549 (0.1%)
All	All	1.20	18/16647 (0.1%)	1.31	13/22417 (0.1%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	HIS	CE1-NE2	7.58	1.40	1.32
1	C	327	HIS	CE1-NE2	7.43	1.40	1.32
1	C	42	PRO	C-O	-6.50	1.16	1.23
1	B	482	HIS	CE1-NE2	6.22	1.38	1.32
1	C	45	ILE	C-O	6.16	1.30	1.24

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	GLU	CB-CG-CD	6.38	123.44	112.60
1	B	277	GLU	CB-CG-CD	6.26	123.24	112.60
1	C	213	ASP	CB-CA-C	-5.82	108.19	116.34
1	A	277	GLU	CB-CG-CD	5.75	122.37	112.60
1	B	363	VAL	CA-C-O	-5.70	114.48	120.57

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	4040	0	4052	49	0
1	B	4119	0	4143	38	0
1	C	4111	0	4133	52	0
1	D	4033	0	4045	44	0
2	A	60	0	24	1	0
2	B	60	0	24	5	0
2	C	60	0	24	3	0
2	D	60	0	24	2	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
3	C	32	0	12	0	0
3	D	32	0	12	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	16	0	8	2	0
5	B	16	0	8	7	0
5	C	16	0	8	5	0
6	A	362	0	0	13	0
6	B	385	0	0	5	0
6	C	381	0	0	14	0
6	D	354	0	0	11	0
All	All	18205	0	16541	183	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 6.

The worst 5 of 183 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:A:469:MET:HE3	1:A:469:MET:HA	1.33	1.08
1:D:469:MET:HE3	1:D:469:MET:HA	1.34	1.06
2:C:601:DTP:O2G	6:C:701:HOH:O	1.76	1.02
2:B:601:DTP:O2G	2:B:601:DTP:H5'1	1.63	0.99
1:A:376[B]:TYR:OH	1:D:376[B]:TYR:OH	1.55	0.95

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	502/526 (95%)	494 (98%)	8 (2%)	0	100	100
1	B	511/526 (97%)	500 (98%)	11 (2%)	0	100	100
1	C	510/526 (97%)	499 (98%)	11 (2%)	0	100	100
1	D	501/526 (95%)	494 (99%)	7 (1%)	0	100	100
All	All	2024/2104 (96%)	1987 (98%)	37 (2%)	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	452/467 (97%)	445 (98%)	7 (2%)	57	46
1	B	460/467 (98%)	449 (98%)	11 (2%)	43	27
1	C	459/467 (98%)	444 (97%)	15 (3%)	33	15
1	D	451/467 (97%)	441 (98%)	10 (2%)	45	30
All	All	1822/1868 (98%)	1779 (98%)	43 (2%)	43	27

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	40	MET
1	C	225	GLU
1	C	41	GLU
1	C	216	LYS
1	C	356	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	326	GLN
1	C	172	ASN
1	D	402	GLN
1	C	210	GLN
1	B	172	ASN

5.3.3 RNA [i](#)

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 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	603	4	31,32,32	1.00	1 (3%)	46,50,50	0.77	0
2	DTP	C	603	4	31,32,32	1.03	3 (9%)	46,50,50	0.72	0
2	DTP	D	602	-	31,32,32	0.83	1 (3%)	46,50,50	0.65	0
2	DTP	B	601	-	31,32,32	0.87	2 (6%)	46,50,50	0.70	0
3	GTP	A	602	4	33,34,34	0.90	1 (3%)	50,54,54	0.96	2 (4%)
3	GTP	C	602	4	33,34,34	1.13	3 (9%)	50,54,54	0.86	2 (4%)
5	SIN	A	607	-	7,7,7	1.47	1 (14%)	8,8,8	1.07	1 (12%)
5	SIN	B	605	-	7,7,7	0.83	0	8,8,8	1.32	1 (12%)
5	SIN	C	604	-	7,7,7	1.03	0	8,8,8	1.21	0
2	DTP	C	601	-	31,32,32	0.89	2 (6%)	46,50,50	0.80	0
2	DTP	A	603	4	31,32,32	1.21	2 (6%)	46,50,50	1.04	2 (4%)
3	GTP	B	602	4	33,34,34	1.07	2 (6%)	50,54,54	0.81	1 (2%)
5	SIN	C	605	-	7,7,7	1.64	2 (28%)	8,8,8	1.09	1 (12%)
3	GTP	D	603	4	33,34,34	0.82	2 (6%)	50,54,54	0.94	3 (6%)
5	SIN	B	606	-	7,7,7	1.09	0	8,8,8	1.15	0
2	DTP	A	601	-	31,32,32	0.65	0	46,50,50	0.80	1 (2%)
5	SIN	A	606	-	7,7,7	1.25	0	8,8,8	1.92	3 (37%)
2	DTP	D	604	4	31,32,32	1.08	1 (3%)	46,50,50	0.86	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	603	4	-	3/22/34/34	0/3/3/3
2	DTP	C	603	4	-	4/22/34/34	0/3/3/3
2	DTP	D	602	-	-	2/22/34/34	0/3/3/3
2	DTP	B	601	-	-	1/22/34/34	0/3/3/3
3	GTP	A	602	4	-	4/22/38/38	0/3/3/3
3	GTP	C	602	4	-	3/22/38/38	0/3/3/3
5	SIN	A	607	-	-	2/5/5/5	-
5	SIN	B	605	-	-	2/5/5/5	-
5	SIN	C	604	-	-	1/5/5/5	-
2	DTP	C	601	-	-	2/22/34/34	0/3/3/3
2	DTP	A	603	4	-	4/22/34/34	0/3/3/3
3	GTP	B	602	4	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SIN	C	605	-	-	3/5/5/5	-
3	GTP	D	603	4	-	4/22/38/38	0/3/3/3
5	SIN	B	606	-	-	0/5/5/5	-
2	DTP	A	601	-	-	3/22/34/34	0/3/3/3
5	SIN	A	606	-	-	2/5/5/5	-
2	DTP	D	604	4	-	4/22/34/34	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	DTP	PA-O3A	4.27	1.64	1.59
2	D	604	DTP	PB-O3B	3.91	1.63	1.59
3	A	602	GTP	PB-O3A	3.40	1.63	1.59
3	B	602	GTP	PB-O3A	3.40	1.63	1.59
3	C	602	GTP	PB-O3A	3.19	1.62	1.59

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	SIN	C2-C3-C4	3.14	122.00	113.67
3	A	602	GTP	O2B-PB-O3B	2.83	114.93	107.27
3	D	603	GTP	O2G-PG-O3B	2.74	113.83	104.64
3	A	602	GTP	O2G-PG-O3B	2.72	113.77	104.64
2	A	603	DTP	O3A-PA-O1A	-2.71	102.54	110.70

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	605	SIN	C1-C2-C3-C4
5	C	605	SIN	C1-C2-C3-C4
5	A	606	SIN	C1-C2-C3-C4
5	A	607	SIN	C1-C2-C3-C4
2	C	601	DTP	PB-O3B-PG-O1G

There are no ring outliers.

10 monomers are involved in 23 short contacts:

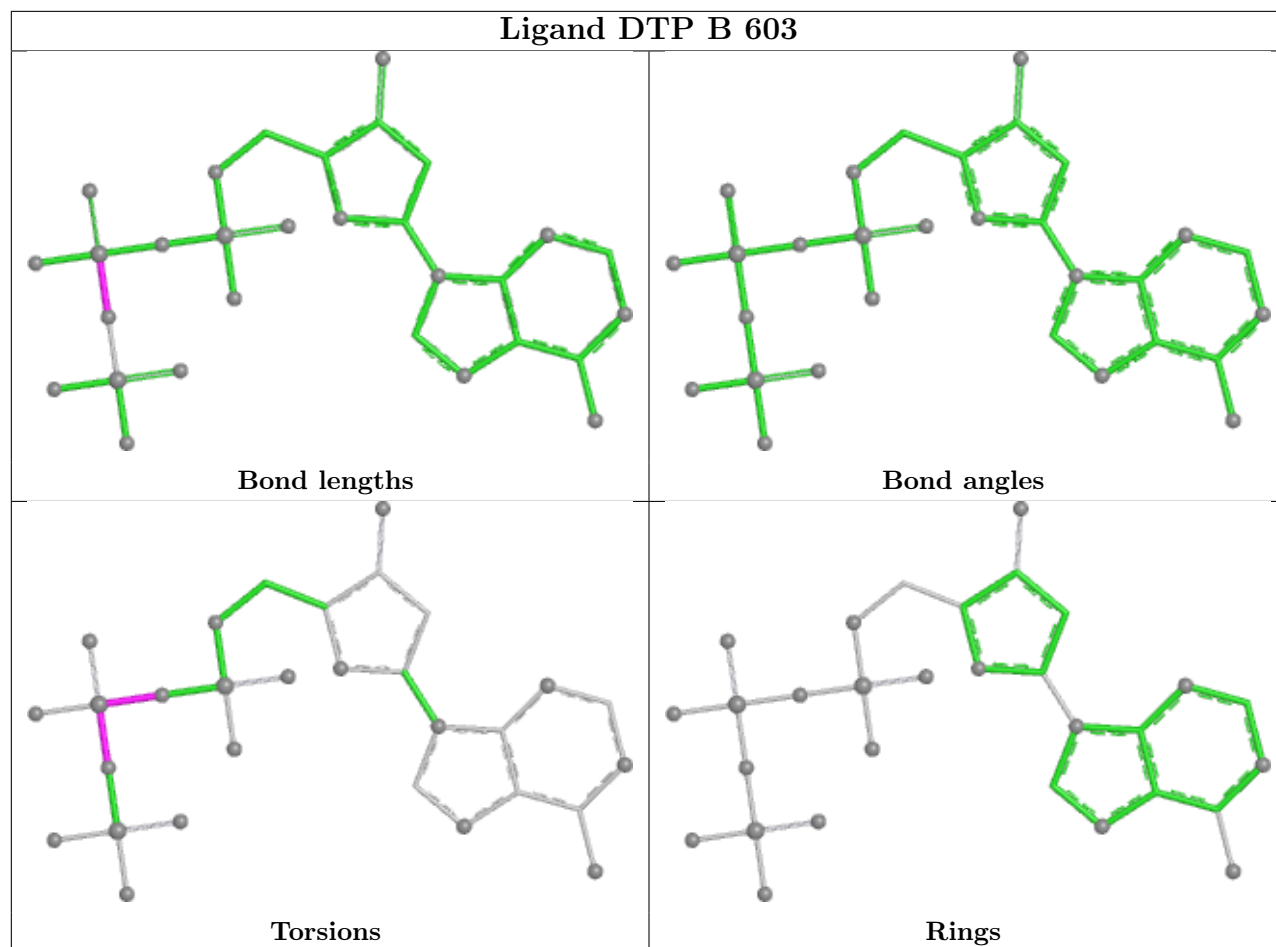
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	602	DTP	2	0

