Full wwPDB EM Validation Report (i)

May 5, 2025 – 10:38 PM EDT

PDB ID	:	9D5N / pdb_00009d5n
EMDB ID	:	EMD-46580
Title	:	48-nm doublet microtubule from Trichomonas vaginalis strain G3
Authors	:	Stevens, A.; Zhou, H.Z.; Kashyap, S.; Crofut, E.J.
Deposited on	:	2024-08-13
Resolution	:	4.20 Å(reported)
Based on initial model	:	.

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 1449349 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	427	3369	2127	577	644	21	0	0
1	Fl	427	3369	2127	577	644	21	0	0
1	Fm	427	3369	2127	577	644	21	0	0
1	Fn	427	3369	2127	577	644	21	0	0
1	Fo	427	3369	2127	577	644	21	0	0
1	Fp	427	3369	2127	577	644	21	0	0
1	Fq	427	3369	2127	577	644	21	0	0
1	Fr	427	3369	2127	577	644	21	0	0
1	Fs	427	3369	2127	577	644	21	0	0
1	A0	427	3369	2127	577	644	21	0	0
1	Ft	427	3369	2127	577	644	21	0	0
1	Fu	427	3369	2127	577	644	21	0	0
1	Fv	427	3369	2127	577	644	21	0	0
1	Fw	427	3369	2127	577	644	21	0	0
1	Fx	427	3369	2127	577	644	21	0	0
1	Fy	427	3369	2127	577	644	21	0	0
1	Fz	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	GH	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	GU	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	GV	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	GW	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	GX	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	GY	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	GZ	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Ga	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gb	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gc	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gd	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Ge	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gf	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gg	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gh	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gi	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gj	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gk	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Gm	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	O	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	P	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	U	427	3369	2127	577	644	21	0	0
1	X	427	3369	2127	577	644	21	0	0
1	A3	427	3369	2127	577	644	21	0	0
1	m	427	3369	2127	577	644	21	0	0
1	n	427	3369	2127	577	644	21	0	0
1	r	427	3369	2127	577	644	21	0	0
1	AA	427	3369	2127	577	644	21	0	0
1	AB	427	3369	2127	577	644	21	0	0
1	AC	427	3369	2127	577	644	21	0	0
1	AD	427	3369	2127	577	644	21	0	0
1	AE	427	3369	2127	577	644	21	0	0
1	AF	427	3369	2127	577	644	21	0	0
1	AG	427	3369	2127	577	644	21	0	0
1	AH	427	3369	2127	577	644	21	0	0
1	AL	427	3369	2127	577	644	21	0	0
1	AM	427	3369	2127	577	644	21	0	0
1	AN	427	3369	2127	577	644	21	0	0
1	AO	427	3369	2127	577	644	21	0	0
1	AP	427	3369	2127	577	644	21	0	0
1	AQ	427	3369	2127	577	644	21	0	0
1	AR	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AS	427	3369	2127	577	644	21	0	0
1	AT	427	3369	2127	577	644	21	0	0
1	AU	427	3369	2127	577	644	21	0	0
1	AV	427	3369	2127	577	644	21	0	0
1	AW	427	3369	2127	577	644	21	0	0
1	AX	427	3369	2127	577	644	21	0	0
1	AY	427	3369	2127	577	644	21	0	0
1	AZ	427	3369	2127	577	644	21	0	0
1	Aa	427	3369	2127	577	644	21	0	0
1	Ab	427	3369	2127	577	644	21	0	0
1	Ac	427	3369	2127	577	644	21	0	0
1	Ad	427	3369	2127	577	644	21	0	0
1	Ae	427	3369	2127	577	644	21	0	0
1	Af	427	3369	2127	577	644	21	0	0
1	Ag	427	3369	2127	577	644	21	0	0
1	Ah	427	3369	2127	577	644	21	0	0
1	Ai	427	3369	2127	577	644	21	0	0
1	Am	427	3369	2127	577	644	21	0	0
1	An	427	3369	2127	577	644	21	0	0
1	Ao	427	3369	2127	577	644	21	0	0
1	Ap	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Aq	427	3369	2127	577	644	21	0	0
1	Ar	427	3369	2127	577	644	21	0	0
1	As	427	3369	2127	577	644	21	0	0
1	At	427	3369	2127	577	644	21	0	0
1	Au	427	3369	2127	577	644	21	0	0
1	Av	427	3369	2127	577	644	21	0	0
1	Az	427	3369	2127	577	644	21	0	0
1	BA	427	3369	2127	577	644	21	0	0
1	BB	427	3369	2127	577	644	21	0	0
1	BC	427	3369	2127	577	644	21	0	0
1	BD	427	3369	2127	577	644	21	0	0
1	BE	427	3369	2127	577	644	21	0	0
1	BF	427	3369	2127	577	644	21	0	0
1	BG	427	3369	2127	577	644	21	0	0
1	BH	427	3369	2127	577	644	21	0	0
1	BW	427	3369	2127	577	644	21	0	0
1	BZ	427	3369	2127	577	644	21	0	0
1	Ba	427	3369	2127	577	644	21	0	0
1	Bb	427	3369	2127	577	644	21	0	0
1	Be	427	3369	2127	577	644	21	0	0
1	Bf	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Bg	427	3369	2127	577	644	21	0	0
1	Bh	427	3369	2127	577	644	21	0	0
1	Bi	427	3369	2127	577	644	21	0	0
1	Bj	427	3369	2127	577	644	21	0	0
1	Bk	427	3369	2127	577	644	21	0	0
1	Bl	427	3369	2127	577	644	21	0	0
1	Bm	427	3369	2127	577	644	21	0	0
1	Bn	427	3369	2127	577	644	21	0	0
1	Bo	427	3369	2127	577	644	21	0	0
1	Bp	427	3369	2127	577	644	21	0	0
1	Bq	427	3369	2127	577	644	21	0	0
1	Br	427	3369	2127	577	644	21	0	0
1	Bs	427	3369	2127	577	644	21	0	0
1	Bt	427	3369	2127	577	644	21	0	0
1	DL	427	3369	2127	577	644	21	0	0
1	DM	427	3369	2127	577	644	21	0	0
1	DN	427	3369	2127	577	644	21	0	0
1	DO	427	3369	2127	577	644	21	0	0
1	DP	427	3369	2127	577	644	21	0	0
1	DQ	427	3369	2127	577	644	21	0	0
1	DR	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DS	427	3369	2127	577	644	21	0	0
1	DT	427	3369	2127	577	644	21	0	0
1	DU	427	3369	2127	577	644	21	0	0
1	DV	427	3369	2127	577	644	21	0	0
1	DW	427	3369	2127	577	644	21	0	0
1	DX	427	3369	2127	577	644	21	0	0
1	DY	427	3369	2127	577	644	21	0	0
1	DZ	427	3369	2127	577	644	21	0	0
1	Da	427	3369	2127	577	644	21	0	0
1	Db	427	3369	2127	577	644	21	0	0
1	Dc	427	3369	2127	577	644	21	0	0
1	Dd	427	3369	2127	577	644	21	0	0
1	De	427	3369	2127	577	644	21	0	0
1	Df	427	3369	2127	577	644	21	0	0
1	Dg	427	3369	2127	577	644	21	0	0
1	Dh	427	3369	2127	577	644	21	0	0
1	Di	427	3369	2127	577	644	21	0	0
1	Dj	427	3369	2127	577	644	21	0	0
1	Dk	427	3369	2127	577	644	21	0	0
1	Dq	427	3369	2127	577	644	21	0	0
1	Dr	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Ds	427	3369	2127	577	644	21	0	0
1	Dt	427	3369	2127	577	644	21	0	0
1	Du	427	3369	2127	577	644	21	0	0
1	Dv	427	3369	2127	577	644	21	0	0
1	Dw	427	3369	2127	577	644	21	0	0
1	Dx	427	3369	2127	577	644	21	0	0
1	E0	427	3369	2127	577	644	21	0	0
1	E9	427	3369	2127	577	644	21	0	0
1	EL	427	3369	2127	577	644	21	0	0
1	EM	427	3369	2127	577	644	21	0	0
1	EN	427	3369	2127	577	644	21	0	0
1	EO	427	3369	2127	577	644	21	0	0
1	EP	427	3369	2127	577	644	21	0	0
1	EQ	427	3369	2127	577	644	21	0	0
1	ER	427	3369	2127	577	644	21	0	0
1	ES	427	3369	2127	577	644	21	0	0
1	ET	427	3369	2127	577	644	21	0	0
1	EU	427	3369	2127	577	644	21	0	0
1	EV	427	3369	2127	577	644	21	0	0
1	EW	427	3369	2127	577	644	21	0	0
1	EX	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	EY	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	EZ	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Ea	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Eb	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Ec	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Ed	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Ef	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	7	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	Ev	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	F1	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	F2	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	8	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	F4	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	FA	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	FB	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	FC	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	FD	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	FE	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	FF	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	FG	427	3369	2127	577	644	21	0	0
			Total	C	N	O	S		
1	FH	427	3369	2127	577	644	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	FI	427	3369	2127	577	644	21	0	0
1	FJ	427	3369	2127	577	644	21	0	0
1	FK	427	3369	2127	577	644	21	0	0
1	FL	427	3369	2127	577	644	21	0	0
1	FN	427	3369	2127	577	644	21	0	0
1	9	427	3369	2127	577	644	21	0	0

- Molecule 2 is a protein called FAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	55	451	280	83	86	2	0	0

- Molecule 3 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Fi	430	3365	2140	570	635	20	0	0
3	Fj	430	3365	2140	570	635	20	0	0
3	Fk	430	3365	2140	570	635	20	0	0
3	G1	430	3365	2140	570	635	20	0	0
3	G2	430	3365	2140	570	635	20	0	0
3	G3	430	3365	2140	570	635	20	0	0
3	G4	430	3365	2140	570	635	20	0	0
3	G5	430	3365	2140	570	635	20	0	0
3	G6	430	3365	2140	570	635	20	0	0
3	GA	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	GB	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GC	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GD	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GE	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	A1	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GF	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GG	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GI	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GJ	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GK	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GL	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GM	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GN	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GO	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GP	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GQ	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GR	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GS	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	GT	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	A2	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	Gl	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Gn	430	3365	2140	570	635	20	0	0
3	Go	430	3365	2140	570	635	20	0	0
3	Gp	430	3365	2140	570	635	20	0	0
3	Gq	430	3365	2140	570	635	20	0	0
3	Gr	430	3365	2140	570	635	20	0	0
3	Gs	430	3365	2140	570	635	20	0	0
3	Gt	430	3365	2140	570	635	20	0	0
3	Gu	430	3365	2140	570	635	20	0	0
3	Gv	430	3365	2140	570	635	20	0	0
3	Gw	430	3365	2140	570	635	20	0	0
3	Gx	430	3365	2140	570	635	20	0	0
3	Gy	430	3365	2140	570	635	20	0	0
3	Gz	430	3365	2140	570	635	20	0	0
3	Q	430	3365	2140	570	635	20	0	0
3	R	430	3365	2140	570	635	20	0	0
3	S	430	3365	2140	570	635	20	0	0
3	T	430	3365	2140	570	635	20	0	0
3	V	430	3365	2140	570	635	20	0	0
3	W	430	3365	2140	570	635	20	0	0
3	Y	430	3365	2140	570	635	20	0	0
3	Z	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	a	430	3365	2140	570	635	20	0	0
3	b	430	3365	2140	570	635	20	0	0
3	c	430	3365	2140	570	635	20	0	0
3	d	430	3365	2140	570	635	20	0	0
3	e	430	3365	2140	570	635	20	0	0
3	f	430	3365	2140	570	635	20	0	0
3	g	430	3365	2140	570	635	20	0	0
3	h	430	3365	2140	570	635	20	0	0
3	i	430	3365	2140	570	635	20	0	0
3	j	430	3365	2140	570	635	20	0	0
3	k	430	3365	2140	570	635	20	0	0
3	l	430	3365	2140	570	635	20	0	0
3	o	430	3365	2140	570	635	20	0	0
3	p	430	3365	2140	570	635	20	0	0
3	A4	430	3365	2140	570	635	20	0	0
3	q	430	3365	2140	570	635	20	0	0
3	s	430	3365	2140	570	635	20	0	0
3	t	430	3365	2140	570	635	20	0	0
3	u	430	3365	2140	570	635	20	0	0
3	v	430	3365	2140	570	635	20	0	0
3	w	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	x	430	3365	2140	570	635	20	0	0
3	y	430	3365	2140	570	635	20	0	0
3	z	430	3365	2140	570	635	20	0	0
3	A5	430	3365	2140	570	635	20	0	0
3	A6	430	3365	2140	570	635	20	0	0
3	A7	430	3365	2140	570	635	20	0	0
3	A8	430	3365	2140	570	635	20	0	0
3	A9	430	3365	2140	570	635	20	0	0
3	AI	430	3365	2140	570	635	20	0	0
3	AJ	430	3365	2140	570	635	20	0	0
3	AK	430	3365	2140	570	635	20	0	0
3	1	430	3365	2140	570	635	20	0	0
3	Aj	430	3365	2140	570	635	20	0	0
3	Ak	430	3365	2140	570	635	20	0	0
3	Al	430	3365	2140	570	635	20	0	0
3	2	430	3365	2140	570	635	20	0	0
3	Aw	430	3365	2140	570	635	20	0	0
3	Ax	430	3365	2140	570	635	20	0	0
3	Ay	430	3365	2140	570	635	20	0	0
3	B0	430	3365	2140	570	635	20	0	0
3	B1	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B2	430	3365	2140	570	635	20	0	0
3	B3	430	3365	2140	570	635	20	0	0
3	B4	430	3365	2140	570	635	20	0	0
3	B5	430	3365	2140	570	635	20	0	0
3	B6	430	3365	2140	570	635	20	0	0
3	B7	430	3365	2140	570	635	20	0	0
3	B8	430	3365	2140	570	635	20	0	0
3	B9	430	3365	2140	570	635	20	0	0
3	BI	430	3365	2140	570	635	20	0	0
3	BJ	430	3365	2140	570	635	20	0	0
3	BK	430	3365	2140	570	635	20	0	0
3	BL	430	3365	2140	570	635	20	0	0
3	BM	430	3365	2140	570	635	20	0	0
3	BN	430	3365	2140	570	635	20	0	0
3	BO	430	3365	2140	570	635	20	0	0
3	3	430	3365	2140	570	635	20	0	0
3	BP	430	3365	2140	570	635	20	0	0
3	BQ	430	3365	2140	570	635	20	0	0
3	BR	430	3365	2140	570	635	20	0	0
3	BS	430	3365	2140	570	635	20	0	0
3	BT	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	BU	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	BV	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	BX	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	BY	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	Bc	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	Bd	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	Bu	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	4	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	Bv	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	Bw	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	Bx	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	By	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	Bz	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	CA	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	CB	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	5	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	E1	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	E2	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	E3	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	6	430	3365	2140	570	635	20	0	0
			Total	C	N	O	S		
3	E4	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E5	430	3365	2140	570	635	20	0	0
3	E6	430	3365	2140	570	635	20	0	0
3	E7	430	3365	2140	570	635	20	0	0
3	E8	430	3365	2140	570	635	20	0	0
3	Ee	430	3365	2140	570	635	20	0	0
3	Eg	430	3365	2140	570	635	20	0	0
3	Eh	430	3365	2140	570	635	20	0	0
3	Ei	430	3365	2140	570	635	20	0	0
3	Ej	430	3365	2140	570	635	20	0	0
3	Ek	430	3365	2140	570	635	20	0	0
3	El	430	3365	2140	570	635	20	0	0
3	Em	430	3365	2140	570	635	20	0	0
3	En	430	3365	2140	570	635	20	0	0
3	Eo	430	3365	2140	570	635	20	0	0
3	Ep	430	3365	2140	570	635	20	0	0
3	Eq	430	3365	2140	570	635	20	0	0
3	Er	430	3365	2140	570	635	20	0	0
3	Es	430	3365	2140	570	635	20	0	0
3	Et	430	3365	2140	570	635	20	0	0
3	Eu	430	3365	2140	570	635	20	0	0
3	Ew	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Ex	430	3365	2140	570	635	20	0	0
3	Ey	430	3365	2140	570	635	20	0	0
3	Ez	430	3365	2140	570	635	20	0	0
3	F0	430	3365	2140	570	635	20	0	0
3	F3	430	3365	2140	570	635	20	0	0
3	F5	430	3365	2140	570	635	20	0	0
3	F6	430	3365	2140	570	635	20	0	0
3	F7	430	3365	2140	570	635	20	0	0
3	F8	430	3365	2140	570	635	20	0	0
3	F9	430	3365	2140	570	635	20	0	0
3	FM	430	3365	2140	570	635	20	0	0
3	FO	430	3365	2140	570	635	20	0	0
3	FP	430	3365	2140	570	635	20	0	0
3	FQ	430	3365	2140	570	635	20	0	0
3	FR	430	3365	2140	570	635	20	0	0
3	FS	430	3365	2140	570	635	20	0	0
3	FT	430	3365	2140	570	635	20	0	0
3	FU	430	3365	2140	570	635	20	0	0
3	FV	430	3365	2140	570	635	20	0	0
3	FW	430	3365	2140	570	635	20	0	0
3	FX	430	3365	2140	570	635	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	FY	430	3365	2140	570	635	20	0	0
3	FZ	430	3365	2140	570	635	20	0	0
3	Fa	430	3365	2140	570	635	20	0	0
3	Fb	430	3365	2140	570	635	20	0	0
3	Fc	430	3365	2140	570	635	20	0	0
3	Fd	430	3365	2140	570	635	20	0	0
3	Fe	430	3365	2140	570	635	20	0	0
3	Ff	430	3365	2140	570	635	20	0	0
3	Fg	430	3365	2140	570	635	20	0	0
3	Fh	430	3365	2140	570	635	20	0	0

- Molecule 4 is a protein called IQ calmodulin-binding motif family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	291	2367	1461	450	451	5	0	0
4	CD	291	2367	1461	450	451	5	0	0
4	Ca	291	2367	1461	450	451	5	0	0
4	Cb	291	2367	1461	450	451	5	0	0

- Molecule 5 is a protein called Flagellar protofilament ribbon protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G0	319	2691	1629	514	538	10	0	0
5	G7	151	1252	740	252	256	4	0	0
5	G8	287	2415	1452	469	486	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G9	181	1544	947	292	300	5	0	0

- Molecule 6 is a protein called TvFAP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	377	3065	1888	582	581	14	0	0
6	CE	377	3065	1888	582	581	14	0	0
6	Cm	377	3065	1888	582	581	14	0	0
6	Cn	377	3065	1888	582	581	14	0	0

- Molecule 7 is a protein called Parkin co-regulated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	HA	208	1704	1093	302	303	6	0	0
7	HB	208	1704	1093	302	303	6	0	0
7	HC	208	1704	1093	302	303	6	0	0
7	HD	208	1704	1093	302	303	6	0	0

- Molecule 8 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	302	2520	1522	488	497	13	0	0
8	CJ	136	1128	696	209	216	7	0	0
8	CK	358	2981	1807	575	584	15	0	0
8	CL	154	1289	783	248	255	3	0	0

- Molecule 9 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	184	1547	1001	265	273	8	0	0
9	C1	184	1547	1001	265	273	8	0	0
9	CI	184	1547	1001	265	273	8	0	0
9	Cu	184	1547	1001	265	273	8	0	0
9	Cv	184	1547	1001	265	273	8	0	0
9	Cw	184	1547	1001	265	273	8	0	0
9	Cx	184	1547	1001	265	273	8	0	0
9	Cy	184	1547	1001	265	273	8	0	0

- Molecule 10 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	95	809	486	164	157	2	0	0
10	CV	226	1881	1136	360	379	6	0	0
10	CX	221	1871	1128	373	365	5	0	0

- Molecule 11 is a protein called Trichohyalin-plectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	243	2042	1240	397	399	6	0	0
11	C	181	1531	928	288	310	5	0	0

- Molecule 12 is a protein called Parkin co-regulated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	C2	192	1589	1032	262	290	5	0	0
12	C3	192	1589	1032	262	290	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Cz	192	1589	1032	262	290	5	0	0

- Molecule 13 is a protein called Enkurin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	CC	239	1971	1249	341	375	6	0	0
13	CY	239	1971	1249	341	375	6	0	0
13	CZ	239	1971	1249	341	375	6	0	0
13	F	239	1971	1249	341	375	6	0	0

- Molecule 14 is a protein called FAP77.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	CF	213	1691	1048	319	317	7	0	0
14	Cc	213	1691	1048	319	317	7	0	0
14	Cf	213	1691	1048	319	317	7	0	0
14	Cg	213	1691	1048	319	317	7	0	0

- Molecule 15 is a protein called EF hand family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	CG	193	1607	1034	264	302	7	0	0
15	Ch	193	1607	1034	264	302	7	0	0
15	Ci	193	1607	1034	264	302	7	0	0
15	Cj	193	1607	1034	264	302	7	0	0
15	Ck	193	1607	1034	264	302	7	0	0
15	Cl	193	1607	1034	264	302	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	E	193	1607	1034	264	302	7	0	0

- Molecule 16 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	CH	605	4612	2889	812	884	27	0	0
16	Cd	605	4612	2889	812	884	27	0	0
16	Ce	605	4612	2889	812	884	27	0	0
16	D	605	4612	2889	812	884	27	0	0

- Molecule 17 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	CM	375	2975	1899	495	571	10	0	0
17	CO	375	2975	1899	495	571	10	0	0
17	CP	375	2975	1899	495	571	10	0	0

- Molecule 18 is a protein called FAP161.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CN	232	1836	1148	315	358	15	0	0
18	CQ	232	1836	1148	315	358	15	0	0

- Molecule 19 is a protein called RIIa domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CR	48	407	257	72	76	2	0	0

- Molecule 20 is a protein called FAP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	CS	97	780	477	153	148	2	0	0

- Molecule 21 is a protein called Meiosis-specific nuclear structural protein 1.

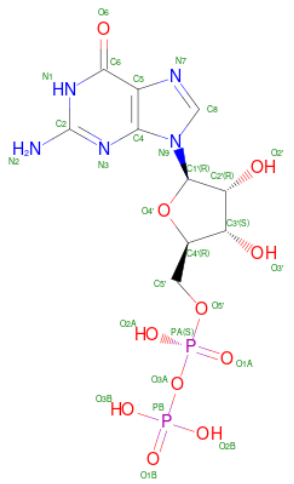
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	CT	400	3402	2038	675	672	17	0	0
			Total	C	N	O	S		
21	CU	163	1382	850	263	263	6	0	0

- Molecule 22 is a protein called MGC84469 protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	CW	500	4099	2602	713	772	12	0	0
			Total	C	N	O	S		
22	Co	500	4099	2602	713	772	12	0	0
			Total	C	N	O	S		
22	Cp	500	4099	2602	713	772	12	0	0
			Total	C	N	O	S		
22	Cq	500	4099	2602	713	772	12	0	0
			Total	C	N	O	S		
22	Cr	500	4099	2602	713	772	12	0	0
			Total	C	N	O	S		
22	Cs	500	4099	2602	713	772	12	0	0
			Total	C	N	O	S		
22	Ct	500	4099	2602	713	772	12	0	0

- Molecule 23 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

GDP



Mol	Chain	Residues	Atoms					AltConf
23	0	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fl	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fm	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fn	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fo	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fp	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fq	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fr	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fs	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	A0	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Ft	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fu	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fv	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fw	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	Fx	1	28	10	5	11	2	0
23	Fy	1	28	10	5	11	2	0
23	Fz	1	28	10	5	11	2	0
23	GH	1	28	10	5	11	2	0
23	GU	1	28	10	5	11	2	0
23	GV	1	28	10	5	11	2	0
23	GW	1	28	10	5	11	2	0
23	GX	1	28	10	5	11	2	0
23	GY	1	28	10	5	11	2	0
23	GZ	1	28	10	5	11	2	0
23	Ga	1	28	10	5	11	2	0
23	Gb	1	28	10	5	11	2	0
23	Gc	1	28	10	5	11	2	0
23	Gd	1	28	10	5	11	2	0
23	Ge	1	28	10	5	11	2	0
23	Gf	1	28	10	5	11	2	0
23	Gg	1	28	10	5	11	2	0
23	Gh	1	28	10	5	11	2	0
23	Gi	1	28	10	5	11	2	0
23	Gj	1	28	10	5	11	2	0
23	Gk	1	28	10	5	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	Gm	1	28	10	5	11	2	0
23	O	1	28	10	5	11	2	0
23	P	1	28	10	5	11	2	0
23	U	1	28	10	5	11	2	0
23	X	1	28	10	5	11	2	0
23	A3	1	28	10	5	11	2	0
23	m	1	28	10	5	11	2	0
23	n	1	28	10	5	11	2	0
23	r	1	28	10	5	11	2	0
23	AA	1	28	10	5	11	2	0
23	AB	1	28	10	5	11	2	0
23	AC	1	28	10	5	11	2	0
23	AD	1	28	10	5	11	2	0
23	AE	1	28	10	5	11	2	0
23	AF	1	28	10	5	11	2	0
23	AG	1	28	10	5	11	2	0
23	AH	1	28	10	5	11	2	0
23	AL	1	28	10	5	11	2	0
23	AM	1	28	10	5	11	2	0
23	AN	1	28	10	5	11	2	0
23	AO	1	28	10	5	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	AP	1	28	10	5	11	2	0
23	AQ	1	28	10	5	11	2	0
23	AR	1	28	10	5	11	2	0
23	AS	1	28	10	5	11	2	0
23	AT	1	28	10	5	11	2	0
23	AU	1	28	10	5	11	2	0
23	AV	1	28	10	5	11	2	0
23	AW	1	28	10	5	11	2	0
23	AX	1	28	10	5	11	2	0
23	AY	1	28	10	5	11	2	0
23	AZ	1	28	10	5	11	2	0
23	Aa	1	28	10	5	11	2	0
23	Ab	1	28	10	5	11	2	0
23	Ac	1	28	10	5	11	2	0
23	Ad	1	28	10	5	11	2	0
23	Ae	1	28	10	5	11	2	0
23	Af	1	28	10	5	11	2	0
23	Ag	1	28	10	5	11	2	0
23	Ah	1	28	10	5	11	2	0
23	Ai	1	28	10	5	11	2	0
23	Am	1	28	10	5	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	An	1	28	10	5	11	2	0
23	Ao	1	28	10	5	11	2	0
23	Ap	1	28	10	5	11	2	0
23	Aq	1	28	10	5	11	2	0
23	Ar	1	28	10	5	11	2	0
23	As	1	28	10	5	11	2	0
23	At	1	28	10	5	11	2	0
23	Au	1	28	10	5	11	2	0
23	Av	1	28	10	5	11	2	0
23	Az	1	28	10	5	11	2	0
23	BA	1	28	10	5	11	2	0
23	BB	1	28	10	5	11	2	0
23	BC	1	28	10	5	11	2	0
23	BD	1	28	10	5	11	2	0
23	BE	1	28	10	5	11	2	0
23	BF	1	28	10	5	11	2	0
23	BG	1	28	10	5	11	2	0
23	BH	1	28	10	5	11	2	0
23	BW	1	28	10	5	11	2	0
23	BZ	1	28	10	5	11	2	0
23	Ba	1	28	10	5	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	Bb	1	28	10	5	11	2	0
23	Be	1	28	10	5	11	2	0
23	Bf	1	28	10	5	11	2	0
23	Bg	1	28	10	5	11	2	0
23	Bh	1	28	10	5	11	2	0
23	Bi	1	28	10	5	11	2	0
23	Bj	1	28	10	5	11	2	0
23	Bk	1	28	10	5	11	2	0
23	Bl	1	28	10	5	11	2	0
23	Bm	1	28	10	5	11	2	0
23	Bn	1	28	10	5	11	2	0
23	Bo	1	28	10	5	11	2	0
23	Bp	1	28	10	5	11	2	0
23	Bq	1	28	10	5	11	2	0
23	Br	1	28	10	5	11	2	0
23	Bs	1	28	10	5	11	2	0
23	Bt	1	28	10	5	11	2	0
23	DL	1	28	10	5	11	2	0
23	DM	1	28	10	5	11	2	0
23	DN	1	28	10	5	11	2	0
23	DO	1	28	10	5	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	DP	1	28	10	5	11	2	0
23	DQ	1	28	10	5	11	2	0
23	DR	1	28	10	5	11	2	0
23	DS	1	28	10	5	11	2	0
23	DT	1	28	10	5	11	2	0
23	DU	1	28	10	5	11	2	0
23	DV	1	28	10	5	11	2	0
23	DW	1	28	10	5	11	2	0
23	DX	1	28	10	5	11	2	0
23	DY	1	28	10	5	11	2	0
23	DZ	1	28	10	5	11	2	0
23	Da	1	28	10	5	11	2	0
23	Db	1	28	10	5	11	2	0
23	Dc	1	28	10	5	11	2	0
23	Dd	1	28	10	5	11	2	0
23	De	1	28	10	5	11	2	0
23	Df	1	28	10	5	11	2	0
23	Dg	1	28	10	5	11	2	0
23	Dh	1	28	10	5	11	2	0
23	Di	1	28	10	5	11	2	0
23	Dj	1	28	10	5	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	Dk	1	28	10	5	11	2	0
23	Dq	1	28	10	5	11	2	0
23	Dr	1	28	10	5	11	2	0
23	Ds	1	28	10	5	11	2	0
23	Dt	1	28	10	5	11	2	0
23	Du	1	28	10	5	11	2	0
23	Dv	1	28	10	5	11	2	0
23	Dw	1	28	10	5	11	2	0
23	Dx	1	28	10	5	11	2	0
23	E0	1	28	10	5	11	2	0
23	E9	1	28	10	5	11	2	0
23	EL	1	28	10	5	11	2	0
23	EM	1	28	10	5	11	2	0
23	EN	1	28	10	5	11	2	0
23	EO	1	28	10	5	11	2	0
23	EP	1	28	10	5	11	2	0
23	EQ	1	28	10	5	11	2	0
23	ER	1	28	10	5	11	2	0
23	ES	1	28	10	5	11	2	0
23	ET	1	28	10	5	11	2	0
23	EU	1	28	10	5	11	2	0

Continued on next page...

Continued from previous page...

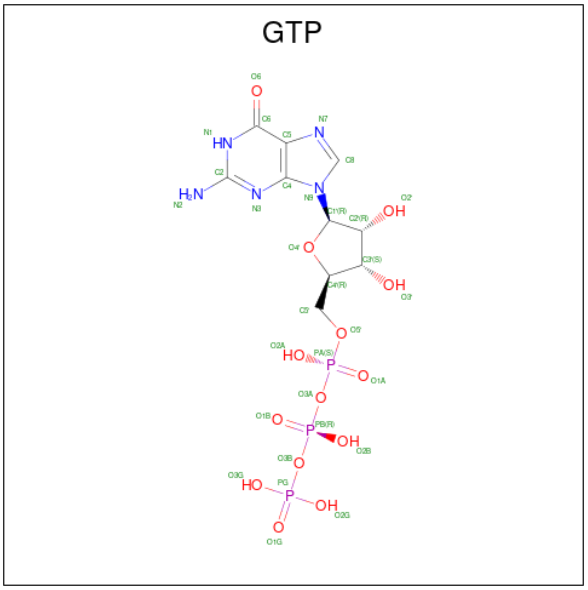
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	EV	1	28	10	5	11	2	0
23	EW	1	28	10	5	11	2	0
23	EX	1	28	10	5	11	2	0
23	EY	1	28	10	5	11	2	0
23	EZ	1	28	10	5	11	2	0
23	Ea	1	28	10	5	11	2	0
23	Eb	1	28	10	5	11	2	0
23	Ec	1	28	10	5	11	2	0
23	Ed	1	28	10	5	11	2	0
23	Ef	1	28	10	5	11	2	0
23	7	1	28	10	5	11	2	0
23	Ev	1	28	10	5	11	2	0
23	F1	1	28	10	5	11	2	0
23	F2	1	28	10	5	11	2	0
23	8	1	28	10	5	11	2	0
23	F4	1	28	10	5	11	2	0
23	FA	1	28	10	5	11	2	0
23	FB	1	28	10	5	11	2	0
23	FC	1	28	10	5	11	2	0
23	FD	1	28	10	5	11	2	0
23	FE	1	28	10	5	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	FF	1	28	10	5	11	2	0
23	FG	1	28	10	5	11	2	0
23	FH	1	28	10	5	11	2	0
23	FI	1	28	10	5	11	2	0
23	FJ	1	28	10	5	11	2	0
23	FK	1	28	10	5	11	2	0
23	FL	1	28	10	5	11	2	0
23	FN	1	28	10	5	11	2	0
23	9	1	28	10	5	11	2	0

- Molecule 24 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	Fi	1	32	10	5	14	3	0
24	Fj	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	Fk	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	G1	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	G2	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	G3	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	G4	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	G5	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	G6	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GA	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GB	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GC	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GD	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GE	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	A1	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GF	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GG	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GI	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GJ	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GK	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GL	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GM	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GN	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	GO	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GP	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GQ	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GR	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GS	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	GT	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	A2	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gl	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gn	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Go	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gp	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gq	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gr	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gs	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gt	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gu	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gv	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gw	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gx	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gy	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Gz	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	Q	1	32	10	5	14	3	0
24	S	1	32	10	5	14	3	0
24	T	1	32	10	5	14	3	0
24	V	1	32	10	5	14	3	0
24	W	1	32	10	5	14	3	0
24	Y	1	32	10	5	14	3	0
24	Z	1	32	10	5	14	3	0
24	a	1	32	10	5	14	3	0
24	b	1	32	10	5	14	3	0
24	c	1	32	10	5	14	3	0
24	d	1	32	10	5	14	3	0
24	e	1	32	10	5	14	3	0
24	f	1	32	10	5	14	3	0
24	g	1	32	10	5	14	3	0
24	h	1	32	10	5	14	3	0
24	i	1	32	10	5	14	3	0
24	j	1	32	10	5	14	3	0
24	k	1	32	10	5	14	3	0
24	l	1	32	10	5	14	3	0
24	o	1	32	10	5	14	3	0
24	p	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	A4	1	32	10	5	14	3	0
24	q	1	32	10	5	14	3	0
24	s	1	32	10	5	14	3	0
24	t	1	32	10	5	14	3	0
24	u	1	32	10	5	14	3	0
24	v	1	32	10	5	14	3	0
24	w	1	32	10	5	14	3	0
24	x	1	32	10	5	14	3	0
24	y	1	32	10	5	14	3	0
24	z	1	32	10	5	14	3	0
24	A5	1	32	10	5	14	3	0
24	A6	1	32	10	5	14	3	0
24	A7	1	32	10	5	14	3	0
24	A8	1	32	10	5	14	3	0
24	A9	1	32	10	5	14	3	0
24	AI	1	32	10	5	14	3	0
24	AJ	1	32	10	5	14	3	0
24	AK	1	32	10	5	14	3	0
24	1	1	32	10	5	14	3	0
24	AS	1	32	10	5	14	3	0
24	Aj	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	Ak	1	32	10	5	14	3	0
24	Al	1	32	10	5	14	3	0
24	2	1	32	10	5	14	3	0
24	Aw	1	32	10	5	14	3	0
24	Ax	1	32	10	5	14	3	0
24	Ay	1	32	10	5	14	3	0
24	B0	1	32	10	5	14	3	0
24	B1	1	32	10	5	14	3	0
24	B2	1	32	10	5	14	3	0
24	B3	1	32	10	5	14	3	0
24	B4	1	32	10	5	14	3	0
24	B5	1	32	10	5	14	3	0
24	B6	1	32	10	5	14	3	0
24	B7	1	32	10	5	14	3	0
24	B8	1	32	10	5	14	3	0
24	B9	1	32	10	5	14	3	0
24	BI	1	32	10	5	14	3	0
24	BJ	1	32	10	5	14	3	0
24	BK	1	32	10	5	14	3	0
24	BL	1	32	10	5	14	3	0
24	BM	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	BN	1	32	10	5	14	3	0
24	BO	1	32	10	5	14	3	0
24	3	1	32	10	5	14	3	0
24	BP	1	32	10	5	14	3	0
24	BQ	1	32	10	5	14	3	0
24	BR	1	32	10	5	14	3	0
24	BS	1	32	10	5	14	3	0
24	BT	1	32	10	5	14	3	0
24	BU	1	32	10	5	14	3	0
24	BV	1	32	10	5	14	3	0
24	BX	1	32	10	5	14	3	0
24	BY	1	32	10	5	14	3	0
24	Bc	1	32	10	5	14	3	0
24	Bd	1	32	10	5	14	3	0
24	Bu	1	32	10	5	14	3	0
24	4	1	32	10	5	14	3	0
24	Bv	1	32	10	5	14	3	0
24	Bw	1	32	10	5	14	3	0
24	Bx	1	32	10	5	14	3	0
24	By	1	32	10	5	14	3	0
24	Bz	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	CA	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	CB	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	5	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	E1	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	E2	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	E3	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	6	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	E4	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	E5	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	E6	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	E7	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	E8	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Ee	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Eg	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Eh	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Ei	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Ej	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Ek	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	El	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	Em	1	32	10	5	14	3	0
			Total	C	N	O	P	
24	En	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	Eo	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Ep	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Eq	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Er	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Es	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Et	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Eu	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Ew	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Ex	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Ey	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Ez	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	F3	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	F5	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	F6	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	F7	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	F8	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	F9	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FM	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FO	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FP	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	FQ	1	32	10	5	14	3	0
24	FR	1	32	10	5	14	3	0
24	FS	1	32	10	5	14	3	0
24	FT	1	32	10	5	14	3	0
24	FU	1	32	10	5	14	3	0
24	FV	1	32	10	5	14	3	0
24	FW	1	32	10	5	14	3	0
24	FX	1	32	10	5	14	3	0
24	FY	1	32	10	5	14	3	0
24	FZ	1	32	10	5	14	3	0
24	Fa	1	32	10	5	14	3	0
24	Fb	1	32	10	5	14	3	0
24	Fc	1	32	10	5	14	3	0
24	Fd	1	32	10	5	14	3	0
24	Fe	1	32	10	5	14	3	0
24	Ff	1	32	10	5	14	3	0
24	Fg	1	32	10	5	14	3	0
24	Fh	1	32	10	5	14	3	0

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	Fi	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	Fj	1	1	1	0
25	Fk	1	1	1	0
25	G1	1	1	1	0
25	G2	1	1	1	0
25	G3	1	1	1	0
25	G4	1	1	1	0
25	G5	1	1	1	0
25	G6	1	1	1	0
25	GA	1	1	1	0
25	GB	1	1	1	0
25	GC	1	1	1	0
25	GD	1	1	1	0
25	GE	1	1	1	0
25	A1	1	1	1	0
25	GF	1	1	1	0
25	GG	1	1	1	0
25	GI	1	1	1	0
25	GJ	1	1	1	0
25	GK	1	1	1	0
25	GL	1	1	1	0
25	GM	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	GN	1	1	1	0
25	GO	1	1	1	0
25	GP	1	1	1	0
25	GQ	1	1	1	0
25	GR	1	1	1	0
25	GS	1	1	1	0
25	GT	1	1	1	0
25	A2	1	1	1	0
25	Gl	1	1	1	0
25	Gn	1	1	1	0
25	Go	1	1	1	0
25	Gp	1	1	1	0
25	Gq	1	1	1	0
25	Gr	1	1	1	0
25	Gs	1	1	1	0
25	Gt	1	1	1	0
25	Gu	1	1	1	0
25	Gv	1	1	1	0
25	Gw	1	1	1	0
25	Gx	1	1	1	0
25	Gy	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	Gz	1	1	1	0
25	Q	1	1	1	0
25	R	1	1	1	0
25	S	1	1	1	0
25	T	1	1	1	0
25	V	1	1	1	0
25	W	1	1	1	0
25	Y	1	1	1	0
25	Z	1	1	1	0
25	a	1	1	1	0
25	b	1	1	1	0
25	c	1	1	1	0
25	d	1	1	1	0
25	e	1	1	1	0
25	f	1	1	1	0
25	g	1	1	1	0
25	h	1	1	1	0
25	i	1	1	1	0
25	j	1	1	1	0
25	k	1	1	1	0
25	l	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	o	1	1	1	0
25	p	1	1	1	0
25	A4	1	1	1	0
25	q	1	1	1	0
25	s	1	1	1	0
25	t	1	1	1	0
25	v	1	1	1	0
25	w	1	1	1	0
25	y	1	1	1	0
25	z	1	1	1	0
25	A5	1	1	1	0
25	A6	1	1	1	0
25	A7	1	1	1	0
25	A8	1	1	1	0
25	A9	1	1	1	0
25	AJ	1	1	1	0
25	AK	1	1	1	0
25	1	1	1	1	0
25	AQ	1	1	1	0
25	AV	1	1	1	0
25	Ac	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	Ah	1	1	1	0
25	Ak	1	1	1	0
25	Al	1	1	1	0
25	Au	1	1	1	0
25	2	1	1	1	0
25	Aw	1	1	1	0
25	Ax	1	1	1	0
25	Ay	1	1	1	0
25	B1	1	1	1	0
25	B2	1	1	1	0
25	B3	1	1	1	0
25	B4	1	1	1	0
25	B5	1	1	1	0
25	B6	1	1	1	0
25	B8	1	1	1	0
25	B9	1	1	1	0
25	BG	1	1	1	0
25	BI	1	1	1	0
25	BJ	1	1	1	0
25	BK	1	1	1	0
25	BL	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	BM	1	1	1	0
25	BN	1	1	1	0
25	BO	1	1	1	0
25	3	1	1	1	0
25	BP	1	1	1	0
25	BQ	1	1	1	0
25	BS	1	1	1	0
25	BU	1	1	1	0
25	BV	1	1	1	0
25	BX	1	1	1	0
25	BY	1	1	1	0
25	Bc	1	1	1	0
25	Bd	1	1	1	0
25	Bl	1	1	1	0
25	Bq	1	1	1	0
25	Bu	1	1	1	0
25	4	1	1	1	0
25	Bv	1	1	1	0
25	Bw	1	1	1	0
25	Bx	1	1	1	0
25	By	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	Bz	1	1	1	0
25	CA	1	1	1	0
25	CB	1	1	1	0
25	5	1	1	1	0
25	E1	1	1	1	0
25	E2	1	1	1	0
25	E3	1	1	1	0
25	6	1	1	1	0
25	E4	1	1	1	0
25	E5	1	1	1	0
25	E6	1	1	1	0
25	E7	1	1	1	0
25	E8	1	1	1	0
25	Ee	1	1	1	0
25	Eg	1	1	1	0
25	Eh	1	1	1	0
25	Ei	1	1	1	0
25	Ej	1	1	1	0
25	Ek	1	1	1	0
25	El	1	1	1	0
25	Em	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	En	1	1	1	0
25	Eo	1	1	1	0
25	Ep	1	1	1	0
25	Eq	1	1	1	0
25	Er	1	1	1	0
25	Es	1	1	1	0
25	Et	1	1	1	0
25	Eu	1	1	1	0
25	Ew	1	1	1	0
25	Ex	1	1	1	0
25	Ey	1	1	1	0
25	Ez	1	1	1	0
25	F0	1	1	1	0
25	F3	1	1	1	0
25	F5	1	1	1	0
25	F6	1	1	1	0
25	F7	1	1	1	0
25	F8	1	1	1	0
25	F9	1	1	1	0
25	FM	1	1	1	0
25	FO	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
25	FP	1	1	1	0
25	FQ	1	1	1	0
25	FR	1	1	1	0
25	FS	1	1	1	0
25	FT	1	1	1	0
25	FU	1	1	1	0
25	FV	1	1	1	0
25	FW	1	1	1	0
25	FX	1	1	1	0
25	FY	1	1	1	0
25	FZ	1	1	1	0
25	Fa	1	1	1	0
25	Fb	1	1	1	0
25	Fc	1	1	1	0
25	Fd	1	1	1	0
25	Fe	1	1	1	0
25	Ff	1	1	1	0
25	Fg	1	1	1	0
25	Fh	1	1	1	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	409692	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.899	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.128	Depositor
Map size (Å)	717.2, 731.5, 1054.9	wwPDB
Map dimensions	652, 665, 959	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

4.6 Ligand geometry (i)

Of 567 ligands modelled in this entry, 188 are monoatomic - leaving 379 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	$\#\|Z\| > 2$
24	GTP	B6	602	25	29,34,34	1.27	3 (10%)	35,54,54	1.35	5 (14%)
24	GTP	Ek	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.25	3 (8%)
23	GDP	AO	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
24	GTP	BU	602	25	29,34,34	1.24	2 (6%)	35,54,54	1.30	3 (8%)
23	GDP	Az	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
24	GTP	E3	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.35	5 (14%)
24	GTP	Al	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.29	4 (11%)
24	GTP	BX	602	25	29,34,34	1.22	2 (6%)	35,54,54	1.35	4 (11%)
24	GTP	Ff	501	25	29,34,34	1.30	3 (10%)	35,54,54	1.30	3 (8%)
24	GTP	Et	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.32	4 (11%)
23	GDP	FF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.24	3 (10%)
23	GDP	Ec	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.33	5 (16%)
24	GTP	A9	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.26	3 (8%)
24	GTP	BY	602	25	29,34,34	1.20	2 (6%)	35,54,54	1.40	7 (20%)
24	GTP	F7	501	25	29,34,34	1.30	5 (17%)	35,54,54	1.27	4 (11%)
23	GDP	Bo	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.00	1 (3%)
23	GDP	DZ	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	3 (10%)
23	GDP	Df	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.19	4 (13%)
24	GTP	By	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.35	5 (14%)
23	GDP	X	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	1 (3%)
23	GDP	DO	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.14	2 (6%)
23	GDP	Fm	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.16	4 (13%)
23	GDP	Gk	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.16	4 (13%)
23	GDP	AW	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	2 (6%)
23	GDP	Gh	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
23	GDP	AZ	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.04	2 (6%)
23	GDP	EQ	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.28	5 (16%)
24	GTP	s	602	25	29,34,34	1.28	3 (10%)	35,54,54	1.36	5 (14%)
23	GDP	Ev	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.30	5 (16%)
24	GTP	T	602	25	29,34,34	1.26	3 (10%)	35,54,54	1.37	5 (14%)
24	GTP	A1	602	25	29,34,34	1.23	2 (6%)	35,54,54	1.34	4 (11%)
23	GDP	Ga	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.22	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	GTP	FR	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.25	3 (8%)
24	GTP	GM	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.31	4 (11%)
23	GDP	BA	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.03	2 (6%)
24	GTP	Fh	501	25	29,34,34	1.34	5 (17%)	35,54,54	1.47	4 (11%)
24	GTP	A5	501	25	29,34,34	1.30	3 (10%)	35,54,54	1.25	3 (8%)
23	GDP	AD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.22	4 (13%)
24	GTP	FS	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.28	3 (8%)
23	GDP	GX	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.20	2 (6%)
23	GDP	FG	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.20	3 (10%)
24	GTP	AK	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.28	4 (11%)
23	GDP	Ab	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.19	3 (10%)
24	GTP	S	602	25	29,34,34	1.25	2 (6%)	35,54,54	1.35	4 (11%)
23	GDP	AN	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.04	2 (6%)
24	GTP	GT	501	25	29,34,34	1.30	3 (10%)	35,54,54	1.26	4 (11%)
24	GTP	AJ	602	25	29,34,34	1.22	2 (6%)	35,54,54	1.28	3 (8%)
24	GTP	Ex	501	25	29,34,34	1.35	4 (13%)	35,54,54	1.33	3 (8%)
24	GTP	y	602	25	29,34,34	1.27	4 (13%)	35,54,54	1.29	4 (11%)
23	GDP	FL	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
23	GDP	Bk	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.18	3 (10%)
23	GDP	Bm	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.09	1 (3%)
24	GTP	F6	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.23	3 (8%)
23	GDP	Fs	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	3 (10%)
24	GTP	AS	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.38	5 (14%)
24	GTP	FW	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.29	3 (8%)
23	GDP	BZ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.27	4 (13%)
24	GTP	Gv	501	25	29,34,34	1.30	3 (10%)	35,54,54	1.29	3 (8%)
24	GTP	Ez	501	25	29,34,34	1.30	5 (17%)	35,54,54	1.24	3 (8%)
24	GTP	A7	501	25	29,34,34	1.29	3 (10%)	35,54,54	1.24	3 (8%)
23	GDP	9	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.02	1 (3%)
24	GTP	5	602	25	29,34,34	1.27	3 (10%)	35,54,54	1.34	5 (14%)
23	GDP	EM	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.20	4 (13%)
23	GDP	Gb	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.11	3 (10%)
23	GDP	Fv	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.13	2 (6%)
23	GDP	Eb	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
24	GTP	Bz	602	25	29,34,34	1.29	5 (17%)	35,54,54	1.33	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	GTP	Fk	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.27	3 (8%)
24	GTP	GP	501	25	29,34,34	1.33	5 (17%)	35,54,54	1.24	3 (8%)
23	GDP	AQ	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.05	1 (3%)
23	GDP	DU	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	3 (10%)
23	GDP	AM	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.08	2 (6%)
24	GTP	Fb	501	25	29,34,34	1.31	4 (13%)	35,54,54	1.27	3 (8%)
24	GTP	FT	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.24	3 (8%)
23	GDP	Dx	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.17	2 (6%)
23	GDP	Dq	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.21	3 (10%)
24	GTP	b	602	25	29,34,34	1.29	4 (13%)	35,54,54	1.32	3 (8%)
24	GTP	k	602	25	29,34,34	1.27	3 (10%)	35,54,54	1.26	3 (8%)
24	GTP	A6	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.25	3 (8%)
24	GTP	BS	602	25	29,34,34	1.23	2 (6%)	35,54,54	1.27	3 (8%)
23	GDP	F2	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	1 (3%)
24	GTP	Gl	501	25	29,34,34	1.26	3 (10%)	35,54,54	1.27	3 (8%)
24	GTP	GE	501	25	29,34,34	1.35	4 (13%)	35,54,54	1.34	4 (11%)
23	GDP	Ag	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.15	2 (6%)
24	GTP	Fd	602	25	29,34,34	1.35	5 (17%)	35,54,54	1.29	3 (8%)
23	GDP	DY	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	3 (10%)
23	GDP	Dd	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	3 (10%)
24	GTP	q	602	25	29,34,34	1.27	4 (13%)	35,54,54	1.36	5 (14%)
23	GDP	Ge	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.17	4 (13%)
24	GTP	Bw	602	25	29,34,34	1.27	4 (13%)	35,54,54	1.34	4 (11%)
24	GTP	Bu	602	25	29,34,34	1.24	3 (10%)	35,54,54	1.31	3 (8%)
24	GTP	Fe	501	25	29,34,34	1.32	4 (13%)	35,54,54	1.32	3 (8%)
24	GTP	F5	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.28	4 (11%)
24	GTP	FQ	501	25	29,34,34	1.30	3 (10%)	35,54,54	1.24	3 (8%)
24	GTP	FM	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.26	4 (11%)
24	GTP	BQ	602	25	29,34,34	1.26	3 (10%)	35,54,54	1.33	5 (14%)
24	GTP	E7	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.32	5 (14%)
23	GDP	Ae	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	2 (6%)
23	GDP	AP	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.17	2 (6%)
23	GDP	7	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.17	3 (10%)
24	GTP	Fj	501	25	29,34,34	1.39	5 (17%)	35,54,54	1.35	4 (11%)
24	GTP	GF	501	25	29,34,34	1.37	5 (17%)	35,54,54	1.36	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	GTP	BL	602	25	29,34,34	1.30	4 (13%)	35,54,54	1.37	6 (17%)
23	GDP	P	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	1 (3%)
23	GDP	Av	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	2 (6%)
23	GDP	Br	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.17	2 (6%)
23	GDP	FD	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.14	2 (6%)
24	GTP	GC	501	25	29,34,34	1.27	4 (13%)	35,54,54	1.27	4 (11%)
23	GDP	Du	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	2 (6%)
23	GDP	EX	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.15	3 (10%)
24	GTP	Gz	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.27	4 (11%)
24	GTP	BM	602	25	29,34,34	1.30	4 (13%)	35,54,54	1.31	4 (11%)
23	GDP	ET	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.11	2 (6%)
23	GDP	E9	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.22	4 (13%)
24	GTP	u	501	25	29,34,34	1.28	4 (13%)	35,54,54	1.29	4 (11%)
23	GDP	An	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.05	2 (6%)
24	GTP	F3	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.30	4 (11%)
24	GTP	f	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.22	3 (8%)
24	GTP	Gq	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.25	3 (8%)
23	GDP	n	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.02	2 (6%)
24	GTP	Go	501	25	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
24	GTP	Aw	602	25	29,34,34	1.26	3 (10%)	35,54,54	1.32	5 (14%)
23	GDP	Dc	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.19	4 (13%)
23	GDP	FJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	3 (10%)
23	GDP	0	501	-	25,30,30	0.96	2 (8%)	30,47,47	1.07	1 (3%)
24	GTP	GJ	501	25	29,34,34	1.31	4 (13%)	35,54,54	1.24	4 (11%)
23	GDP	Ac	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
23	GDP	DT	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)
23	GDP	BG	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	1 (3%)
24	GTP	x	501	25	29,34,34	1.27	2 (6%)	35,54,54	1.31	4 (11%)
24	GTP	W	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.32	5 (14%)
24	GTP	F8	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.26	4 (11%)
24	GTP	Es	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.26	4 (11%)
23	GDP	Au	602	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
24	GTP	B1	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
24	GTP	h	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.32	5 (14%)
24	GTP	B8	602	25	29,34,34	1.26	4 (13%)	35,54,54	1.29	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	GDP	Dv	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.32	4 (13%)
24	GTP	A8	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.26	3 (8%)
23	GDP	AB	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.04	2 (6%)
23	GDP	Dk	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	2 (6%)
23	GDP	GH	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
24	GTP	Eq	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.31	5 (14%)
24	GTP	1	602	25	29,34,34	1.21	2 (6%)	35,54,54	1.35	3 (8%)
24	GTP	BN	602	25	29,34,34	1.29	4 (13%)	35,54,54	1.28	4 (11%)
24	GTP	Em	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.24	3 (8%)
24	GTP	i	602	25	29,34,34	1.27	4 (13%)	35,54,54	1.31	3 (8%)
24	GTP	BK	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.33	4 (11%)
23	GDP	DL	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.17	4 (13%)
23	GDP	FE	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.16	4 (13%)
23	GDP	A3	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.14	3 (10%)
23	GDP	AA	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
24	GTP	FX	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.25	4 (11%)
24	GTP	FV	602	25	29,34,34	1.29	3 (10%)	35,54,54	1.25	3 (8%)
24	GTP	Eh	501	25	29,34,34	1.29	3 (10%)	35,54,54	1.26	4 (11%)
24	GTP	B2	602	25	29,34,34	1.29	4 (13%)	35,54,54	1.27	4 (11%)
24	GTP	Bx	602	25	29,34,34	1.29	4 (13%)	35,54,54	1.43	5 (14%)
23	GDP	Bq	602	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
23	GDP	Am	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	2 (6%)
23	GDP	Ds	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	1 (3%)
24	GTP	FU	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.26	3 (8%)
24	GTP	FZ	501	25	29,34,34	1.27	4 (13%)	35,54,54	1.28	4 (11%)
23	GDP	BC	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.12	1 (3%)
23	GDP	Fx	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	2 (6%)
23	GDP	Bp	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.20	3 (10%)
23	GDP	FC	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.14	2 (6%)
24	GTP	Eg	501	25	29,34,34	1.29	3 (10%)	35,54,54	1.25	3 (8%)
23	GDP	Ba	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	2 (6%)
23	GDP	DM	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	2 (6%)
24	GTP	Bv	602	25	29,34,34	1.23	2 (6%)	35,54,54	1.35	3 (8%)
24	GTP	BP	602	25	29,34,34	1.31	4 (13%)	35,54,54	1.30	3 (8%)
23	GDP	EP	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.16	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	GDP	Dj	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.11	2 (6%)
24	GTP	GR	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.47	5 (14%)
24	GTP	Ej	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.26	4 (11%)
23	GDP	Dr	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	2 (6%)
24	GTP	Gt	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.22	3 (8%)
23	GDP	Bb	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.02	2 (6%)
23	GDP	FB	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	1 (3%)
24	GTP	GB	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.30	4 (11%)
24	GTP	GK	501	25	29,34,34	1.31	4 (13%)	35,54,54	1.25	4 (11%)
24	GTP	Er	501	25	29,34,34	1.25	3 (10%)	35,54,54	1.28	3 (8%)
24	GTP	Aj	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.26	4 (11%)
24	GTP	GI	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.25	4 (11%)
24	GTP	CB	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.31	5 (14%)
23	GDP	EV	501	-	25,30,30	1.05	1 (4%)	30,47,47	1.24	4 (13%)
23	GDP	Da	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.12	3 (10%)
23	GDP	ES	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.17	2 (6%)
23	GDP	Gj	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.31	4 (13%)
24	GTP	Gy	501	25	29,34,34	1.27	4 (13%)	35,54,54	1.28	4 (11%)
23	GDP	FK	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.18	3 (10%)
23	GDP	Fw	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.15	3 (10%)
24	GTP	BR	501	25	29,34,34	1.28	5 (17%)	35,54,54	1.29	4 (11%)
23	GDP	Ea	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
24	GTP	d	602	25	29,34,34	1.26	3 (10%)	35,54,54	1.34	5 (14%)
24	GTP	GA	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.25	4 (11%)
24	GTP	Ax	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.28	4 (11%)
23	GDP	Gm	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.25	3 (10%)
23	GDP	BW	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.29	4 (13%)
23	GDP	Fz	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.13	2 (6%)
23	GDP	ER	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.29	3 (10%)
23	GDP	AF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.02	1 (3%)
23	GDP	Ed	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
24	GTP	Gu	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.26	4 (11%)
23	GDP	As	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	1 (3%)
23	GDP	r	501	-	25,30,30	1.07	2 (8%)	30,47,47	1.01	2 (6%)
24	GTP	Ay	602	25	29,34,34	1.26	4 (13%)	35,54,54	1.27	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	GTP	BJ	602	25	29,34,34	1.26	3 (10%)	35,54,54	1.34	5 (14%)
24	GTP	Z	602	25	29,34,34	1.24	2 (6%)	35,54,54	1.37	4 (11%)
23	GDP	Di	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.18	3 (10%)
23	GDP	Af	501	-	25,30,30	0.98	1 (4%)	30,47,47	0.99	1 (3%)
24	GTP	6	602	25	29,34,34	1.27	3 (10%)	35,54,54	1.35	5 (14%)
24	GTP	A2	602	25	29,34,34	1.24	2 (6%)	35,54,54	1.35	4 (11%)
24	GTP	Eu	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.26	3 (8%)
24	GTP	GG	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.27	3 (8%)
24	GTP	GO	602	25	29,34,34	1.28	3 (10%)	35,54,54	1.26	4 (11%)
23	GDP	EY	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.19	3 (10%)
24	GTP	B0	501	25	29,34,34	1.28	4 (13%)	35,54,54	1.29	4 (11%)
24	GTP	Gn	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.24	3 (8%)
24	GTP	En	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.26	3 (8%)
24	GTP	E4	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.26	3 (8%)
24	GTP	F0	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.30	3 (8%)
24	GTP	BT	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.26	4 (11%)
23	GDP	AX	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.18	3 (10%)
24	GTP	Fc	501	25	29,34,34	1.29	3 (10%)	35,54,54	1.28	3 (8%)
23	GDP	Gd	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.28	4 (13%)
23	GDP	Bf	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.02	2 (6%)
23	GDP	AG	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	1 (3%)
24	GTP	Ee	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.25	3 (8%)
24	GTP	B4	602	25	29,34,34	1.27	3 (10%)	35,54,54	1.25	3 (8%)
23	GDP	Bi	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.02	2 (6%)
24	GTP	e	602	25	29,34,34	1.27	4 (13%)	35,54,54	1.26	3 (8%)
23	GDP	DR	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.29	5 (16%)
23	GDP	GZ	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.25	2 (6%)
23	GDP	EO	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.30	5 (16%)
24	GTP	Ei	501	25	29,34,34	1.32	5 (17%)	35,54,54	1.31	3 (8%)
24	GTP	El	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.24	3 (8%)
23	GDP	DQ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	3 (10%)
24	GTP	B3	602	25	29,34,34	1.28	3 (10%)	35,54,54	1.25	3 (8%)
24	GTP	BO	602	25	29,34,34	1.27	3 (10%)	35,54,54	1.27	4 (11%)
24	GTP	F9	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.25	3 (8%)
23	GDP	A0	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	GDP	E0	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.20	4 (13%)
23	GDP	At	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	2 (6%)
24	GTP	FO	501	25	29,34,34	1.29	3 (10%)	35,54,54	1.24	3 (8%)
24	GTP	Ak	602	25	29,34,34	1.27	4 (13%)	35,54,54	1.29	4 (11%)
23	GDP	AV	602	-	25,30,30	1.05	2 (8%)	30,47,47	1.07	2 (6%)
23	GDP	Fp	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.27	3 (10%)
24	GTP	Ep	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.25	3 (8%)
24	GTP	GN	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.31	5 (14%)
24	GTP	Gw	501	25	29,34,34	1.28	4 (13%)	35,54,54	1.26	4 (11%)
24	GTP	Ew	501	25	29,34,34	1.34	5 (17%)	35,54,54	1.30	3 (8%)
24	GTP	B7	501	25	29,34,34	1.28	4 (13%)	35,54,54	1.26	4 (11%)
23	GDP	EL	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.17	3 (10%)
23	GDP	DV	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	3 (10%)
23	GDP	Ft	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.11	2 (6%)
23	GDP	GY	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.24	4 (13%)
24	GTP	a	602	25	29,34,34	1.28	4 (13%)	35,54,54	1.29	3 (8%)
23	GDP	BB	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.17	2 (6%)
24	GTP	Bc	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.27	3 (8%)
23	GDP	AC	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.27	4 (13%)
24	GTP	c	602	25	29,34,34	1.28	5 (17%)	35,54,54	1.31	3 (8%)
23	GDP	Bj	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
23	GDP	EU	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	3 (10%)
23	GDP	Dw	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
23	GDP	Gg	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.21	2 (6%)
24	GTP	BV	602	25	29,34,34	1.28	3 (10%)	35,54,54	1.32	5 (14%)
24	GTP	Y	602	25	29,34,34	1.25	3 (10%)	35,54,54	1.30	3 (8%)
23	GDP	Ar	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.06	1 (3%)
23	GDP	DN	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.15	3 (10%)
24	GTP	E6	602	25	29,34,34	1.31	4 (13%)	35,54,54	1.42	5 (14%)
24	GTP	GS	501	25	29,34,34	1.25	2 (6%)	35,54,54	1.31	4 (11%)
23	GDP	AT	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.00	1 (3%)
24	GTP	G6	501	25	29,34,34	1.26	2 (6%)	35,54,54	1.26	3 (8%)
23	GDP	AS	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	3 (10%)
24	GTP	o	501	25	29,34,34	1.27	4 (13%)	35,54,54	1.30	4 (11%)
23	GDP	AE	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.05	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	GDP	Gf	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.31	5 (16%)
23	GDP	BF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.14	2 (6%)
23	GDP	AR	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.11	1 (3%)
24	GTP	G4	602	25	29,34,34	1.33	4 (13%)	35,54,54	1.32	3 (8%)
24	GTP	GQ	602	25	29,34,34	1.31	4 (13%)	35,54,54	1.46	4 (11%)
23	GDP	F4	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	2 (6%)
23	GDP	BH	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.18	2 (6%)
23	GDP	Ef	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.13	2 (6%)
23	GDP	DX	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.15	1 (3%)
24	GTP	B9	602	25	29,34,34	1.27	4 (13%)	35,54,54	1.30	4 (11%)
23	GDP	Fn	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.20	3 (10%)
23	GDP	AL	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.18	3 (10%)
23	GDP	GW	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.26	5 (16%)
24	GTP	Bd	501	25	29,34,34	1.29	3 (10%)	35,54,54	1.24	3 (8%)
24	GTP	FY	501	25	29,34,34	1.26	3 (10%)	35,54,54	1.31	5 (14%)
23	GDP	DP	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.17	3 (10%)
23	GDP	8	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
24	GTP	V	602	25	29,34,34	1.27	4 (13%)	35,54,54	1.35	4 (11%)
24	GTP	G3	602	25	29,34,34	1.36	5 (17%)	35,54,54	1.30	4 (11%)
23	GDP	FH	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	2 (6%)
23	GDP	Bt	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.02	1 (3%)
23	GDP	Db	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	2 (6%)
24	GTP	4	602	25	29,34,34	1.22	2 (6%)	35,54,54	1.37	6 (17%)
23	GDP	BD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
23	GDP	O	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.01	2 (6%)
23	GDP	Bs	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	2 (6%)
23	GDP	Ad	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.12	2 (6%)
23	GDP	DW	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.10	1 (3%)
24	GTP	GL	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.27	4 (11%)
23	GDP	Bh	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.06	2 (6%)
24	GTP	Gp	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.26	3 (8%)
24	GTP	BI	602	25	29,34,34	1.24	2 (6%)	35,54,54	1.39	4 (11%)
23	GDP	Fr	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.19	2 (6%)
24	GTP	2	602	25	29,34,34	1.22	2 (6%)	35,54,54	1.37	5 (14%)
24	GTP	v	602	25	29,34,34	1.26	4 (13%)	35,54,54	1.28	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	GDP	AY	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.07	1 (3%)
23	GDP	Gi	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	1 (3%)
23	GDP	DS	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	3 (10%)
24	GTP	Gr	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.24	3 (8%)
23	GDP	Aq	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	2 (6%)
23	GDP	Gc	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	3 (10%)
23	GDP	m	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.04	1 (3%)
23	GDP	Fo	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	3 (10%)
23	GDP	GV	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.21	3 (10%)
24	GTP	Fi	501	25	29,34,34	1.34	4 (13%)	35,54,54	1.37	3 (8%)
23	GDP	AU	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.20	3 (10%)
23	GDP	Be	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.04	2 (6%)
24	GTP	G1	501	25	29,34,34	1.31	4 (13%)	35,54,54	1.28	4 (11%)
23	GDP	Ao	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.04	1 (3%)
24	GTP	j	602	25	29,34,34	1.30	4 (13%)	35,54,54	1.30	3 (8%)
23	GDP	EW	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	1 (3%)
24	GTP	E2	501	25	29,34,34	1.32	4 (13%)	35,54,54	1.36	3 (8%)
24	GTP	3	602	25	29,34,34	1.20	2 (6%)	35,54,54	1.37	4 (11%)
23	GDP	De	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.20	4 (13%)
23	GDP	Ai	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.16	2 (6%)
24	GTP	E8	501	25	29,34,34	1.26	3 (10%)	35,54,54	1.27	3 (8%)
24	GTP	G2	501	25	29,34,34	1.29	4 (13%)	35,54,54	1.27	3 (8%)
23	GDP	FN	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.22	4 (13%)
23	GDP	Bl	602	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	3 (10%)
23	GDP	Ap	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.05	1 (3%)
23	GDP	BE	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.00	1 (3%)
23	GDP	F1	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.24	4 (13%)
24	GTP	Gs	501	25	29,34,34	1.28	4 (13%)	35,54,54	1.25	3 (8%)
24	GTP	B5	602	25	29,34,34	1.26	3 (10%)	35,54,54	1.34	5 (14%)
24	GTP	E5	501	25	29,34,34	1.34	5 (17%)	35,54,54	1.45	5 (14%)
23	GDP	EZ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.15	2 (6%)
23	GDP	Aa	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
24	GTP	t	602	25	29,34,34	1.28	3 (10%)	35,54,54	1.37	5 (14%)
23	GDP	Fq	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.19	3 (10%)
24	GTP	l	602	25	29,34,34	1.31	4 (13%)	35,54,54	1.21	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	GDP	Fy	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
24	GTP	Gx	501	25	29,34,34	1.28	4 (13%)	35,54,54	1.31	5 (14%)
24	GTP	G5	501	25	29,34,34	1.25	3 (10%)	35,54,54	1.31	3 (8%)
23	GDP	U	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.02	1 (3%)
24	GTP	w	602	25	29,34,34	1.25	3 (10%)	35,54,54	1.27	4 (11%)
24	GTP	Fa	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.25	4 (11%)
24	GTP	Q	602	25	29,34,34	1.28	3 (10%)	35,54,54	1.32	3 (8%)
23	GDP	Fl	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	3 (10%)
24	GTP	z	602	25	29,34,34	1.28	3 (10%)	35,54,54	1.30	5 (14%)
24	GTP	E1	501	25	29,34,34	1.34	5 (17%)	35,54,54	1.48	4 (11%)
23	GDP	Bg	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	3 (10%)
23	GDP	FA	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.28	4 (13%)
23	GDP	FI	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	1 (3%)
24	GTP	GD	501	25	29,34,34	1.35	5 (17%)	35,54,54	1.30	4 (11%)
23	GDP	Ah	602	-	25,30,30	0.98	1 (4%)	30,47,47	1.05	1 (3%)
23	GDP	Dh	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	3 (10%)
24	GTP	A4	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.25	3 (8%)
23	GDP	EN	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.24	4 (13%)
24	GTP	CA	602	25	29,34,34	1.26	3 (10%)	35,54,54	1.28	3 (8%)
23	GDP	GU	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.30	4 (13%)
24	GTP	Ey	602	25	29,34,34	1.31	4 (13%)	35,54,54	1.35	5 (14%)
24	GTP	FP	501	25	29,34,34	1.30	4 (13%)	35,54,54	1.25	3 (8%)
23	GDP	Dg	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	2 (6%)
24	GTP	p	602	25	29,34,34	1.25	2 (6%)	35,54,54	1.38	5 (14%)
24	GTP	g	602	25	29,34,34	1.26	3 (10%)	35,54,54	1.37	5 (14%)
24	GTP	Fg	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.26	3 (8%)
23	GDP	Bn	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	2 (6%)
24	GTP	Eo	501	25	29,34,34	1.27	3 (10%)	35,54,54	1.30	3 (8%)
24	GTP	AI	501	25	29,34,34	1.28	3 (10%)	35,54,54	1.28	4 (11%)
23	GDP	Dt	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)
23	GDP	Fu	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.17	2 (6%)
23	GDP	AH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.04	1 (3%)

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
24	GTP	B6	602	25	-	5/18/38/38	0/3/3/3
24	GTP	Ek	501	25	-	3/18/38/38	0/3/3/3
23	GDP	AO	501	-	-	6/12/32/32	0/3/3/3
24	GTP	BU	602	25	-	6/18/38/38	0/3/3/3
23	GDP	Az	501	-	-	3/12/32/32	0/3/3/3
24	GTP	E3	501	25	-	4/18/38/38	0/3/3/3
24	GTP	Al	602	25	-	6/18/38/38	0/3/3/3
24	GTP	BX	602	25	-	3/18/38/38	0/3/3/3
24	GTP	Ff	501	25	-	7/18/38/38	0/3/3/3
24	GTP	Et	501	25	-	4/18/38/38	0/3/3/3
23	GDP	FF	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Ec	501	-	-	3/12/32/32	0/3/3/3
24	GTP	A9	501	25	-	5/18/38/38	0/3/3/3
24	GTP	BY	602	25	-	3/18/38/38	0/3/3/3
24	GTP	F7	501	25	-	5/18/38/38	0/3/3/3
23	GDP	Bo	501	-	-	3/12/32/32	0/3/3/3
23	GDP	DZ	501	-	-	5/12/32/32	0/3/3/3
23	GDP	Df	501	-	-	7/12/32/32	0/3/3/3
24	GTP	By	602	25	-	3/18/38/38	0/3/3/3
23	GDP	X	501	-	-	2/12/32/32	0/3/3/3
23	GDP	DO	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Fm	501	-	-	4/12/32/32	0/3/3/3
23	GDP	Gk	501	-	-	1/12/32/32	0/3/3/3
23	GDP	AW	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Gh	501	-	-	8/12/32/32	0/3/3/3
23	GDP	AZ	501	-	-	4/12/32/32	0/3/3/3
23	GDP	EQ	501	-	-	5/12/32/32	0/3/3/3
24	GTP	s	602	25	-	3/18/38/38	0/3/3/3
23	GDP	Ev	501	-	-	2/12/32/32	0/3/3/3
24	GTP	T	602	25	-	2/18/38/38	0/3/3/3
24	GTP	A1	602	25	-	3/18/38/38	0/3/3/3
23	GDP	Ga	501	-	-	2/12/32/32	0/3/3/3
24	GTP	FR	501	25	-	5/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	GM	501	25	-	4/18/38/38	0/3/3/3
23	GDP	BA	501	-	-	5/12/32/32	0/3/3/3
24	GTP	Fh	501	25	-	6/18/38/38	0/3/3/3
24	GTP	A5	501	25	-	5/18/38/38	0/3/3/3
23	GDP	AD	501	-	-	1/12/32/32	0/3/3/3
24	GTP	FS	501	25	-	3/18/38/38	0/3/3/3
23	GDP	GX	501	-	-	3/12/32/32	0/3/3/3
23	GDP	FG	501	-	-	5/12/32/32	0/3/3/3
24	GTP	AK	602	25	-	4/18/38/38	0/3/3/3
23	GDP	Ab	501	-	-	6/12/32/32	0/3/3/3
24	GTP	S	602	25	-	9/18/38/38	0/3/3/3
23	GDP	AN	501	-	-	4/12/32/32	0/3/3/3
24	GTP	GT	501	25	-	4/18/38/38	0/3/3/3
24	GTP	AJ	602	25	-	5/18/38/38	0/3/3/3
24	GTP	Ex	501	25	-	7/18/38/38	0/3/3/3
24	GTP	y	602	25	-	5/18/38/38	0/3/3/3
23	GDP	FL	501	-	-	8/12/32/32	0/3/3/3
23	GDP	Bk	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Bm	501	-	-	4/12/32/32	0/3/3/3
24	GTP	F6	501	25	-	5/18/38/38	0/3/3/3
23	GDP	Fs	501	-	-	6/12/32/32	0/3/3/3
24	GTP	AS	501	25	-	2/18/38/38	0/3/3/3
24	GTP	FW	501	25	-	5/18/38/38	0/3/3/3
23	GDP	BZ	501	-	-	2/12/32/32	0/3/3/3
24	GTP	Gv	501	25	-	4/18/38/38	0/3/3/3
24	GTP	Ez	501	25	-	7/18/38/38	0/3/3/3
24	GTP	A7	501	25	-	4/18/38/38	0/3/3/3
23	GDP	9	501	-	-	3/12/32/32	0/3/3/3
24	GTP	5	602	25	-	3/18/38/38	0/3/3/3
23	GDP	EM	501	-	-	5/12/32/32	0/3/3/3
23	GDP	Gb	501	-	-	7/12/32/32	0/3/3/3
23	GDP	Fv	501	-	-	4/12/32/32	0/3/3/3
23	GDP	Eb	501	-	-	6/12/32/32	0/3/3/3
24	GTP	Bz	602	25	-	5/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	Fk	501	25	-	3/18/38/38	0/3/3/3
24	GTP	GP	501	25	-	9/18/38/38	0/3/3/3
23	GDP	AQ	501	-	-	2/12/32/32	0/3/3/3
23	GDP	DU	501	-	-	2/12/32/32	0/3/3/3
23	GDP	AM	501	-	-	5/12/32/32	0/3/3/3
24	GTP	Fb	501	25	-	4/18/38/38	0/3/3/3
24	GTP	FT	501	25	-	4/18/38/38	0/3/3/3
23	GDP	Dx	501	-	-	3/12/32/32	0/3/3/3
23	GDP	Dq	501	-	-	1/12/32/32	0/3/3/3
24	GTP	b	602	25	-	6/18/38/38	0/3/3/3
24	GTP	k	602	25	-	4/18/38/38	0/3/3/3
24	GTP	A6	501	25	-	4/18/38/38	0/3/3/3
24	GTP	BS	602	25	-	6/18/38/38	0/3/3/3
23	GDP	F2	501	-	-	6/12/32/32	0/3/3/3
24	GTP	Gl	501	25	-	3/18/38/38	0/3/3/3
24	GTP	GE	501	25	-	7/18/38/38	0/3/3/3
23	GDP	Ag	501	-	-	5/12/32/32	0/3/3/3
24	GTP	Fd	602	25	-	6/18/38/38	0/3/3/3
23	GDP	DY	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Dd	501	-	-	8/12/32/32	0/3/3/3
24	GTP	q	602	25	-	4/18/38/38	0/3/3/3
23	GDP	Ge	501	-	-	2/12/32/32	0/3/3/3
24	GTP	Bw	602	25	-	11/18/38/38	0/3/3/3
24	GTP	Bu	602	25	-	6/18/38/38	0/3/3/3
24	GTP	Fe	501	25	-	9/18/38/38	0/3/3/3
24	GTP	F5	501	25	-	4/18/38/38	0/3/3/3
24	GTP	FQ	501	25	-	5/18/38/38	0/3/3/3
24	GTP	FM	501	25	-	4/18/38/38	0/3/3/3
24	GTP	BQ	602	25	-	3/18/38/38	0/3/3/3
24	GTP	E7	501	25	-	1/18/38/38	0/3/3/3
23	GDP	Ae	501	-	-	4/12/32/32	0/3/3/3
23	GDP	AP	501	-	-	6/12/32/32	0/3/3/3
23	GDP	7	501	-	-	0/12/32/32	0/3/3/3
24	GTP	Fj	501	25	-	6/18/38/38	0/3/3/3
24	GTP	GF	501	25	-	10/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	BL	602	25	-	7/18/38/38	0/3/3/3
23	GDP	P	501	-	-	2/12/32/32	0/3/3/3
23	GDP	Av	501	-	-	5/12/32/32	0/3/3/3
23	GDP	Br	501	-	-	5/12/32/32	0/3/3/3
23	GDP	FD	501	-	-	6/12/32/32	0/3/3/3
24	GTP	GC	501	25	-	4/18/38/38	0/3/3/3
23	GDP	Du	501	-	-	0/12/32/32	0/3/3/3
23	GDP	EX	501	-	-	5/12/32/32	0/3/3/3
24	GTP	Gz	501	25	-	4/18/38/38	0/3/3/3
24	GTP	BM	602	25	-	6/18/38/38	0/3/3/3
23	GDP	ET	501	-	-	6/12/32/32	0/3/3/3
23	GDP	E9	501	-	-	3/12/32/32	0/3/3/3
24	GTP	u	501	25	-	4/18/38/38	0/3/3/3
23	GDP	An	501	-	-	3/12/32/32	0/3/3/3
24	GTP	F3	501	25	-	4/18/38/38	0/3/3/3
24	GTP	f	602	25	-	3/18/38/38	0/3/3/3
24	GTP	Gq	501	25	-	4/18/38/38	0/3/3/3
23	GDP	n	501	-	-	2/12/32/32	0/3/3/3
24	GTP	Go	501	25	-	3/18/38/38	0/3/3/3
24	GTP	Aw	602	25	-	5/18/38/38	0/3/3/3
23	GDP	Dc	501	-	-	5/12/32/32	0/3/3/3
23	GDP	FJ	501	-	-	6/12/32/32	0/3/3/3
23	GDP	0	501	-	-	7/12/32/32	0/3/3/3
24	GTP	GJ	501	25	-	5/18/38/38	0/3/3/3
23	GDP	Ac	501	-	-	1/12/32/32	0/3/3/3
23	GDP	DT	501	-	-	7/12/32/32	0/3/3/3
23	GDP	BG	501	-	-	2/12/32/32	0/3/3/3
24	GTP	x	501	25	-	3/18/38/38	0/3/3/3
24	GTP	W	602	25	-	6/18/38/38	0/3/3/3
24	GTP	F8	501	25	-	6/18/38/38	0/3/3/3
24	GTP	Es	501	25	-	4/18/38/38	0/3/3/3
23	GDP	Au	602	-	-	0/12/32/32	0/3/3/3
24	GTP	B1	602	25	-	5/18/38/38	0/3/3/3
24	GTP	h	602	25	-	6/18/38/38	0/3/3/3
24	GTP	B8	602	25	-	5/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	Dv	501	-	-	1/12/32/32	0/3/3/3
24	GTP	A8	501	25	-	5/18/38/38	0/3/3/3
23	GDP	AB	501	-	-	1/12/32/32	0/3/3/3
23	GDP	Dk	501	-	-	6/12/32/32	0/3/3/3
23	GDP	GH	501	-	-	4/12/32/32	0/3/3/3
24	GTP	Eq	501	25	-	4/18/38/38	0/3/3/3
24	GTP	1	602	25	-	3/18/38/38	0/3/3/3
24	GTP	BN	602	25	-	6/18/38/38	0/3/3/3
24	GTP	Em	501	25	-	7/18/38/38	0/3/3/3
24	GTP	i	602	25	-	6/18/38/38	0/3/3/3
24	GTP	BK	602	25	-	3/18/38/38	0/3/3/3
23	GDP	DL	501	-	-	8/12/32/32	0/3/3/3
23	GDP	FE	501	-	-	3/12/32/32	0/3/3/3
23	GDP	A3	501	-	-	1/12/32/32	0/3/3/3
23	GDP	AA	501	-	-	2/12/32/32	0/3/3/3
24	GTP	FX	501	25	-	4/18/38/38	0/3/3/3
24	GTP	FV	602	25	-	4/18/38/38	0/3/3/3
24	GTP	Eh	501	25	-	4/18/38/38	0/3/3/3
24	GTP	B2	602	25	-	5/18/38/38	0/3/3/3
24	GTP	Bx	602	25	-	4/18/38/38	0/3/3/3
23	GDP	Bq	602	-	-	2/12/32/32	0/3/3/3
23	GDP	Am	501	-	-	1/12/32/32	0/3/3/3
23	GDP	Ds	501	-	-	0/12/32/32	0/3/3/3
24	GTP	FU	501	25	-	5/18/38/38	0/3/3/3
24	GTP	FZ	501	25	-	5/18/38/38	0/3/3/3
23	GDP	BC	501	-	-	4/12/32/32	0/3/3/3
23	GDP	Fx	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Bp	501	-	-	3/12/32/32	0/3/3/3
23	GDP	FC	501	-	-	1/12/32/32	0/3/3/3
24	GTP	Eg	501	25	-	5/18/38/38	0/3/3/3
23	GDP	Ba	501	-	-	2/12/32/32	0/3/3/3
23	GDP	DM	501	-	-	6/12/32/32	0/3/3/3
24	GTP	Bv	602	25	-	2/18/38/38	0/3/3/3
24	GTP	BP	602	25	-	4/18/38/38	0/3/3/3
23	GDP	EP	501	-	-	4/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	Dj	501	-	-	6/12/32/32	0/3/3/3
24	GTP	GR	501	25	-	7/18/38/38	0/3/3/3
24	GTP	Ej	501	25	-	5/18/38/38	0/3/3/3
23	GDP	Dr	501	-	-	4/12/32/32	0/3/3/3
24	GTP	Gt	501	25	-	7/18/38/38	0/3/3/3
23	GDP	Bb	501	-	-	3/12/32/32	0/3/3/3
23	GDP	FB	501	-	-	2/12/32/32	0/3/3/3
24	GTP	GB	501	25	-	4/18/38/38	0/3/3/3
24	GTP	GK	501	25	-	4/18/38/38	0/3/3/3
24	GTP	Er	501	25	-	4/18/38/38	0/3/3/3
24	GTP	Aj	501	25	-	3/18/38/38	0/3/3/3
24	GTP	GI	501	25	-	4/18/38/38	0/3/3/3
24	GTP	CB	602	25	-	5/18/38/38	0/3/3/3
23	GDP	EV	501	-	-	3/12/32/32	0/3/3/3
23	GDP	Da	501	-	-	8/12/32/32	0/3/3/3
23	GDP	ES	501	-	-	3/12/32/32	0/3/3/3
23	GDP	Gj	501	-	-	6/12/32/32	0/3/3/3
24	GTP	Gy	501	25	-	4/18/38/38	0/3/3/3
23	GDP	FK	501	-	-	7/12/32/32	0/3/3/3
23	GDP	Fw	501	-	-	6/12/32/32	0/3/3/3
24	GTP	BR	501	25	-	5/18/38/38	0/3/3/3
23	GDP	Ea	501	-	-	8/12/32/32	0/3/3/3
24	GTP	d	602	25	-	2/18/38/38	0/3/3/3
24	GTP	GA	501	25	-	3/18/38/38	0/3/3/3
24	GTP	Ax	602	25	-	4/18/38/38	0/3/3/3
23	GDP	Gm	501	-	-	4/12/32/32	0/3/3/3
23	GDP	BW	501	-	-	1/12/32/32	0/3/3/3
23	GDP	Fz	501	-	-	6/12/32/32	0/3/3/3
23	GDP	ER	501	-	-	4/12/32/32	0/3/3/3
23	GDP	AF	501	-	-	4/12/32/32	0/3/3/3
23	GDP	Ed	501	-	-	6/12/32/32	0/3/3/3
24	GTP	Gu	501	25	-	6/18/38/38	0/3/3/3
23	GDP	As	501	-	-	4/12/32/32	0/3/3/3
23	GDP	r	501	-	-	2/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	Ay	602	25	-	4/18/38/38	0/3/3/3
24	GTP	BJ	602	25	-	2/18/38/38	0/3/3/3
24	GTP	Z	602	25	-	2/18/38/38	0/3/3/3
23	GDP	Di	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Af	501	-	-	3/12/32/32	0/3/3/3
24	GTP	6	602	25	-	3/18/38/38	0/3/3/3
24	GTP	A2	602	25	-	3/18/38/38	0/3/3/3
24	GTP	Eu	501	25	-	4/18/38/38	0/3/3/3
24	GTP	GG	501	25	-	4/18/38/38	0/3/3/3
24	GTP	GO	602	25	-	4/18/38/38	0/3/3/3
23	GDP	EY	501	-	-	8/12/32/32	0/3/3/3
24	GTP	B0	501	25	-	4/18/38/38	0/3/3/3
24	GTP	Gn	501	25	-	4/18/38/38	0/3/3/3
24	GTP	En	501	25	-	4/18/38/38	0/3/3/3
24	GTP	E4	501	25	-	5/18/38/38	0/3/3/3
24	GTP	F0	501	25	-	5/18/38/38	0/3/3/3
24	GTP	BT	501	25	-	3/18/38/38	0/3/3/3
23	GDP	AX	501	-	-	4/12/32/32	0/3/3/3
24	GTP	Fc	501	25	-	4/18/38/38	0/3/3/3
23	GDP	Gd	501	-	-	3/12/32/32	0/3/3/3
23	GDP	Bf	501	-	-	3/12/32/32	0/3/3/3
23	GDP	AG	501	-	-	3/12/32/32	0/3/3/3
24	GTP	Ee	501	25	-	5/18/38/38	0/3/3/3
24	GTP	B4	602	25	-	3/18/38/38	0/3/3/3
23	GDP	Bi	501	-	-	4/12/32/32	0/3/3/3
24	GTP	e	602	25	-	4/18/38/38	0/3/3/3
23	GDP	DR	501	-	-	1/12/32/32	0/3/3/3
23	GDP	GZ	501	-	-	5/12/32/32	0/3/3/3
23	GDP	EO	501	-	-	3/12/32/32	0/3/3/3
24	GTP	Ei	501	25	-	7/18/38/38	0/3/3/3
24	GTP	El	501	25	-	5/18/38/38	0/3/3/3
23	GDP	DQ	501	-	-	6/12/32/32	0/3/3/3
24	GTP	B3	602	25	-	4/18/38/38	0/3/3/3
24	GTP	BO	602	25	-	4/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	F9	501	25	-	5/18/38/38	0/3/3/3
23	GDP	A0	501	-	-	3/12/32/32	0/3/3/3
23	GDP	E0	501	-	-	5/12/32/32	0/3/3/3
23	GDP	At	501	-	-	5/12/32/32	0/3/3/3
24	GTP	FO	501	25	-	4/18/38/38	0/3/3/3
24	GTP	Ak	602	25	-	6/18/38/38	0/3/3/3
23	GDP	AV	602	-	-	1/12/32/32	0/3/3/3
23	GDP	Fp	501	-	-	5/12/32/32	0/3/3/3
24	GTP	Ep	501	25	-	4/18/38/38	0/3/3/3
24	GTP	GN	501	25	-	6/18/38/38	0/3/3/3
24	GTP	Gw	501	25	-	4/18/38/38	0/3/3/3
24	GTP	Ew	501	25	-	6/18/38/38	0/3/3/3
24	GTP	B7	501	25	-	3/18/38/38	0/3/3/3
23	GDP	EL	501	-	-	5/12/32/32	0/3/3/3
23	GDP	DV	501	-	-	8/12/32/32	0/3/3/3
23	GDP	Ft	501	-	-	6/12/32/32	0/3/3/3
23	GDP	GY	501	-	-	3/12/32/32	0/3/3/3
24	GTP	a	602	25	-	5/18/38/38	0/3/3/3
23	GDP	BB	501	-	-	7/12/32/32	0/3/3/3
24	GTP	Bc	501	25	-	4/18/38/38	0/3/3/3
23	GDP	AC	501	-	-	3/12/32/32	0/3/3/3
24	GTP	c	602	25	-	11/18/38/38	0/3/3/3
23	GDP	Bj	501	-	-	5/12/32/32	0/3/3/3
23	GDP	EU	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Dw	501	-	-	0/12/32/32	0/3/3/3
23	GDP	Gg	501	-	-	6/12/32/32	0/3/3/3
24	GTP	BV	602	25	-	5/18/38/38	0/3/3/3
24	GTP	Y	602	25	-	8/18/38/38	0/3/3/3
23	GDP	Ar	501	-	-	5/12/32/32	0/3/3/3
23	GDP	DN	501	-	-	8/12/32/32	0/3/3/3
24	GTP	E6	602	25	-	5/18/38/38	0/3/3/3
24	GTP	GS	501	25	-	4/18/38/38	0/3/3/3
23	GDP	AT	501	-	-	4/12/32/32	0/3/3/3
24	GTP	G6	501	25	-	3/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	AS	502	-	-	5/12/32/32	0/3/3/3
24	GTP	o	501	25	-	10/18/38/38	0/3/3/3
23	GDP	AE	501	-	-	3/12/32/32	0/3/3/3
23	GDP	Gf	501	-	-	2/12/32/32	0/3/3/3
23	GDP	BF	501	-	-	6/12/32/32	0/3/3/3
23	GDP	AR	501	-	-	7/12/32/32	0/3/3/3
24	GTP	G4	602	25	-	10/18/38/38	0/3/3/3
24	GTP	GQ	602	25	-	6/18/38/38	0/3/3/3
23	GDP	F4	501	-	-	8/12/32/32	0/3/3/3
23	GDP	BH	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Ef	501	-	-	6/12/32/32	0/3/3/3
23	GDP	DX	501	-	-	4/12/32/32	0/3/3/3
24	GTP	B9	602	25	-	4/18/38/38	0/3/3/3
23	GDP	Fn	501	-	-	5/12/32/32	0/3/3/3
23	GDP	AL	501	-	-	5/12/32/32	0/3/3/3
23	GDP	GW	501	-	-	3/12/32/32	0/3/3/3
24	GTP	Bd	501	25	-	5/18/38/38	0/3/3/3
24	GTP	FY	501	25	-	4/18/38/38	0/3/3/3
23	GDP	DP	501	-	-	5/12/32/32	0/3/3/3
23	GDP	8	501	-	-	3/12/32/32	0/3/3/3
24	GTP	V	602	25	-	3/18/38/38	0/3/3/3
24	GTP	G3	602	25	-	6/18/38/38	0/3/3/3
23	GDP	FH	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Bt	501	-	-	2/12/32/32	0/3/3/3
23	GDP	Db	501	-	-	8/12/32/32	0/3/3/3
24	GTP	4	602	25	-	3/18/38/38	0/3/3/3
23	GDP	BD	501	-	-	6/12/32/32	0/3/3/3
23	GDP	O	501	-	-	2/12/32/32	0/3/3/3
23	GDP	Bs	501	-	-	4/12/32/32	0/3/3/3
23	GDP	Ad	501	-	-	7/12/32/32	0/3/3/3
23	GDP	DW	501	-	-	6/12/32/32	0/3/3/3
24	GTP	GL	501	25	-	3/18/38/38	0/3/3/3
23	GDP	Bh	501	-	-	5/12/32/32	0/3/3/3
24	GTP	Gp	501	25	-	4/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	BI	602	25	-	11/18/38/38	0/3/3/3
23	GDP	Fr	501	-	-	2/12/32/32	0/3/3/3
24	GTP	2	602	25	-	3/18/38/38	0/3/3/3
24	GTP	v	602	25	-	5/18/38/38	0/3/3/3
23	GDP	AY	501	-	-	3/12/32/32	0/3/3/3
23	GDP	Gi	501	-	-	6/12/32/32	0/3/3/3
23	GDP	DS	501	-	-	6/12/32/32	0/3/3/3
24	GTP	Gr	501	25	-	4/18/38/38	0/3/3/3
23	GDP	Aq	501	-	-	4/12/32/32	0/3/3/3
23	GDP	Gc	501	-	-	6/12/32/32	0/3/3/3
23	GDP	m	501	-	-	2/12/32/32	0/3/3/3
23	GDP	Fo	501	-	-	3/12/32/32	0/3/3/3
23	GDP	GV	501	-	-	5/12/32/32	0/3/3/3
24	GTP	Fi	501	25	-	6/18/38/38	0/3/3/3
23	GDP	AU	501	-	-	2/12/32/32	0/3/3/3
23	GDP	Be	501	-	-	4/12/32/32	0/3/3/3
24	GTP	G1	501	25	-	4/18/38/38	0/3/3/3
23	GDP	Ao	501	-	-	3/12/32/32	0/3/3/3
24	GTP	j	602	25	-	5/18/38/38	0/3/3/3
23	GDP	EW	501	-	-	6/12/32/32	0/3/3/3
24	GTP	E2	501	25	-	6/18/38/38	0/3/3/3
24	GTP	3	602	25	-	3/18/38/38	0/3/3/3
23	GDP	De	501	-	-	3/12/32/32	0/3/3/3
23	GDP	Ai	501	-	-	5/12/32/32	0/3/3/3
24	GTP	E8	501	25	-	4/18/38/38	0/3/3/3
24	GTP	G2	501	25	-	5/18/38/38	0/3/3/3
23	GDP	FN	501	-	-	3/12/32/32	0/3/3/3
23	GDP	Bl	602	-	-	4/12/32/32	0/3/3/3
23	GDP	Ap	501	-	-	4/12/32/32	0/3/3/3
23	GDP	BE	501	-	-	3/12/32/32	0/3/3/3
23	GDP	F1	501	-	-	7/12/32/32	0/3/3/3
24	GTP	Gs	501	25	-	3/18/38/38	0/3/3/3
24	GTP	B5	602	25	-	3/18/38/38	0/3/3/3
24	GTP	E5	501	25	-	7/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	EZ	501	-	-	6/12/32/32	0/3/3/3
23	GDP	Aa	501	-	-	7/12/32/32	0/3/3/3
24	GTP	t	602	25	-	3/18/38/38	0/3/3/3
23	GDP	Fq	501	-	-	4/12/32/32	0/3/3/3
24	GTP	l	602	25	-	4/18/38/38	0/3/3/3
23	GDP	Fy	501	-	-	8/12/32/32	0/3/3/3
24	GTP	Gx	501	25	-	5/18/38/38	0/3/3/3
24	GTP	G5	501	25	-	3/18/38/38	0/3/3/3
23	GDP	U	501	-	-	2/12/32/32	0/3/3/3
24	GTP	w	602	25	-	4/18/38/38	0/3/3/3
24	GTP	Fa	501	25	-	4/18/38/38	0/3/3/3
24	GTP	Q	602	25	-	7/18/38/38	0/3/3/3
23	GDP	Fl	501	-	-	6/12/32/32	0/3/3/3
24	GTP	z	602	25	-	6/18/38/38	0/3/3/3
24	GTP	E1	501	25	-	7/18/38/38	0/3/3/3
23	GDP	Bg	501	-	-	5/12/32/32	0/3/3/3
23	GDP	FA	501	-	-	4/12/32/32	0/3/3/3
23	GDP	FI	501	-	-	6/12/32/32	0/3/3/3
24	GTP	GD	501	25	-	6/18/38/38	0/3/3/3
23	GDP	Ah	602	-	-	2/12/32/32	0/3/3/3
23	GDP	Dh	501	-	-	3/12/32/32	0/3/3/3
24	GTP	A4	501	25	-	4/18/38/38	0/3/3/3
23	GDP	EN	501	-	-	3/12/32/32	0/3/3/3
24	GTP	CA	602	25	-	5/18/38/38	0/3/3/3
23	GDP	GU	501	-	-	3/12/32/32	0/3/3/3
24	GTP	Ey	602	25	-	7/18/38/38	0/3/3/3
24	GTP	FP	501	25	-	4/18/38/38	0/3/3/3
23	GDP	Dg	501	-	-	3/12/32/32	0/3/3/3
24	GTP	p	602	25	-	2/18/38/38	0/3/3/3
24	GTP	g	602	25	-	3/18/38/38	0/3/3/3
24	GTP	Fg	501	25	-	3/18/38/38	0/3/3/3
23	GDP	Bn	501	-	-	5/12/32/32	0/3/3/3
24	GTP	Eo	501	25	-	4/18/38/38	0/3/3/3
24	GTP	AI	501	25	-	4/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	Dt	501	-	-	0/12/32/32	0/3/3/3
23	GDP	Fu	501	-	-	1/12/32/32	0/3/3/3
23	GDP	AH	501	-	-	4/12/32/32	0/3/3/3

All (863) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	GT	501	GTP	C5-C6	-4.34	1.38	1.47
24	Bd	501	GTP	C5-C6	-4.31	1.38	1.47
24	FO	501	GTP	C5-C6	-4.30	1.38	1.47
24	Et	501	GTP	C5-C6	-4.29	1.39	1.47
24	A2	602	GTP	C5-C6	-4.29	1.39	1.47
24	GB	501	GTP	C5-C6	-4.29	1.39	1.47
24	Fb	501	GTP	C5-C6	-4.29	1.39	1.47
24	Fg	501	GTP	C5-C6	-4.28	1.39	1.47
24	GS	501	GTP	C5-C6	-4.27	1.39	1.47
24	Eg	501	GTP	C5-C6	-4.27	1.39	1.47
24	Gz	501	GTP	C5-C6	-4.27	1.39	1.47
24	FS	501	GTP	C5-C6	-4.27	1.39	1.47
24	Gl	501	GTP	C5-C6	-4.27	1.39	1.47
24	G1	501	GTP	C5-C6	-4.26	1.39	1.47
24	Ey	602	GTP	C5-C6	-4.25	1.39	1.47
24	GE	501	GTP	C5-C6	-4.25	1.39	1.47
24	E7	501	GTP	C5-C6	-4.25	1.39	1.47
24	Fa	501	GTP	C5-C6	-4.25	1.39	1.47
24	FV	602	GTP	C5-C6	-4.25	1.39	1.47
24	GJ	501	GTP	C5-C6	-4.25	1.39	1.47
24	BV	602	GTP	C5-C6	-4.25	1.39	1.47
24	t	602	GTP	C5-C6	-4.25	1.39	1.47
24	FR	501	GTP	C5-C6	-4.25	1.39	1.47
24	Gr	501	GTP	C5-C6	-4.25	1.39	1.47
24	E5	501	GTP	C5-C6	-4.25	1.39	1.47
24	A5	501	GTP	C5-C6	-4.24	1.39	1.47
24	z	602	GTP	C5-C6	-4.24	1.39	1.47
24	Fd	602	GTP	C5-C6	-4.23	1.39	1.47
24	A8	501	GTP	C5-C6	-4.23	1.39	1.47
24	BP	602	GTP	C5-C6	-4.23	1.39	1.47
24	Aj	501	GTP	C5-C6	-4.23	1.39	1.47
24	GN	501	GTP	C5-C6	-4.23	1.39	1.47
24	Ek	501	GTP	C5-C6	-4.23	1.39	1.47
24	By	602	GTP	C5-C6	-4.23	1.39	1.47
24	G5	501	GTP	C5-C6	-4.22	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A1	602	GTP	C5-C6	-4.22	1.39	1.47
24	Gs	501	GTP	C5-C6	-4.22	1.39	1.47
24	Ep	501	GTP	C5-C6	-4.22	1.39	1.47
24	Ej	501	GTP	C5-C6	-4.22	1.39	1.47
24	G6	501	GTP	C5-C6	-4.22	1.39	1.47
24	x	501	GTP	C5-C6	-4.22	1.39	1.47
24	GO	602	GTP	C5-C6	-4.22	1.39	1.47
24	GK	501	GTP	C5-C6	-4.21	1.39	1.47
24	s	602	GTP	C5-C6	-4.21	1.39	1.47
24	E4	501	GTP	C5-C6	-4.21	1.39	1.47
24	Gt	501	GTP	C5-C6	-4.21	1.39	1.47
24	FT	501	GTP	C5-C6	-4.21	1.39	1.47
24	Fk	501	GTP	C5-C6	-4.21	1.39	1.47
24	AK	602	GTP	C5-C6	-4.21	1.39	1.47
24	GF	501	GTP	C5-C6	-4.21	1.39	1.47
24	g	602	GTP	C5-C6	-4.21	1.39	1.47
24	V	602	GTP	C5-C6	-4.21	1.39	1.47
24	FQ	501	GTP	C5-C6	-4.21	1.39	1.47
24	A7	501	GTP	C5-C6	-4.21	1.39	1.47
24	G2	501	GTP	C5-C6	-4.21	1.39	1.47
24	FY	501	GTP	C5-C6	-4.21	1.39	1.47
24	Fj	501	GTP	C5-C6	-4.21	1.39	1.47
24	E8	501	GTP	C5-C6	-4.21	1.39	1.47
24	En	501	GTP	C5-C6	-4.21	1.39	1.47
24	FM	501	GTP	C5-C6	-4.20	1.39	1.47
24	B3	602	GTP	C5-C6	-4.20	1.39	1.47
24	E3	501	GTP	C5-C6	-4.20	1.39	1.47
24	BN	602	GTP	C5-C6	-4.20	1.39	1.47
24	Gp	501	GTP	C5-C6	-4.20	1.39	1.47
24	FW	501	GTP	C5-C6	-4.20	1.39	1.47
24	6	602	GTP	C5-C6	-4.20	1.39	1.47
24	El	501	GTP	C5-C6	-4.20	1.39	1.47
24	Q	602	GTP	C5-C6	-4.20	1.39	1.47
24	E1	501	GTP	C5-C6	-4.20	1.39	1.47
24	Ee	501	GTP	C5-C6	-4.20	1.39	1.47
24	Fc	501	GTP	C5-C6	-4.20	1.39	1.47
24	F3	501	GTP	C5-C6	-4.20	1.39	1.47
24	Gn	501	GTP	C5-C6	-4.20	1.39	1.47
24	Eh	501	GTP	C5-C6	-4.19	1.39	1.47
24	Ei	501	GTP	C5-C6	-4.19	1.39	1.47
24	Eu	501	GTP	C5-C6	-4.19	1.39	1.47
24	Aw	602	GTP	C5-C6	-4.19	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	GQ	602	GTP	C5-C6	-4.19	1.39	1.47
24	FP	501	GTP	C5-C6	-4.19	1.39	1.47
24	A4	501	GTP	C5-C6	-4.19	1.39	1.47
24	F0	501	GTP	C5-C6	-4.19	1.39	1.47
24	Eo	501	GTP	C5-C6	-4.19	1.39	1.47
24	GG	501	GTP	C5-C6	-4.19	1.39	1.47
24	w	602	GTP	C5-C6	-4.18	1.39	1.47
24	G3	602	GTP	C5-C6	-4.18	1.39	1.47
24	GM	501	GTP	C5-C6	-4.18	1.39	1.47
24	GD	501	GTP	C5-C6	-4.18	1.39	1.47
24	G4	602	GTP	C5-C6	-4.18	1.39	1.47
24	Ff	501	GTP	C5-C6	-4.18	1.39	1.47
24	Al	602	GTP	C5-C6	-4.18	1.39	1.47
24	BR	501	GTP	C5-C6	-4.18	1.39	1.47
24	BS	602	GTP	C5-C6	-4.18	1.39	1.47
24	F9	501	GTP	C5-C6	-4.18	1.39	1.47
24	Bc	501	GTP	C5-C6	-4.18	1.39	1.47
24	Er	501	GTP	C5-C6	-4.18	1.39	1.47
24	B2	602	GTP	C5-C6	-4.17	1.39	1.47
24	Em	501	GTP	C5-C6	-4.17	1.39	1.47
24	BL	602	GTP	C5-C6	-4.17	1.39	1.47
24	F5	501	GTP	C5-C6	-4.17	1.39	1.47
24	B4	602	GTP	C5-C6	-4.17	1.39	1.47
24	Ez	501	GTP	C5-C6	-4.17	1.39	1.47
24	j	602	GTP	C5-C6	-4.17	1.39	1.47
24	Es	501	GTP	C5-C6	-4.17	1.39	1.47
24	Bz	602	GTP	C5-C6	-4.16	1.39	1.47
24	B5	602	GTP	C5-C6	-4.16	1.39	1.47
24	5	602	GTP	C5-C6	-4.16	1.39	1.47
24	Gy	501	GTP	C5-C6	-4.16	1.39	1.47
24	B7	501	GTP	C5-C6	-4.16	1.39	1.47
24	AI	501	GTP	C5-C6	-4.16	1.39	1.47
24	i	602	GTP	C5-C6	-4.16	1.39	1.47
24	Bx	602	GTP	C5-C6	-4.16	1.39	1.47
24	Ex	501	GTP	C5-C6	-4.16	1.39	1.47
24	l	602	GTP	C5-C6	-4.16	1.39	1.47
24	Gu	501	GTP	C5-C6	-4.16	1.39	1.47
24	GL	501	GTP	C5-C6	-4.16	1.39	1.47
24	B6	602	GTP	C5-C6	-4.16	1.39	1.47
24	B1	602	GTP	C5-C6	-4.15	1.39	1.47
24	Eq	501	GTP	C5-C6	-4.15	1.39	1.47
24	Go	501	GTP	C5-C6	-4.15	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Ew	501	GTP	C5-C6	-4.15	1.39	1.47
24	FU	501	GTP	C5-C6	-4.15	1.39	1.47
24	b	602	GTP	C5-C6	-4.15	1.39	1.47
24	T	602	GTP	C5-C6	-4.15	1.39	1.47
24	Y	602	GTP	C5-C6	-4.15	1.39	1.47
24	Ay	602	GTP	C5-C6	-4.15	1.39	1.47
24	Gq	501	GTP	C5-C6	-4.15	1.39	1.47
24	GR	501	GTP	C5-C6	-4.15	1.39	1.47
24	d	602	GTP	C5-C6	-4.15	1.39	1.47
24	A6	501	GTP	C5-C6	-4.15	1.39	1.47
24	CA	602	GTP	C5-C6	-4.15	1.39	1.47
24	f	602	GTP	C5-C6	-4.15	1.39	1.47
24	a	602	GTP	C5-C6	-4.15	1.39	1.47
24	BQ	602	GTP	C5-C6	-4.15	1.39	1.47
24	u	501	GTP	C5-C6	-4.14	1.39	1.47
24	AS	501	GTP	C5-C6	-4.14	1.39	1.47
24	Ax	602	GTP	C5-C6	-4.14	1.39	1.47
24	v	602	GTP	C5-C6	-4.14	1.39	1.47
24	BO	602	GTP	C5-C6	-4.14	1.39	1.47
24	CB	602	GTP	C5-C6	-4.14	1.39	1.47
24	B0	501	GTP	C5-C6	-4.14	1.39	1.47
24	Bw	602	GTP	C5-C6	-4.14	1.39	1.47
24	BM	602	GTP	C5-C6	-4.14	1.39	1.47
24	F6	501	GTP	C5-C6	-4.14	1.39	1.47
24	BU	602	GTP	C5-C6	-4.14	1.39	1.47
24	GC	501	GTP	C5-C6	-4.14	1.39	1.47
24	GI	501	GTP	C5-C6	-4.14	1.39	1.47
24	Gv	501	GTP	C5-C6	-4.14	1.39	1.47
24	BK	602	GTP	C5-C6	-4.13	1.39	1.47
24	E6	602	GTP	C5-C6	-4.13	1.39	1.47
24	Fe	501	GTP	C5-C6	-4.13	1.39	1.47
24	B9	602	GTP	C5-C6	-4.13	1.39	1.47
24	B8	602	GTP	C5-C6	-4.13	1.39	1.47
24	3	602	GTP	C5-C6	-4.13	1.39	1.47
24	Gx	501	GTP	C5-C6	-4.13	1.39	1.47
24	F8	501	GTP	C5-C6	-4.13	1.39	1.47
24	Fh	501	GTP	C5-C6	-4.12	1.39	1.47
24	Gw	501	GTP	C5-C6	-4.12	1.39	1.47
24	q	602	GTP	C5-C6	-4.12	1.39	1.47
24	k	602	GTP	C5-C6	-4.12	1.39	1.47
24	Bu	602	GTP	C5-C6	-4.12	1.39	1.47
24	h	602	GTP	C5-C6	-4.12	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BT	501	GTP	C5-C6	-4.12	1.39	1.47
24	2	602	GTP	C5-C6	-4.12	1.39	1.47
24	F7	501	GTP	C5-C6	-4.11	1.39	1.47
24	FZ	501	GTP	C5-C6	-4.11	1.39	1.47
24	Z	602	GTP	C5-C6	-4.11	1.39	1.47
24	GA	501	GTP	C5-C6	-4.11	1.39	1.47
24	Fi	501	GTP	C5-C6	-4.11	1.39	1.47
24	e	602	GTP	C5-C6	-4.10	1.39	1.47
24	E2	501	GTP	C5-C6	-4.10	1.39	1.47
24	p	602	GTP	C5-C6	-4.10	1.39	1.47
24	Bv	602	GTP	C5-C6	-4.10	1.39	1.47
24	FX	501	GTP	C5-C6	-4.09	1.39	1.47
24	BJ	602	GTP	C5-C6	-4.09	1.39	1.47
24	y	602	GTP	C5-C6	-4.09	1.39	1.47
24	1	602	GTP	C5-C6	-4.09	1.39	1.47
24	GP	501	GTP	C5-C6	-4.09	1.39	1.47
24	W	602	GTP	C5-C6	-4.09	1.39	1.47
24	AJ	602	GTP	C5-C6	-4.08	1.39	1.47
24	A9	501	GTP	C5-C6	-4.08	1.39	1.47
24	BY	602	GTP	C5-C6	-4.08	1.39	1.47
24	4	602	GTP	C5-C6	-4.08	1.39	1.47
24	S	602	GTP	C5-C6	-4.07	1.39	1.47
24	Ak	602	GTP	C5-C6	-4.07	1.39	1.47
24	o	501	GTP	C5-C6	-4.07	1.39	1.47
24	c	602	GTP	C5-C6	-4.07	1.39	1.47
24	BX	602	GTP	C5-C6	-4.07	1.39	1.47
24	BI	602	GTP	C5-C6	-4.07	1.39	1.47
24	Fj	501	GTP	PB-O3A	3.11	1.62	1.59
24	Ex	501	GTP	PB-O3A	2.94	1.62	1.59
24	GF	501	GTP	PB-O3A	2.92	1.62	1.59
24	GE	501	GTP	PB-O3A	2.89	1.62	1.59
24	G3	602	GTP	PB-O3A	2.77	1.62	1.59
24	Fi	501	GTP	PB-O3A	2.75	1.62	1.59
24	Fe	501	GTP	PB-O3A	2.74	1.62	1.59
24	G4	602	GTP	PB-O3A	2.71	1.62	1.59
24	GP	501	GTP	PB-O3A	2.70	1.62	1.59
24	GD	501	GTP	PB-O3A	2.70	1.62	1.59
23	EV	501	GDP	C6-N1	-2.69	1.33	1.37
24	Ew	501	GTP	PB-O3A	2.68	1.62	1.59
24	Fh	501	GTP	PB-O3A	2.68	1.62	1.59
24	Fd	602	GTP	PB-O3A	2.67	1.62	1.59
23	Gk	501	GDP	C6-N1	-2.67	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Gd	501	GDP	C6-N1	-2.65	1.33	1.37
24	E1	501	GTP	PB-O3A	2.64	1.62	1.59
23	AV	602	GDP	C6-N1	-2.63	1.33	1.37
23	r	501	GDP	C6-N1	-2.63	1.33	1.37
24	E2	501	GTP	PB-O3A	2.62	1.62	1.59
24	E5	501	GTP	PB-O3A	2.62	1.62	1.59
23	DR	501	GDP	C6-N1	-2.58	1.33	1.37
24	Fj	501	GTP	PA-O3A	2.58	1.62	1.59
24	GQ	602	GTP	PB-O3A	2.57	1.62	1.59
24	GR	501	GTP	PB-O3A	2.53	1.62	1.59
24	Ex	501	GTP	PA-O3A	2.52	1.62	1.59
24	A4	501	GTP	PB-O3A	2.51	1.62	1.59
24	G4	602	GTP	PA-O3A	2.51	1.62	1.59
24	Fi	501	GTP	PA-O3A	2.50	1.62	1.59
24	GK	501	GTP	PB-O3A	2.49	1.62	1.59
23	FI	501	GDP	C6-N1	-2.48	1.34	1.37
23	AR	501	GDP	C6-N1	-2.47	1.34	1.37
24	Gv	501	GTP	PB-O3A	2.46	1.62	1.59
24	Ei	501	GTP	PB-O3A	2.46	1.62	1.59
24	G1	501	GTP	PB-O3A	2.46	1.62	1.59
24	E6	602	GTP	PB-O3A	2.45	1.62	1.59
23	DS	501	GDP	C6-N1	-2.45	1.34	1.37
23	EX	501	GDP	C6-N1	-2.45	1.34	1.37
24	Ez	501	GTP	PB-O3A	2.44	1.62	1.59
24	F8	501	GTP	PB-O3A	2.44	1.62	1.59
24	Fh	501	GTP	PA-O3A	2.44	1.62	1.59
23	Df	501	GDP	C6-N1	-2.44	1.34	1.37
24	Ey	602	GTP	PB-O3A	2.44	1.62	1.59
24	FU	501	GTP	PB-O3A	2.44	1.62	1.59
24	GL	501	GTP	PB-O3A	2.44	1.62	1.59
24	BM	602	GTP	PB-O3B	2.43	1.62	1.59
24	BP	602	GTP	PB-O3A	2.43	1.62	1.59
23	Af	501	GDP	C6-N1	-2.43	1.34	1.37
24	GA	501	GTP	PB-O3A	2.43	1.62	1.59
24	A9	501	GTP	PB-O3A	2.43	1.62	1.59
24	E3	501	GTP	PB-O3A	2.43	1.62	1.59
24	FQ	501	GTP	PB-O3A	2.42	1.62	1.59
23	FG	501	GDP	C6-N1	-2.42	1.34	1.37
23	Fv	501	GDP	C6-N1	-2.42	1.34	1.37
23	FD	501	GDP	C6-N1	-2.42	1.34	1.37
24	GE	501	GTP	PA-O3A	2.42	1.62	1.59
23	Bt	501	GDP	C6-N1	-2.42	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DO	501	GDP	C6-N1	-2.42	1.34	1.37
23	Gf	501	GDP	C6-N1	-2.41	1.34	1.37
24	GI	501	GTP	PB-O3A	2.41	1.62	1.59
24	El	501	GTP	PB-O3A	2.41	1.62	1.59
24	FX	501	GTP	PB-O3A	2.41	1.62	1.59
23	DW	501	GDP	C6-N1	-2.41	1.34	1.37
24	l	602	GTP	PB-O3A	2.41	1.62	1.59
23	Bl	602	GDP	C6-N1	-2.40	1.34	1.37
23	Dk	501	GDP	C6-N1	-2.40	1.34	1.37
23	DP	501	GDP	C6-N1	-2.40	1.34	1.37
24	Ff	501	GTP	PB-O3A	2.40	1.62	1.59
23	DX	501	GDP	C6-N1	-2.40	1.34	1.37
23	Du	501	GDP	C6-N1	-2.40	1.34	1.37
24	Em	501	GTP	PB-O3A	2.40	1.62	1.59
24	Gp	501	GTP	PB-O3A	2.40	1.62	1.59
24	F9	501	GTP	PB-O3A	2.40	1.62	1.59
23	Ai	501	GDP	C6-N1	-2.40	1.34	1.37
23	EL	501	GDP	C6-N1	-2.39	1.34	1.37
24	FP	501	GTP	PB-O3A	2.39	1.62	1.59
24	A7	501	GTP	PB-O3A	2.39	1.62	1.59
24	AS	501	GTP	PB-O3B	2.39	1.62	1.59
23	FH	501	GDP	C6-N1	-2.39	1.34	1.37
23	AP	501	GDP	C6-N1	-2.39	1.34	1.37
24	F7	501	GTP	PB-O3A	2.39	1.62	1.59
23	Ag	501	GDP	C6-N1	-2.39	1.34	1.37
23	BH	501	GDP	C6-N1	-2.39	1.34	1.37
23	Fu	501	GDP	C6-N1	-2.39	1.34	1.37
24	A6	501	GTP	PB-O3A	2.39	1.62	1.59
23	GX	501	GDP	C6-N1	-2.39	1.34	1.37
23	FL	501	GDP	C6-N1	-2.39	1.34	1.37
23	BC	501	GDP	C6-N1	-2.39	1.34	1.37
23	Dv	501	GDP	C6-N1	-2.38	1.34	1.37
23	Bm	501	GDP	C6-N1	-2.38	1.34	1.37
23	DL	501	GDP	C6-N1	-2.38	1.34	1.37
24	Ee	501	GTP	PB-O3A	2.38	1.62	1.59
23	Dc	501	GDP	C6-N1	-2.38	1.34	1.37
24	Fb	501	GTP	PB-O3A	2.38	1.62	1.59
23	Fl	501	GDP	C6-N1	-2.38	1.34	1.37
23	Dw	501	GDP	C6-N1	-2.38	1.34	1.37
23	Br	501	GDP	C6-N1	-2.37	1.34	1.37
23	BG	501	GDP	C6-N1	-2.37	1.34	1.37
23	9	501	GDP	C6-N1	-2.37	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Gu	501	GTP	PB-O3A	2.37	1.62	1.59
23	E9	501	GDP	C6-N1	-2.37	1.34	1.37
23	Bp	501	GDP	C6-N1	-2.37	1.34	1.37
23	Gh	501	GDP	C6-N1	-2.37	1.34	1.37
24	Gt	501	GTP	PB-O3A	2.37	1.62	1.59
23	Ab	501	GDP	C6-N1	-2.37	1.34	1.37
24	Gw	501	GTP	PB-O3A	2.37	1.62	1.59
24	E7	501	GTP	PB-O3A	2.36	1.62	1.59
23	Az	501	GDP	C6-N1	-2.36	1.34	1.37
23	Da	501	GDP	C6-N1	-2.36	1.34	1.37
23	EM	501	GDP	C6-N1	-2.36	1.34	1.37
23	Di	501	GDP	C6-N1	-2.36	1.34	1.37
23	DM	501	GDP	C6-N1	-2.36	1.34	1.37
23	O	501	GDP	C6-N1	-2.36	1.34	1.37
23	EW	501	GDP	C6-N1	-2.36	1.34	1.37
23	Ge	501	GDP	C6-N1	-2.36	1.34	1.37
23	EQ	501	GDP	C6-N1	-2.36	1.34	1.37
23	AW	501	GDP	C6-N1	-2.36	1.34	1.37
23	FF	501	GDP	C6-N1	-2.36	1.34	1.37
23	Bk	501	GDP	C6-N1	-2.36	1.34	1.37
23	Ah	602	GDP	C6-N1	-2.36	1.34	1.37
23	DT	501	GDP	C6-N1	-2.36	1.34	1.37
23	8	501	GDP	C6-N1	-2.36	1.34	1.37
24	GJ	501	GTP	PB-O3A	2.36	1.62	1.59
23	BB	501	GDP	C6-N1	-2.35	1.34	1.37
24	GF	501	GTP	PA-O3A	2.35	1.62	1.59
23	AF	501	GDP	C6-N1	-2.35	1.34	1.37
23	DN	501	GDP	C6-N1	-2.35	1.34	1.37
23	EY	501	GDP	C6-N1	-2.35	1.34	1.37
23	F1	501	GDP	C6-N1	-2.35	1.34	1.37
23	F2	501	GDP	C6-N1	-2.35	1.34	1.37
24	Fe	501	GTP	PA-O3A	2.35	1.62	1.59
23	Fw	501	GDP	C6-N1	-2.35	1.34	1.37
23	Ae	501	GDP	C6-N1	-2.35	1.34	1.37
23	BE	501	GDP	C6-N1	-2.35	1.34	1.37
24	GD	501	GTP	PA-O3A	2.35	1.62	1.59
23	Aa	501	GDP	C6-N1	-2.35	1.34	1.37
23	EZ	501	GDP	C6-N1	-2.35	1.34	1.37
23	Ft	501	GDP	C6-N1	-2.35	1.34	1.37
23	Dj	501	GDP	C6-N1	-2.35	1.34	1.37
24	Gr	501	GTP	PB-O3A	2.35	1.62	1.59
24	j	602	GTP	PA-O3A	2.35	1.62	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Bh	501	GDP	C6-N1	-2.34	1.34	1.37
24	BM	602	GTP	PA-O3A	2.34	1.62	1.59
24	A5	501	GTP	PB-O3A	2.34	1.62	1.59
23	Fr	501	GDP	C6-N1	-2.34	1.34	1.37
24	G3	602	GTP	PA-O3A	2.34	1.62	1.59
23	Fy	501	GDP	C6-N1	-2.34	1.34	1.37
24	Bx	602	GTP	PA-O3A	2.34	1.62	1.59
23	GV	501	GDP	C6-N1	-2.34	1.34	1.37
23	Gj	501	GDP	C6-N1	-2.34	1.34	1.37
23	BD	501	GDP	C6-N1	-2.34	1.34	1.37
23	Bo	501	GDP	C6-N1	-2.34	1.34	1.37
23	ES	501	GDP	C6-N1	-2.34	1.34	1.37
23	FC	501	GDP	C6-N1	-2.34	1.34	1.37
24	FM	501	GTP	PB-O3A	2.34	1.62	1.59
23	Fn	501	GDP	C6-N1	-2.33	1.34	1.37
23	DY	501	GDP	C6-N1	-2.33	1.34	1.37
24	Gs	501	GTP	PB-O3A	2.33	1.62	1.59
24	Bc	501	GTP	PB-O3A	2.33	1.62	1.59
23	AH	501	GDP	C6-N1	-2.33	1.34	1.37
23	Fz	501	GDP	C6-N1	-2.33	1.34	1.37
23	FJ	501	GDP	C6-N1	-2.33	1.34	1.37
23	AT	501	GDP	C6-N1	-2.33	1.34	1.37
23	Bi	501	GDP	C6-N1	-2.33	1.34	1.37
23	AQ	501	GDP	C6-N1	-2.33	1.34	1.37
23	P	501	GDP	C6-N1	-2.33	1.34	1.37
23	Dr	501	GDP	C6-N1	-2.33	1.34	1.37
23	X	501	GDP	C6-N1	-2.33	1.34	1.37
23	U	501	GDP	C6-N1	-2.33	1.34	1.37
23	FB	501	GDP	C6-N1	-2.33	1.34	1.37
23	AL	501	GDP	C6-N1	-2.33	1.34	1.37
24	W	602	GTP	PB-O3B	2.33	1.62	1.59
24	Gx	501	GTP	PB-O3A	2.32	1.62	1.59
23	Ad	501	GDP	C6-N1	-2.32	1.34	1.37
23	AN	501	GDP	C6-N1	-2.32	1.34	1.37
23	AY	501	GDP	C6-N1	-2.32	1.34	1.37
24	E1	501	GTP	PA-O3A	2.32	1.62	1.59
23	DU	501	GDP	C6-N1	-2.32	1.34	1.37
24	Ep	501	GTP	PB-O3A	2.32	1.62	1.59
23	AA	501	GDP	C6-N1	-2.32	1.34	1.37
23	Ar	501	GDP	C6-N1	-2.32	1.34	1.37
23	EO	501	GDP	C6-N1	-2.32	1.34	1.37
23	Bb	501	GDP	C6-N1	-2.32	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	GN	501	GTP	PB-O3A	2.32	1.62	1.59
24	BL	602	GTP	PB-O3B	2.32	1.62	1.59
23	AE	501	GDP	C6-N1	-2.32	1.34	1.37
23	AG	501	GDP	C6-N1	-2.32	1.34	1.37
23	GU	501	GDP	C6-N1	-2.32	1.34	1.37
23	FK	501	GDP	C6-N1	-2.32	1.34	1.37
23	An	501	GDP	C6-N1	-2.32	1.34	1.37
24	A8	501	GTP	PB-O3A	2.32	1.62	1.59
23	Ef	501	GDP	C6-N1	-2.32	1.34	1.37
23	Bf	501	GDP	C6-N1	-2.31	1.34	1.37
23	EU	501	GDP	C6-N1	-2.31	1.34	1.37
24	GT	501	GTP	PB-O3A	2.31	1.62	1.59
23	At	501	GDP	C6-N1	-2.31	1.34	1.37
23	Dh	501	GDP	C6-N1	-2.31	1.34	1.37
23	Eb	501	GDP	C6-N1	-2.31	1.34	1.37
24	E2	501	GTP	PA-O3A	2.31	1.62	1.59
23	Bn	501	GDP	C6-N1	-2.31	1.34	1.37
24	F6	501	GTP	PB-O3A	2.31	1.62	1.59
23	Gi	501	GDP	C6-N1	-2.31	1.34	1.37
23	Au	602	GDP	C6-N1	-2.31	1.34	1.37
23	Ed	501	GDP	C6-N1	-2.31	1.34	1.37
23	m	501	GDP	C6-N1	-2.31	1.34	1.37
23	AU	501	GDP	C6-N1	-2.31	1.34	1.37
23	Gb	501	GDP	C6-N1	-2.31	1.34	1.37
24	FT	501	GTP	PB-O3A	2.30	1.62	1.59
23	DQ	501	GDP	C6-N1	-2.30	1.34	1.37
23	Gm	501	GDP	C6-N1	-2.30	1.34	1.37
23	Ac	501	GDP	C6-N1	-2.30	1.34	1.37
23	Am	501	GDP	C6-N1	-2.30	1.34	1.37
24	Ey	602	GTP	C2-N3	2.30	1.38	1.33
23	BF	501	GDP	C6-N1	-2.30	1.34	1.37
23	ET	501	GDP	C6-N1	-2.30	1.34	1.37
23	BA	501	GDP	C6-N1	-2.30	1.34	1.37
24	Bx	602	GTP	PB-O3A	2.30	1.62	1.59
24	E6	602	GTP	PA-O3A	2.30	1.62	1.59
23	Db	501	GDP	C6-N1	-2.30	1.34	1.37
24	Fj	501	GTP	C2-N3	2.30	1.38	1.33
23	Fm	501	GDP	C6-N1	-2.30	1.34	1.37
23	AZ	501	GDP	C6-N1	-2.30	1.34	1.37
23	Ea	501	GDP	C6-N1	-2.30	1.34	1.37
23	Gc	501	GDP	C6-N1	-2.30	1.34	1.37
23	AM	501	GDP	C6-N1	-2.30	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DV	501	GDP	C6-N1	-2.29	1.34	1.37
23	Gg	501	GDP	C6-N1	-2.29	1.34	1.37
23	As	501	GDP	C6-N1	-2.29	1.34	1.37
23	De	501	GDP	C6-N1	-2.29	1.34	1.37
24	GM	501	GTP	PB-O3A	2.29	1.62	1.59
23	Fx	501	GDP	C6-N1	-2.29	1.34	1.37
24	Fd	602	GTP	PA-O3A	2.29	1.62	1.59
23	EN	501	GDP	C6-N1	-2.29	1.34	1.37
23	Bg	501	GDP	C6-N1	-2.29	1.34	1.37
23	AX	501	GDP	C6-N1	-2.29	1.34	1.37
23	Ev	501	GDP	C6-N1	-2.28	1.34	1.37
23	GZ	501	GDP	C6-N1	-2.28	1.34	1.37
23	A3	501	GDP	C6-N1	-2.28	1.34	1.37
23	Bq	602	GDP	C6-N1	-2.28	1.34	1.37
23	Ga	501	GDP	C6-N1	-2.28	1.34	1.37
23	Av	501	GDP	C6-N1	-2.28	1.34	1.37
23	FE	501	GDP	C6-N1	-2.28	1.34	1.37
24	E5	501	GTP	PA-O3A	2.28	1.62	1.59
23	E0	501	GDP	C6-N1	-2.28	1.34	1.37
23	FA	501	GDP	C6-N1	-2.28	1.34	1.37
24	Go	501	GTP	PB-O3A	2.28	1.62	1.59
23	AS	502	GDP	C6-N1	-2.28	1.34	1.37
24	FV	602	GTP	PB-O3A	2.28	1.62	1.59
23	Ao	501	GDP	C6-N1	-2.28	1.34	1.37
24	h	602	GTP	PB-O3B	2.27	1.62	1.59
23	Ap	501	GDP	C6-N1	-2.27	1.34	1.37
23	Dd	501	GDP	C6-N1	-2.27	1.34	1.37
23	A0	501	GDP	C6-N1	-2.27	1.34	1.37
24	F0	501	GTP	PB-O3A	2.27	1.61	1.59
24	Fc	501	GTP	PB-O3A	2.27	1.61	1.59
23	Fs	501	GDP	C6-N1	-2.27	1.34	1.37
23	Be	501	GDP	C6-N1	-2.27	1.34	1.37
23	F4	501	GDP	C6-N1	-2.26	1.34	1.37
24	j	602	GTP	PB-O3A	2.26	1.61	1.59
24	Ew	501	GTP	PA-O3A	2.26	1.61	1.59
23	EP	501	GDP	C6-N1	-2.26	1.34	1.37
23	Dt	501	GDP	C6-N1	-2.26	1.34	1.37
24	Eq	501	GTP	C2-N3	2.26	1.38	1.33
24	Ff	501	GTP	C2-N3	2.26	1.38	1.33
23	Fo	501	GDP	C6-N1	-2.26	1.34	1.37
23	Fq	501	GDP	C6-N1	-2.26	1.34	1.37
23	Bs	501	GDP	C6-N1	-2.26	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DZ	501	GDP	C6-N1	-2.26	1.34	1.37
24	GL	501	GTP	C2-N3	2.25	1.38	1.33
24	B2	602	GTP	PA-O3A	2.25	1.61	1.59
23	AB	501	GDP	C6-N1	-2.25	1.34	1.37
24	Eh	501	GTP	PB-O3A	2.25	1.61	1.59
23	Dg	501	GDP	C6-N1	-2.25	1.34	1.37
23	Fp	501	GDP	C6-N1	-2.25	1.34	1.37
24	Eq	501	GTP	PB-O3A	2.25	1.61	1.59
24	FS	501	GTP	PB-O3A	2.25	1.61	1.59
24	Gz	501	GTP	PB-O3A	2.25	1.61	1.59
24	Es	501	GTP	PB-O3A	2.25	1.61	1.59
23	Ba	501	GDP	C6-N1	-2.25	1.34	1.37
23	ER	501	GDP	C6-N1	-2.25	1.34	1.37
23	Dq	501	GDP	C6-N1	-2.25	1.34	1.37
24	Bd	501	GTP	PB-O3A	2.24	1.61	1.59
24	x	501	GTP	C2-N3	2.24	1.38	1.33
23	Bj	501	GDP	C6-N1	-2.24	1.34	1.37
23	n	501	GDP	C6-N1	-2.24	1.34	1.37
24	F8	501	GTP	C2-N3	2.24	1.38	1.33
23	GH	501	GDP	C6-N1	-2.24	1.34	1.37
24	Ek	501	GTP	PB-O3A	2.24	1.61	1.59
24	En	501	GTP	PB-O3A	2.24	1.61	1.59
23	Dx	501	GDP	C6-N1	-2.24	1.34	1.37
24	Gn	501	GTP	PB-O3A	2.24	1.61	1.59
24	Gu	501	GTP	PA-O3A	2.24	1.61	1.59
24	F3	501	GTP	PB-O3A	2.24	1.61	1.59
23	0	501	GDP	C6-N1	-2.24	1.34	1.37
23	GW	501	GDP	C6-N1	-2.24	1.34	1.37
24	E3	501	GTP	C2-N3	2.23	1.38	1.33
24	FO	501	GTP	PB-O3A	2.23	1.61	1.59
24	E7	501	GTP	C2-N3	2.23	1.38	1.33
23	AO	501	GDP	C6-N1	-2.23	1.34	1.37
24	Ak	602	GTP	PA-O3A	2.23	1.61	1.59
24	Eh	501	GTP	C2-N3	2.23	1.38	1.33
24	BV	602	GTP	C2-N3	2.23	1.38	1.33
24	Gx	501	GTP	C2-N3	2.22	1.38	1.33
24	Fk	501	GTP	PB-O3A	2.22	1.61	1.59
24	F8	501	GTP	PA-O3A	2.22	1.61	1.59
24	G2	501	GTP	PB-O3A	2.22	1.61	1.59
24	CB	602	GTP	PB-O3A	2.22	1.61	1.59
24	t	602	GTP	C2-N3	2.22	1.38	1.33
24	Eg	501	GTP	PB-O3A	2.22	1.61	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Fh	501	GTP	PB-O3B	2.22	1.61	1.59
24	l	602	GTP	PA-O3A	2.22	1.61	1.59
24	T	602	GTP	C2-N3	2.22	1.38	1.33
23	AD	501	GDP	C6-N1	-2.22	1.34	1.37
24	A9	501	GTP	C2-N3	2.22	1.38	1.33
23	BW	501	GDP	C6-N1	-2.22	1.34	1.37
24	Go	501	GTP	C2-N3	2.22	1.38	1.33
24	GF	501	GTP	PB-O3B	2.22	1.61	1.59
24	FM	501	GTP	C2-N3	2.22	1.38	1.33
24	FX	501	GTP	C2-N3	2.22	1.38	1.33
23	FN	501	GDP	C6-N1	-2.21	1.34	1.37
24	Eu	501	GTP	PB-O3A	2.21	1.61	1.59
24	F7	501	GTP	C2-N3	2.21	1.38	1.33
24	En	501	GTP	C2-N3	2.21	1.38	1.33
24	B1	602	GTP	PB-O3A	2.21	1.61	1.59
24	GN	501	GTP	C2-N3	2.21	1.38	1.33
24	Gq	501	GTP	PB-O3A	2.21	1.61	1.59
24	Fg	501	GTP	PB-O3A	2.21	1.61	1.59
24	Aw	602	GTP	C2-N3	2.21	1.38	1.33
24	GC	501	GTP	C2-N3	2.21	1.38	1.33
24	z	602	GTP	C2-N3	2.21	1.38	1.33
24	GO	602	GTP	PB-O3A	2.21	1.61	1.59
24	GM	501	GTP	C2-N3	2.21	1.38	1.33
24	FZ	501	GTP	C2-N3	2.21	1.38	1.33
24	b	602	GTP	C2-N3	2.20	1.38	1.33
24	Aj	501	GTP	C2-N3	2.20	1.38	1.33
24	B3	602	GTP	PB-O3A	2.20	1.61	1.59
24	BK	602	GTP	PA-O3A	2.20	1.61	1.59
23	BZ	501	GDP	C6-N1	-2.20	1.34	1.37
24	Es	501	GTP	C2-N3	2.20	1.38	1.33
24	BQ	602	GTP	C2-N3	2.20	1.38	1.33
24	Fh	501	GTP	C2-N3	2.20	1.38	1.33
24	GA	501	GTP	PA-O3A	2.20	1.61	1.59
24	FX	501	GTP	PA-O3A	2.20	1.61	1.59
24	GA	501	GTP	C2-N3	2.20	1.38	1.33
24	BP	602	GTP	C2-N3	2.20	1.38	1.33
24	B0	501	GTP	C2-N3	2.20	1.38	1.33
24	BO	602	GTP	PB-O3A	2.20	1.61	1.59
24	Ej	501	GTP	PB-O3A	2.20	1.61	1.59
24	F7	501	GTP	PA-O3A	2.20	1.61	1.59
23	GY	501	GDP	C6-N1	-2.20	1.34	1.37
24	b	602	GTP	PB-O3A	2.20	1.61	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	602	GTP	C2-N3	2.20	1.38	1.33
24	a	602	GTP	PB-O3A	2.20	1.61	1.59
24	GJ	501	GTP	C2-N3	2.19	1.38	1.33
24	BN	602	GTP	PA-O3A	2.19	1.61	1.59
24	Ew	501	GTP	C2-N3	2.19	1.38	1.33
24	G3	602	GTP	C2-N3	2.19	1.38	1.33
24	Gw	501	GTP	C2-N3	2.19	1.38	1.33
24	By	602	GTP	PA-O3A	2.19	1.61	1.59
24	Er	501	GTP	C2-N3	2.19	1.38	1.33
24	Al	602	GTP	C2-N3	2.19	1.38	1.33
24	Bz	602	GTP	PB-O3B	2.19	1.61	1.59
23	7	501	GDP	C6-N1	-2.19	1.34	1.37
24	y	602	GTP	PB-O3A	2.19	1.61	1.59
24	Eo	501	GTP	PB-O3A	2.19	1.61	1.59
24	B7	501	GTP	C2-N3	2.19	1.38	1.33
24	k	602	GTP	PB-O3A	2.19	1.61	1.59
24	FV	602	GTP	C2-N3	2.19	1.38	1.33
24	B6	602	GTP	C2-N3	2.18	1.38	1.33
24	G1	501	GTP	C2-N3	2.18	1.38	1.33
24	s	602	GTP	PA-O3A	2.18	1.61	1.59
24	G2	501	GTP	C2-N3	2.18	1.38	1.33
24	Eu	501	GTP	C2-N3	2.18	1.38	1.33
23	AC	501	GDP	C6-N1	-2.18	1.34	1.37
24	B2	602	GTP	PB-O3A	2.18	1.61	1.59
24	BN	602	GTP	PB-O3A	2.18	1.61	1.59
24	f	602	GTP	C2-N3	2.18	1.38	1.33
24	AK	602	GTP	C2-N3	2.18	1.38	1.33
24	B5	602	GTP	C2-N3	2.18	1.38	1.33
24	GG	501	GTP	PB-O3A	2.18	1.61	1.59
24	Eq	501	GTP	PB-O3B	2.18	1.61	1.59
23	Ds	501	GDP	C6-N1	-2.18	1.34	1.37
24	A6	501	GTP	C2-N3	2.18	1.38	1.33
24	Ax	602	GTP	C2-N3	2.18	1.38	1.33
24	GC	501	GTP	PB-O3B	2.18	1.61	1.59
24	BJ	602	GTP	PA-O3A	2.18	1.61	1.59
24	Ei	501	GTP	PA-O3A	2.18	1.61	1.59
24	GO	602	GTP	C2-N3	2.18	1.38	1.33
24	CB	602	GTP	C2-N3	2.18	1.38	1.33
24	Al	602	GTP	PB-O3A	2.18	1.61	1.59
24	Gv	501	GTP	C2-N3	2.18	1.38	1.33
24	E1	501	GTP	C2-N3	2.18	1.38	1.33
24	E4	501	GTP	PB-O3A	2.18	1.61	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BT	501	GTP	C2-N3	2.18	1.38	1.33
24	GI	501	GTP	C2-N3	2.18	1.38	1.33
24	s	602	GTP	C2-N3	2.18	1.38	1.33
24	GK	501	GTP	C2-N3	2.17	1.38	1.33
24	Ek	501	GTP	C2-N3	2.17	1.38	1.33
24	Ep	501	GTP	C2-N3	2.17	1.38	1.33
24	By	602	GTP	PB-O3A	2.17	1.61	1.59
24	5	602	GTP	C2-N3	2.17	1.38	1.33
24	6	602	GTP	C2-N3	2.17	1.38	1.33
24	Eo	501	GTP	C2-N3	2.17	1.38	1.33
24	B4	602	GTP	PB-O3A	2.17	1.61	1.59
24	GB	501	GTP	PB-O3A	2.17	1.61	1.59
24	Fc	501	GTP	C2-N3	2.17	1.38	1.33
24	G3	602	GTP	PB-O3B	2.17	1.61	1.59
24	E5	501	GTP	PB-O3B	2.17	1.61	1.59
24	i	602	GTP	C2-N3	2.17	1.38	1.33
24	d	602	GTP	C2-N3	2.17	1.38	1.33
24	B9	602	GTP	C2-N3	2.17	1.38	1.33
24	f	602	GTP	PB-O3A	2.17	1.61	1.59
23	Ec	501	GDP	C6-N1	-2.17	1.34	1.37
24	FR	501	GTP	PB-O3A	2.17	1.61	1.59
24	Gy	501	GTP	C2-N3	2.17	1.38	1.33
24	A8	501	GTP	C2-N3	2.17	1.38	1.33
24	FT	501	GTP	C2-N3	2.16	1.38	1.33
24	GD	501	GTP	PB-O3B	2.16	1.61	1.59
24	Gq	501	GTP	C2-N3	2.16	1.38	1.33
24	e	602	GTP	C2-N3	2.16	1.38	1.33
24	Ay	602	GTP	C2-N3	2.16	1.38	1.33
24	v	602	GTP	C2-N3	2.16	1.38	1.33
24	FU	501	GTP	C2-N3	2.16	1.38	1.33
24	B6	602	GTP	PA-O3A	2.16	1.61	1.59
24	FY	501	GTP	PB-O3A	2.16	1.61	1.59
24	q	602	GTP	PB-O3A	2.16	1.61	1.59
24	F5	501	GTP	C2-N3	2.16	1.38	1.33
24	B3	602	GTP	C2-N3	2.16	1.38	1.33
24	BM	602	GTP	C2-N3	2.16	1.38	1.33
24	Bx	602	GTP	C2-N3	2.16	1.38	1.33
24	B4	602	GTP	C2-N3	2.16	1.38	1.33
24	Gu	501	GTP	C2-N3	2.16	1.38	1.33
24	Es	501	GTP	PA-O3A	2.16	1.61	1.59
24	GD	501	GTP	C2-N3	2.16	1.38	1.33
24	GQ	602	GTP	C2-N3	2.16	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B1	602	GTP	C2-N3	2.16	1.38	1.33
24	F0	501	GTP	C2-N3	2.16	1.38	1.33
24	V	602	GTP	C2-N3	2.16	1.38	1.33
24	BK	602	GTP	C2-N3	2.16	1.38	1.33
24	G5	501	GTP	C2-N3	2.15	1.38	1.33
24	AI	501	GTP	C2-N3	2.15	1.38	1.33
24	GI	501	GTP	PA-O3A	2.15	1.61	1.59
24	GB	501	GTP	C2-N3	2.15	1.38	1.33
24	GP	501	GTP	PA-O3A	2.15	1.61	1.59
24	Ak	602	GTP	C2-N3	2.15	1.38	1.33
24	q	602	GTP	C2-N3	2.15	1.38	1.33
24	u	501	GTP	C2-N3	2.15	1.38	1.33
24	Bd	501	GTP	C2-N3	2.15	1.38	1.33
24	El	501	GTP	C2-N3	2.15	1.38	1.33
24	A9	501	GTP	PA-O3A	2.15	1.61	1.59
24	Ei	501	GTP	C2-N3	2.15	1.38	1.33
24	b	602	GTP	PA-O3A	2.15	1.61	1.59
24	A5	501	GTP	C2-N3	2.15	1.38	1.33
24	a	602	GTP	C2-N3	2.15	1.38	1.33
24	A4	501	GTP	C2-N3	2.15	1.38	1.33
24	y	602	GTP	C2-N3	2.15	1.38	1.33
24	GP	501	GTP	PB-O3B	2.15	1.61	1.59
24	Gy	501	GTP	PB-O3A	2.15	1.61	1.59
24	A7	501	GTP	C2-N3	2.14	1.38	1.33
24	FY	501	GTP	C2-N3	2.14	1.38	1.33
24	Em	501	GTP	C2-N3	2.14	1.38	1.33
24	GP	501	GTP	C2-N3	2.14	1.38	1.33
24	Ax	602	GTP	PA-O3A	2.14	1.61	1.59
24	B9	602	GTP	PB-O3A	2.14	1.61	1.59
24	BR	501	GTP	C2-N3	2.14	1.38	1.33
24	Fa	501	GTP	PB-O3A	2.14	1.61	1.59
24	Gl	501	GTP	C2-N3	2.14	1.38	1.33
24	k	602	GTP	C2-N3	2.14	1.38	1.33
23	Aq	501	GDP	C6-N1	-2.14	1.34	1.37
24	GR	501	GTP	PA-O3A	2.14	1.61	1.59
24	AS	501	GTP	C2-N3	2.14	1.38	1.33
24	BO	602	GTP	C2-N3	2.14	1.38	1.33
24	GB	501	GTP	PB-O3B	2.14	1.61	1.59
24	Gr	501	GTP	C2-N3	2.14	1.38	1.33
24	BN	602	GTP	C2-N3	2.14	1.38	1.33
24	Fd	602	GTP	C2-N3	2.14	1.38	1.33
24	Ez	501	GTP	C2-N3	2.14	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CA	602	GTP	C2-N3	2.14	1.38	1.33
24	FQ	501	GTP	C2-N3	2.14	1.38	1.33
24	GE	501	GTP	C2-N3	2.14	1.38	1.33
24	Bc	501	GTP	C2-N3	2.14	1.38	1.33
24	Ew	501	GTP	PB-O3B	2.14	1.61	1.59
24	F9	501	GTP	C2-N3	2.14	1.38	1.33
24	A1	602	GTP	C2-N3	2.14	1.38	1.33
24	Bv	602	GTP	C2-N3	2.14	1.38	1.33
24	AI	501	GTP	PA-O3A	2.14	1.61	1.59
24	e	602	GTP	PA-O3A	2.13	1.61	1.59
24	u	501	GTP	PB-O3A	2.13	1.61	1.59
24	B9	602	GTP	PA-O3A	2.13	1.61	1.59
24	Fa	501	GTP	C2-N3	2.13	1.38	1.33
24	o	501	GTP	PA-O3A	2.13	1.61	1.59
24	BR	501	GTP	PA-O3A	2.13	1.61	1.59
24	Eg	501	GTP	C2-N3	2.13	1.38	1.33
24	w	602	GTP	C2-N3	2.13	1.38	1.33
24	c	602	GTP	PA-O3A	2.13	1.61	1.59
24	BK	602	GTP	PB-O3A	2.13	1.61	1.59
24	Fi	501	GTP	C2-N3	2.13	1.38	1.33
24	Et	501	GTP	C2-N3	2.13	1.38	1.33
24	BV	602	GTP	PB-O3A	2.13	1.61	1.59
24	g	602	GTP	C2-N3	2.13	1.38	1.33
24	AK	602	GTP	PB-O3A	2.13	1.61	1.59
24	B8	602	GTP	C2-N3	2.13	1.38	1.33
24	l	602	GTP	C2-N3	2.13	1.38	1.33
24	FO	501	GTP	C2-N3	2.13	1.38	1.33
24	W	602	GTP	C2-N3	2.13	1.38	1.33
24	GS	501	GTP	C2-N3	2.12	1.38	1.33
24	Ee	501	GTP	C2-N3	2.12	1.38	1.33
24	e	602	GTP	PB-O3A	2.12	1.61	1.59
24	BY	602	GTP	C2-N3	2.12	1.38	1.33
24	Ej	501	GTP	C2-N3	2.12	1.38	1.33
24	Fk	501	GTP	C2-N3	2.12	1.38	1.33
24	FW	501	GTP	C2-N3	2.12	1.38	1.33
24	BS	602	GTP	C2-N3	2.12	1.38	1.33
24	E2	501	GTP	C2-N3	2.12	1.38	1.33
24	B2	602	GTP	C2-N3	2.12	1.38	1.33
24	Et	501	GTP	PB-O3A	2.12	1.61	1.59
24	o	501	GTP	C2-N3	2.12	1.38	1.33
24	u	501	GTP	PA-O3A	2.12	1.61	1.59
24	5	602	GTP	PA-O3A	2.12	1.61	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	FM	501	GTP	PA-O3A	2.12	1.61	1.59
24	AJ	602	GTP	C2-N3	2.12	1.38	1.33
24	Bz	602	GTP	C2-N3	2.12	1.38	1.33
24	F3	501	GTP	C2-N3	2.12	1.38	1.33
24	Gr	501	GTP	PA-O3A	2.12	1.61	1.59
24	BL	602	GTP	PB-O3A	2.12	1.61	1.59
24	BQ	602	GTP	PA-O3A	2.12	1.61	1.59
24	Gp	501	GTP	C2-N3	2.12	1.38	1.33
24	Gs	501	GTP	C2-N3	2.11	1.38	1.33
24	h	602	GTP	C2-N3	2.11	1.38	1.33
24	j	602	GTP	C2-N3	2.11	1.38	1.33
24	V	602	GTP	PA-O3A	2.11	1.61	1.59
24	F5	501	GTP	PB-O3A	2.11	1.61	1.59
24	E6	602	GTP	C2-N3	2.11	1.38	1.33
24	G4	602	GTP	C2-N3	2.11	1.38	1.33
24	GF	501	GTP	C2-N3	2.11	1.38	1.33
24	2	602	GTP	C2-N3	2.11	1.38	1.33
24	Fd	602	GTP	PB-O3B	2.11	1.61	1.59
24	1	602	GTP	C2-N3	2.11	1.38	1.33
24	Ak	602	GTP	PB-O3A	2.11	1.61	1.59
24	FW	501	GTP	PB-O3A	2.11	1.61	1.59
24	B7	501	GTP	PA-O3A	2.11	1.61	1.59
24	Bu	602	GTP	C2-N3	2.11	1.38	1.33
24	3	602	GTP	C2-N3	2.11	1.38	1.33
24	F6	501	GTP	C2-N3	2.11	1.38	1.33
24	GN	501	GTP	PB-O3B	2.11	1.61	1.59
24	FZ	501	GTP	PB-O3A	2.11	1.61	1.59
24	FP	501	GTP	C2-N3	2.11	1.38	1.33
24	Ax	602	GTP	PB-O3A	2.11	1.61	1.59
24	BU	602	GTP	C2-N3	2.10	1.38	1.33
24	c	602	GTP	C2-N3	2.10	1.38	1.33
24	By	602	GTP	C2-N3	2.10	1.38	1.33
24	BJ	602	GTP	C2-N3	2.10	1.38	1.33
24	FR	501	GTP	C2-N3	2.10	1.38	1.33
24	Al	602	GTP	PB-O3B	2.10	1.61	1.59
24	Q	602	GTP	C2-N3	2.10	1.38	1.33
24	Z	602	GTP	C2-N3	2.10	1.38	1.33
24	Ex	501	GTP	C2-N3	2.10	1.38	1.33
24	FS	501	GTP	C2-N3	2.10	1.38	1.33
24	z	602	GTP	PB-O3A	2.10	1.61	1.59
24	Gt	501	GTP	C2-N3	2.10	1.38	1.33
24	Gz	501	GTP	C2-N3	2.10	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Gx	501	GTP	PB-O3B	2.09	1.61	1.59
24	i	602	GTP	PB-O3A	2.09	1.61	1.59
24	Ee	501	GTP	PA-O3A	2.09	1.61	1.59
24	Gn	501	GTP	C2-N3	2.09	1.38	1.33
24	E5	501	GTP	C2-N3	2.09	1.38	1.33
24	Aj	501	GTP	PA-O3A	2.09	1.61	1.59
24	E4	501	GTP	C2-N3	2.09	1.38	1.33
24	GQ	602	GTP	PA-O3A	2.09	1.61	1.59
24	GG	501	GTP	C2-N3	2.09	1.38	1.33
24	4	602	GTP	C2-N3	2.09	1.38	1.33
24	Gw	501	GTP	PA-O3A	2.09	1.61	1.59
24	GK	501	GTP	PA-O3A	2.09	1.61	1.59
24	Gq	501	GTP	PA-O3A	2.09	1.61	1.59
24	GL	501	GTP	PA-O3A	2.09	1.61	1.59
24	Bz	602	GTP	PB-O3A	2.08	1.61	1.59
24	Ei	501	GTP	PB-O3B	2.08	1.61	1.59
24	BL	602	GTP	C2-N3	2.08	1.38	1.33
24	B1	602	GTP	PA-O3A	2.08	1.61	1.59
24	CA	602	GTP	PB-O3A	2.08	1.61	1.59
24	Fb	501	GTP	PB-O3B	2.08	1.61	1.59
24	BX	602	GTP	C2-N3	2.08	1.38	1.33
24	GC	501	GTP	PB-O3A	2.08	1.61	1.59
24	c	602	GTP	PB-O3A	2.08	1.61	1.59
23	E9	501	GDP	O4'-C1'	2.08	1.43	1.40
24	6	602	GTP	PA-O3A	2.08	1.61	1.59
24	E8	501	GTP	PB-O3A	2.08	1.61	1.59
23	r	501	GDP	C5-C4	2.08	1.48	1.43
23	0	501	GDP	O4'-C1'	2.07	1.43	1.40
24	G1	501	GTP	PA-O3A	2.07	1.61	1.59
24	GM	501	GTP	PB-O3B	2.07	1.61	1.59
24	T	602	GTP	PA-O3A	2.07	1.61	1.59
24	Fj	501	GTP	PB-O3B	2.07	1.61	1.59
24	V	602	GTP	PB-O3A	2.07	1.61	1.59
24	B7	501	GTP	PB-O3A	2.07	1.61	1.59
24	El	501	GTP	PA-O3A	2.07	1.61	1.59
24	AK	602	GTP	PA-O3A	2.07	1.61	1.59
24	FZ	501	GTP	PB-O3B	2.07	1.61	1.59
24	S	602	GTP	C2-N3	2.06	1.38	1.33
24	G6	501	GTP	C2-N3	2.06	1.38	1.33
24	f	602	GTP	PB-O3B	2.06	1.61	1.59
24	E8	501	GTP	C2-N3	2.06	1.38	1.33
24	B5	602	GTP	PA-O3A	2.06	1.61	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B8	602	GTP	PB-O3A	2.06	1.61	1.59
24	Y	602	GTP	C2-N3	2.06	1.38	1.33
24	BI	602	GTP	C2-N3	2.06	1.38	1.33
24	A6	501	GTP	PA-O3A	2.06	1.61	1.59
24	BP	602	GTP	PA-O3A	2.06	1.61	1.59
24	a	602	GTP	PA-O3A	2.06	1.61	1.59
24	Ay	602	GTP	PB-O3A	2.06	1.61	1.59
24	Bw	602	GTP	C2-N3	2.06	1.38	1.33
24	FP	501	GTP	PA-O3A	2.06	1.61	1.59
24	q	602	GTP	PA-O3A	2.06	1.61	1.59
24	A2	602	GTP	C2-N3	2.06	1.38	1.33
24	E1	501	GTP	PB-O3B	2.06	1.61	1.59
23	AV	602	GDP	PA-O3A	2.05	1.61	1.59
24	d	602	GTP	PA-O3A	2.05	1.61	1.59
24	Fb	501	GTP	C2-N3	2.05	1.38	1.33
24	Bw	602	GTP	PA-O3A	2.05	1.61	1.59
24	Em	501	GTP	PA-O3A	2.05	1.61	1.59
24	B0	501	GTP	PA-O3A	2.05	1.61	1.59
24	Er	501	GTP	PB-O3A	2.05	1.61	1.59
24	BR	501	GTP	PB-O3A	2.05	1.61	1.59
24	Fe	501	GTP	C2-N3	2.05	1.38	1.33
24	Gy	501	GTP	PB-O3B	2.05	1.61	1.59
24	BT	501	GTP	PA-O3A	2.04	1.61	1.59
24	o	501	GTP	PB-O3A	2.04	1.61	1.59
24	FS	501	GTP	PB-O3B	2.04	1.61	1.59
24	Fg	501	GTP	C2-N3	2.04	1.38	1.33
24	t	602	GTP	PA-O3A	2.04	1.61	1.59
24	Ez	501	GTP	PB-O3B	2.04	1.61	1.59
23	AY	501	GDP	PA-O3A	2.04	1.61	1.59
24	v	602	GTP	PA-O3A	2.04	1.61	1.59
23	A3	501	GDP	O4'-C1'	2.04	1.43	1.40
24	y	602	GTP	PA-O3A	2.04	1.61	1.59
24	Aw	602	GTP	PA-O3A	2.04	1.61	1.59
24	G5	501	GTP	PB-O3A	2.04	1.61	1.59
24	Gs	501	GTP	PA-O3A	2.04	1.61	1.59
24	B0	501	GTP	PB-O3A	2.04	1.61	1.59
24	FT	501	GTP	PB-O3B	2.04	1.61	1.59
24	c	602	GTP	PB-O3B	2.03	1.61	1.59
24	Go	501	GTP	PA-O3A	2.03	1.61	1.59
24	Bu	602	GTP	PB-O3B	2.03	1.61	1.59
24	BR	501	GTP	PB-O3B	2.03	1.61	1.59
24	FU	501	GTP	PA-O3A	2.03	1.61	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	h	602	GTP	PB-O3A	2.03	1.61	1.59
24	Gl	501	GTP	PB-O3A	2.03	1.61	1.59
23	BE	501	GDP	O4'-C1'	2.03	1.43	1.40
24	GR	501	GTP	C2-N3	2.02	1.38	1.33
24	CB	602	GTP	PB-O3B	2.02	1.61	1.59
24	G2	501	GTP	PB-O3B	2.02	1.61	1.59
24	g	602	GTP	PA-O3A	2.02	1.61	1.59
24	w	602	GTP	PB-O3A	2.02	1.61	1.59
24	Ey	602	GTP	PA-O3A	2.02	1.61	1.59
24	W	602	GTP	PB-O3A	2.02	1.61	1.59
24	F7	501	GTP	PB-O3B	2.02	1.61	1.59
23	AC	501	GDP	O4'-C1'	2.01	1.43	1.40
23	AT	501	GDP	O4'-C1'	2.01	1.43	1.40
24	Ez	501	GTP	PA-O3A	2.01	1.61	1.59
24	B8	602	GTP	PA-O3A	2.01	1.61	1.59
24	E7	501	GTP	PA-O3A	2.01	1.61	1.59
24	En	501	GTP	PA-O3A	2.01	1.61	1.59
24	Gp	501	GTP	PA-O3A	2.01	1.61	1.59
23	GX	501	GDP	O4'-C1'	2.01	1.43	1.40
24	Bz	602	GTP	PA-O3A	2.01	1.61	1.59
24	GT	501	GTP	C2-N3	2.01	1.38	1.33
24	v	602	GTP	PB-O3A	2.01	1.61	1.59
24	i	602	GTP	PA-O3A	2.01	1.61	1.59
23	Ar	501	GDP	PA-O3A	2.00	1.61	1.59
24	A4	501	GTP	PA-O3A	2.00	1.61	1.59
24	Bw	602	GTP	PB-O3A	2.00	1.61	1.59
24	GJ	501	GTP	PA-O3A	2.00	1.61	1.59
24	Q	602	GTP	PA-O3A	2.00	1.61	1.59
24	Ay	602	GTP	PA-O3A	2.00	1.61	1.59
24	Y	602	GTP	PB-O3B	2.00	1.61	1.59