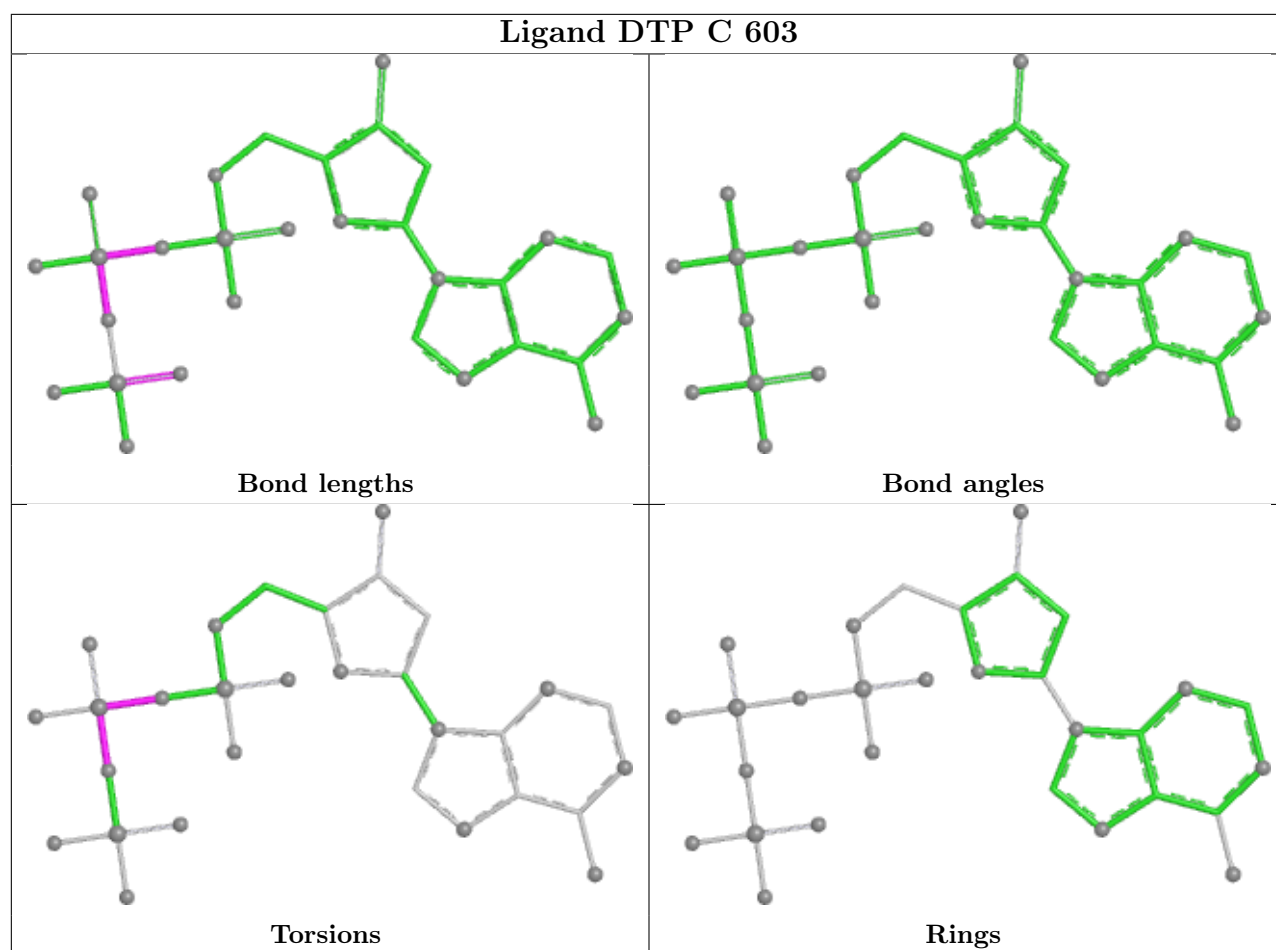
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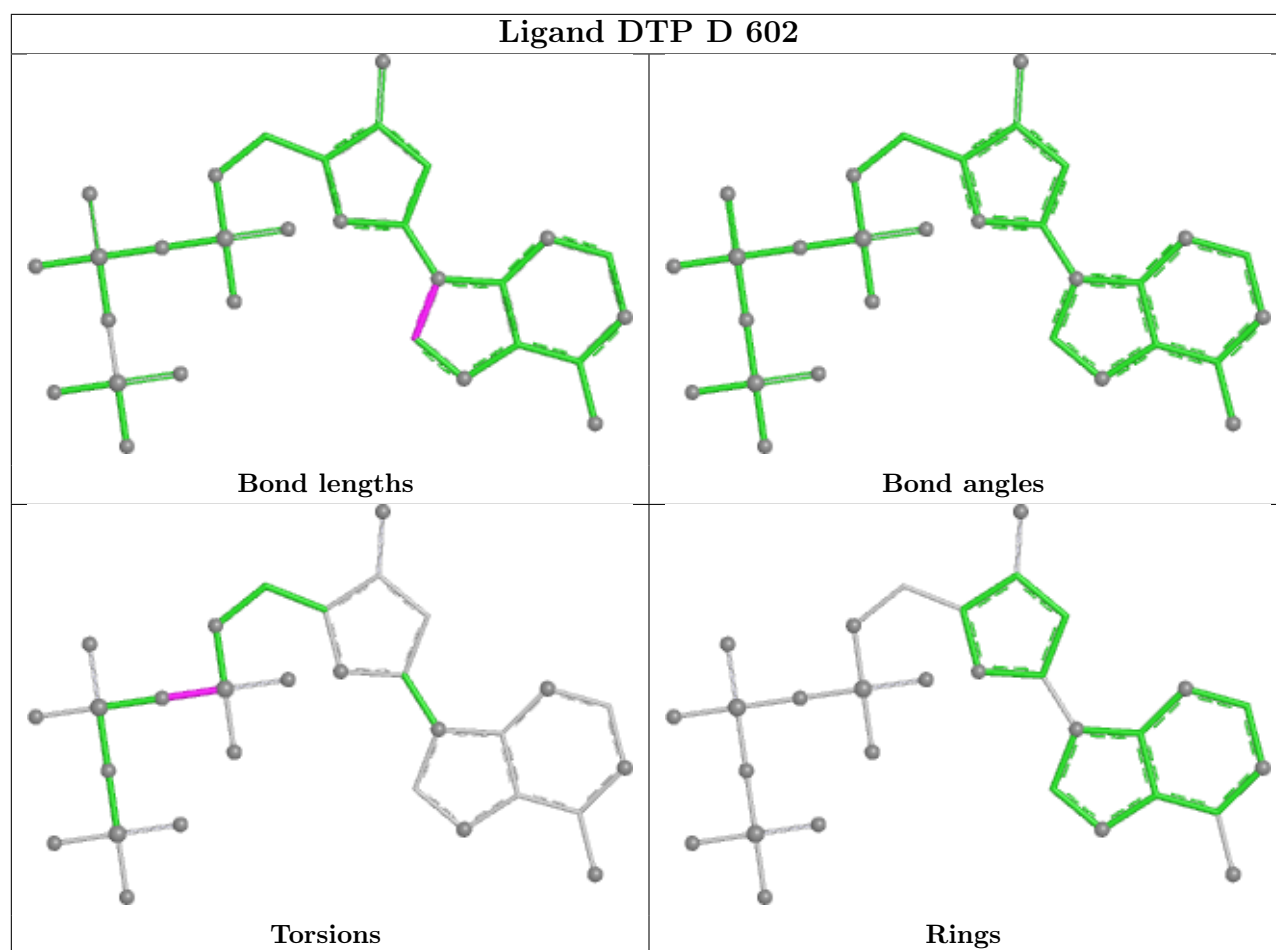
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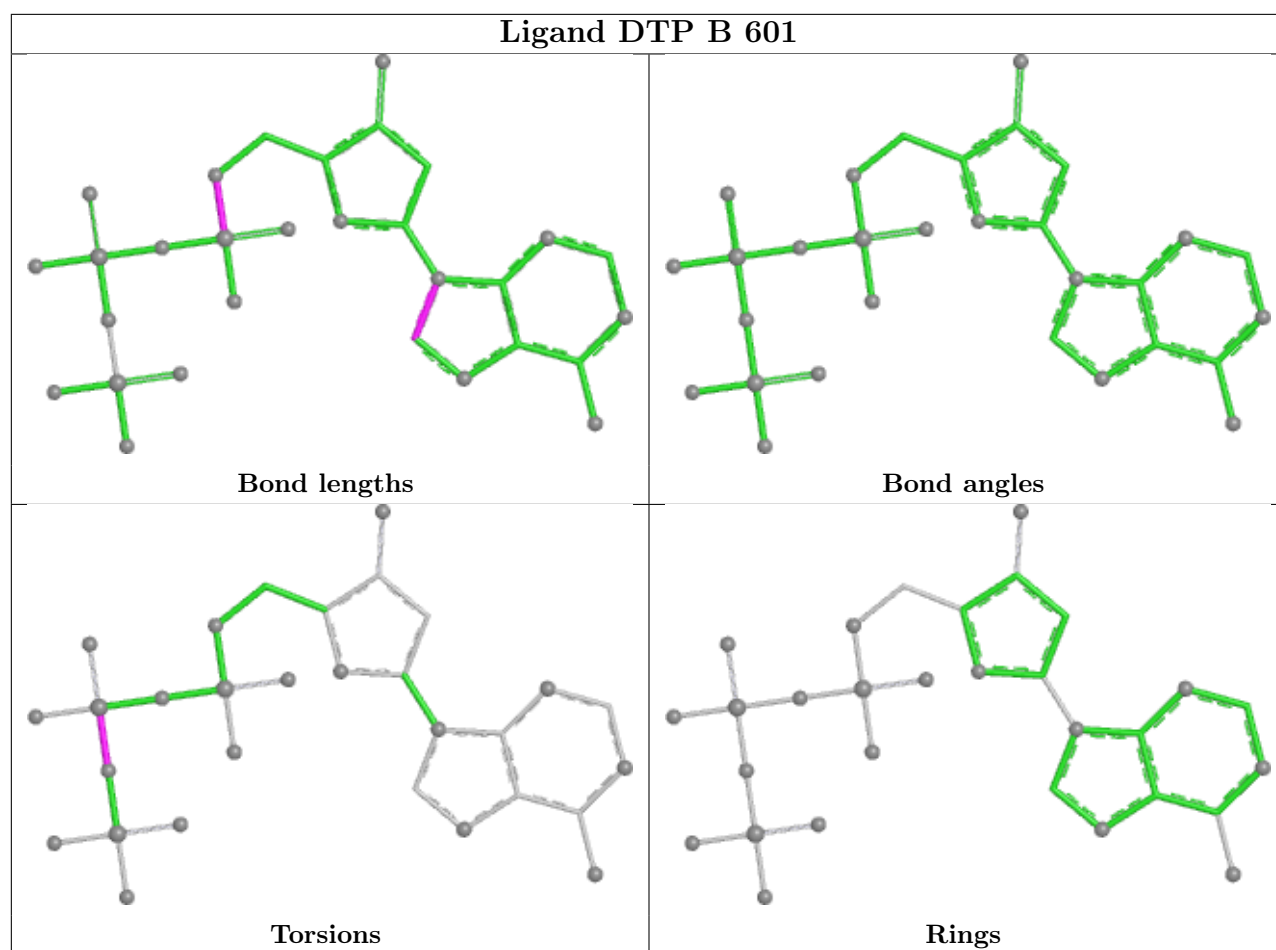
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	DTP	5	0
5	A	607	SIN	1	0
5	B	605	SIN	4	0
5	C	604	SIN	2	0
2	C	601	DTP	3	0
5	C	605	SIN	3	0
5	B	606	SIN	3	0
2	A	601	DTP	1	0
5	A	606	SIN	1	0

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.

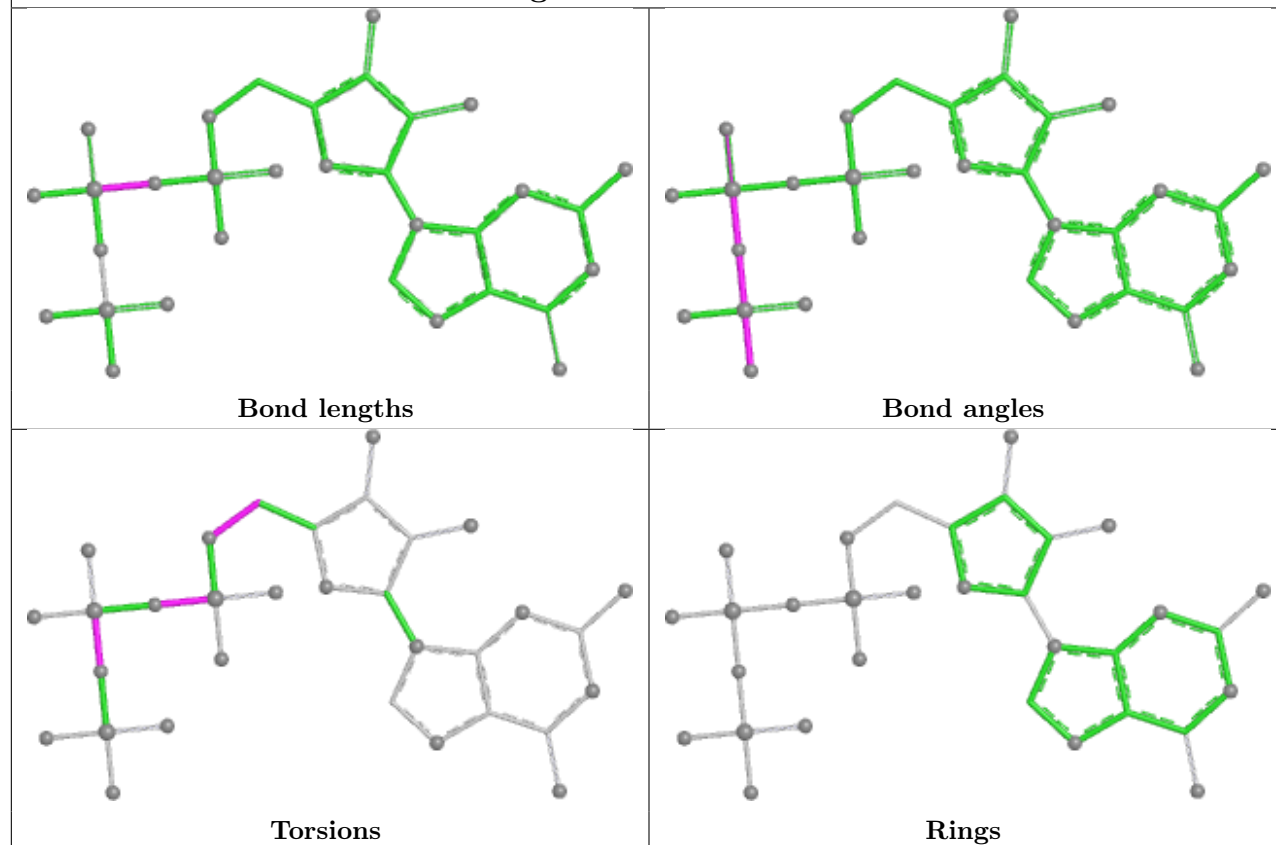




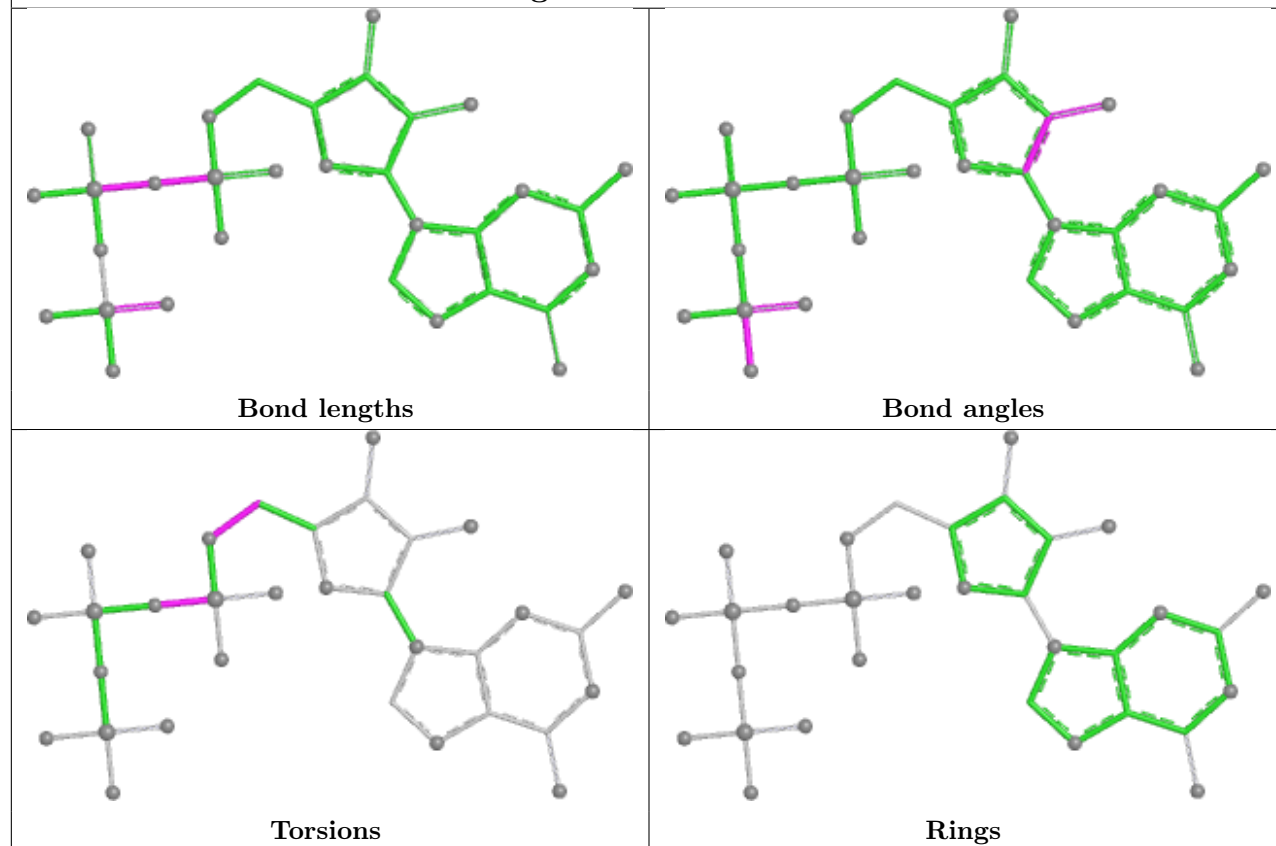


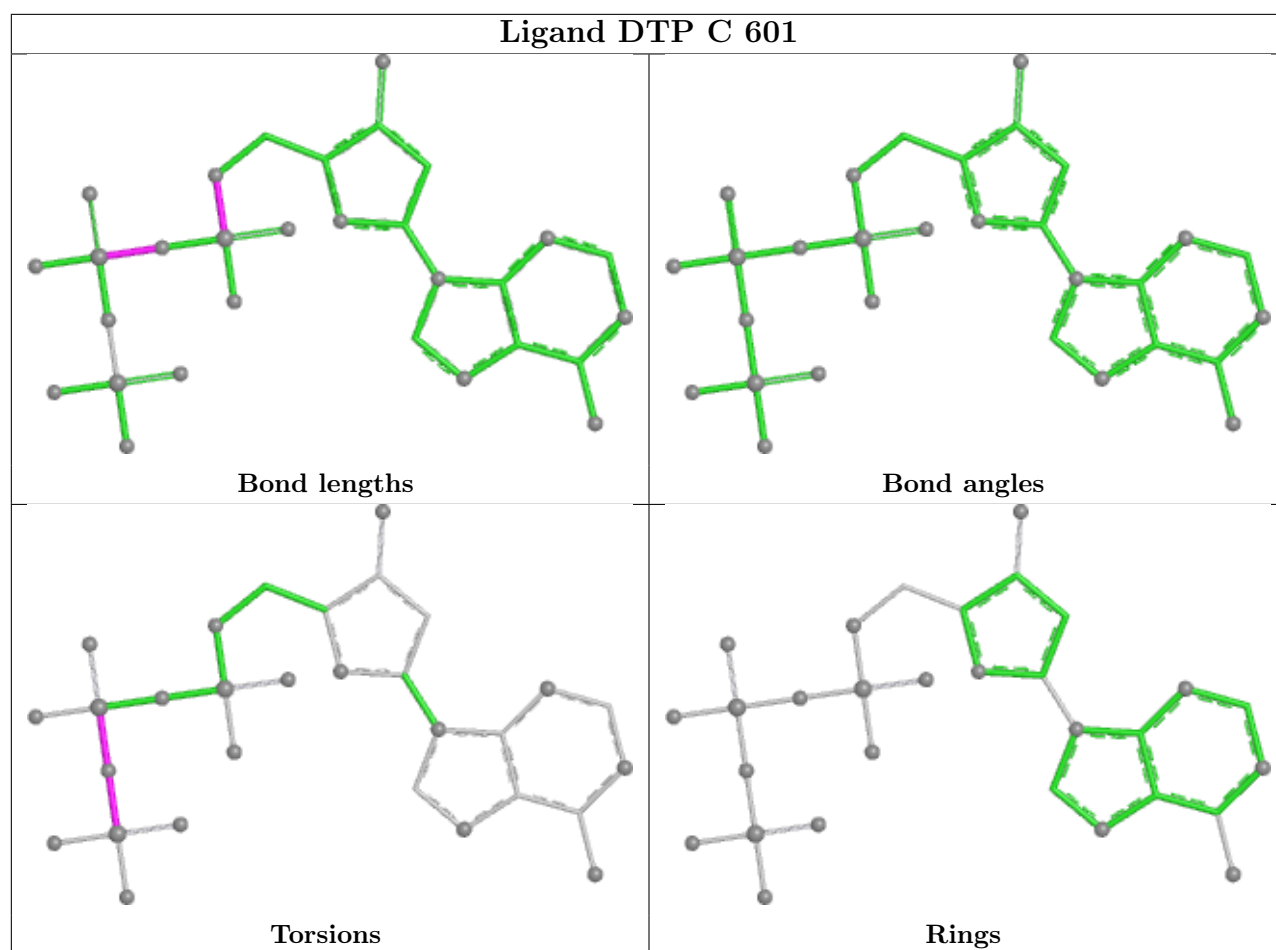


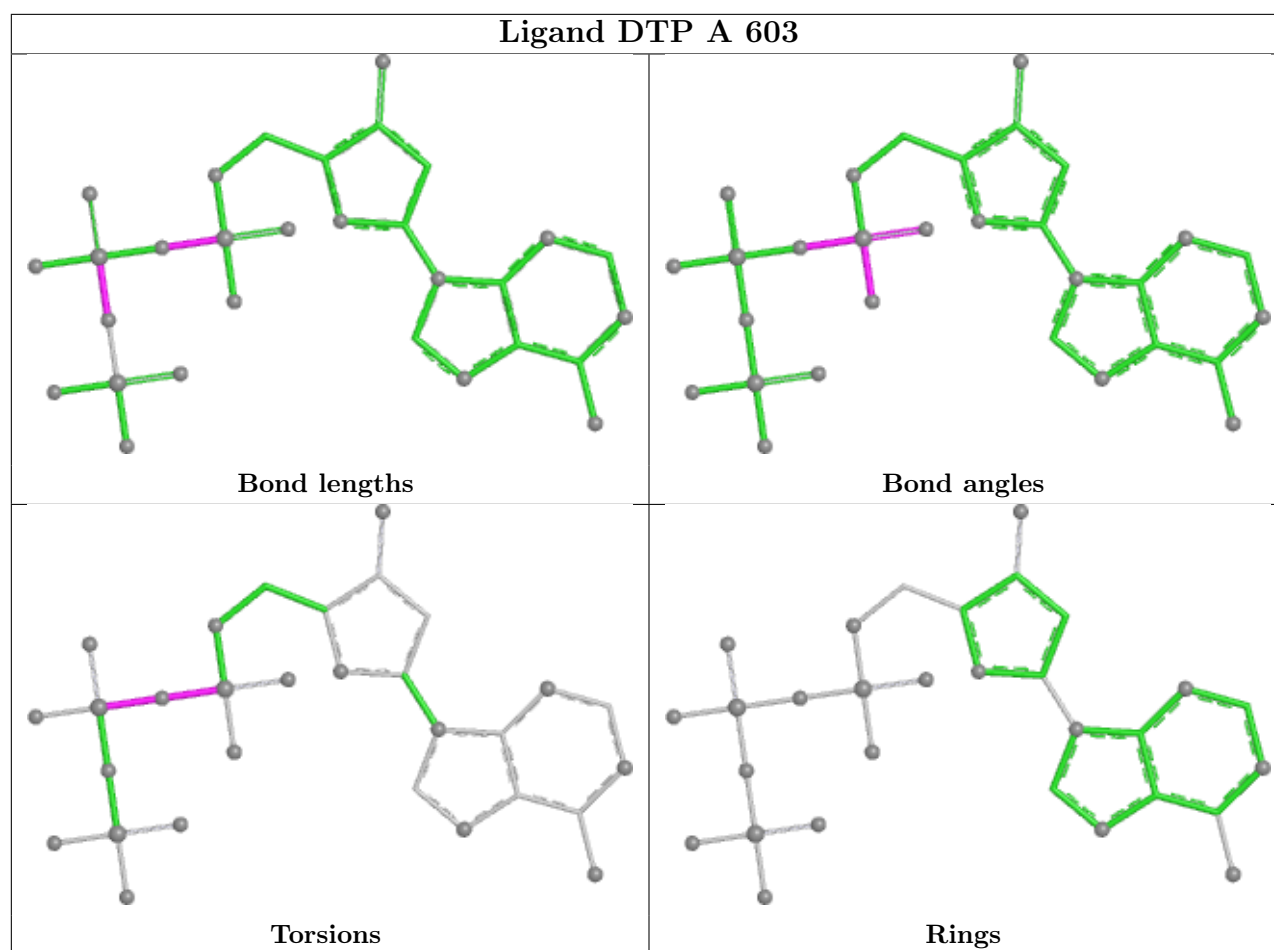
Ligand GTP A 602



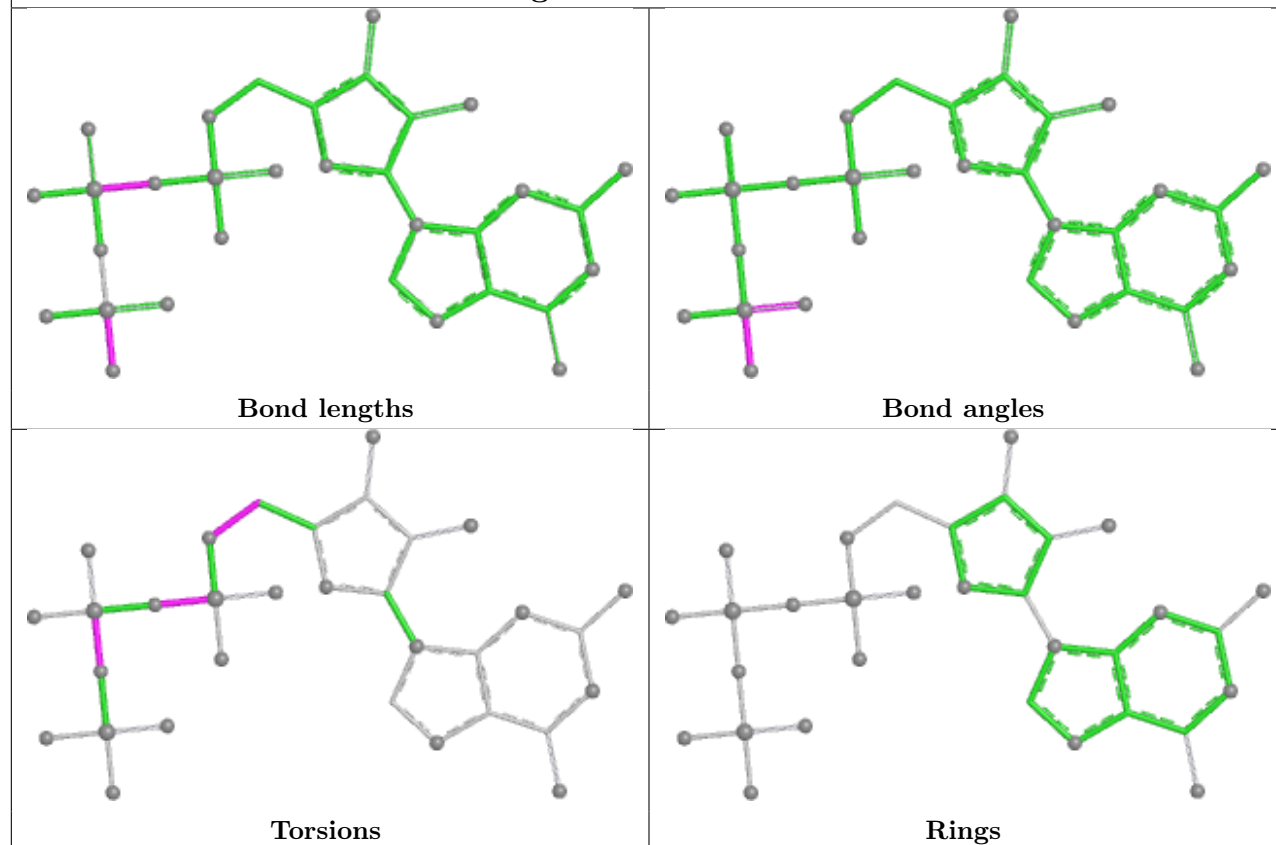
Ligand GTP C 602



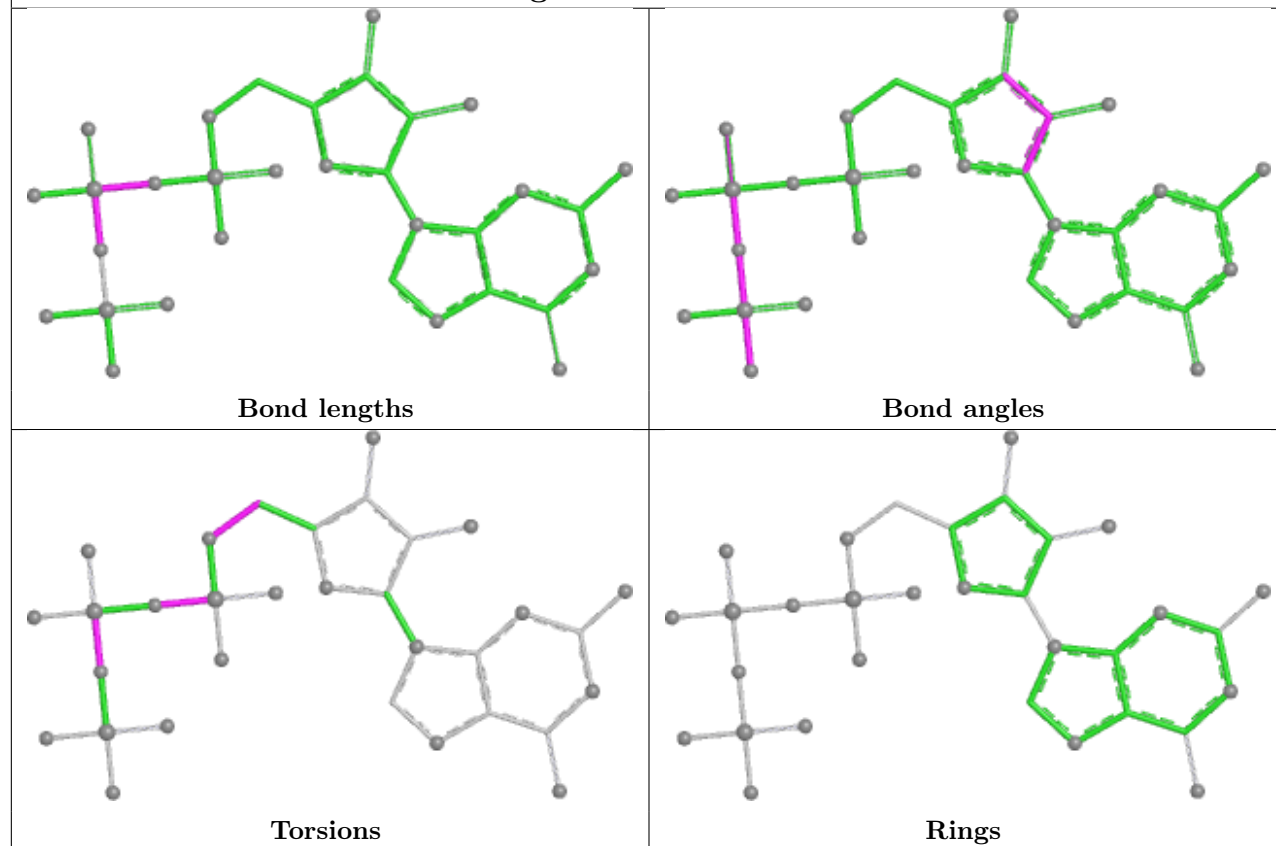


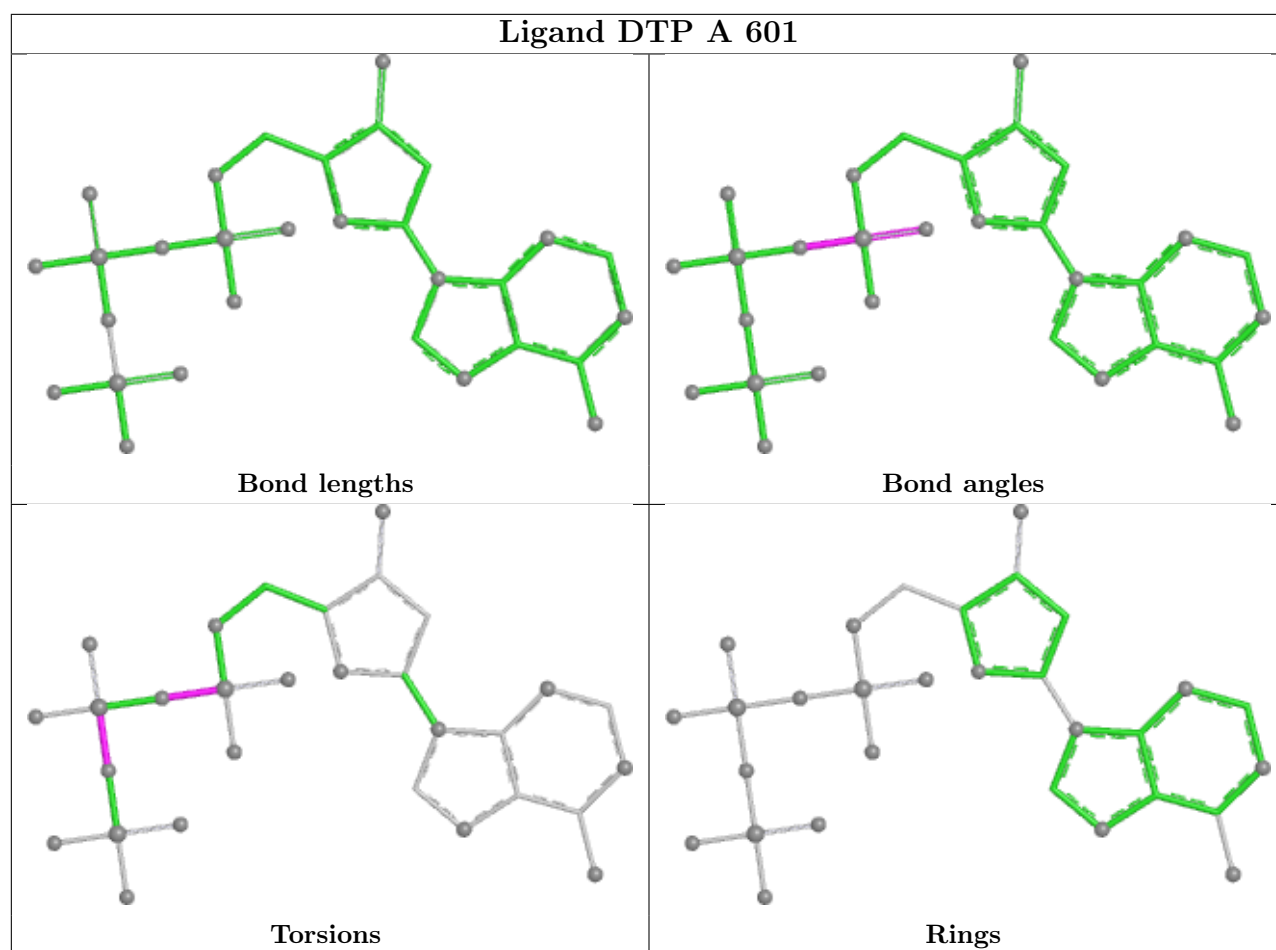


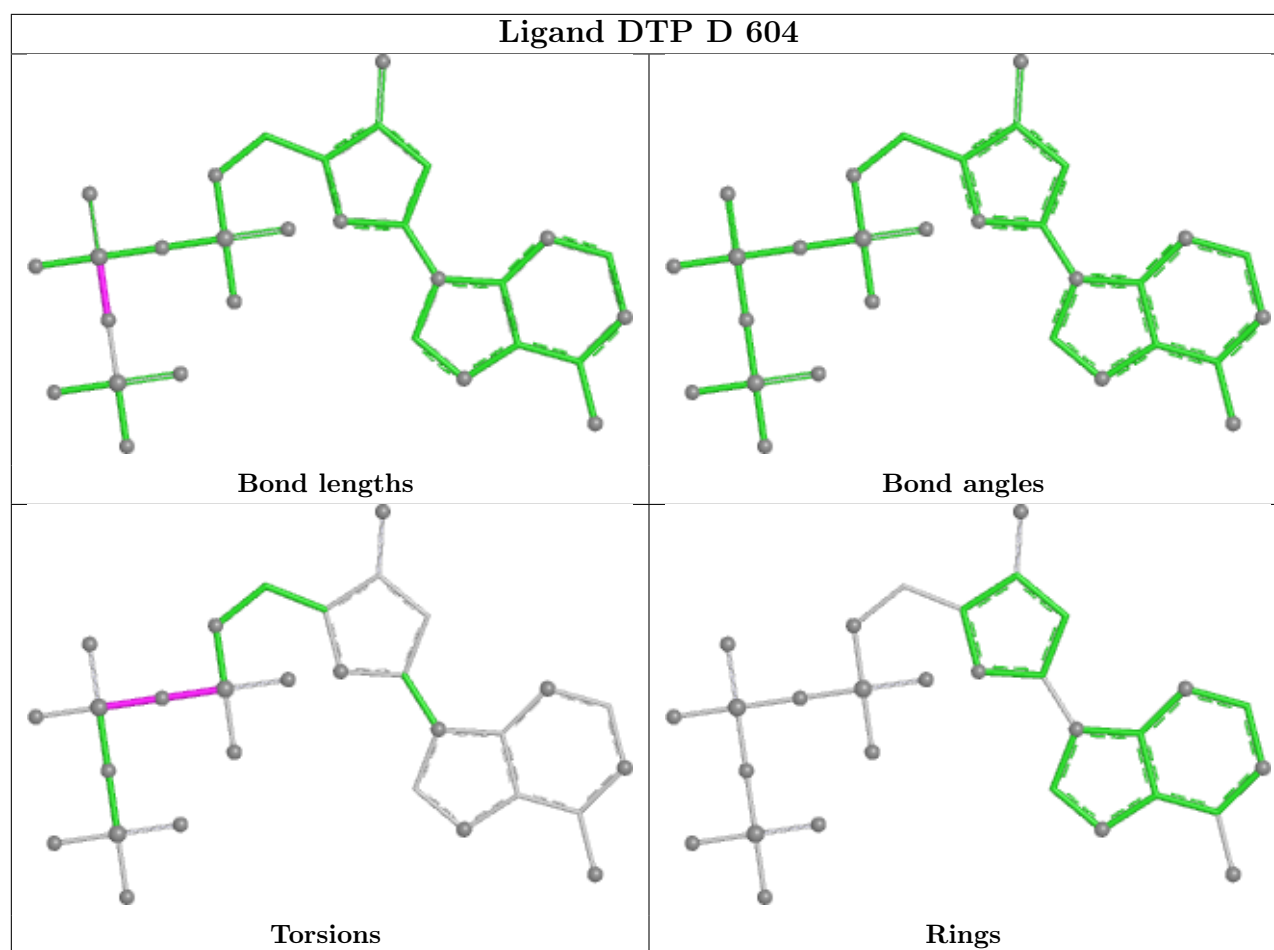
Ligand GTP B 602



Ligand GTP D 603







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	504/526 (95%)	-1.10	0 100 100	10, 26, 66, 92	4 (0%)