All (1178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G5	501	GTP	C8-N7-C5	3.86	109.12	102.55
24	E3	501	GTP	C8-N7-C5	3.82	109.05	102.55
24	Ff	501	GTP	C8-N7-C5	3.79	109.00	102.55
24	Ey	602	GTP	C8-N7-C5	3.76	108.95	102.55
24	GR	501	GTP	C8-N7-C5	3.76	108.94	102.55
24	E7	501	GTP	C8-N7-C5	3.73	108.90	102.55
24	BM	602	GTP	C8-N7-C5	3.72	108.88	102.55
24	E6	602	GTP	C8-N7-C5	3.71	108.87	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Fe	501	GTP	C8-N7-C5	3.71	108.86	102.55
24	x	501	GTP	C8-N7-C5	3.71	108.86	102.55
24	B9	602	GTP	C8-N7-C5	3.70	108.85	102.55
24	Fi	501	GTP	C8-N7-C5	3.70	108.84	102.55
24	Ex	501	GTP	C8-N7-C5	3.69	108.84	102.55
24	Bu	602	GTP	C8-N7-C5	3.69	108.84	102.55
24	G4	602	GTP	C8-N7-C5	3.69	108.83	102.55
24	S	602	GTP	C8-N7-C5	3.69	108.83	102.55
24	2	602	GTP	C8-N7-C5	3.69	108.83	102.55
24	BU	602	GTP	C8-N7-C5	3.69	108.83	102.55
24	o	501	GTP	C8-N7-C5	3.69	108.83	102.55
24	B4	602	GTP	C8-N7-C5	3.69	108.83	102.55
24	BX	602	GTP	C8-N7-C5	3.68	108.82	102.55
24	GF	501	GTP	C8-N7-C5	3.68	108.81	102.55
24	b	602	GTP	C8-N7-C5	3.67	108.80	102.55
24	E2	501	GTP	C8-N7-C5	3.67	108.80	102.55
24	CA	602	GTP	C8-N7-C5	3.67	108.80	102.55
24	Ez	501	GTP	C8-N7-C5	3.67	108.80	102.55
24	GQ	602	GTP	C8-N7-C5	3.67	108.79	102.55
24	Ei	501	GTP	C8-N7-C5	3.67	108.79	102.55
24	Gv	501	GTP	C8-N7-C5	3.66	108.78	102.55
24	Bw	602	GTP	C8-N7-C5	3.66	108.78	102.55
24	3	602	GTP	C8-N7-C5	3.66	108.78	102.55
24	F3	501	GTP	C8-N7-C5	3.66	108.78	102.55
24	Ak	602	GTP	C8-N7-C5	3.66	108.78	102.55
24	BP	602	GTP	C8-N7-C5	3.66	108.78	102.55
24	Bz	602	GTP	C8-N7-C5	3.66	108.78	102.55
24	FX	501	GTP	C8-N7-C5	3.66	108.78	102.55
24	v	602	GTP	C8-N7-C5	3.66	108.78	102.55
24	Ew	501	GTP	C8-N7-C5	3.66	108.78	102.55
24	A1	602	GTP	C8-N7-C5	3.65	108.77	102.55
24	Y	602	GTP	C8-N7-C5	3.65	108.77	102.55
24	F6	501	GTP	C8-N7-C5	3.65	108.77	102.55
24	A2	602	GTP	C8-N7-C5	3.65	108.77	102.55
24	1	602	GTP	C8-N7-C5	3.65	108.77	102.55
24	BS	602	GTP	C8-N7-C5	3.65	108.77	102.55
24	BN	602	GTP	C8-N7-C5	3.65	108.76	102.55
24	B7	501	GTP	C8-N7-C5	3.65	108.76	102.55
24	Eo	501	GTP	C8-N7-C5	3.65	108.76	102.55
24	GE	501	GTP	C8-N7-C5	3.65	108.76	102.55
24	El	501	GTP	C8-N7-C5	3.65	108.76	102.55
24	AS	501	GTP	C8-N7-C5	3.64	108.75	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BL	602	GTP	C8-N7-C5	3.64	108.75	102.55
24	c	602	GTP	C8-N7-C5	3.64	108.75	102.55
24	AI	501	GTP	C8-N7-C5	3.64	108.75	102.55
24	Fk	501	GTP	C8-N7-C5	3.64	108.75	102.55
24	A4	501	GTP	C8-N7-C5	3.64	108.75	102.55
24	4	602	GTP	C8-N7-C5	3.64	108.75	102.55
24	FU	501	GTP	C8-N7-C5	3.64	108.75	102.55
24	a	602	GTP	C8-N7-C5	3.64	108.75	102.55
24	AJ	602	GTP	C8-N7-C5	3.64	108.75	102.55
24	BI	602	GTP	C8-N7-C5	3.64	108.74	102.55
24	W	602	GTP	C8-N7-C5	3.63	108.74	102.55
24	y	602	GTP	C8-N7-C5	3.63	108.74	102.55
24	GP	501	GTP	C8-N7-C5	3.63	108.73	102.55
24	GM	501	GTP	C8-N7-C5	3.63	108.73	102.55
24	j	602	GTP	C8-N7-C5	3.63	108.73	102.55
24	E8	501	GTP	C8-N7-C5	3.63	108.73	102.55
24	h	602	GTP	C8-N7-C5	3.63	108.73	102.55
24	F7	501	GTP	C8-N7-C5	3.63	108.73	102.55
24	G3	602	GTP	C8-N7-C5	3.63	108.72	102.55
24	Gq	501	GTP	C8-N7-C5	3.63	108.72	102.55
24	BY	602	GTP	C8-N7-C5	3.63	108.72	102.55
24	F8	501	GTP	C8-N7-C5	3.62	108.72	102.55
24	FP	501	GTP	C8-N7-C5	3.62	108.72	102.55
24	AK	602	GTP	C8-N7-C5	3.62	108.72	102.55
24	A8	501	GTP	C8-N7-C5	3.62	108.72	102.55
24	i	602	GTP	C8-N7-C5	3.62	108.72	102.55
24	Gu	501	GTP	C8-N7-C5	3.62	108.71	102.55
24	F0	501	GTP	C8-N7-C5	3.62	108.71	102.55
24	FQ	501	GTP	C8-N7-C5	3.62	108.71	102.55
24	G2	501	GTP	C8-N7-C5	3.62	108.71	102.55
24	B8	602	GTP	C8-N7-C5	3.62	108.71	102.55
24	B2	602	GTP	C8-N7-C5	3.62	108.71	102.55
24	BR	501	GTP	C8-N7-C5	3.62	108.71	102.55
24	s	602	GTP	C8-N7-C5	3.62	108.70	102.55
24	FT	501	GTP	C8-N7-C5	3.62	108.70	102.55
24	BO	602	GTP	C8-N7-C5	3.61	108.70	102.55
24	GN	501	GTP	C8-N7-C5	3.61	108.70	102.55
24	Al	602	GTP	C8-N7-C5	3.61	108.70	102.55
24	GI	501	GTP	C8-N7-C5	3.61	108.70	102.55
24	Q	602	GTP	C8-N7-C5	3.61	108.70	102.55
24	Gp	501	GTP	C8-N7-C5	3.61	108.70	102.55
23	BW	501	GDP	O4'-C1'-N9	3.61	113.53	108.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	e	602	GTP	C8-N7-C5	3.61	108.70	102.55
24	A7	501	GTP	C8-N7-C5	3.61	108.69	102.55
24	A5	501	GTP	C8-N7-C5	3.61	108.69	102.55
24	Eu	501	GTP	C8-N7-C5	3.61	108.69	102.55
24	Fg	501	GTP	C8-N7-C5	3.61	108.69	102.55
24	l	602	GTP	C8-N7-C5	3.61	108.69	102.55
23	Ec	501	GDP	O4'-C1'-N9	3.61	113.53	108.75
24	Ax	602	GTP	C8-N7-C5	3.61	108.69	102.55
24	FZ	501	GTP	C8-N7-C5	3.61	108.69	102.55
24	FR	501	GTP	C8-N7-C5	3.60	108.69	102.55
24	GS	501	GTP	C8-N7-C5	3.60	108.69	102.55
24	Eh	501	GTP	C8-N7-C5	3.60	108.68	102.55
24	BQ	602	GTP	C8-N7-C5	3.60	108.68	102.55
24	BT	501	GTP	C8-N7-C5	3.60	108.68	102.55
24	Ej	501	GTP	C8-N7-C5	3.60	108.68	102.55
24	A9	501	GTP	C8-N7-C5	3.60	108.68	102.55
24	GL	501	GTP	C8-N7-C5	3.60	108.68	102.55
24	f	602	GTP	C8-N7-C5	3.60	108.68	102.55
24	En	501	GTP	C8-N7-C5	3.60	108.68	102.55
24	Fa	501	GTP	C8-N7-C5	3.60	108.68	102.55
24	Fd	602	GTP	C8-N7-C5	3.60	108.68	102.55
24	A6	501	GTP	C8-N7-C5	3.60	108.68	102.55
24	Gy	501	GTP	C8-N7-C5	3.60	108.67	102.55
24	GA	501	GTP	C8-N7-C5	3.60	108.67	102.55
24	G6	501	GTP	C8-N7-C5	3.60	108.67	102.55
23	Gj	501	GDP	O4'-C1'-N9	3.60	113.51	108.75
24	Bx	602	GTP	C8-N7-C5	3.59	108.67	102.55
24	BV	602	GTP	C8-N7-C5	3.59	108.67	102.55
24	Gs	501	GTP	C8-N7-C5	3.59	108.66	102.55
24	Gt	501	GTP	C8-N7-C5	3.59	108.66	102.55
24	G1	501	GTP	C8-N7-C5	3.59	108.66	102.55
24	V	602	GTP	C8-N7-C5	3.59	108.65	102.55
24	B1	602	GTP	C8-N7-C5	3.59	108.65	102.55
24	FS	501	GTP	C8-N7-C5	3.59	108.65	102.55
24	CB	602	GTP	C8-N7-C5	3.58	108.65	102.55
24	Gx	501	GTP	C8-N7-C5	3.58	108.65	102.55
24	Ay	602	GTP	C8-N7-C5	3.58	108.65	102.55
24	Go	501	GTP	C8-N7-C5	3.58	108.65	102.55
24	FM	501	GTP	C8-N7-C5	3.58	108.64	102.55
24	p	602	GTP	C8-N7-C5	3.58	108.64	102.55
24	z	602	GTP	C8-N7-C5	3.58	108.64	102.55
24	w	602	GTP	C8-N7-C5	3.58	108.64	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	602	GTP	C8-N7-C5	3.58	108.64	102.55
24	GK	501	GTP	C8-N7-C5	3.58	108.64	102.55
24	Z	602	GTP	C8-N7-C5	3.57	108.64	102.55
24	5	602	GTP	C8-N7-C5	3.57	108.63	102.55
24	FY	501	GTP	C8-N7-C5	3.57	108.63	102.55
24	GD	501	GTP	C8-N7-C5	3.57	108.63	102.55
24	FV	602	GTP	C8-N7-C5	3.57	108.63	102.55
24	Em	501	GTP	C8-N7-C5	3.57	108.63	102.55
24	Gl	501	GTP	C8-N7-C5	3.57	108.63	102.55
24	Bv	602	GTP	C8-N7-C5	3.57	108.63	102.55
24	Eq	501	GTP	C8-N7-C5	3.57	108.62	102.55
24	Gz	501	GTP	C8-N7-C5	3.57	108.62	102.55
24	k	602	GTP	C8-N7-C5	3.57	108.62	102.55
24	E4	501	GTP	C8-N7-C5	3.57	108.62	102.55
24	Gw	501	GTP	C8-N7-C5	3.57	108.62	102.55
24	B3	602	GTP	C8-N7-C5	3.57	108.62	102.55
24	BJ	602	GTP	C8-N7-C5	3.57	108.62	102.55
24	Fc	501	GTP	C8-N7-C5	3.57	108.62	102.55
24	GC	501	GTP	C8-N7-C5	3.57	108.62	102.55
24	g	602	GTP	C8-N7-C5	3.57	108.62	102.55
24	u	501	GTP	C8-N7-C5	3.57	108.62	102.55
24	E1	501	GTP	C8-N7-C5	3.57	108.62	102.55
24	Gr	501	GTP	C8-N7-C5	3.56	108.62	102.55
24	B0	501	GTP	C8-N7-C5	3.56	108.62	102.55
24	Eg	501	GTP	C8-N7-C5	3.56	108.62	102.55
24	Er	501	GTP	C8-N7-C5	3.56	108.62	102.55
24	Es	501	GTP	C8-N7-C5	3.56	108.61	102.55
24	d	602	GTP	C8-N7-C5	3.56	108.61	102.55
24	FO	501	GTP	C8-N7-C5	3.56	108.61	102.55
24	Fh	501	GTP	C8-N7-C5	3.56	108.61	102.55
24	Bd	501	GTP	C8-N7-C5	3.56	108.61	102.55
24	F5	501	GTP	C8-N7-C5	3.56	108.60	102.55
24	F9	501	GTP	C8-N7-C5	3.56	108.60	102.55
24	GJ	501	GTP	C8-N7-C5	3.56	108.60	102.55
24	Aw	602	GTP	C8-N7-C5	3.55	108.60	102.55
24	BK	602	GTP	C8-N7-C5	3.55	108.60	102.55
24	FW	501	GTP	C8-N7-C5	3.55	108.60	102.55
24	T	602	GTP	C8-N7-C5	3.55	108.59	102.55
24	q	602	GTP	C8-N7-C5	3.55	108.59	102.55
24	Gn	501	GTP	C8-N7-C5	3.54	108.58	102.55
24	t	602	GTP	C8-N7-C5	3.54	108.58	102.55
24	E5	501	GTP	C8-N7-C5	3.54	108.57	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	GO	602	GTP	C8-N7-C5	3.54	108.57	102.55
24	Ep	501	GTP	C8-N7-C5	3.53	108.57	102.55
24	Et	501	GTP	C8-N7-C5	3.53	108.57	102.55
24	Ee	501	GTP	C8-N7-C5	3.53	108.57	102.55
24	By	602	GTP	C8-N7-C5	3.53	108.56	102.55
23	Gf	501	GDP	O4'-C1'-N9	3.53	113.42	108.75
24	B6	602	GTP	C8-N7-C5	3.53	108.56	102.55
24	GT	501	GTP	C8-N7-C5	3.53	108.55	102.55
24	GG	501	GTP	C8-N7-C5	3.53	108.55	102.55
24	B5	602	GTP	C8-N7-C5	3.52	108.55	102.55
24	Aj	501	GTP	C8-N7-C5	3.52	108.54	102.55
24	Bc	501	GTP	C8-N7-C5	3.51	108.52	102.55
24	Fb	501	GTP	C8-N7-C5	3.51	108.52	102.55
24	Fj	501	GTP	C8-N7-C5	3.51	108.52	102.55
24	Ek	501	GTP	C8-N7-C5	3.51	108.52	102.55
24	GB	501	GTP	C8-N7-C5	3.50	108.50	102.55
23	FA	501	GDP	O4'-C1'-N9	3.49	113.37	108.75
23	AC	501	GDP	O4'-C1'-N9	3.39	113.25	108.75
23	BZ	501	GDP	O4'-C1'-N9	3.26	113.07	108.75
23	ER	501	GDP	O4'-C1'-N9	3.25	113.05	108.75
23	Ev	501	GDP	O4'-C1'-N9	3.24	113.04	108.75
23	Dv	501	GDP	O4'-C1'-N9	3.22	113.02	108.75
23	Fp	501	GDP	O4'-C1'-N9	3.21	113.00	108.75
24	Fh	501	GTP	C4'-O4'-C1'	3.14	112.80	109.92
23	Gd	501	GDP	O4'-C1'-N9	3.14	112.90	108.75
23	F1	501	GDP	O4'-C1'-N9	3.11	112.87	108.75
24	E1	501	GTP	C4'-O4'-C1'	3.10	112.77	109.92
24	E5	501	GTP	C4'-O4'-C1'	3.10	112.77	109.92
23	EO	501	GDP	O4'-C1'-N9	3.10	112.86	108.75
23	GZ	501	GDP	O4'-C1'-N9	3.09	112.84	108.75
24	Fj	501	GTP	C2-N1-C6	-3.01	119.59	125.11
24	GQ	602	GTP	C4'-O4'-C1'	3.01	112.69	109.92
23	DR	501	GDP	O4'-C1'-N9	2.99	112.72	108.75
23	ER	501	GDP	C8-N7-C5	2.99	107.64	102.55
23	Dv	501	GDP	C8-N7-C5	2.99	107.64	102.55
23	GY	501	GDP	C8-N7-C5	2.99	107.64	102.55
23	E9	501	GDP	C8-N7-C5	2.99	107.64	102.55
24	E3	501	GTP	C2-N1-C6	-2.99	119.64	125.11
23	EQ	501	GDP	C8-N7-C5	2.99	107.63	102.55
23	FA	501	GDP	C8-N7-C5	2.97	107.61	102.55
23	BW	501	GDP	C8-N7-C5	2.97	107.60	102.55
24	Fj	501	GTP	C5-C6-N1	2.96	119.72	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Ff	501	GTP	C2-N1-C6	-2.96	119.69	125.11
24	t	602	GTP	C2-N1-C6	-2.96	119.69	125.11
24	A9	501	GTP	C5-C6-N1	2.96	119.72	114.07
24	E7	501	GTP	C2-N1-C6	-2.96	119.69	125.11
23	GX	501	GDP	C8-N7-C5	2.96	107.59	102.55
23	7	501	GDP	C8-N7-C5	2.96	107.59	102.55
23	Ga	501	GDP	O4'-C1'-N9	2.96	112.67	108.75
24	Eh	501	GTP	C2-N1-C6	-2.96	119.70	125.11
24	Go	501	GTP	C2-N1-C6	-2.96	119.70	125.11
23	AD	501	GDP	C8-N7-C5	2.95	107.58	102.55
24	Eq	501	GTP	C2-N1-C6	-2.95	119.70	125.11
24	F3	501	GTP	C2-N1-C6	-2.95	119.70	125.11
24	p	602	GTP	C4'-O4'-C1'	2.95	112.63	109.92
23	GW	501	GDP	C8-N7-C5	2.95	107.57	102.55
24	Bv	602	GTP	C5-C6-N1	2.95	119.70	114.07
24	G2	501	GTP	C2-N1-C6	-2.95	119.71	125.11
23	GZ	501	GDP	C8-N7-C5	2.94	107.56	102.55
23	Gm	501	GDP	O4'-C1'-N9	2.94	112.65	108.75
24	GL	501	GTP	C2-N1-C6	-2.94	119.72	125.11
24	F8	501	GTP	C5-C6-N1	2.94	119.69	114.07
23	Bp	501	GDP	C8-N7-C5	2.94	107.56	102.55
23	EO	501	GDP	C8-N7-C5	2.94	107.56	102.55
23	AL	501	GDP	C8-N7-C5	2.94	107.56	102.55
23	AU	501	GDP	C8-N7-C5	2.94	107.56	102.55
23	Gf	501	GDP	C8-N7-C5	2.94	107.56	102.55
24	x	501	GTP	C2-N1-C6	-2.94	119.73	125.11
24	Eu	501	GTP	C2-N1-C6	-2.94	119.73	125.11
23	Ev	501	GDP	C8-N7-C5	2.94	107.56	102.55
23	A3	501	GDP	C8-N7-C5	2.94	107.55	102.55
23	Fo	501	GDP	C8-N7-C5	2.94	107.55	102.55
23	DX	501	GDP	C8-N7-C5	2.94	107.55	102.55
24	BV	602	GTP	C2-N1-C6	-2.94	119.73	125.11
24	BV	602	GTP	C5-C6-N1	2.93	119.67	114.07
23	Bs	501	GDP	C8-N7-C5	2.93	107.54	102.55
24	Bx	602	GTP	C4'-O4'-C1'	2.93	112.61	109.92
23	Dq	501	GDP	C8-N7-C5	2.93	107.54	102.55
23	Ec	501	GDP	C8-N7-C5	2.93	107.54	102.55
24	En	501	GTP	C2-N1-C6	-2.93	119.74	125.11
24	F7	501	GTP	C2-N1-C6	-2.93	119.74	125.11
23	GV	501	GDP	C8-N7-C5	2.93	107.54	102.55
24	B0	501	GTP	C5-C6-N1	2.93	119.66	114.07
23	BF	501	GDP	C8-N7-C5	2.93	107.54	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	GC	501	GTP	C2-N1-C6	-2.93	119.75	125.11
24	Es	501	GTP	C2-N1-C6	-2.93	119.75	125.11
23	FG	501	GDP	C8-N7-C5	2.93	107.53	102.55
24	Gx	501	GTP	C2-N1-C6	-2.93	119.75	125.11
24	A9	501	GTP	C2-N1-C6	-2.93	119.75	125.11
24	z	602	GTP	C2-N1-C6	-2.93	119.75	125.11
24	Fc	501	GTP	C2-N1-C6	-2.93	119.75	125.11
24	Fh	501	GTP	C2-N1-C6	-2.92	119.76	125.11
24	Ey	602	GTP	C2-N1-C6	-2.92	119.76	125.11
24	b	602	GTP	C5-C6-N1	2.92	119.65	114.07
24	A6	501	GTP	C2-N1-C6	-2.92	119.76	125.11
24	t	602	GTP	C5-C6-N1	2.92	119.65	114.07
23	Fx	501	GDP	C8-N7-C5	2.92	107.53	102.55
23	EN	501	GDP	C8-N7-C5	2.92	107.52	102.55
24	Eq	501	GTP	C5-C6-N1	2.92	119.64	114.07
24	G5	501	GTP	C2-N1-C6	-2.92	119.76	125.11
24	z	602	GTP	C5-C6-N1	2.92	119.64	114.07
24	B5	602	GTP	C2-N1-C6	-2.92	119.76	125.11
23	Fn	501	GDP	C8-N7-C5	2.92	107.52	102.55
23	An	501	GDP	C8-N7-C5	2.92	107.52	102.55
23	AX	501	GDP	C8-N7-C5	2.92	107.52	102.55
23	FJ	501	GDP	C8-N7-C5	2.92	107.52	102.55
24	Eo	501	GTP	C2-N1-C6	-2.92	119.77	125.11
23	Ga	501	GDP	C8-N7-C5	2.92	107.52	102.55
24	A4	501	GTP	C2-N1-C6	-2.92	119.77	125.11
24	El	501	GTP	C2-N1-C6	-2.92	119.77	125.11
24	GO	602	GTP	C2-N1-C6	-2.92	119.77	125.11
24	s	602	GTP	C2-N1-C6	-2.92	119.77	125.11
24	B0	501	GTP	C2-N1-C6	-2.92	119.77	125.11
23	Gg	501	GDP	C8-N7-C5	2.92	107.52	102.55
24	o	501	GTP	C5-C6-N1	2.92	119.64	114.07
24	E1	501	GTP	C5-C6-N1	2.92	119.64	114.07
24	Er	501	GTP	C2-N1-C6	-2.92	119.77	125.11
24	F7	501	GTP	C5-C6-N1	2.92	119.63	114.07
24	6	602	GTP	C2-N1-C6	-2.92	119.77	125.11
24	F5	501	GTP	C2-N1-C6	-2.92	119.77	125.11
23	Fp	501	GDP	C8-N7-C5	2.91	107.51	102.55
23	Aq	501	GDP	C8-N7-C5	2.91	107.51	102.55
24	Ei	501	GTP	C2-N1-C6	-2.91	119.77	125.11
24	T	602	GTP	C4'-O4'-C1'	2.91	112.59	109.92
23	AC	501	GDP	C8-N7-C5	2.91	107.51	102.55
23	BB	501	GDP	C8-N7-C5	2.91	107.51	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A4	501	GTP	C5-C6-N1	2.91	119.63	114.07
24	CB	602	GTP	C2-N1-C6	-2.91	119.78	125.11
23	GW	501	GDP	O4'-C1'-N9	2.91	112.61	108.75
24	El	501	GTP	C5-C6-N1	2.91	119.63	114.07
24	FM	501	GTP	C2-N1-C6	-2.91	119.78	125.11
24	Bv	602	GTP	C2-N1-C6	-2.91	119.78	125.11
24	Fi	501	GTP	C5-C6-N1	2.91	119.62	114.07
23	GU	501	GDP	C8-N7-C5	2.91	107.50	102.55
23	ET	501	GDP	C8-N7-C5	2.91	107.50	102.55
24	Gs	501	GTP	C5-C6-N1	2.91	119.62	114.07
24	Es	501	GTP	C5-C6-N1	2.91	119.62	114.07
24	GF	501	GTP	C5-C6-N1	2.91	119.62	114.07
24	BY	602	GTP	C5-C6-N1	2.91	119.62	114.07
24	Gs	501	GTP	C2-N1-C6	-2.91	119.78	125.11
24	FY	501	GTP	C2-N1-C6	-2.91	119.79	125.11
23	Ds	501	GDP	C8-N7-C5	2.91	107.50	102.55
24	A5	501	GTP	C2-N1-C6	-2.91	119.79	125.11
24	Fh	501	GTP	C5-C6-N1	2.91	119.62	114.07
23	Fu	501	GDP	C8-N7-C5	2.91	107.50	102.55
23	Dx	501	GDP	C8-N7-C5	2.91	107.50	102.55
24	BJ	602	GTP	C2-N1-C6	-2.91	119.79	125.11
24	BP	602	GTP	C2-N1-C6	-2.91	119.79	125.11
24	A6	501	GTP	C5-C6-N1	2.91	119.62	114.07
23	Fm	501	GDP	C8-N7-C5	2.91	107.50	102.55
24	B4	602	GTP	C2-N1-C6	-2.91	119.79	125.11
24	GP	501	GTP	C2-N1-C6	-2.91	119.79	125.11
24	b	602	GTP	C2-N1-C6	-2.91	119.79	125.11
24	FZ	501	GTP	C2-N1-C6	-2.91	119.79	125.11
24	i	602	GTP	C2-N1-C6	-2.90	119.79	125.11
23	AE	501	GDP	C8-N7-C5	2.90	107.49	102.55
24	Ak	602	GTP	C5-C6-N1	2.90	119.61	114.07
24	GI	501	GTP	C2-N1-C6	-2.90	119.79	125.11
24	F8	501	GTP	C2-N1-C6	-2.90	119.79	125.11
24	FU	501	GTP	C2-N1-C6	-2.90	119.79	125.11
23	Gd	501	GDP	C8-N7-C5	2.90	107.49	102.55
24	AK	602	GTP	C2-N1-C6	-2.90	119.80	125.11
24	GA	501	GTP	C5-C6-N1	2.90	119.61	114.07
24	Fi	501	GTP	C2-N1-C6	-2.90	119.80	125.11
24	GN	501	GTP	C2-N1-C6	-2.90	119.80	125.11
24	BO	602	GTP	C2-N1-C6	-2.90	119.80	125.11
24	Gn	501	GTP	C2-N1-C6	-2.90	119.80	125.11
24	6	602	GTP	C5-C6-N1	2.90	119.61	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Em	501	GTP	C2-N1-C6	-2.90	119.80	125.11
23	ES	501	GDP	C8-N7-C5	2.90	107.49	102.55
23	FC	501	GDP	C8-N7-C5	2.90	107.49	102.55
24	BT	501	GTP	C2-N1-C6	-2.90	119.80	125.11
24	BQ	602	GTP	C2-N1-C6	-2.90	119.80	125.11
24	e	602	GTP	C2-N1-C6	-2.90	119.80	125.11
23	FN	501	GDP	C8-N7-C5	2.90	107.48	102.55
24	W	602	GTP	C5-C6-N1	2.90	119.60	114.07
24	Ej	501	GTP	C2-N1-C6	-2.90	119.81	125.11
23	P	501	GDP	C8-N7-C5	2.90	107.48	102.55
24	AS	501	GTP	C2-N1-C6	-2.90	119.81	125.11
24	Bd	501	GTP	C2-N1-C6	-2.90	119.81	125.11
23	Db	501	GDP	C8-N7-C5	2.90	107.48	102.55
23	FH	501	GDP	C8-N7-C5	2.90	107.48	102.55
24	F0	501	GTP	C2-N1-C6	-2.90	119.81	125.11
23	Fq	501	GDP	C8-N7-C5	2.90	107.48	102.55
23	DY	501	GDP	C8-N7-C5	2.90	107.48	102.55
23	Dt	501	GDP	C8-N7-C5	2.90	107.48	102.55
24	GD	501	GTP	C2-N1-C6	-2.90	119.81	125.11
24	GQ	602	GTP	C2-N1-C6	-2.90	119.81	125.11
24	A8	501	GTP	C2-N1-C6	-2.90	119.81	125.11
24	Ak	602	GTP	C2-N1-C6	-2.90	119.81	125.11
24	FX	501	GTP	C2-N1-C6	-2.90	119.81	125.11
24	A1	602	GTP	C5-C6-N1	2.90	119.59	114.07
23	Da	501	GDP	C8-N7-C5	2.90	107.48	102.55
24	f	602	GTP	C2-N1-C6	-2.89	119.81	125.11
23	Fs	501	GDP	C8-N7-C5	2.89	107.48	102.55
24	T	602	GTP	C2-N1-C6	-2.89	119.81	125.11
23	Gj	501	GDP	C8-N7-C5	2.89	107.48	102.55
23	De	501	GDP	C8-N7-C5	2.89	107.47	102.55
24	CB	602	GTP	C5-C6-N1	2.89	119.59	114.07
23	DT	501	GDP	C8-N7-C5	2.89	107.47	102.55
24	Ee	501	GTP	C2-N1-C6	-2.89	119.81	125.11
24	GM	501	GTP	C2-N1-C6	-2.89	119.82	125.11
24	u	501	GTP	C2-N1-C6	-2.89	119.82	125.11
24	E1	501	GTP	C2-N1-C6	-2.89	119.82	125.11
24	FZ	501	GTP	C5-C6-N1	2.89	119.59	114.07
23	Fr	501	GDP	C8-N7-C5	2.89	107.47	102.55
23	EY	501	GDP	C8-N7-C5	2.89	107.47	102.55
23	FF	501	GDP	C8-N7-C5	2.89	107.47	102.55
24	q	602	GTP	C2-N1-C6	-2.89	119.82	125.11
24	j	602	GTP	C2-N1-C6	-2.89	119.82	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Ew	501	GTP	C2-N1-C6	-2.89	119.82	125.11
23	Gi	501	GDP	C8-N7-C5	2.89	107.47	102.55
24	GS	501	GTP	C2-N1-C6	-2.89	119.82	125.11
24	Gw	501	GTP	C5-C6-N1	2.89	119.58	114.07
24	Gl	501	GTP	C2-N1-C6	-2.89	119.82	125.11
24	B7	501	GTP	C2-N1-C6	-2.89	119.82	125.11
23	Dh	501	GDP	C8-N7-C5	2.89	107.47	102.55
23	GU	501	GDP	O4'-C1'-N9	2.89	112.58	108.75
24	Z	602	GTP	C2-N1-C6	-2.89	119.82	125.11
24	G2	501	GTP	C5-C6-N1	2.89	119.58	114.07
24	FM	501	GTP	C5-C6-N1	2.89	119.58	114.07
23	EN	501	GDP	O4'-C1'-N9	2.89	112.57	108.75
24	a	602	GTP	C2-N1-C6	-2.89	119.83	125.11
24	2	602	GTP	C2-N1-C6	-2.89	119.83	125.11
24	FS	501	GTP	C2-N1-C6	-2.89	119.83	125.11
23	Be	501	GDP	C8-N7-C5	2.89	107.46	102.55
24	Ay	602	GTP	C5-C6-N1	2.89	119.58	114.07
23	BH	501	GDP	C8-N7-C5	2.89	107.46	102.55
24	G1	501	GTP	C2-N1-C6	-2.88	119.83	125.11
24	B6	602	GTP	C2-N1-C6	-2.88	119.83	125.11
23	Fl	501	GDP	C8-N7-C5	2.88	107.46	102.55
24	Gv	501	GTP	C2-N1-C6	-2.88	119.83	125.11
24	k	602	GTP	C2-N1-C6	-2.88	119.83	125.11
24	BK	602	GTP	C2-N1-C6	-2.88	119.83	125.11
24	w	602	GTP	C5-C6-N1	2.88	119.57	114.07
24	Ei	501	GTP	C5-C6-N1	2.88	119.57	114.07
24	F3	501	GTP	C5-C6-N1	2.88	119.57	114.07
24	Bx	602	GTP	C2-N1-C6	-2.88	119.83	125.11
24	Aw	602	GTP	C5-C6-N1	2.88	119.57	114.07
24	Ej	501	GTP	C5-C6-N1	2.88	119.57	114.07
24	l	602	GTP	C2-N1-C6	-2.88	119.83	125.11
24	5	602	GTP	C2-N1-C6	-2.88	119.83	125.11
23	Gm	501	GDP	C8-N7-C5	2.88	107.46	102.55
23	E0	501	GDP	C8-N7-C5	2.88	107.46	102.55
24	GM	501	GTP	C5-C6-N1	2.88	119.57	114.07
23	EP	501	GDP	C8-N7-C5	2.88	107.45	102.55
23	Eb	501	GDP	C8-N7-C5	2.88	107.45	102.55
24	q	602	GTP	C5-C6-N1	2.88	119.57	114.07
24	B7	501	GTP	C5-C6-N1	2.88	119.57	114.07
24	BY	602	GTP	C2-N1-C6	-2.88	119.84	125.11
24	x	501	GTP	C5-C6-N1	2.88	119.57	114.07
24	Ez	501	GTP	C5-C6-N1	2.88	119.57	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Gb	501	GDP	C8-N7-C5	2.88	107.45	102.55
24	y	602	GTP	C2-N1-C6	-2.88	119.84	125.11
24	Bc	501	GTP	C2-N1-C6	-2.88	119.84	125.11
24	c	602	GTP	C5-C6-N1	2.88	119.56	114.07
23	Ge	501	GDP	C8-N7-C5	2.88	107.45	102.55
23	8	501	GDP	C8-N7-C5	2.88	107.45	102.55
24	AJ	602	GTP	C2-N1-C6	-2.88	119.84	125.11
23	Dc	501	GDP	C8-N7-C5	2.88	107.45	102.55
24	Gy	501	GTP	C2-N1-C6	-2.88	119.84	125.11
24	AI	501	GTP	C2-N1-C6	-2.88	119.84	125.11
23	Dr	501	GDP	C8-N7-C5	2.88	107.45	102.55
24	Aj	501	GTP	C2-N1-C6	-2.88	119.84	125.11
24	B2	602	GTP	C2-N1-C6	-2.88	119.84	125.11
23	Bk	501	GDP	C8-N7-C5	2.88	107.45	102.55
23	Bq	602	GDP	C8-N7-C5	2.88	107.45	102.55
24	FV	602	GTP	C5-C6-N1	2.88	119.56	114.07
24	FX	501	GTP	C5-C6-N1	2.88	119.56	114.07
24	B9	602	GTP	C2-N1-C6	-2.88	119.84	125.11
24	Go	501	GTP	C5-C6-N1	2.88	119.56	114.07
24	B9	602	GTP	C5-C6-N1	2.88	119.56	114.07
23	A0	501	GDP	C8-N7-C5	2.88	107.45	102.55
23	Fw	501	GDP	C8-N7-C5	2.88	107.44	102.55
23	DO	501	GDP	C8-N7-C5	2.88	107.44	102.55
23	Dd	501	GDP	C8-N7-C5	2.88	107.44	102.55
24	FT	501	GTP	C2-N1-C6	-2.88	119.85	125.11
24	GO	602	GTP	C5-C6-N1	2.88	119.56	114.07
24	Gp	501	GTP	C2-N1-C6	-2.88	119.85	125.11
24	Gr	501	GTP	C2-N1-C6	-2.88	119.85	125.11
24	Aw	602	GTP	C2-N1-C6	-2.88	119.85	125.11
24	Eg	501	GTP	C2-N1-C6	-2.88	119.85	125.11
23	DV	501	GDP	C8-N7-C5	2.88	107.44	102.55
24	A1	602	GTP	C2-N1-C6	-2.87	119.85	125.11
24	GL	501	GTP	C5-C6-N1	2.87	119.55	114.07
23	E9	501	GDP	O4'-C1'-N9	2.87	112.56	108.75
23	AT	501	GDP	C8-N7-C5	2.87	107.44	102.55
23	Bg	501	GDP	C8-N7-C5	2.87	107.44	102.55
23	DQ	501	GDP	C8-N7-C5	2.87	107.44	102.55
23	EM	501	GDP	C8-N7-C5	2.87	107.44	102.55
24	AK	602	GTP	C5-C6-N1	2.87	119.55	114.07
24	BT	501	GTP	C5-C6-N1	2.87	119.55	114.07
24	Ax	602	GTP	C2-N1-C6	-2.87	119.85	125.11
24	Ex	501	GTP	C2-N1-C6	-2.87	119.85	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Ba	501	GDP	C8-N7-C5	2.87	107.44	102.55
24	AI	501	GTP	C5-C6-N1	2.87	119.55	114.07
24	GA	501	GTP	C2-N1-C6	-2.87	119.85	125.11
24	o	501	GTP	C2-N1-C6	-2.87	119.85	125.11
24	E4	501	GTP	C2-N1-C6	-2.87	119.86	125.11
24	FR	501	GTP	C2-N1-C6	-2.87	119.86	125.11
24	Ey	602	GTP	C5-C6-N1	2.87	119.54	114.07
23	AA	501	GDP	C8-N7-C5	2.87	107.43	102.55
23	AQ	501	GDP	C8-N7-C5	2.87	107.43	102.55
24	Gq	501	GTP	C2-N1-C6	-2.87	119.86	125.11
24	G3	602	GTP	C2-N1-C6	-2.87	119.86	125.11
24	2	602	GTP	C5-C6-N1	2.87	119.54	114.07
24	GF	501	GTP	C2-N1-C6	-2.87	119.86	125.11
23	Df	501	GDP	C8-N7-C5	2.87	107.43	102.55
24	B8	602	GTP	C2-N1-C6	-2.87	119.86	125.11
23	FD	501	GDP	C8-N7-C5	2.87	107.43	102.55
23	Gc	501	GDP	C8-N7-C5	2.87	107.43	102.55
23	Dj	501	GDP	C8-N7-C5	2.87	107.43	102.55
23	FK	501	GDP	C8-N7-C5	2.87	107.43	102.55
24	B6	602	GTP	C5-C6-N1	2.87	119.54	114.07
23	Av	501	GDP	C8-N7-C5	2.87	107.43	102.55
23	DU	501	GDP	C8-N7-C5	2.87	107.43	102.55
24	B5	602	GTP	C5-C6-N1	2.87	119.54	114.07
24	FT	501	GTP	C5-C6-N1	2.87	119.54	114.07
24	E2	501	GTP	C2-N1-C6	-2.87	119.86	125.11
23	EU	501	GDP	C8-N7-C5	2.87	107.43	102.55
23	FL	501	GDP	C8-N7-C5	2.87	107.43	102.55
24	Gu	501	GTP	C5-C6-N1	2.86	119.54	114.07
24	BK	602	GTP	C5-C6-N1	2.86	119.54	114.07
24	Bu	602	GTP	C5-C6-N1	2.86	119.54	114.07
24	Gw	501	GTP	C2-N1-C6	-2.86	119.87	125.11
23	FE	501	GDP	C8-N7-C5	2.86	107.43	102.55
24	Gr	501	GTP	C5-C6-N1	2.86	119.53	114.07
24	B8	602	GTP	C5-C6-N1	2.86	119.53	114.07
24	Gu	501	GTP	C2-N1-C6	-2.86	119.87	125.11
24	B3	602	GTP	C2-N1-C6	-2.86	119.87	125.11
24	FV	602	GTP	C2-N1-C6	-2.86	119.87	125.11
23	Ag	501	GDP	C8-N7-C5	2.86	107.42	102.55
23	Dg	501	GDP	C8-N7-C5	2.86	107.42	102.55
23	Dw	501	GDP	C8-N7-C5	2.86	107.42	102.55
23	X	501	GDP	C8-N7-C5	2.86	107.42	102.55
23	AG	501	GDP	C8-N7-C5	2.86	107.42	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	GC	501	GTP	C5-C6-N1	2.86	119.53	114.07
24	GN	501	GTP	C5-C6-N1	2.86	119.53	114.07
24	Ek	501	GTP	C2-N1-C6	-2.86	119.87	125.11
24	v	602	GTP	C5-C6-N1	2.86	119.53	114.07
24	Al	602	GTP	C2-N1-C6	-2.86	119.87	125.11
24	d	602	GTP	C2-N1-C6	-2.86	119.87	125.11
23	Fq	501	GDP	O4'-C1'-N9	2.86	112.54	108.75
23	Ab	501	GDP	C8-N7-C5	2.86	107.42	102.55
24	GK	501	GTP	C2-N1-C6	-2.86	119.87	125.11
24	p	602	GTP	C2-N1-C6	-2.86	119.87	125.11
24	BM	602	GTP	C2-N1-C6	-2.86	119.87	125.11
24	G3	602	GTP	C5-C6-N1	2.86	119.53	114.07
24	Fe	501	GTP	C2-N1-C6	-2.86	119.88	125.11
24	Ex	501	GTP	C5-C6-N1	2.86	119.53	114.07
24	V	602	GTP	C2-N1-C6	-2.86	119.88	125.11
24	GI	501	GTP	C5-C6-N1	2.86	119.53	114.07
24	Ek	501	GTP	C5-C6-N1	2.86	119.53	114.07
24	GB	501	GTP	C2-N1-C6	-2.86	119.88	125.11
24	Et	501	GTP	C2-N1-C6	-2.86	119.88	125.11
23	Di	501	GDP	C8-N7-C5	2.86	107.42	102.55
24	u	501	GTP	C5-C6-N1	2.86	119.52	114.07
24	Bd	501	GTP	C5-C6-N1	2.86	119.52	114.07
24	F5	501	GTP	C5-C6-N1	2.86	119.52	114.07
24	Ay	602	GTP	C2-N1-C6	-2.86	119.88	125.11
24	g	602	GTP	C5-C6-N1	2.86	119.52	114.07
24	Eh	501	GTP	C5-C6-N1	2.86	119.52	114.07
24	Ez	501	GTP	C2-N1-C6	-2.86	119.88	125.11
24	Fg	501	GTP	C2-N1-C6	-2.86	119.88	125.11
24	3	602	GTP	C5-C6-N1	2.86	119.52	114.07
24	Bx	602	GTP	C5-C6-N1	2.86	119.52	114.07
24	Z	602	GTP	C5-C6-N1	2.86	119.52	114.07
24	BX	602	GTP	C5-C6-N1	2.86	119.52	114.07
23	Fz	501	GDP	C8-N7-C5	2.86	107.41	102.55
24	Ep	501	GTP	C5-C6-N1	2.86	119.52	114.07
23	Az	501	GDP	C8-N7-C5	2.86	107.41	102.55
24	Q	602	GTP	C5-C6-N1	2.86	119.52	114.07
24	FY	501	GTP	C5-C6-N1	2.86	119.52	114.07
23	At	501	GDP	C8-N7-C5	2.86	107.41	102.55
24	GJ	501	GTP	C2-N1-C6	-2.85	119.88	125.11
24	BN	602	GTP	C2-N1-C6	-2.85	119.88	125.11
24	Ep	501	GTP	C2-N1-C6	-2.85	119.88	125.11
24	Gv	501	GTP	C5-C6-N1	2.85	119.52	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AM	501	GDP	C8-N7-C5	2.85	107.41	102.55
23	Ea	501	GDP	C8-N7-C5	2.85	107.41	102.55
23	Gh	501	GDP	C8-N7-C5	2.85	107.41	102.55
24	y	602	GTP	C5-C6-N1	2.85	119.51	114.07
24	g	602	GTP	C2-N1-C6	-2.85	119.89	125.11
23	Bi	501	GDP	C8-N7-C5	2.85	107.41	102.55
24	G1	501	GTP	C5-C6-N1	2.85	119.51	114.07
24	AS	501	GTP	C5-C6-N1	2.85	119.51	114.07
23	BE	501	GDP	C8-N7-C5	2.85	107.41	102.55
24	w	602	GTP	C2-N1-C6	-2.85	119.89	125.11
24	By	602	GTP	C2-N1-C6	-2.85	119.89	125.11
24	A7	501	GTP	C2-N1-C6	-2.85	119.89	125.11
24	CA	602	GTP	C2-N1-C6	-2.85	119.89	125.11
23	Bt	501	GDP	C8-N7-C5	2.85	107.40	102.55
24	Y	602	GTP	C5-C6-N1	2.85	119.51	114.07
24	BJ	602	GTP	C5-C6-N1	2.85	119.51	114.07
24	Bw	602	GTP	C5-C6-N1	2.85	119.51	114.07
23	EX	501	GDP	C8-N7-C5	2.85	107.40	102.55
24	A7	501	GTP	C5-C6-N1	2.85	119.51	114.07
24	BM	602	GTP	C5-C6-N1	2.85	119.51	114.07
23	Bn	501	GDP	C8-N7-C5	2.85	107.40	102.55
23	Br	501	GDP	C8-N7-C5	2.85	107.40	102.55
23	EZ	501	GDP	C8-N7-C5	2.85	107.40	102.55
23	Aa	501	GDP	C8-N7-C5	2.85	107.40	102.55
24	GE	501	GTP	C5-C6-N1	2.85	119.51	114.07
23	Bb	501	GDP	C8-N7-C5	2.85	107.40	102.55
24	E8	501	GTP	C2-N1-C6	-2.85	119.89	125.11
23	Ac	501	GDP	C8-N7-C5	2.85	107.40	102.55
23	FI	501	GDP	C8-N7-C5	2.85	107.40	102.55
24	Eu	501	GTP	C5-C6-N1	2.85	119.50	114.07
24	FQ	501	GTP	C5-C6-N1	2.85	119.50	114.07
24	v	602	GTP	C2-N1-C6	-2.85	119.90	125.11
23	DM	501	GDP	C8-N7-C5	2.85	107.40	102.55
23	DP	501	GDP	C8-N7-C5	2.85	107.40	102.55
23	Ef	501	GDP	C8-N7-C5	2.85	107.40	102.55
24	V	602	GTP	C5-C6-N1	2.85	119.50	114.07
24	f	602	GTP	C5-C6-N1	2.85	119.50	114.07
24	A8	501	GTP	C5-C6-N1	2.85	119.50	114.07
24	E2	501	GTP	C5-C6-N1	2.85	119.50	114.07
23	AN	501	GDP	C8-N7-C5	2.85	107.39	102.55
24	GR	501	GTP	C5-C6-N1	2.85	119.50	114.07
24	1	602	GTP	C5-C6-N1	2.85	119.50	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	501	GDP	C8-N7-C5	2.85	107.39	102.55
23	BA	501	GDP	C8-N7-C5	2.85	107.39	102.55
23	EV	501	GDP	C8-N7-C5	2.85	107.39	102.55
23	F1	501	GDP	C8-N7-C5	2.85	107.39	102.55
24	BI	602	GTP	C5-C6-N1	2.84	119.50	114.07
23	AO	501	GDP	C8-N7-C5	2.84	107.39	102.55
24	GG	501	GTP	C5-C6-N1	2.84	119.50	114.07
24	Bc	501	GTP	C5-C6-N1	2.84	119.50	114.07
23	Fy	501	GDP	C8-N7-C5	2.84	107.39	102.55
23	AP	501	GDP	C8-N7-C5	2.84	107.39	102.55
23	Du	501	GDP	C8-N7-C5	2.84	107.39	102.55
24	G4	602	GTP	C2-N1-C6	-2.84	119.91	125.11
24	Gz	501	GTP	C5-C6-N1	2.84	119.49	114.07
23	GH	501	GDP	C8-N7-C5	2.84	107.39	102.55
24	d	602	GTP	C5-C6-N1	2.84	119.49	114.07
24	4	602	GTP	C5-C6-N1	2.84	119.49	114.07
23	Bo	501	GDP	C8-N7-C5	2.84	107.39	102.55
24	Gx	501	GTP	C5-C6-N1	2.84	119.49	114.07
24	s	602	GTP	C5-C6-N1	2.84	119.49	114.07
24	F6	501	GTP	C2-N1-C6	-2.84	119.91	125.11
23	DW	501	GDP	C8-N7-C5	2.84	107.38	102.55
24	GE	501	GTP	C2-N1-C6	-2.84	119.91	125.11
24	FO	501	GTP	C2-N1-C6	-2.84	119.91	125.11
23	AZ	501	GDP	C8-N7-C5	2.84	107.38	102.55
24	Fk	501	GTP	C2-N1-C6	-2.84	119.91	125.11
23	Bh	501	GDP	C8-N7-C5	2.84	107.38	102.55
24	3	602	GTP	C2-N1-C6	-2.84	119.92	125.11
24	Fa	501	GTP	C2-N1-C6	-2.84	119.92	125.11
24	Ax	602	GTP	C5-C6-N1	2.84	119.48	114.07
24	Eo	501	GTP	C5-C6-N1	2.84	119.48	114.07
23	Ap	501	GDP	C8-N7-C5	2.84	107.38	102.55
23	Dq	501	GDP	O4'-C1'-N9	2.84	112.51	108.75
23	EW	501	GDP	C8-N7-C5	2.84	107.38	102.55
24	5	602	GTP	C5-C6-N1	2.84	119.48	114.07
23	Fv	501	GDP	C8-N7-C5	2.84	107.38	102.55
24	Aj	501	GTP	C5-C6-N1	2.84	119.48	114.07
23	AW	501	GDP	C8-N7-C5	2.84	107.38	102.55
23	FB	501	GDP	C8-N7-C5	2.84	107.38	102.55
24	Fg	501	GTP	C5-C6-N1	2.84	119.48	114.07
24	Fb	501	GTP	C2-N1-C6	-2.84	119.92	125.11
23	m	501	GDP	C8-N7-C5	2.83	107.38	102.55
23	Dk	501	GDP	C8-N7-C5	2.83	107.37	102.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Al	602	GTP	C5-C6-N1	2.83	119.48	114.07
23	n	501	GDP	C8-N7-C5	2.83	107.37	102.55
24	Fk	501	GTP	C5-C6-N1	2.83	119.48	114.07
24	FU	501	GTP	C5-C6-N1	2.83	119.47	114.07
23	Au	602	GDP	C8-N7-C5	2.83	107.37	102.55
23	F2	501	GDP	C8-N7-C5	2.83	107.37	102.55
24	Gz	501	GTP	C2-N1-C6	-2.83	119.92	125.11
24	CA	602	GTP	C5-C6-N1	2.83	119.47	114.07
24	S	602	GTP	C5-C6-N1	2.83	119.47	114.07
24	Er	501	GTP	C5-C6-N1	2.83	119.47	114.07
24	W	602	GTP	C2-N1-C6	-2.83	119.93	125.11
24	GQ	602	GTP	C5-C6-N1	2.83	119.47	114.07
24	GK	501	GTP	C5-C6-N1	2.83	119.47	114.07
24	T	602	GTP	C5-C6-N1	2.83	119.47	114.07
23	BG	501	GDP	C8-N7-C5	2.83	107.37	102.55
24	BR	501	GTP	C2-N1-C6	-2.83	119.93	125.11
24	4	602	GTP	C2-N1-C6	-2.83	119.93	125.11
24	En	501	GTP	C5-C6-N1	2.83	119.47	114.07
23	AB	501	GDP	C8-N7-C5	2.83	107.37	102.55
24	B1	602	GTP	C2-N1-C6	-2.83	119.93	125.11
23	0	501	GDP	C8-N7-C5	2.83	107.37	102.55
23	DL	501	GDP	C8-N7-C5	2.83	107.37	102.55
24	c	602	GTP	C2-N1-C6	-2.83	119.93	125.11
23	BC	501	GDP	C8-N7-C5	2.83	107.36	102.55
24	GS	501	GTP	C5-C6-N1	2.83	119.47	114.07
24	FR	501	GTP	C5-C6-N1	2.83	119.47	114.07
23	EL	501	GDP	C8-N7-C5	2.83	107.36	102.55
24	GJ	501	GTP	C5-C6-N1	2.83	119.47	114.07
24	A2	602	GTP	C5-C6-N1	2.83	119.46	114.07
24	Em	501	GTP	C5-C6-N1	2.83	119.46	114.07
24	E4	501	GTP	C5-C6-N1	2.83	119.46	114.07
24	E8	501	GTP	C5-C6-N1	2.83	119.46	114.07
24	Ee	501	GTP	C5-C6-N1	2.83	119.46	114.07
24	Fc	501	GTP	C5-C6-N1	2.83	119.46	114.07
24	Bz	602	GTP	C2-N1-C6	-2.83	119.94	125.11
23	EV	501	GDP	O4'-C1'-N9	2.82	112.49	108.75
23	F4	501	GDP	C8-N7-C5	2.82	107.36	102.55
24	Gq	501	GTP	C5-C6-N1	2.82	119.46	114.07
24	Gy	501	GTP	C5-C6-N1	2.82	119.46	114.07
24	e	602	GTP	C5-C6-N1	2.82	119.46	114.07
24	i	602	GTP	C5-C6-N1	2.82	119.46	114.07
24	BS	602	GTP	C5-C6-N1	2.82	119.46	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	FP	501	GTP	C2-N1-C6	-2.82	119.94	125.11
24	a	602	GTP	C5-C6-N1	2.82	119.46	114.07
23	Ao	501	GDP	C8-N7-C5	2.82	107.35	102.55
23	Gg	501	GDP	O4'-C1'-N9	2.82	112.49	108.75
23	AY	501	GDP	C8-N7-C5	2.82	107.35	102.55
23	BZ	501	GDP	C8-N7-C5	2.82	107.35	102.55
24	BU	602	GTP	C2-N1-C6	-2.82	119.95	125.11
24	GG	501	GTP	C2-N1-C6	-2.82	119.95	125.11
24	p	602	GTP	C5-C6-N1	2.82	119.45	114.07
24	F9	501	GTP	C5-C6-N1	2.82	119.45	114.07
23	U	501	GDP	C8-N7-C5	2.82	107.35	102.55
23	Ed	501	GDP	C8-N7-C5	2.82	107.35	102.55
24	BX	602	GTP	C2-N1-C6	-2.82	119.95	125.11
24	AJ	602	GTP	C5-C6-N1	2.82	119.45	114.07
24	BQ	602	GTP	C5-C6-N1	2.82	119.45	114.07
23	9	501	GDP	C8-N7-C5	2.82	107.35	102.55
24	BN	602	GTP	C5-C6-N1	2.82	119.45	114.07
24	Bz	602	GTP	C5-C6-N1	2.82	119.45	114.07
24	Fd	602	GTP	C2-N1-C6	-2.82	119.95	125.11
24	B2	602	GTP	C5-C6-N1	2.82	119.45	114.07
24	Bu	602	GTP	C2-N1-C6	-2.82	119.95	125.11
24	G4	602	GTP	C5-C6-N1	2.82	119.44	114.07
24	By	602	GTP	C5-C6-N1	2.82	119.44	114.07
24	Ew	501	GTP	C5-C6-N1	2.82	119.44	114.07
24	F9	501	GTP	C2-N1-C6	-2.82	119.95	125.11
24	BO	602	GTP	C5-C6-N1	2.82	119.44	114.07
23	Ah	602	GDP	C8-N7-C5	2.82	107.34	102.55
24	h	602	GTP	C5-C6-N1	2.82	119.44	114.07
24	B4	602	GTP	C5-C6-N1	2.82	119.44	114.07
23	Bj	501	GDP	C8-N7-C5	2.82	107.34	102.55
24	AS	501	GTP	C4'-O4'-C1'	2.82	112.50	109.92
24	Gp	501	GTP	C5-C6-N1	2.81	119.44	114.07
24	Gt	501	GTP	C2-N1-C6	-2.81	119.96	125.11
24	E6	602	GTP	C2-N1-C6	-2.81	119.96	125.11
24	E6	602	GTP	C5-C6-N1	2.81	119.44	114.07
23	DR	501	GDP	C8-N7-C5	2.81	107.34	102.55
23	Bm	501	GDP	C8-N7-C5	2.81	107.34	102.55
24	Gn	501	GTP	C5-C6-N1	2.81	119.44	114.07
24	Fa	501	GTP	C5-C6-N1	2.81	119.44	114.07
23	Ar	501	GDP	C8-N7-C5	2.81	107.34	102.55
24	GB	501	GTP	C5-C6-N1	2.81	119.44	114.07
24	FQ	501	GTP	C2-N1-C6	-2.81	119.96	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	E7	501	GTP	C5-C6-N1	2.81	119.43	114.07
23	DS	501	GDP	C8-N7-C5	2.81	107.33	102.55
24	1	602	GTP	C2-N1-C6	-2.81	119.97	125.11
24	h	602	GTP	C2-N1-C6	-2.81	119.97	125.11
24	BR	501	GTP	C5-C6-N1	2.81	119.42	114.07
24	BS	602	GTP	C2-N1-C6	-2.81	119.97	125.11
24	F0	501	GTP	C5-C6-N1	2.81	119.42	114.07
24	Y	602	GTP	C2-N1-C6	-2.80	119.98	125.11
24	BU	602	GTP	C5-C6-N1	2.80	119.42	114.07
23	Ft	501	GDP	C8-N7-C5	2.80	107.32	102.55
23	AH	501	GDP	C8-N7-C5	2.80	107.32	102.55
23	DN	501	GDP	C8-N7-C5	2.80	107.32	102.55
24	A5	501	GTP	C5-C6-N1	2.80	119.42	114.07
24	E5	501	GTP	C2-N1-C6	-2.80	119.98	125.11
23	Ae	501	GDP	C8-N7-C5	2.80	107.32	102.55
24	GD	501	GTP	C5-C6-N1	2.80	119.41	114.07
24	j	602	GTP	C5-C6-N1	2.80	119.41	114.07
24	G6	501	GTP	C5-C6-N1	2.80	119.41	114.07
24	k	602	GTP	C5-C6-N1	2.80	119.41	114.07
23	Gk	501	GDP	C8-N7-C5	2.80	107.31	102.55
23	r	501	GDP	C8-N7-C5	2.80	107.31	102.55
24	GR	501	GTP	C2-N1-C6	-2.80	119.99	125.11
24	BL	602	GTP	C5-C6-N1	2.80	119.41	114.07
24	GT	501	GTP	C2-N1-C6	-2.80	119.99	125.11
24	Et	501	GTP	C5-C6-N1	2.80	119.41	114.07
23	As	501	GDP	C8-N7-C5	2.80	107.31	102.55
24	B3	602	GTP	C5-C6-N1	2.80	119.41	114.07
24	FP	501	GTP	C5-C6-N1	2.80	119.40	114.07
24	Fe	501	GTP	C5-C6-N1	2.80	119.40	114.07
23	E0	501	GDP	O4'-C1'-N9	2.79	112.45	108.75
23	AF	501	GDP	C8-N7-C5	2.79	107.31	102.55
24	G5	501	GTP	C5-C6-N1	2.79	119.40	114.07
24	Bw	602	GTP	C2-N1-C6	-2.79	120.00	125.11
24	FW	501	GTP	C2-N1-C6	-2.79	120.00	125.11
24	BL	602	GTP	C2-N1-C6	-2.79	120.00	125.11
24	FS	501	GTP	C5-C6-N1	2.79	119.39	114.07
24	Eg	501	GTP	C5-C6-N1	2.79	119.39	114.07
23	AV	602	GDP	C8-N7-C5	2.79	107.30	102.55
23	Bf	501	GDP	C8-N7-C5	2.79	107.30	102.55
24	G6	501	GTP	C2-N1-C6	-2.79	120.00	125.11
24	A2	602	GTP	C2-N1-C6	-2.79	120.01	125.11
24	Ff	501	GTP	C5-C6-N1	2.79	119.38	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	602	GTP	C2-N1-C6	-2.78	120.01	125.11
24	GT	501	GTP	C5-C6-N1	2.78	119.38	114.07
23	Ab	501	GDP	O4'-C1'-N9	2.78	112.44	108.75
23	Ai	501	GDP	C8-N7-C5	2.78	107.29	102.55
24	B1	602	GTP	C5-C6-N1	2.78	119.38	114.07
23	Ad	501	GDP	C8-N7-C5	2.78	107.28	102.55
24	Fd	602	GTP	C5-C6-N1	2.78	119.37	114.07
24	GP	501	GTP	C5-C6-N1	2.78	119.37	114.07
24	F6	501	GTP	C5-C6-N1	2.77	119.36	114.07
23	GX	501	GDP	O4'-C1'-N9	2.77	112.42	108.75
23	BD	501	GDP	C8-N7-C5	2.77	107.27	102.55
24	Gl	501	GTP	C5-C6-N1	2.77	119.36	114.07
24	FO	501	GTP	C5-C6-N1	2.77	119.36	114.07
24	E3	501	GTP	C5-C6-N1	2.77	119.35	114.07
23	Af	501	GDP	C8-N7-C5	2.77	107.26	102.55
23	Am	501	GDP	C8-N7-C5	2.77	107.26	102.55
24	Z	602	GTP	C4'-O4'-C1'	2.77	112.46	109.92
24	S	602	GTP	C2-N1-C6	-2.76	120.05	125.11
23	AR	501	GDP	C8-N7-C5	2.76	107.25	102.55
23	AS	502	GDP	C8-N7-C5	2.76	107.25	102.55
24	E5	501	GTP	C5-C6-N1	2.76	119.33	114.07
24	BP	602	GTP	C5-C6-N1	2.76	119.33	114.07
24	Gt	501	GTP	C5-C6-N1	2.74	119.30	114.07
24	GR	501	GTP	C4'-O4'-C1'	-2.73	107.42	109.92
23	Dv	501	GDP	C4'-O4'-C1'	-2.73	107.42	109.92
24	BI	602	GTP	C2-N1-C6	-2.73	120.11	125.11
24	FW	501	GTP	C5-C6-N1	2.73	119.28	114.07
23	FF	501	GDP	O4'-C1'-N9	2.73	112.36	108.75
24	Fb	501	GTP	C5-C6-N1	2.73	119.27	114.07
24	l	602	GTP	C5-C6-N1	2.72	119.27	114.07
24	t	602	GTP	C4'-O4'-C1'	2.72	112.41	109.92
23	AU	501	GDP	O4'-C1'-N9	2.72	112.35	108.75
24	s	602	GTP	C4'-O4'-C1'	2.71	112.41	109.92
23	AD	501	GDP	O4'-C1'-N9	2.70	112.33	108.75
23	Fu	501	GDP	O4'-C1'-N9	2.70	112.32	108.75
23	EQ	501	GDP	O4'-C1'-N9	2.69	112.32	108.75
24	GR	501	GTP	O4'-C1'-N9	2.68	112.30	108.75
23	GV	501	GDP	O4'-C1'-N9	2.67	112.28	108.75
23	GU	501	GDP	C4'-O4'-C1'	-2.66	107.49	109.92
23	DZ	501	GDP	C8-N7-C5	2.66	107.08	102.55
23	AL	501	GDP	O4'-C1'-N9	2.65	112.26	108.75
23	FN	501	GDP	O4'-C1'-N9	2.64	112.24	108.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B6	602	GTP	C4'-O4'-C1'	2.63	112.33	109.92
23	Bp	501	GDP	O4'-C1'-N9	2.63	112.23	108.75
23	7	501	GDP	O4'-C1'-N9	2.62	112.22	108.75
23	Fr	501	GDP	O4'-C1'-N9	2.62	112.22	108.75
24	5	602	GTP	C4'-O4'-C1'	2.60	112.31	109.92
23	GY	501	GDP	O4'-C1'-N9	2.59	112.19	108.75
23	AX	501	GDP	O4'-C1'-N9	2.58	112.16	108.75
24	B5	602	GTP	C4'-O4'-C1'	2.57	112.28	109.92
23	Gm	501	GDP	C4'-O4'-C1'	-2.57	107.58	109.92
24	BI	602	GTP	O4'-C1'-N9	2.55	112.13	108.75
23	FG	501	GDP	O4'-C1'-N9	2.53	112.11	108.75
24	6	602	GTP	C4'-O4'-C1'	2.52	112.24	109.92
23	ES	501	GDP	O4'-C1'-N9	2.52	112.09	108.75
23	Fo	501	GDP	O4'-C1'-N9	2.52	112.09	108.75
23	Bk	501	GDP	O4'-C1'-N9	2.52	112.09	108.75
23	Fn	501	GDP	O4'-C1'-N9	2.51	112.07	108.75
24	W	602	GTP	O3G-PG-O3B	2.50	113.01	104.64
24	BY	602	GTP	C4'-O4'-C1'	-2.50	107.64	109.92
23	EY	501	GDP	O4'-C1'-N9	2.49	112.05	108.75
23	EO	501	GDP	C4'-O4'-C1'	-2.49	107.64	109.92
23	FE	501	GDP	O4'-C1'-N9	2.49	112.05	108.75
23	AW	501	GDP	C4'-O4'-C1'	2.49	112.20	109.92
23	EQ	501	GDP	C4'-O4'-C1'	-2.49	107.65	109.92
23	AP	501	GDP	O4'-C1'-N9	2.48	112.04	108.75
23	At	501	GDP	O4'-C1'-N9	2.46	112.01	108.75
23	Dc	501	GDP	O4'-C1'-N9	2.46	112.00	108.75
23	Ec	501	GDP	C4'-O4'-C1'	-2.45	107.68	109.92
23	Br	501	GDP	C4'-O4'-C1'	2.45	112.17	109.92
24	BL	602	GTP	O3G-PG-O3B	2.44	112.83	104.64
23	A3	501	GDP	O4'-C1'-N9	2.44	111.98	108.75
23	FK	501	GDP	O4'-C1'-N9	2.44	111.98	108.75
24	CB	602	GTP	C4'-O4'-C1'	2.42	112.14	109.92
23	FC	501	GDP	O2A-PA-O3A	2.42	113.81	107.27
24	BY	602	GTP	O4'-C1'-N9	2.42	111.95	108.75
23	Bg	501	GDP	O4'-C1'-N9	2.41	111.94	108.75
23	Gf	501	GDP	C4'-O4'-C1'	-2.41	107.72	109.92
23	BH	501	GDP	C4'-O4'-C1'	2.41	112.13	109.92
23	FF	501	GDP	C4'-O4'-C1'	-2.40	107.73	109.92
24	h	602	GTP	O3G-PG-O3B	2.40	112.67	104.64
24	BQ	602	GTP	C4'-O4'-C1'	2.39	112.11	109.92
23	BZ	501	GDP	C4'-O4'-C1'	-2.37	107.75	109.92
23	Gj	501	GDP	C4'-O4'-C1'	-2.37	107.75	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	FY	501	GTP	C4'-O4'-C1'	2.37	112.09	109.92
23	EM	501	GDP	O4'-C1'-N9	2.36	111.88	108.75
23	EV	501	GDP	O2A-PA-O3A	2.36	113.65	107.27
24	E3	501	GTP	C4'-O4'-C1'	2.36	112.08	109.92
23	Ge	501	GDP	O4'-C1'-N9	2.35	111.86	108.75
23	Gb	501	GDP	O2A-PA-O3A	2.35	113.62	107.27
24	E6	602	GTP	C4'-O4'-C1'	-2.34	107.78	109.92
23	Ag	501	GDP	O4'-C1'-N9	2.34	111.85	108.75
24	S	602	GTP	O4'-C1'-N9	2.34	111.84	108.75
24	BV	602	GTP	C4'-O4'-C1'	2.33	112.06	109.92
23	Gc	501	GDP	O2A-PA-O3A	2.32	113.53	107.27
23	Ai	501	GDP	C4'-O4'-C1'	2.32	112.05	109.92
23	GH	501	GDP	O2A-PA-O3A	2.31	113.53	107.27
24	Bz	602	GTP	O3G-PG-O3B	2.31	112.37	104.64
23	BW	501	GDP	C4'-O4'-C1'	-2.31	107.81	109.92
23	De	501	GDP	O4'-C1'-N9	2.30	111.80	108.75
23	FN	501	GDP	O2A-PA-O3A	2.30	113.49	107.27
23	Di	501	GDP	O4'-C1'-N9	2.30	111.79	108.75
23	ET	501	GDP	O2A-PA-O3A	2.30	113.48	107.27
23	DY	501	GDP	O2A-PA-O3A	2.30	113.48	107.27
23	Df	501	GDP	O2A-PA-O3A	2.29	113.46	107.27
23	DR	501	GDP	O2A-PA-O3A	2.29	113.46	107.27
24	Aw	602	GTP	C4'-O4'-C1'	2.28	112.02	109.92
23	FH	501	GDP	O4'-C1'-N9	2.28	111.77	108.75
23	Ea	501	GDP	O2A-PA-O3A	2.28	113.44	107.27
23	Fs	501	GDP	O2A-PA-O3A	2.28	113.43	107.27
24	4	602	GTP	C4'-O4'-C1'	-2.28	107.84	109.92
23	GW	501	GDP	C4'-O4'-C1'	-2.27	107.84	109.92
23	DO	501	GDP	O2A-PA-O3A	2.27	113.40	107.27
23	DU	501	GDP	O2A-PA-O3A	2.26	113.38	107.27
24	z	602	GTP	C4'-O4'-C1'	2.26	111.99	109.92
23	GW	501	GDP	O2A-PA-O3A	2.26	113.37	107.27
23	EO	501	GDP	O2A-PA-O3A	2.26	113.37	107.27
24	Bw	602	GTP	O4'-C1'-N9	2.25	111.73	108.75
23	DM	501	GDP	O2A-PA-O3A	2.25	113.37	107.27
23	DL	501	GDP	O2A-PA-O3A	2.25	113.36	107.27
23	EP	501	GDP	O4'-C1'-N9	2.25	111.73	108.75
23	Bj	501	GDP	O4'-C1'-N9	2.25	111.72	108.75
23	E0	501	GDP	O2A-PA-O3A	2.24	113.34	107.27
23	FA	501	GDP	C4'-O4'-C1'	-2.24	107.87	109.92
23	EU	501	GDP	O2A-PA-O3A	2.24	113.33	107.27
23	Gd	501	GDP	O2A-PA-O3A	2.24	113.32	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AV	602	GDP	C5-C6-N1	2.23	118.33	114.07
23	De	501	GDP	O2A-PA-O3A	2.23	113.31	107.27
23	EZ	501	GDP	O4'-C1'-N9	2.23	111.70	108.75
24	d	602	GTP	C4'-O4'-C1'	2.23	111.97	109.92
23	DR	501	GDP	C5-C6-N1	2.23	118.32	114.07
23	Gk	501	GDP	O2A-PA-O3A	2.23	113.29	107.27
23	DN	501	GDP	O2A-PA-O3A	2.23	113.29	107.27
23	Fv	501	GDP	O2A-PA-O3A	2.23	113.29	107.27
23	Fx	501	GDP	O4'-C1'-N9	2.23	111.70	108.75
23	FD	501	GDP	O2A-PA-O3A	2.23	113.29	107.27
23	DR	501	GDP	C4'-O4'-C1'	-2.22	107.89	109.92
23	Bn	501	GDP	O2A-PA-O3A	2.22	113.28	107.27
23	Ft	501	GDP	O2A-PA-O3A	2.22	113.28	107.27
23	Bl	602	GDP	C8-N7-C5	2.22	106.33	102.55
23	Df	501	GDP	O4'-C1'-N9	2.22	111.69	108.75
23	Ev	501	GDP	C4'-O4'-C1'	-2.22	107.89	109.92
23	FL	501	GDP	O2A-PA-O3A	2.21	113.26	107.27
24	2	602	GTP	C4'-O4'-C1'	-2.21	107.90	109.92
23	GV	501	GDP	O2A-PA-O3A	2.20	113.22	107.27
24	Et	501	GTP	C4'-O4'-C1'	2.20	111.94	109.92
23	EL	501	GDP	O2A-PA-O3A	2.20	113.22	107.27
23	Fm	501	GDP	O2A-PA-O3A	2.20	113.22	107.27
23	Aq	501	GDP	O4'-C1'-N9	2.20	111.66	108.75
23	EQ	501	GDP	O2A-PA-O3A	2.20	113.21	107.27
24	Gx	501	GTP	C4'-O4'-C1'	2.19	111.94	109.92
23	DP	501	GDP	O2A-PA-O3A	2.19	113.20	107.27
23	F1	501	GDP	O2A-PA-O3A	2.19	113.20	107.27
23	DZ	501	GDP	O2A-PA-O3A	2.19	113.20	107.27
23	Fl	501	GDP	O2A-PA-O3A	2.19	113.19	107.27
24	t	602	GTP	O6-C6-C5	-2.19	119.98	124.32
24	q	602	GTP	C4'-O4'-C1'	2.19	111.93	109.92
24	3	602	GTP	O4'-C1'-N9	2.19	111.65	108.75
24	BX	602	GTP	O4'-C1'-N9	2.19	111.64	108.75
23	DS	501	GDP	O2A-PA-O3A	2.19	113.18	107.27
23	Dc	501	GDP	O2A-PA-O3A	2.19	113.18	107.27
23	EX	501	GDP	O4'-C1'-N9	2.19	111.64	108.75
23	AC	501	GDP	C4'-O4'-C1'	-2.18	107.93	109.92
23	Dd	501	GDP	O2A-PA-O3A	2.18	113.16	107.27
23	DZ	501	GDP	C5-C6-N1	2.17	118.22	114.07
23	Ge	501	GDP	O2A-PA-O3A	2.17	113.14	107.27
24	E6	602	GTP	O4'-C1'-N9	2.17	111.62	108.75
23	Fz	501	GDP	O4'-C1'-N9	2.17	111.62	108.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Ae	501	GDP	O2A-PA-O3A	2.17	113.13	107.27
23	Dx	501	GDP	O4'-C1'-N9	2.16	111.61	108.75
23	BF	501	GDP	O4'-C1'-N9	2.16	111.61	108.75
23	Dh	501	GDP	O2A-PA-O3A	2.16	113.11	107.27
24	BJ	602	GTP	C4'-O4'-C1'	2.16	111.90	109.92
23	FJ	501	GDP	O4'-C1'-N9	2.16	111.60	108.75
23	Di	501	GDP	O2A-PA-O3A	2.16	113.10	107.27
23	DP	501	GDP	O4'-C1'-N9	2.16	111.60	108.75
23	EL	501	GDP	O4'-C1'-N9	2.15	111.60	108.75
23	FK	501	GDP	O2A-PA-O3A	2.15	113.08	107.27
24	g	602	GTP	C4'-O4'-C1'	2.15	111.89	109.92
23	EV	501	GDP	C5-C6-N1	2.15	118.17	114.07
23	Gk	501	GDP	C5-C6-N1	2.15	118.17	114.07
23	Ad	501	GDP	C4'-O4'-C1'	2.15	111.89	109.92
23	Ec	501	GDP	O2A-PA-O3A	2.15	113.08	107.27
23	AD	501	GDP	C4'-O4'-C1'	-2.15	107.96	109.92
23	AS	502	GDP	O2A-PA-O3A	2.15	113.07	107.27
23	Fp	501	GDP	C4'-O4'-C1'	-2.14	107.96	109.92
23	Da	501	GDP	O2A-PA-O3A	2.14	113.07	107.27
24	x	501	GTP	O6-C6-C5	-2.14	120.08	124.32
24	Aw	602	GTP	O6-C6-C5	-2.14	120.08	124.32
23	BB	501	GDP	C5-C6-N1	2.14	118.14	114.07
24	AI	501	GTP	O6-C6-C5	-2.13	120.09	124.32
24	6	602	GTP	O6-C6-C5	-2.13	120.09	124.32
24	B5	602	GTP	O6-C6-C5	-2.13	120.09	124.32
24	Ey	602	GTP	O6-C6-C5	-2.13	120.09	124.32
23	EM	501	GDP	O2A-PA-O3A	2.13	113.03	107.27
24	Ay	602	GTP	O6-C6-C5	-2.13	120.10	124.32
23	Fm	501	GDP	C5-C6-N1	2.13	118.12	114.07
24	A2	602	GTP	C4'-O4'-C1'	-2.12	107.98	109.92
23	GU	501	GDP	O2A-PA-O3A	2.12	113.01	107.27
23	FN	501	GDP	C4'-O4'-C1'	-2.12	107.98	109.92
24	Eq	501	GTP	C4'-O4'-C1'	2.12	111.87	109.92
24	w	602	GTP	O6-C6-C5	-2.12	120.12	124.32
24	V	602	GTP	C4'-O4'-C1'	2.12	111.86	109.92
23	Eb	501	GDP	O4'-C1'-N9	2.12	111.55	108.75
23	Gd	501	GDP	C5-C6-N1	2.11	118.10	114.07
23	Db	501	GDP	O2A-PA-O3A	2.11	112.98	107.27
24	BV	602	GTP	O6-C6-C5	-2.11	120.14	124.32
24	B6	602	GTP	O6-C6-C5	-2.11	120.14	124.32
24	Fj	501	GTP	O6-C6-C5	-2.11	120.14	124.32
23	Bl	602	GDP	O6-C6-C5	-2.11	120.14	124.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Fm	501	GDP	O4'-C1'-N9	2.11	111.54	108.75
23	GY	501	GDP	C5-C6-N1	2.10	118.08	114.07
23	r	501	GDP	C5-C6-N1	2.10	118.08	114.07
24	Al	602	GTP	C4'-O4'-C1'	2.10	111.85	109.92
23	Dj	501	GDP	O2A-PA-O3A	2.10	112.95	107.27
24	G3	602	GTP	O6-C6-C5	-2.10	120.16	124.32
23	DQ	501	GDP	O2A-PA-O3A	2.10	112.95	107.27
24	Aj	501	GTP	O6-C6-C5	-2.10	120.16	124.32
24	B0	501	GTP	O6-C6-C5	-2.10	120.16	124.32
23	Dg	501	GDP	O2A-PA-O3A	2.10	112.94	107.27
23	EP	501	GDP	O2A-PA-O3A	2.10	112.94	107.27
24	T	602	GTP	O6-C6-C5	-2.09	120.17	124.32
23	EY	501	GDP	O2A-PA-O3A	2.09	112.93	107.27
23	FG	501	GDP	O2A-PA-O3A	2.09	112.93	107.27
24	F8	501	GTP	O6-C6-C5	-2.09	120.17	124.32
23	DV	501	GDP	O2A-PA-O3A	2.09	112.92	107.27
24	s	602	GTP	O6-C6-C5	-2.09	120.18	124.32
23	EX	501	GDP	O2A-PA-O3A	2.09	112.91	107.27
23	GY	501	GDP	O2A-PA-O3A	2.09	112.91	107.27
23	7	501	GDP	C5-C6-N1	2.08	118.05	114.07
23	Aa	501	GDP	C5-C6-N1	2.08	118.04	114.07
24	Gw	501	GTP	O6-C6-C5	-2.08	120.20	124.32
24	Eq	501	GTP	O6-C6-C5	-2.08	120.20	124.32
24	BK	602	GTP	O6-C6-C5	-2.08	120.20	124.32
23	Gj	501	GDP	O2A-PA-O3A	2.07	112.88	107.27
23	Ed	501	GDP	O2A-PA-O3A	2.07	112.88	107.27
23	ER	501	GDP	C5-C6-N1	2.07	118.03	114.07
23	Ab	501	GDP	C4'-O4'-C1'	-2.07	108.03	109.92
23	DT	501	GDP	O2A-PA-O3A	2.07	112.87	107.27
24	z	602	GTP	O6-C6-C5	-2.07	120.21	124.32
24	W	602	GTP	O6-C6-C5	-2.07	120.22	124.32
24	AK	602	GTP	O6-C6-C5	-2.07	120.22	124.32
23	Dv	501	GDP	O2A-PA-O3A	2.07	112.87	107.27
24	F7	501	GTP	O6-C6-C5	-2.07	120.22	124.32
23	Ev	501	GDP	C5-C6-N1	2.07	118.02	114.07
24	5	602	GTP	O6-C6-C5	-2.07	120.22	124.32
23	F4	501	GDP	O2A-PA-O3A	2.07	112.86	107.27
23	De	501	GDP	C5-C6-N1	2.07	118.01	114.07
23	Gh	501	GDP	O2A-PA-O3A	2.07	112.86	107.27
24	Ey	602	GTP	C4'-O4'-C1'	2.06	111.81	109.92
24	q	602	GTP	O6-C6-C5	-2.06	120.23	124.32
23	EN	501	GDP	C5-C6-N1	2.06	118.00	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Ef	501	GDP	O2A-PA-O3A	2.06	112.84	107.27
23	BZ	501	GDP	C5-C6-N1	2.06	118.00	114.07
23	Fy	501	GDP	O2A-PA-O3A	2.06	112.84	107.27
24	4	602	GTP	O4'-C1'-N9	2.06	111.48	108.75
24	2	602	GTP	O4'-C1'-N9	2.06	111.47	108.75
23	Fw	501	GDP	C5-C6-N1	2.06	118.00	114.07
23	Dq	501	GDP	C5-C6-N1	2.06	118.00	114.07
23	Fo	501	GDP	C5-C6-N1	2.06	117.99	114.07
23	AX	501	GDP	C5-C6-N1	2.06	117.99	114.07
23	BD	501	GDP	O2A-PA-O3A	2.05	112.83	107.27
23	A0	501	GDP	C5-C6-N1	2.05	117.99	114.07
23	Bq	602	GDP	C5-C6-N1	2.05	117.99	114.07
23	Dd	501	GDP	C5-C6-N1	2.05	117.99	114.07
23	Av	501	GDP	C5-C6-N1	2.05	117.99	114.07
23	Am	501	GDP	C5-C6-N1	2.05	117.99	114.07
23	BW	501	GDP	C5-C6-N1	2.05	117.99	114.07
23	AU	501	GDP	C4'-O4'-C1'	-2.05	108.05	109.92
23	F1	501	GDP	C4'-O4'-C1'	-2.05	108.05	109.92
23	Fs	501	GDP	C5-C6-N1	2.05	117.98	114.07
23	AO	501	GDP	C5-C6-N1	2.05	117.98	114.07
24	GC	501	GTP	O6-C6-C5	-2.05	120.26	124.32
23	Ga	501	GDP	C5-C6-N1	2.05	117.98	114.07
23	n	501	GDP	C5-C6-N1	2.05	117.98	114.07
24	BL	602	GTP	C4'-O4'-C1'	-2.05	108.05	109.92
24	GO	602	GTP	O6-C6-C5	-2.05	120.26	124.32
24	BT	501	GTP	O6-C6-C5	-2.05	120.26	124.32
24	Ej	501	GTP	O6-C6-C5	-2.05	120.26	124.32
23	AD	501	GDP	C5-C6-N1	2.05	117.98	114.07
23	Bl	602	GDP	C5-C6-N1	2.05	117.98	114.07
24	Gx	501	GTP	O6-C6-C5	-2.05	120.26	124.32
24	d	602	GTP	O6-C6-C5	-2.05	120.26	124.32
24	FM	501	GTP	O6-C6-C5	-2.05	120.27	124.32
23	Dt	501	GDP	C5-C6-N1	2.05	117.97	114.07
24	BY	602	GTP	O2B-PB-O3A	2.05	112.80	107.27
24	Go	501	GTP	O6-C6-C5	-2.04	120.27	124.32
24	BM	602	GTP	O6-C6-C5	-2.04	120.27	124.32
23	Ev	501	GDP	O2A-PA-O3A	2.04	112.80	107.27
23	Bb	501	GDP	C5-C6-N1	2.04	117.97	114.07
24	BQ	602	GTP	O6-C6-C5	-2.04	120.27	124.32
24	F3	501	GTP	O6-C6-C5	-2.04	120.27	124.32
24	Bx	602	GTP	O6-C6-C5	-2.04	120.27	124.32
23	AB	501	GDP	C5-C6-N1	2.04	117.96	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Gz	501	GTP	O6-C6-C5	-2.04	120.28	124.32
23	FE	501	GDP	C5-C6-N1	2.04	117.96	114.07
24	GN	501	GTP	O6-C6-C5	-2.04	120.28	124.32
23	Dw	501	GDP	C5-C6-N1	2.04	117.96	114.07
23	EQ	501	GDP	C5-C6-N1	2.04	117.96	114.07
23	GW	501	GDP	C5-C6-N1	2.04	117.96	114.07
23	Ge	501	GDP	C5-C6-N1	2.04	117.96	114.07
23	DU	501	GDP	C5-C6-N1	2.04	117.96	114.07
24	E7	501	GTP	C4'-O4'-C1'	2.04	111.79	109.92
23	AM	501	GDP	C5-C6-N1	2.04	117.95	114.07
23	Ac	501	GDP	C5-C6-N1	2.04	117.95	114.07
24	Es	501	GTP	O6-C6-C5	-2.04	120.28	124.32
23	Fl	501	GDP	C5-C6-N1	2.04	117.95	114.07
23	AZ	501	GDP	C5-C6-N1	2.04	117.95	114.07
24	B2	602	GTP	O6-C6-C5	-2.04	120.29	124.32
24	GE	501	GTP	O6-C6-C5	-2.03	120.29	124.32
24	o	501	GTP	O6-C6-C5	-2.03	120.29	124.32
24	GN	501	GTP	C4'-O4'-C1'	2.03	111.79	109.92
23	EM	501	GDP	C5-C6-N1	2.03	117.95	114.07
24	BR	501	GTP	O6-C6-C5	-2.03	120.29	124.32
23	8	501	GDP	C5-C6-N1	2.03	117.95	114.07
23	A3	501	GDP	C5-C6-N1	2.03	117.95	114.07
24	FX	501	GTP	O6-C6-C5	-2.03	120.29	124.32
24	Bz	602	GTP	O6-C6-C5	-2.03	120.29	124.32
24	E5	501	GTP	C2'-C3'-C4'	2.03	106.53	102.61
24	GI	501	GTP	O6-C6-C5	-2.03	120.29	124.32
24	A1	602	GTP	O2B-PB-O3A	2.03	112.76	107.27
24	By	602	GTP	C4'-O4'-C1'	2.03	111.78	109.92
23	Bs	501	GDP	C5-C6-N1	2.03	117.94	114.07
23	Dr	501	GDP	C5-C6-N1	2.03	117.94	114.07
24	F5	501	GTP	O6-C6-C5	-2.03	120.30	124.32
23	Fw	501	GDP	O2A-PA-O3A	2.03	112.76	107.27
23	E9	501	GDP	C5-C6-N1	2.03	117.94	114.07
23	EN	501	GDP	O2A-PA-O3A	2.03	112.76	107.27
23	Dk	501	GDP	O2A-PA-O3A	2.03	112.76	107.27
23	DL	501	GDP	C5-C6-N1	2.03	117.94	114.07
23	Gf	501	GDP	O2A-PA-O3A	2.03	112.75	107.27
23	DS	501	GDP	C5-C6-N1	2.03	117.94	114.07
24	GD	501	GTP	O6-C6-C5	-2.03	120.30	124.32
24	h	602	GTP	O6-C6-C5	-2.03	120.30	124.32
23	Gc	501	GDP	C5-C6-N1	2.03	117.93	114.07
23	AC	501	GDP	C5-C6-N1	2.03	117.93	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	501	GDP	C5-C6-N1	2.02	117.93	114.07
23	Dh	501	GDP	C5-C6-N1	2.02	117.93	114.07
24	GS	501	GTP	O6-C6-C5	-2.02	120.31	124.32
24	Ax	602	GTP	O6-C6-C5	-2.02	120.31	124.32
23	DL	501	GDP	O4'-C1'-N9	2.02	111.43	108.75
24	g	602	GTP	O6-C6-C5	-2.02	120.31	124.32
24	CB	602	GTP	O6-C6-C5	-2.02	120.31	124.32
23	Fn	501	GDP	C5-C6-N1	2.02	117.93	114.07
24	B7	501	GTP	O6-C6-C5	-2.02	120.31	124.32
24	u	501	GTP	O6-C6-C5	-2.02	120.31	124.32
24	E3	501	GTP	O6-C6-C5	-2.02	120.31	124.32
24	E7	501	GTP	O6-C6-C5	-2.02	120.31	124.32
24	G1	501	GTP	O6-C6-C5	-2.02	120.31	124.32
23	AE	501	GDP	C5-C6-N1	2.02	117.93	114.07
24	Gy	501	GTP	O6-C6-C5	-2.02	120.31	124.32
23	AA	501	GDP	C2'-C3'-C4'	2.02	106.51	102.61
24	AS	501	GTP	O6-C6-C5	-2.02	120.31	124.32
23	Ec	501	GDP	C5-C6-N1	2.02	117.92	114.07
23	E9	501	GDP	C4'-O4'-C1'	-2.02	108.08	109.92
23	Az	501	GDP	C5-C6-N1	2.02	117.92	114.07
24	B1	602	GTP	O6-C6-C5	-2.02	120.32	124.32
24	FY	501	GTP	O6-C6-C5	-2.02	120.32	124.32
23	AL	501	GDP	C5-C6-N1	2.02	117.92	114.07
23	DQ	501	GDP	C5-C6-N1	2.02	117.92	114.07
23	Da	501	GDP	C5-C6-N1	2.02	117.92	114.07
23	Df	501	GDP	C5-C6-N1	2.02	117.92	114.07
23	AS	502	GDP	C5-C6-N1	2.02	117.92	114.07
23	Bh	501	GDP	C5-C6-N1	2.02	117.92	114.07
24	GB	501	GTP	O6-C6-C5	-2.02	120.32	124.32
23	EU	501	GDP	C5-C6-N1	2.02	117.92	114.07
23	FJ	501	GDP	C5-C6-N1	2.02	117.92	114.07
23	Be	501	GDP	C5-C6-N1	2.02	117.91	114.07
23	Bp	501	GDP	C5-C6-N1	2.02	117.91	114.07
23	Gk	501	GDP	O6-C6-C5	-2.02	120.33	124.32
24	BY	602	GTP	O6-C6-C5	-2.02	120.33	124.32
23	An	501	GDP	C5-C6-N1	2.01	117.91	114.07
23	Du	501	GDP	C5-C6-N1	2.01	117.91	114.07
24	BL	602	GTP	O6-C6-C5	-2.01	120.33	124.32
24	GM	501	GTP	O6-C6-C5	-2.01	120.33	124.32
23	Dc	501	GDP	C5-C6-N1	2.01	117.91	114.07
24	FZ	501	GTP	O6-C6-C5	-2.01	120.33	124.32
23	Au	602	GDP	C5-C6-N1	2.01	117.91	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Bk	501	GDP	C5-C6-N1	2.01	117.91	114.07
24	p	602	GTP	O6-C6-C5	-2.01	120.33	124.32
24	B9	602	GTP	O6-C6-C5	-2.01	120.33	124.32
23	Bg	501	GDP	C5-C6-N1	2.01	117.91	114.07
23	DV	501	GDP	C5-C6-N1	2.01	117.91	114.07
24	BJ	602	GTP	O6-C6-C5	-2.01	120.33	124.32
24	By	602	GTP	O6-C6-C5	-2.01	120.33	124.32
23	BA	501	GDP	C5-C6-N1	2.01	117.91	114.07
23	Fq	501	GDP	O2A-PA-O3A	2.01	112.71	107.27
23	E0	501	GDP	C5-C6-N1	2.01	117.91	114.07
23	DY	501	GDP	C5-C6-N1	2.01	117.90	114.07
24	GK	501	GTP	O6-C6-C5	-2.01	120.34	124.32
24	GL	501	GTP	O6-C6-C5	-2.01	120.34	124.32
23	Gf	501	GDP	C5-C6-N1	2.01	117.90	114.07
23	DN	501	GDP	C5-C6-N1	2.01	117.90	114.07
23	FA	501	GDP	C5-C6-N1	2.01	117.90	114.07
23	FE	501	GDP	O2A-PA-O3A	2.01	112.70	107.27
24	GA	501	GTP	O6-C6-C5	-2.01	120.34	124.32
23	AN	501	GDP	C5-C6-N1	2.01	117.90	114.07
24	GT	501	GTP	O6-C6-C5	-2.01	120.34	124.32
23	Gb	501	GDP	C5-C6-N1	2.01	117.90	114.07
24	BO	602	GTP	O6-C6-C5	-2.01	120.34	124.32
24	Fa	501	GTP	O6-C6-C5	-2.01	120.34	124.32
24	Gu	501	GTP	O6-C6-C5	-2.01	120.34	124.32
24	BN	602	GTP	O6-C6-C5	-2.01	120.34	124.32
24	GJ	501	GTP	O6-C6-C5	-2.00	120.35	124.32
24	Ak	602	GTP	O6-C6-C5	-2.00	120.35	124.32
24	4	602	GTP	O6-C6-C5	-2.00	120.35	124.32
24	v	602	GTP	O6-C6-C5	-2.00	120.35	124.32
23	Bi	501	GDP	C5-C6-N1	2.00	117.89	114.07
23	EP	501	GDP	C5-C6-N1	2.00	117.89	114.07
23	Bf	501	GDP	C5-C6-N1	2.00	117.89	114.07
23	EO	501	GDP	C5-C6-N1	2.00	117.89	114.07
24	y	602	GTP	O6-C6-C5	-2.00	120.35	124.32
24	Eh	501	GTP	O6-C6-C5	-2.00	120.35	124.32
23	Ba	501	GDP	C5-C6-N1	2.00	117.89	114.07

There are no chirality outliers.