1	B	513/526 (97%)	-1.12	0 100 100	9, 24, 66, 102	4 (0%)
1	C	513/526 (97%)	-1.10	0 100 100	10, 24, 67, 102	3 (0%)
1	D	503/526 (95%)	-1.11	0 100 100	10, 26, 64, 93	4 (0%)
All	All	2033/2104 (96%)	-1.11	0 100 100	9, 25, 67, 102	15 (0%)

There are no RSRZ outliers to report.

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
5	SIN	B	605	8/8	0.94	0.13	50,52,55,66	0
5	SIN	A	606	8/8	0.95	0.10	34,48,59,62	0
5	SIN	C	605	8/8	0.95	0.12	48,52,58,64	0
5	SIN	B	606	8/8	0.96	0.12	36,54,70,72	0

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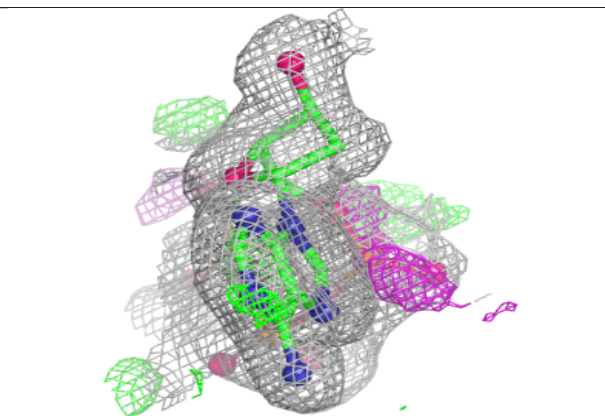
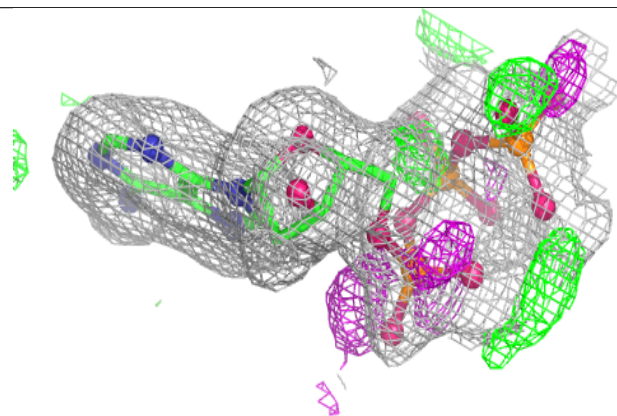
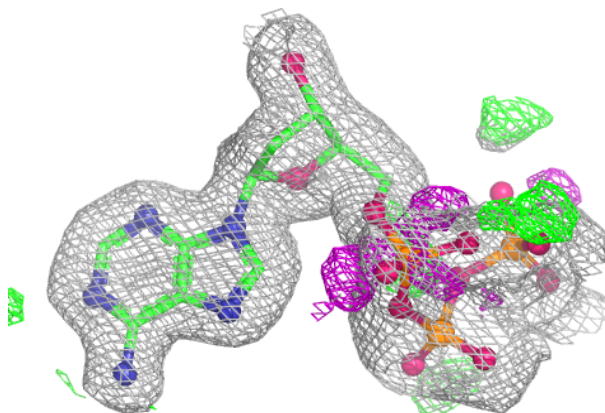
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SIN	C	604	8/8	0.96	0.10	37,45,57,72	0
5	SIN	A	607	8/8	0.96	0.11	30,45,61,62	0
2	DTP	A	601	30/30	0.98	0.05	19,22,125,128	0
2	DTP	B	601	30/30	0.98	0.05	14,20,90,103	0
2	DTP	D	602	30/30	0.98	0.05	17,25,120,129	0
2	DTP	C	601	30/30	0.99	0.05	16,20,93,102	0
3	GTP	D	603	32/32	0.99	0.02	12,15,22,23	0
4	MG	D	601	1/1	0.99	0.02	15,15,15,15	0
4	MG	A	604	1/1	1.00	0.02	12,12,12,12	0