All (1688) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	0	501	GDP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	0	501	GDP	C5'-O5'-PA-O3A
23	0	501	GDP	C5'-O5'-PA-O1A
23	0	501	GDP	C5'-O5'-PA-O2A
23	Fo	501	GDP	PA-O3A-PB-O3B
23	Fq	501	GDP	PA-O3A-PB-O2B
23	Fq	501	GDP	C5'-O5'-PA-O3A
23	Fq	501	GDP	C5'-O5'-PA-O2A
23	Fs	501	GDP	C5'-O5'-PA-O3A
23	Fs	501	GDP	C5'-O5'-PA-O1A
23	Fs	501	GDP	C5'-O5'-PA-O2A
23	A0	501	GDP	C5'-O5'-PA-O3A
23	Ft	501	GDP	C5'-O5'-PA-O3A
23	Ft	501	GDP	C5'-O5'-PA-O1A
23	Ft	501	GDP	C5'-O5'-PA-O2A
23	Fu	501	GDP	PA-O3A-PB-O3B
23	Fw	501	GDP	C5'-O5'-PA-O3A
23	Fw	501	GDP	C5'-O5'-PA-O1A
23	Fw	501	GDP	C5'-O5'-PA-O2A
23	Fx	501	GDP	PA-O3A-PB-O2B
23	Fx	501	GDP	C5'-O5'-PA-O3A
23	Fx	501	GDP	C5'-O5'-PA-O1A
23	Fx	501	GDP	C5'-O5'-PA-O2A
23	Fx	501	GDP	O4'-C4'-C5'-O5'
23	Fy	501	GDP	C5'-O5'-PA-O3A
23	Fy	501	GDP	C5'-O5'-PA-O1A
23	Fy	501	GDP	C5'-O5'-PA-O2A
23	Fz	501	GDP	C5'-O5'-PA-O3A
23	Fz	501	GDP	C5'-O5'-PA-O1A
23	Fz	501	GDP	C5'-O5'-PA-O2A
23	Fz	501	GDP	O4'-C4'-C5'-O5'
23	Ga	501	GDP	PA-O3A-PB-O3B
23	Gb	501	GDP	PA-O3A-PB-O3B
23	Gb	501	GDP	C5'-O5'-PA-O3A
23	Gb	501	GDP	C5'-O5'-PA-O1A
23	Gb	501	GDP	C5'-O5'-PA-O2A
23	Gb	501	GDP	O4'-C4'-C5'-O5'
23	Gc	501	GDP	C5'-O5'-PA-O3A
23	Gc	501	GDP	C5'-O5'-PA-O1A
23	Gc	501	GDP	C5'-O5'-PA-O2A
23	Gg	501	GDP	PA-O3A-PB-O2B
23	Gg	501	GDP	C5'-O5'-PA-O3A
23	Gg	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Gg	501	GDP	C5'-O5'-PA-O2A
23	Gg	501	GDP	O4'-C4'-C5'-O5'
23	Gh	501	GDP	C5'-O5'-PA-O3A
23	Gh	501	GDP	C5'-O5'-PA-O1A
23	Gh	501	GDP	C5'-O5'-PA-O2A
23	Gi	501	GDP	C5'-O5'-PA-O3A
23	Gi	501	GDP	C5'-O5'-PA-O1A
23	Gi	501	GDP	C5'-O5'-PA-O2A
23	Gi	501	GDP	O4'-C4'-C5'-O5'
23	Gj	501	GDP	PA-O3A-PB-O2B
23	Gj	501	GDP	C5'-O5'-PA-O3A
23	Gj	501	GDP	C5'-O5'-PA-O1A
23	Gj	501	GDP	C5'-O5'-PA-O2A
23	Gj	501	GDP	O4'-C4'-C5'-O5'
23	Gm	501	GDP	C5'-O5'-PA-O2A
23	O	501	GDP	C5'-O5'-PA-O3A
23	O	501	GDP	C5'-O5'-PA-O2A
23	P	501	GDP	C5'-O5'-PA-O3A
23	P	501	GDP	C5'-O5'-PA-O2A
23	U	501	GDP	C5'-O5'-PA-O3A
23	U	501	GDP	C5'-O5'-PA-O2A
23	X	501	GDP	C5'-O5'-PA-O3A
23	X	501	GDP	C5'-O5'-PA-O2A
23	m	501	GDP	C5'-O5'-PA-O3A
23	m	501	GDP	C5'-O5'-PA-O2A
23	n	501	GDP	C5'-O5'-PA-O3A
23	n	501	GDP	C5'-O5'-PA-O2A
23	r	501	GDP	C5'-O5'-PA-O3A
23	r	501	GDP	C5'-O5'-PA-O2A
23	AA	501	GDP	C5'-O5'-PA-O3A
23	AC	501	GDP	PB-O3A-PA-O5'
23	AC	501	GDP	C5'-O5'-PA-O3A
23	AC	501	GDP	C5'-O5'-PA-O2A
23	AD	501	GDP	PB-O3A-PA-O5'
23	AE	501	GDP	C5'-O5'-PA-O3A
23	AF	501	GDP	C5'-O5'-PA-O3A
23	AF	501	GDP	C5'-O5'-PA-O1A
23	AF	501	GDP	C5'-O5'-PA-O2A
23	AG	501	GDP	C5'-O5'-PA-O3A
23	AH	501	GDP	C5'-O5'-PA-O3A
23	AH	501	GDP	C5'-O5'-PA-O1A
23	AH	501	GDP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	AL	501	GDP	C5'-O5'-PA-O3A
23	AL	501	GDP	C5'-O5'-PA-O1A
23	AL	501	GDP	O4'-C4'-C5'-O5'
23	AM	501	GDP	C5'-O5'-PA-O3A
23	AM	501	GDP	C5'-O5'-PA-O2A
23	AN	501	GDP	C5'-O5'-PA-O1A
23	AO	501	GDP	C5'-O5'-PA-O1A
23	AP	501	GDP	C5'-O5'-PA-O3A
23	AP	501	GDP	C5'-O5'-PA-O1A
23	AP	501	GDP	C5'-O5'-PA-O2A
23	AQ	501	GDP	PA-O3A-PB-O3B
23	AR	501	GDP	PA-O3A-PB-O3B
23	AR	501	GDP	C5'-O5'-PA-O3A
23	AR	501	GDP	C5'-O5'-PA-O1A
23	AR	501	GDP	C5'-O5'-PA-O2A
23	AR	501	GDP	O4'-C4'-C5'-O5'
23	AS	502	GDP	C5'-O5'-PA-O3A
23	AS	502	GDP	C5'-O5'-PA-O2A
23	AT	501	GDP	C5'-O5'-PA-O1A
23	AV	602	GDP	C5'-O5'-PA-O1A
23	AW	501	GDP	PA-O3A-PB-O3B
23	AW	501	GDP	C5'-O5'-PA-O3A
23	AW	501	GDP	C5'-O5'-PA-O1A
23	AW	501	GDP	C5'-O5'-PA-O2A
23	AX	501	GDP	C5'-O5'-PA-O3A
23	AX	501	GDP	C5'-O5'-PA-O1A
23	AX	501	GDP	O4'-C4'-C5'-O5'
23	AY	501	GDP	C5'-O5'-PA-O3A
23	AY	501	GDP	C5'-O5'-PA-O2A
23	AZ	501	GDP	C5'-O5'-PA-O1A
23	Aa	501	GDP	C5'-O5'-PA-O3A
23	Aa	501	GDP	C5'-O5'-PA-O1A
23	Aa	501	GDP	O4'-C4'-C5'-O5'
23	Ab	501	GDP	C5'-O5'-PA-O3A
23	Ab	501	GDP	C5'-O5'-PA-O2A
23	Ad	501	GDP	PA-O3A-PB-O3B
23	Ad	501	GDP	C5'-O5'-PA-O3A
23	Ad	501	GDP	C5'-O5'-PA-O1A
23	Ad	501	GDP	C5'-O5'-PA-O2A
23	Ae	501	GDP	C5'-O5'-PA-O3A
23	Af	501	GDP	C5'-O5'-PA-O3A
23	Af	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Ai	501	GDP	PA-O3A-PB-O3B
23	Ai	501	GDP	C5'-O5'-PA-O3A
23	Ai	501	GDP	C5'-O5'-PA-O2A
23	An	501	GDP	C5'-O5'-PA-O3A
23	Ao	501	GDP	C5'-O5'-PA-O3A
23	Ao	501	GDP	C5'-O5'-PA-O1A
23	Ao	501	GDP	C5'-O5'-PA-O2A
23	Ap	501	GDP	C5'-O5'-PA-O3A
23	Aq	501	GDP	C5'-O5'-PA-O3A
23	Aq	501	GDP	O4'-C4'-C5'-O5'
23	Ar	501	GDP	C5'-O5'-PA-O3A
23	As	501	GDP	C5'-O5'-PA-O1A
23	At	501	GDP	C5'-O5'-PA-O2A
23	Av	501	GDP	PA-O3A-PB-O3B
23	Az	501	GDP	PB-O3A-PA-O5'
23	Az	501	GDP	O4'-C4'-C5'-O5'
23	BA	501	GDP	C5'-O5'-PA-O3A
23	BA	501	GDP	C5'-O5'-PA-O1A
23	BA	501	GDP	C5'-O5'-PA-O2A
23	BB	501	GDP	C5'-O5'-PA-O3A
23	BB	501	GDP	O4'-C4'-C5'-O5'
23	BB	501	GDP	C3'-C4'-C5'-O5'
23	BC	501	GDP	PA-O3A-PB-O3B
23	BC	501	GDP	C3'-C4'-C5'-O5'
23	BD	501	GDP	C5'-O5'-PA-O3A
23	BD	501	GDP	C5'-O5'-PA-O2A
23	BE	501	GDP	C5'-O5'-PA-O3A
23	BE	501	GDP	C5'-O5'-PA-O1A
23	BG	501	GDP	PA-O3A-PB-O3B
23	BH	501	GDP	PA-O3A-PB-O3B
23	BH	501	GDP	C5'-O5'-PA-O3A
23	BH	501	GDP	C5'-O5'-PA-O2A
23	BZ	501	GDP	C5'-O5'-PA-O3A
23	Ba	501	GDP	C5'-O5'-PA-O3A
23	Bb	501	GDP	C5'-O5'-PA-O3A
23	Bb	501	GDP	C5'-O5'-PA-O1A
23	Bb	501	GDP	C5'-O5'-PA-O2A
23	Be	501	GDP	C5'-O5'-PA-O3A
23	Be	501	GDP	C5'-O5'-PA-O2A
23	Bf	501	GDP	C5'-O5'-PA-O3A
23	Bf	501	GDP	C5'-O5'-PA-O1A
23	Bf	501	GDP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Bg	501	GDP	C5'-O5'-PA-O3A
23	Bg	501	GDP	C5'-O5'-PA-O1A
23	Bg	501	GDP	O4'-C4'-C5'-O5'
23	Bh	501	GDP	C5'-O5'-PA-O3A
23	Bi	501	GDP	C5'-O5'-PA-O1A
23	Bk	501	GDP	C5'-O5'-PA-O3A
23	Bk	501	GDP	C5'-O5'-PA-O2A
23	Bl	602	GDP	PA-O3A-PB-O3B
23	Bm	501	GDP	PA-O3A-PB-O3B
23	Bn	501	GDP	C5'-O5'-PA-O3A
23	Bo	501	GDP	C5'-O5'-PA-O3A
23	Bo	501	GDP	C5'-O5'-PA-O1A
23	Bq	602	GDP	PA-O3A-PB-O3B
23	Br	501	GDP	PA-O3A-PB-O3B
23	Br	501	GDP	C5'-O5'-PA-O3A
23	Br	501	GDP	C5'-O5'-PA-O2A
23	Bs	501	GDP	C5'-O5'-PA-O3A
23	Bs	501	GDP	C5'-O5'-PA-O1A
23	Bs	501	GDP	C5'-O5'-PA-O2A
23	Bt	501	GDP	C5'-O5'-PA-O3A
23	Bt	501	GDP	C5'-O5'-PA-O2A
23	DL	501	GDP	C5'-O5'-PA-O3A
23	DL	501	GDP	C5'-O5'-PA-O2A
23	DM	501	GDP	PA-O3A-PB-O3B
23	DM	501	GDP	C5'-O5'-PA-O3A
23	DM	501	GDP	C5'-O5'-PA-O2A
23	DN	501	GDP	C5'-O5'-PA-O3A
23	DN	501	GDP	C5'-O5'-PA-O2A
23	DO	501	GDP	PA-O3A-PB-O3B
23	DO	501	GDP	C5'-O5'-PA-O3A
23	DO	501	GDP	C5'-O5'-PA-O2A
23	DR	501	GDP	PA-O3A-PB-O3B
23	DS	501	GDP	PA-O3A-PB-O3B
23	DS	501	GDP	C5'-O5'-PA-O3A
23	DS	501	GDP	C5'-O5'-PA-O2A
23	DU	501	GDP	PA-O3A-PB-O3B
23	DV	501	GDP	C5'-O5'-PA-O3A
23	DV	501	GDP	C5'-O5'-PA-O2A
23	DW	501	GDP	PA-O3A-PB-O3B
23	DW	501	GDP	C5'-O5'-PA-O3A
23	DW	501	GDP	C5'-O5'-PA-O2A
23	DY	501	GDP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	DY	501	GDP	C5'-O5'-PA-O3A
23	DY	501	GDP	C5'-O5'-PA-O2A
23	Da	501	GDP	C5'-O5'-PA-O3A
23	Da	501	GDP	C5'-O5'-PA-O2A
23	Db	501	GDP	C5'-O5'-PA-O3A
23	Db	501	GDP	C5'-O5'-PA-O2A
23	Dd	501	GDP	C5'-O5'-PA-O3A
23	Dd	501	GDP	C5'-O5'-PA-O2A
23	Dg	501	GDP	PA-O3A-PB-O3B
23	Dh	501	GDP	PA-O3A-PB-O3B
23	Di	501	GDP	C5'-O5'-PA-O3A
23	Di	501	GDP	C5'-O5'-PA-O1A
23	Di	501	GDP	C5'-O5'-PA-O2A
23	Di	501	GDP	O4'-C4'-C5'-O5'
23	Dj	501	GDP	PA-O3A-PB-O3B
23	Dj	501	GDP	C5'-O5'-PA-O3A
23	Dj	501	GDP	C5'-O5'-PA-O2A
23	Dj	501	GDP	O4'-C4'-C5'-O5'
23	Dk	501	GDP	C5'-O5'-PA-O3A
23	Dk	501	GDP	C5'-O5'-PA-O2A
23	Dq	501	GDP	PA-O3A-PB-O3B
23	E0	501	GDP	PA-O3A-PB-O2B
23	E9	501	GDP	PA-O3A-PB-O3B
23	E9	501	GDP	O4'-C4'-C5'-O5'
23	ET	501	GDP	C5'-O5'-PA-O3A
23	ET	501	GDP	C5'-O5'-PA-O1A
23	ET	501	GDP	C5'-O5'-PA-O2A
23	EU	501	GDP	PA-O3A-PB-O3B
23	EU	501	GDP	C5'-O5'-PA-O3A
23	EU	501	GDP	C5'-O5'-PA-O1A
23	EU	501	GDP	C5'-O5'-PA-O2A
23	EW	501	GDP	C5'-O5'-PA-O3A
23	EW	501	GDP	C5'-O5'-PA-O2A
23	EY	501	GDP	C5'-O5'-PA-O3A
23	EY	501	GDP	C5'-O5'-PA-O2A
23	EZ	501	GDP	PA-O3A-PB-O2B
23	EZ	501	GDP	C5'-O5'-PA-O3A
23	EZ	501	GDP	C5'-O5'-PA-O1A
23	EZ	501	GDP	C5'-O5'-PA-O2A
23	EZ	501	GDP	O4'-C4'-C5'-O5'
23	Ea	501	GDP	C5'-O5'-PA-O3A
23	Ea	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Ea	501	GDP	C5'-O5'-PA-O2A
23	Eb	501	GDP	PA-O3A-PB-O2B
23	Eb	501	GDP	C5'-O5'-PA-O3A
23	Eb	501	GDP	C5'-O5'-PA-O1A
23	Eb	501	GDP	C5'-O5'-PA-O2A
23	Ec	501	GDP	PA-O3A-PB-O2B
23	Ed	501	GDP	C5'-O5'-PA-O3A
23	Ed	501	GDP	C5'-O5'-PA-O1A
23	Ed	501	GDP	C5'-O5'-PA-O2A
23	Ef	501	GDP	C5'-O5'-PA-O3A
23	Ef	501	GDP	C5'-O5'-PA-O1A
23	Ef	501	GDP	C5'-O5'-PA-O2A
23	Ev	501	GDP	PA-O3A-PB-O3B
23	F1	501	GDP	PA-O3A-PB-O2B
23	F1	501	GDP	C5'-O5'-PA-O3A
23	F1	501	GDP	C5'-O5'-PA-O1A
23	F1	501	GDP	C5'-O5'-PA-O2A
23	F1	501	GDP	O4'-C4'-C5'-O5'
23	F2	501	GDP	C5'-O5'-PA-O3A
23	F2	501	GDP	C5'-O5'-PA-O1A
23	F2	501	GDP	C5'-O5'-PA-O2A
23	8	501	GDP	C5'-O5'-PA-O3A
23	F4	501	GDP	C5'-O5'-PA-O3A
23	F4	501	GDP	C5'-O5'-PA-O1A
23	F4	501	GDP	C5'-O5'-PA-O2A
23	FC	501	GDP	PA-O3A-PB-O3B
23	FD	501	GDP	PA-O3A-PB-O3B
23	FD	501	GDP	C5'-O5'-PA-O3A
23	FD	501	GDP	C5'-O5'-PA-O1A
23	FD	501	GDP	C5'-O5'-PA-O2A
23	FF	501	GDP	PA-O3A-PB-O2B
23	FF	501	GDP	C5'-O5'-PA-O3A
23	FF	501	GDP	C5'-O5'-PA-O2A
23	FH	501	GDP	PA-O3A-PB-O2B
23	FH	501	GDP	C5'-O5'-PA-O3A
23	FH	501	GDP	C5'-O5'-PA-O1A
23	FH	501	GDP	C5'-O5'-PA-O2A
23	FH	501	GDP	O4'-C4'-C5'-O5'
23	FI	501	GDP	C5'-O5'-PA-O3A
23	FI	501	GDP	C5'-O5'-PA-O1A
23	FI	501	GDP	C5'-O5'-PA-O2A
23	FJ	501	GDP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	FJ	501	GDP	C5'-O5'-PA-O3A
23	FJ	501	GDP	C5'-O5'-PA-O1A
23	FJ	501	GDP	C5'-O5'-PA-O2A
23	FK	501	GDP	C5'-O5'-PA-O3A
23	FK	501	GDP	O4'-C4'-C5'-O5'
23	FK	501	GDP	C3'-C4'-C5'-O5'
23	FL	501	GDP	C5'-O5'-PA-O3A
23	FL	501	GDP	C5'-O5'-PA-O1A
23	FL	501	GDP	C5'-O5'-PA-O2A
23	9	501	GDP	C5'-O5'-PA-O3A
23	9	501	GDP	C5'-O5'-PA-O1A
23	9	501	GDP	C5'-O5'-PA-O2A
24	Fk	501	GTP	C5'-O5'-PA-O3A
24	Fk	501	GTP	C5'-O5'-PA-O1A
24	G1	501	GTP	C5'-O5'-PA-O3A
24	G4	602	GTP	C5'-O5'-PA-O3A
24	G4	602	GTP	C5'-O5'-PA-O1A
24	G6	501	GTP	C5'-O5'-PA-O3A
24	G6	501	GTP	C5'-O5'-PA-O1A
24	GA	501	GTP	C5'-O5'-PA-O3A
24	GA	501	GTP	C5'-O5'-PA-O1A
24	GB	501	GTP	C5'-O5'-PA-O3A
24	GC	501	GTP	C5'-O5'-PA-O3A
24	GC	501	GTP	C5'-O5'-PA-O1A
24	A1	602	GTP	O4'-C4'-C5'-O5'
24	A1	602	GTP	C3'-C4'-C5'-O5'
24	GG	501	GTP	C5'-O5'-PA-O3A
24	GI	501	GTP	C5'-O5'-PA-O3A
24	GI	501	GTP	C5'-O5'-PA-O1A
24	GJ	501	GTP	C5'-O5'-PA-O3A
24	GK	501	GTP	C5'-O5'-PA-O3A
24	GK	501	GTP	C5'-O5'-PA-O1A
24	GL	501	GTP	C5'-O5'-PA-O3A
24	GM	501	GTP	C5'-O5'-PA-O3A
24	GM	501	GTP	C5'-O5'-PA-O1A
24	GN	501	GTP	C5'-O5'-PA-O3A
24	GO	602	GTP	C5'-O5'-PA-O3A
24	GO	602	GTP	C5'-O5'-PA-O1A
24	GR	501	GTP	C5'-O5'-PA-O1A
24	GS	501	GTP	C5'-O5'-PA-O3A
24	GS	501	GTP	C5'-O5'-PA-O1A
24	GT	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	GT	501	GTP	C5'-O5'-PA-O1A
24	A2	602	GTP	O4'-C4'-C5'-O5'
24	Gl	501	GTP	C5'-O5'-PA-O3A
24	Gl	501	GTP	C5'-O5'-PA-O1A
24	Gn	501	GTP	C5'-O5'-PA-O3A
24	Gn	501	GTP	C5'-O5'-PA-O1A
24	Go	501	GTP	C5'-O5'-PA-O3A
24	Go	501	GTP	C5'-O5'-PA-O1A
24	Gp	501	GTP	C5'-O5'-PA-O3A
24	Gp	501	GTP	C5'-O5'-PA-O1A
24	Gq	501	GTP	C5'-O5'-PA-O3A
24	Gq	501	GTP	C5'-O5'-PA-O1A
24	Gr	501	GTP	C5'-O5'-PA-O3A
24	Gr	501	GTP	C5'-O5'-PA-O1A
24	Gs	501	GTP	C5'-O5'-PA-O3A
24	Gs	501	GTP	C5'-O5'-PA-O1A
24	Gt	501	GTP	C5'-O5'-PA-O3A
24	Gt	501	GTP	C5'-O5'-PA-O1A
24	Gu	501	GTP	C5'-O5'-PA-O3A
24	Gu	501	GTP	C5'-O5'-PA-O1A
24	Gv	501	GTP	C5'-O5'-PA-O3A
24	Gv	501	GTP	C5'-O5'-PA-O1A
24	Gw	501	GTP	C5'-O5'-PA-O3A
24	Gw	501	GTP	C5'-O5'-PA-O1A
24	Gx	501	GTP	C5'-O5'-PA-O3A
24	Gy	501	GTP	C5'-O5'-PA-O3A
24	Gz	501	GTP	C5'-O5'-PA-O3A
24	Gz	501	GTP	C5'-O5'-PA-O1A
24	Q	602	GTP	C5'-O5'-PA-O3A
24	Q	602	GTP	C5'-O5'-PA-O1A
24	Q	602	GTP	C5'-O5'-PA-O2A
24	S	602	GTP	C5'-O5'-PA-O3A
24	S	602	GTP	C5'-O5'-PA-O1A
24	S	602	GTP	C5'-O5'-PA-O2A
24	V	602	GTP	O4'-C4'-C5'-O5'
24	V	602	GTP	C3'-C4'-C5'-O5'
24	W	602	GTP	C5'-O5'-PA-O3A
24	W	602	GTP	C5'-O5'-PA-O1A
24	Y	602	GTP	C5'-O5'-PA-O3A
24	Y	602	GTP	C5'-O5'-PA-O1A
24	Y	602	GTP	C5'-O5'-PA-O2A
24	c	602	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	c	602	GTP	C5'-O5'-PA-O1A
24	c	602	GTP	C5'-O5'-PA-O2A
24	e	602	GTP	C5'-O5'-PA-O3A
24	e	602	GTP	C5'-O5'-PA-O1A
24	f	602	GTP	C5'-O5'-PA-O1A
24	g	602	GTP	O4'-C4'-C5'-O5'
24	h	602	GTP	C5'-O5'-PA-O3A
24	h	602	GTP	C5'-O5'-PA-O1A
24	k	602	GTP	C5'-O5'-PA-O3A
24	k	602	GTP	C5'-O5'-PA-O1A
24	l	602	GTP	C5'-O5'-PA-O1A
24	o	501	GTP	C5'-O5'-PA-O3A
24	o	501	GTP	C5'-O5'-PA-O1A
24	o	501	GTP	C5'-O5'-PA-O2A
24	A4	501	GTP	C5'-O5'-PA-O3A
24	A4	501	GTP	C5'-O5'-PA-O1A
24	q	602	GTP	O4'-C4'-C5'-O5'
24	q	602	GTP	C3'-C4'-C5'-O5'
24	u	501	GTP	C5'-O5'-PA-O3A
24	u	501	GTP	C5'-O5'-PA-O2A
24	x	501	GTP	PB-O3B-PG-O2G
24	x	501	GTP	C5'-O5'-PA-O3A
24	z	602	GTP	C5'-O5'-PA-O3A
24	z	602	GTP	C5'-O5'-PA-O1A
24	A5	501	GTP	C5'-O5'-PA-O3A
24	A5	501	GTP	C5'-O5'-PA-O1A
24	A6	501	GTP	C5'-O5'-PA-O3A
24	A6	501	GTP	C5'-O5'-PA-O1A
24	A7	501	GTP	C5'-O5'-PA-O3A
24	A7	501	GTP	C5'-O5'-PA-O1A
24	A8	501	GTP	C5'-O5'-PA-O3A
24	A8	501	GTP	C5'-O5'-PA-O1A
24	A9	501	GTP	C5'-O5'-PA-O3A
24	AI	501	GTP	PB-O3B-PG-O2G
24	AI	501	GTP	C5'-O5'-PA-O3A
24	AI	501	GTP	C5'-O5'-PA-O2A
24	1	602	GTP	PB-O3B-PG-O3G
24	1	602	GTP	O4'-C4'-C5'-O5'
24	Aj	501	GTP	PB-O3B-PG-O2G
24	Aj	501	GTP	C5'-O5'-PA-O3A
24	Al	602	GTP	C5'-O5'-PA-O3A
24	Al	602	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	2	602	GTP	PB-O3B-PG-O3G
24	2	602	GTP	O4'-C4'-C5'-O5'
24	2	602	GTP	C3'-C4'-C5'-O5'
24	Ax	602	GTP	PB-O3B-PG-O2G
24	Ax	602	GTP	C5'-O5'-PA-O3A
24	Ax	602	GTP	C5'-O5'-PA-O2A
24	B0	501	GTP	PB-O3B-PG-O2G
24	B0	501	GTP	C5'-O5'-PA-O3A
24	B1	602	GTP	C5'-O5'-PA-O1A
24	B3	602	GTP	C5'-O5'-PA-O3A
24	B3	602	GTP	C5'-O5'-PA-O1A
24	B4	602	GTP	C5'-O5'-PA-O3A
24	B4	602	GTP	C5'-O5'-PA-O1A
24	B7	501	GTP	C5'-O5'-PA-O3A
24	BI	602	GTP	C5'-O5'-PA-O3A
24	BI	602	GTP	C5'-O5'-PA-O1A
24	BI	602	GTP	C5'-O5'-PA-O2A
24	BK	602	GTP	C3'-C4'-C5'-O5'
24	BL	602	GTP	PB-O3B-PG-O3G
24	BL	602	GTP	C5'-O5'-PA-O3A
24	BL	602	GTP	C5'-O5'-PA-O1A
24	BO	602	GTP	C5'-O5'-PA-O3A
24	BO	602	GTP	C5'-O5'-PA-O1A
24	3	602	GTP	O4'-C4'-C5'-O5'
24	3	602	GTP	C3'-C4'-C5'-O5'
24	BP	602	GTP	C5'-O5'-PA-O3A
24	BP	602	GTP	C5'-O5'-PA-O1A
24	BR	501	GTP	PB-O3B-PG-O2G
24	BR	501	GTP	C5'-O5'-PA-O3A
24	BR	501	GTP	C5'-O5'-PA-O1A
24	BR	501	GTP	C5'-O5'-PA-O2A
24	BT	501	GTP	PB-O3B-PG-O2G
24	BT	501	GTP	C5'-O5'-PA-O3A
24	BV	602	GTP	C5'-O5'-PA-O3A
24	BV	602	GTP	C5'-O5'-PA-O1A
24	BX	602	GTP	PB-O3B-PG-O3G
24	BX	602	GTP	O4'-C4'-C5'-O5'
24	BY	602	GTP	PB-O3B-PG-O3G
24	BY	602	GTP	O4'-C4'-C5'-O5'
24	BY	602	GTP	C3'-C4'-C5'-O5'
24	Bc	501	GTP	C5'-O5'-PA-O3A
24	Bc	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Bd	501	GTP	C5'-O5'-PA-O3A
24	Bu	602	GTP	C5'-O5'-PA-O3A
24	Bu	602	GTP	C5'-O5'-PA-O1A
24	Bu	602	GTP	C5'-O5'-PA-O2A
24	4	602	GTP	PB-O3B-PG-O3G
24	4	602	GTP	O4'-C4'-C5'-O5'
24	4	602	GTP	C3'-C4'-C5'-O5'
24	Bw	602	GTP	C5'-O5'-PA-O3A
24	Bw	602	GTP	C5'-O5'-PA-O1A
24	Bw	602	GTP	C5'-O5'-PA-O2A
24	By	602	GTP	O4'-C4'-C5'-O5'
24	By	602	GTP	C3'-C4'-C5'-O5'
24	Bz	602	GTP	C5'-O5'-PA-O3A
24	Bz	602	GTP	C5'-O5'-PA-O1A
24	CB	602	GTP	C5'-O5'-PA-O3A
24	CB	602	GTP	C5'-O5'-PA-O1A
24	E3	501	GTP	C5'-O5'-PA-O3A
24	E3	501	GTP	C5'-O5'-PA-O1A
24	E4	501	GTP	C5'-O5'-PA-O3A
24	E4	501	GTP	C5'-O5'-PA-O1A
24	E8	501	GTP	C5'-O5'-PA-O3A
24	Ee	501	GTP	C5'-O5'-PA-O3A
24	Ee	501	GTP	C5'-O5'-PA-O1A
24	Eg	501	GTP	C5'-O5'-PA-O3A
24	Eg	501	GTP	C5'-O5'-PA-O1A
24	Eh	501	GTP	C5'-O5'-PA-O3A
24	Eh	501	GTP	C5'-O5'-PA-O1A
24	Ei	501	GTP	C5'-O5'-PA-O3A
24	Ei	501	GTP	C5'-O5'-PA-O1A
24	Ej	501	GTP	C5'-O5'-PA-O3A
24	Ek	501	GTP	C5'-O5'-PA-O3A
24	Ek	501	GTP	C5'-O5'-PA-O1A
24	El	501	GTP	C5'-O5'-PA-O3A
24	El	501	GTP	C5'-O5'-PA-O1A
24	Em	501	GTP	C5'-O5'-PA-O3A
24	Em	501	GTP	C5'-O5'-PA-O1A
24	En	501	GTP	C5'-O5'-PA-O3A
24	Eo	501	GTP	C5'-O5'-PA-O3A
24	Eo	501	GTP	C5'-O5'-PA-O1A
24	Ep	501	GTP	C5'-O5'-PA-O3A
24	Ep	501	GTP	C5'-O5'-PA-O1A
24	Eq	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Eq	501	GTP	C5'-O5'-PA-O1A
24	Er	501	GTP	C5'-O5'-PA-O3A
24	Es	501	GTP	C5'-O5'-PA-O3A
24	Es	501	GTP	C5'-O5'-PA-O1A
24	Et	501	GTP	C5'-O5'-PA-O3A
24	Eu	501	GTP	C5'-O5'-PA-O3A
24	Eu	501	GTP	C5'-O5'-PA-O1A
24	Ew	501	GTP	C5'-O5'-PA-O1A
24	Ex	501	GTP	C5'-O5'-PA-O1A
24	Ey	602	GTP	PB-O3B-PG-O2G
24	Ey	602	GTP	PB-O3B-PG-O3G
24	Ey	602	GTP	C5'-O5'-PA-O3A
24	Ey	602	GTP	C5'-O5'-PA-O1A
24	Ez	501	GTP	C5'-O5'-PA-O3A
24	Ez	501	GTP	C5'-O5'-PA-O1A
24	F0	501	GTP	C5'-O5'-PA-O3A
24	F3	501	GTP	C5'-O5'-PA-O3A
24	F5	501	GTP	C5'-O5'-PA-O3A
24	F6	501	GTP	C5'-O5'-PA-O3A
24	F7	501	GTP	C5'-O5'-PA-O3A
24	F7	501	GTP	C5'-O5'-PA-O1A
24	F8	501	GTP	C5'-O5'-PA-O3A
24	F9	501	GTP	C5'-O5'-PA-O3A
24	F9	501	GTP	C5'-O5'-PA-O1A
24	FM	501	GTP	C5'-O5'-PA-O3A
24	FO	501	GTP	C5'-O5'-PA-O3A
24	FO	501	GTP	C5'-O5'-PA-O1A
24	FP	501	GTP	C5'-O5'-PA-O3A
24	FP	501	GTP	C5'-O5'-PA-O1A
24	FQ	501	GTP	C5'-O5'-PA-O3A
24	FQ	501	GTP	C5'-O5'-PA-O1A
24	FR	501	GTP	C5'-O5'-PA-O3A
24	FR	501	GTP	C5'-O5'-PA-O1A
24	FS	501	GTP	C5'-O5'-PA-O3A
24	FT	501	GTP	C5'-O5'-PA-O3A
24	FU	501	GTP	C5'-O5'-PA-O3A
24	FU	501	GTP	C5'-O5'-PA-O1A
24	FV	602	GTP	C5'-O5'-PA-O3A
24	FV	602	GTP	C5'-O5'-PA-O1A
24	FW	501	GTP	C5'-O5'-PA-O3A
24	FW	501	GTP	C5'-O5'-PA-O1A
24	FX	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	FX	501	GTP	C5'-O5'-PA-O1A
24	FY	501	GTP	C5'-O5'-PA-O3A
24	FZ	501	GTP	C5'-O5'-PA-O3A
24	Fa	501	GTP	C5'-O5'-PA-O3A
24	Fa	501	GTP	C5'-O5'-PA-O1A
24	Fb	501	GTP	C5'-O5'-PA-O3A
24	Fb	501	GTP	C5'-O5'-PA-O1A
24	Fc	501	GTP	C5'-O5'-PA-O3A
24	Fc	501	GTP	C5'-O5'-PA-O1A
24	Ff	501	GTP	PB-O3B-PG-O3G
24	Ff	501	GTP	C5'-O5'-PA-O3A
24	Ff	501	GTP	C5'-O5'-PA-O1A
24	Fg	501	GTP	C5'-O5'-PA-O3A
24	Fg	501	GTP	C5'-O5'-PA-O1A
23	Fo	501	GDP	O4'-C4'-C5'-O5'
23	Fr	501	GDP	O4'-C4'-C5'-O5'
23	Fs	501	GDP	O4'-C4'-C5'-O5'
23	Fw	501	GDP	O4'-C4'-C5'-O5'
23	Fy	501	GDP	O4'-C4'-C5'-O5'
23	Gh	501	GDP	O4'-C4'-C5'-O5'
23	AL	501	GDP	C3'-C4'-C5'-O5'
23	AO	501	GDP	O4'-C4'-C5'-O5'
23	AO	501	GDP	C3'-C4'-C5'-O5'
23	AP	501	GDP	O4'-C4'-C5'-O5'
23	AR	501	GDP	C3'-C4'-C5'-O5'
23	Aa	501	GDP	C3'-C4'-C5'-O5'
23	Ab	501	GDP	O4'-C4'-C5'-O5'
23	Ag	501	GDP	O4'-C4'-C5'-O5'
23	Av	501	GDP	C3'-C4'-C5'-O5'
23	Az	501	GDP	C3'-C4'-C5'-O5'
23	BF	501	GDP	O4'-C4'-C5'-O5'
23	Bg	501	GDP	C3'-C4'-C5'-O5'
23	Bk	501	GDP	O4'-C4'-C5'-O5'
23	Bm	501	GDP	C3'-C4'-C5'-O5'
23	DL	501	GDP	O4'-C4'-C5'-O5'
23	DM	501	GDP	O4'-C4'-C5'-O5'
23	DO	501	GDP	O4'-C4'-C5'-O5'
23	DS	501	GDP	O4'-C4'-C5'-O5'
23	DW	501	GDP	O4'-C4'-C5'-O5'
23	Da	501	GDP	O4'-C4'-C5'-O5'
23	Dc	501	GDP	O4'-C4'-C5'-O5'
23	Dd	501	GDP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	EL	501	GDP	O4'-C4'-C5'-O5'
23	EM	501	GDP	O4'-C4'-C5'-O5'
23	ET	501	GDP	O4'-C4'-C5'-O5'
23	EW	501	GDP	O4'-C4'-C5'-O5'
23	Ea	501	GDP	O4'-C4'-C5'-O5'
23	Eb	501	GDP	O4'-C4'-C5'-O5'
23	Ed	501	GDP	O4'-C4'-C5'-O5'
23	F2	501	GDP	O4'-C4'-C5'-O5'
23	F4	501	GDP	O4'-C4'-C5'-O5'
23	FB	501	GDP	O4'-C4'-C5'-O5'
23	FH	501	GDP	C3'-C4'-C5'-O5'
23	FJ	501	GDP	O4'-C4'-C5'-O5'
23	FL	501	GDP	O4'-C4'-C5'-O5'
24	Fi	501	GTP	O4'-C4'-C5'-O5'
24	A2	602	GTP	C3'-C4'-C5'-O5'
24	g	602	GTP	C3'-C4'-C5'-O5'
24	1	602	GTP	C3'-C4'-C5'-O5'
24	BI	602	GTP	C3'-C4'-C5'-O5'
24	BX	602	GTP	C3'-C4'-C5'-O5'
24	E6	602	GTP	O4'-C4'-C5'-O5'
23	0	501	GDP	C3'-C4'-C5'-O5'
23	Fn	501	GDP	O4'-C4'-C5'-O5'
23	Ft	501	GDP	O4'-C4'-C5'-O5'
23	GX	501	GDP	O4'-C4'-C5'-O5'
23	Gg	501	GDP	C3'-C4'-C5'-O5'
23	AU	501	GDP	O4'-C4'-C5'-O5'
23	At	501	GDP	O4'-C4'-C5'-O5'
23	Av	501	GDP	O4'-C4'-C5'-O5'
23	BC	501	GDP	O4'-C4'-C5'-O5'
23	Bj	501	GDP	O4'-C4'-C5'-O5'
23	Bj	501	GDP	C3'-C4'-C5'-O5'
23	Bm	501	GDP	O4'-C4'-C5'-O5'
23	Bp	501	GDP	O4'-C4'-C5'-O5'
23	DQ	501	GDP	O4'-C4'-C5'-O5'
23	DV	501	GDP	O4'-C4'-C5'-O5'
23	DY	501	GDP	O4'-C4'-C5'-O5'
23	DZ	501	GDP	O4'-C4'-C5'-O5'
23	Db	501	GDP	O4'-C4'-C5'-O5'
23	Dk	501	GDP	O4'-C4'-C5'-O5'
23	ES	501	GDP	O4'-C4'-C5'-O5'
23	EY	501	GDP	O4'-C4'-C5'-O5'
23	Ef	501	GDP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	FG	501	GDP	O4'-C4'-C5'-O5'
23	FI	501	GDP	O4'-C4'-C5'-O5'
24	Fi	501	GTP	C3'-C4'-C5'-O5'
24	G3	602	GTP	O4'-C4'-C5'-O5'
24	G3	602	GTP	C3'-C4'-C5'-O5'
24	GR	501	GTP	O4'-C4'-C5'-O5'
24	p	602	GTP	O4'-C4'-C5'-O5'
24	v	602	GTP	O4'-C4'-C5'-O5'
24	AS	501	GTP	O4'-C4'-C5'-O5'
24	BI	602	GTP	O4'-C4'-C5'-O5'
24	BK	602	GTP	O4'-C4'-C5'-O5'
24	BL	602	GTP	O4'-C4'-C5'-O5'
24	E6	602	GTP	C3'-C4'-C5'-O5'
23	Fx	501	GDP	C3'-C4'-C5'-O5'
23	Fz	501	GDP	C3'-C4'-C5'-O5'
23	Gb	501	GDP	C3'-C4'-C5'-O5'
23	Gi	501	GDP	C3'-C4'-C5'-O5'
23	Gj	501	GDP	C3'-C4'-C5'-O5'
23	AX	501	GDP	C3'-C4'-C5'-O5'
23	Aq	501	GDP	C3'-C4'-C5'-O5'
23	F1	501	GDP	C3'-C4'-C5'-O5'
24	GR	501	GTP	C3'-C4'-C5'-O5'
24	T	602	GTP	O4'-C4'-C5'-O5'
24	T	602	GTP	C3'-C4'-C5'-O5'
24	Z	602	GTP	O4'-C4'-C5'-O5'
24	Z	602	GTP	C3'-C4'-C5'-O5'
24	d	602	GTP	C3'-C4'-C5'-O5'
24	v	602	GTP	C3'-C4'-C5'-O5'
24	BJ	602	GTP	O4'-C4'-C5'-O5'
24	BJ	602	GTP	C3'-C4'-C5'-O5'
24	BS	602	GTP	O4'-C4'-C5'-O5'
24	Bv	602	GTP	C3'-C4'-C5'-O5'
23	Fo	501	GDP	C3'-C4'-C5'-O5'
23	Fr	501	GDP	C3'-C4'-C5'-O5'
23	Fs	501	GDP	C3'-C4'-C5'-O5'
23	Fy	501	GDP	C3'-C4'-C5'-O5'
23	GX	501	GDP	C3'-C4'-C5'-O5'
23	AP	501	GDP	C3'-C4'-C5'-O5'
23	Ad	501	GDP	C3'-C4'-C5'-O5'
23	Ag	501	GDP	C3'-C4'-C5'-O5'
23	DM	501	GDP	C3'-C4'-C5'-O5'
23	Dd	501	GDP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Di	501	GDP	C3'-C4'-C5'-O5'
23	Dj	501	GDP	C3'-C4'-C5'-O5'
23	E9	501	GDP	C3'-C4'-C5'-O5'
23	EL	501	GDP	C3'-C4'-C5'-O5'
23	EZ	501	GDP	C3'-C4'-C5'-O5'
23	Ed	501	GDP	C3'-C4'-C5'-O5'
23	F4	501	GDP	C3'-C4'-C5'-O5'
23	FB	501	GDP	C3'-C4'-C5'-O5'
23	FL	501	GDP	C3'-C4'-C5'-O5'
24	d	602	GTP	O4'-C4'-C5'-O5'
24	p	602	GTP	C3'-C4'-C5'-O5'
24	s	602	GTP	C3'-C4'-C5'-O5'
24	AJ	602	GTP	C3'-C4'-C5'-O5'
24	AS	501	GTP	C3'-C4'-C5'-O5'
24	Aw	602	GTP	O4'-C4'-C5'-O5'
24	B8	602	GTP	C3'-C4'-C5'-O5'
24	BL	602	GTP	C3'-C4'-C5'-O5'
24	BM	602	GTP	C3'-C4'-C5'-O5'
24	BS	602	GTP	C3'-C4'-C5'-O5'
24	BU	602	GTP	C3'-C4'-C5'-O5'
24	Bv	602	GTP	O4'-C4'-C5'-O5'
24	Bw	602	GTP	C3'-C4'-C5'-O5'
24	E1	501	GTP	O4'-C4'-C5'-O5'
24	E2	501	GTP	C3'-C4'-C5'-O5'
23	Fp	501	GDP	O4'-C4'-C5'-O5'
23	Fw	501	GDP	C3'-C4'-C5'-O5'
23	GH	501	GDP	O4'-C4'-C5'-O5'
23	GZ	501	GDP	O4'-C4'-C5'-O5'
23	Gc	501	GDP	O4'-C4'-C5'-O5'
23	BF	501	GDP	C3'-C4'-C5'-O5'
23	DL	501	GDP	C3'-C4'-C5'-O5'
23	DO	501	GDP	C3'-C4'-C5'-O5'
23	DS	501	GDP	C3'-C4'-C5'-O5'
23	DW	501	GDP	C3'-C4'-C5'-O5'
23	Dc	501	GDP	C3'-C4'-C5'-O5'
23	EM	501	GDP	C3'-C4'-C5'-O5'
23	EQ	501	GDP	O4'-C4'-C5'-O5'
23	ET	501	GDP	C3'-C4'-C5'-O5'
23	EW	501	GDP	C3'-C4'-C5'-O5'
23	Ea	501	GDP	C3'-C4'-C5'-O5'
23	Eb	501	GDP	C3'-C4'-C5'-O5'
23	Ec	501	GDP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	F2	501	GDP	C3'-C4'-C5'-O5'
23	FJ	501	GDP	C3'-C4'-C5'-O5'
24	GD	501	GTP	C3'-C4'-C5'-O5'
24	y	602	GTP	C3'-C4'-C5'-O5'
24	AJ	602	GTP	O4'-C4'-C5'-O5'
24	Aw	602	GTP	C3'-C4'-C5'-O5'
24	B8	602	GTP	O4'-C4'-C5'-O5'
24	Bx	602	GTP	C3'-C4'-C5'-O5'
24	E1	501	GTP	C3'-C4'-C5'-O5'
24	Fh	501	GTP	C3'-C4'-C5'-O5'
23	Gh	501	GDP	C3'-C4'-C5'-O5'
23	Ab	501	GDP	C3'-C4'-C5'-O5'
23	Ad	501	GDP	O4'-C4'-C5'-O5'
23	As	501	GDP	C3'-C4'-C5'-O5'
23	Bk	501	GDP	C3'-C4'-C5'-O5'
23	DN	501	GDP	O4'-C4'-C5'-O5'
23	Df	501	GDP	O4'-C4'-C5'-O5'
23	Dg	501	GDP	O4'-C4'-C5'-O5'
24	S	602	GTP	C3'-C4'-C5'-O5'
24	s	602	GTP	O4'-C4'-C5'-O5'
24	Ak	602	GTP	C3'-C4'-C5'-O5'
24	B5	602	GTP	O4'-C4'-C5'-O5'
24	B5	602	GTP	C3'-C4'-C5'-O5'
24	B6	602	GTP	O4'-C4'-C5'-O5'
24	B6	602	GTP	C3'-C4'-C5'-O5'
24	BU	602	GTP	O4'-C4'-C5'-O5'
24	Bx	602	GTP	O4'-C4'-C5'-O5'
24	E2	501	GTP	O4'-C4'-C5'-O5'
24	Fh	501	GTP	O4'-C4'-C5'-O5'
24	W	602	GTP	PB-O3B-PG-O1G
24	h	602	GTP	PB-O3B-PG-O1G
23	GU	501	GDP	O4'-C4'-C5'-O5'
23	GY	501	GDP	O4'-C4'-C5'-O5'
23	AU	501	GDP	C3'-C4'-C5'-O5'
23	Bp	501	GDP	C3'-C4'-C5'-O5'
23	Bs	501	GDP	C3'-C4'-C5'-O5'
23	DV	501	GDP	C3'-C4'-C5'-O5'
23	Da	501	GDP	C3'-C4'-C5'-O5'
23	E0	501	GDP	O4'-C4'-C5'-O5'
23	ES	501	GDP	C3'-C4'-C5'-O5'
23	FD	501	GDP	O4'-C4'-C5'-O5'
24	GF	501	GTP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	i	602	GTP	C3'-C4'-C5'-O5'
24	j	602	GTP	C3'-C4'-C5'-O5'
24	BM	602	GTP	O4'-C4'-C5'-O5'
24	BN	602	GTP	C3'-C4'-C5'-O5'
24	Bw	602	GTP	O4'-C4'-C5'-O5'
24	6	602	GTP	O4'-C4'-C5'-O5'
24	G3	602	GTP	PA-O3A-PB-O1B
24	GD	501	GTP	PA-O3A-PB-O1B
24	GR	501	GTP	PA-O3A-PB-O1B
24	a	602	GTP	PA-O3A-PB-O1B
24	b	602	GTP	PA-O3A-PB-O1B
24	i	602	GTP	PA-O3A-PB-O1B
24	j	602	GTP	PA-O3A-PB-O1B
24	B2	602	GTP	PA-O3A-PB-O1B
24	BS	602	GTP	PB-O3A-PA-O1A
24	Bx	602	GTP	PA-O3A-PB-O1B
24	E2	501	GTP	PA-O3A-PB-O1B
24	Ew	501	GTP	PA-O3A-PB-O1B
23	DP	501	GDP	O4'-C4'-C5'-O5'
23	DZ	501	GDP	C3'-C4'-C5'-O5'
23	Db	501	GDP	C3'-C4'-C5'-O5'
23	Dh	501	GDP	O4'-C4'-C5'-O5'
23	EN	501	GDP	O4'-C4'-C5'-O5'
23	EU	501	GDP	O4'-C4'-C5'-O5'
23	EY	501	GDP	C3'-C4'-C5'-O5'
23	Ef	501	GDP	C3'-C4'-C5'-O5'
24	GD	501	GTP	O4'-C4'-C5'-O5'
24	GQ	602	GTP	O4'-C4'-C5'-O5'
24	GQ	602	GTP	C3'-C4'-C5'-O5'
24	t	602	GTP	O4'-C4'-C5'-O5'
24	y	602	GTP	O4'-C4'-C5'-O5'
24	BQ	602	GTP	O4'-C4'-C5'-O5'
24	5	602	GTP	O4'-C4'-C5'-O5'
24	6	602	GTP	C3'-C4'-C5'-O5'
24	E5	501	GTP	O4'-C4'-C5'-O5'
24	E5	501	GTP	C3'-C4'-C5'-O5'
24	Ei	501	GTP	PA-O3A-PB-O3B
23	Ft	501	GDP	C3'-C4'-C5'-O5'
23	GV	501	GDP	O4'-C4'-C5'-O5'
23	At	501	GDP	C3'-C4'-C5'-O5'
23	DT	501	GDP	O4'-C4'-C5'-O5'
23	DY	501	GDP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Dr	501	GDP	O4'-C4'-C5'-O5'
23	FA	501	GDP	O4'-C4'-C5'-O5'
23	FG	501	GDP	C3'-C4'-C5'-O5'
23	FI	501	GDP	C3'-C4'-C5'-O5'
24	GF	501	GTP	O4'-C4'-C5'-O5'
24	S	602	GTP	O4'-C4'-C5'-O5'
24	t	602	GTP	C3'-C4'-C5'-O5'
24	Ak	602	GTP	O4'-C4'-C5'-O5'
24	BQ	602	GTP	C3'-C4'-C5'-O5'
24	5	602	GTP	C3'-C4'-C5'-O5'
24	Fe	501	GTP	C3'-C4'-C5'-O5'
23	0	501	GDP	PB-O3A-PA-O5'
23	A3	501	GDP	PB-O3A-PA-O5'
23	BW	501	GDP	PB-O3A-PA-O5'
23	BZ	501	GDP	PB-O3A-PA-O5'
23	0	501	GDP	O4'-C4'-C5'-O5'
23	Fn	501	GDP	C3'-C4'-C5'-O5'
23	DQ	501	GDP	C3'-C4'-C5'-O5'
23	Dk	501	GDP	C3'-C4'-C5'-O5'
24	B2	602	GTP	C3'-C4'-C5'-O5'
23	Fl	501	GDP	PA-O3A-PB-O1B
23	Fm	501	GDP	PA-O3A-PB-O1B
23	Fy	501	GDP	PA-O3A-PB-O1B
23	GV	501	GDP	PA-O3A-PB-O1B
23	GZ	501	GDP	PA-O3A-PB-O1B
23	Gh	501	GDP	PA-O3A-PB-O1B
23	AM	501	GDP	PA-O3A-PB-O1B
23	AO	501	GDP	PA-O3A-PB-O1B
23	Aa	501	GDP	PA-O3A-PB-O1B
23	BB	501	GDP	PA-O3A-PB-O1B
23	DV	501	GDP	PA-O3A-PB-O1B
23	DX	501	GDP	PA-O3A-PB-O1B
23	Db	501	GDP	PA-O3A-PB-O1B
23	Dd	501	GDP	PA-O3A-PB-O1B
23	De	501	GDP	PA-O3A-PB-O1B
23	Dx	501	GDP	PA-O3A-PB-O1B
23	ER	501	GDP	PA-O3A-PB-O1B
23	EY	501	GDP	PA-O3A-PB-O1B
23	Ea	501	GDP	PA-O3A-PB-O1B
23	F4	501	GDP	PA-O3A-PB-O1B
23	FA	501	GDP	PA-O3A-PB-O1B
23	FE	501	GDP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	FG	501	GDP	PA-O3A-PB-O1B
23	FN	501	GDP	PA-O3A-PB-O1B
24	o	501	GTP	PB-O3B-PG-O1G
24	B6	602	GTP	PB-O3B-PG-O1G
24	BI	602	GTP	PB-O3B-PG-O1G
24	Ay	602	GTP	PA-O3A-PB-O3B
23	Fs	501	GDP	PA-O3A-PB-O3B
23	Ft	501	GDP	PA-O3A-PB-O3B
23	Fv	501	GDP	PA-O3A-PB-O2B
23	GX	501	GDP	PA-O3A-PB-O3B
23	GY	501	GDP	PA-O3A-PB-O3B
23	Gc	501	GDP	PA-O3A-PB-O3B
23	Ge	501	GDP	PA-O3A-PB-O2B
23	Gf	501	GDP	PA-O3A-PB-O3B
23	Gm	501	GDP	PA-O3A-PB-O2B
23	AY	501	GDP	PA-O3A-PB-O3B
23	Ah	602	GDP	PA-O3A-PB-O3B
23	DZ	501	GDP	PA-O3A-PB-O3B
23	Dc	501	GDP	PA-O3A-PB-O3B
23	Di	501	GDP	PA-O3A-PB-O3B
23	Dk	501	GDP	PA-O3A-PB-O2B
23	Dv	501	GDP	PA-O3A-PB-O3B
23	EL	501	GDP	PA-O3A-PB-O3B
23	EN	501	GDP	PA-O3A-PB-O3B
23	EW	501	GDP	PA-O3A-PB-O2B
23	Ed	501	GDP	PA-O3A-PB-O2B
24	A1	602	GTP	PB-O3B-PG-O3G
24	GF	501	GTP	PB-O3B-PG-O3G
24	S	602	GTP	PB-O3B-PG-O3G
24	h	602	GTP	PB-O3B-PG-O3G
24	s	602	GTP	PB-O3B-PG-O2G
24	t	602	GTP	PB-O3B-PG-O2G
24	u	501	GTP	PB-O3B-PG-O2G
24	B5	602	GTP	PB-O3B-PG-O2G
24	B7	501	GTP	PB-O3B-PG-O2G
24	3	602	GTP	PB-O3B-PG-O3G
24	BQ	602	GTP	PB-O3B-PG-O2G
24	CB	602	GTP	PB-O3B-PG-O2G
24	6	602	GTP	PB-O3B-PG-O2G
24	Ff	501	GTP	PB-O3B-PG-O2G
23	AZ	501	GDP	C3'-C4'-C5'-O5'
23	Ev	501	GDP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	FF	501	GDP	O4'-C4'-C5'-O5'
24	a	602	GTP	C3'-C4'-C5'-O5'
24	c	602	GTP	C3'-C4'-C5'-O5'
24	o	501	GTP	C3'-C4'-C5'-O5'
24	BR	501	GTP	C3'-C4'-C5'-O5'
24	Ew	501	GTP	C3'-C4'-C5'-O5'
24	Fd	602	GTP	C3'-C4'-C5'-O5'
24	GA	501	GTP	C4'-C5'-O5'-PA
24	GI	501	GTP	C4'-C5'-O5'-PA
24	Gl	501	GTP	C4'-C5'-O5'-PA
24	Gn	501	GTP	C4'-C5'-O5'-PA
24	Go	501	GTP	C4'-C5'-O5'-PA
24	Gt	501	GTP	C4'-C5'-O5'-PA
24	e	602	GTP	C4'-C5'-O5'-PA
24	k	602	GTP	C4'-C5'-O5'-PA
24	A6	501	GTP	C4'-C5'-O5'-PA
24	A8	501	GTP	C4'-C5'-O5'-PA
24	B3	602	GTP	C4'-C5'-O5'-PA
24	Bd	501	GTP	C4'-C5'-O5'-PA
24	Eg	501	GTP	C4'-C5'-O5'-PA
24	Ek	501	GTP	C4'-C5'-O5'-PA
24	Ep	501	GTP	C4'-C5'-O5'-PA
24	Eu	501	GTP	C4'-C5'-O5'-PA
24	FM	501	GTP	C4'-C5'-O5'-PA
24	FT	501	GTP	C4'-C5'-O5'-PA
24	FX	501	GTP	C4'-C5'-O5'-PA
24	Fa	501	GTP	C4'-C5'-O5'-PA
23	Ae	501	GDP	PB-O3A-PA-O1A
23	BD	501	GDP	PB-O3A-PA-O1A
23	Bn	501	GDP	PB-O3A-PA-O1A
24	Fi	501	GTP	PA-O3A-PB-O1B
24	G2	501	GTP	PB-O3A-PA-O1A
24	G4	602	GTP	PG-O3B-PB-O1B
24	GP	501	GTP	PG-O3B-PB-O1B
24	GQ	602	GTP	PG-O3B-PB-O1B
24	S	602	GTP	PB-O3A-PA-O2A
24	b	602	GTP	PG-O3B-PB-O1B
24	c	602	GTP	PB-O3A-PA-O2A
24	i	602	GTP	PG-O3B-PB-O1B
24	B1	602	GTP	PG-O3B-PB-O1B
24	B1	602	GTP	PA-O3A-PB-O1B
24	BM	602	GTP	PG-O3B-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	BN	602	GTP	PG-O3B-PB-O1B
24	BN	602	GTP	PA-O3A-PB-O1B
24	Ey	602	GTP	PB-O3A-PA-O1A
24	FW	501	GTP	PB-O3A-PA-O1A
24	Fe	501	GTP	PG-O3B-PB-O1B
24	Fh	501	GTP	PA-O3A-PB-O1B
24	G4	602	GTP	PA-O3A-PB-O3B
24	G4	602	GTP	C3'-C4'-C5'-O5'
24	b	602	GTP	C3'-C4'-C5'-O5'
24	h	602	GTP	C3'-C4'-C5'-O5'
24	Fk	501	GTP	C4'-C5'-O5'-PA
24	GG	501	GTP	C4'-C5'-O5'-PA
24	GJ	501	GTP	C4'-C5'-O5'-PA
24	GN	501	GTP	C4'-C5'-O5'-PA
24	GO	602	GTP	C4'-C5'-O5'-PA
24	Gq	501	GTP	C4'-C5'-O5'-PA
24	Gv	501	GTP	C4'-C5'-O5'-PA
24	Gz	501	GTP	C4'-C5'-O5'-PA
24	A5	501	GTP	C4'-C5'-O5'-PA
24	Ay	602	GTP	C4'-C5'-O5'-PA
24	BO	602	GTP	C4'-C5'-O5'-PA
24	Bc	501	GTP	C4'-C5'-O5'-PA
24	CB	602	GTP	C4'-C5'-O5'-PA
24	E8	501	GTP	C4'-C5'-O5'-PA
24	Ee	501	GTP	C4'-C5'-O5'-PA
24	Eh	501	GTP	C4'-C5'-O5'-PA
24	Ej	501	GTP	C4'-C5'-O5'-PA
24	Eo	501	GTP	C4'-C5'-O5'-PA
24	Eq	501	GTP	C4'-C5'-O5'-PA
24	Er	501	GTP	C4'-C5'-O5'-PA
24	F3	501	GTP	C4'-C5'-O5'-PA
24	F5	501	GTP	C4'-C5'-O5'-PA
24	FO	501	GTP	C4'-C5'-O5'-PA
24	FP	501	GTP	C4'-C5'-O5'-PA
24	FQ	501	GTP	C4'-C5'-O5'-PA
24	FR	501	GTP	C4'-C5'-O5'-PA
24	FS	501	GTP	C4'-C5'-O5'-PA
24	FY	501	GTP	C4'-C5'-O5'-PA
24	FZ	501	GTP	C4'-C5'-O5'-PA
24	Fg	501	GTP	C4'-C5'-O5'-PA
23	Fl	501	GDP	O4'-C4'-C5'-O5'
23	DU	501	GDP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	EP	501	GDP	O4'-C4'-C5'-O5'
24	i	602	GTP	O4'-C4'-C5'-O5'
24	j	602	GTP	O4'-C4'-C5'-O5'
24	BN	602	GTP	O4'-C4'-C5'-O5'
24	Fe	501	GTP	O4'-C4'-C5'-O5'
24	Fe	501	GTP	PA-O3A-PB-O3B
23	Fl	501	GDP	C5'-O5'-PA-O3A
23	Fl	501	GDP	C5'-O5'-PA-O1A
23	Fq	501	GDP	C5'-O5'-PA-O1A
23	A0	501	GDP	C5'-O5'-PA-O1A
23	Fv	501	GDP	C5'-O5'-PA-O3A
23	Fv	501	GDP	C5'-O5'-PA-O1A
23	Fv	501	GDP	C5'-O5'-PA-O2A
23	Ge	501	GDP	C5'-O5'-PA-O1A
23	Gm	501	GDP	C5'-O5'-PA-O3A
23	Gm	501	GDP	C5'-O5'-PA-O1A
23	AA	501	GDP	C5'-O5'-PA-O1A
23	AE	501	GDP	C5'-O5'-PA-O1A
23	AG	501	GDP	C5'-O5'-PA-O1A
23	AN	501	GDP	C5'-O5'-PA-O3A
23	AN	501	GDP	C5'-O5'-PA-O2A
23	AQ	501	GDP	C5'-O5'-PA-O1A
23	AS	502	GDP	C5'-O5'-PA-O1A
23	AT	501	GDP	C5'-O5'-PA-O3A
23	AT	501	GDP	C5'-O5'-PA-O2A
23	AZ	501	GDP	C5'-O5'-PA-O3A
23	AZ	501	GDP	C5'-O5'-PA-O2A
23	Ab	501	GDP	C5'-O5'-PA-O1A
23	Ae	501	GDP	C5'-O5'-PA-O1A
23	Af	501	GDP	C5'-O5'-PA-O2A
23	Ag	501	GDP	C5'-O5'-PA-O3A
23	Ag	501	GDP	C5'-O5'-PA-O1A
23	Ah	602	GDP	C5'-O5'-PA-O1A
23	Ai	501	GDP	C5'-O5'-PA-O1A
23	An	501	GDP	C5'-O5'-PA-O1A
23	Ap	501	GDP	C5'-O5'-PA-O1A
23	Aq	501	GDP	C5'-O5'-PA-O1A
23	Ar	501	GDP	C5'-O5'-PA-O2A
23	As	501	GDP	C5'-O5'-PA-O3A
23	As	501	GDP	C5'-O5'-PA-O2A
23	At	501	GDP	C5'-O5'-PA-O3A
23	At	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	BB	501	GDP	C5'-O5'-PA-O1A
23	BD	501	GDP	C5'-O5'-PA-O1A
23	BE	501	GDP	C5'-O5'-PA-O2A
23	BF	501	GDP	C5'-O5'-PA-O3A
23	BF	501	GDP	C5'-O5'-PA-O1A
23	BG	501	GDP	C5'-O5'-PA-O1A
23	BH	501	GDP	C5'-O5'-PA-O1A
23	Ba	501	GDP	C5'-O5'-PA-O1A
23	Be	501	GDP	C5'-O5'-PA-O1A
23	Bh	501	GDP	C5'-O5'-PA-O2A
23	Bi	501	GDP	C5'-O5'-PA-O3A
23	Bi	501	GDP	C5'-O5'-PA-O2A
23	Bj	501	GDP	C5'-O5'-PA-O1A
23	Bk	501	GDP	C5'-O5'-PA-O1A
23	Bl	602	GDP	C5'-O5'-PA-O1A
23	Bn	501	GDP	C5'-O5'-PA-O1A
23	Bo	501	GDP	C5'-O5'-PA-O2A
23	Bq	602	GDP	C5'-O5'-PA-O1A
23	Br	501	GDP	C5'-O5'-PA-O1A
23	DL	501	GDP	C5'-O5'-PA-O1A
23	DM	501	GDP	C5'-O5'-PA-O1A
23	DN	501	GDP	C5'-O5'-PA-O1A
23	DO	501	GDP	C5'-O5'-PA-O1A
23	DQ	501	GDP	C5'-O5'-PA-O1A
23	DS	501	GDP	C5'-O5'-PA-O1A
23	DT	501	GDP	C5'-O5'-PA-O3A
23	DT	501	GDP	C5'-O5'-PA-O1A
23	DV	501	GDP	C5'-O5'-PA-O1A
23	DW	501	GDP	C5'-O5'-PA-O1A
23	DY	501	GDP	C5'-O5'-PA-O1A
23	DZ	501	GDP	C5'-O5'-PA-O3A
23	DZ	501	GDP	C5'-O5'-PA-O1A
23	Da	501	GDP	C5'-O5'-PA-O1A
23	Db	501	GDP	C5'-O5'-PA-O1A
23	Dc	501	GDP	C5'-O5'-PA-O3A
23	Dc	501	GDP	C5'-O5'-PA-O1A
23	Dd	501	GDP	C5'-O5'-PA-O1A
23	Df	501	GDP	C5'-O5'-PA-O3A
23	Df	501	GDP	C5'-O5'-PA-O1A
23	Dj	501	GDP	C5'-O5'-PA-O1A
23	Dk	501	GDP	C5'-O5'-PA-O1A
23	Dr	501	GDP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Dr	501	GDP	C5'-O5'-PA-O1A
23	E0	501	GDP	C5'-O5'-PA-O3A
23	E0	501	GDP	C5'-O5'-PA-O1A
23	EL	501	GDP	C5'-O5'-PA-O3A
23	EL	501	GDP	C5'-O5'-PA-O1A
23	EW	501	GDP	C5'-O5'-PA-O1A
23	EX	501	GDP	C5'-O5'-PA-O3A
23	EX	501	GDP	C5'-O5'-PA-O1A
23	EY	501	GDP	C5'-O5'-PA-O1A
23	8	501	GDP	C5'-O5'-PA-O1A
23	FF	501	GDP	C5'-O5'-PA-O1A
23	FK	501	GDP	C5'-O5'-PA-O1A
24	Fi	501	GTP	C5'-O5'-PA-O1A
24	G1	501	GTP	C5'-O5'-PA-O1A
24	G2	501	GTP	C5'-O5'-PA-O1A
24	G3	602	GTP	C5'-O5'-PA-O1A
24	G5	501	GTP	C5'-O5'-PA-O1A
24	GB	501	GTP	C5'-O5'-PA-O1A
24	GD	501	GTP	C5'-O5'-PA-O1A
24	GE	501	GTP	C5'-O5'-PA-O1A
24	GF	501	GTP	C5'-O5'-PA-O1A
24	GG	501	GTP	C5'-O5'-PA-O1A
24	GJ	501	GTP	C5'-O5'-PA-O1A
24	GL	501	GTP	C5'-O5'-PA-O1A
24	GN	501	GTP	C5'-O5'-PA-O1A
24	GP	501	GTP	C5'-O5'-PA-O1A
24	GR	501	GTP	C5'-O5'-PA-O3A
24	Gx	501	GTP	C5'-O5'-PA-O1A
24	Gy	501	GTP	C5'-O5'-PA-O1A
24	a	602	GTP	C5'-O5'-PA-O1A
24	b	602	GTP	C5'-O5'-PA-O1A
24	i	602	GTP	C5'-O5'-PA-O1A
24	j	602	GTP	C5'-O5'-PA-O1A
24	l	602	GTP	C5'-O5'-PA-O3A
24	u	501	GTP	C5'-O5'-PA-O1A
24	w	602	GTP	C5'-O5'-PA-O1A
24	x	501	GTP	C5'-O5'-PA-O1A
24	A9	501	GTP	C5'-O5'-PA-O1A
24	AI	501	GTP	C5'-O5'-PA-O1A
24	AK	602	GTP	C5'-O5'-PA-O1A
24	Aj	501	GTP	C5'-O5'-PA-O1A
24	Ax	602	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Ay	602	GTP	C5'-O5'-PA-O1A
24	B0	501	GTP	C5'-O5'-PA-O1A
24	B0	501	GTP	C5'-O5'-PA-O2A
24	B1	602	GTP	C5'-O5'-PA-O3A
24	B2	602	GTP	C5'-O5'-PA-O1A
24	B7	501	GTP	C5'-O5'-PA-O1A
24	B9	602	GTP	C5'-O5'-PA-O1A
24	BM	602	GTP	C5'-O5'-PA-O1A
24	BN	602	GTP	C5'-O5'-PA-O1A
24	BT	501	GTP	C5'-O5'-PA-O1A
24	Bd	501	GTP	C5'-O5'-PA-O1A
24	E2	501	GTP	C5'-O5'-PA-O1A
24	E6	602	GTP	C5'-O5'-PA-O1A
24	E8	501	GTP	C5'-O5'-PA-O1A
24	Ej	501	GTP	C5'-O5'-PA-O1A
24	En	501	GTP	C5'-O5'-PA-O1A
24	Er	501	GTP	C5'-O5'-PA-O1A
24	Et	501	GTP	C5'-O5'-PA-O1A
24	F0	501	GTP	C5'-O5'-PA-O1A
24	F3	501	GTP	C5'-O5'-PA-O1A
24	F5	501	GTP	C5'-O5'-PA-O1A
24	F6	501	GTP	C5'-O5'-PA-O1A
24	F8	501	GTP	C5'-O5'-PA-O1A
24	FM	501	GTP	C5'-O5'-PA-O1A
24	FS	501	GTP	C5'-O5'-PA-O1A
24	FT	501	GTP	C5'-O5'-PA-O1A
24	FY	501	GTP	C5'-O5'-PA-O1A
24	FZ	501	GTP	C5'-O5'-PA-O1A
24	Fd	602	GTP	C5'-O5'-PA-O1A
24	Fe	501	GTP	C5'-O5'-PA-O1A
24	G2	501	GTP	C4'-C5'-O5'-PA
24	G5	501	GTP	C4'-C5'-O5'-PA
24	G6	501	GTP	C4'-C5'-O5'-PA
24	GB	501	GTP	C4'-C5'-O5'-PA
24	GC	501	GTP	C4'-C5'-O5'-PA
24	GL	501	GTP	C4'-C5'-O5'-PA
24	GM	501	GTP	C4'-C5'-O5'-PA
24	GS	501	GTP	C4'-C5'-O5'-PA
24	GT	501	GTP	C4'-C5'-O5'-PA
24	Gr	501	GTP	C4'-C5'-O5'-PA
24	Gs	501	GTP	C4'-C5'-O5'-PA
24	Gu	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Gw	501	GTP	C4'-C5'-O5'-PA
24	Gx	501	GTP	C4'-C5'-O5'-PA
24	Gy	501	GTP	C4'-C5'-O5'-PA
24	S	602	GTP	C4'-C5'-O5'-PA
24	c	602	GTP	C4'-C5'-O5'-PA
24	f	602	GTP	C4'-C5'-O5'-PA
24	A4	501	GTP	C4'-C5'-O5'-PA
24	w	602	GTP	C4'-C5'-O5'-PA
24	z	602	GTP	C4'-C5'-O5'-PA
24	A7	501	GTP	C4'-C5'-O5'-PA
24	A9	501	GTP	C4'-C5'-O5'-PA
24	AK	602	GTP	C4'-C5'-O5'-PA
24	Al	602	GTP	C4'-C5'-O5'-PA
24	B9	602	GTP	C4'-C5'-O5'-PA
24	BI	602	GTP	C4'-C5'-O5'-PA
24	BV	602	GTP	C4'-C5'-O5'-PA
24	Bu	602	GTP	C4'-C5'-O5'-PA
24	Bw	602	GTP	C4'-C5'-O5'-PA
24	E4	501	GTP	C4'-C5'-O5'-PA
24	El	501	GTP	C4'-C5'-O5'-PA
24	Em	501	GTP	C4'-C5'-O5'-PA
24	En	501	GTP	C4'-C5'-O5'-PA
24	Es	501	GTP	C4'-C5'-O5'-PA
24	Et	501	GTP	C4'-C5'-O5'-PA
24	Ey	602	GTP	C4'-C5'-O5'-PA
24	F0	501	GTP	C4'-C5'-O5'-PA
24	F6	501	GTP	C4'-C5'-O5'-PA
24	F7	501	GTP	C4'-C5'-O5'-PA
24	F8	501	GTP	C4'-C5'-O5'-PA
24	F9	501	GTP	C4'-C5'-O5'-PA
24	FU	501	GTP	C4'-C5'-O5'-PA
24	FV	602	GTP	C4'-C5'-O5'-PA
24	FW	501	GTP	C4'-C5'-O5'-PA
24	Ff	501	GTP	C4'-C5'-O5'-PA
23	Da	501	GDP	PA-O3A-PB-O1B
24	BL	602	GTP	PB-O3B-PG-O1G
23	BA	501	GDP	C3'-C4'-C5'-O5'
23	Bl	602	GDP	C3'-C4'-C5'-O5'
24	o	501	GTP	O4'-C4'-C5'-O5'
24	G1	501	GTP	C4'-C5'-O5'-PA
24	GK	501	GTP	C4'-C5'-O5'-PA
24	B4	602	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Ei	501	GTP	C4'-C5'-O5'-PA
24	Ez	501	GTP	C4'-C5'-O5'-PA
24	w	602	GTP	PA-O3A-PB-O3B
23	FK	501	GDP	PB-O3A-PA-O2A
24	v	602	GTP	PB-O3A-PA-O2A
24	AJ	602	GTP	PB-O3A-PA-O1A
24	Ak	602	GTP	PB-O3A-PA-O2A
24	B8	602	GTP	PB-O3A-PA-O2A
24	BI	602	GTP	PB-O3A-PA-O2A
24	BM	602	GTP	PA-O3A-PB-O1B
24	BU	602	GTP	PB-O3A-PA-O2A
24	Bw	602	GTP	PB-O3A-PA-O2A
24	CA	602	GTP	PB-O3A-PA-O2A
24	Fd	602	GTP	PA-O3A-PB-O1B
23	GH	501	GDP	C3'-C4'-C5'-O5'
23	AN	501	GDP	C3'-C4'-C5'-O5'
23	Ec	501	GDP	C3'-C4'-C5'-O5'
24	Y	602	GTP	C3'-C4'-C5'-O5'
24	Gp	501	GTP	C4'-C5'-O5'-PA
24	GF	501	GTP	PA-O3A-PB-O3B
24	AK	602	GTP	PA-O3A-PB-O3B
24	B9	602	GTP	PA-O3A-PB-O3B
24	GP	501	GTP	C3'-C4'-C5'-O5'
24	Bz	602	GTP	C3'-C4'-C5'-O5'
24	Q	602	GTP	C4'-C5'-O5'-PA
24	o	501	GTP	C4'-C5'-O5'-PA
23	Fn	501	GDP	PA-O3A-PB-O1B
23	Fp	501	GDP	PA-O3A-PB-O1B
23	Ar	501	GDP	PA-O3A-PB-O1B
23	DN	501	GDP	PA-O3A-PB-O1B
23	DP	501	GDP	PA-O3A-PB-O1B
23	DQ	501	GDP	PA-O3A-PB-O1B
23	Df	501	GDP	PA-O3A-PB-O1B
23	EM	501	GDP	PA-O3A-PB-O1B
23	EP	501	GDP	PA-O3A-PB-O1B
23	ES	501	GDP	PA-O3A-PB-O1B
23	FL	501	GDP	PA-O3A-PB-O1B
24	Aw	602	GTP	PB-O3B-PG-O1G
24	Bw	602	GTP	PB-O3B-PG-O1G
23	Fp	501	GDP	C3'-C4'-C5'-O5'
24	BP	602	GTP	C4'-C5'-O5'-PA
24	E7	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Fc	501	GTP	C4'-C5'-O5'-PA
23	Fm	501	GDP	O4'-C4'-C5'-O5'
23	GZ	501	GDP	C3'-C4'-C5'-O5'
23	Gc	501	GDP	C3'-C4'-C5'-O5'
23	AW	501	GDP	O4'-C4'-C5'-O5'
23	EQ	501	GDP	C3'-C4'-C5'-O5'
24	a	602	GTP	O4'-C4'-C5'-O5'
24	c	602	GTP	O4'-C4'-C5'-O5'
24	B2	602	GTP	O4'-C4'-C5'-O5'
24	Ew	501	GTP	O4'-C4'-C5'-O5'
24	Fd	602	GTP	O4'-C4'-C5'-O5'
23	A0	501	GDP	PB-O3A-PA-O2A
23	Am	501	GDP	PB-O3A-PA-O1A
24	GD	501	GTP	PG-O3B-PB-O2B
24	GN	501	GTP	PB-O3A-PA-O1A
24	y	602	GTP	PB-O3A-PA-O1A
24	AJ	602	GTP	PB-O3A-PA-O2A
24	Ak	602	GTP	PB-O3A-PA-O1A
24	BU	602	GTP	PG-O3B-PB-O2B
24	E1	501	GTP	PB-O3A-PA-O1A
24	E5	501	GTP	PB-O3A-PA-O1A
24	Em	501	GTP	PG-O3B-PB-O1B
24	Eq	501	GTP	PB-O3A-PA-O1A
24	Fc	501	GTP	PB-O3A-PA-O1A
24	Fh	501	GTP	PB-O3A-PA-O1A
24	Y	602	GTP	C4'-C5'-O5'-PA
24	l	602	GTP	C4'-C5'-O5'-PA
24	E3	501	GTP	C4'-C5'-O5'-PA
24	GE	501	GTP	PA-O3A-PB-O3B
24	G4	602	GTP	O4'-C4'-C5'-O5'
24	W	602	GTP	C3'-C4'-C5'-O5'
24	h	602	GTP	O4'-C4'-C5'-O5'
24	Bu	602	GTP	C3'-C4'-C5'-O5'
24	CA	602	GTP	C3'-C4'-C5'-O5'
24	GF	501	GTP	C4'-C5'-O5'-PA
23	GU	501	GDP	C3'-C4'-C5'-O5'
23	GW	501	GDP	O4'-C4'-C5'-O5'
23	EO	501	GDP	O4'-C4'-C5'-O5'
24	b	602	GTP	O4'-C4'-C5'-O5'
23	GH	501	GDP	PA-O3A-PB-O1B
23	GW	501	GDP	PA-O3A-PB-O1B
23	Gd	501	GDP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	AR	501	GDP	PA-O3A-PB-O1B
23	AW	501	GDP	PA-O3A-PB-O1B
23	Ad	501	GDP	PA-O3A-PB-O1B
23	Av	501	GDP	PA-O3A-PB-O1B
23	BH	501	GDP	PA-O3A-PB-O1B
23	Bh	501	GDP	PA-O3A-PB-O1B
23	Bj	501	GDP	PA-O3A-PB-O1B
23	Br	501	GDP	PA-O3A-PB-O1B
23	DL	501	GDP	PA-O3A-PB-O1B
23	DT	501	GDP	PA-O3A-PB-O1B
23	EO	501	GDP	PA-O3A-PB-O1B
23	EQ	501	GDP	PA-O3A-PB-O1B
23	EV	501	GDP	PA-O3A-PB-O1B
24	c	602	GTP	PB-O3B-PG-O1G
24	Ff	501	GTP	PB-O3B-PG-O1G
24	Fj	501	GTP	PA-O3A-PB-O3B
24	GQ	602	GTP	PA-O3A-PB-O3B
24	Ex	501	GTP	PA-O3A-PB-O3B
23	Fl	501	GDP	PA-O3A-PB-O2B
23	Fl	501	GDP	PA-O3A-PB-O3B
23	Fm	501	GDP	PA-O3A-PB-O2B
23	Fm	501	GDP	PA-O3A-PB-O3B
23	Fn	501	GDP	PA-O3A-PB-O2B
23	Fn	501	GDP	PA-O3A-PB-O3B
23	Fp	501	GDP	PA-O3A-PB-O2B
23	Fp	501	GDP	PA-O3A-PB-O3B
23	Fw	501	GDP	PA-O3A-PB-O2B
23	Fy	501	GDP	PA-O3A-PB-O2B
23	Fy	501	GDP	PA-O3A-PB-O3B
23	Fz	501	GDP	PA-O3A-PB-O2B
23	GH	501	GDP	PA-O3A-PB-O3B
23	GU	501	GDP	PA-O3A-PB-O3B
23	GV	501	GDP	PA-O3A-PB-O2B
23	GV	501	GDP	PA-O3A-PB-O3B
23	GW	501	GDP	PA-O3A-PB-O3B
23	GZ	501	GDP	PA-O3A-PB-O2B
23	GZ	501	GDP	PA-O3A-PB-O3B
23	Gd	501	GDP	PA-O3A-PB-O2B
23	Gd	501	GDP	PA-O3A-PB-O3B
23	Gh	501	GDP	PA-O3A-PB-O2B
23	Gh	501	GDP	PA-O3A-PB-O3B
23	Gi	501	GDP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Gk	501	GDP	PA-O3A-PB-O3B
23	AB	501	GDP	PA-O3A-PB-O3B
23	AL	501	GDP	PA-O3A-PB-O2B
23	AM	501	GDP	PA-O3A-PB-O2B
23	AM	501	GDP	PA-O3A-PB-O3B
23	AO	501	GDP	PA-O3A-PB-O2B
23	AO	501	GDP	PA-O3A-PB-O3B
23	AP	501	GDP	PA-O3A-PB-O2B
23	Aa	501	GDP	PA-O3A-PB-O2B
23	Aa	501	GDP	PA-O3A-PB-O3B
23	Ab	501	GDP	PA-O3A-PB-O2B
23	Ac	501	GDP	PA-O3A-PB-O3B
23	Ai	501	GDP	PA-O3A-PB-O2B
23	Ar	501	GDP	PA-O3A-PB-O2B
23	Ar	501	GDP	PA-O3A-PB-O3B
23	Av	501	GDP	PA-O3A-PB-O2B
23	BB	501	GDP	PA-O3A-PB-O2B
23	BB	501	GDP	PA-O3A-PB-O3B
23	BH	501	GDP	PA-O3A-PB-O2B
23	Bg	501	GDP	PA-O3A-PB-O2B
23	Bh	501	GDP	PA-O3A-PB-O2B
23	Bh	501	GDP	PA-O3A-PB-O3B
23	Bj	501	GDP	PA-O3A-PB-O2B
23	Bk	501	GDP	PA-O3A-PB-O2B
23	DL	501	GDP	PA-O3A-PB-O2B
23	DL	501	GDP	PA-O3A-PB-O3B
23	DN	501	GDP	PA-O3A-PB-O2B
23	DN	501	GDP	PA-O3A-PB-O3B
23	DP	501	GDP	PA-O3A-PB-O2B
23	DP	501	GDP	PA-O3A-PB-O3B
23	DQ	501	GDP	PA-O3A-PB-O2B
23	DQ	501	GDP	PA-O3A-PB-O3B
23	DT	501	GDP	PA-O3A-PB-O2B
23	DT	501	GDP	PA-O3A-PB-O3B
23	DV	501	GDP	PA-O3A-PB-O2B
23	DV	501	GDP	PA-O3A-PB-O3B
23	DX	501	GDP	PA-O3A-PB-O2B
23	DX	501	GDP	PA-O3A-PB-O3B
23	Da	501	GDP	PA-O3A-PB-O2B
23	Da	501	GDP	PA-O3A-PB-O3B
23	Db	501	GDP	PA-O3A-PB-O2B
23	Db	501	GDP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Dd	501	GDP	PA-O3A-PB-O2B
23	Dd	501	GDP	PA-O3A-PB-O3B
23	De	501	GDP	PA-O3A-PB-O2B
23	De	501	GDP	PA-O3A-PB-O3B
23	Df	501	GDP	PA-O3A-PB-O2B
23	Df	501	GDP	PA-O3A-PB-O3B
23	Dx	501	GDP	PA-O3A-PB-O2B
23	Dx	501	GDP	PA-O3A-PB-O3B
23	EM	501	GDP	PA-O3A-PB-O2B
23	EM	501	GDP	PA-O3A-PB-O3B
23	EO	501	GDP	PA-O3A-PB-O3B
23	EP	501	GDP	PA-O3A-PB-O2B
23	EP	501	GDP	PA-O3A-PB-O3B
23	EQ	501	GDP	PA-O3A-PB-O2B
23	EQ	501	GDP	PA-O3A-PB-O3B
23	ER	501	GDP	PA-O3A-PB-O2B
23	ER	501	GDP	PA-O3A-PB-O3B
23	ET	501	GDP	PA-O3A-PB-O3B
23	EV	501	GDP	PA-O3A-PB-O2B
23	EV	501	GDP	PA-O3A-PB-O3B
23	EX	501	GDP	PA-O3A-PB-O2B
23	EY	501	GDP	PA-O3A-PB-O2B
23	EY	501	GDP	PA-O3A-PB-O3B
23	Ea	501	GDP	PA-O3A-PB-O2B
23	Ea	501	GDP	PA-O3A-PB-O3B
23	Ef	501	GDP	PA-O3A-PB-O2B
23	F2	501	GDP	PA-O3A-PB-O2B
23	F4	501	GDP	PA-O3A-PB-O2B
23	F4	501	GDP	PA-O3A-PB-O3B
23	FA	501	GDP	PA-O3A-PB-O2B
23	FA	501	GDP	PA-O3A-PB-O3B
23	FE	501	GDP	PA-O3A-PB-O2B
23	FE	501	GDP	PA-O3A-PB-O3B
23	FG	501	GDP	PA-O3A-PB-O2B
23	FG	501	GDP	PA-O3A-PB-O3B
23	FI	501	GDP	PA-O3A-PB-O2B
23	FK	501	GDP	PA-O3A-PB-O2B
23	FL	501	GDP	PA-O3A-PB-O2B
23	FL	501	GDP	PA-O3A-PB-O3B
23	FN	501	GDP	PA-O3A-PB-O2B
23	FN	501	GDP	PA-O3A-PB-O3B
24	Fj	501	GTP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Fj	501	GTP	PB-O3B-PG-O3G
24	G2	501	GTP	PB-O3B-PG-O2G
24	GC	501	GTP	PB-O3B-PG-O2G
24	GF	501	GTP	PB-O3B-PG-O2G
24	GN	501	GTP	PB-O3B-PG-O2G
24	GN	501	GTP	PB-O3B-PG-O3G
24	A2	602	GTP	PB-O3B-PG-O3G
24	Gx	501	GTP	PB-O3B-PG-O2G
24	W	602	GTP	PB-O3B-PG-O3G
24	Y	602	GTP	PB-O3B-PG-O3G
24	c	602	GTP	PB-O3B-PG-O2G
24	c	602	GTP	PB-O3B-PG-O3G
24	o	501	GTP	PB-O3B-PG-O2G
24	o	501	GTP	PB-O3B-PG-O3G
24	q	602	GTP	PB-O3B-PG-O2G
24	Aw	602	GTP	PB-O3B-PG-O2G
24	Aw	602	GTP	PB-O3B-PG-O3G
24	B6	602	GTP	PB-O3B-PG-O2G
24	B6	602	GTP	PB-O3B-PG-O3G
24	BI	602	GTP	PB-O3B-PG-O2G
24	BI	602	GTP	PB-O3B-PG-O3G
24	BK	602	GTP	PB-O3B-PG-O2G
24	Bw	602	GTP	PB-O3B-PG-O2G
24	Bw	602	GTP	PB-O3B-PG-O3G
24	5	602	GTP	PB-O3B-PG-O2G
24	BU	602	GTP	C4'-C5'-O5'-PA
24	Fb	501	GTP	C4'-C5'-O5'-PA
23	Gf	501	GDP	O4'-C4'-C5'-O5'
23	Bi	501	GDP	C3'-C4'-C5'-O5'
23	EN	501	GDP	C3'-C4'-C5'-O5'
23	ER	501	GDP	O4'-C4'-C5'-O5'
24	Y	602	GTP	O4'-C4'-C5'-O5'
24	GP	501	GTP	PA-O3A-PB-O3B
23	AF	501	GDP	C3'-C4'-C5'-O5'
23	AT	501	GDP	C3'-C4'-C5'-O5'
23	BD	501	GDP	C3'-C4'-C5'-O5'
23	Bn	501	GDP	C3'-C4'-C5'-O5'
23	EX	501	GDP	O4'-C4'-C5'-O5'
24	Q	602	GTP	C3'-C4'-C5'-O5'
24	Bz	602	GTP	O4'-C4'-C5'-O5'
24	Ei	501	GTP	C3'-C4'-C5'-O5'
24	Et	501	GTP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	Ex	501	GTP	C3'-C4'-C5'-O5'
24	BS	602	GTP	C4'-C5'-O5'-PA
23	Gb	501	GDP	PB-O3A-PA-O2A
23	AE	501	GDP	PB-O3A-PA-O2A
23	AG	501	GDP	PB-O3A-PA-O2A
23	AS	502	GDP	PB-O3A-PA-O1A
23	AS	502	GDP	PB-O3A-PA-O2A
23	Ag	501	GDP	PB-O3A-PA-O2A
23	Ap	501	GDP	PB-O3A-PA-O2A
23	BF	501	GDP	PB-O3A-PA-O1A
23	BF	501	GDP	PB-O3A-PA-O2A
23	Be	501	GDP	PB-O3A-PA-O2A
23	8	501	GDP	PB-O3A-PA-O2A
23	FK	501	GDP	PB-O3A-PA-O1A
24	Fi	501	GTP	PG-O3B-PB-O1B
24	Fj	501	GTP	PA-O3A-PB-O2B
24	G1	501	GTP	PB-O3A-PA-O2A
24	G3	602	GTP	PG-O3B-PB-O2B
24	G3	602	GTP	PB-O3A-PA-O2A
24	G4	602	GTP	PB-O3A-PA-O2A
24	G5	501	GTP	PB-O3A-PA-O2A
24	GB	501	GTP	PB-O3A-PA-O2A
24	GD	501	GTP	PB-O3A-PA-O2A
24	GE	501	GTP	PG-O3B-PB-O1B
24	GE	501	GTP	PA-O3A-PB-O1B
24	GF	501	GTP	PA-O3A-PB-O1B
24	GF	501	GTP	PB-O3A-PA-O2A
24	GP	501	GTP	PA-O3A-PB-O2B
24	GP	501	GTP	PB-O3A-PA-O2A
24	GQ	602	GTP	PA-O3A-PB-O1B
24	GR	501	GTP	PG-O3B-PB-O2B
24	Gp	501	GTP	PB-O3A-PA-O2A
24	Gt	501	GTP	PG-O3B-PB-O1B
24	Gt	501	GTP	PG-O3B-PB-O2B
24	Gt	501	GTP	PA-O3A-PB-O2B
24	Gu	501	GTP	PG-O3B-PB-O1B
24	Gu	501	GTP	PA-O3A-PB-O2B
24	Gv	501	GTP	PB-O3A-PA-O1A
24	Gy	501	GTP	PB-O3A-PA-O2A
24	Q	602	GTP	PB-O3A-PA-O2A
24	S	602	GTP	PB-O3A-PA-O1A
24	Y	602	GTP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	c	602	GTP	PB-O3A-PA-O1A
24	v	602	GTP	PG-O3B-PB-O2B
24	w	602	GTP	PA-O3A-PB-O1B
24	y	602	GTP	PG-O3B-PB-O2B
24	y	602	GTP	PB-O3A-PA-O2A
24	z	602	GTP	PG-O3B-PB-O2B
24	z	602	GTP	PB-O3A-PA-O1A
24	z	602	GTP	PB-O3A-PA-O2A
24	A5	501	GTP	PB-O3A-PA-O2A
24	AJ	602	GTP	PG-O3B-PB-O2B
24	AK	602	GTP	PA-O3A-PB-O1B
24	Ak	602	GTP	PG-O3B-PB-O2B
24	Al	602	GTP	PB-O3A-PA-O1A
24	B2	602	GTP	PG-O3B-PB-O1B
24	B8	602	GTP	PG-O3B-PB-O2B
24	B9	602	GTP	PA-O3A-PB-O1B
24	BV	602	GTP	PB-O3A-PA-O1A
24	BV	602	GTP	PB-O3A-PA-O2A
24	Bc	501	GTP	PB-O3A-PA-O2A
24	Bd	501	GTP	PB-O3A-PA-O2A
24	Bw	602	GTP	PB-O3A-PA-O1A
24	Bx	602	GTP	PB-O3A-PA-O2A
24	CA	602	GTP	PG-O3B-PB-O2B
24	E2	501	GTP	PG-O3B-PB-O2B
24	E3	501	GTP	PB-O3A-PA-O1A
24	E5	501	GTP	PG-O3B-PB-O2B
24	E5	501	GTP	PB-O3A-PA-O2A
24	E6	602	GTP	PG-O3B-PB-O2B
24	Ee	501	GTP	PG-O3B-PB-O1B
24	Ei	501	GTP	PG-O3B-PB-O1B
24	Em	501	GTP	PA-O3A-PB-O2B
24	Eo	501	GTP	PB-O3A-PA-O2A
24	Ep	501	GTP	PB-O3A-PA-O2A
24	Er	501	GTP	PB-O3A-PA-O2A
24	Ew	501	GTP	PG-O3B-PB-O2B
24	Ew	501	GTP	PB-O3A-PA-O2A
24	Ex	501	GTP	PG-O3B-PB-O1B
24	Ex	501	GTP	PA-O3A-PB-O1B
24	Ez	501	GTP	PG-O3B-PB-O1B
24	F0	501	GTP	PB-O3A-PA-O2A
24	F5	501	GTP	PB-O3A-PA-O2A
24	F7	501	GTP	PG-O3B-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	F9	501	GTP	PB-O3A-PA-O2A
24	FY	501	GTP	PB-O3A-PA-O2A
24	FZ	501	GTP	PB-O3A-PA-O2A
24	Fb	501	GTP	PB-O3A-PA-O2A
24	Fd	602	GTP	PG-O3B-PB-O2B
24	Fd	602	GTP	PB-O3A-PA-O2A
24	Fe	501	GTP	PA-O3A-PB-O1B
24	Fe	501	GTP	PA-O3A-PB-O2B
24	Fe	501	GTP	PB-O3A-PA-O1A
24	Ff	501	GTP	PB-O3A-PA-O1A
24	Fh	501	GTP	PG-O3B-PB-O2B
23	GY	501	GDP	C3'-C4'-C5'-O5'
23	AH	501	GDP	C3'-C4'-C5'-O5'
23	Df	501	GDP	C3'-C4'-C5'-O5'
23	Dg	501	GDP	C3'-C4'-C5'-O5'
23	EU	501	GDP	C3'-C4'-C5'-O5'
23	FD	501	GDP	C3'-C4'-C5'-O5'
24	GE	501	GTP	C3'-C4'-C5'-O5'
24	Ak	602	GTP	C4'-C5'-O5'-PA
24	Ex	501	GTP	C4'-C5'-O5'-PA
24	E1	501	GTP	PA-O3A-PB-O3B
24	E5	501	GTP	PA-O3A-PB-O3B
24	Em	501	GTP	PA-O3A-PB-O3B
23	Ga	501	GDP	PA-O3A-PB-O1B
23	BC	501	GDP	PA-O3A-PB-O1B
23	Bm	501	GDP	PA-O3A-PB-O1B
23	EX	501	GDP	PA-O3A-PB-O1B
23	GV	501	GDP	C3'-C4'-C5'-O5'
23	DN	501	GDP	C3'-C4'-C5'-O5'
23	DX	501	GDP	O4'-C4'-C5'-O5'
23	Dh	501	GDP	C3'-C4'-C5'-O5'
23	Dr	501	GDP	C3'-C4'-C5'-O5'
23	E0	501	GDP	C3'-C4'-C5'-O5'
23	FF	501	GDP	C3'-C4'-C5'-O5'
24	W	602	GTP	O4'-C4'-C5'-O5'
24	CA	602	GTP	O4'-C4'-C5'-O5'
24	G4	602	GTP	C4'-C5'-O5'-PA
24	E2	501	GTP	C4'-C5'-O5'-PA
23	DP	501	GDP	C3'-C4'-C5'-O5'
23	DT	501	GDP	C3'-C4'-C5'-O5'
24	GR	501	GTP	C4'-C5'-O5'-PA
24	E6	602	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Ae	501	GDP	PB-O3A-PA-O2A
23	An	501	GDP	PB-O3A-PA-O2A
23	Ap	501	GDP	PB-O3A-PA-O1A
23	BD	501	GDP	PB-O3A-PA-O2A
23	Bn	501	GDP	PB-O3A-PA-O2A
23	Bp	501	GDP	PB-O3A-PA-O1A
23	F1	501	GDP	PB-O3A-PA-O2A
24	Fi	501	GTP	PG-O3B-PB-O2B
24	Fj	501	GTP	PA-O3A-PB-O1B
24	Fj	501	GTP	PB-O3A-PA-O1A
24	G2	501	GTP	PB-O3A-PA-O2A
24	G4	602	GTP	PG-O3B-PB-O2B
24	G4	602	GTP	PA-O3A-PB-O2B
24	GE	501	GTP	PG-O3B-PB-O2B
24	GE	501	GTP	PB-O3A-PA-O2A
24	GF	501	GTP	PA-O3A-PB-O2B
24	GG	501	GTP	PB-O3A-PA-O2A
24	GI	501	GTP	PB-O3A-PA-O2A
24	GJ	501	GTP	PG-O3B-PB-O2B
24	GJ	501	GTP	PB-O3A-PA-O2A
24	GK	501	GTP	PB-O3A-PA-O2A
24	GM	501	GTP	PB-O3A-PA-O2A
24	GO	602	GTP	PA-O3A-PB-O2B
24	GP	501	GTP	PG-O3B-PB-O2B
24	GP	501	GTP	PA-O3A-PB-O1B
24	GQ	602	GTP	PG-O3B-PB-O2B
24	GS	501	GTP	PB-O3A-PA-O2A
24	GT	501	GTP	PB-O3A-PA-O2A
24	Gn	501	GTP	PB-O3A-PA-O2A
24	Gq	501	GTP	PB-O3A-PA-O2A
24	Gr	501	GTP	PB-O3A-PA-O2A
24	Gt	501	GTP	PB-O3A-PA-O2A
24	Gu	501	GTP	PG-O3B-PB-O2B
24	Gw	501	GTP	PB-O3A-PA-O2A
24	Gx	501	GTP	PB-O3A-PA-O1A
24	Gz	501	GTP	PB-O3A-PA-O2A
24	Q	602	GTP	PB-O3A-PA-O1A
24	V	602	GTP	PB-O3A-PA-O2A
24	a	602	GTP	PG-O3B-PB-O2B
24	b	602	GTP	PG-O3B-PB-O2B
24	e	602	GTP	PA-O3A-PB-O2B
24	f	602	GTP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	g	602	GTP	PB-O3A-PA-O2A
24	i	602	GTP	PG-O3B-PB-O2B
24	j	602	GTP	PG-O3B-PB-O2B
24	k	602	GTP	PA-O3A-PB-O2B
24	l	602	GTP	PA-O3A-PB-O2B
24	o	501	GTP	PB-O3A-PA-O2A
24	A4	501	GTP	PB-O3A-PA-O2A
24	q	602	GTP	PB-O3A-PA-O2A
24	v	602	GTP	PB-O3A-PA-O1A
24	A5	501	GTP	PG-O3B-PB-O2B
24	A6	501	GTP	PB-O3A-PA-O2A
24	A7	501	GTP	PB-O3A-PA-O2A
24	A8	501	GTP	PG-O3B-PB-O2B
24	A8	501	GTP	PB-O3A-PA-O2A
24	A9	501	GTP	PA-O3A-PB-O2B
24	A9	501	GTP	PB-O3A-PA-O2A
24	Al	602	GTP	PG-O3B-PB-O2B
24	Al	602	GTP	PB-O3A-PA-O2A
24	Ay	602	GTP	PA-O3A-PB-O2B
24	B1	602	GTP	PG-O3B-PB-O2B
24	B3	602	GTP	PA-O3A-PB-O2B
24	B8	602	GTP	PB-O3A-PA-O1A
24	BI	602	GTP	PB-O3A-PA-O1A
24	BL	602	GTP	PB-O3A-PA-O2A
24	BM	602	GTP	PG-O3B-PB-O2B
24	BN	602	GTP	PG-O3B-PB-O2B
24	BO	602	GTP	PA-O3A-PB-O2B
24	BP	602	GTP	PA-O3A-PB-O2B
24	BS	602	GTP	PG-O3B-PB-O2B
24	BS	602	GTP	PB-O3A-PA-O2A
24	BU	602	GTP	PB-O3A-PA-O1A
24	Bd	501	GTP	PG-O3B-PB-O2B
24	By	602	GTP	PB-O3A-PA-O2A
24	Bz	602	GTP	PB-O3A-PA-O2A
24	CA	602	GTP	PB-O3A-PA-O1A
24	CB	602	GTP	PG-O3B-PB-O2B
24	E1	501	GTP	PG-O3B-PB-O2B
24	E1	501	GTP	PA-O3A-PB-O1B
24	E1	501	GTP	PB-O3A-PA-O2A
24	E4	501	GTP	PA-O3A-PB-O2B
24	E4	501	GTP	PB-O3A-PA-O2A
24	E5	501	GTP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	E8	501	GTP	PB-O3A-PA-O2A
24	Ee	501	GTP	PA-O3A-PB-O2B
24	Eg	501	GTP	PG-O3B-PB-O2B
24	Eg	501	GTP	PB-O3A-PA-O2A
24	Eh	501	GTP	PA-O3A-PB-O2B
24	Ei	501	GTP	PA-O3A-PB-O2B
24	Ej	501	GTP	PG-O3B-PB-O2B
24	Ej	501	GTP	PB-O3A-PA-O2A
24	El	501	GTP	PG-O3B-PB-O2B
24	El	501	GTP	PB-O3A-PA-O2A
24	Em	501	GTP	PG-O3B-PB-O2B
24	En	501	GTP	PB-O3A-PA-O2A
24	Es	501	GTP	PA-O3A-PB-O2B
24	Eu	501	GTP	PB-O3A-PA-O2A
24	Ex	501	GTP	PG-O3B-PB-O2B
24	Ey	602	GTP	PB-O3A-PA-O2A
24	Ez	501	GTP	PG-O3B-PB-O2B
24	Ez	501	GTP	PA-O3A-PB-O2B
24	F0	501	GTP	PG-O3B-PB-O2B
24	F3	501	GTP	PB-O3A-PA-O2A
24	F6	501	GTP	PG-O3B-PB-O2B
24	F6	501	GTP	PB-O3A-PA-O2A
24	F7	501	GTP	PA-O3A-PB-O2B
24	F8	501	GTP	PG-O3B-PB-O1B
24	F8	501	GTP	PA-O3A-PB-O2B
24	F8	501	GTP	PB-O3A-PA-O2A
24	F9	501	GTP	PG-O3B-PB-O2B
24	FM	501	GTP	PB-O3A-PA-O2A
24	FO	501	GTP	PB-O3A-PA-O2A
24	FP	501	GTP	PB-O3A-PA-O2A
24	FQ	501	GTP	PG-O3B-PB-O2B
24	FQ	501	GTP	PB-O3A-PA-O2A
24	FR	501	GTP	PG-O3B-PB-O2B
24	FR	501	GTP	PB-O3A-PA-O2A
24	FT	501	GTP	PB-O3A-PA-O2A
24	FU	501	GTP	PA-O3A-PB-O2B
24	FU	501	GTP	PB-O3A-PA-O2A
24	FV	602	GTP	PB-O3A-PA-O2A
24	FW	501	GTP	PB-O3A-PA-O2A
24	FX	501	GTP	PB-O3A-PA-O2A
24	FZ	501	GTP	PG-O3B-PB-O2B
24	Fa	501	GTP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

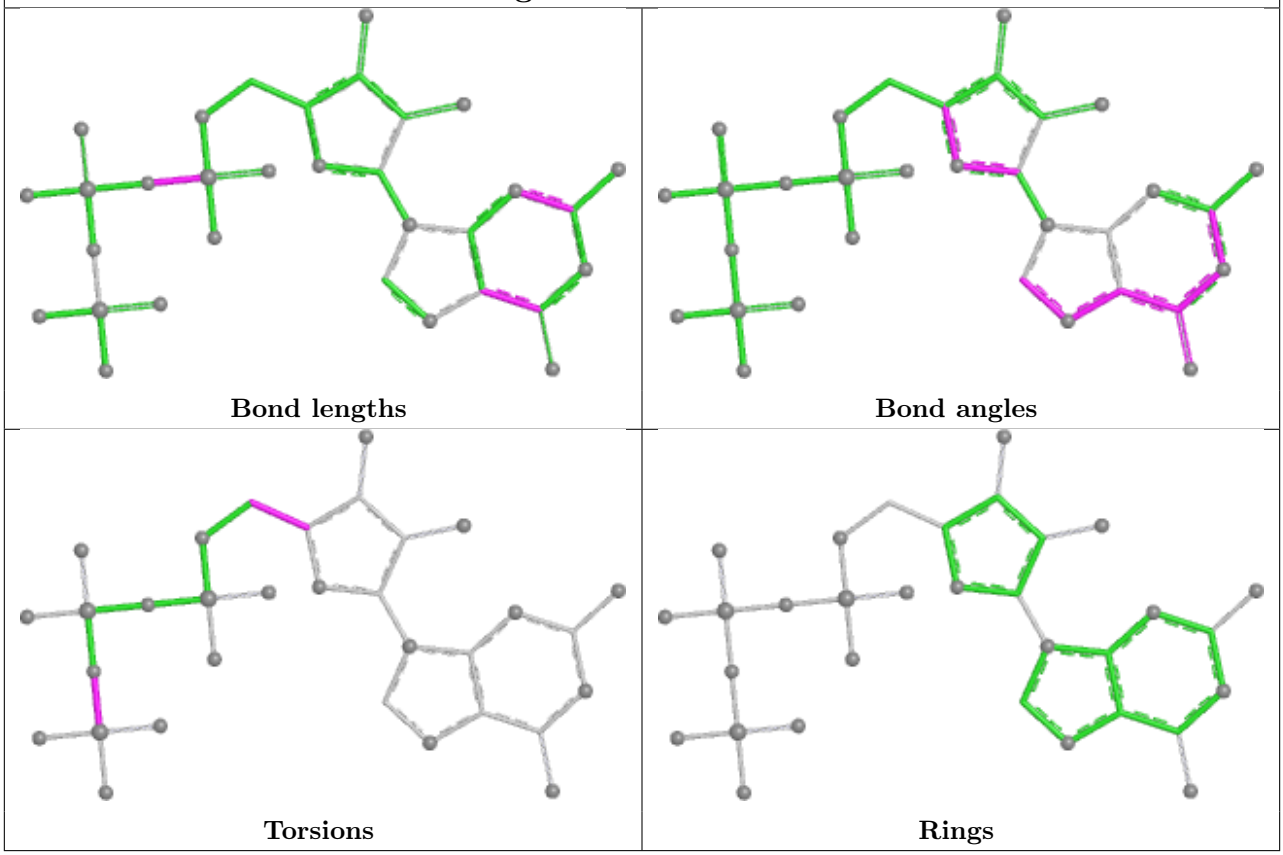
Mol	Chain	Res	Type	Atoms
24	Fe	501	GTP	PG-O3B-PB-O2B
24	Fh	501	GTP	PB-O3A-PA-O2A
23	BA	501	GDP	O4'-C4'-C5'-O5'
23	Bl	602	GDP	O4'-C4'-C5'-O5'
24	GP	501	GTP	O4'-C4'-C5'-O5'
24	Bu	602	GTP	O4'-C4'-C5'-O5'
24	Ez	501	GTP	PA-O3A-PB-O3B

There are no ring outliers.

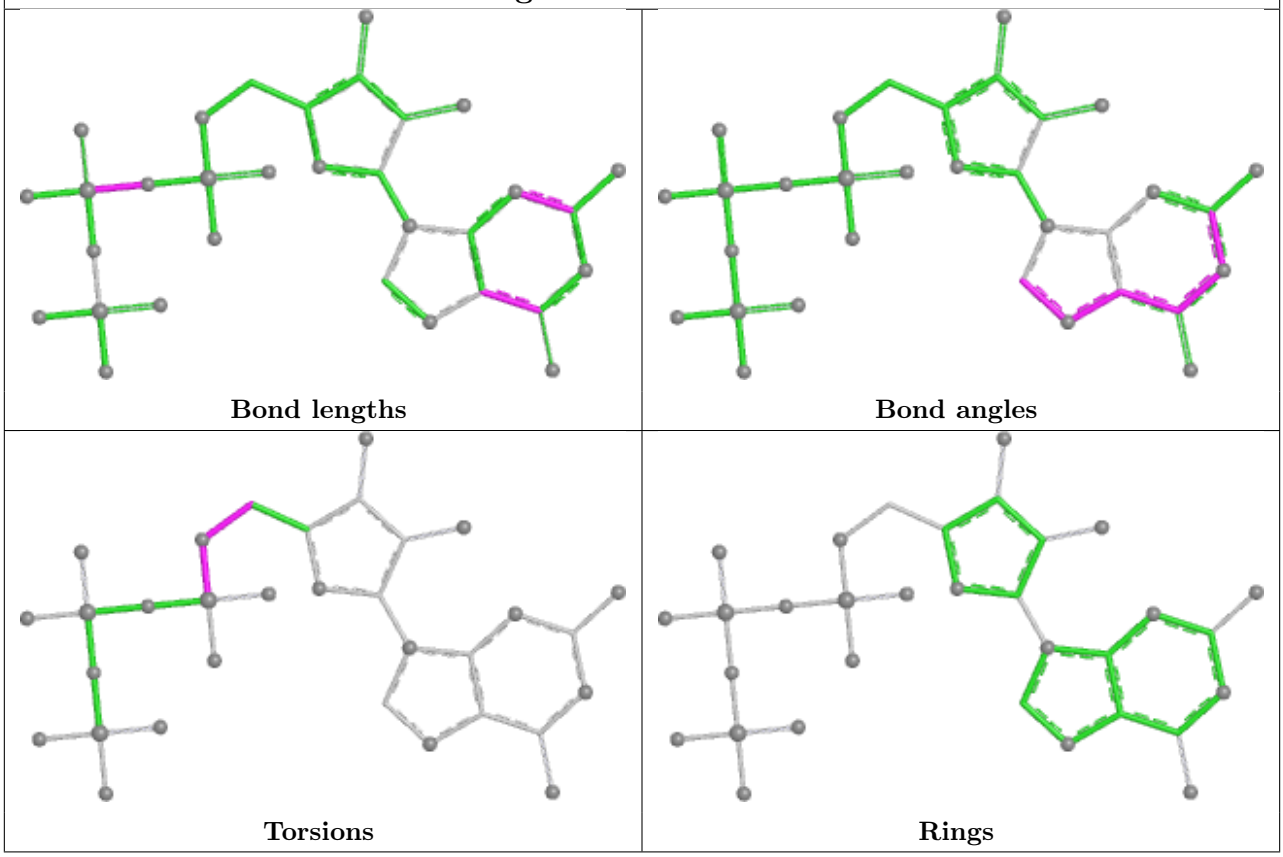
No monomer is involved in short contacts.

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 then 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.

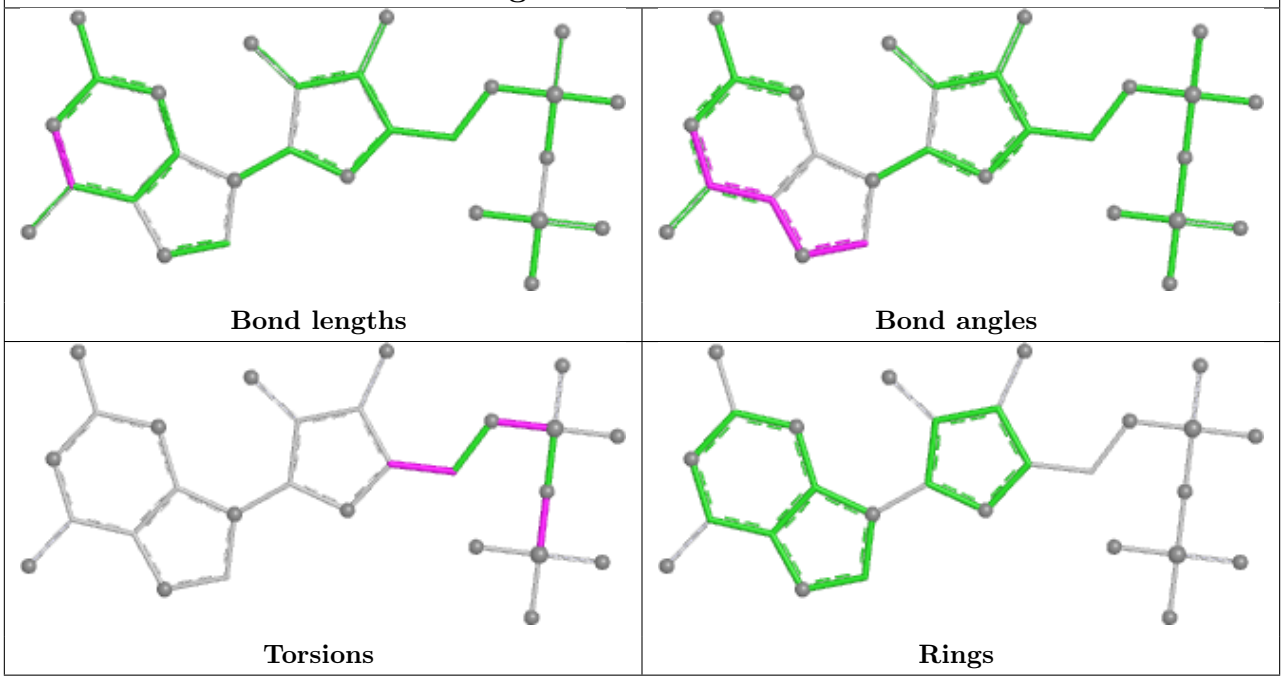
Ligand GTP B6 602



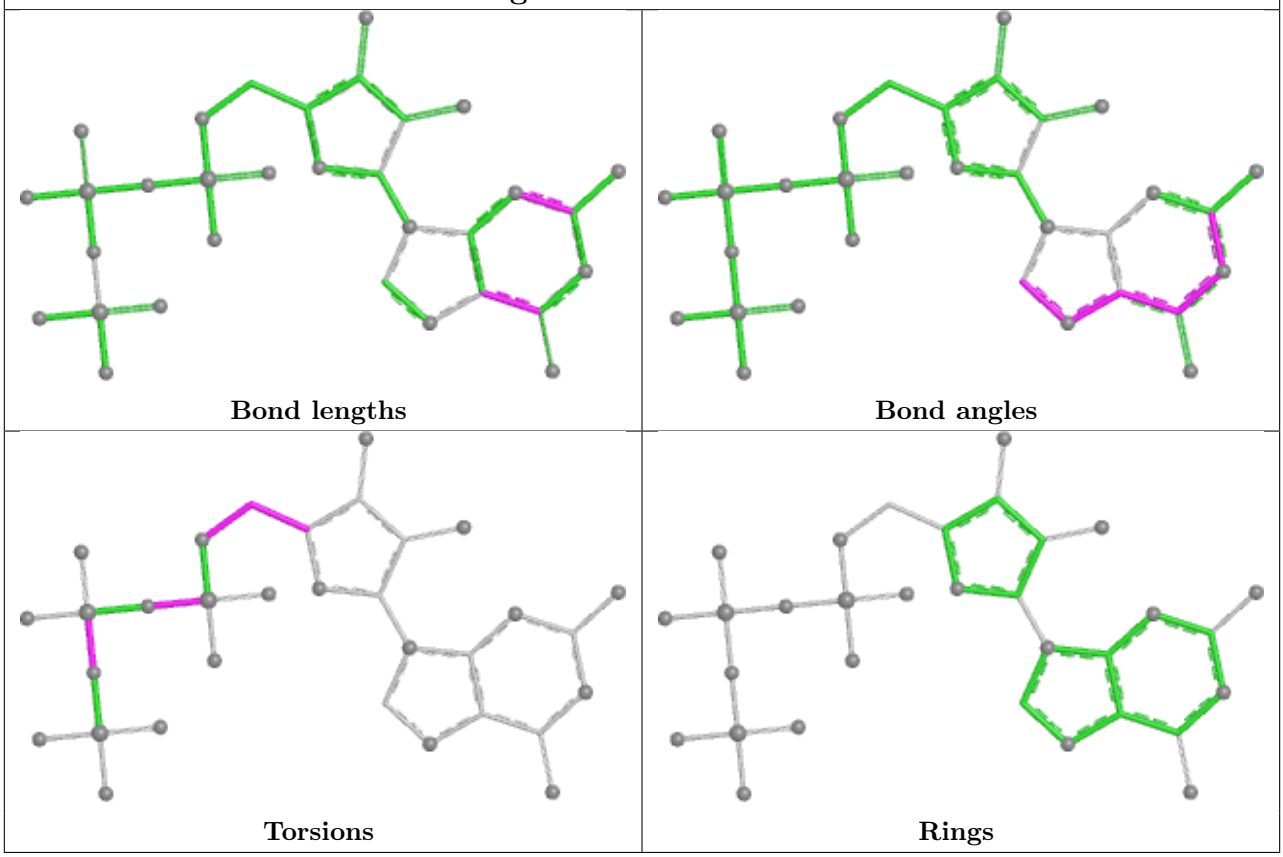
Ligand GTP Ek 501



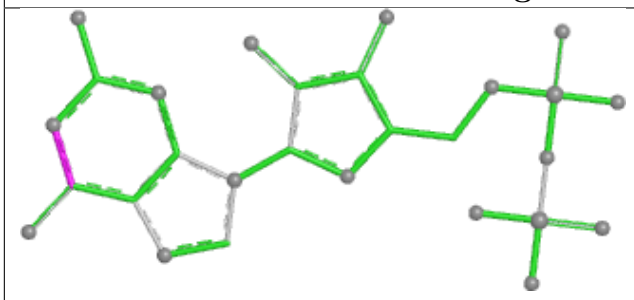
Ligand GDP AO 501



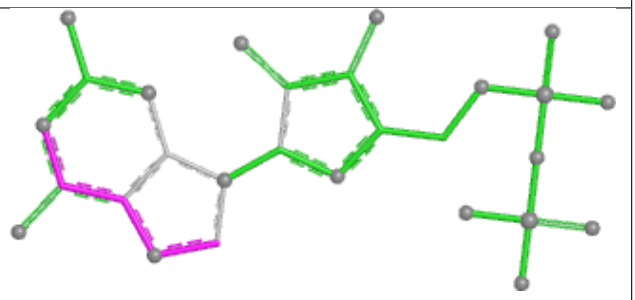
Ligand GTP BU 602



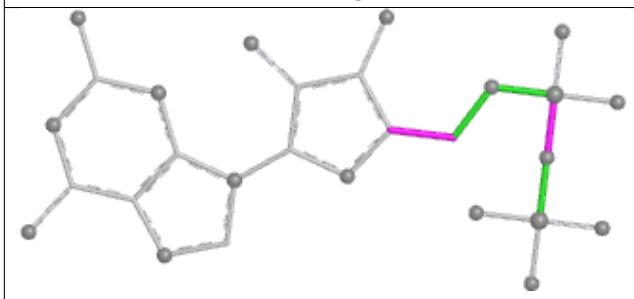
Ligand GDP Az 501



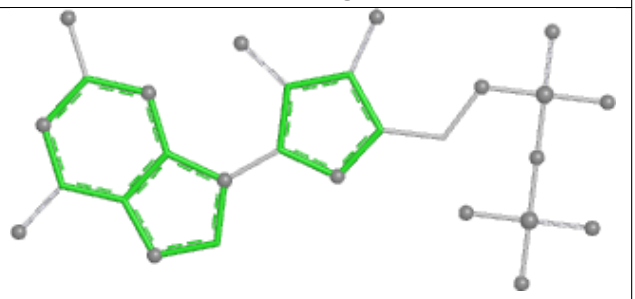
Bond lengths



Bond angles

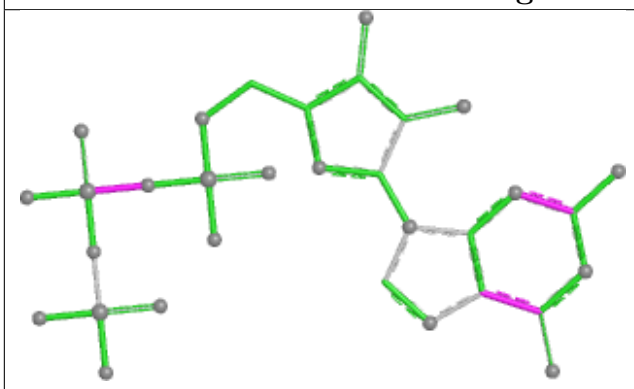


Torsions

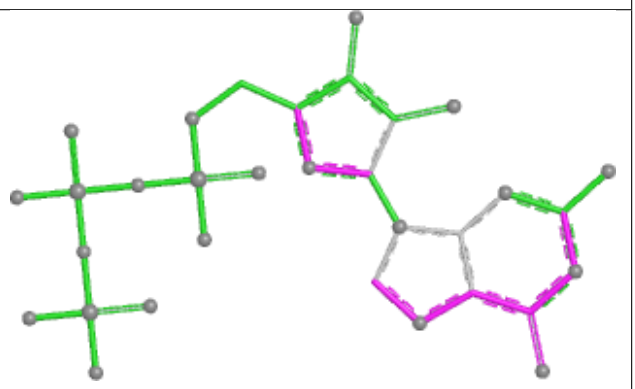


Rings

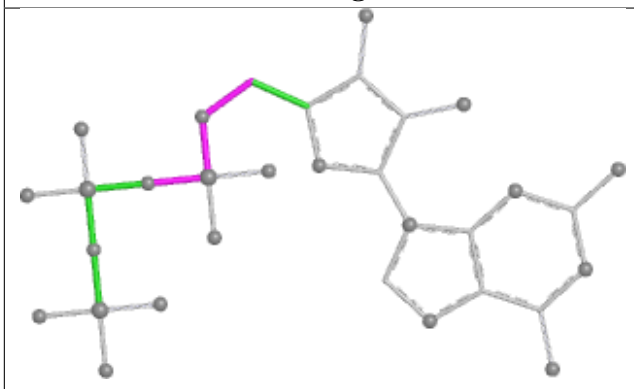
Ligand GTP E3 501



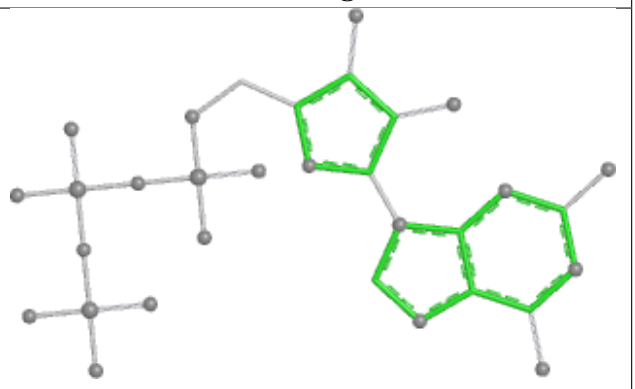
Bond lengths



Bond angles

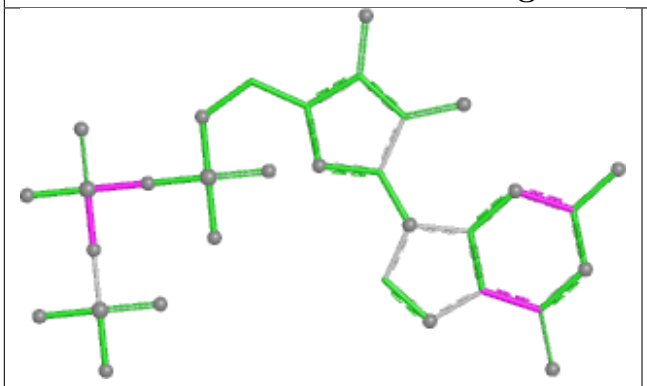


Torsions

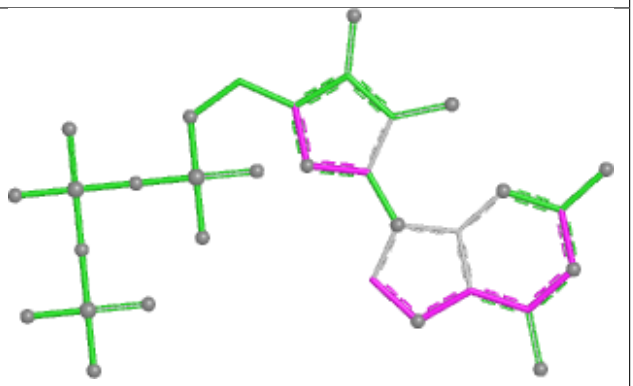


Rings

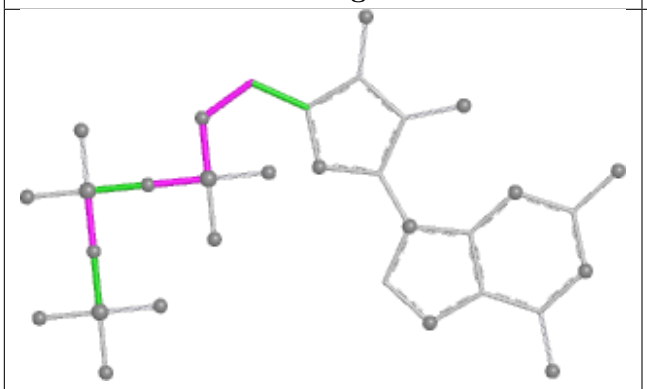
Ligand GTP Al 602



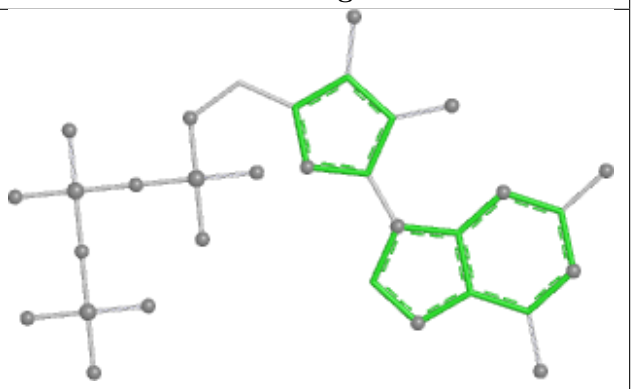
Bond lengths



Bond angles

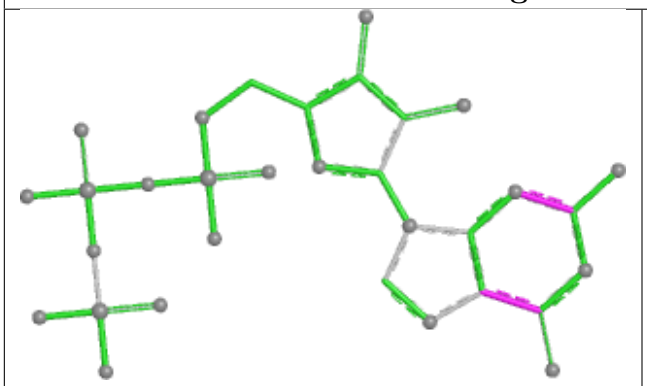


Torsions

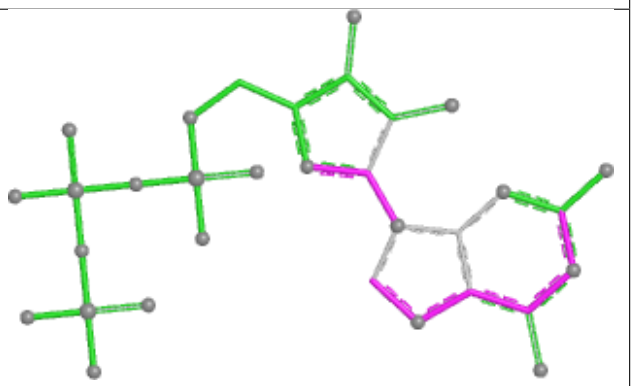


Rings

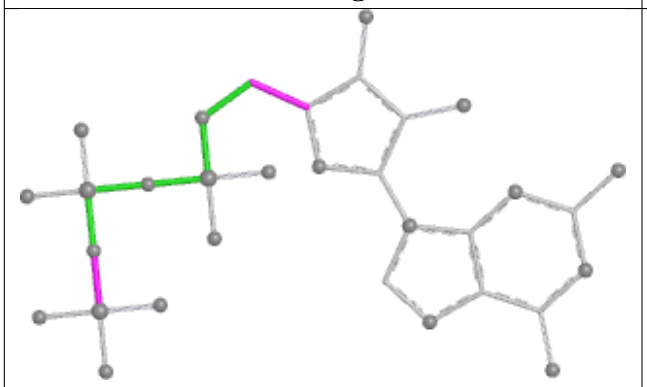
Ligand GTP BX 602



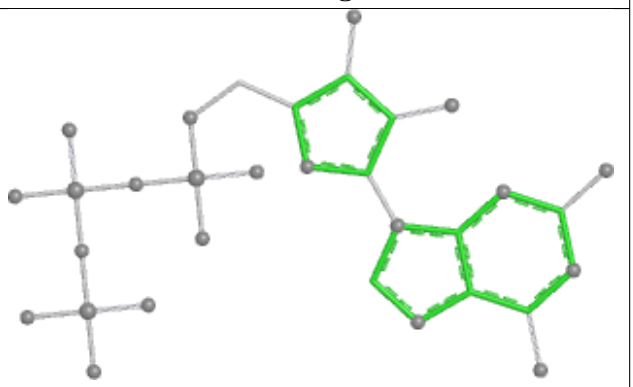
Bond lengths



Bond angles

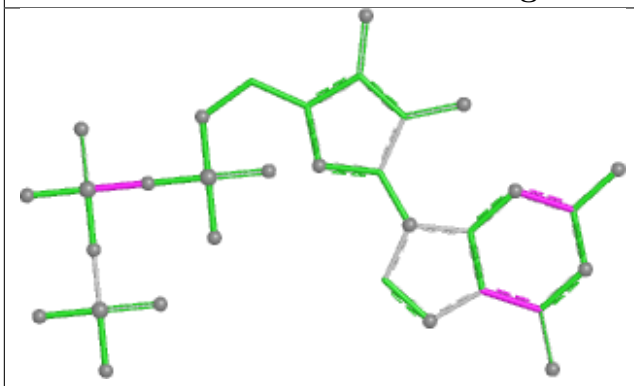


Torsions

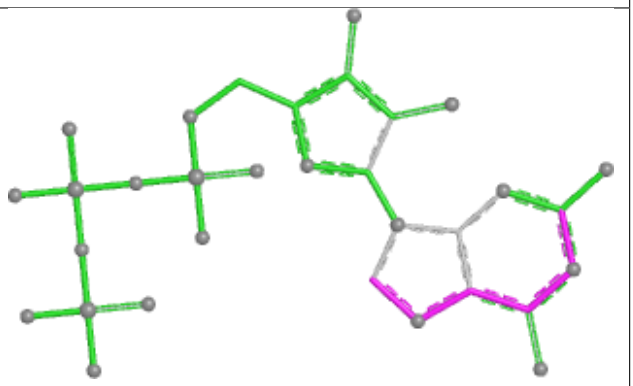


Rings

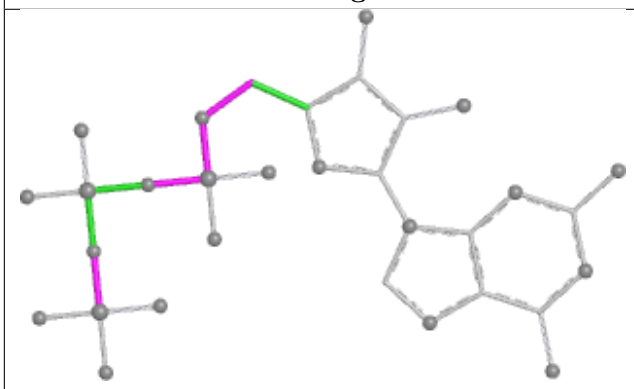
Ligand GTP Ff 501



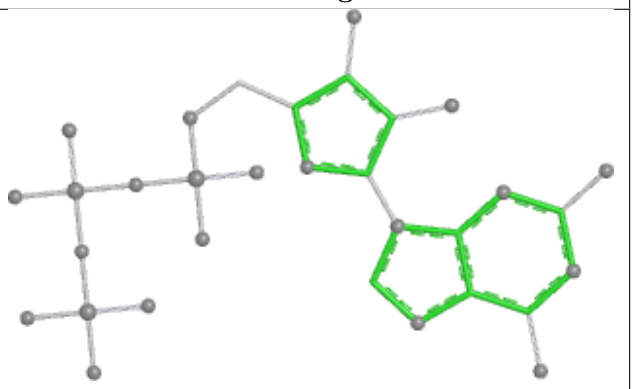
Bond lengths



Bond angles

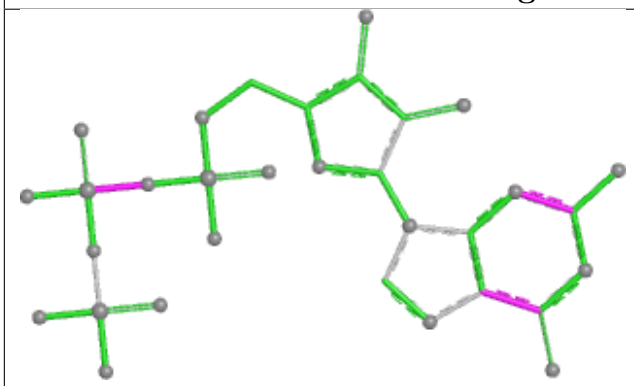


Torsions

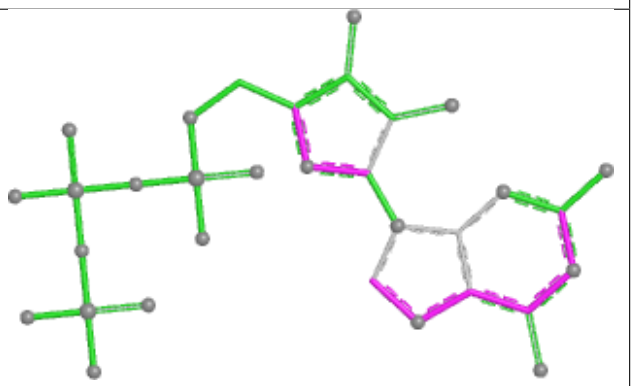


Rings

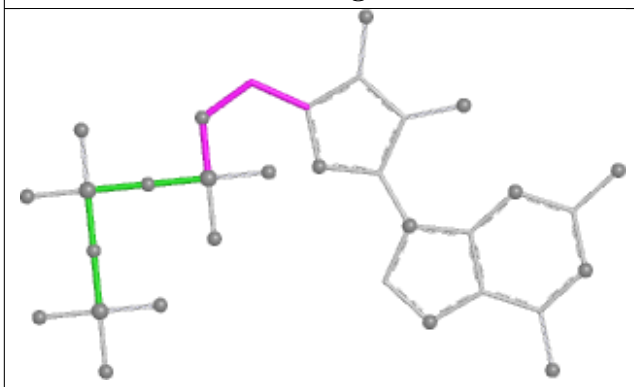
Ligand GTP Et 501



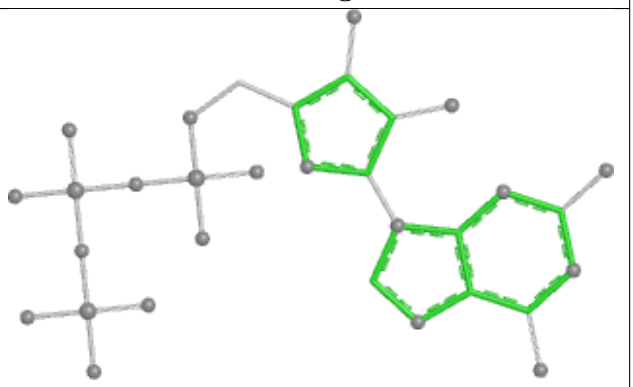
Bond lengths



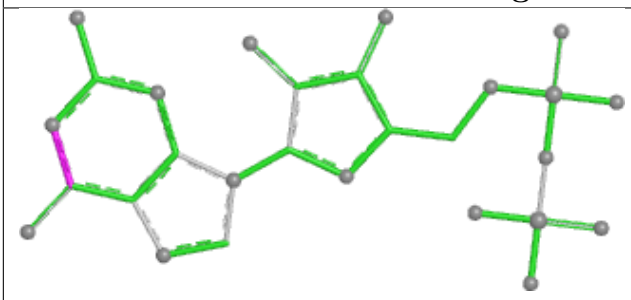
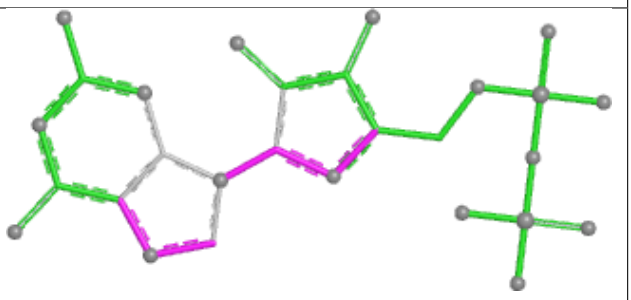
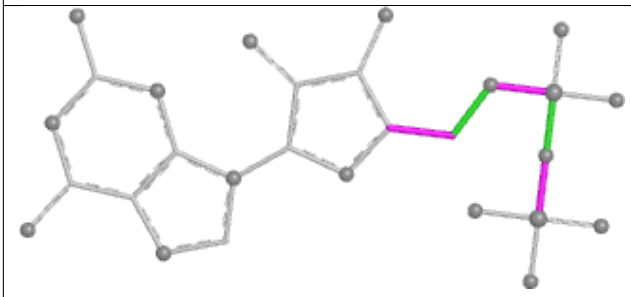
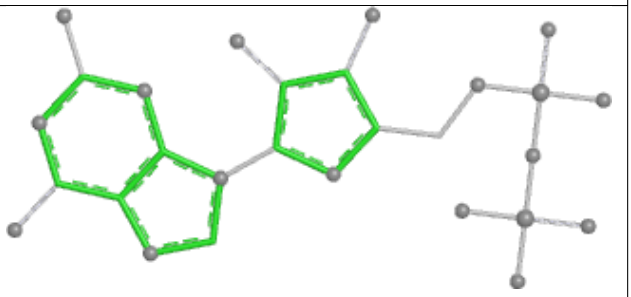
Bond angles

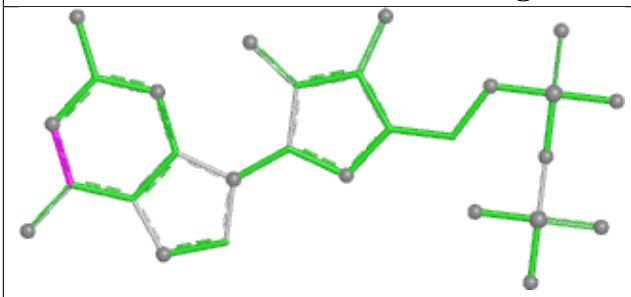
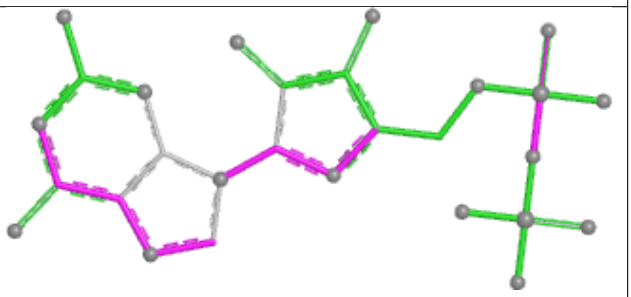
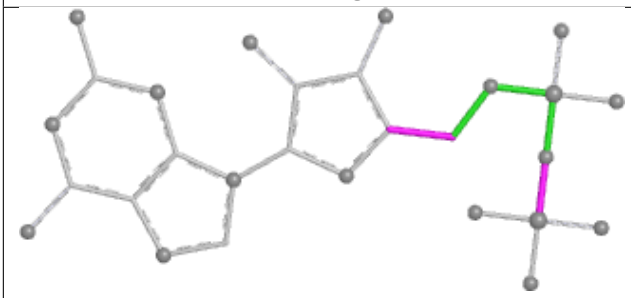
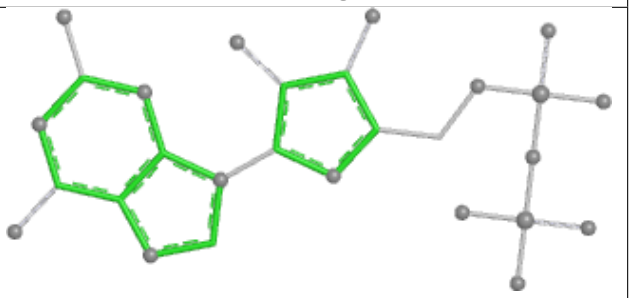


Torsions

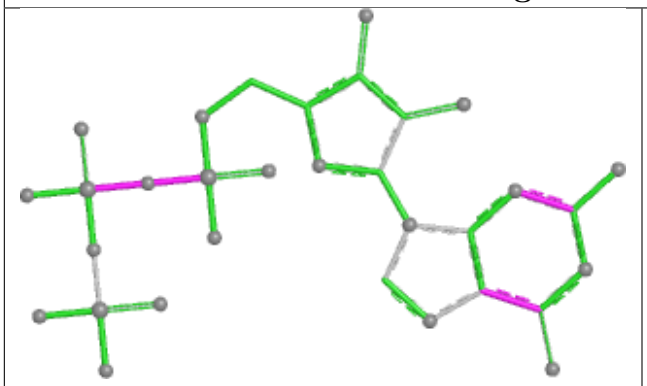


Rings

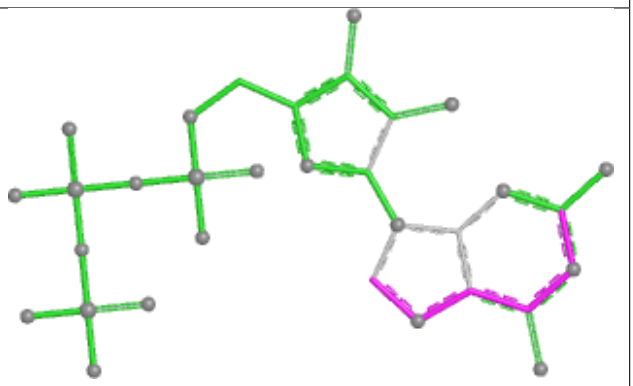
Ligand GDP FF 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP Ec 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

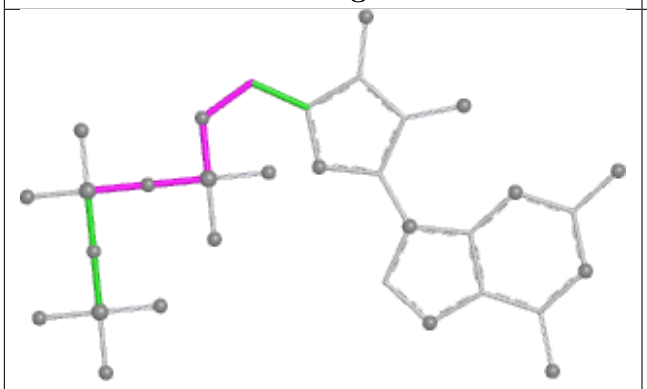
Ligand GTP A9 501



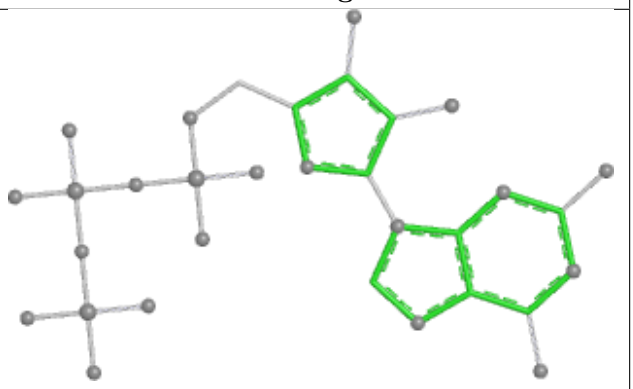
Bond lengths



Bond angles

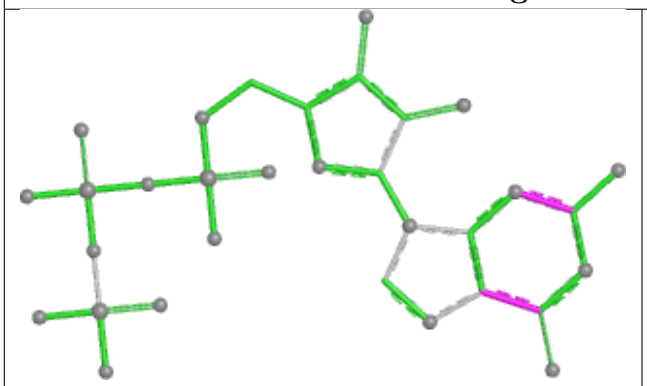


Torsions

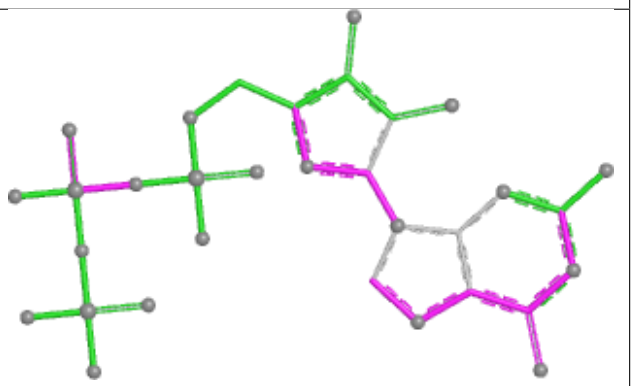


Rings

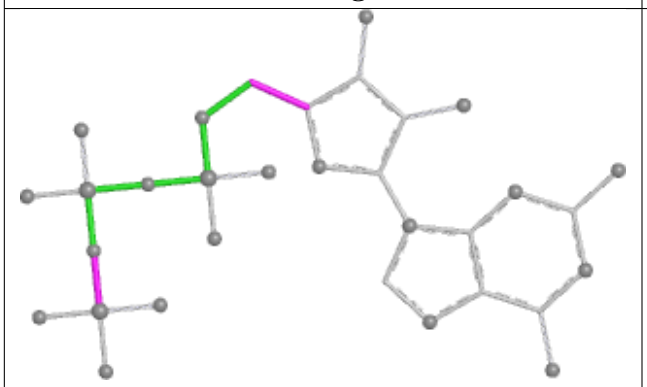
Ligand GTP BY 602



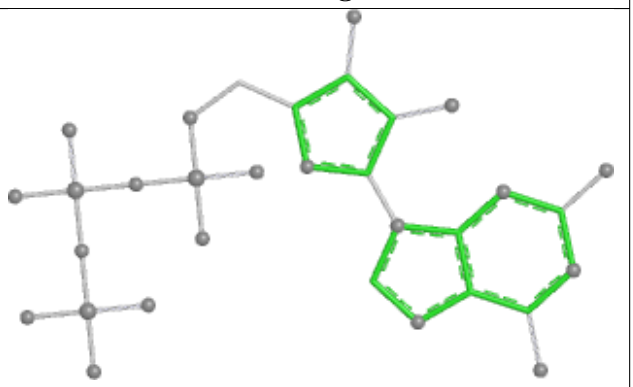
Bond lengths



Bond angles

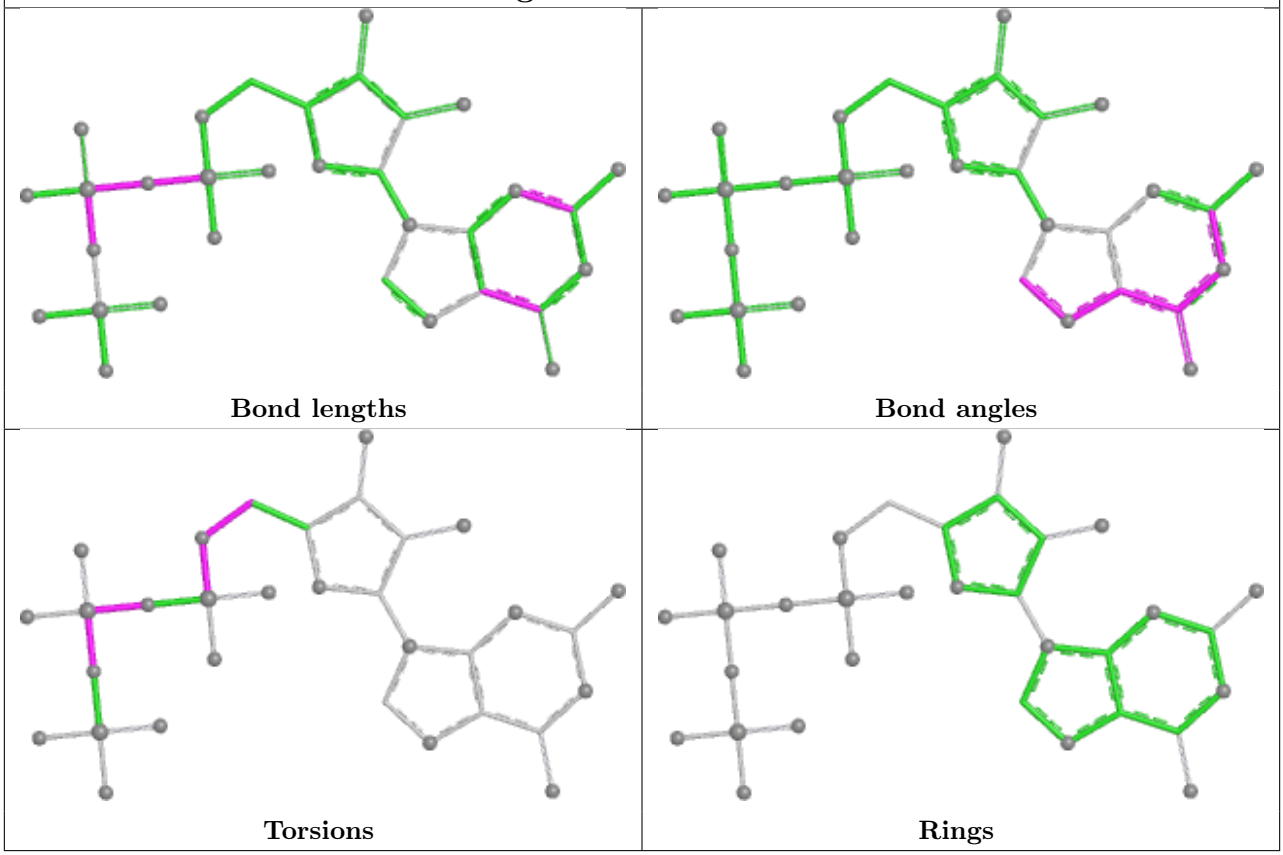


Torsions

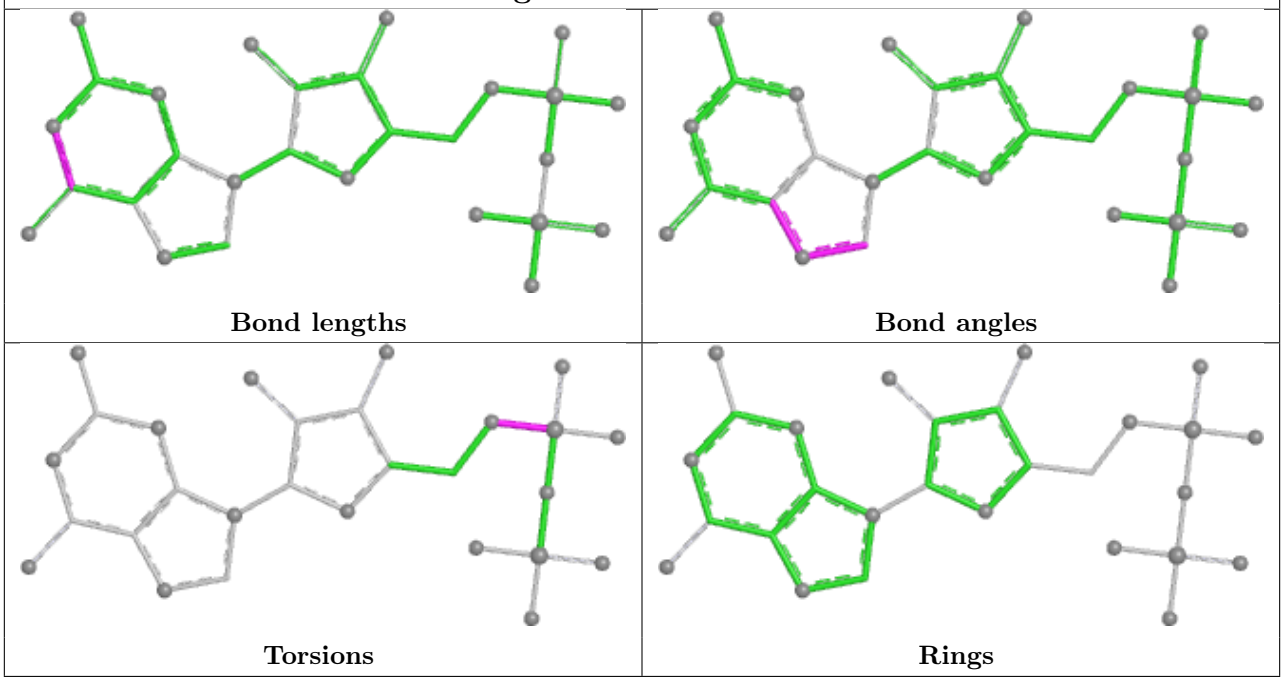


Rings

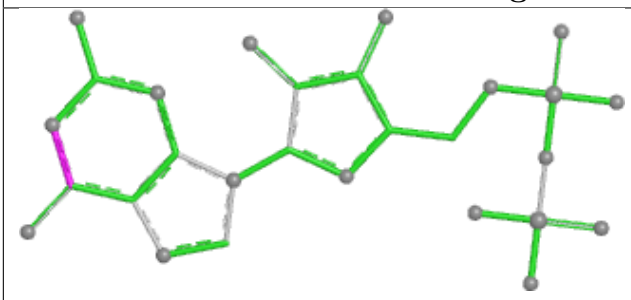
Ligand GTP F7 501



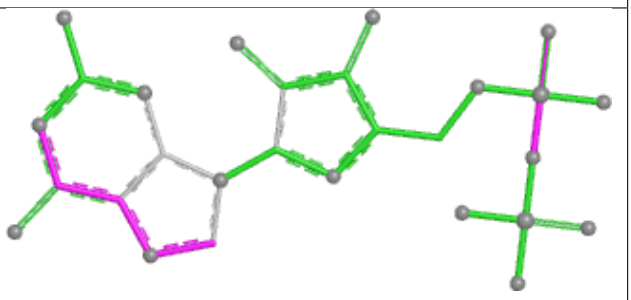
Ligand GDP Bo 501



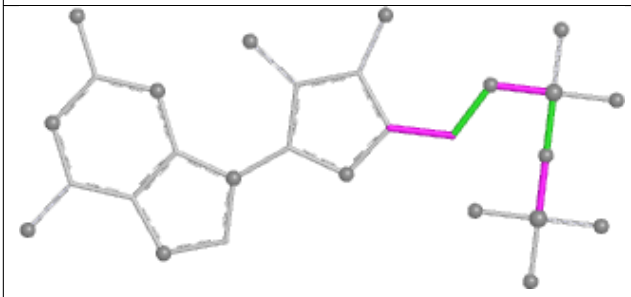
Ligand GDP DZ 501



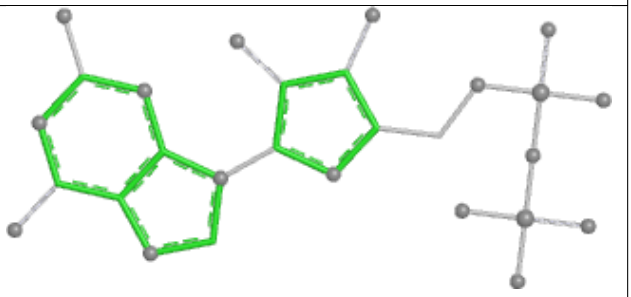
Bond lengths



Bond angles

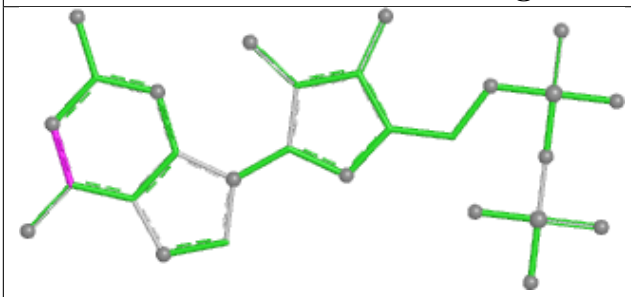


Torsions

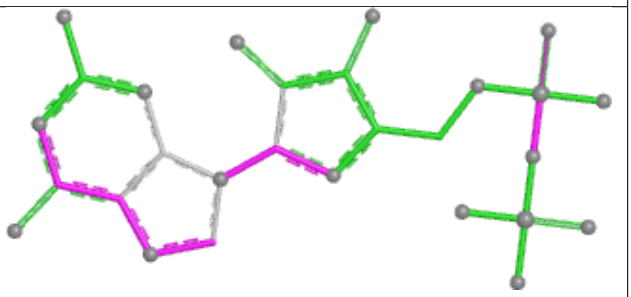


Rings

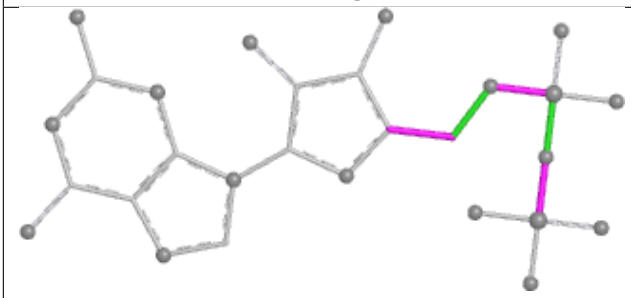
Ligand GDP Df 501



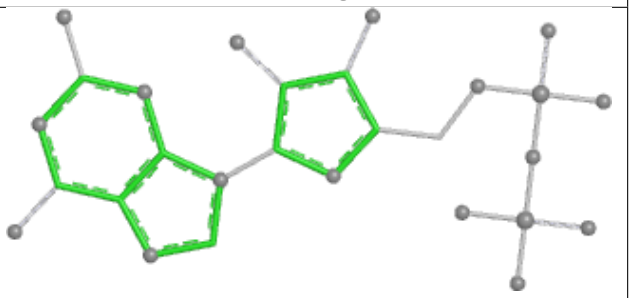
Bond lengths



Bond angles

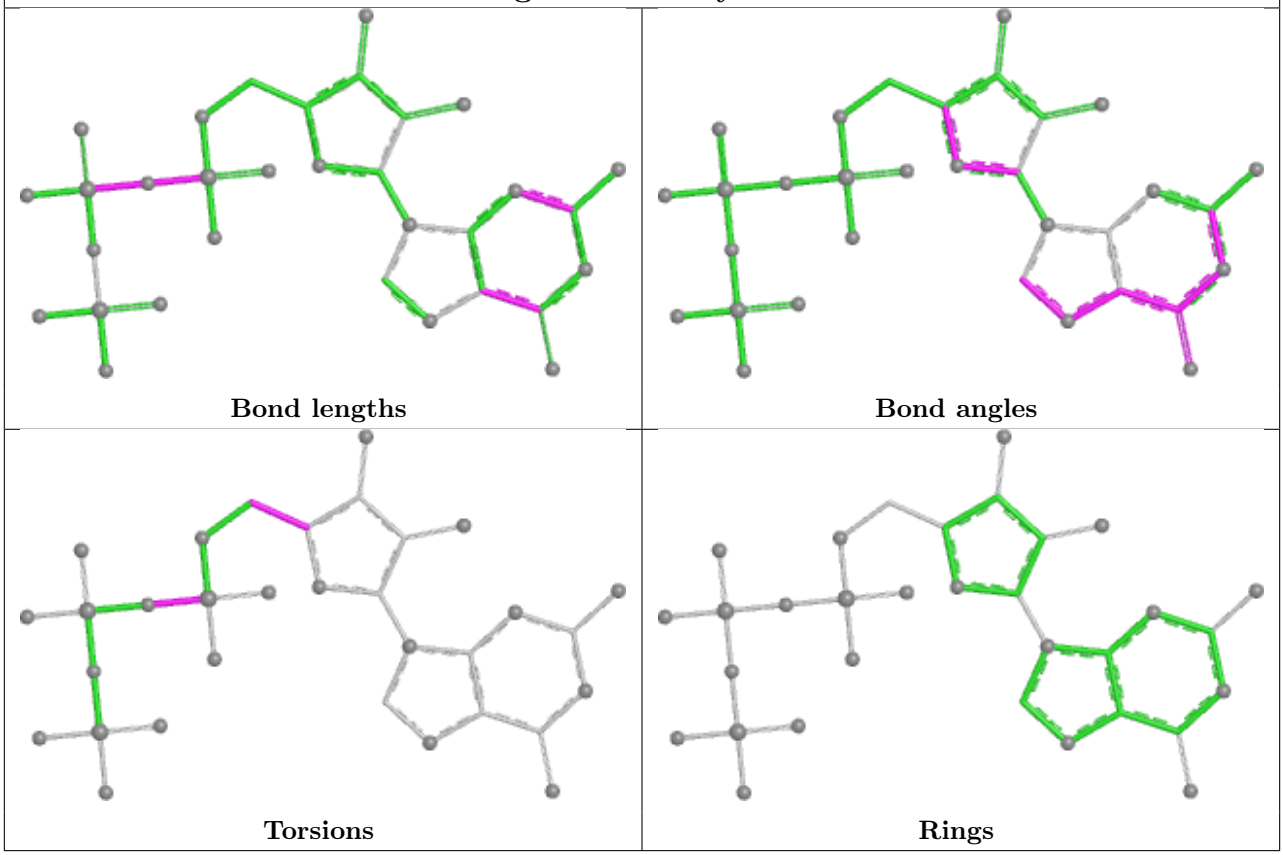


Torsions

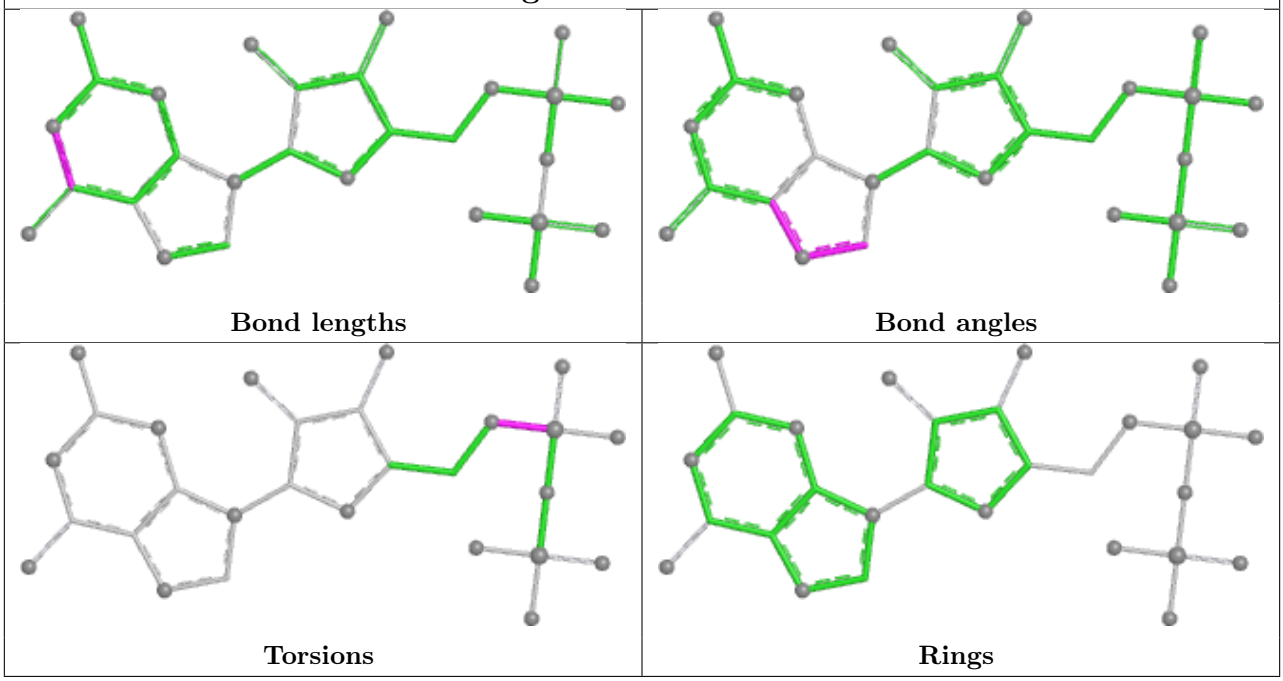


Rings

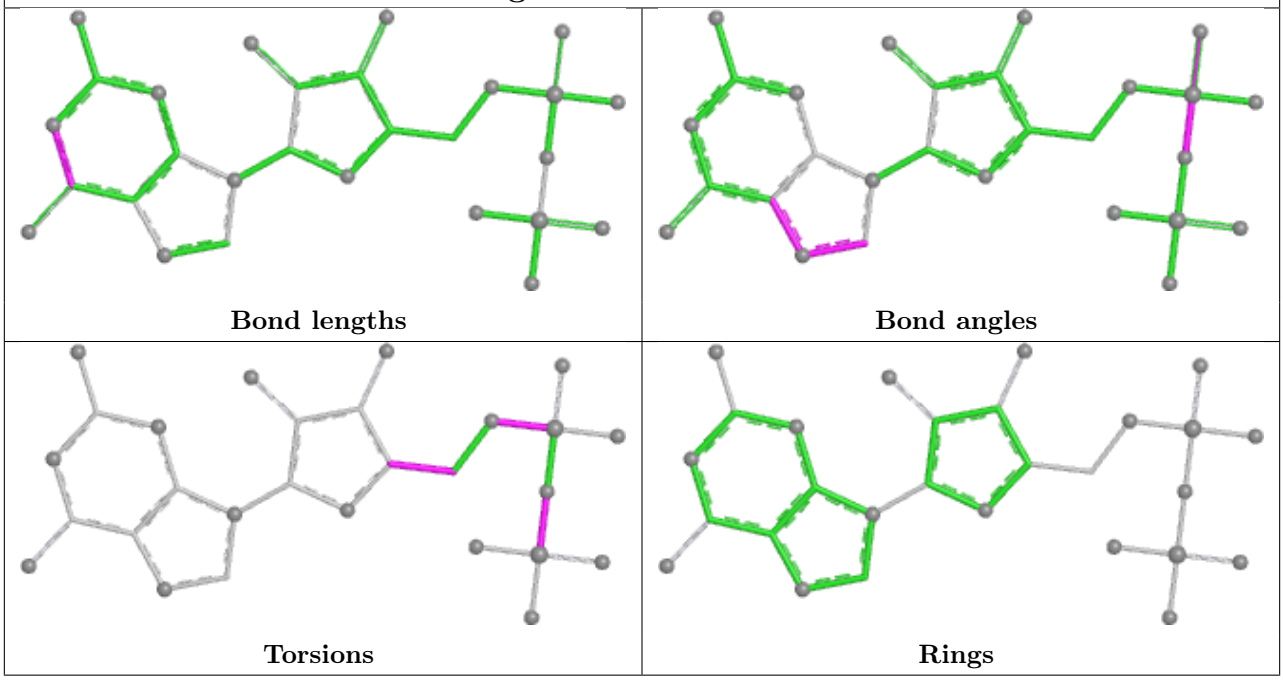
Ligand GTP By 602



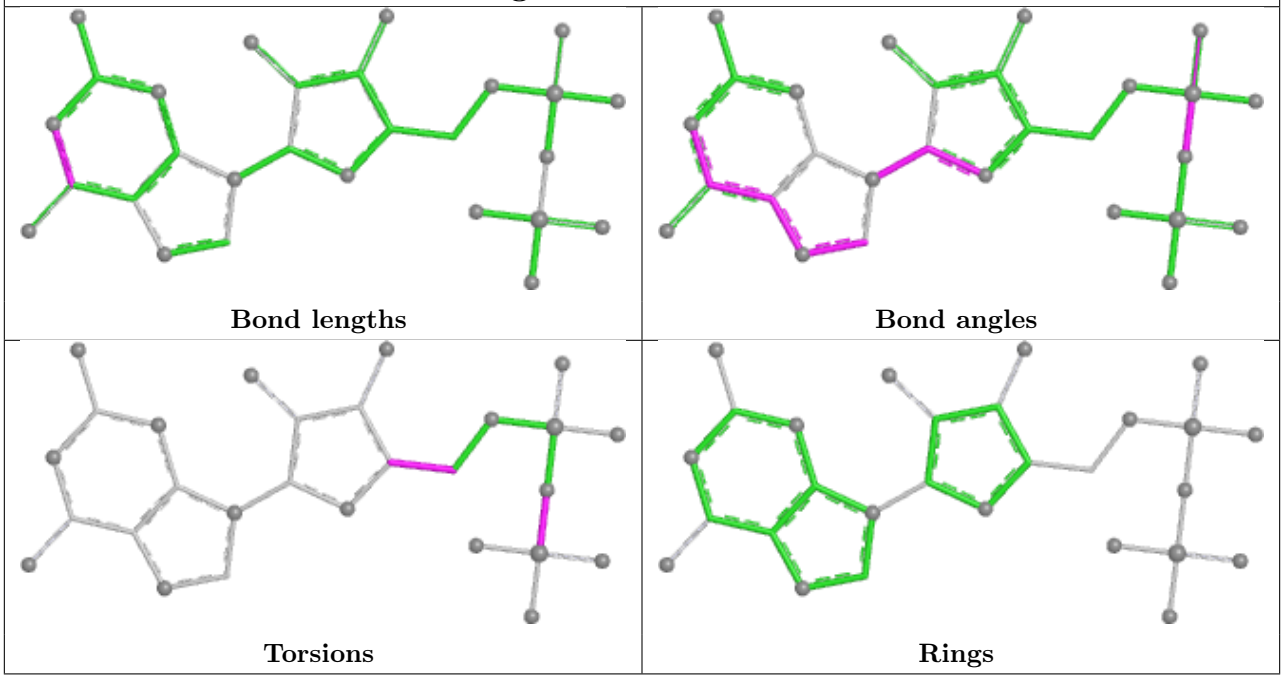
Ligand GDP X 501



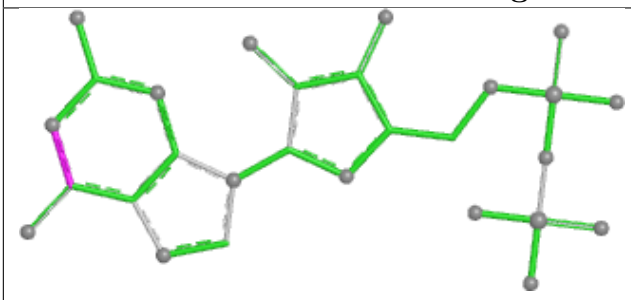
Ligand GDP DO 501



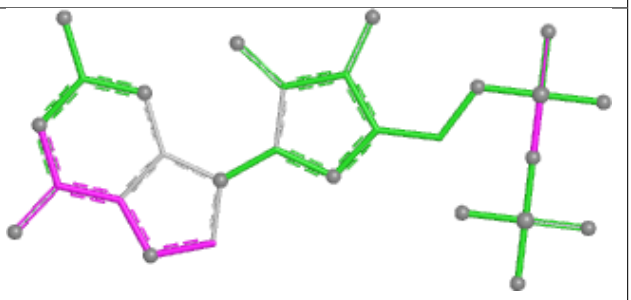
Ligand GDP Fm 501



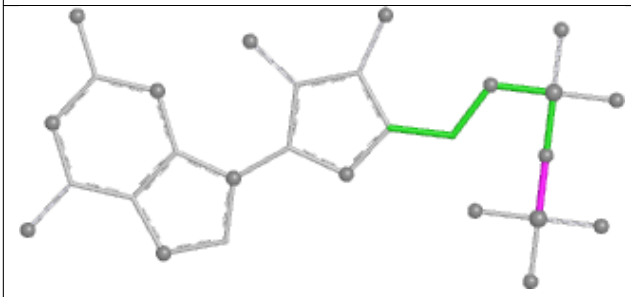
Ligand GDP Gk 501



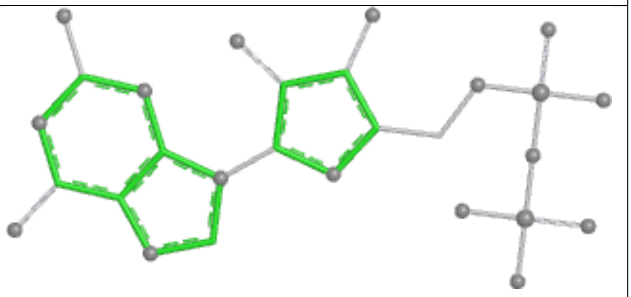
Bond lengths



Bond angles

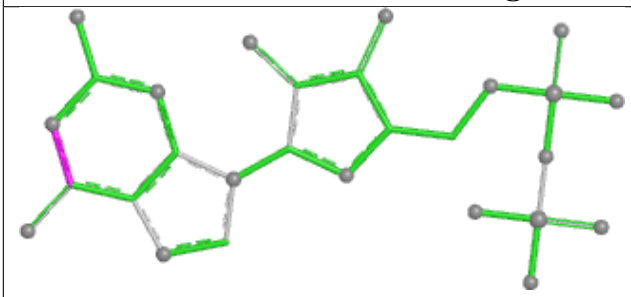


Torsions

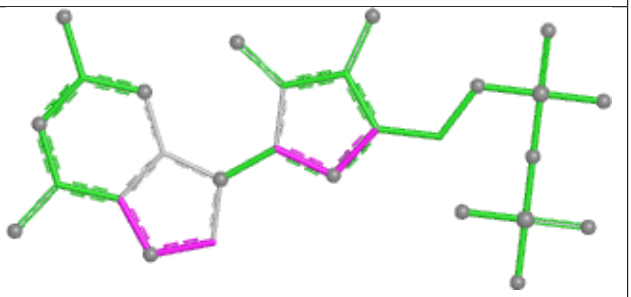


Rings

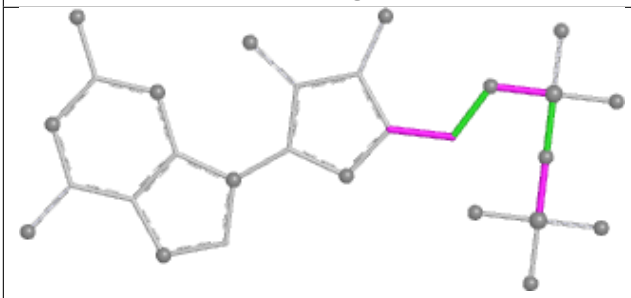
Ligand GDP AW 501



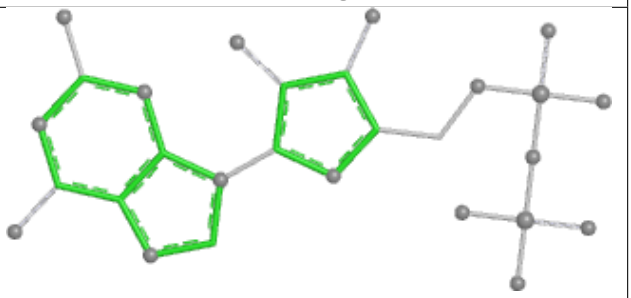
Bond lengths



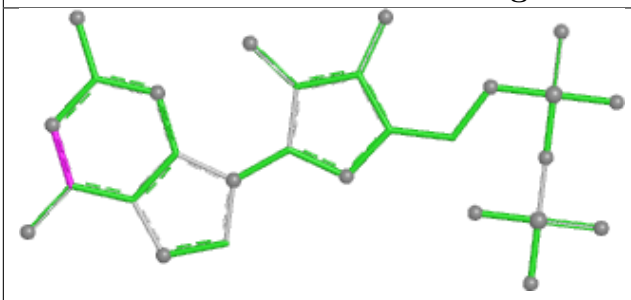
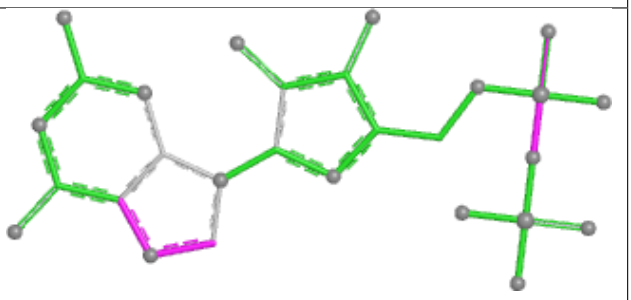
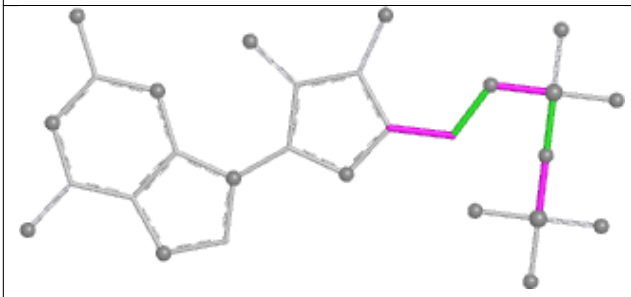
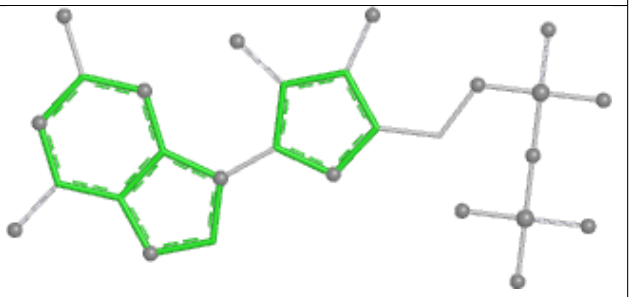
Bond angles

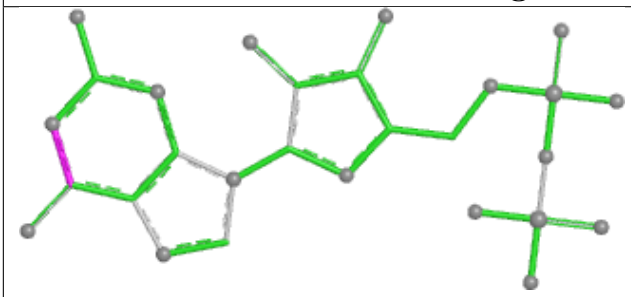
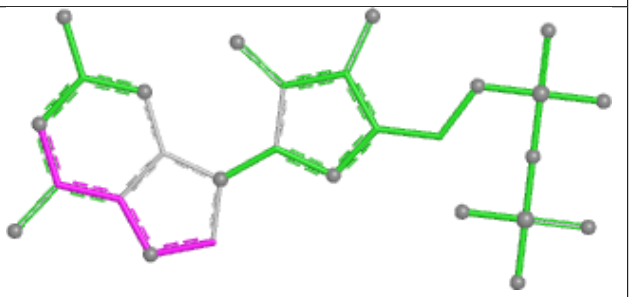
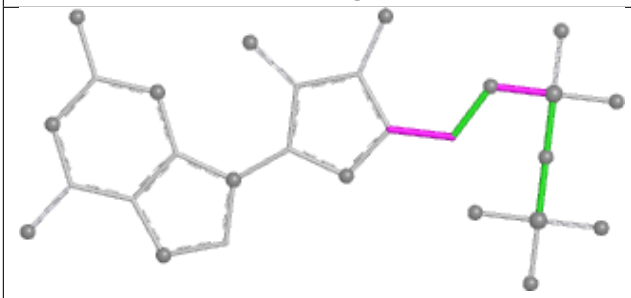
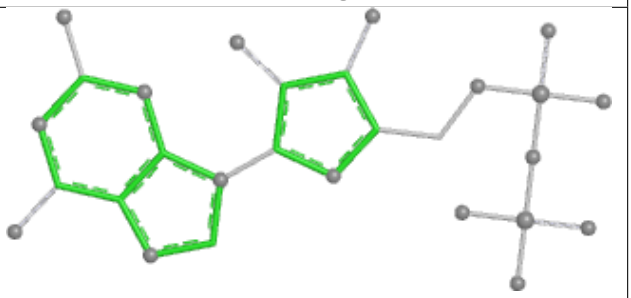


Torsions

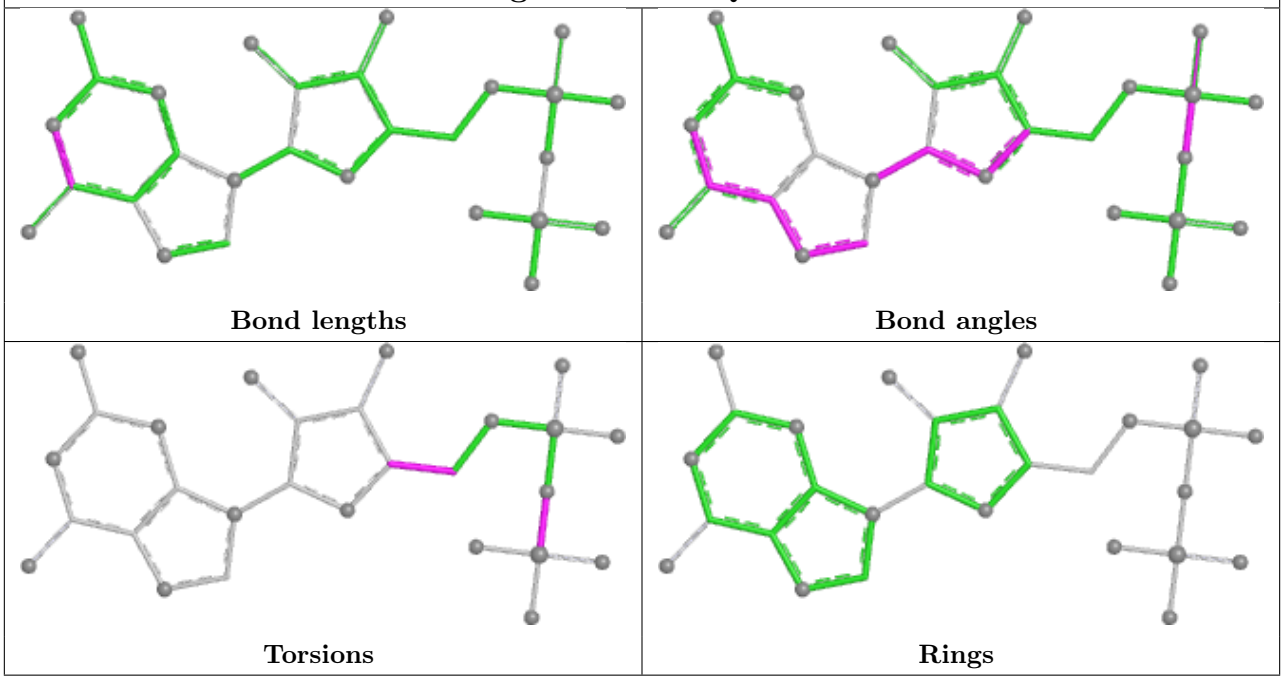


Rings

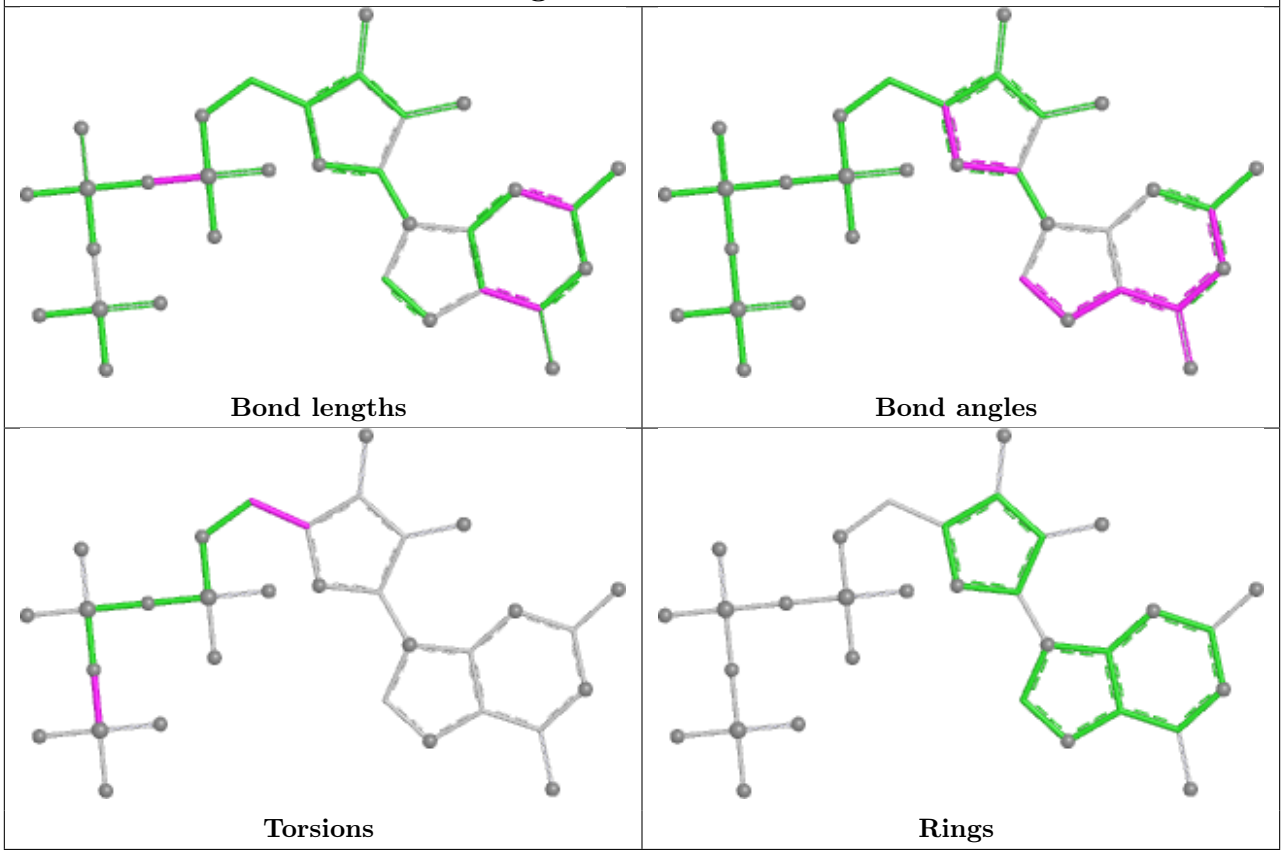
Ligand GDP Gh 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP AZ 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