4	MG	A	605	1/1	1.00	0.02	18,18,18,18	0
4	MG	B	604	1/1	1.00	0.02	13,13,13,13	0
2	DTP	D	604	30/30	1.00	0.02	10,12,14,16	0
2	DTP	B	603	30/30	1.00	0.02	9,11,12,13	0
2	DTP	C	603	30/30	1.00	0.02	9,11,12,13	0
3	GTP	A	602	32/32	1.00	0.02	11,14,22,23	0
3	GTP	B	602	32/32	1.00	0.02	10,11,18,20	0
2	DTP	A	603	30/30	1.00	0.02	11,12,15,16	0
3	GTP	C	602	32/32	1.00	0.02	9,11,17,19	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.

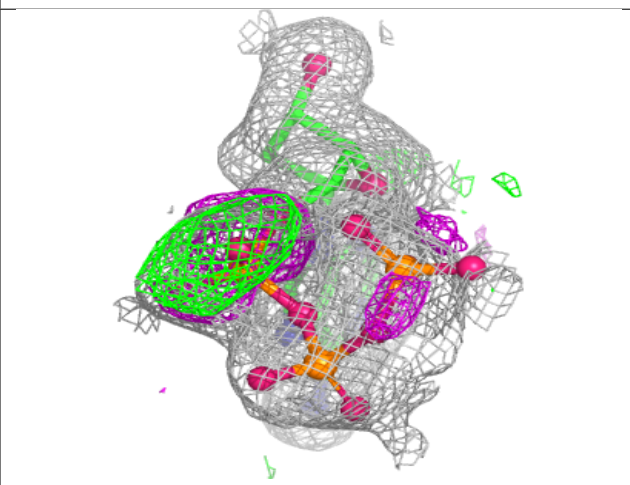
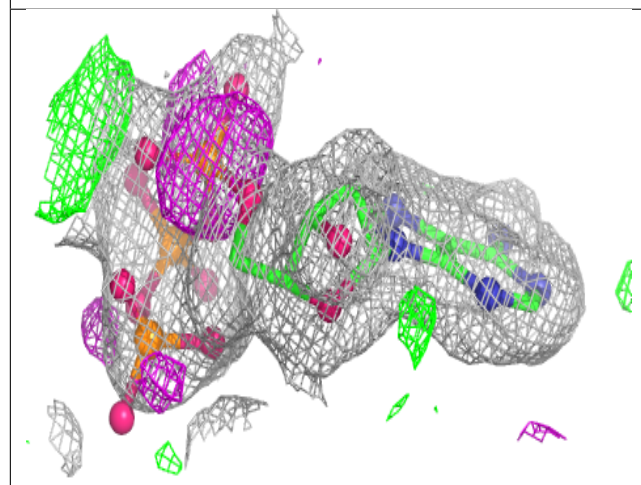
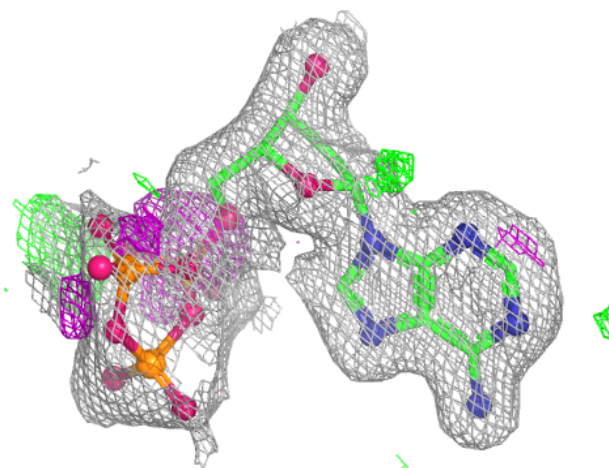
Electron density around DTP A 601:

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



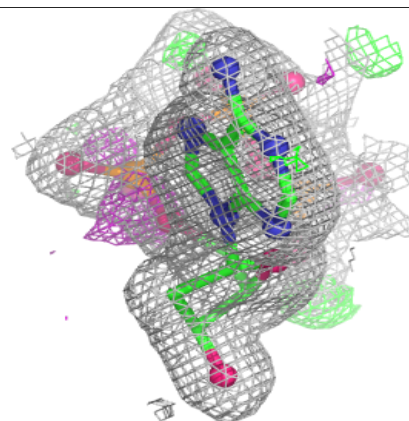
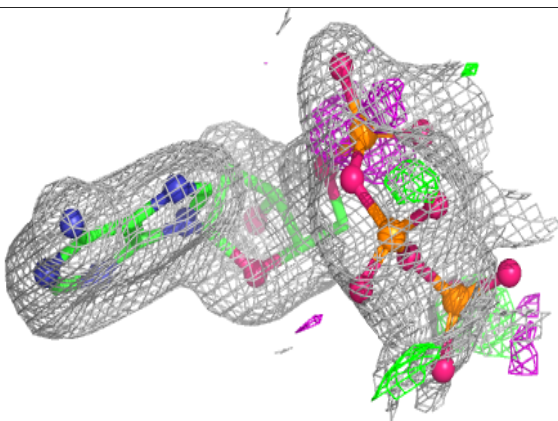
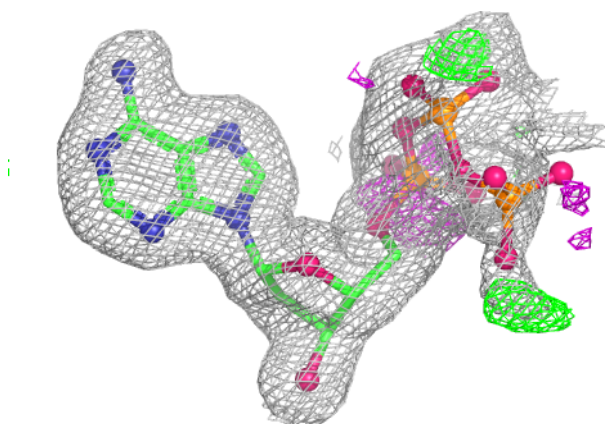
Electron density around DTP B 601:

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



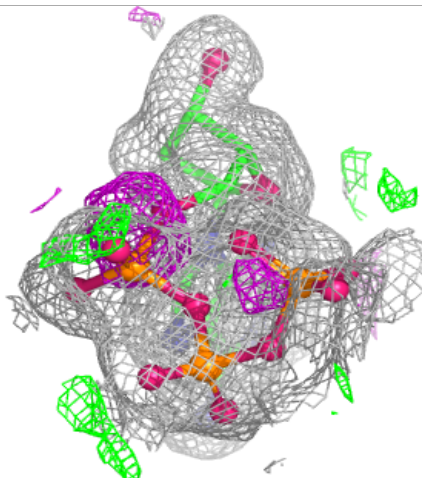
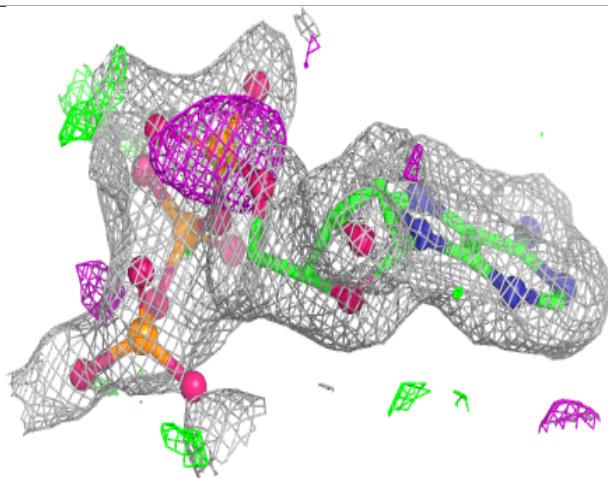
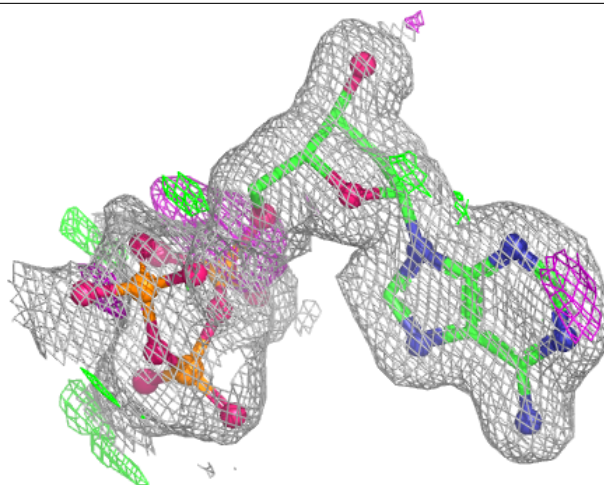
Electron density around DTP D 602:

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



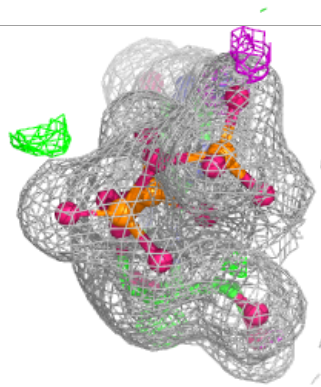
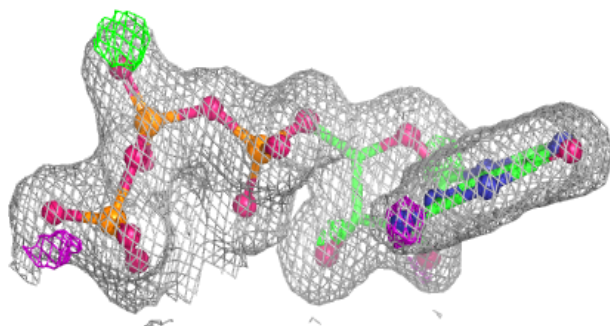
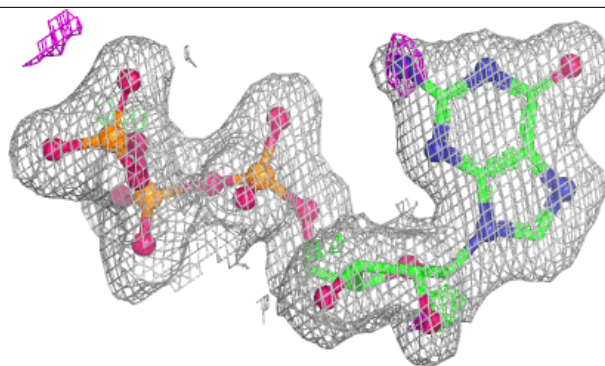
Electron density around DTP C 601:

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

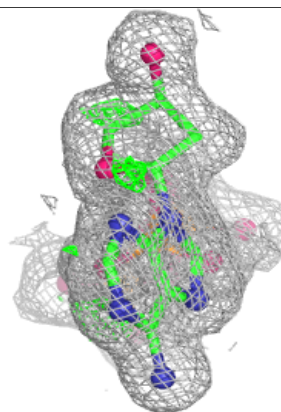
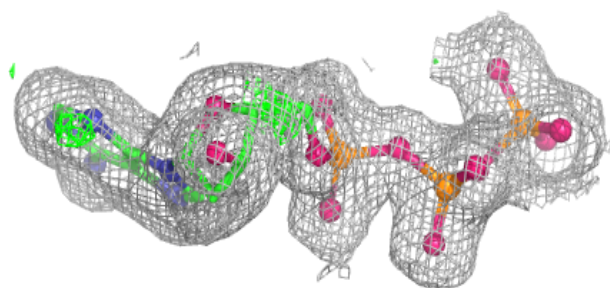
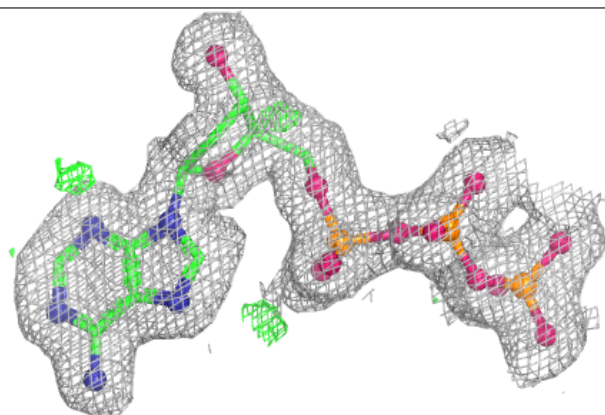


Electron density around GTP D 603:

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

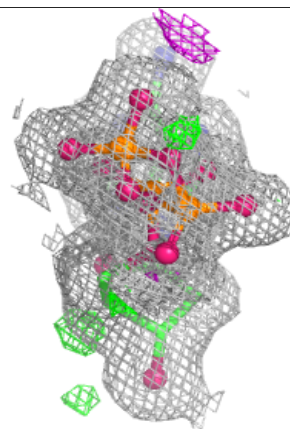
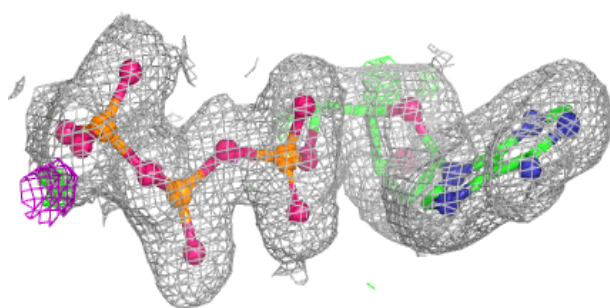
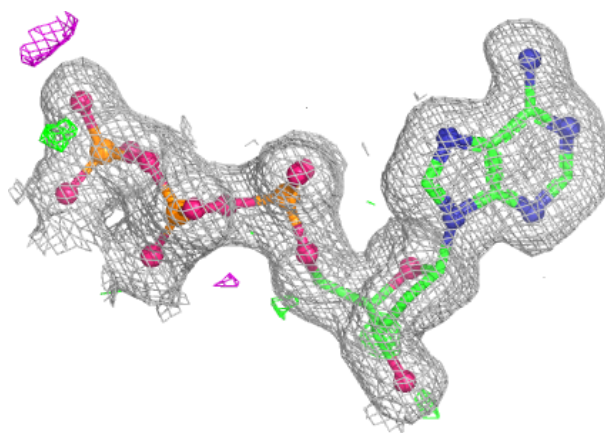
**Electron density around DTP D 604:**