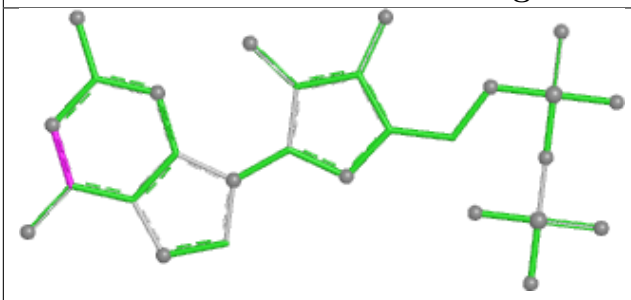
Ligand GDP EQ 501



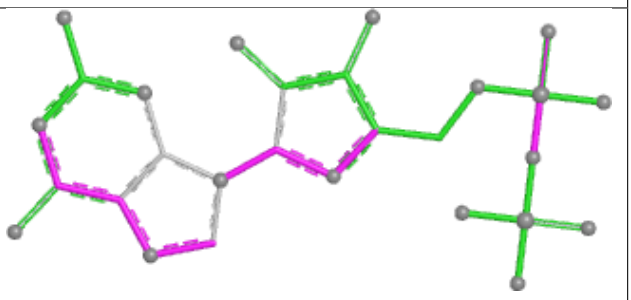
Ligand GTP s 602



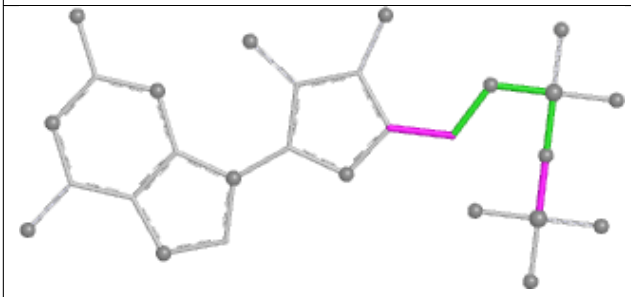
Ligand GDP Ev 501



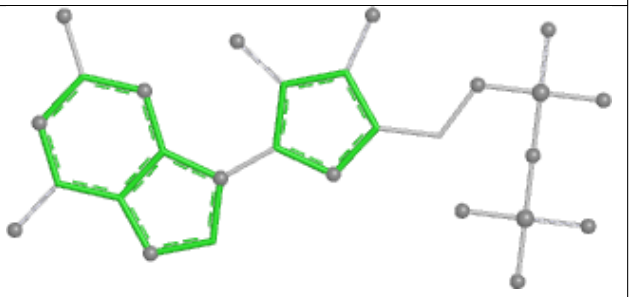
Bond lengths



Bond angles

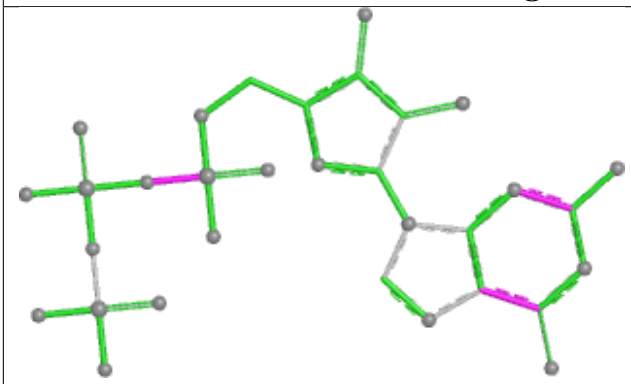


Torsions

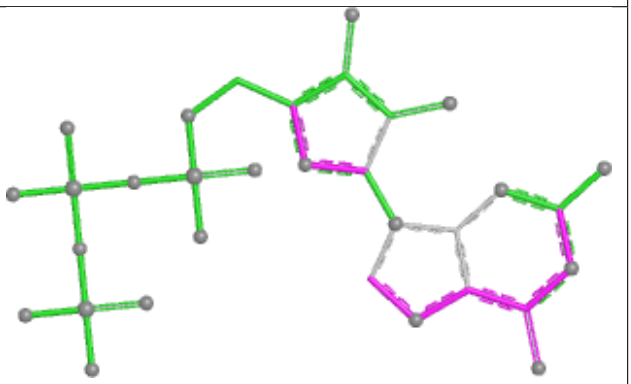


Rings

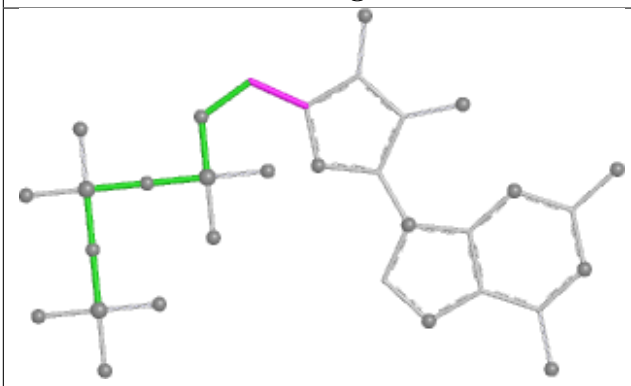
Ligand GTP T 602



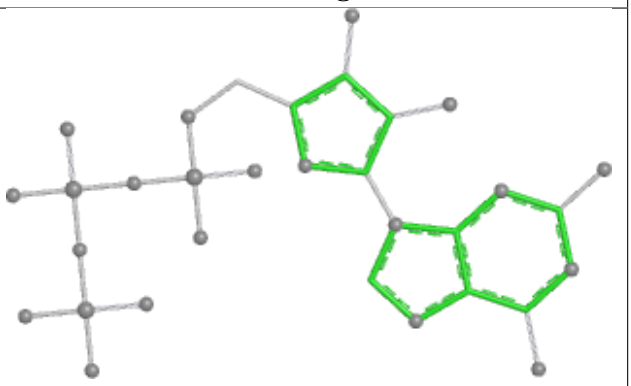
Bond lengths



Bond angles

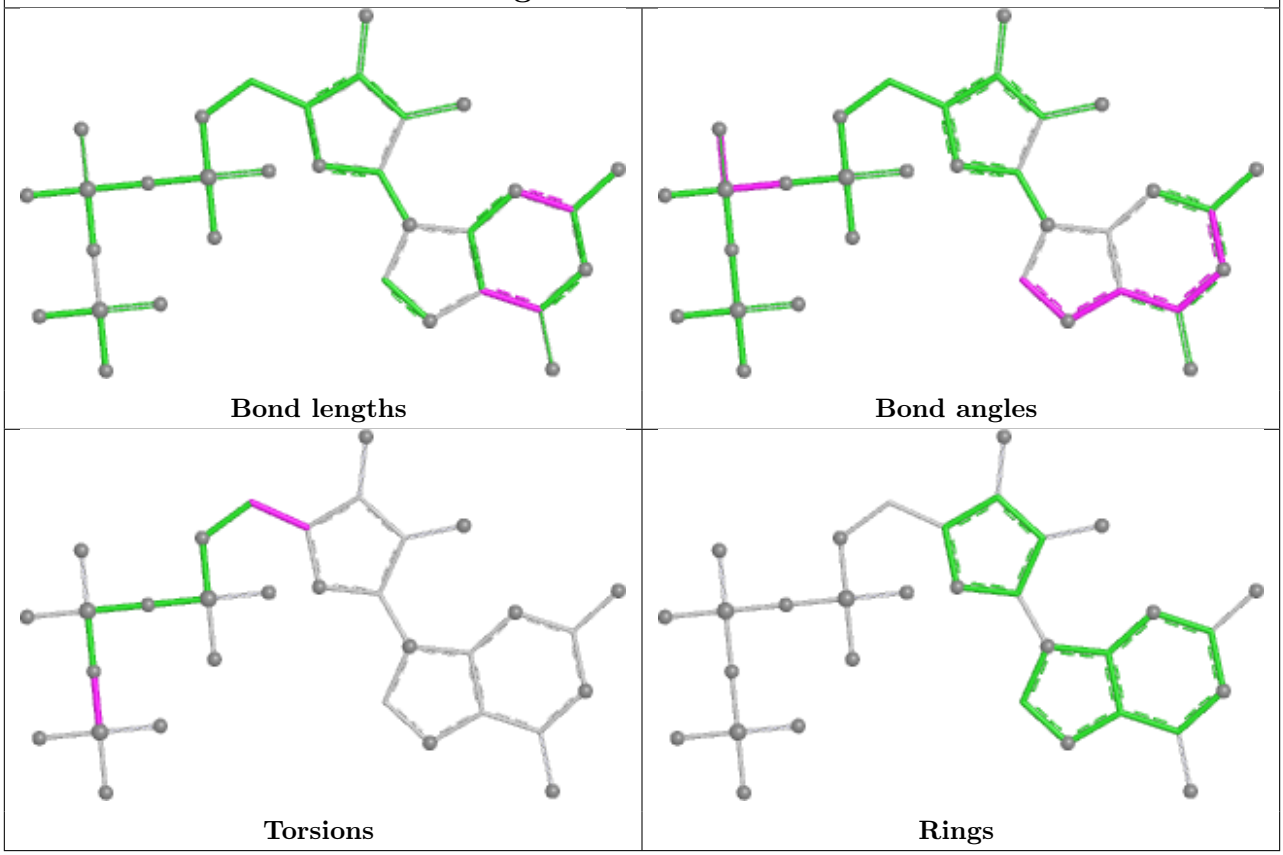


Torsions

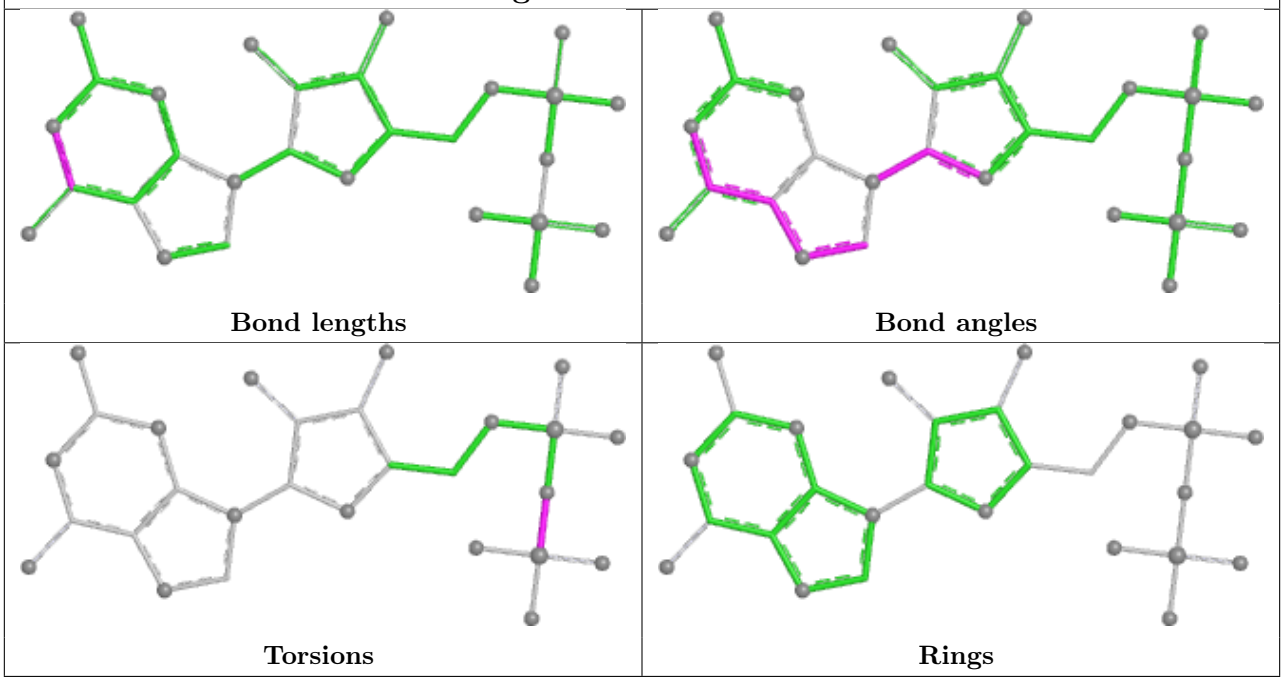


Rings

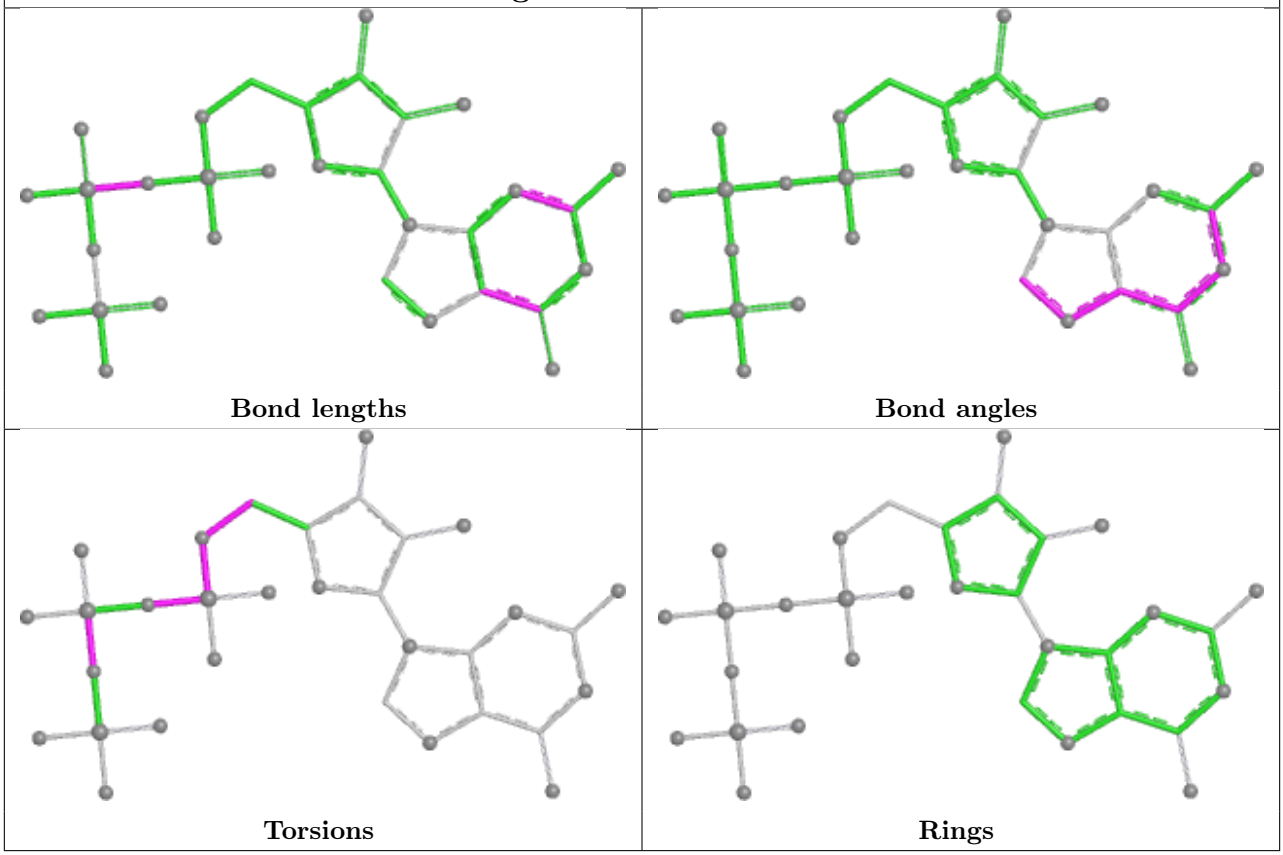
Ligand GTP A1 602



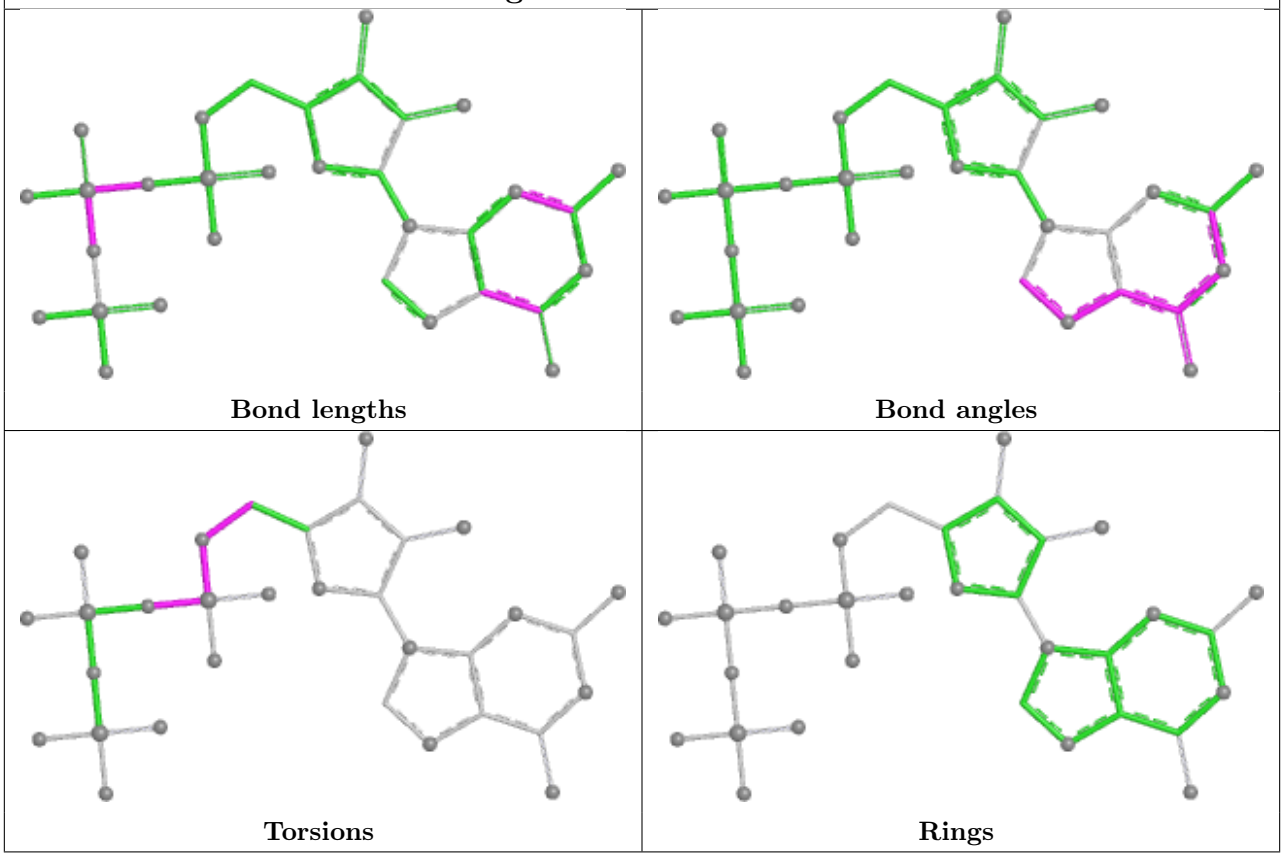
Ligand GDP Ga 501



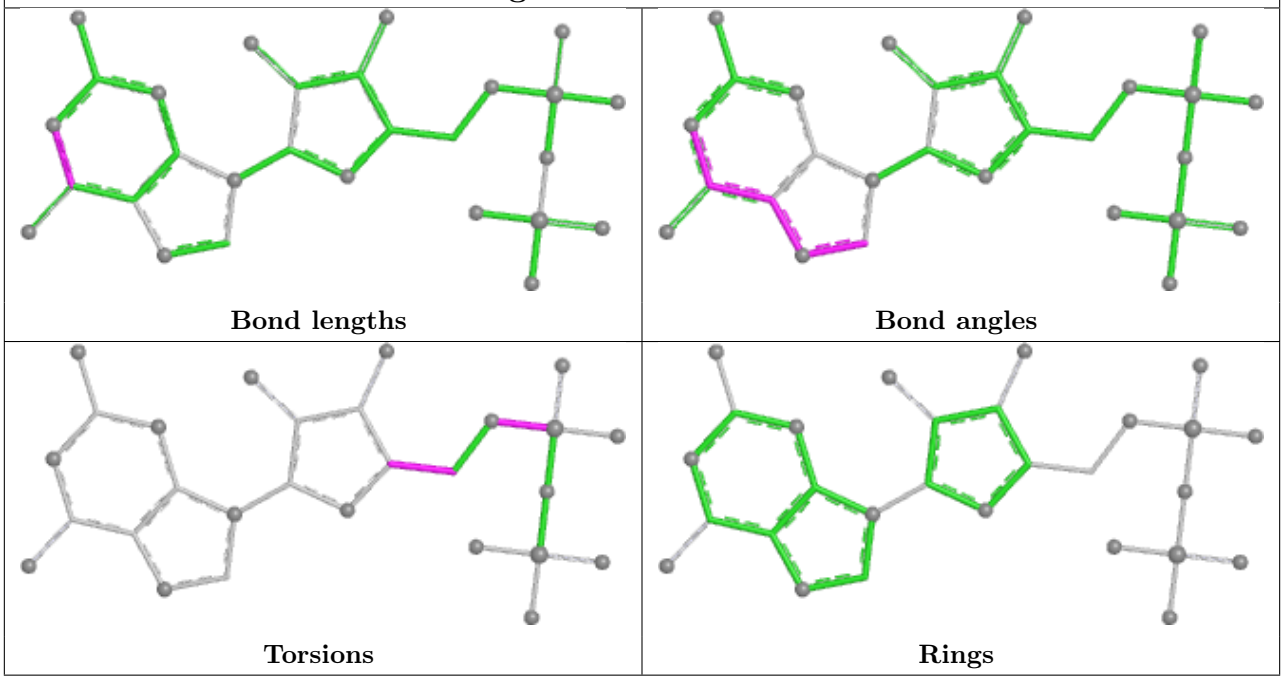
Ligand GTP FR 501



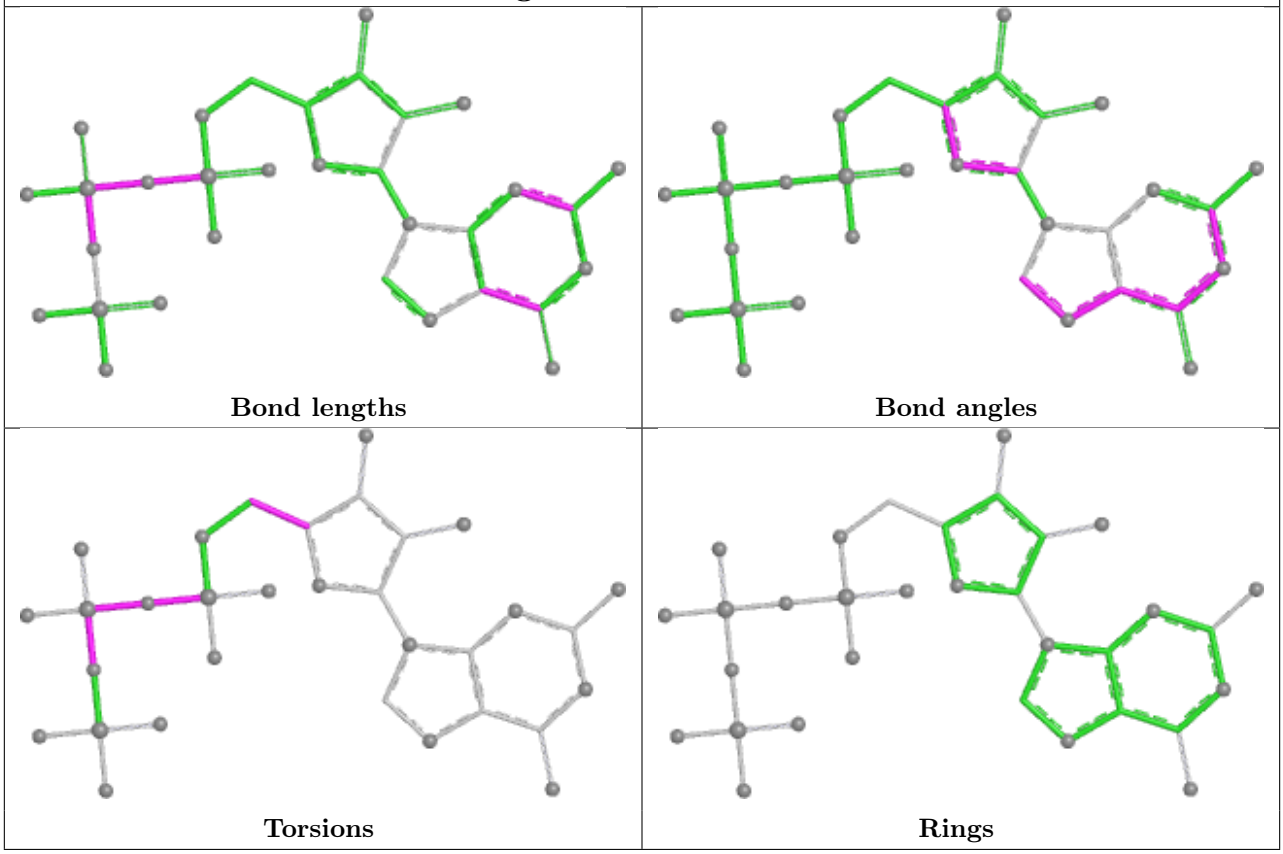
Ligand GTP GM 501



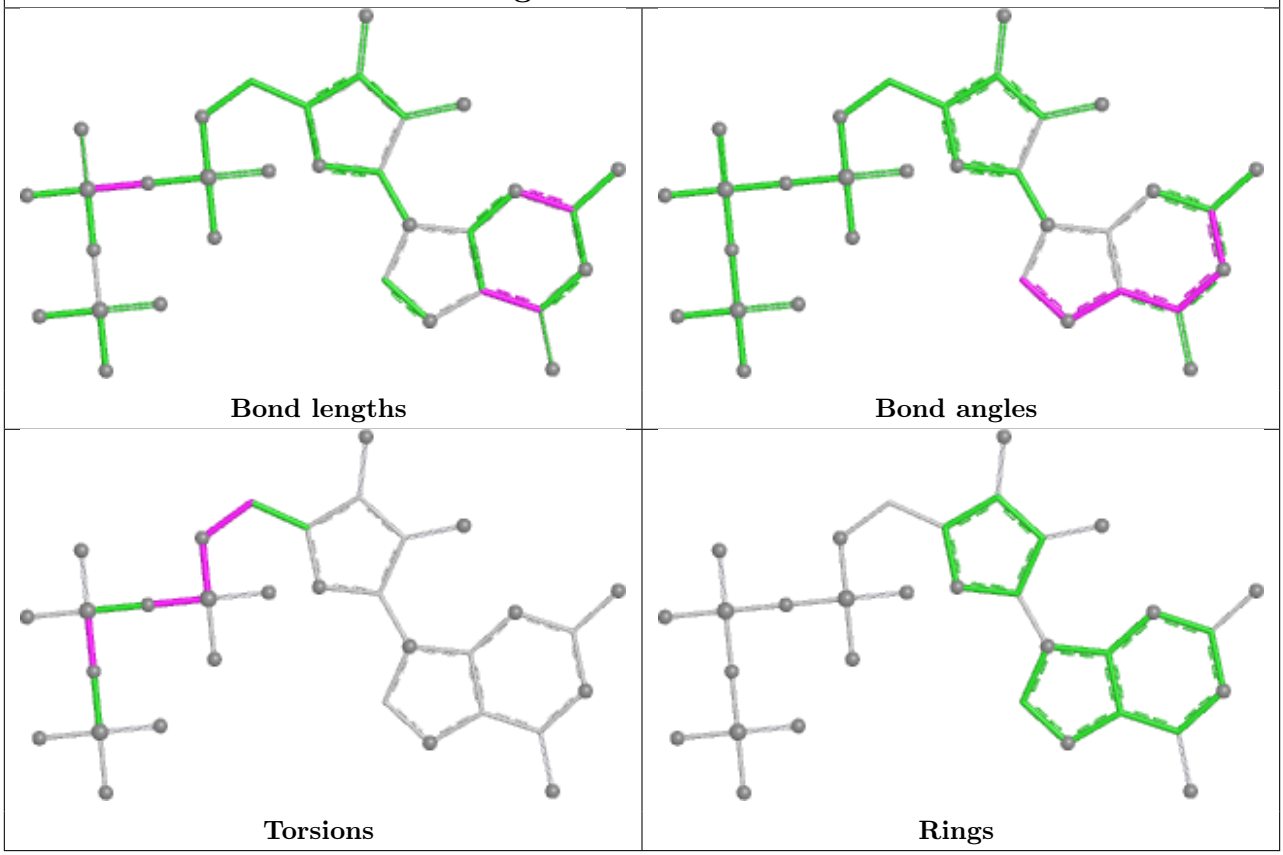
Ligand GDP BA 501



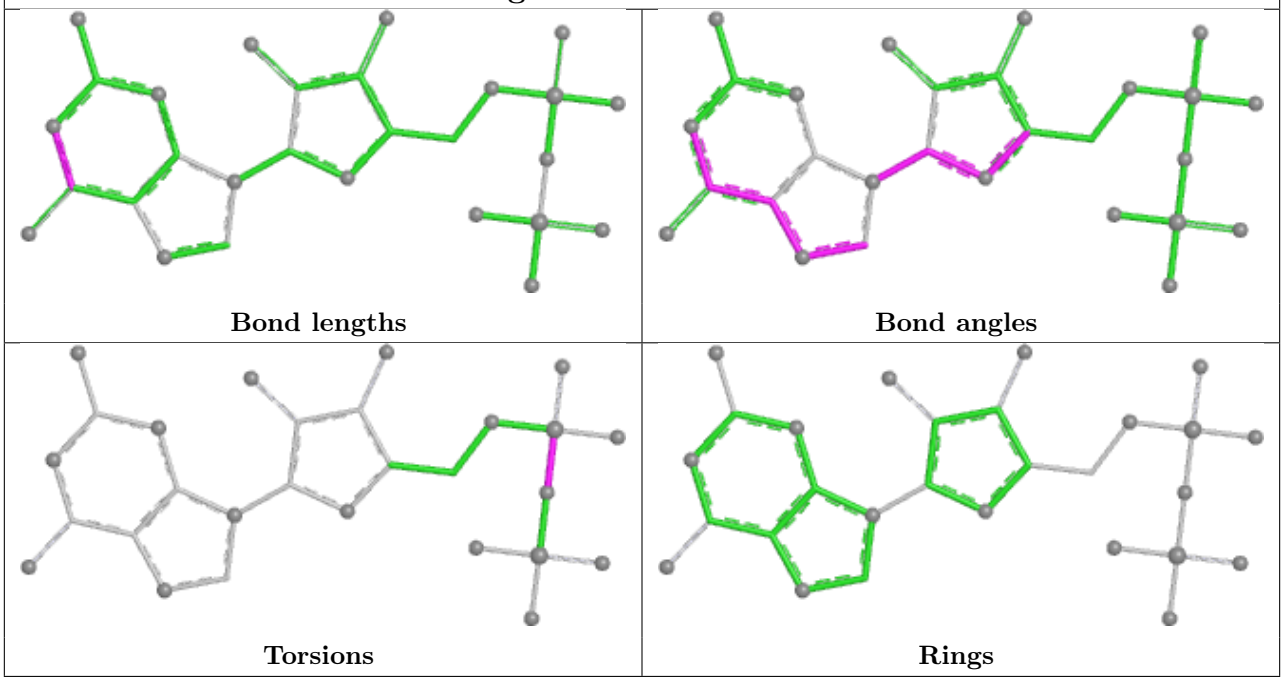
Ligand GTP Fh 501



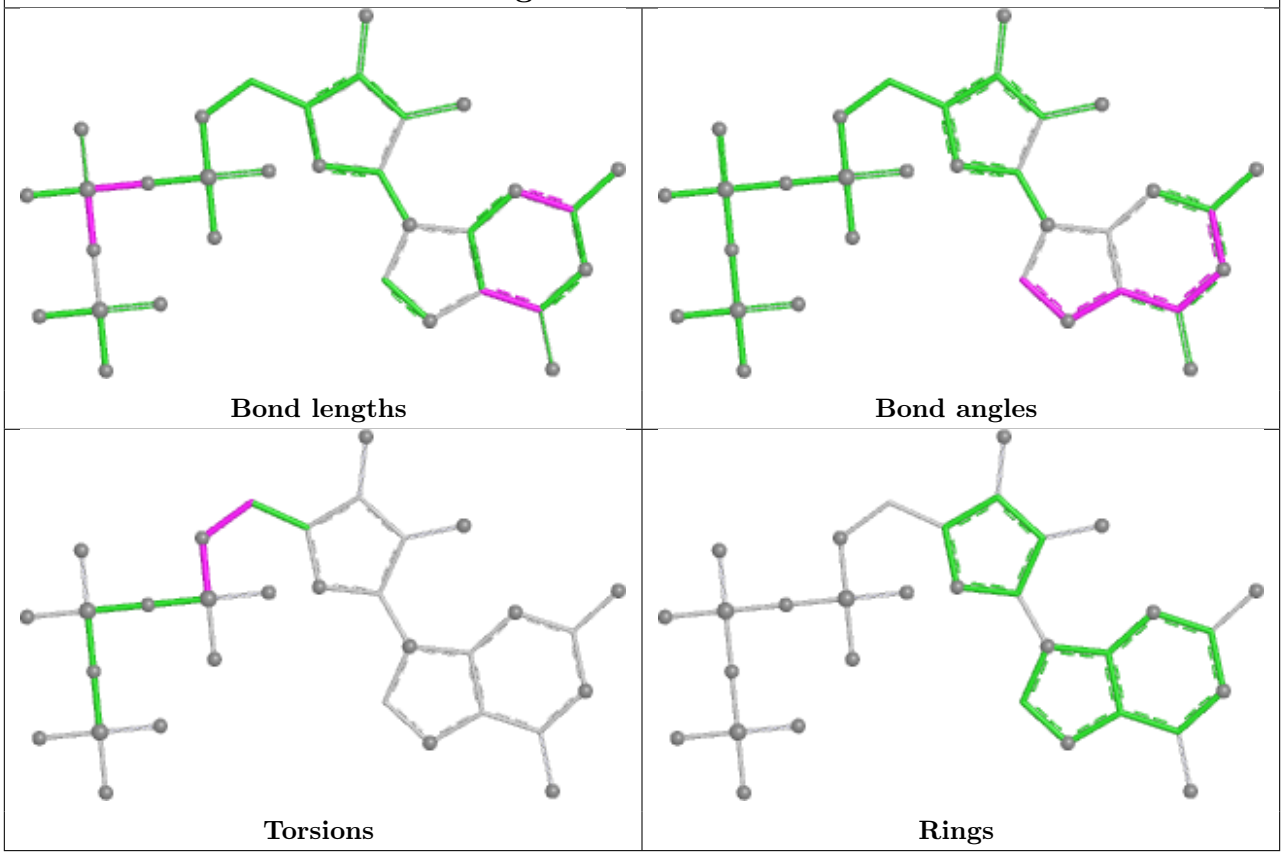
Ligand GTP A5 501



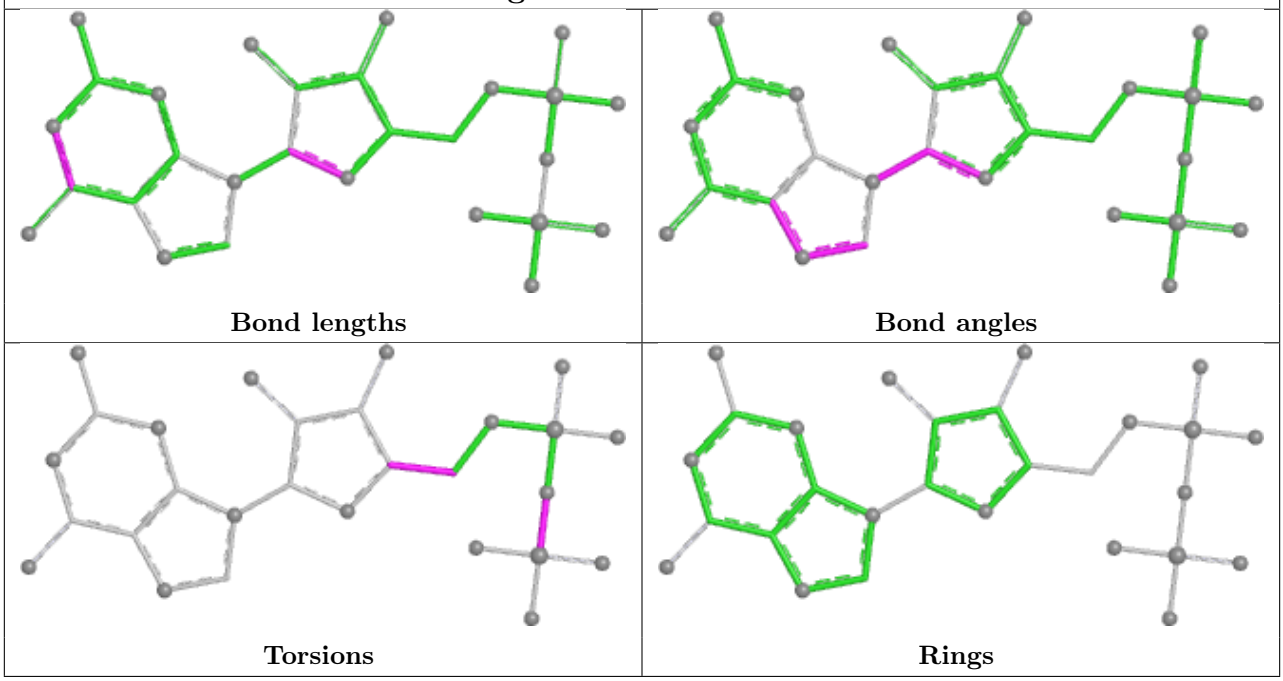
Ligand GDP AD 501



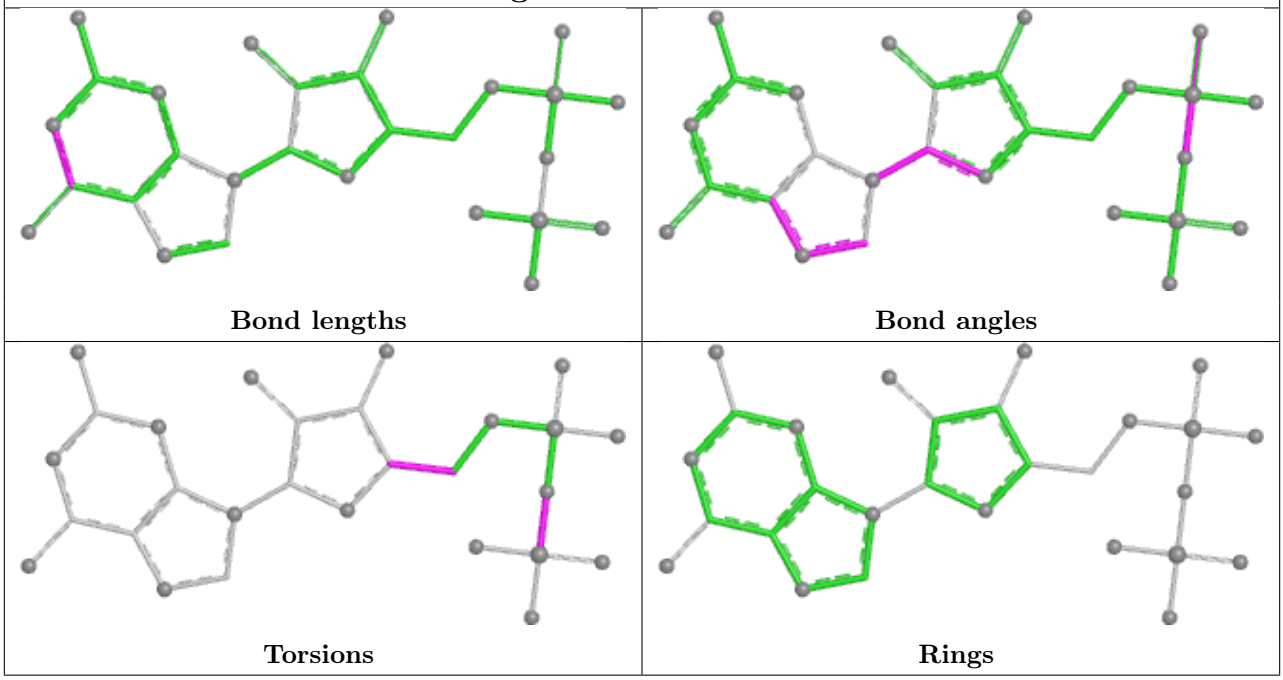
Ligand GTP FS 501



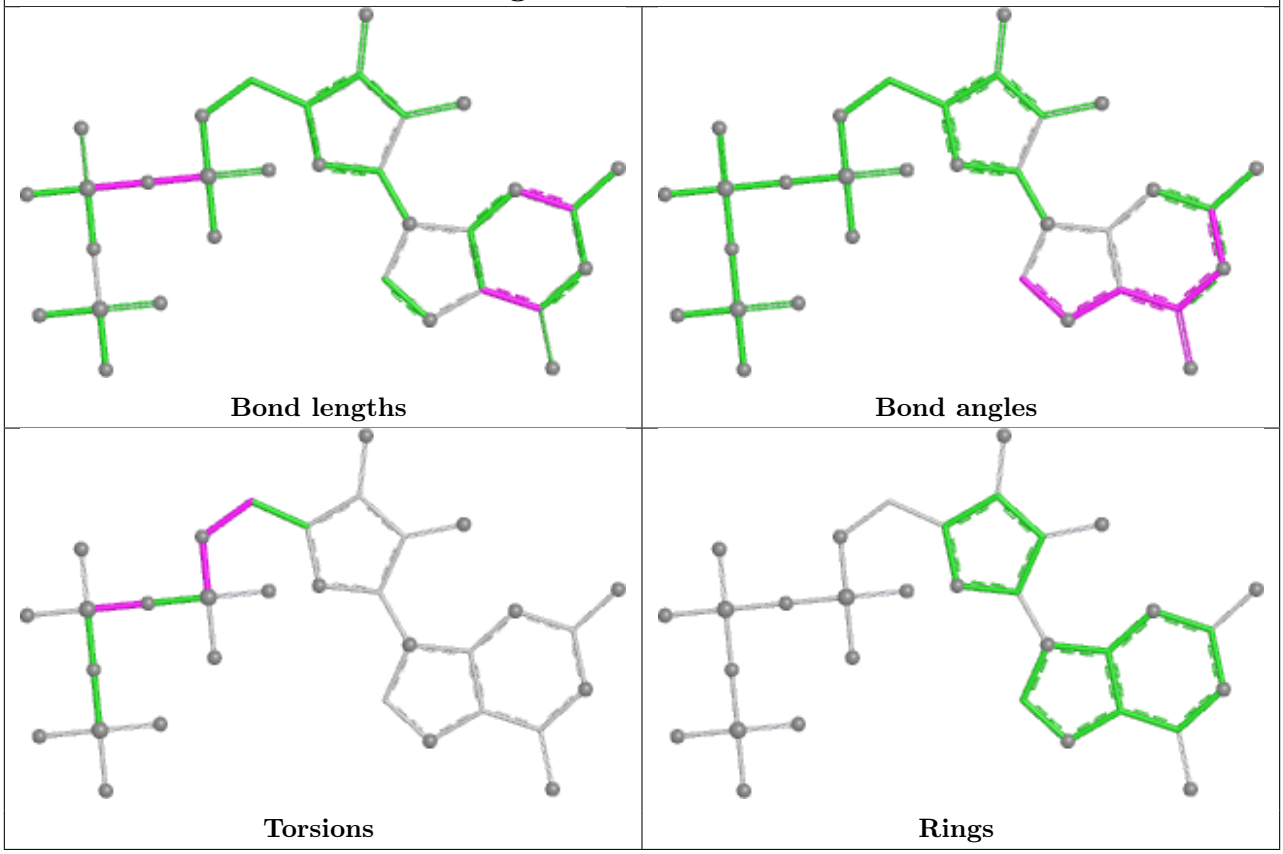
Ligand GDP GX 501



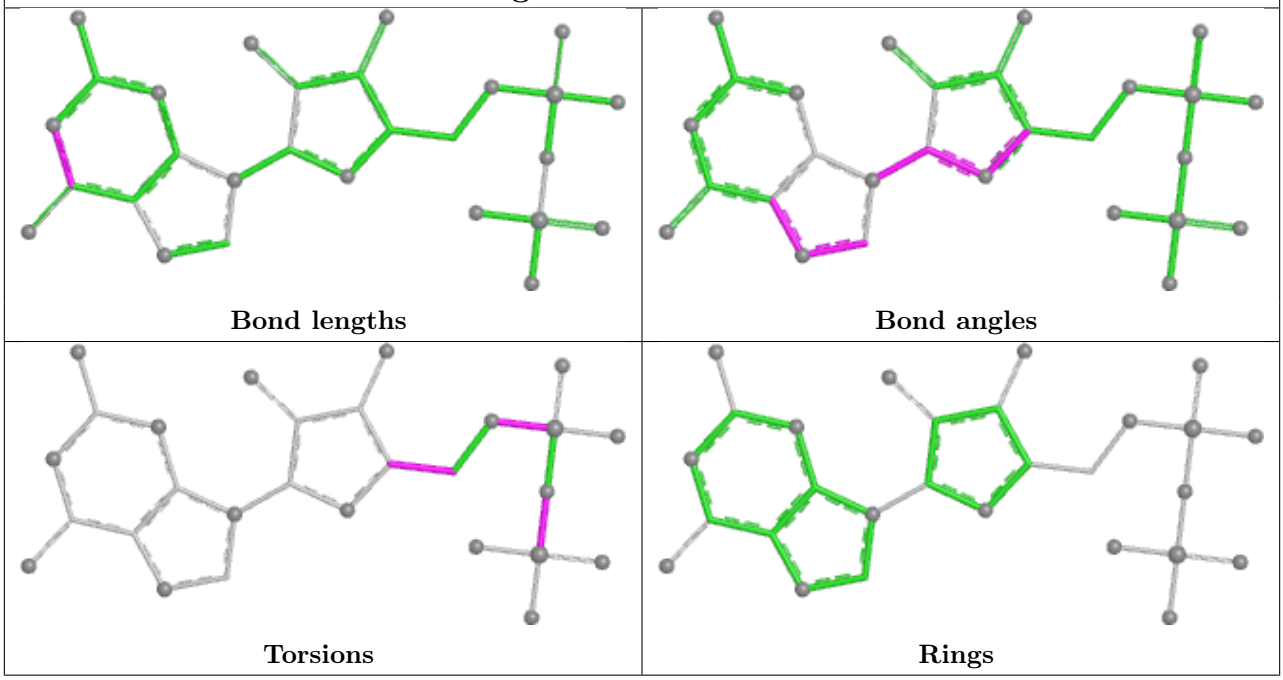
Ligand GDP FG 501



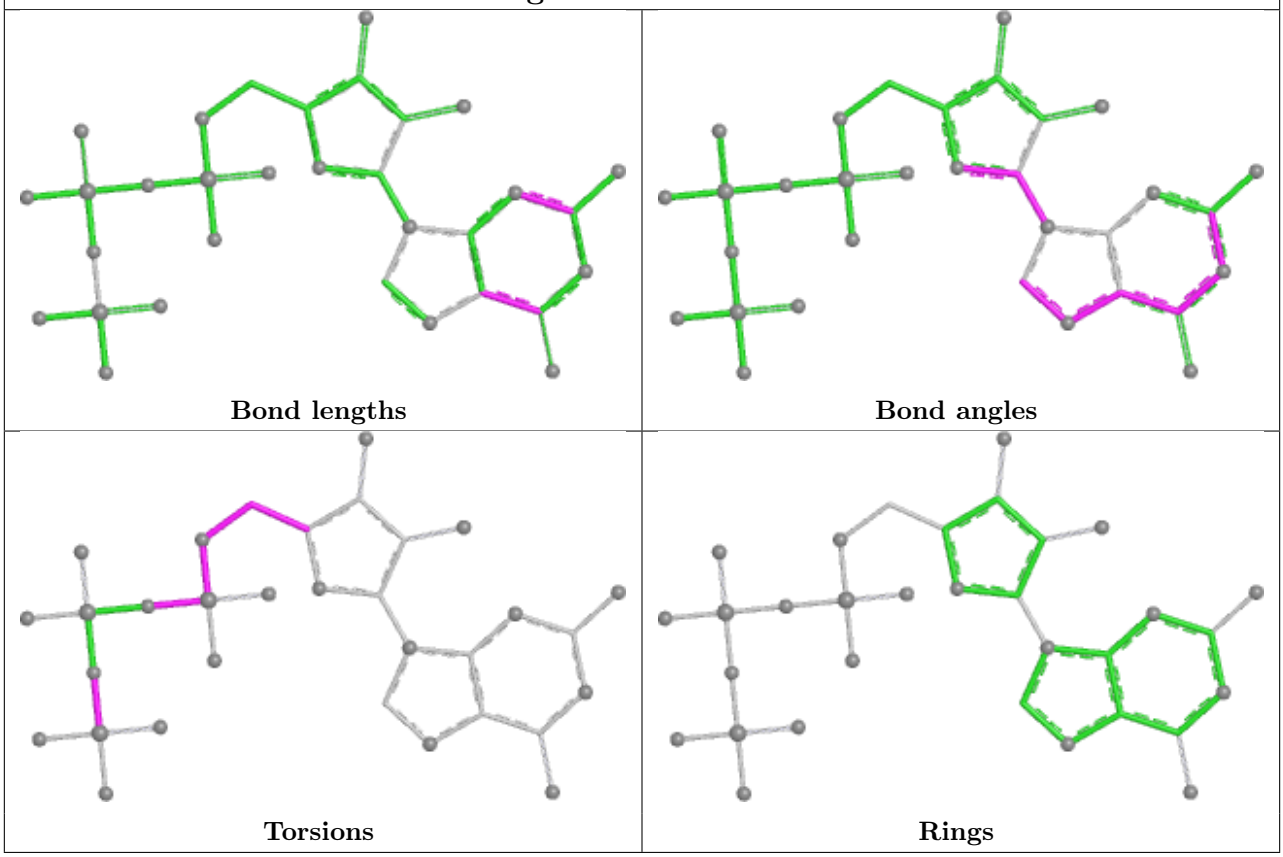
Ligand GTP AK 602



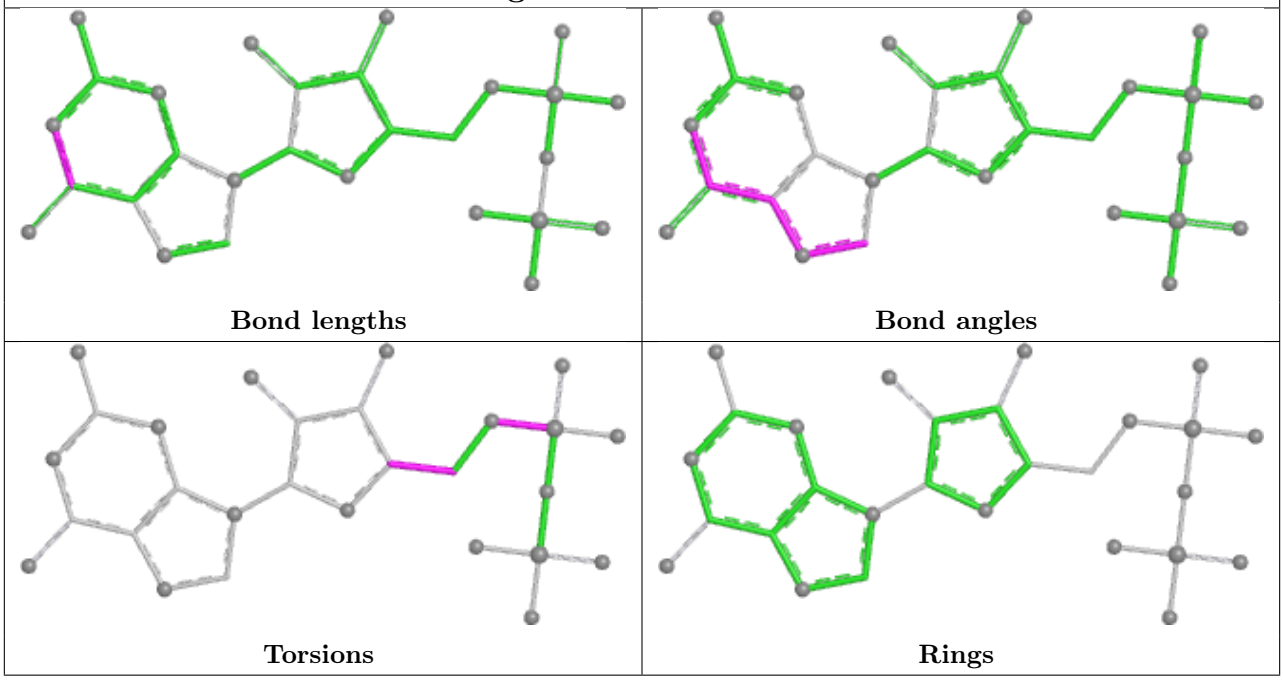
Ligand GDP Ab 501



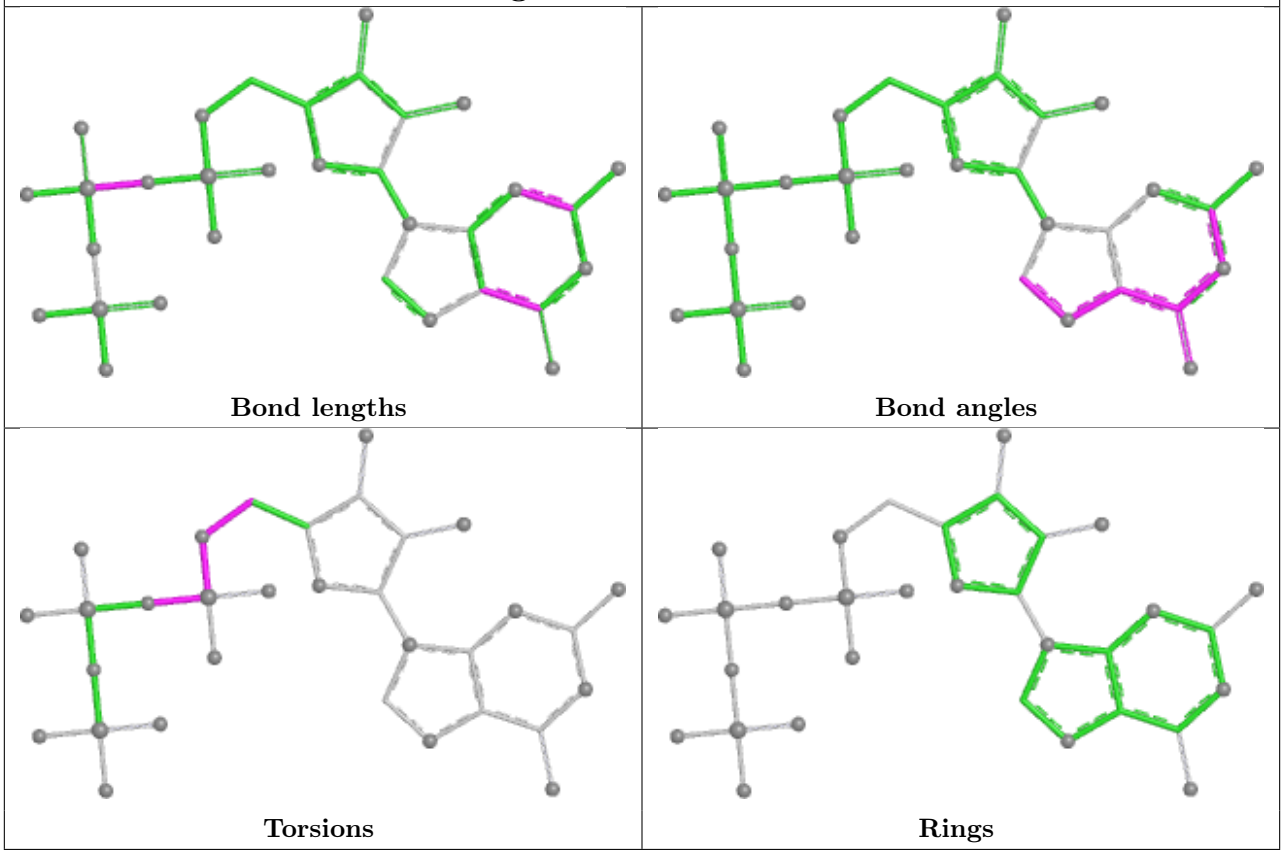
Ligand GTP S 602



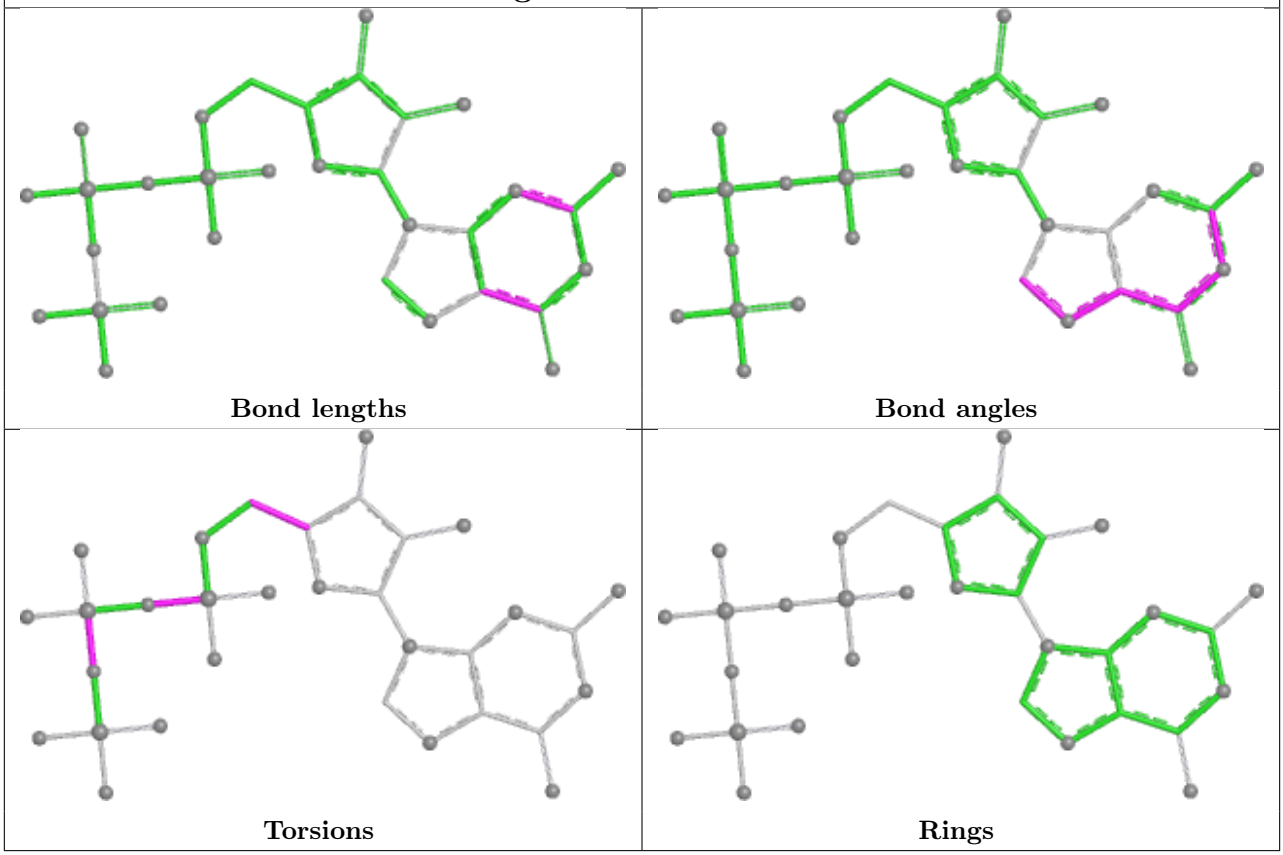
Ligand GDP AN 501



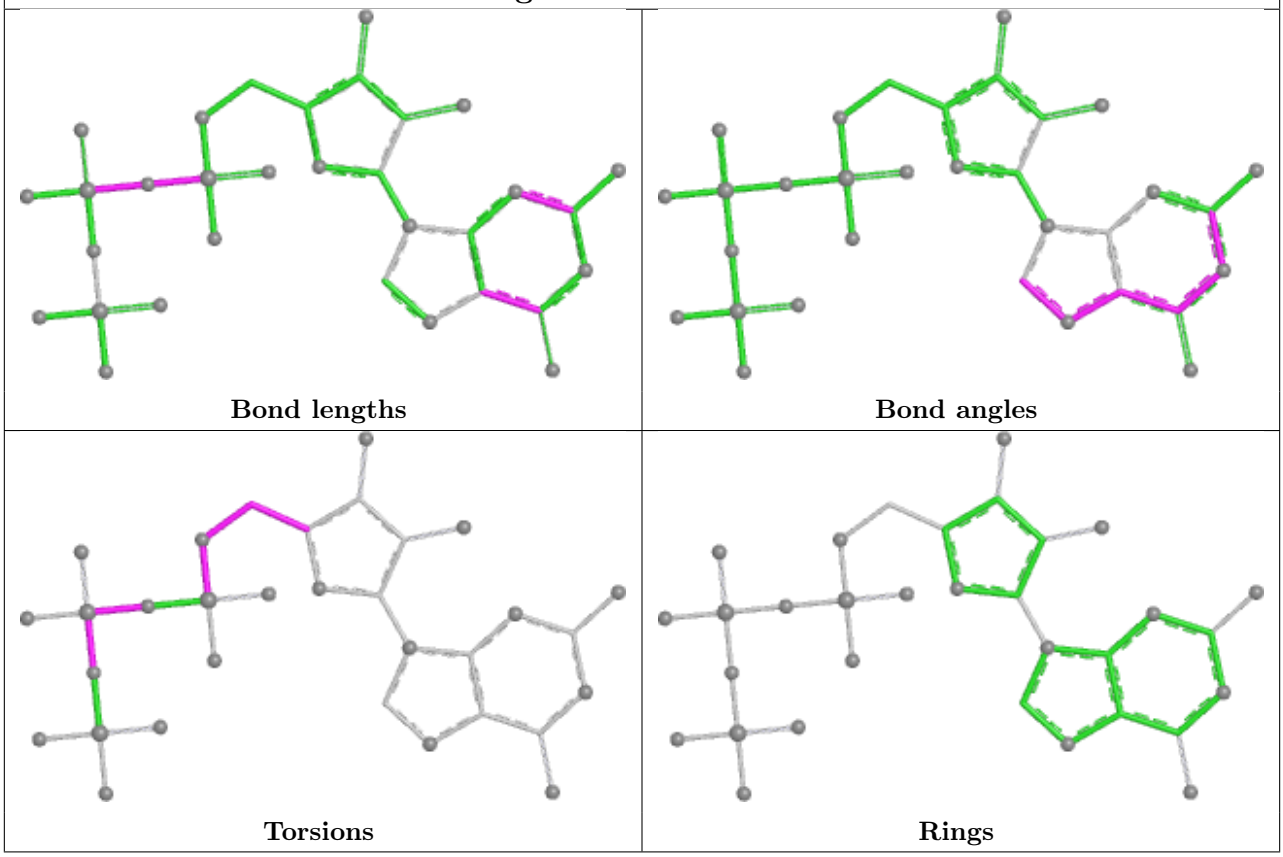
Ligand GTP GT 501



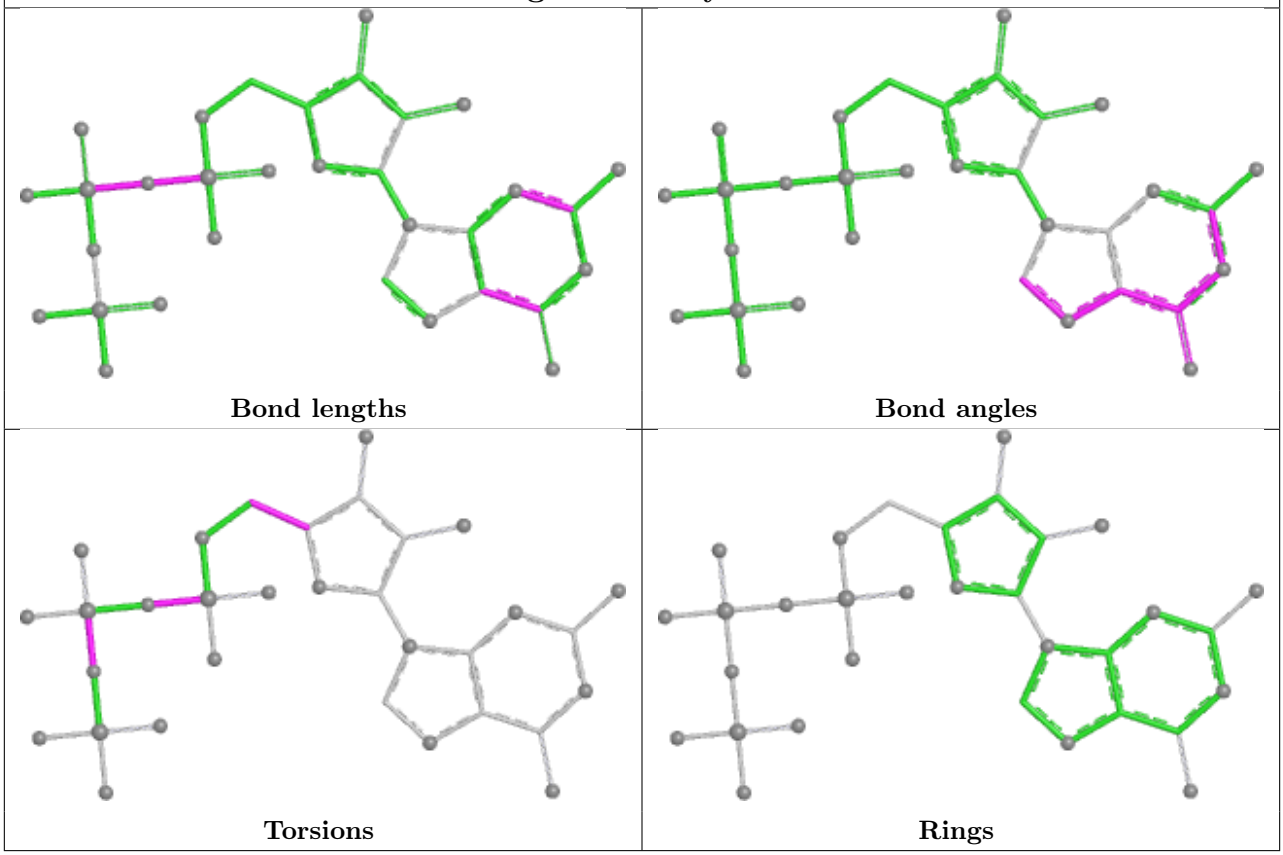
Ligand GTP AJ 602



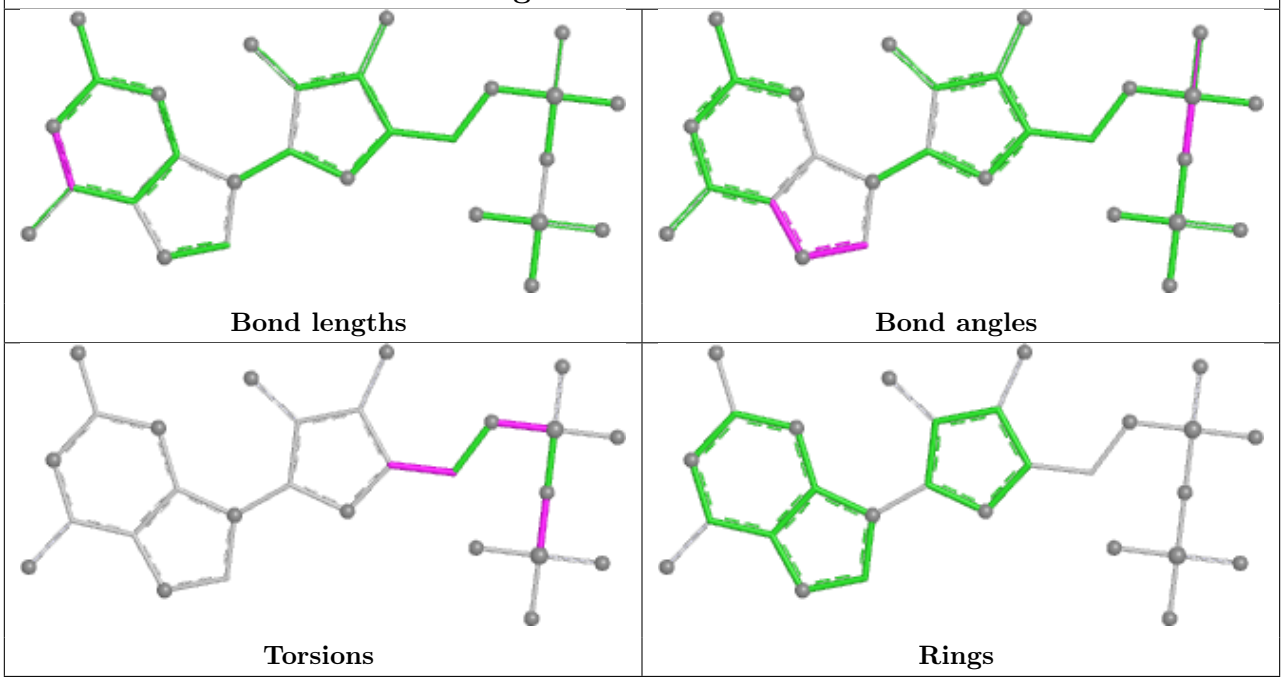
Ligand GTP Ex 501



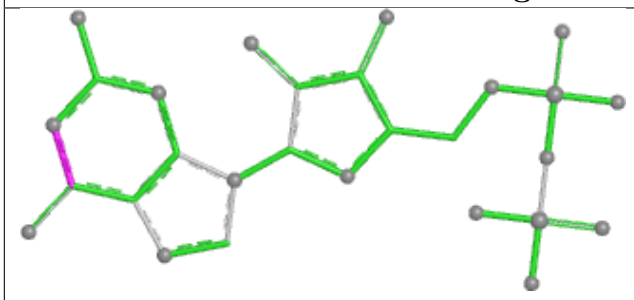
Ligand GTP y 602



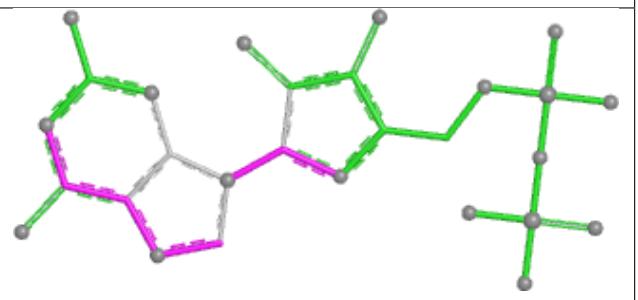
Ligand GDP FL 501



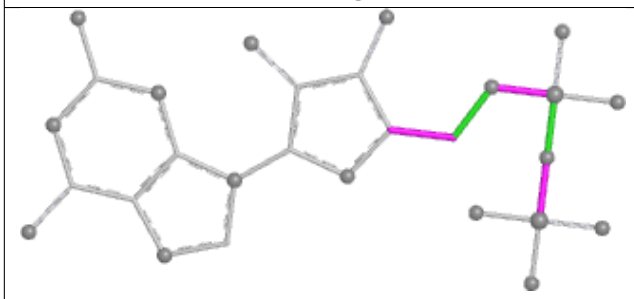
Ligand GDP Bk 501



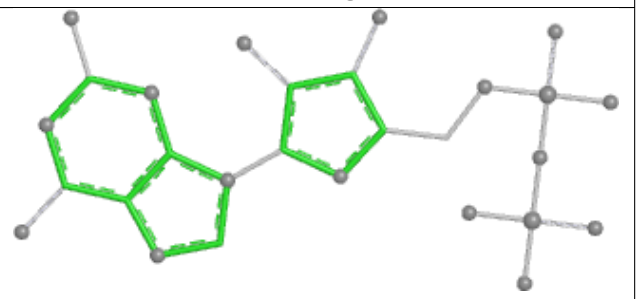
Bond lengths



Bond angles

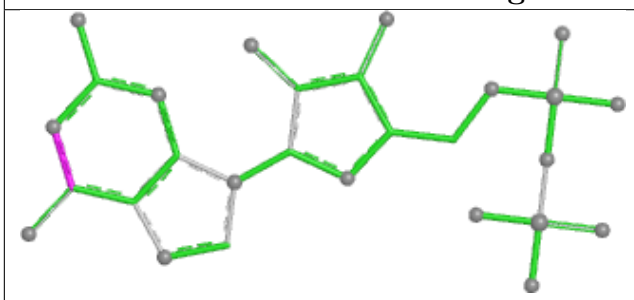


Torsions

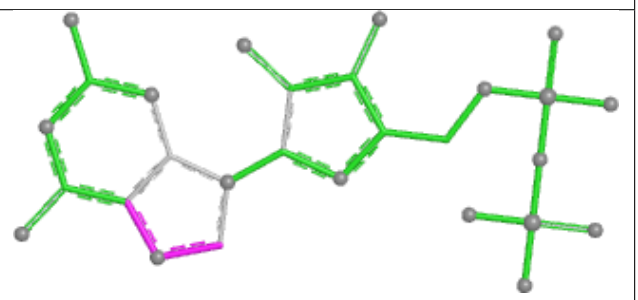


Rings

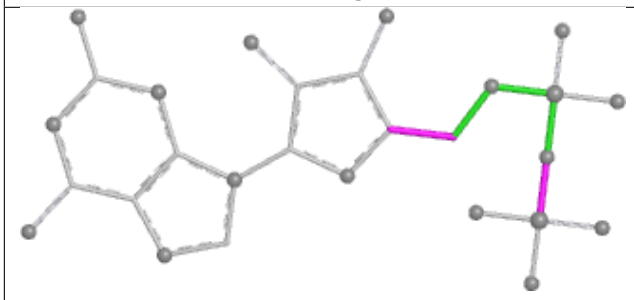
Ligand GDP Bm 501



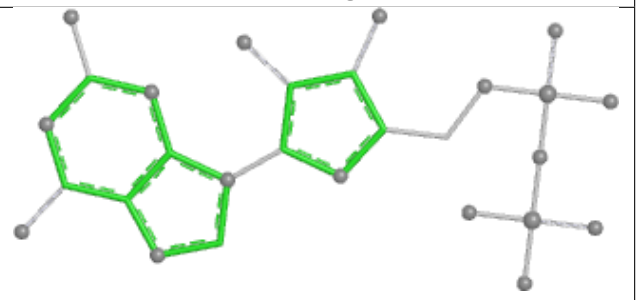
Bond lengths



Bond angles

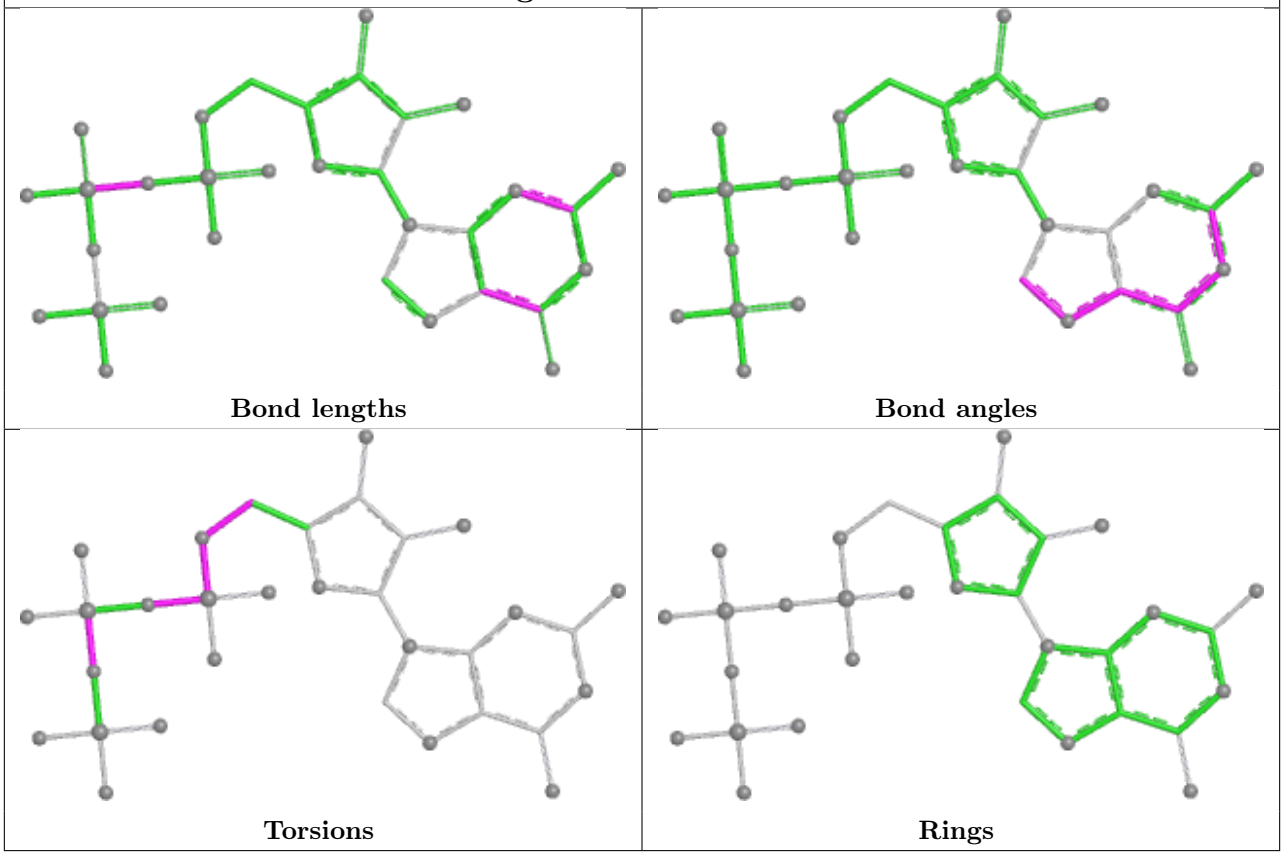


Torsions

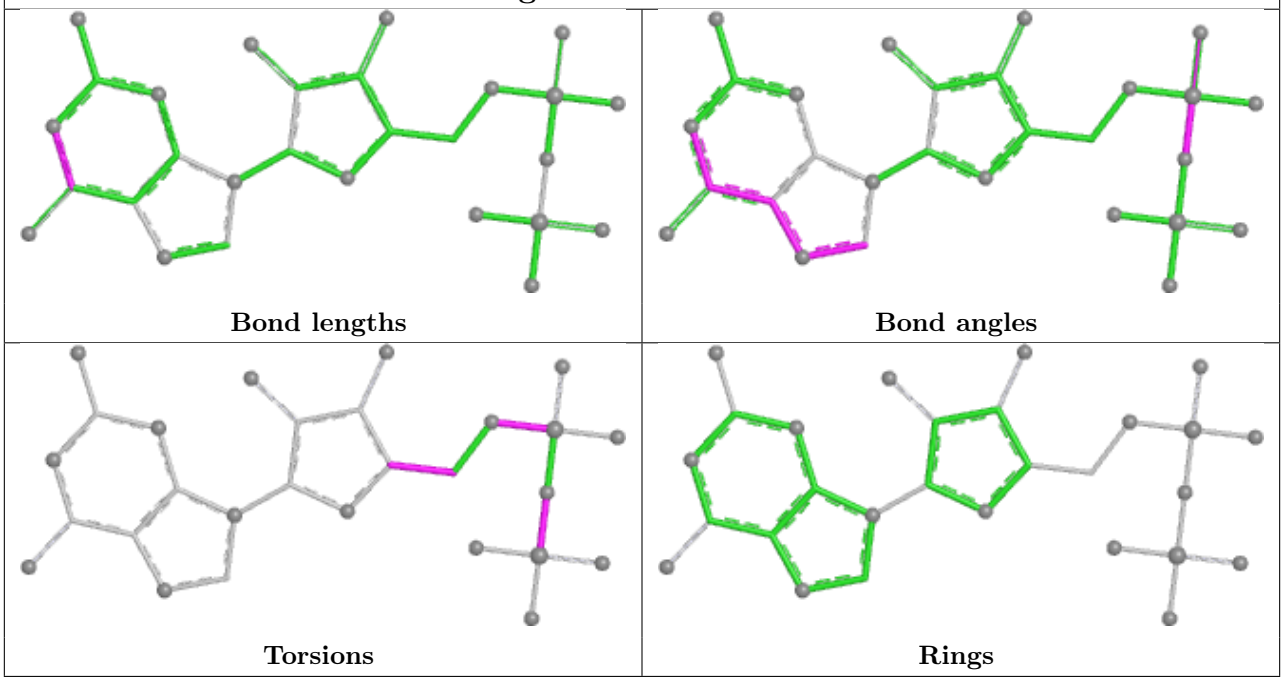


Rings

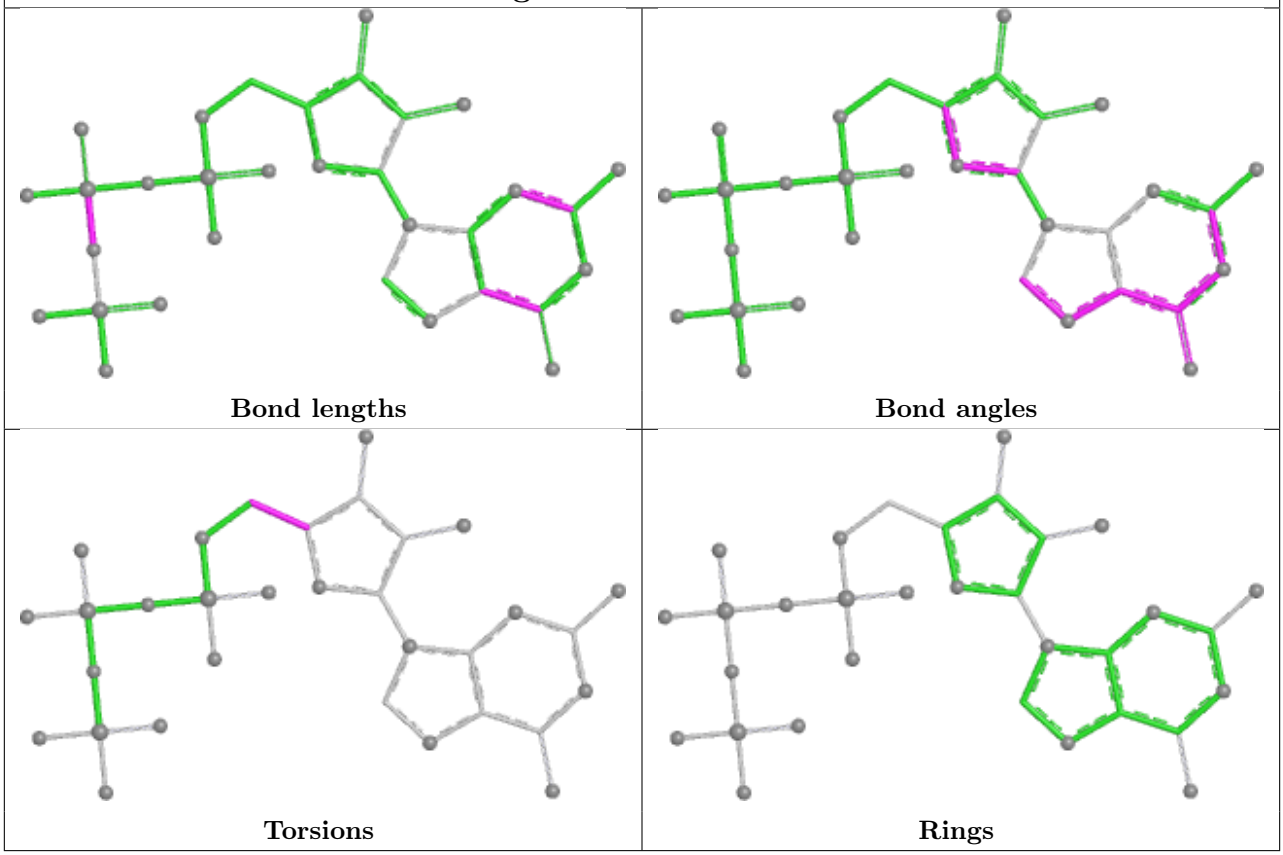
Ligand GTP F6 501



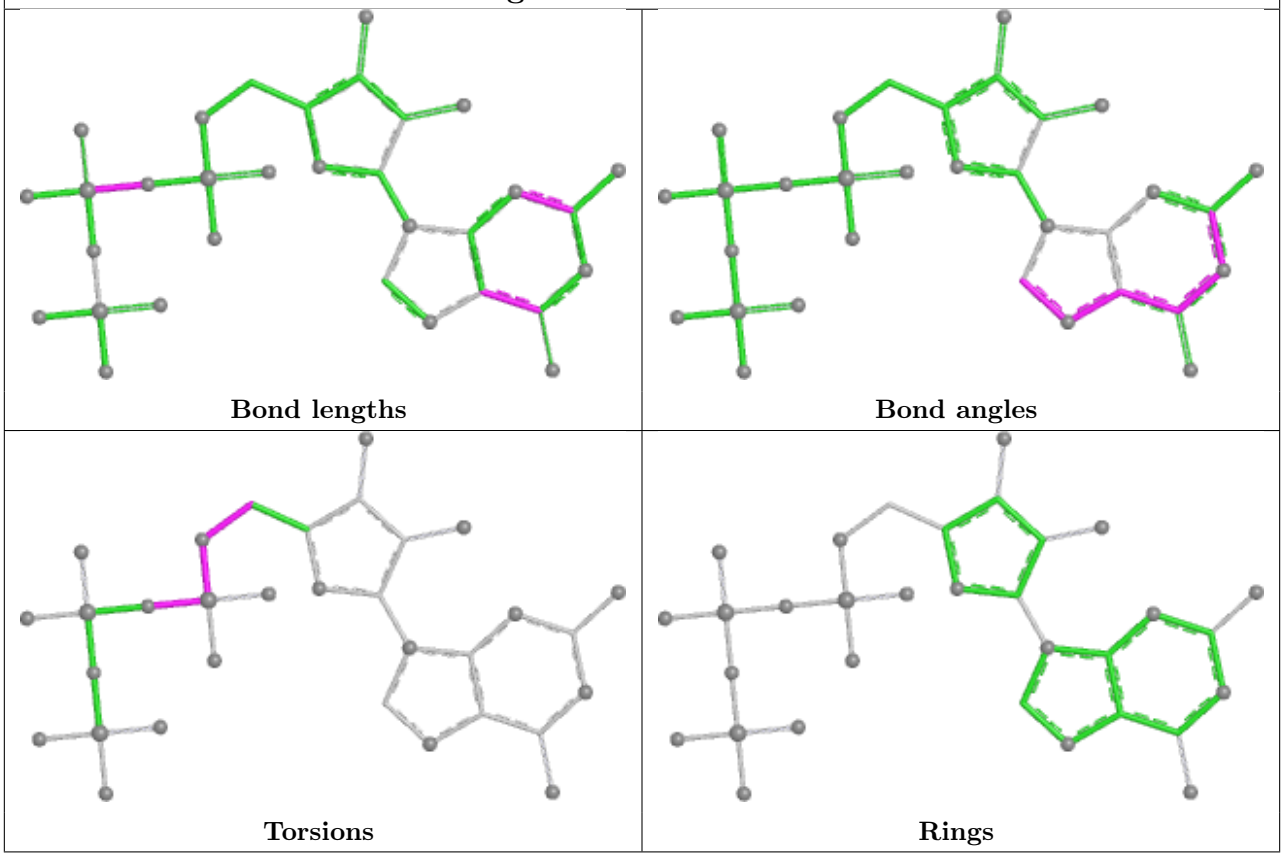
Ligand GDP Fs 501



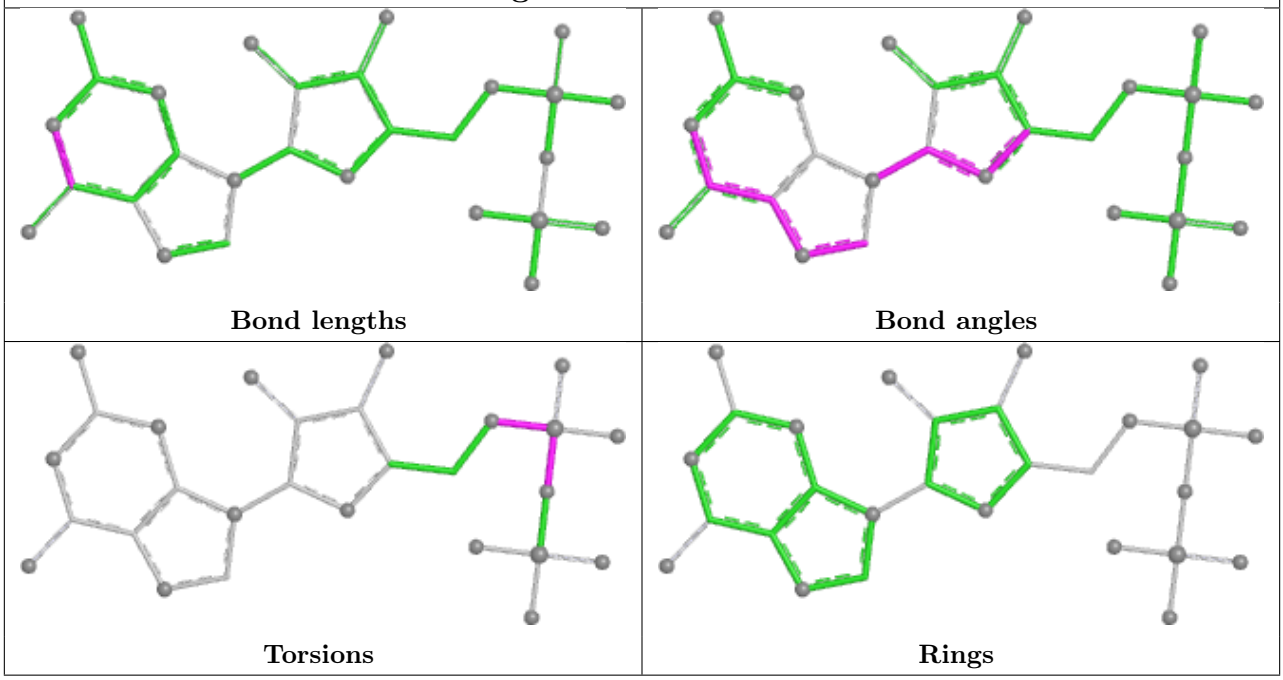
Ligand GTP AS 501



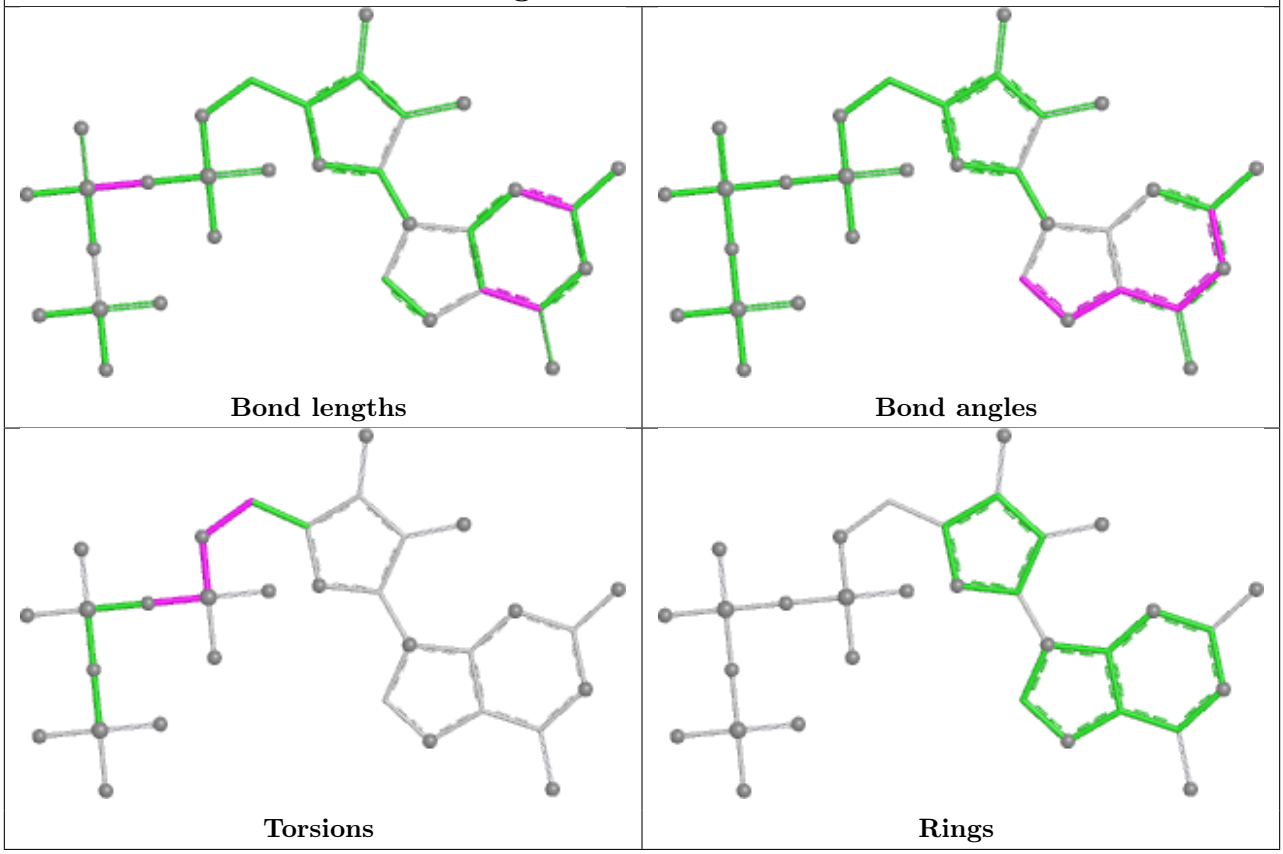
Ligand GTP FW 501



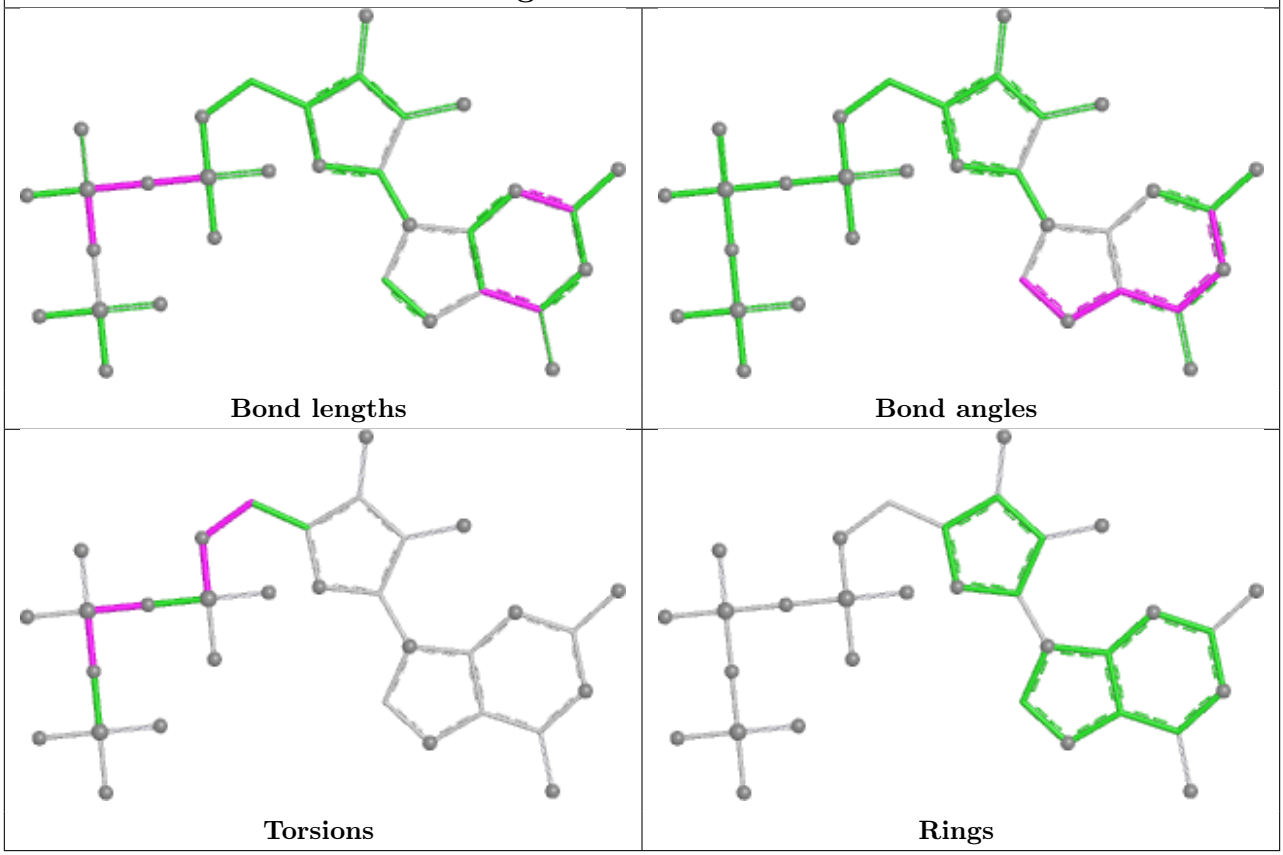
Ligand GDP BZ 501



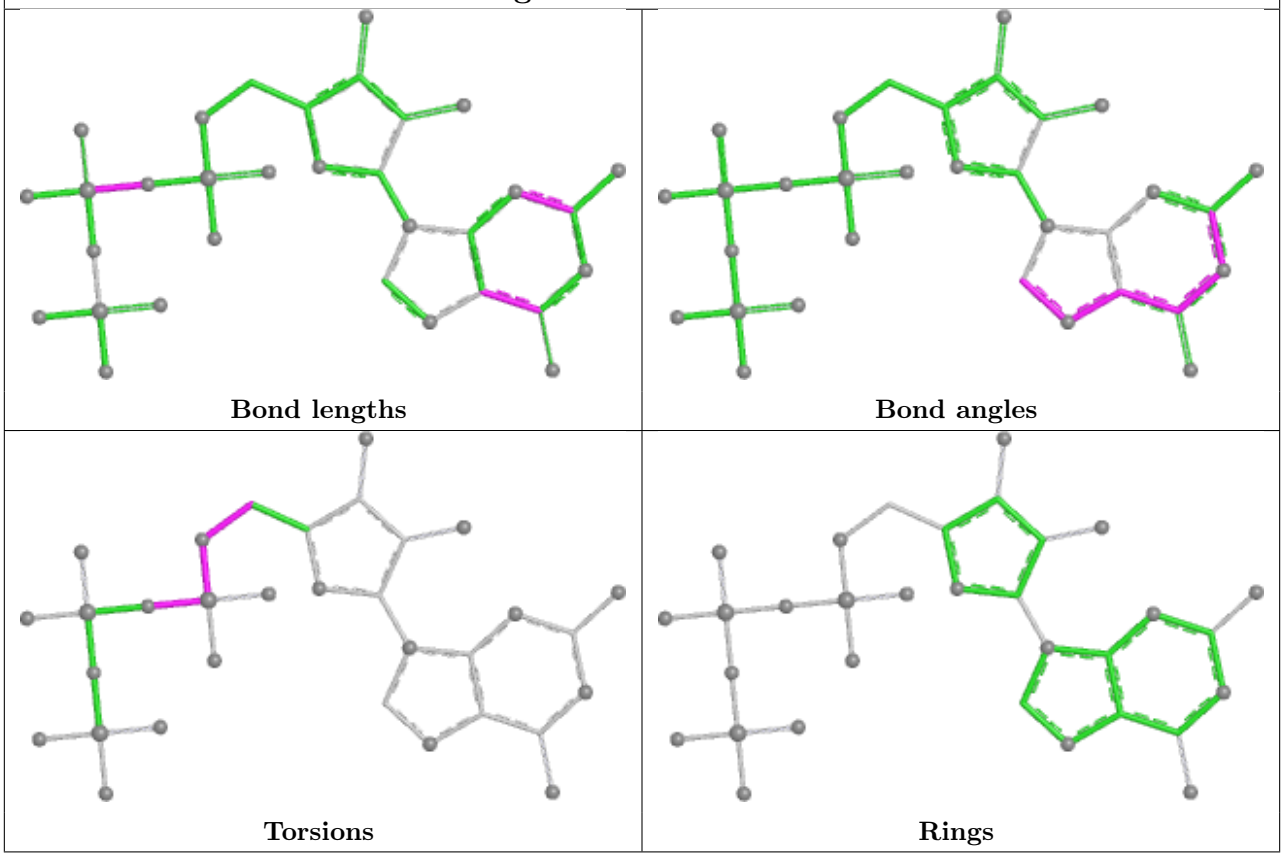
Ligand GTP Gv 501



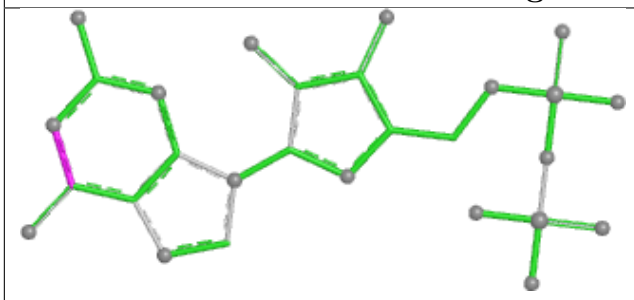
Ligand GTP Ez 501



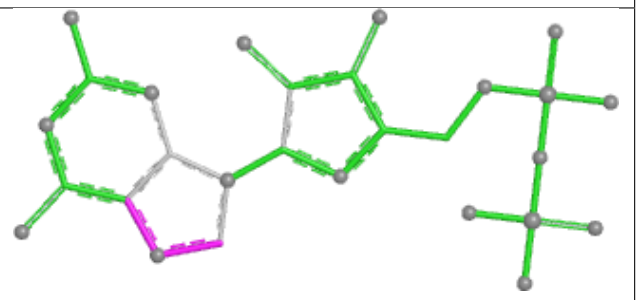
Ligand GTP A7 501



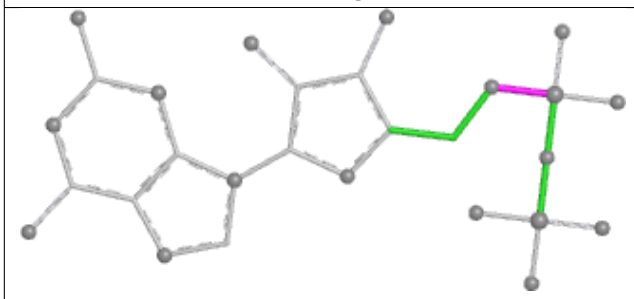
Ligand GDP 9 501



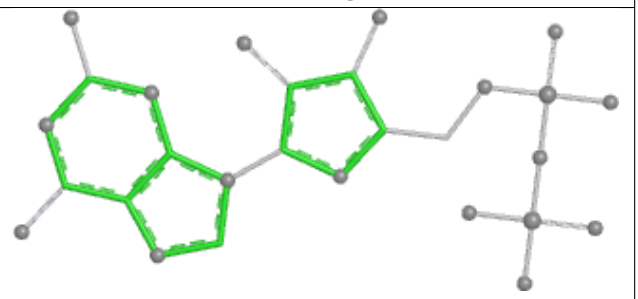
Bond lengths



Bond angles

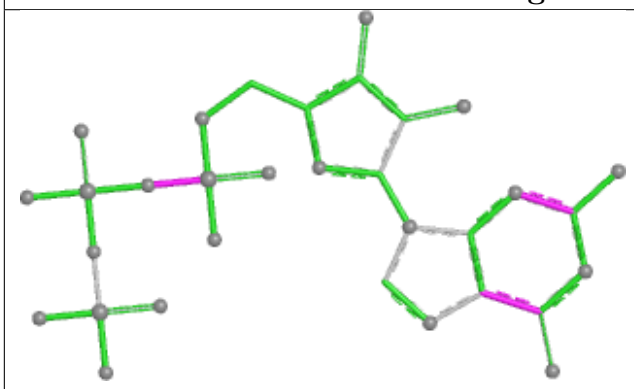


Torsions

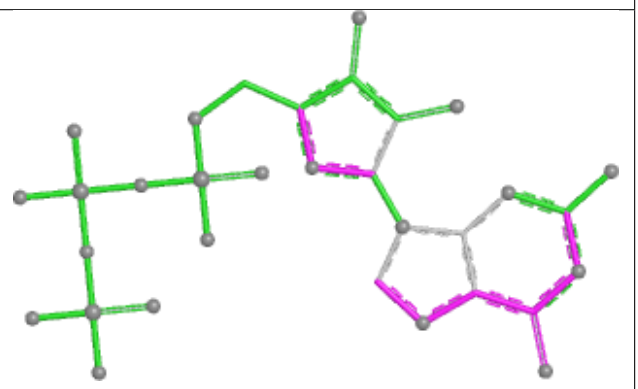


Rings

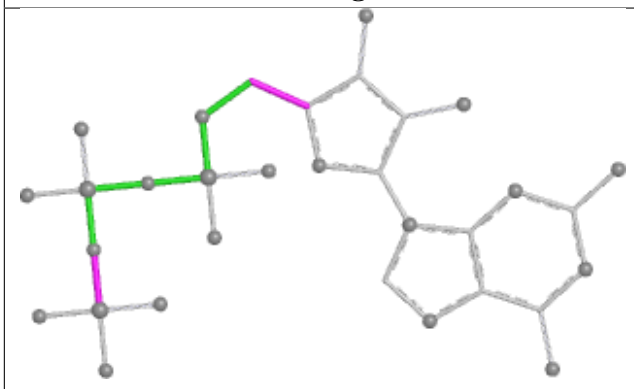
Ligand GTP 5 602



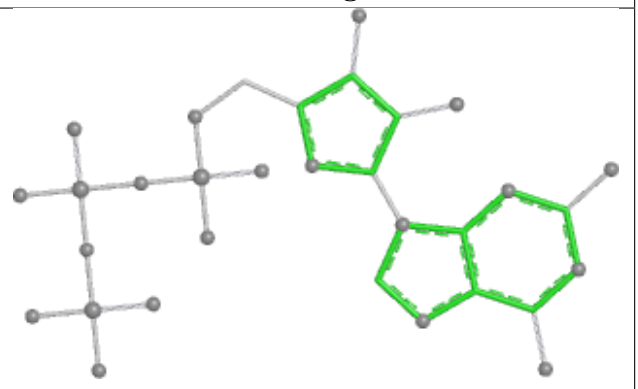
Bond lengths



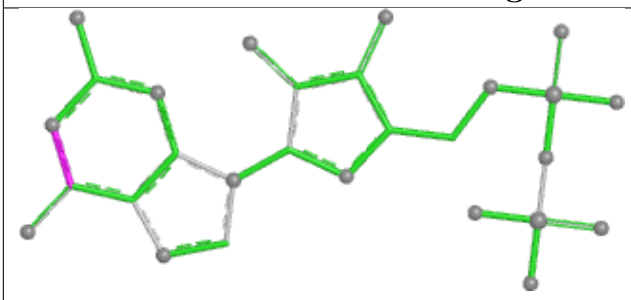
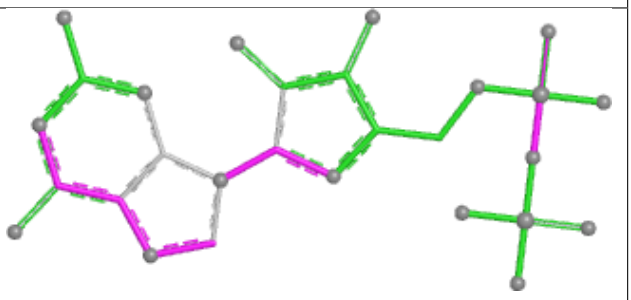
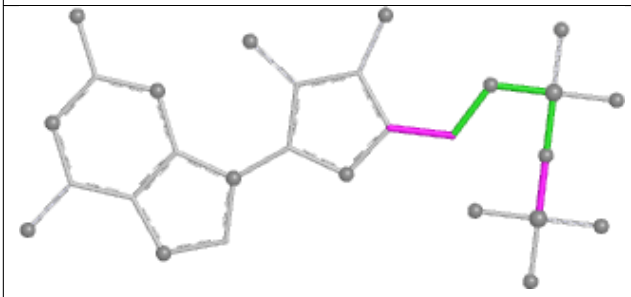
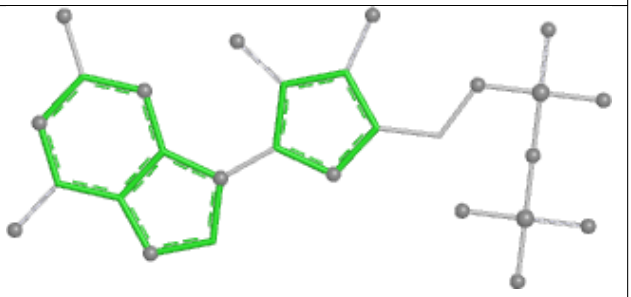
Bond angles

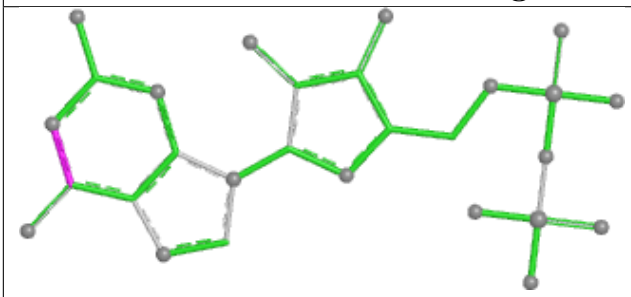
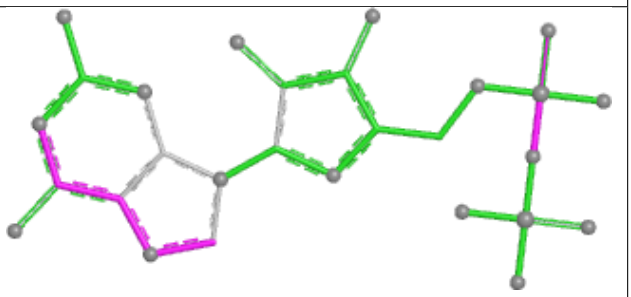
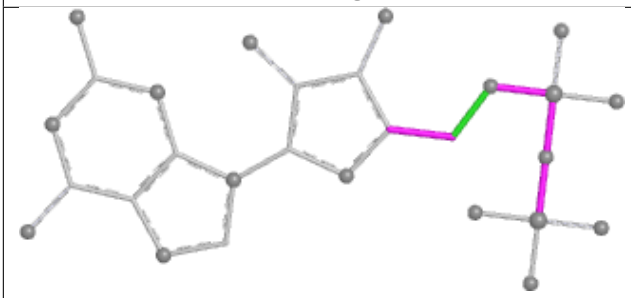
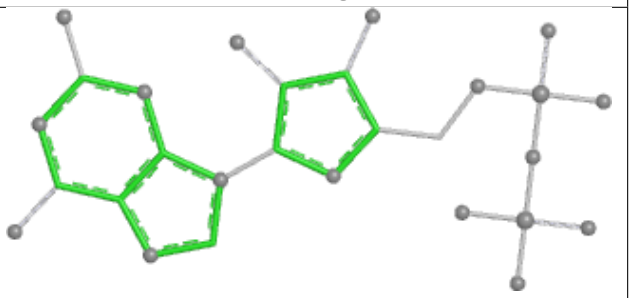


Torsions

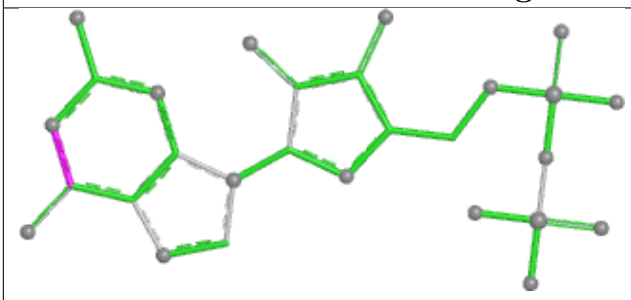


Rings

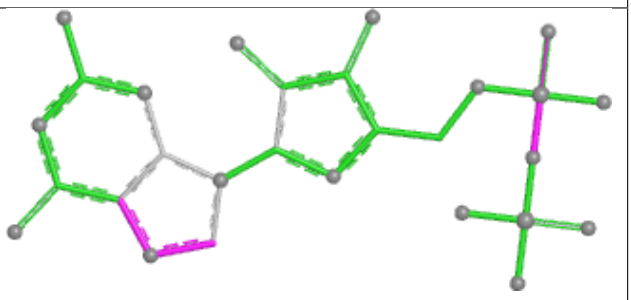
Ligand GDP EM 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP Gb 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