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and green (positive)

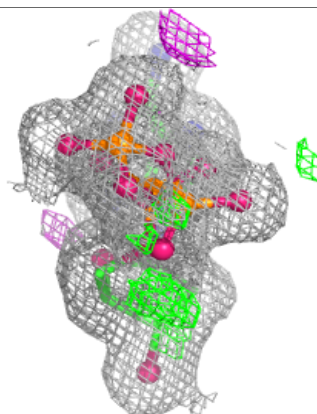
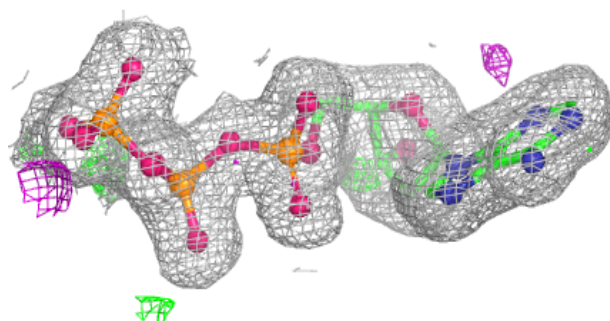
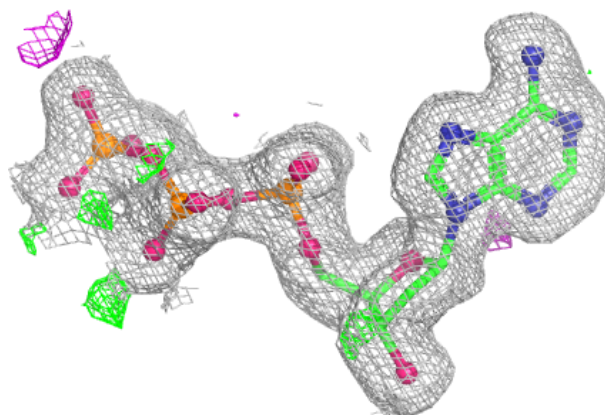


Electron density around DTP B 603:

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

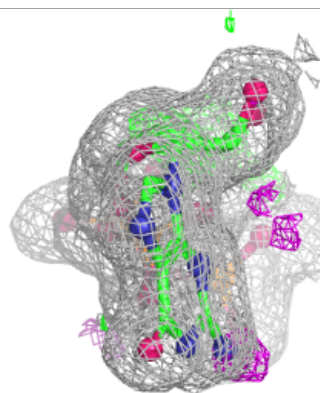
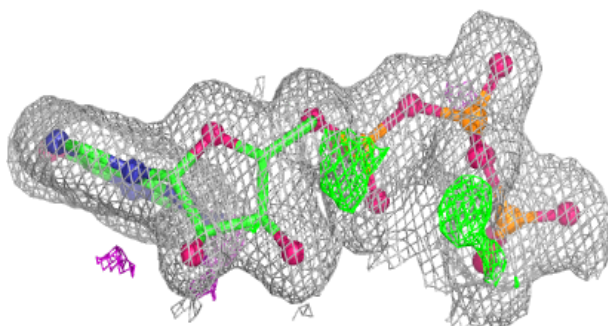
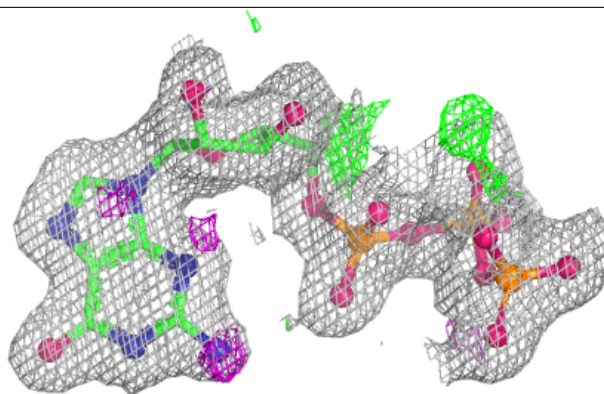
**Electron density around DTP C 603:**

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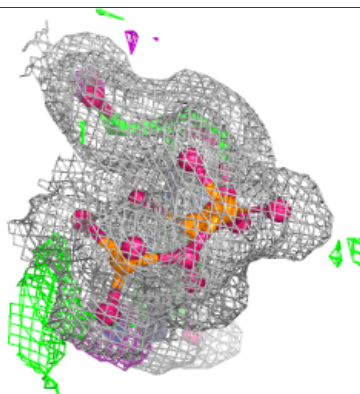
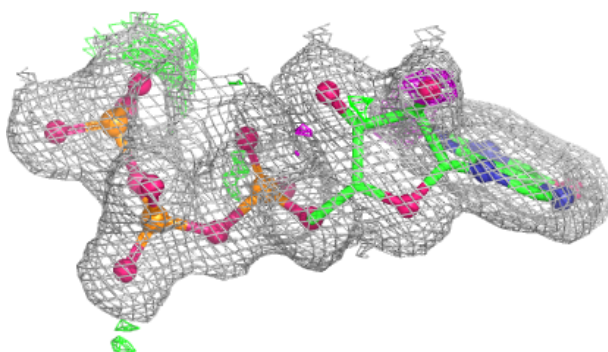
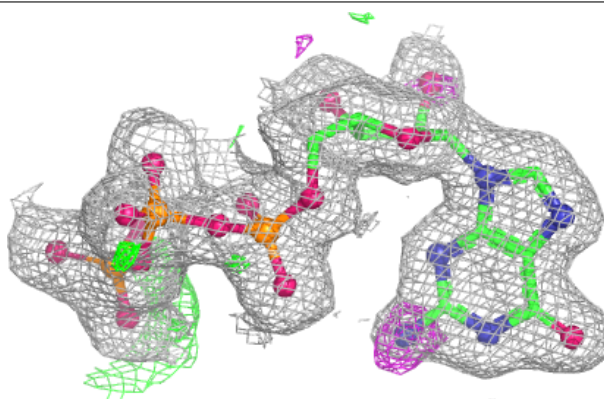


Electron density around GTP A 602:

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and green (positive)

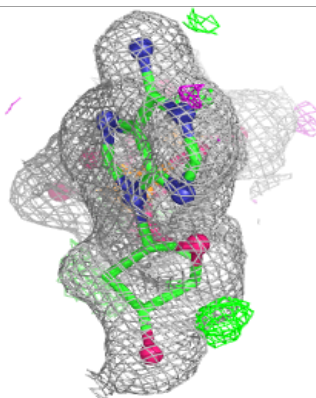
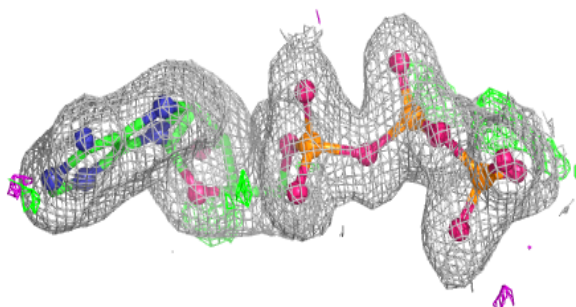
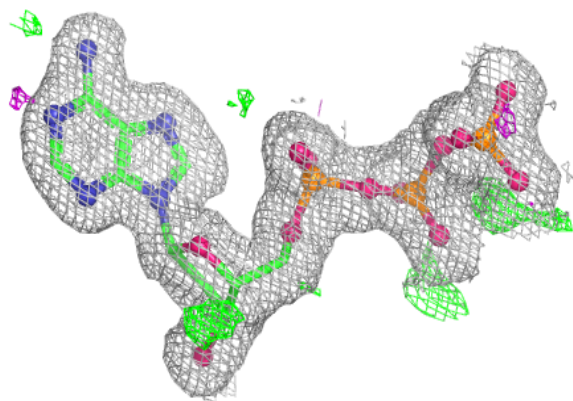
**Electron density around GTP B 602:**

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

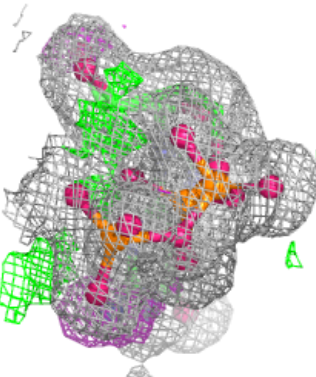
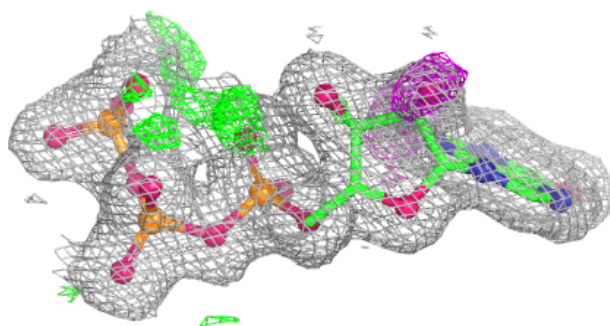
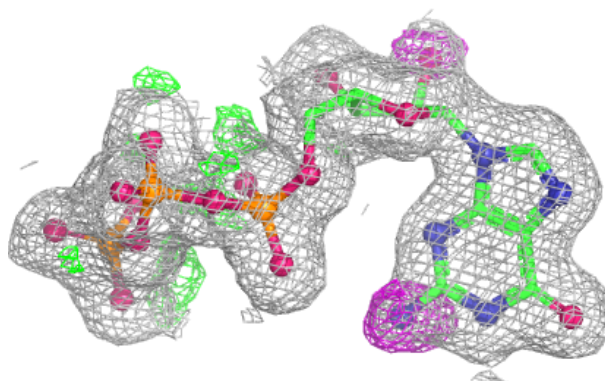


Electron density around DTP A 603:

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

**Electron density around GTP C 602:**

$2mF_o-DF_c$ (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.