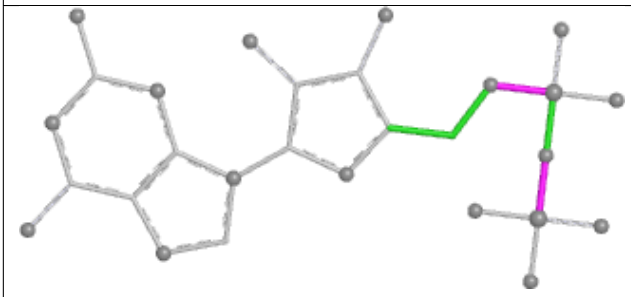
Ligand GDP Fv 501



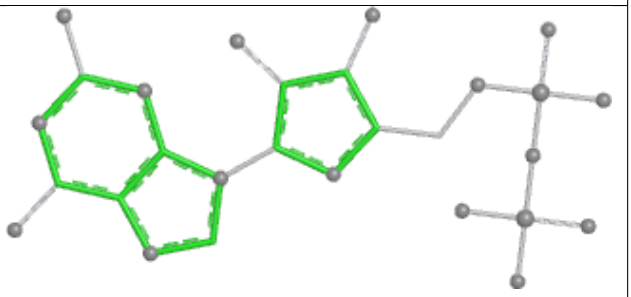
Bond lengths



Bond angles

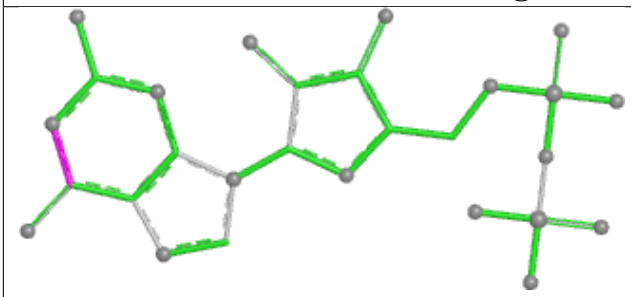


Torsions

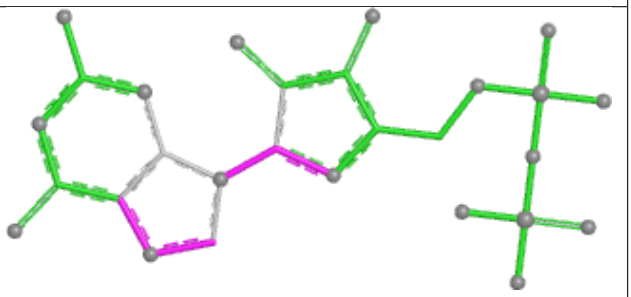


Rings

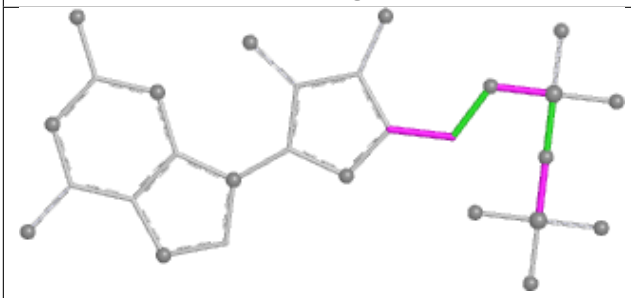
Ligand GDP Eb 501



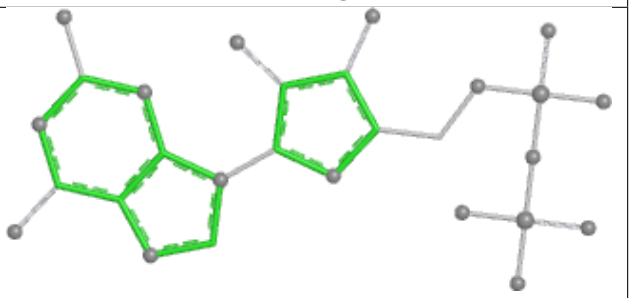
Bond lengths



Bond angles

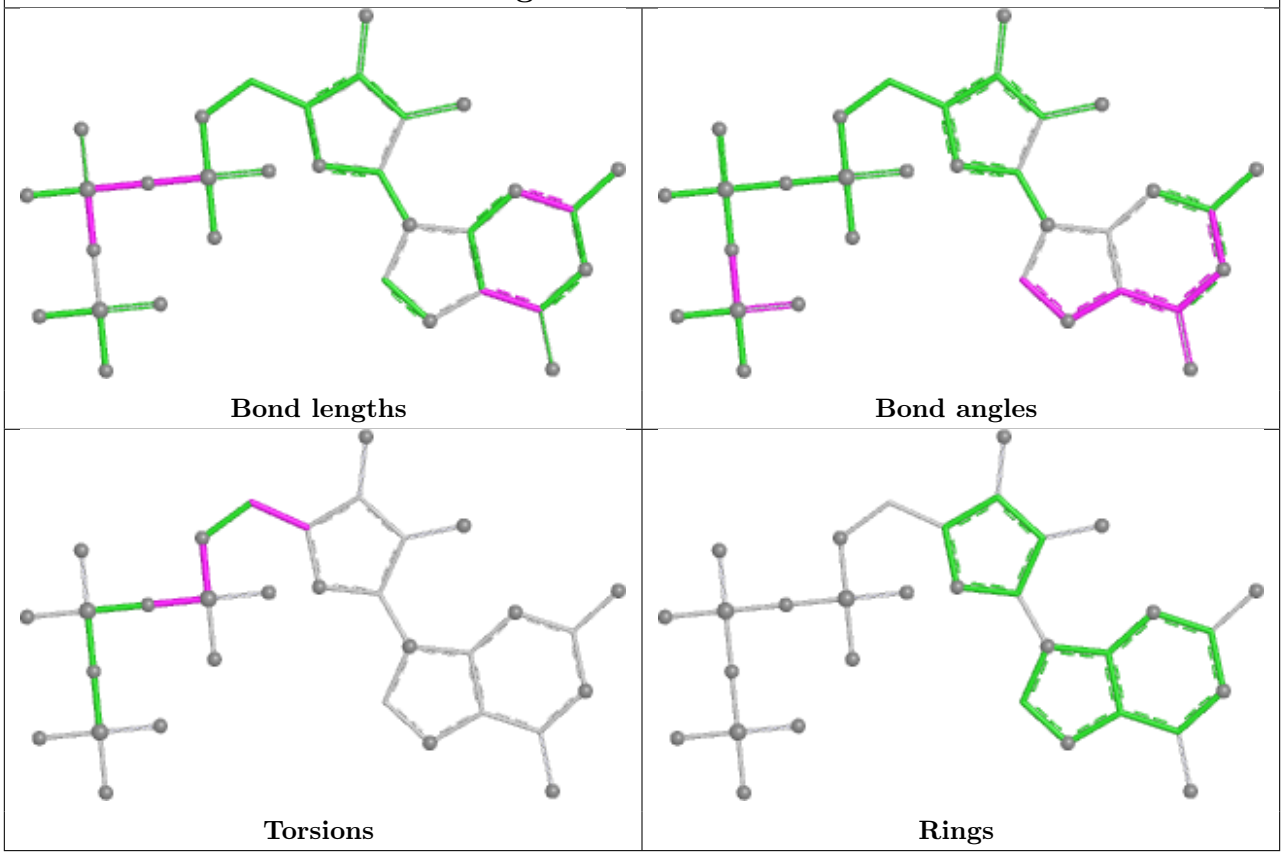


Torsions

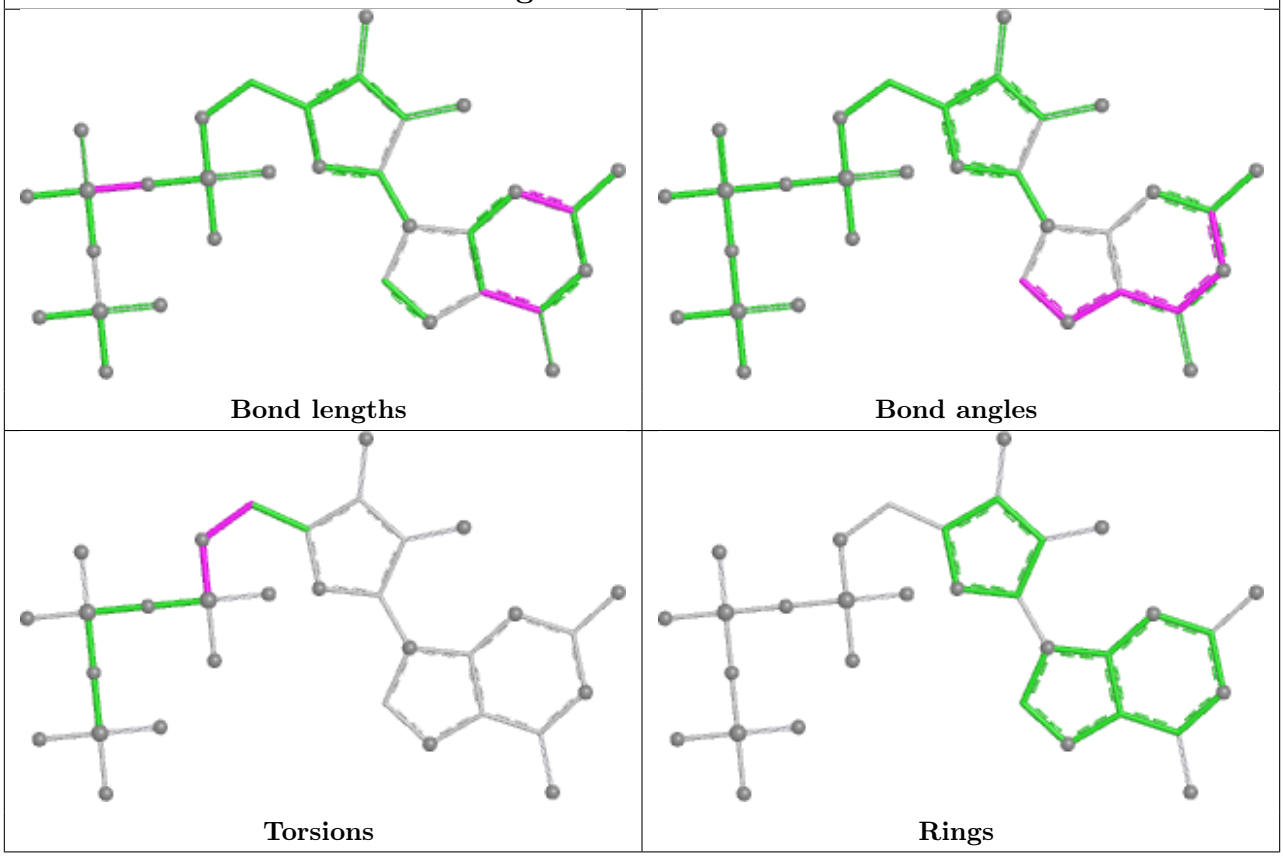


Rings

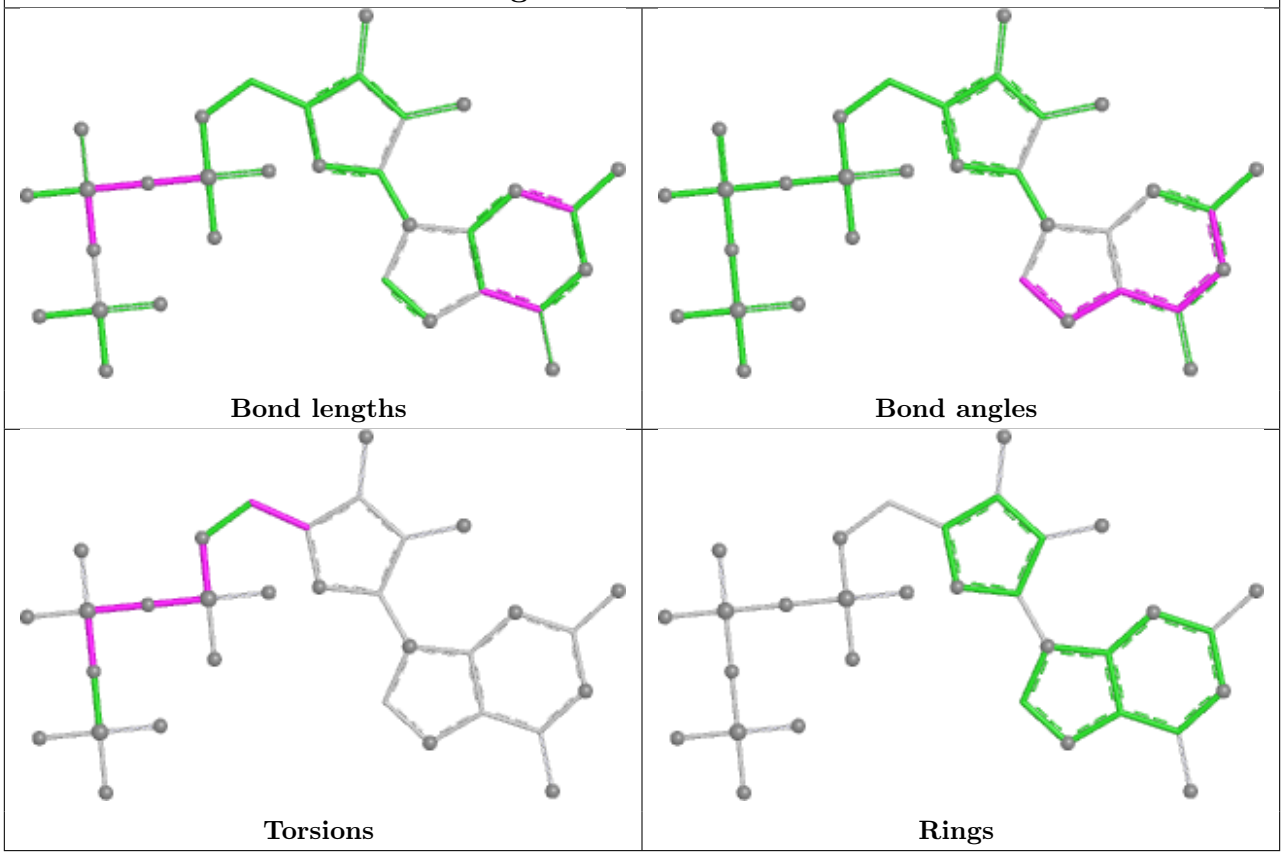
Ligand GTP Bz 602



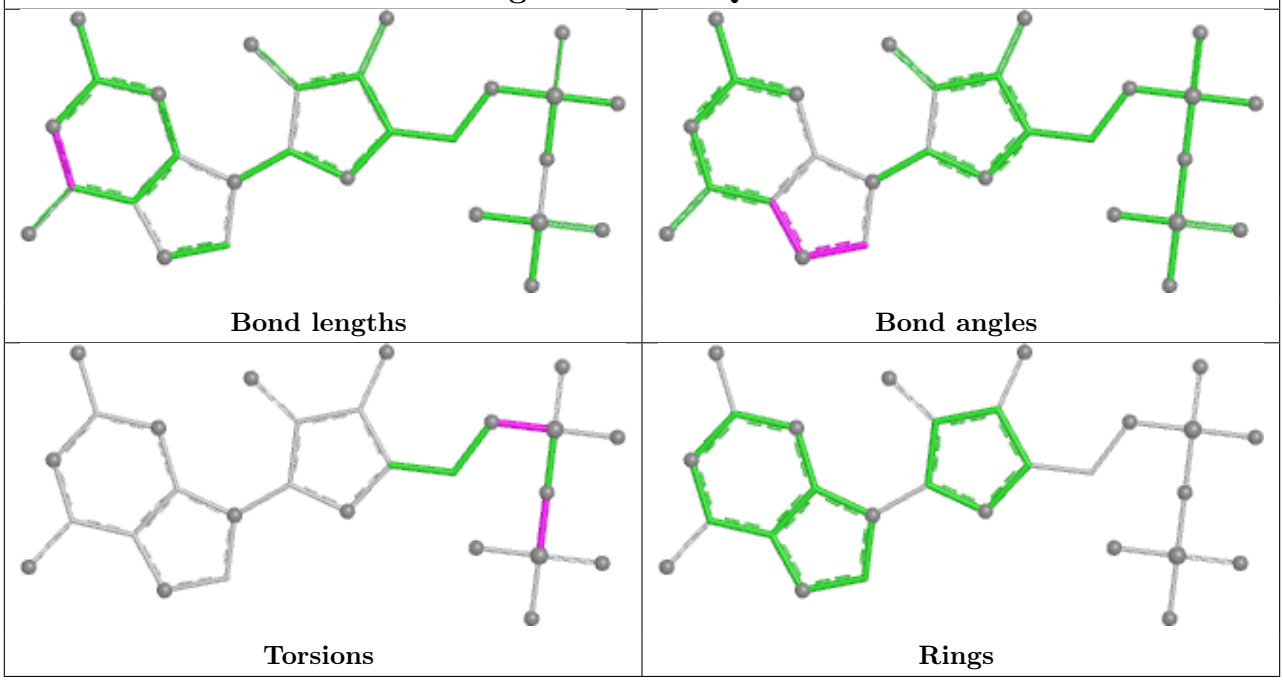
Ligand GTP Fk 501



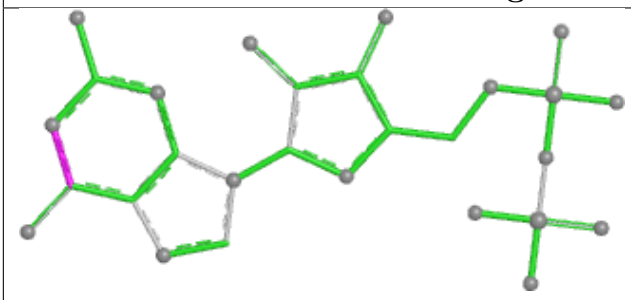
Ligand GTP GP 501



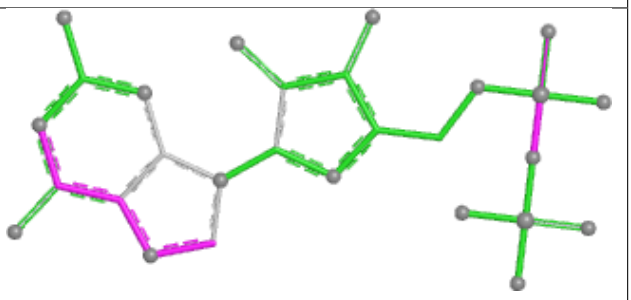
Ligand GDP AQ 501



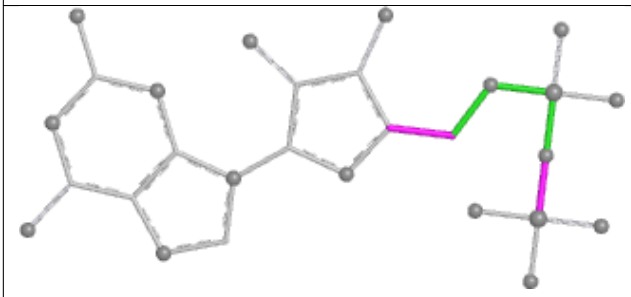
Ligand GDP DU 501



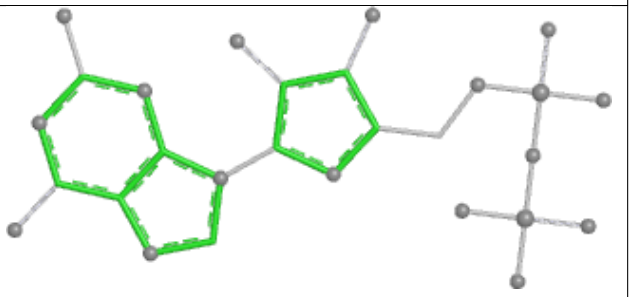
Bond lengths



Bond angles

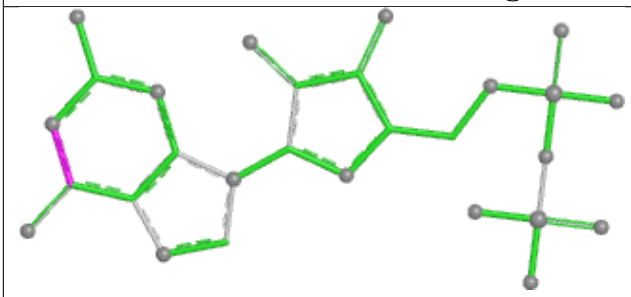


Torsions

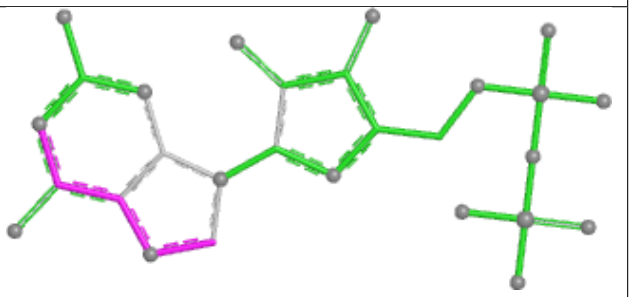


Rings

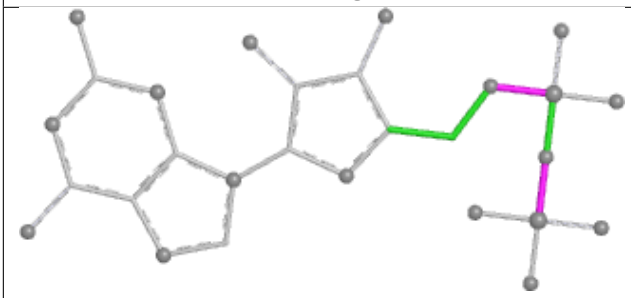
Ligand GDP AM 501



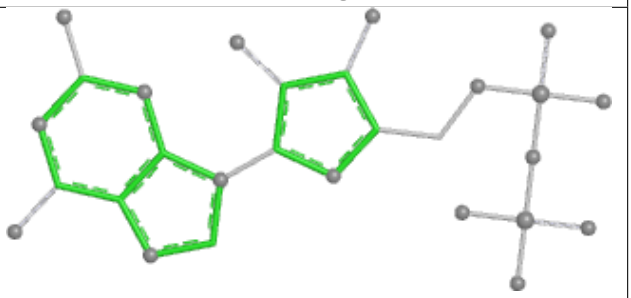
Bond lengths



Bond angles

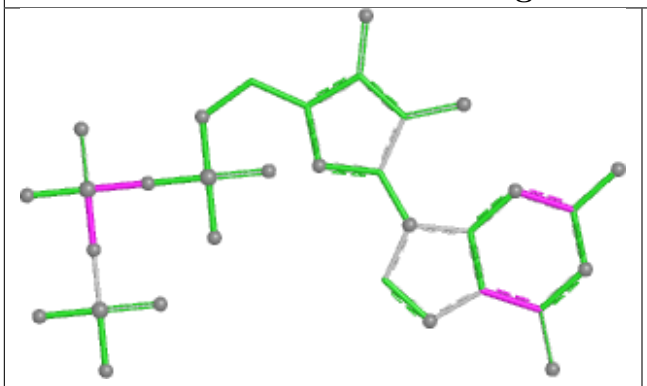


Torsions

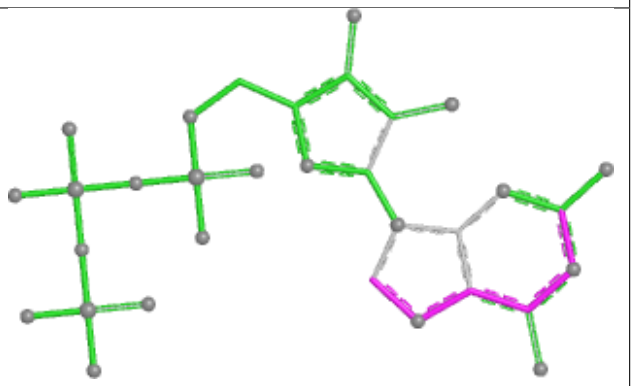


Rings

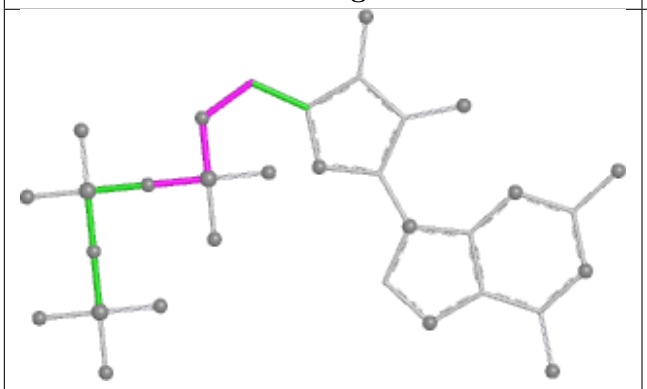
Ligand GTP Fb 501



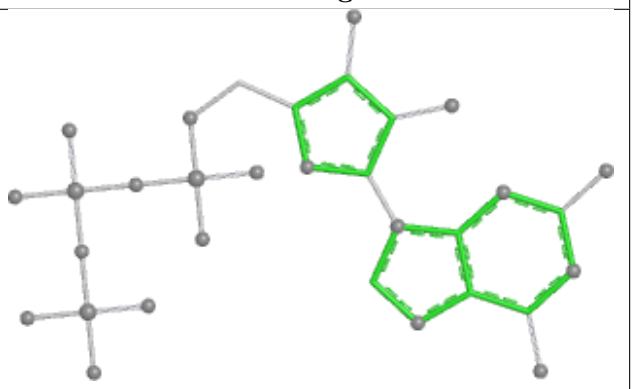
Bond lengths



Bond angles

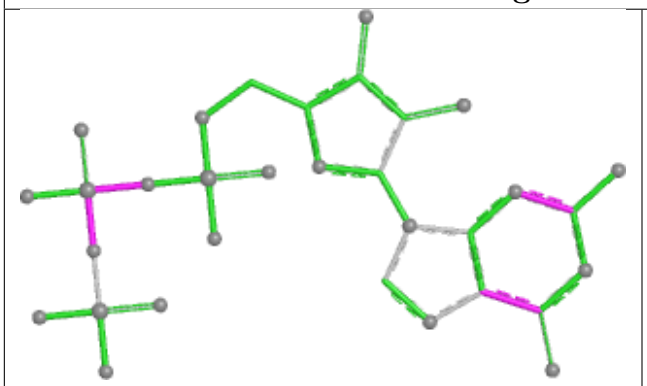


Torsions

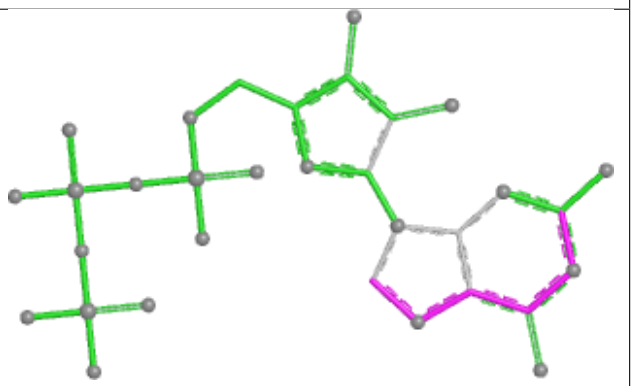


Rings

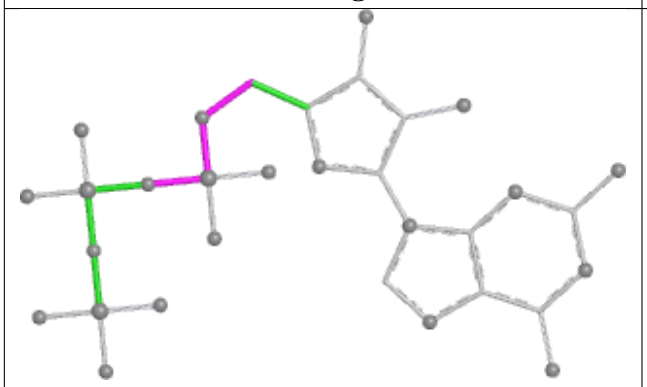
Ligand GTP FT 501



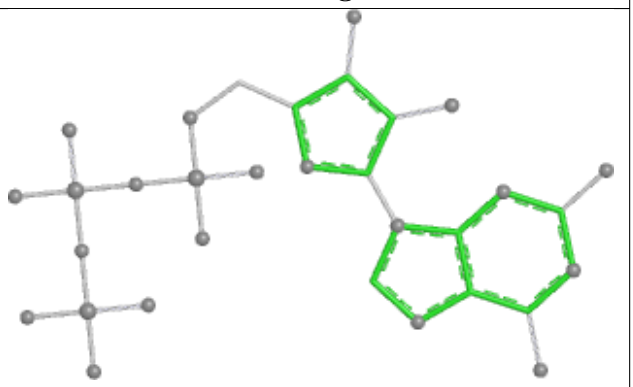
Bond lengths



Bond angles

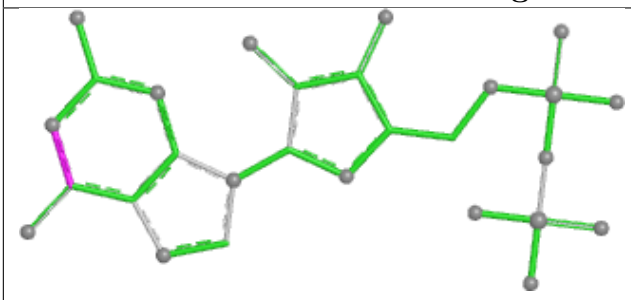


Torsions

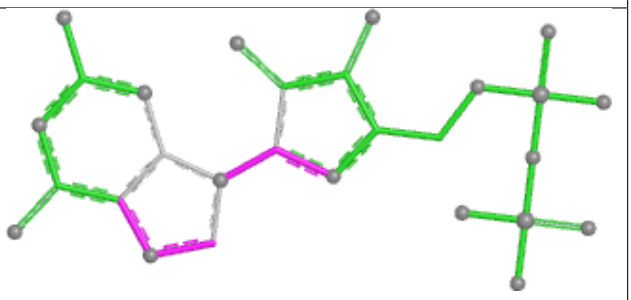


Rings

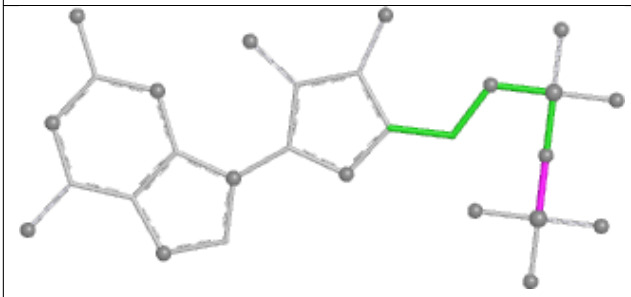
Ligand GDP Dx 501



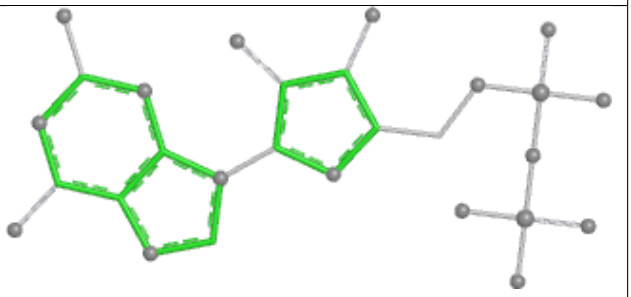
Bond lengths



Bond angles

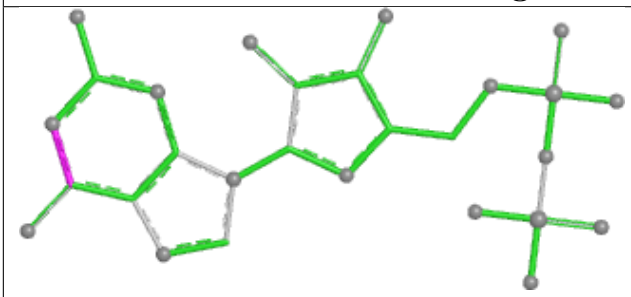


Torsions

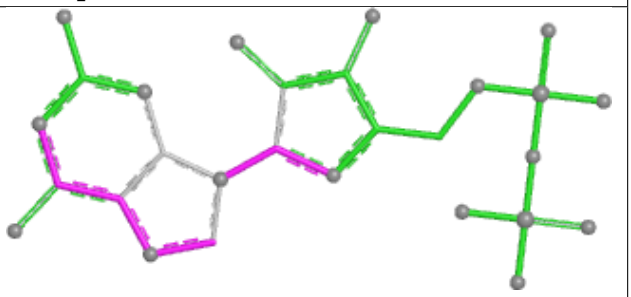


Rings

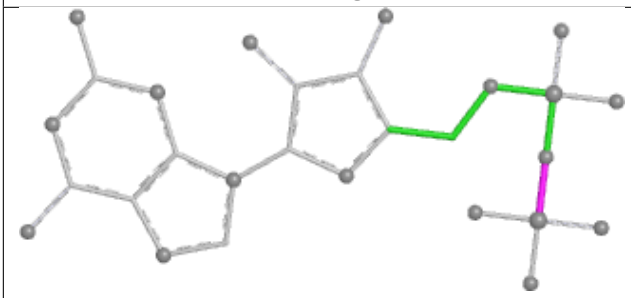
Ligand GDP Dq 501



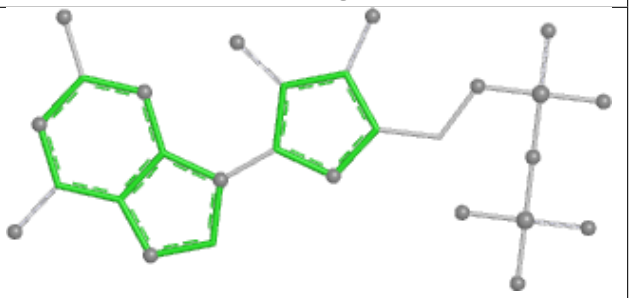
Bond lengths



Bond angles

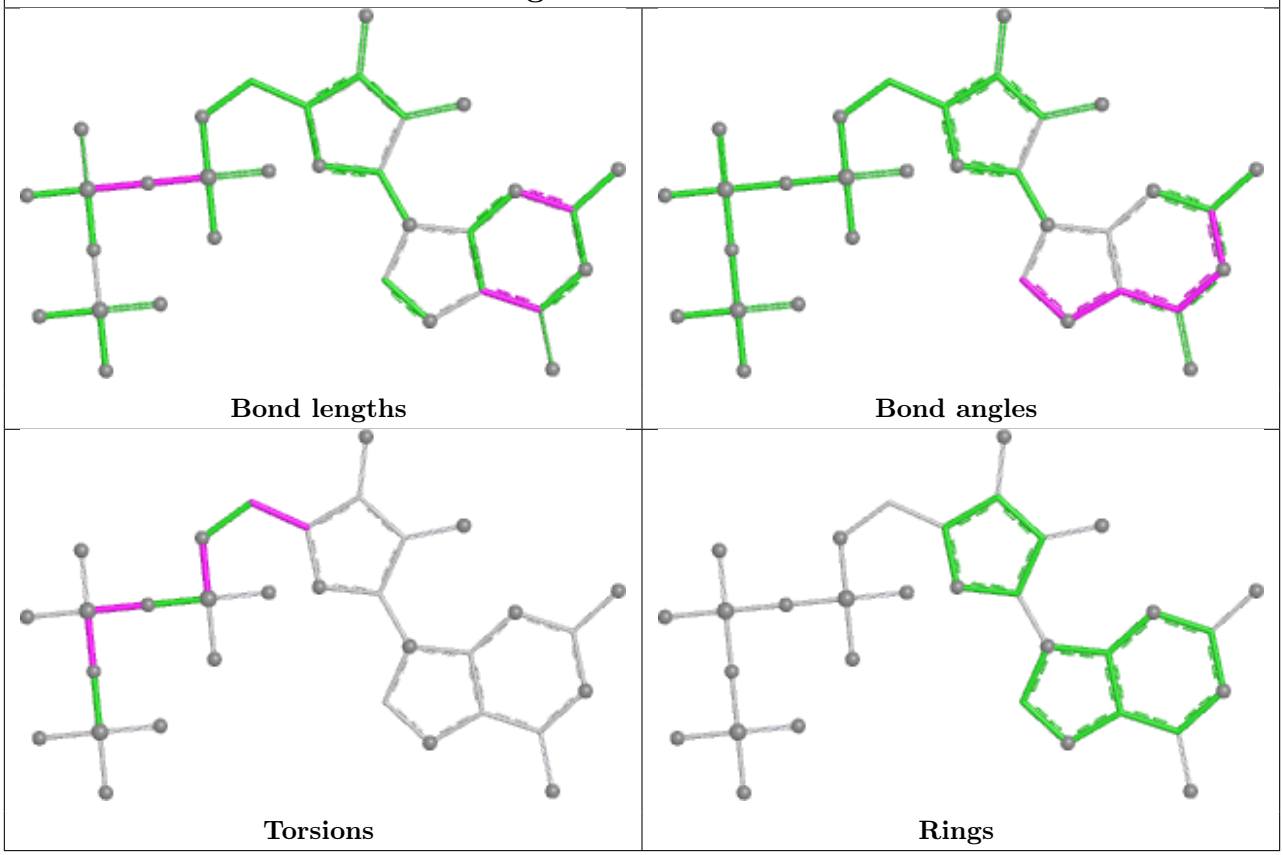


Torsions

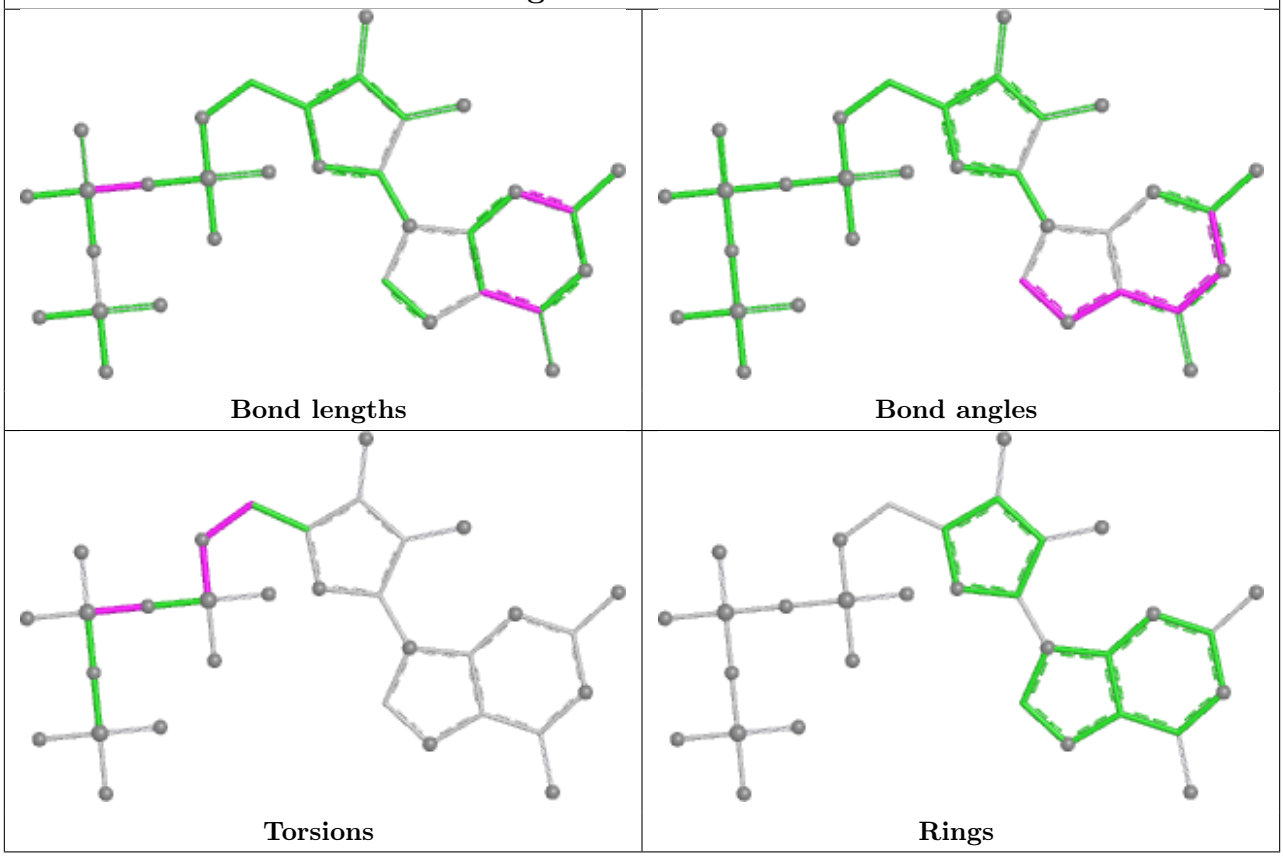


Rings

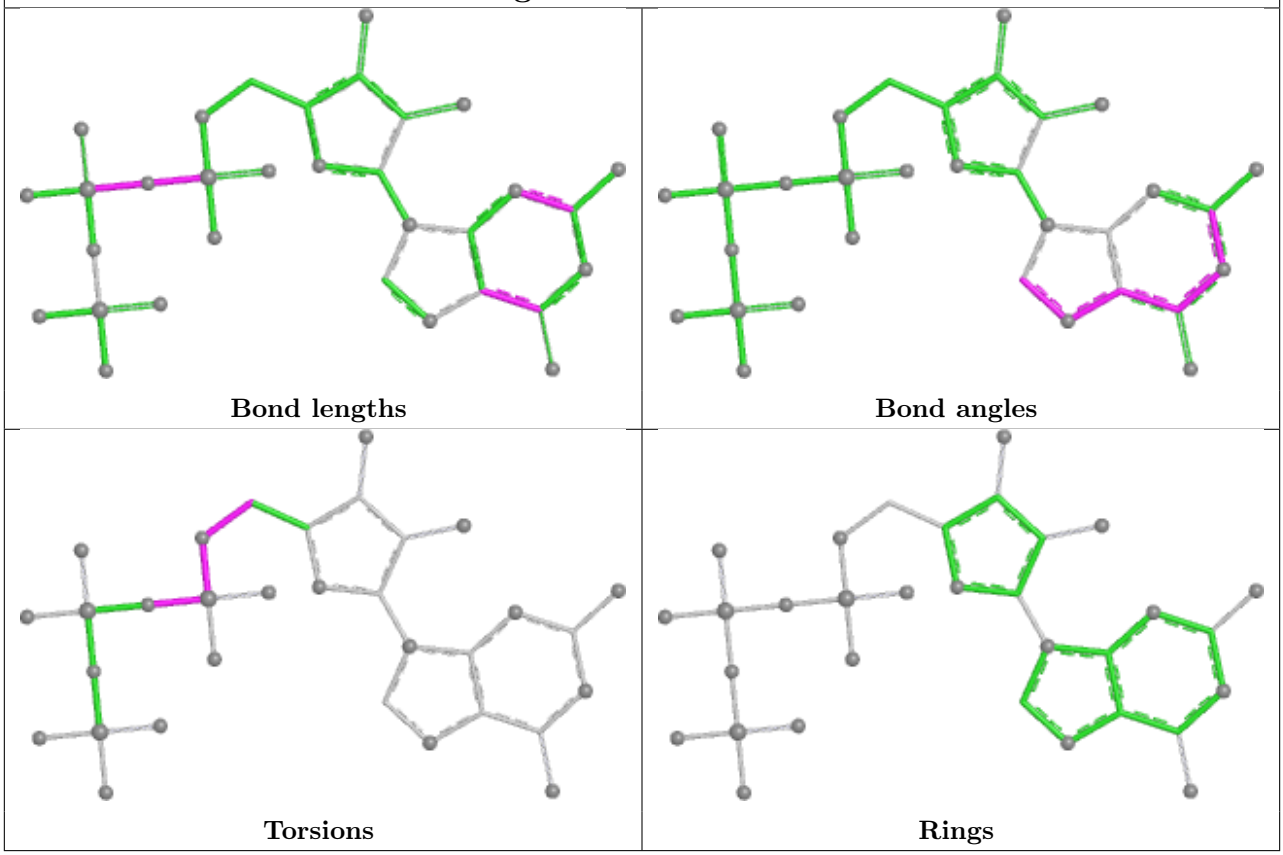
Ligand GTP b 602



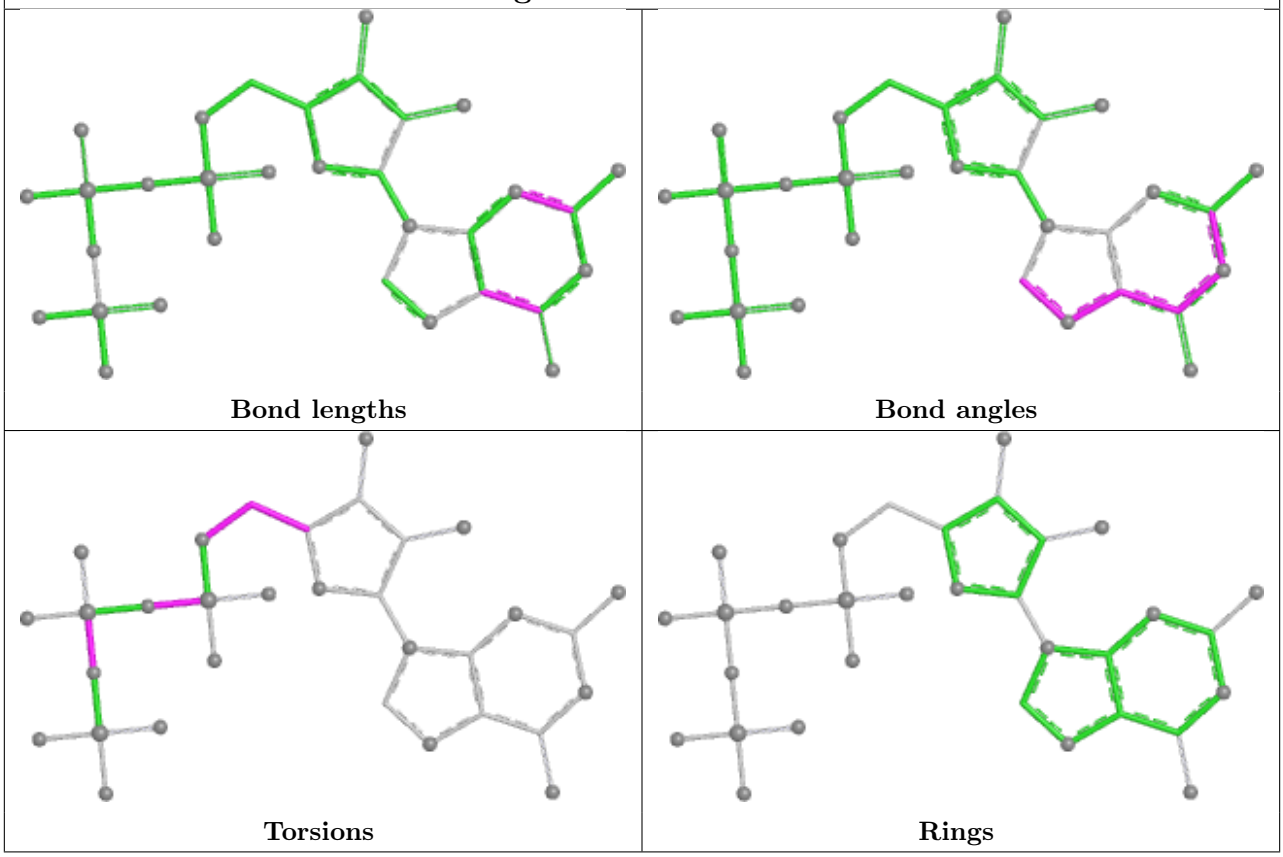
Ligand GTP k 602



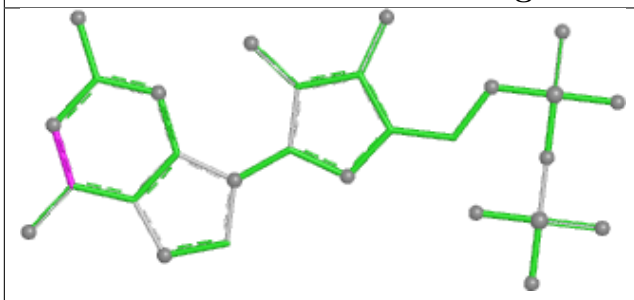
Ligand GTP A6 501



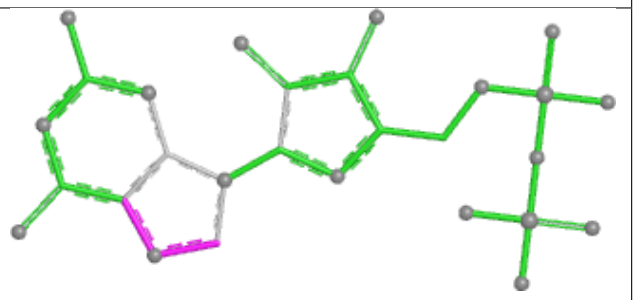
Ligand GTP BS 602



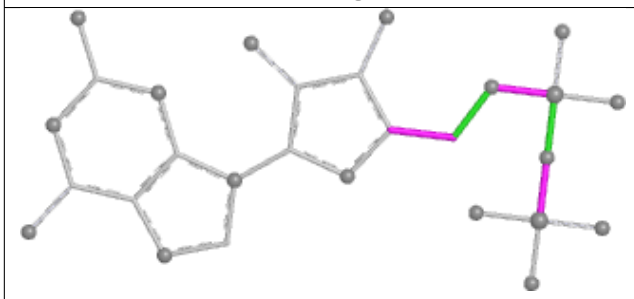
Ligand GDP F2 501



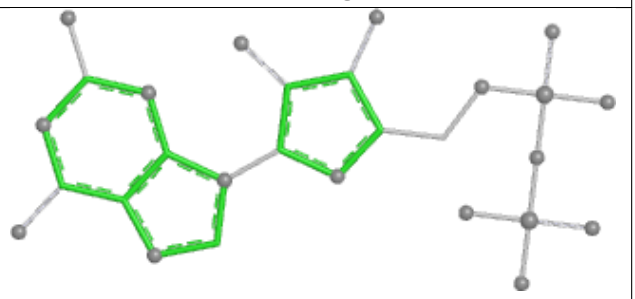
Bond lengths



Bond angles

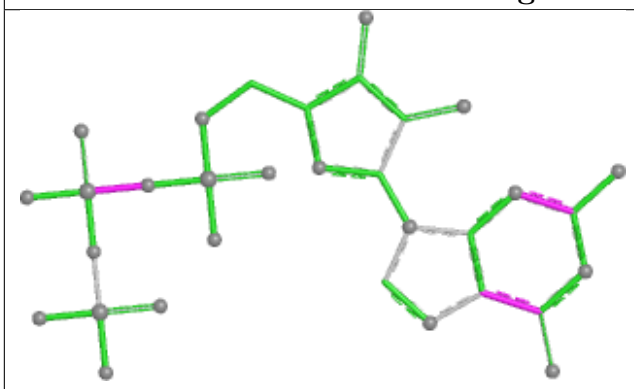


Torsions

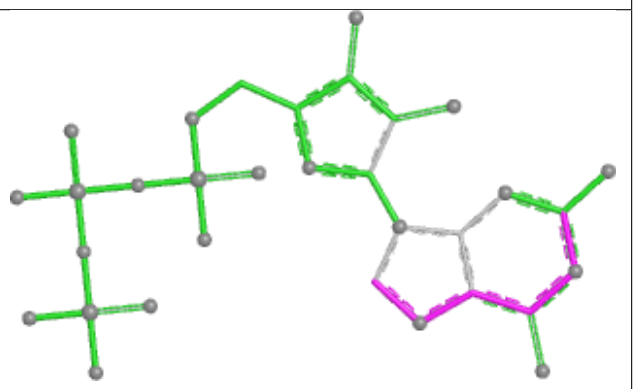


Rings

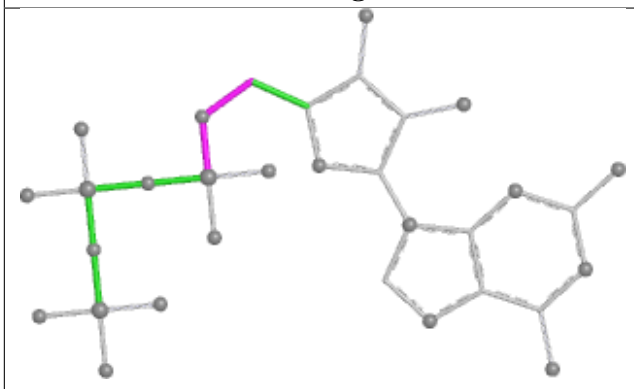
Ligand GTP Gl 501



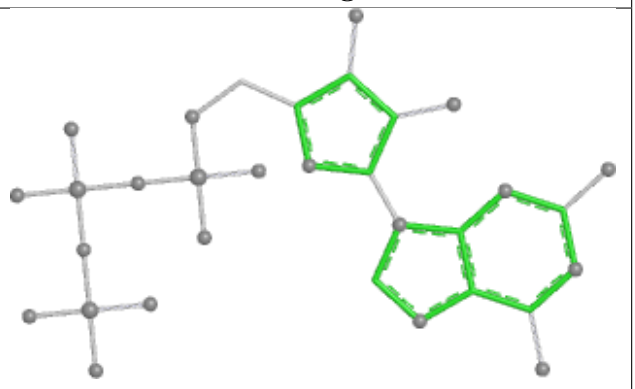
Bond lengths



Bond angles

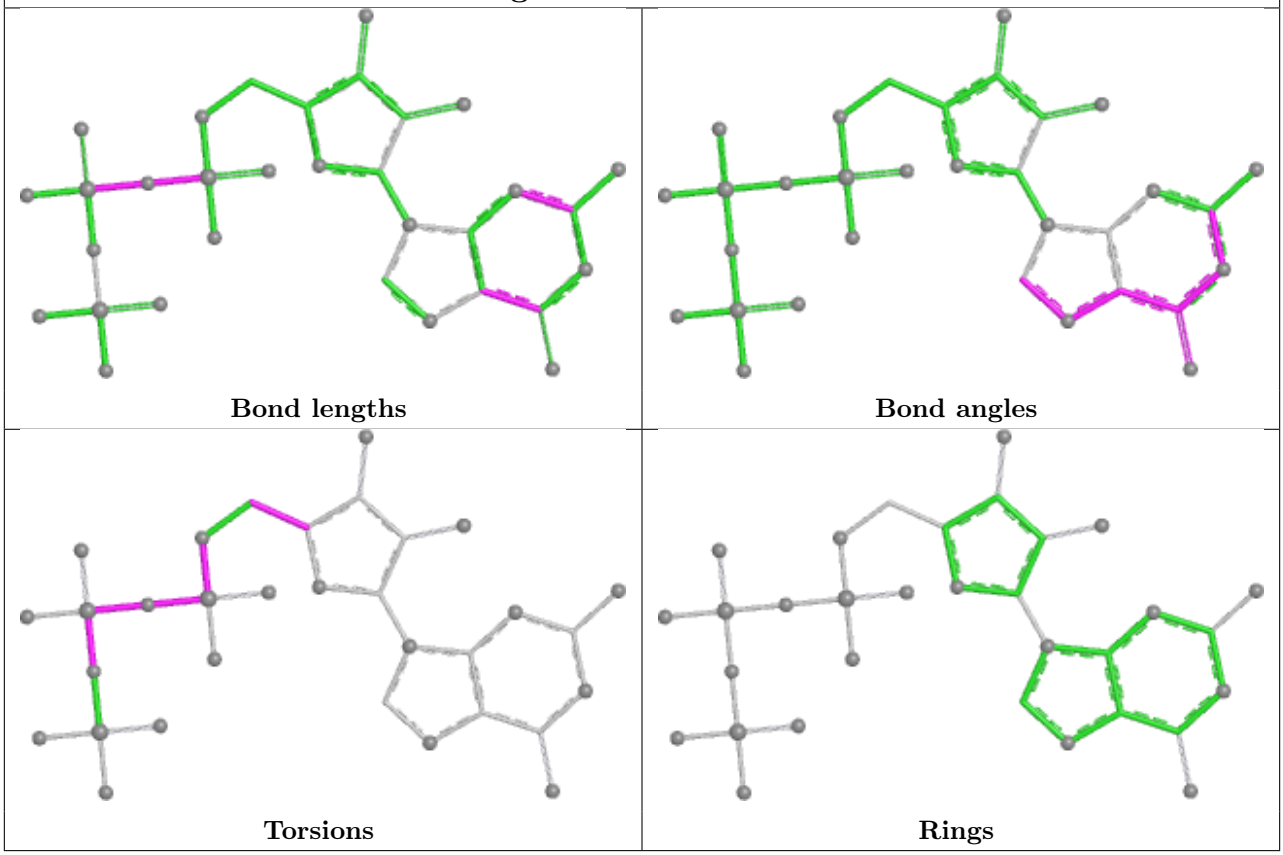


Torsions

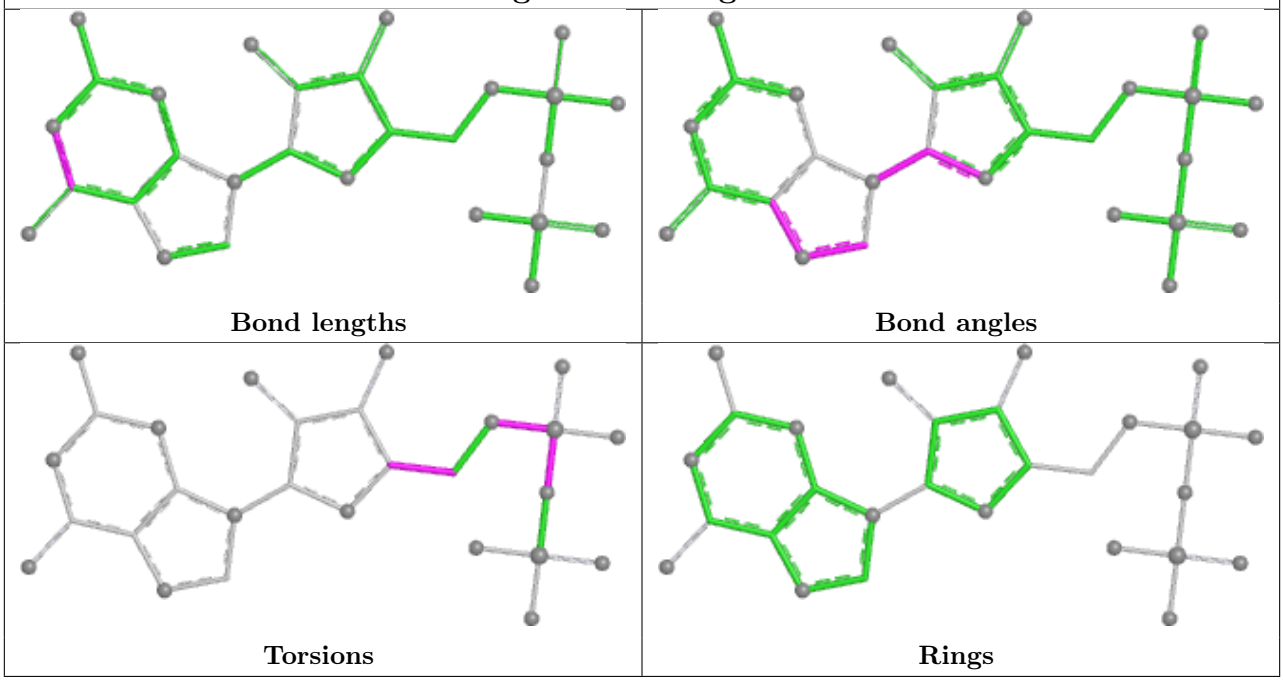


Rings

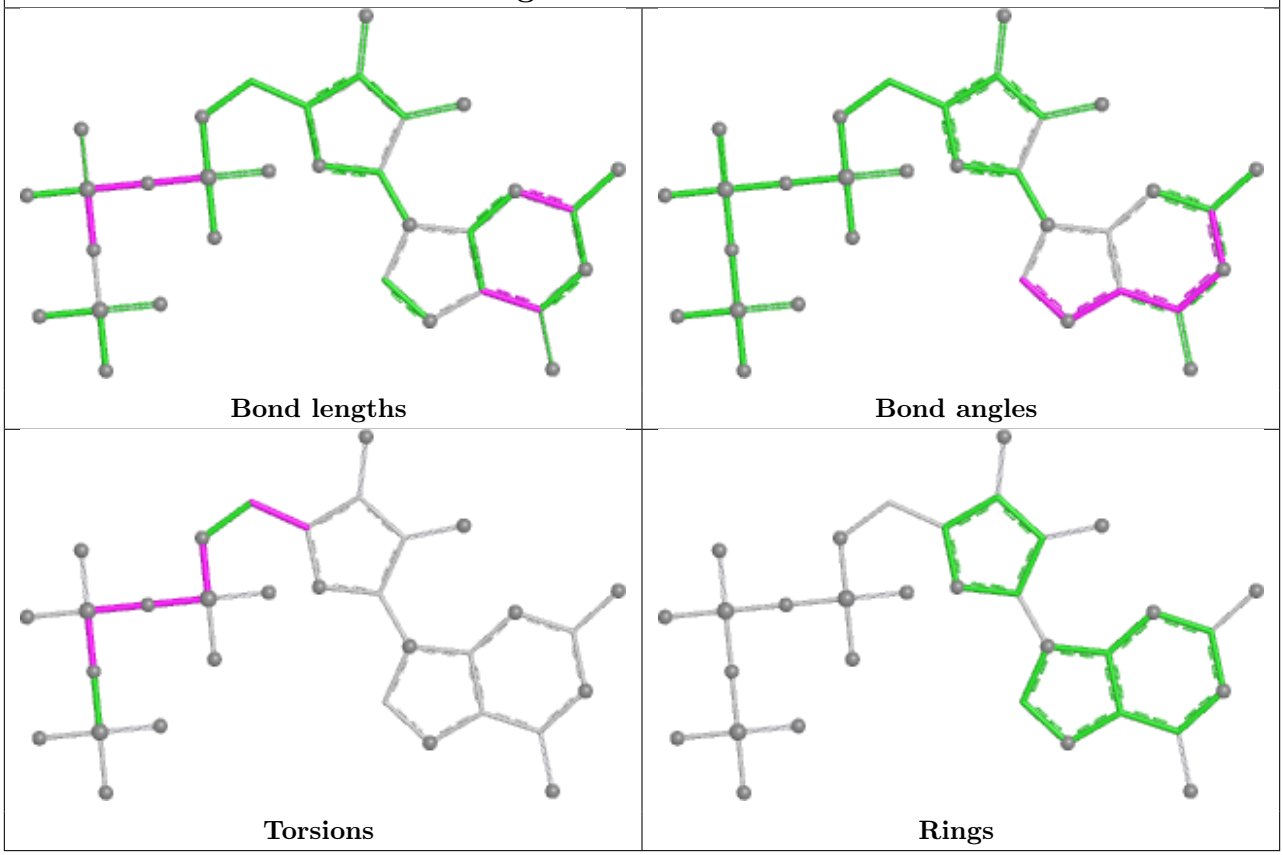
Ligand GTP GE 501



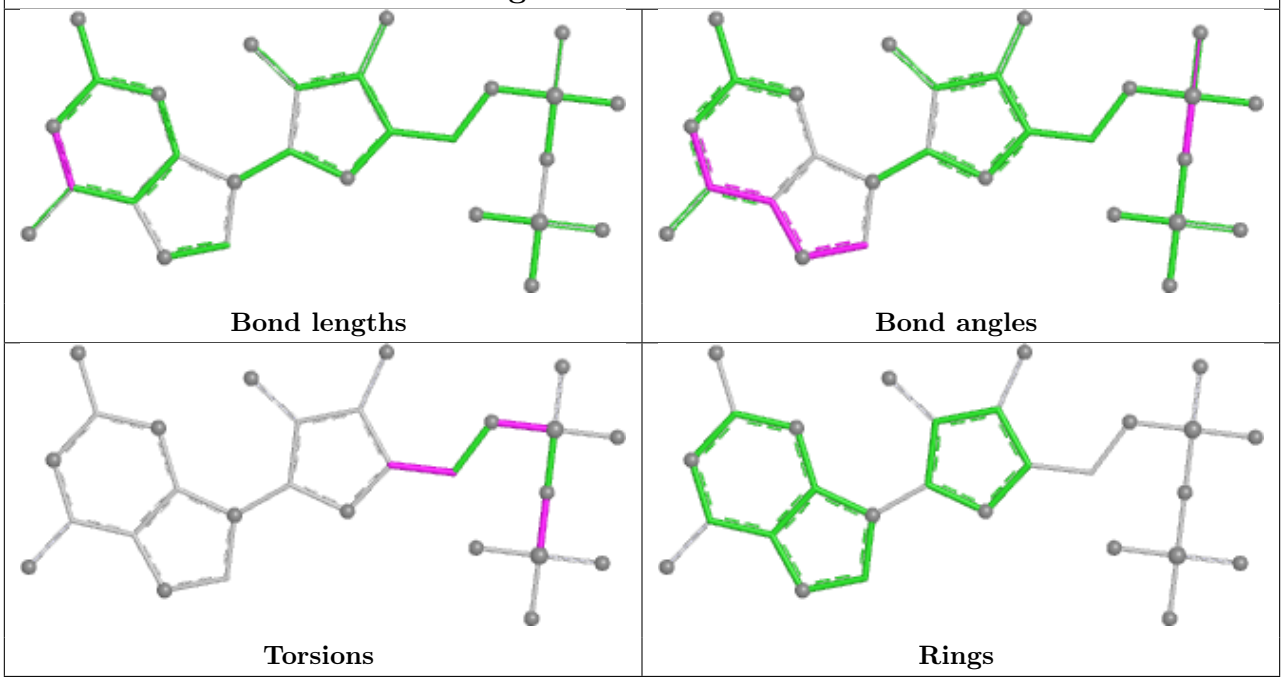
Ligand GDP Ag 501



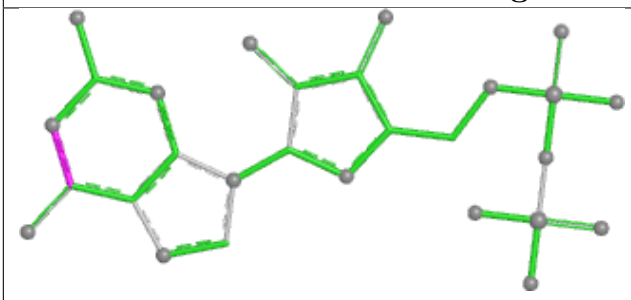
Ligand GTP Fd 602



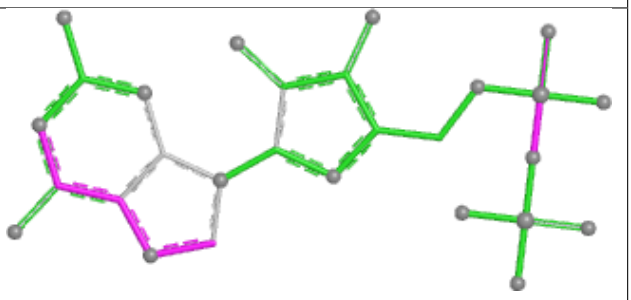
Ligand GDP DY 501



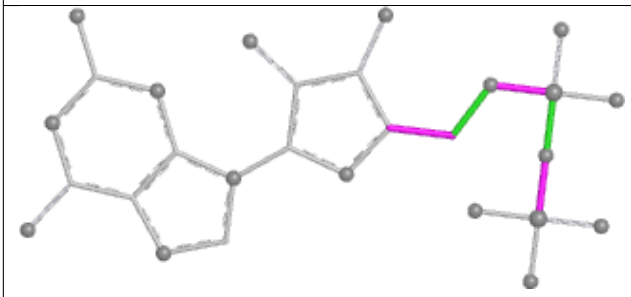
Ligand GDP Dd 501



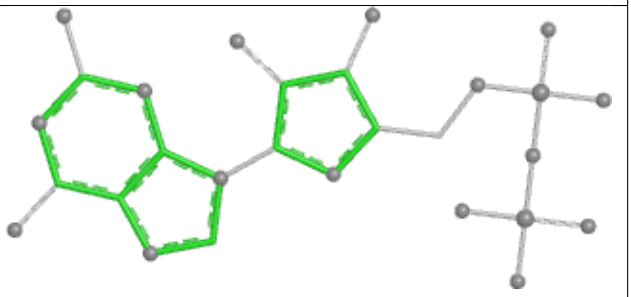
Bond lengths



Bond angles

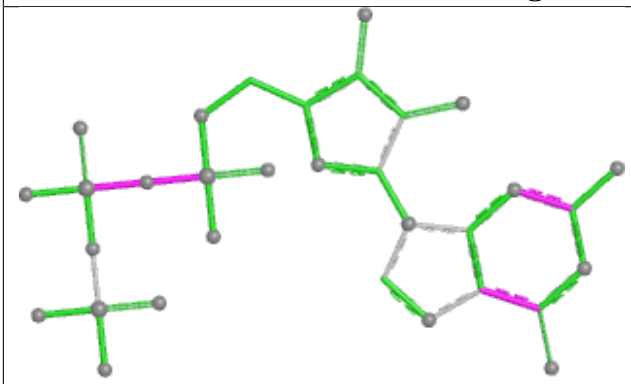


Torsions

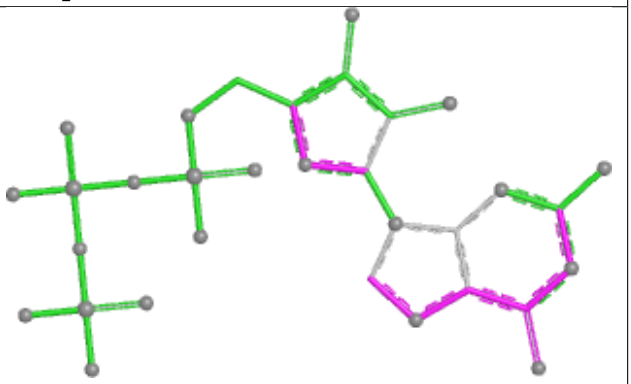


Rings

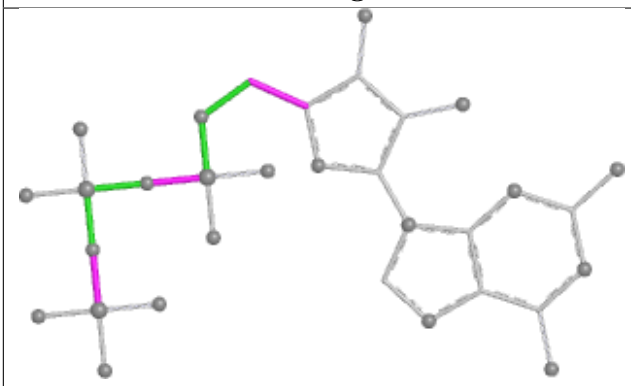
Ligand GTP q 602



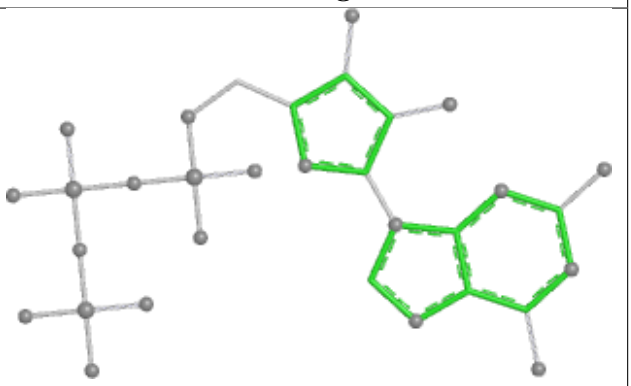
Bond lengths



Bond angles

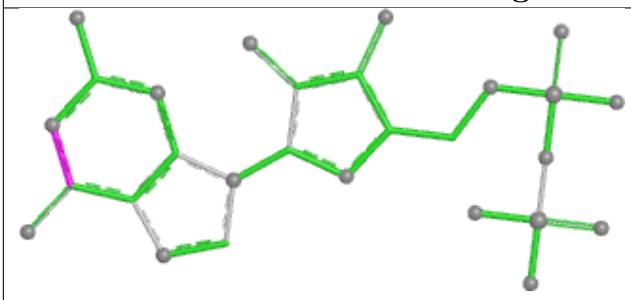


Torsions

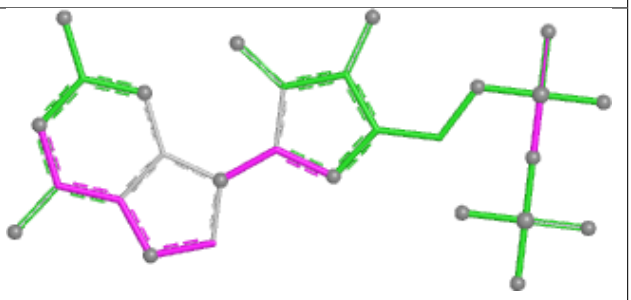


Rings

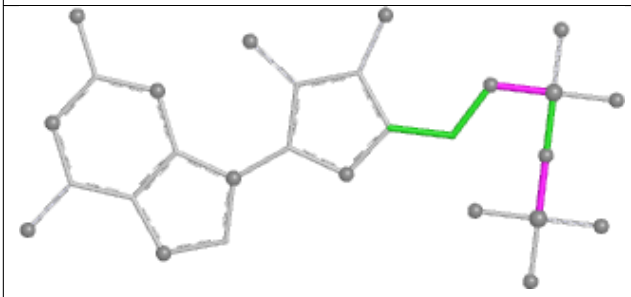
Ligand GDP Ge 501



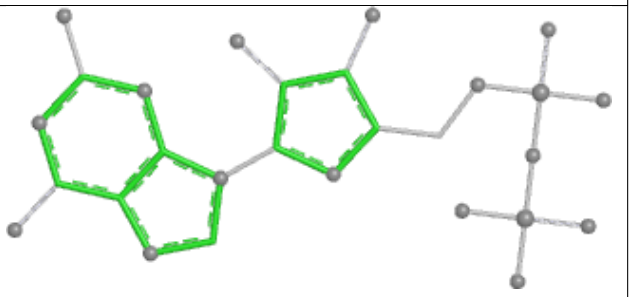
Bond lengths



Bond angles

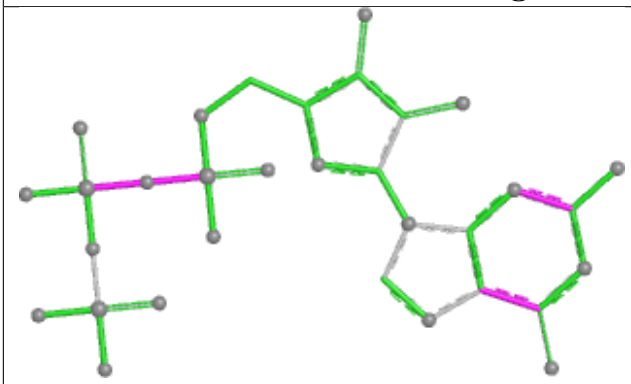


Torsions

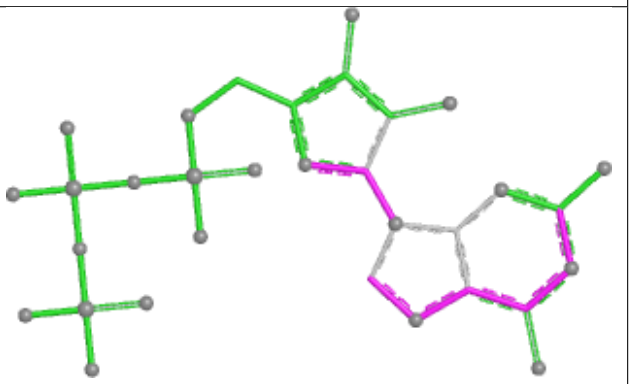


Rings

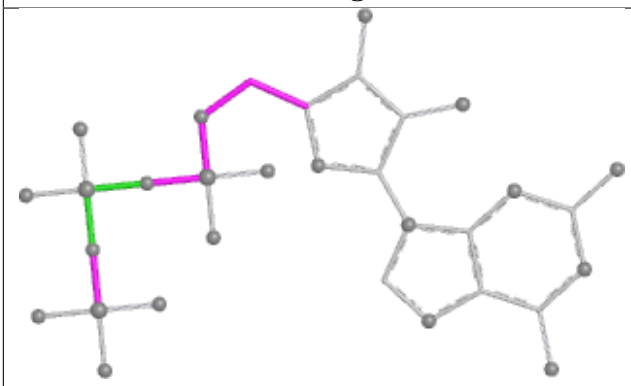
Ligand GTP Bw 602



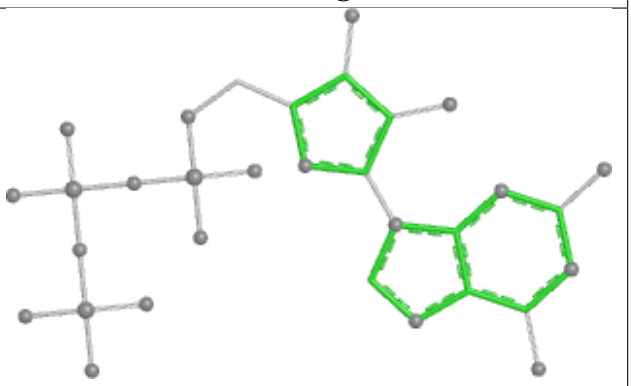
Bond lengths



Bond angles

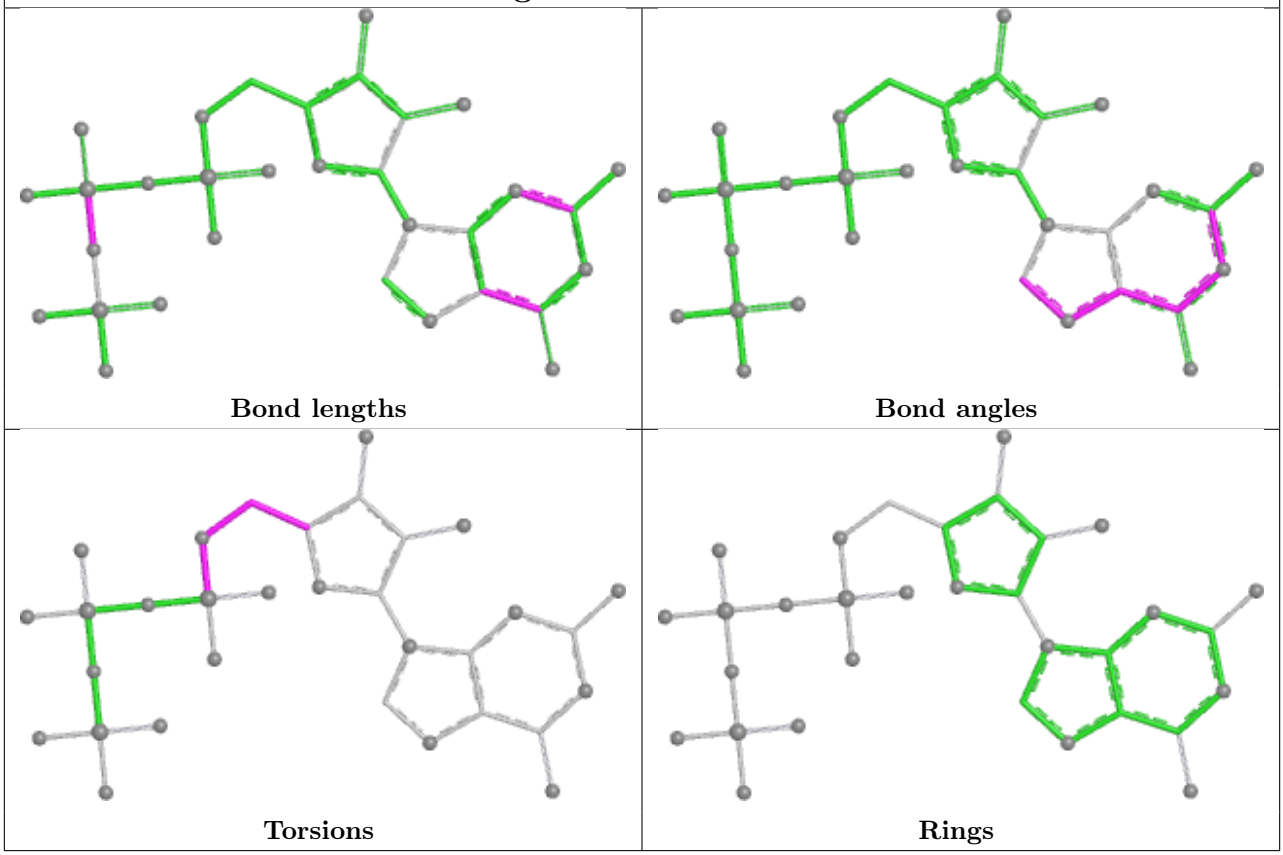


Torsions

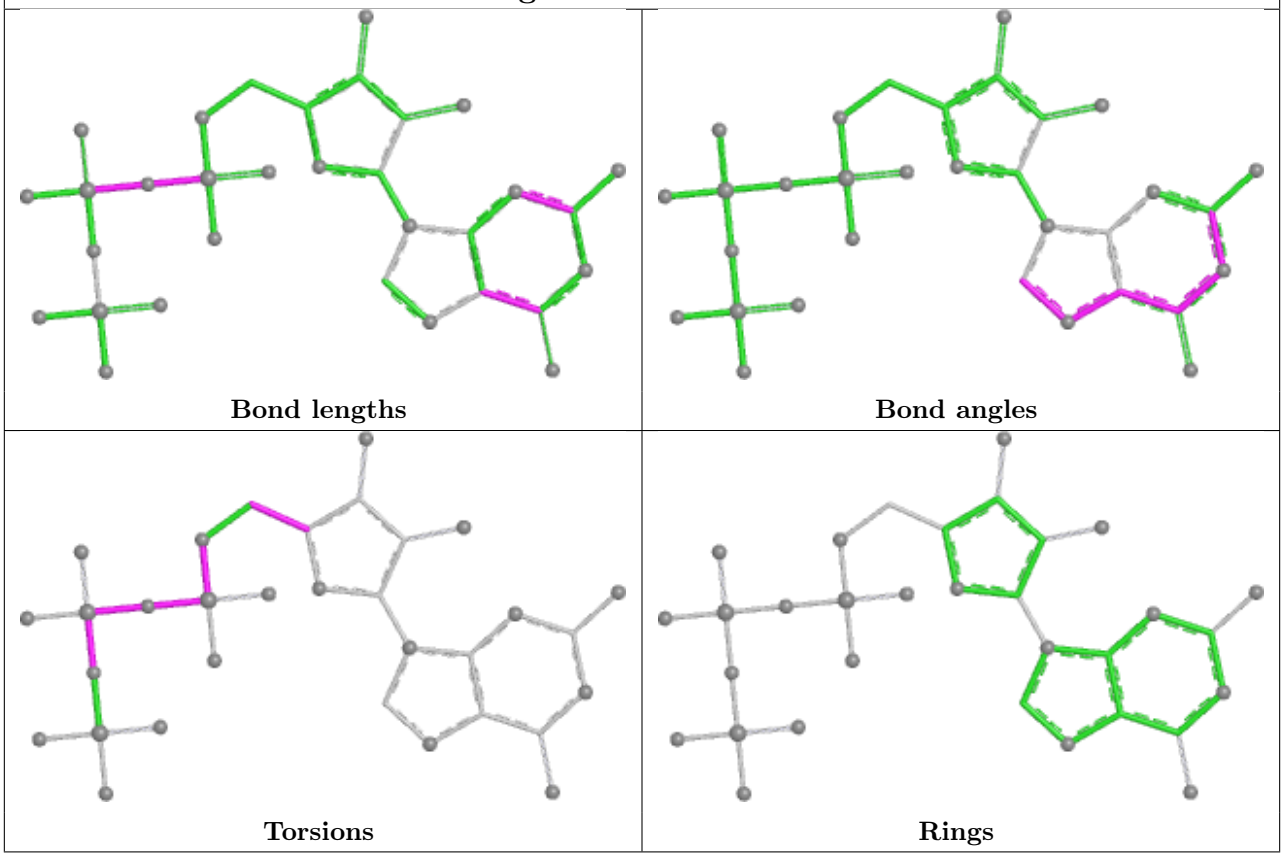


Rings

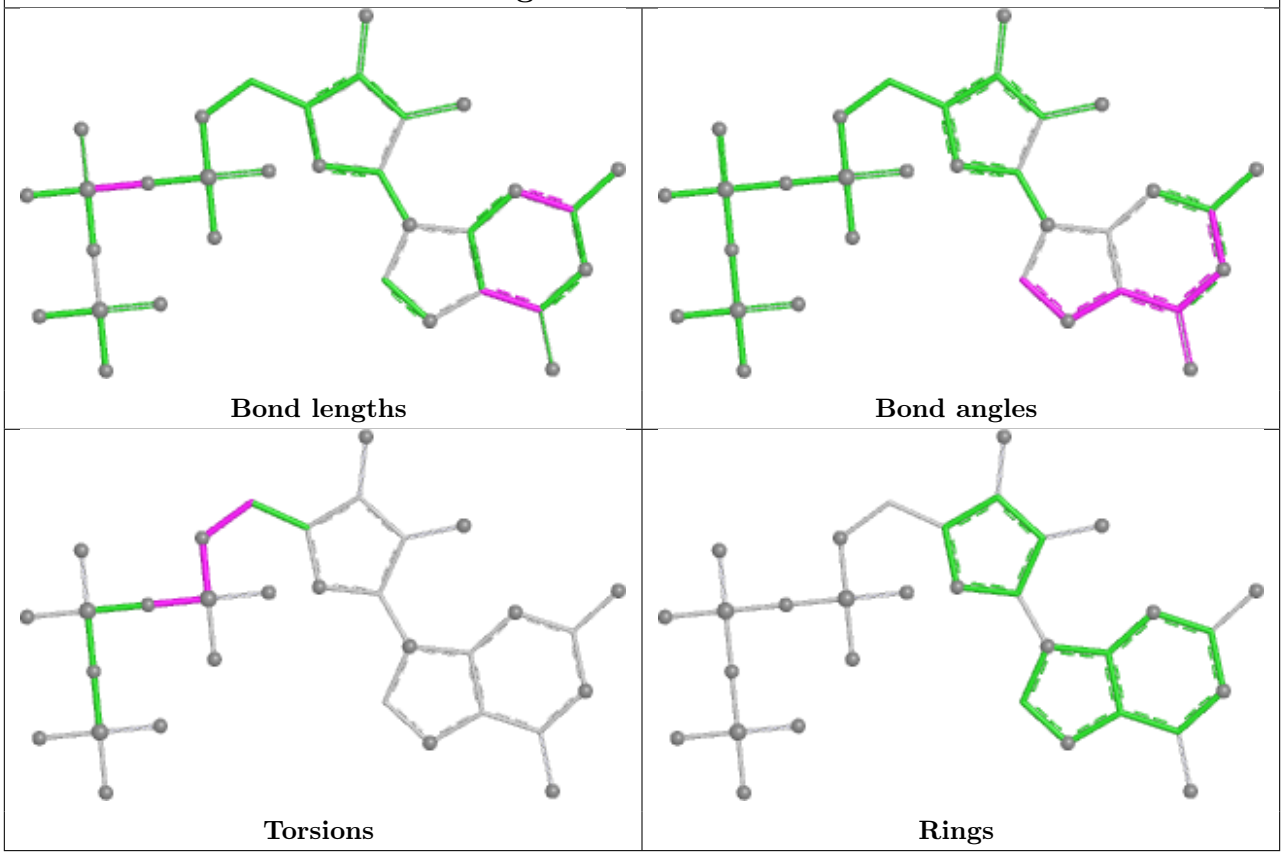
Ligand GTP Bu 602



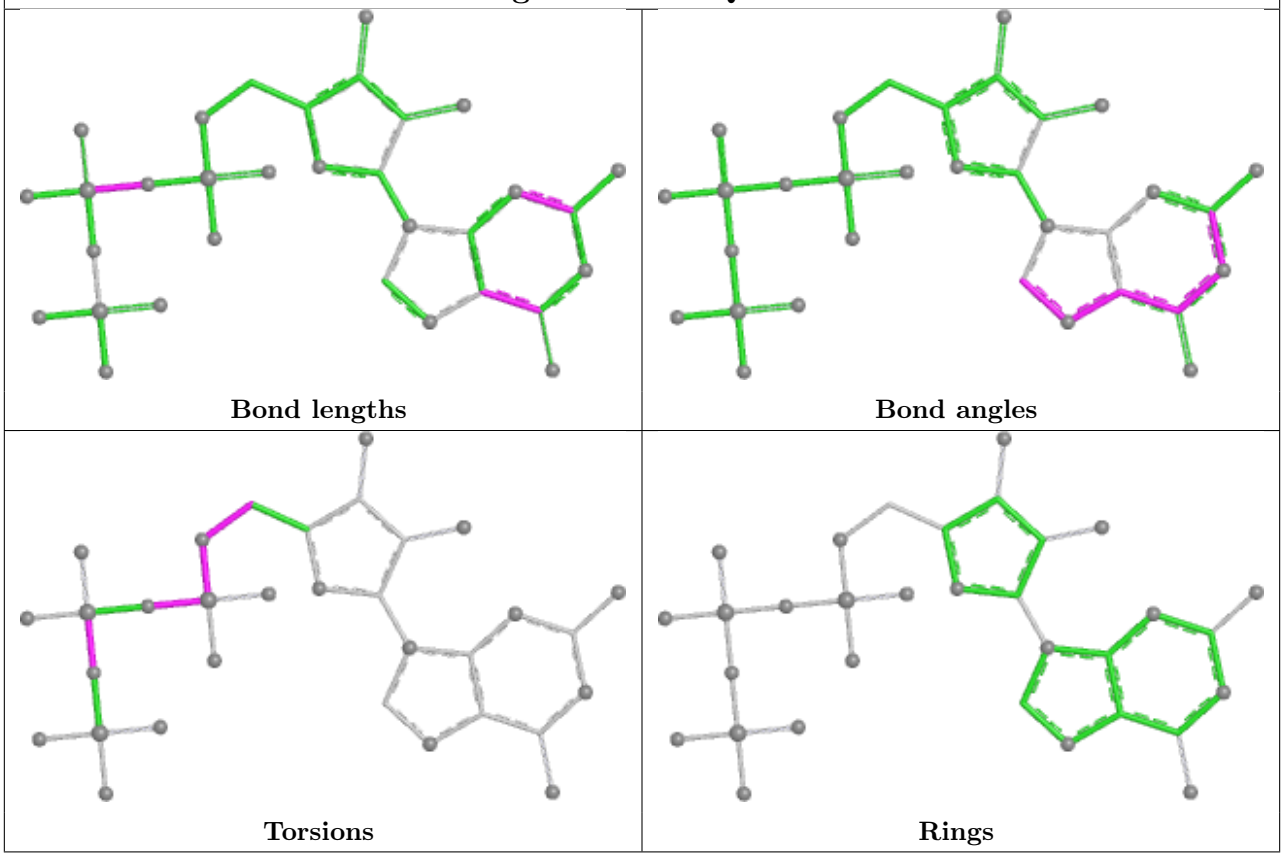
Ligand GTP Fe 501



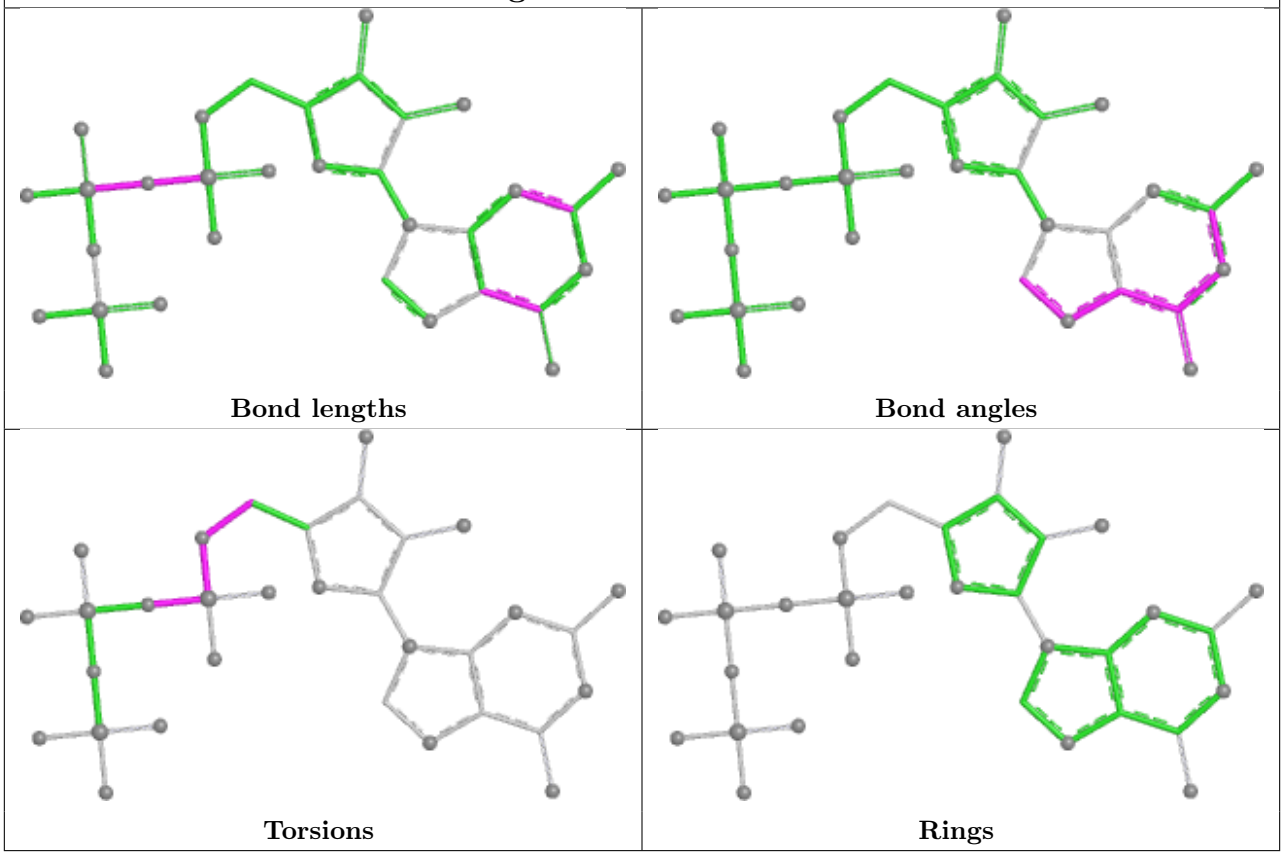
Ligand GTP F5 501



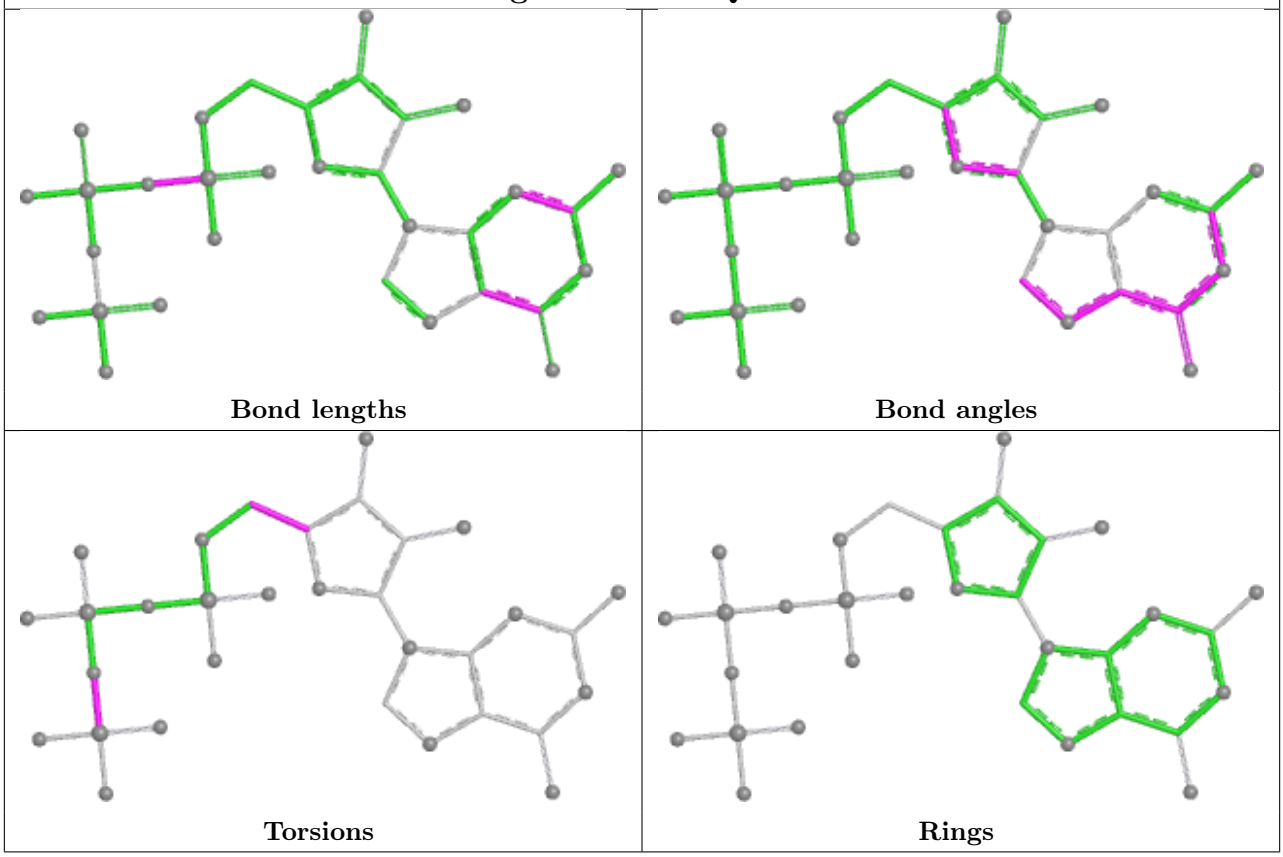
Ligand GTP FQ 501



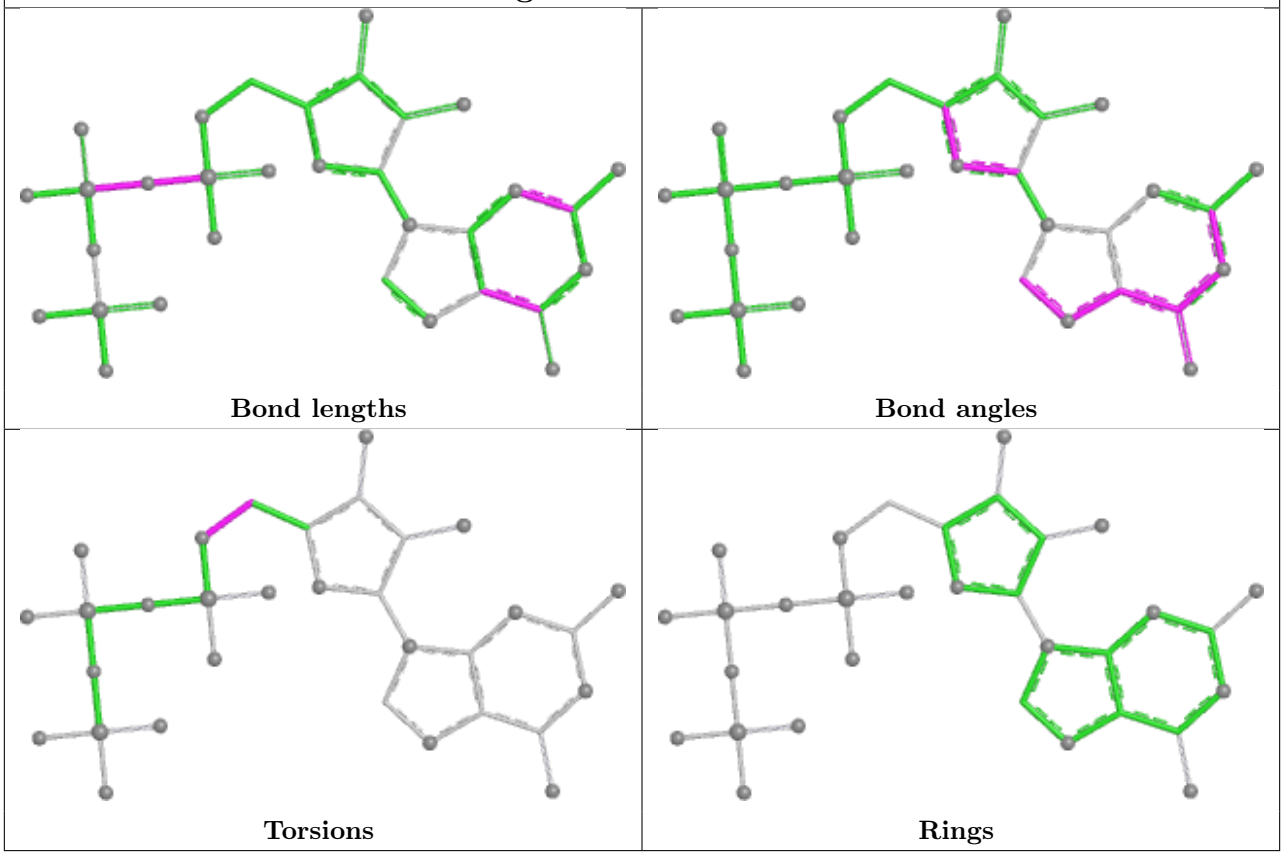
Ligand GTP FM 501



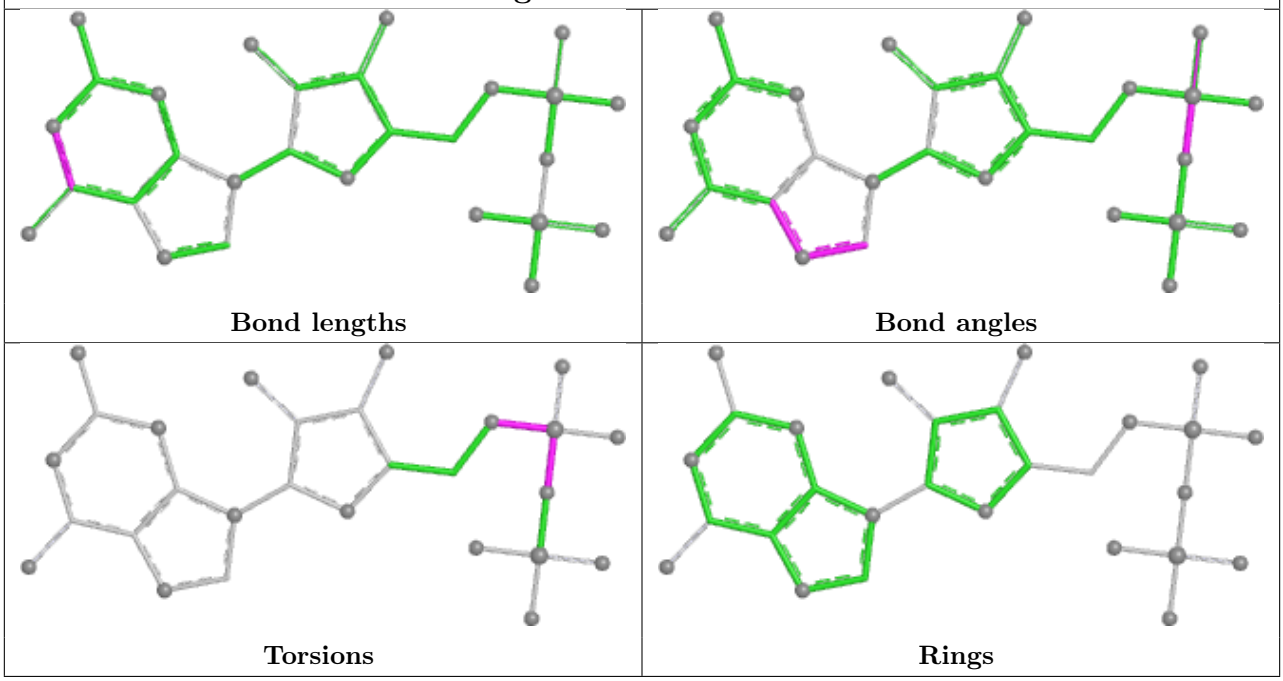
Ligand GTP BQ 602



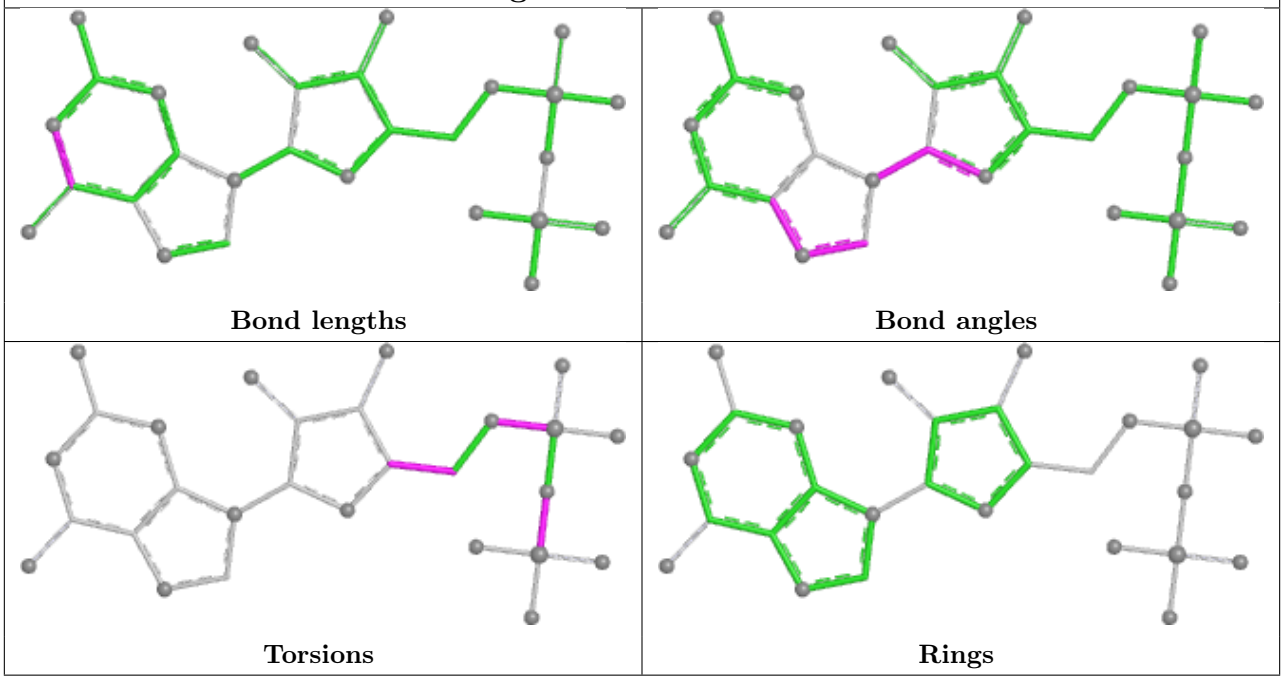
Ligand GTP E7 501



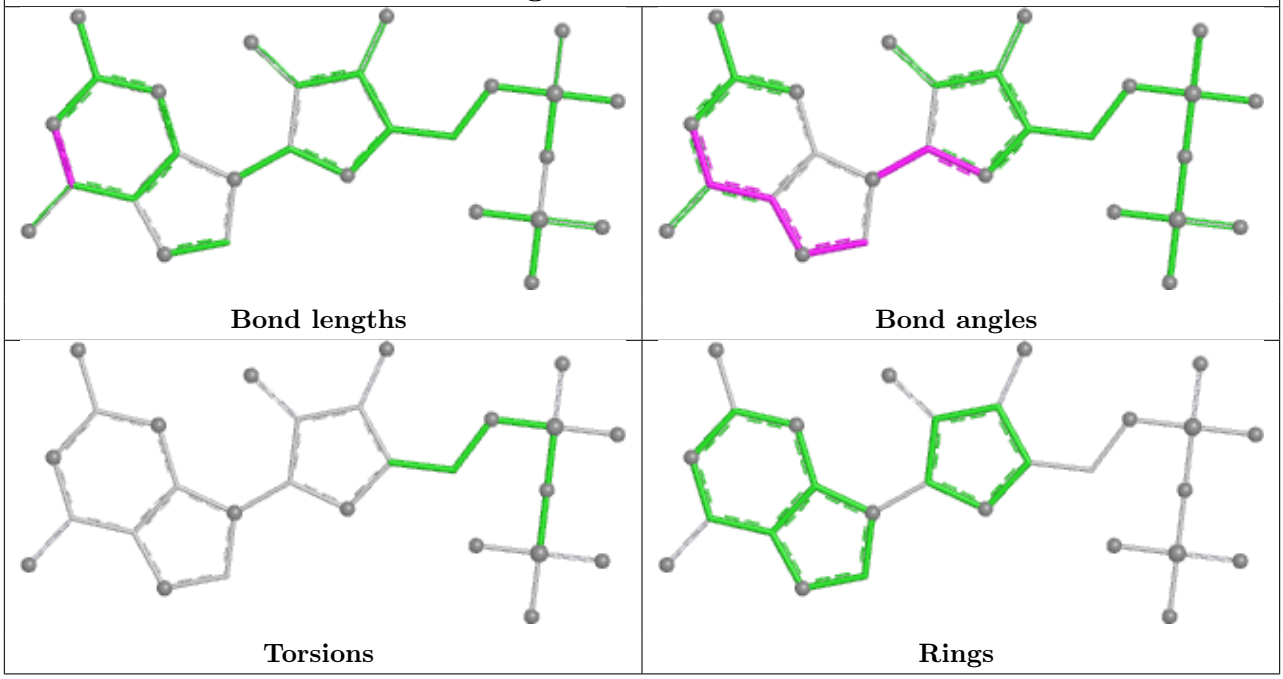
Ligand GDP Ae 501



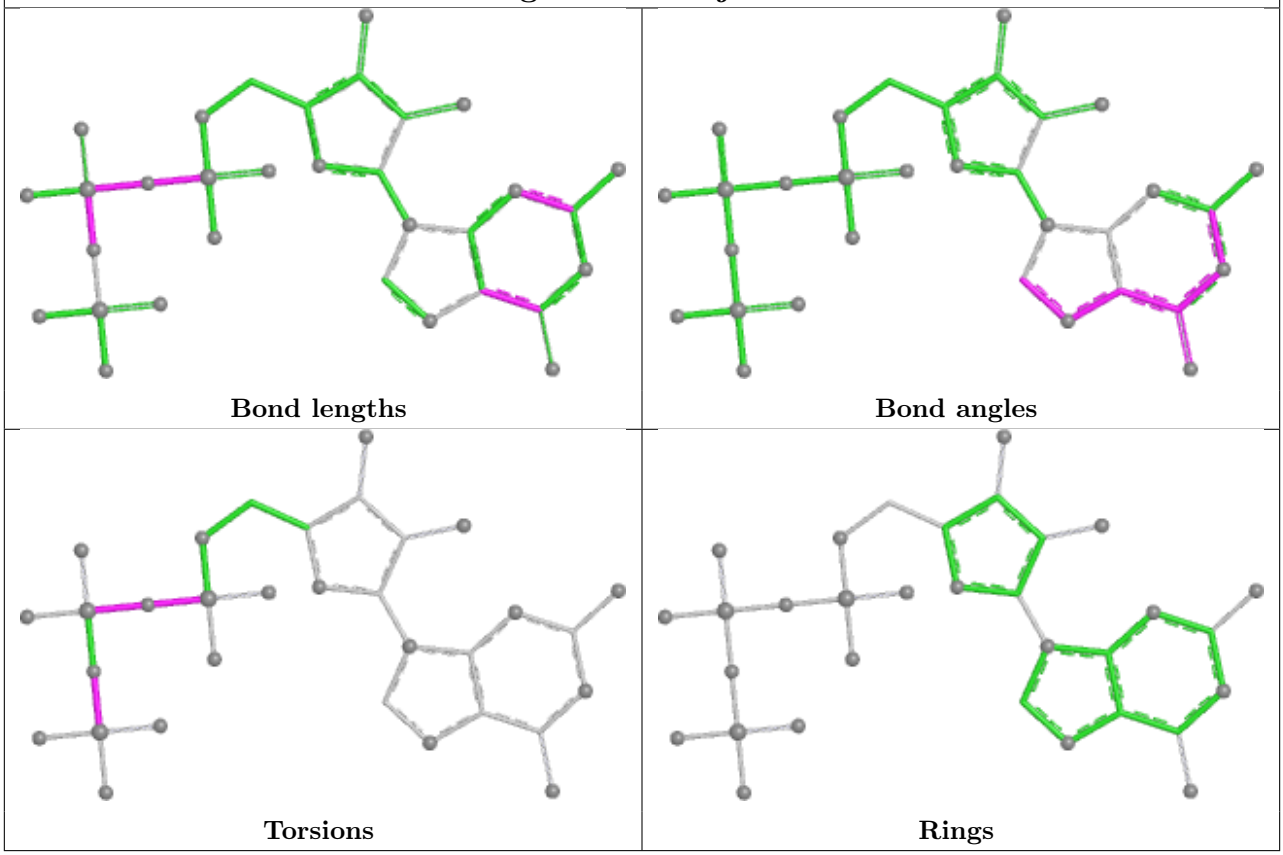
Ligand GDP AP 501



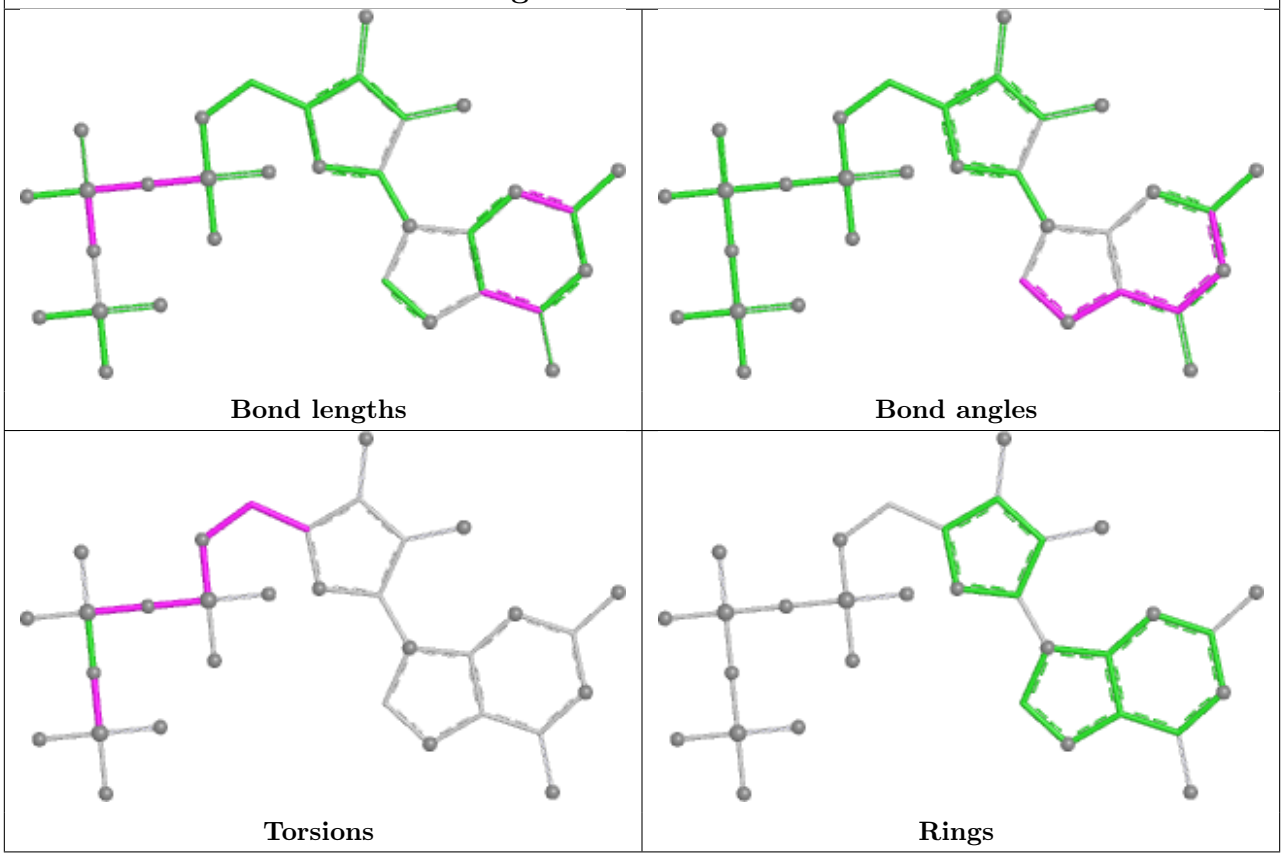
Ligand GDP 7 501



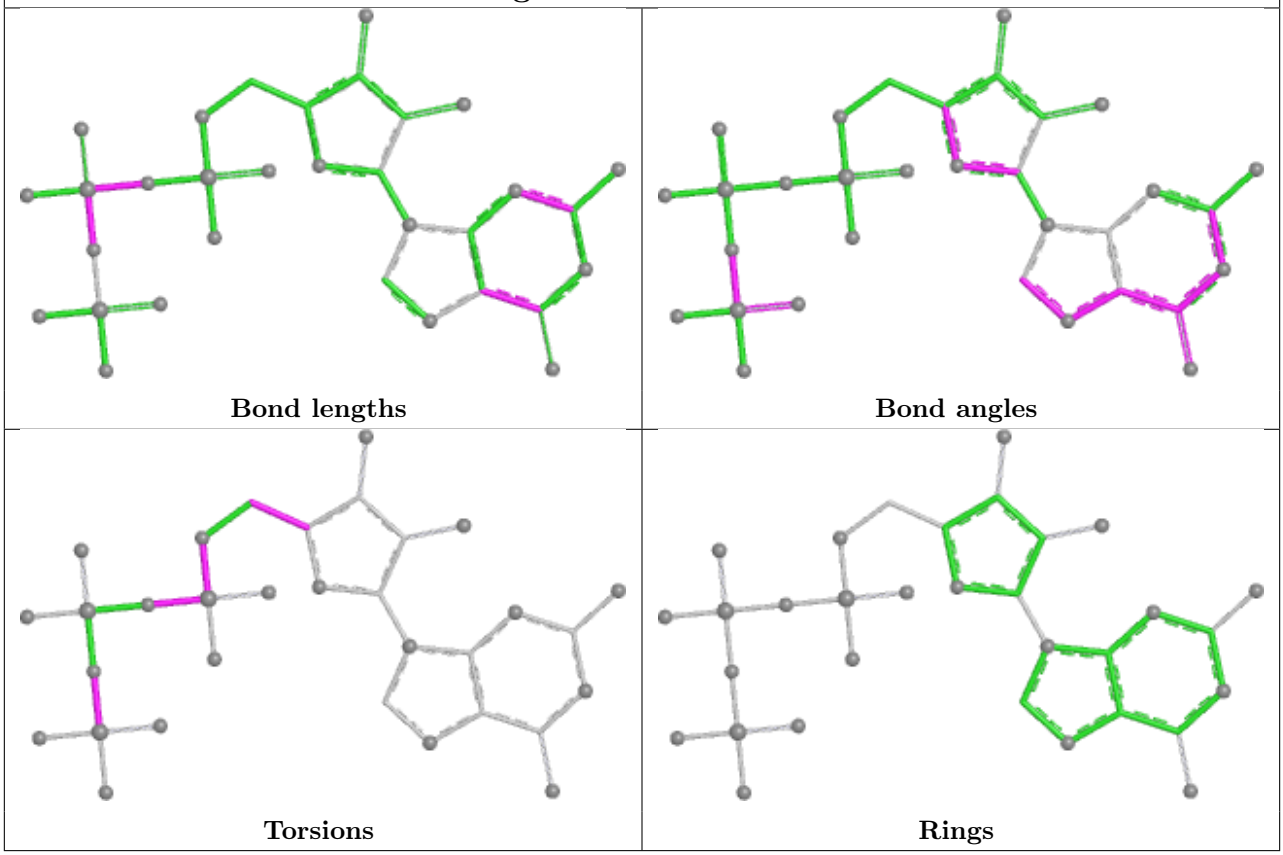
Ligand GTP Fj 501



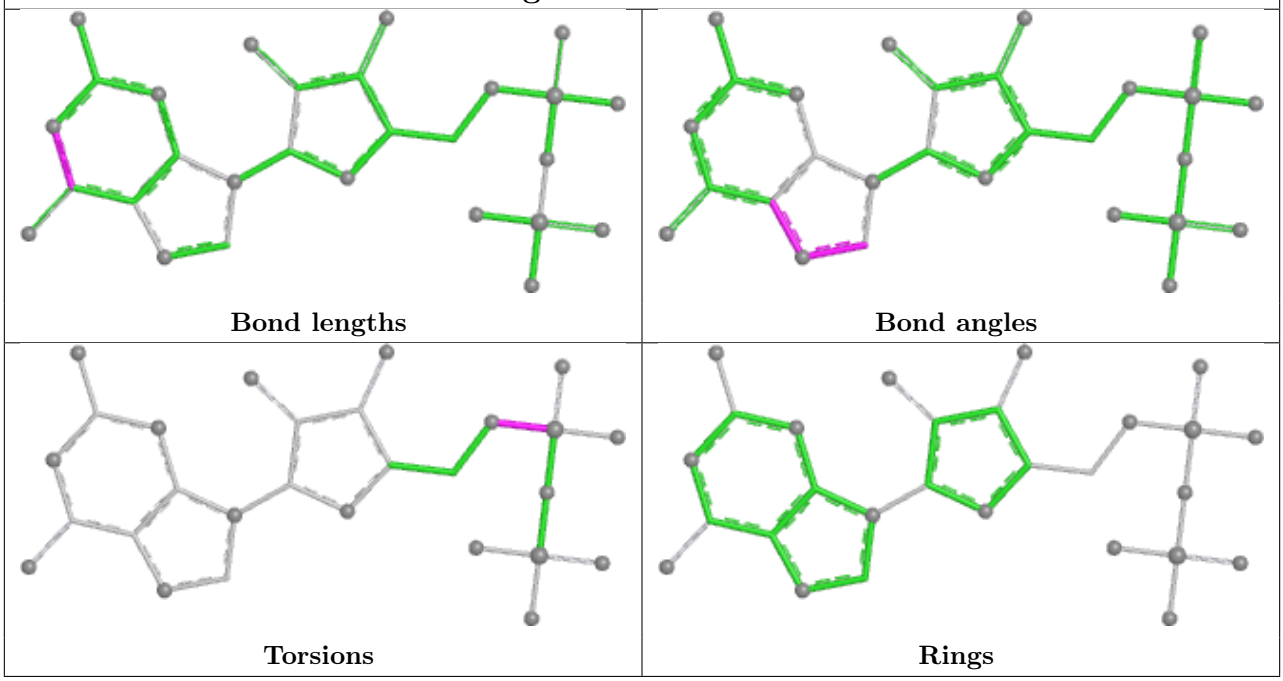
Ligand GTP GF 501



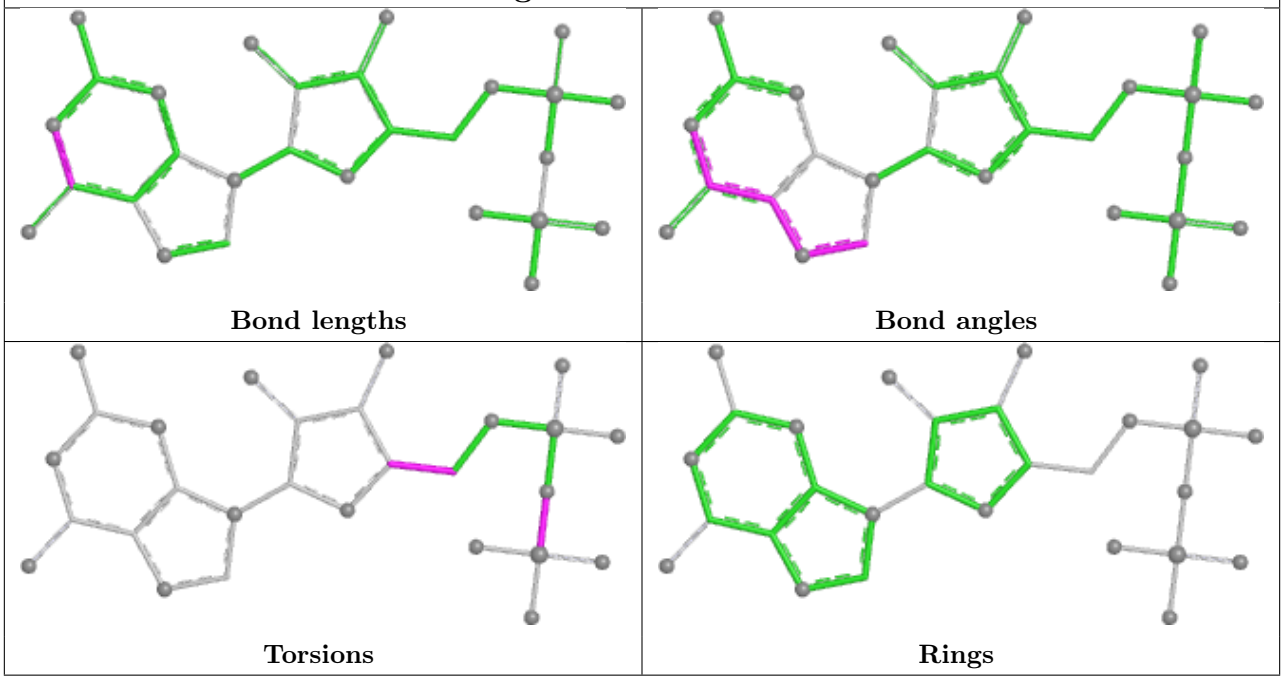
Ligand GTP BL 602



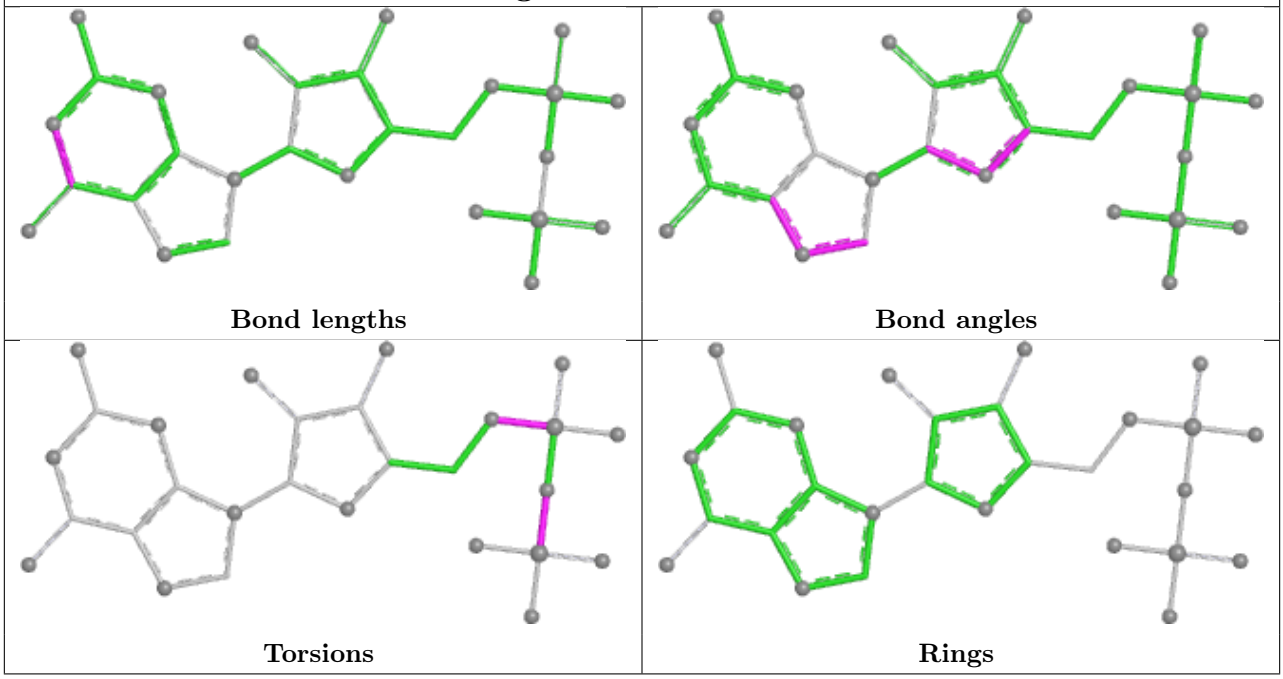
Ligand GDP P 501



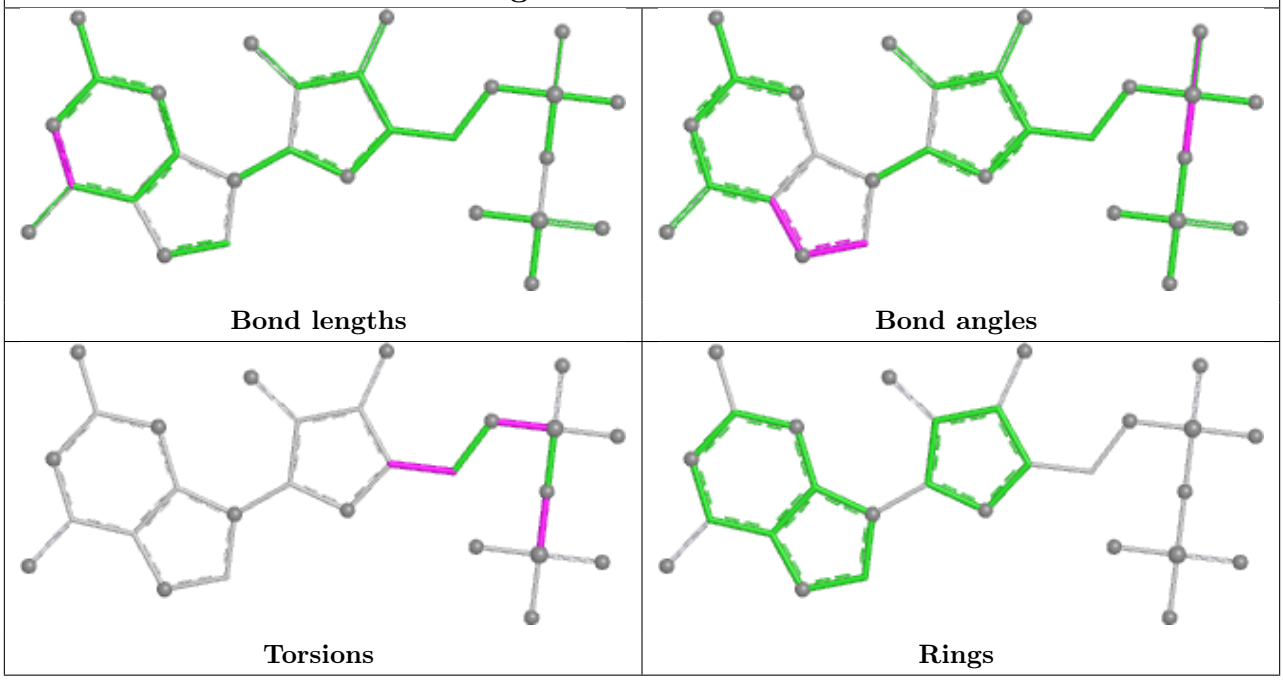
Ligand GDP Av 501



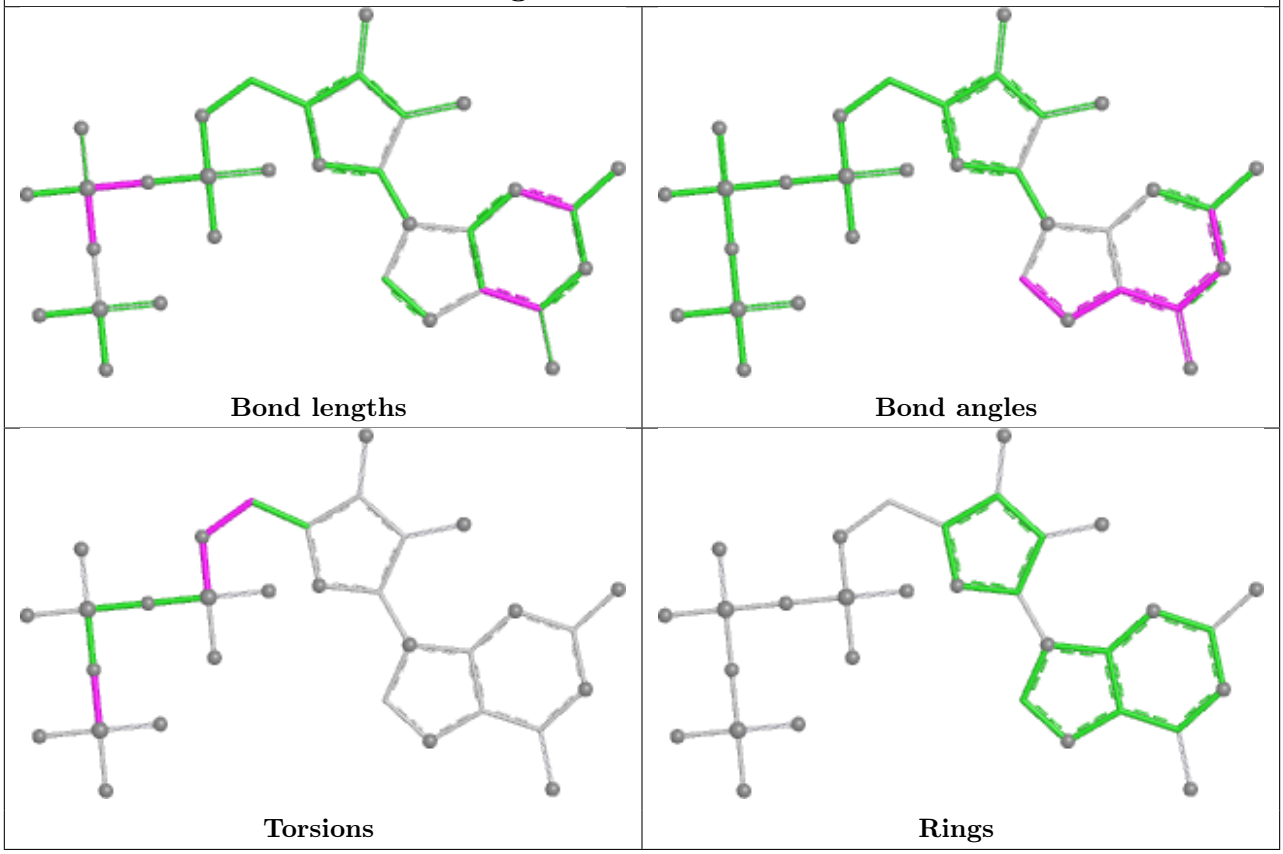
Ligand GDP Br 501



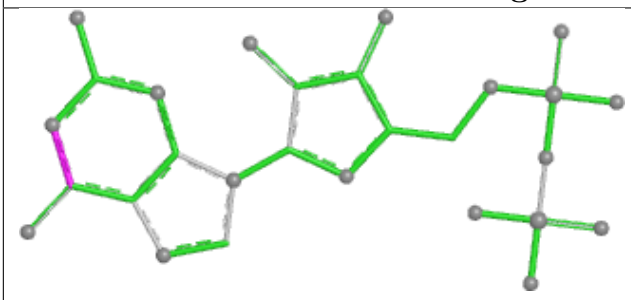
Ligand GDP FD 501



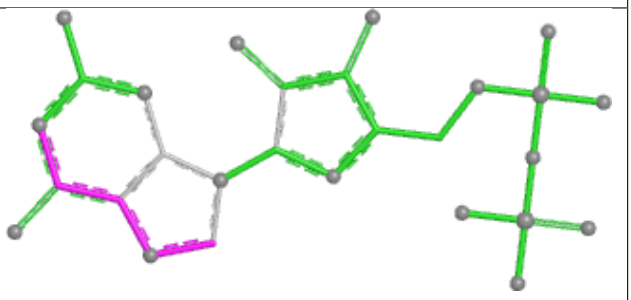
Ligand GTP GC 501



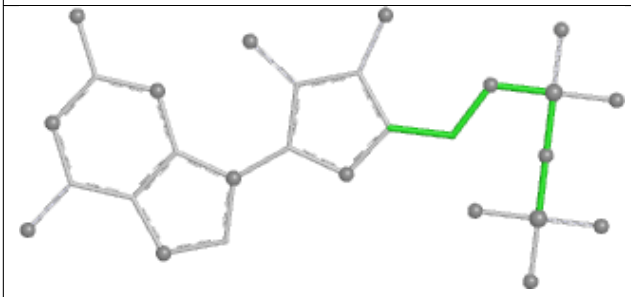
Ligand GDP Du 501



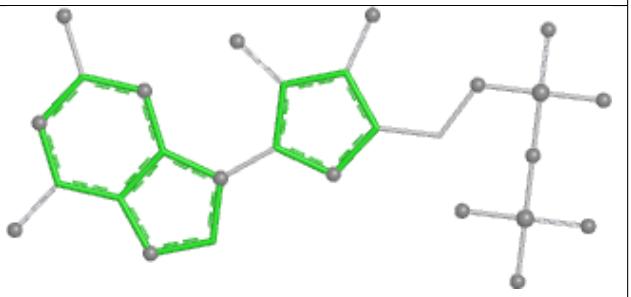
Bond lengths



Bond angles

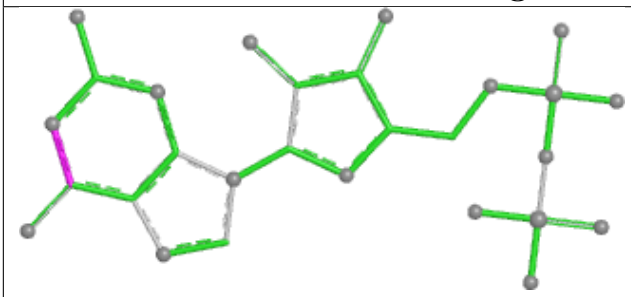


Torsions

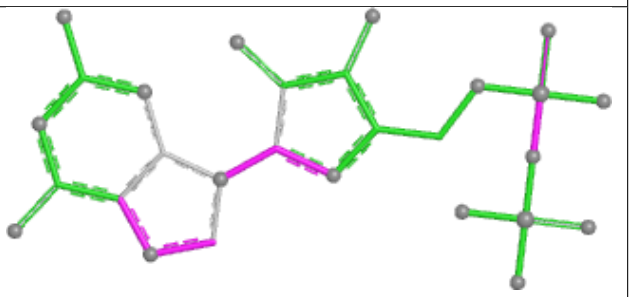


Rings

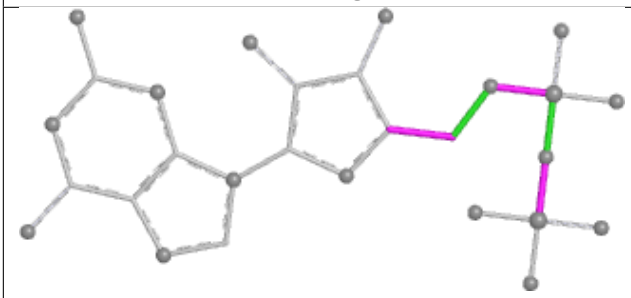
Ligand GDP EX 501



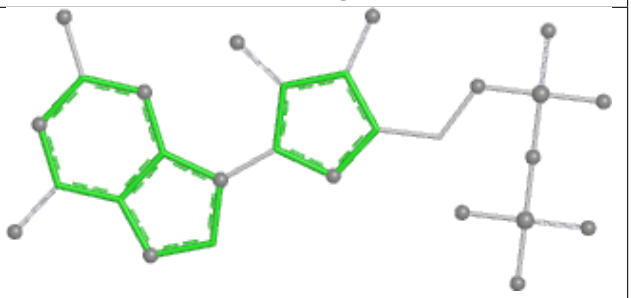
Bond lengths



Bond angles

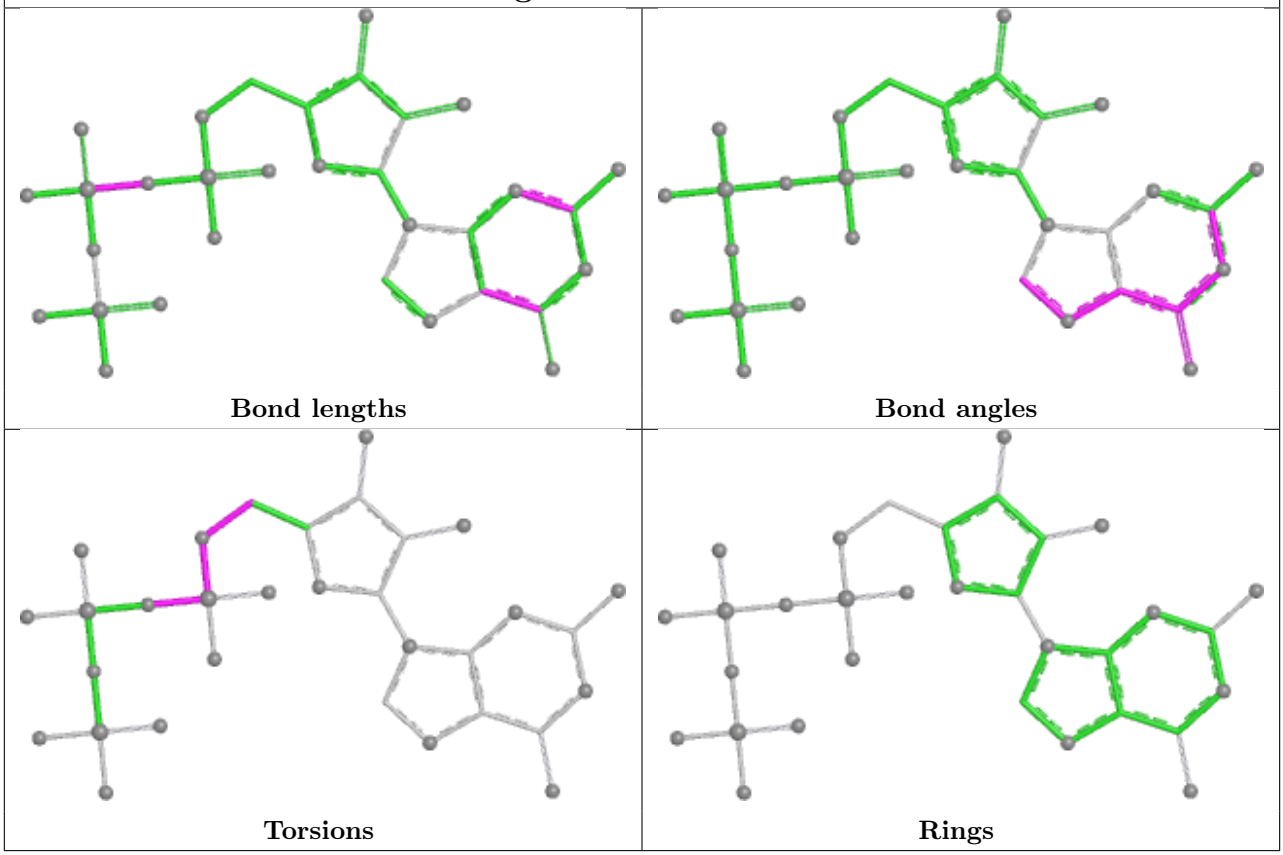


Torsions

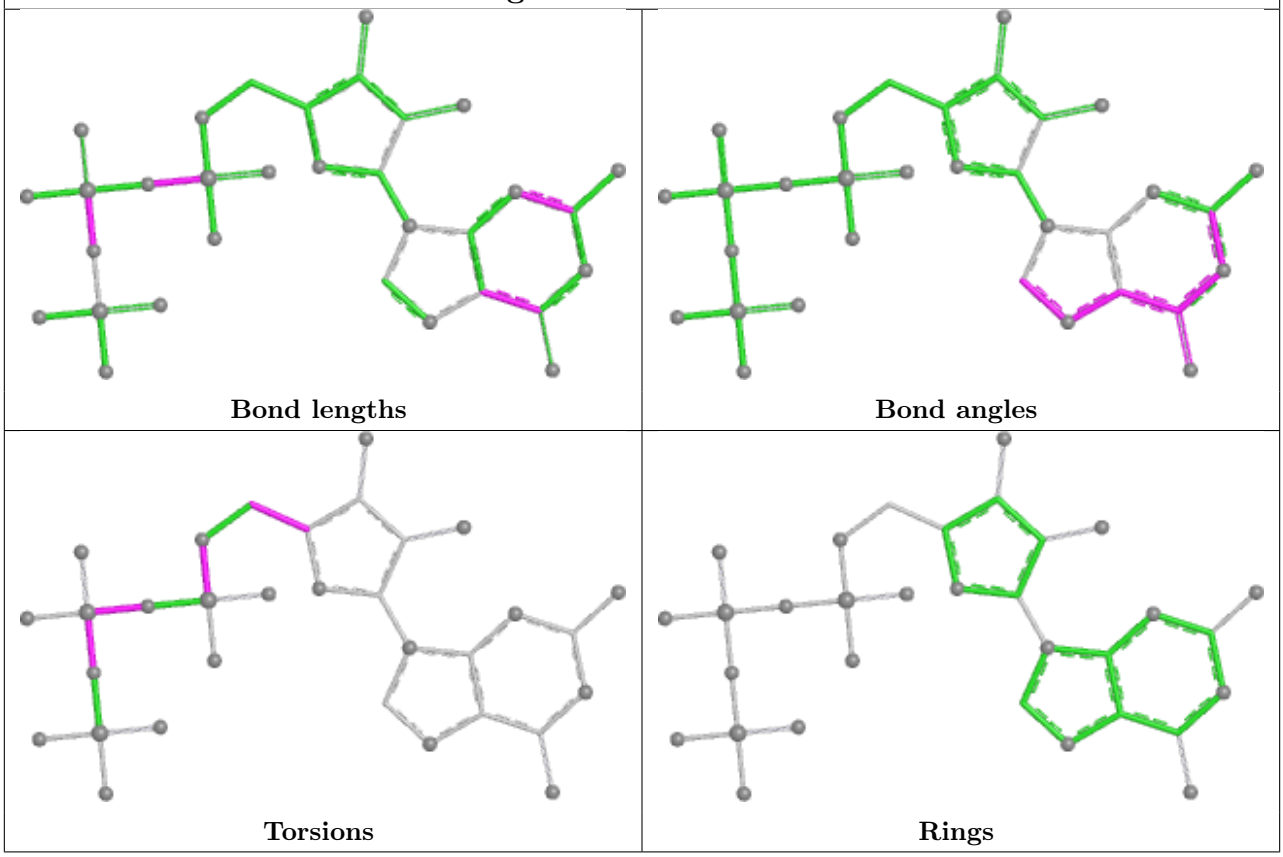


Rings

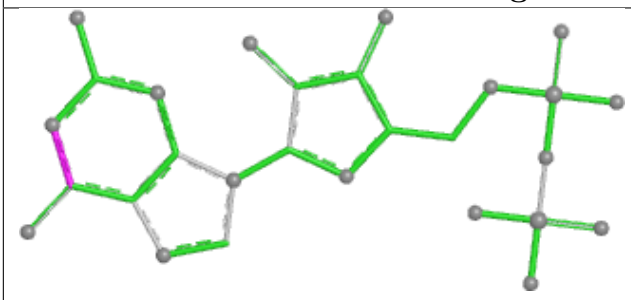
Ligand GTP Gz 501



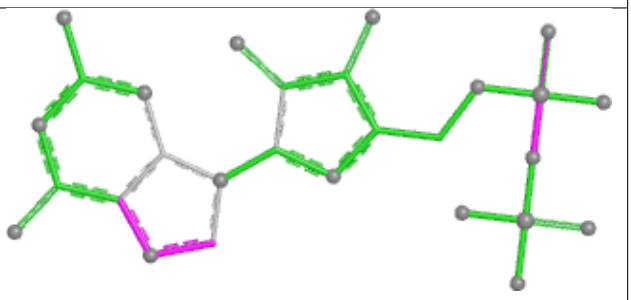
Ligand GTP BM 602



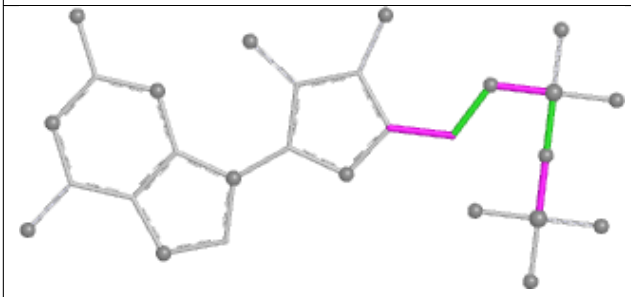
Ligand GDP ET 501



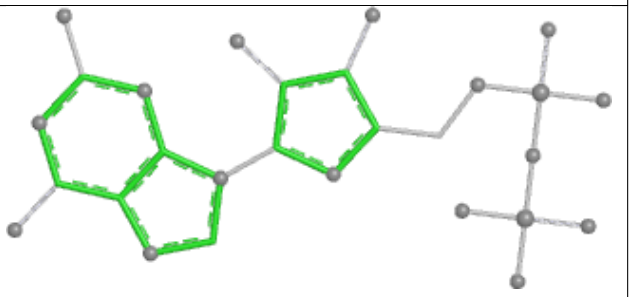
Bond lengths



Bond angles

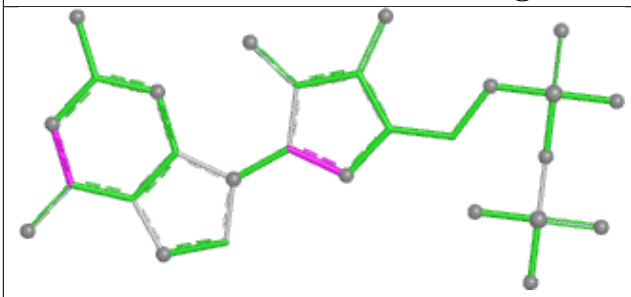


Torsions

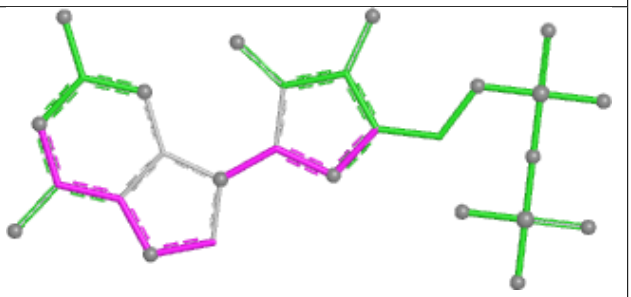


Rings

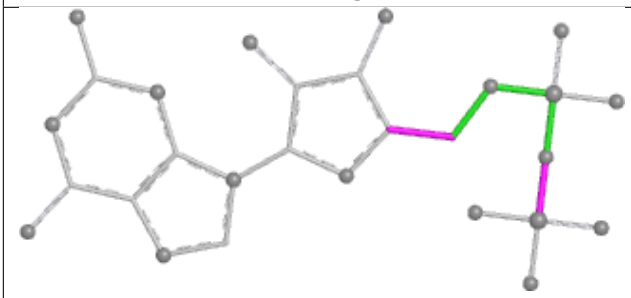
Ligand GDP E9 501



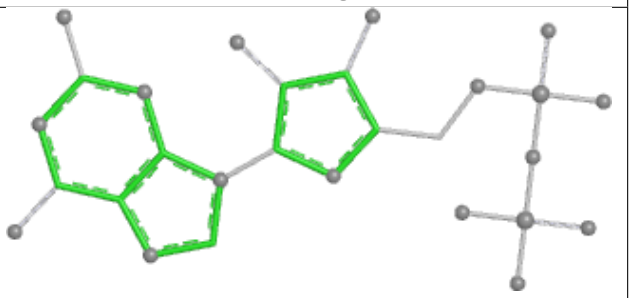
Bond lengths



Bond angles

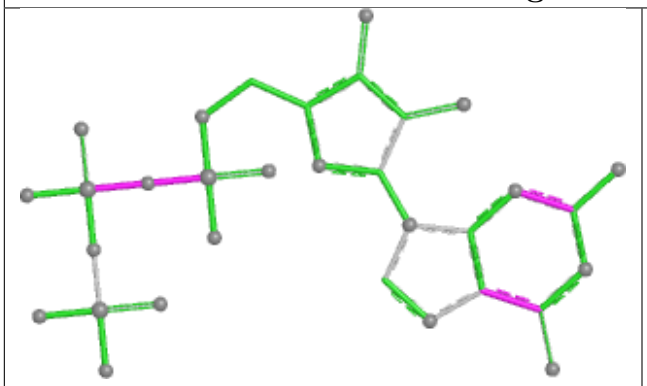


Torsions

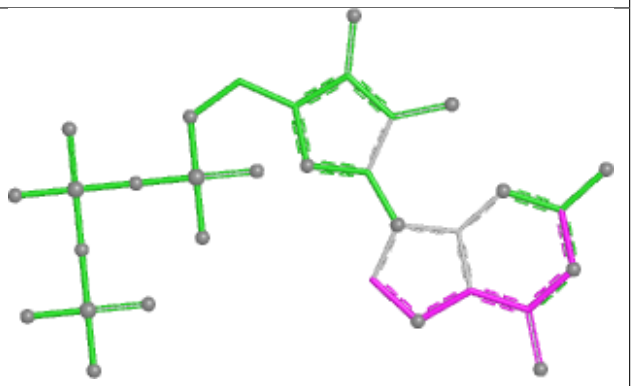


Rings

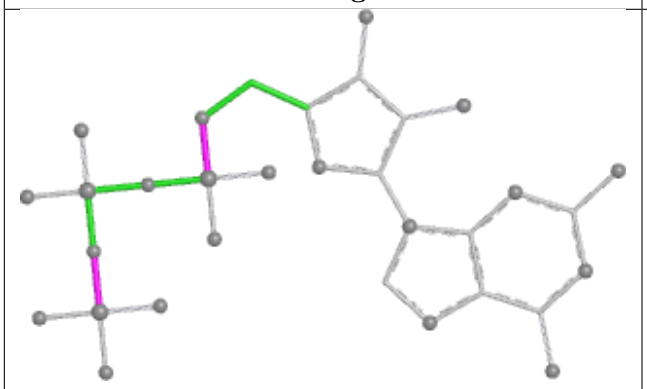
Ligand GTP u 501



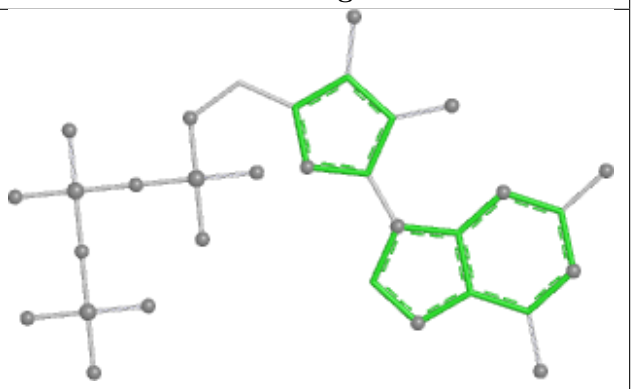
Bond lengths



Bond angles

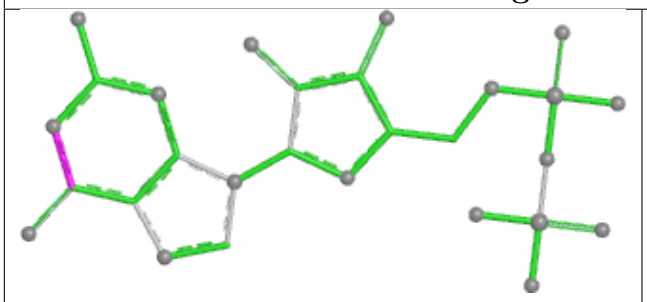


Torsions

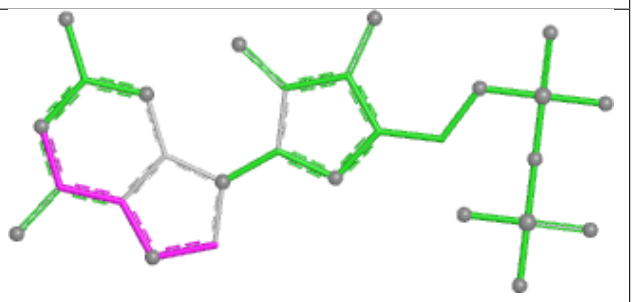


Rings

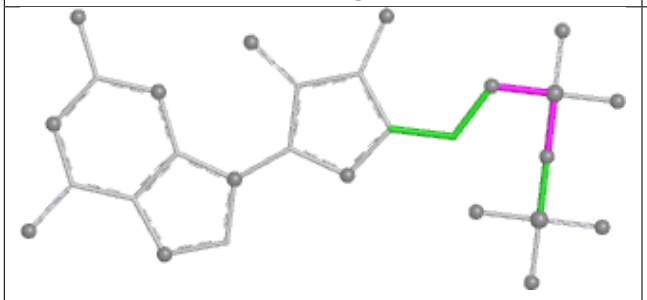
Ligand GDP An 501



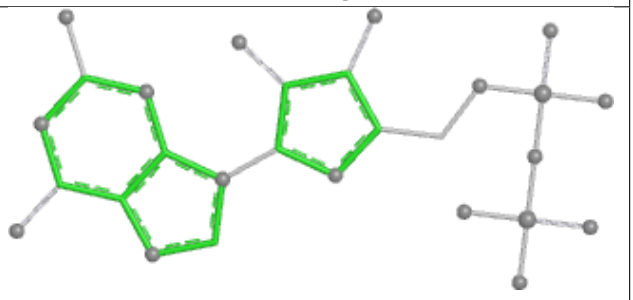
Bond lengths



Bond angles

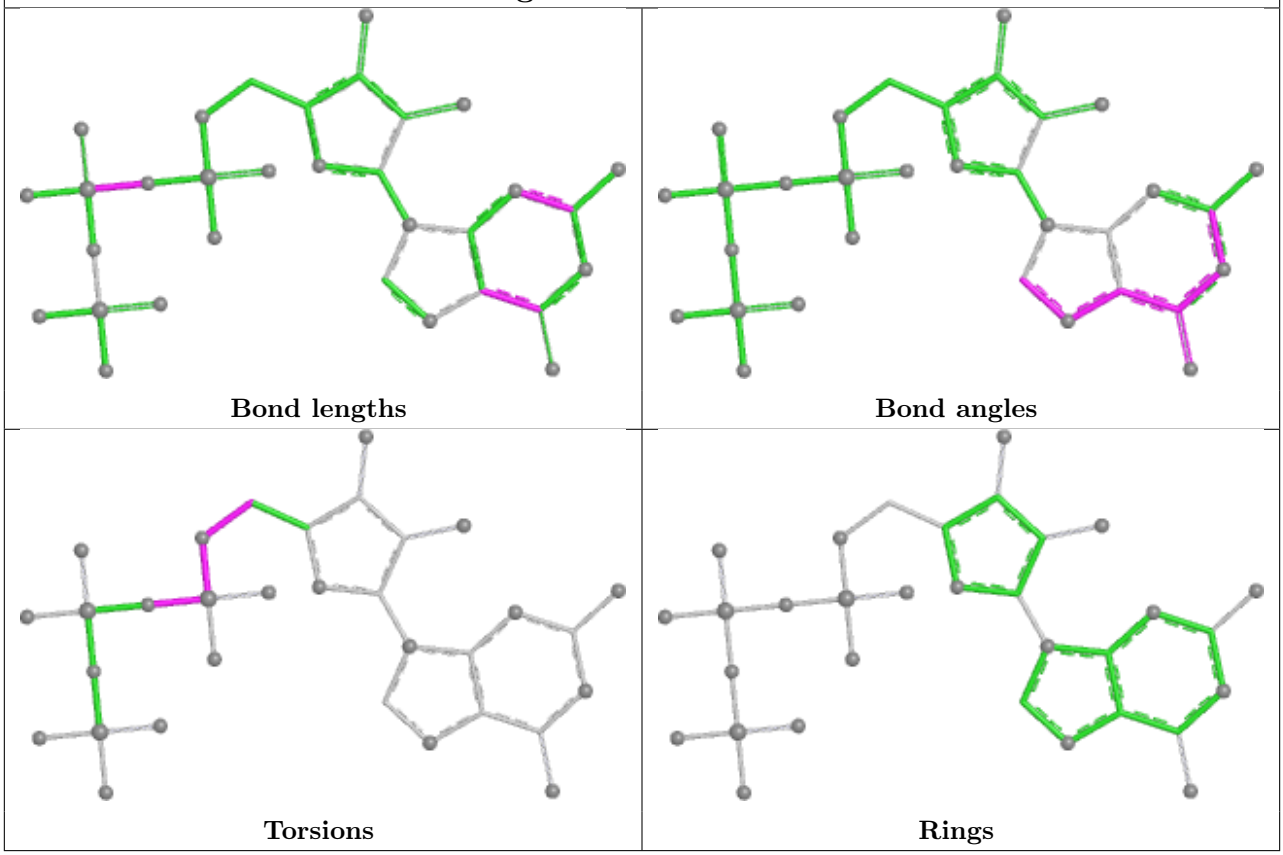


Torsions

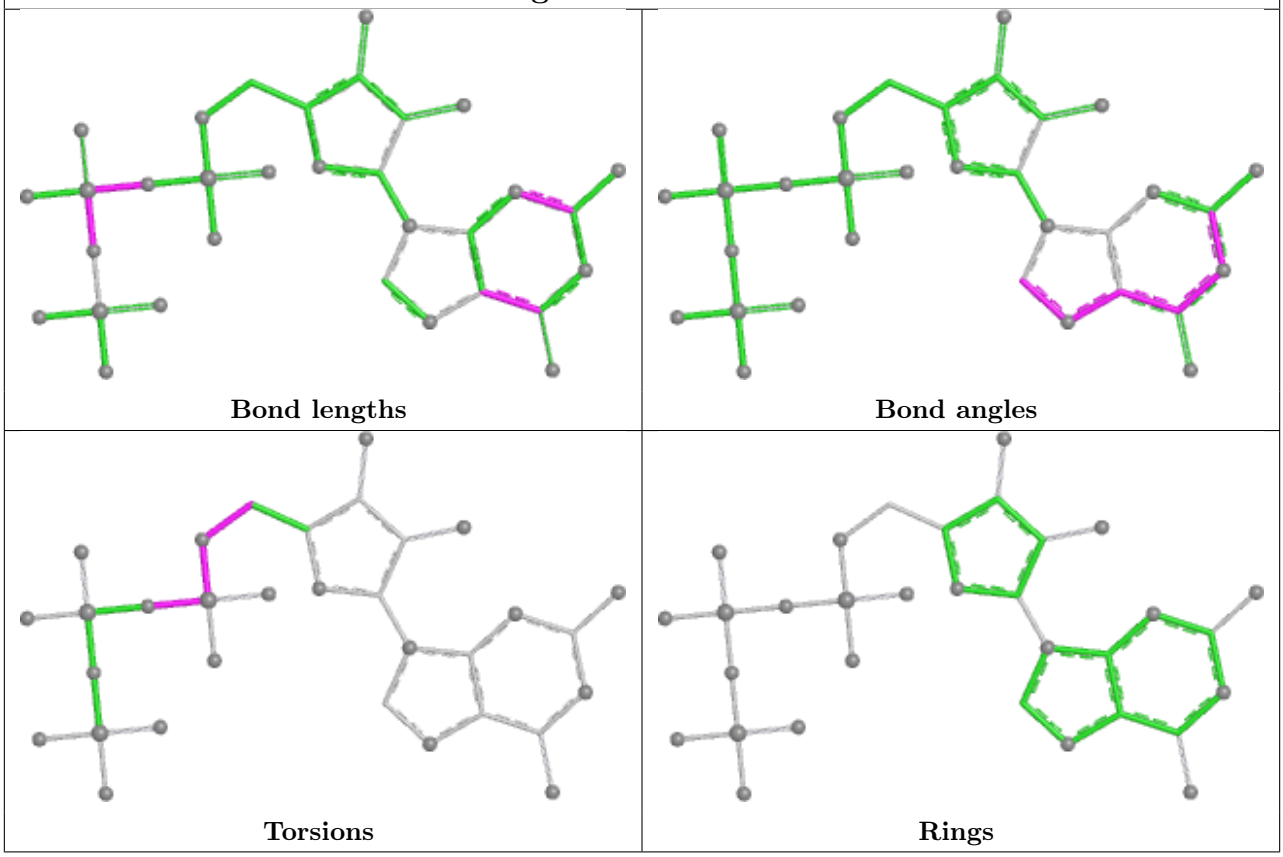


Rings

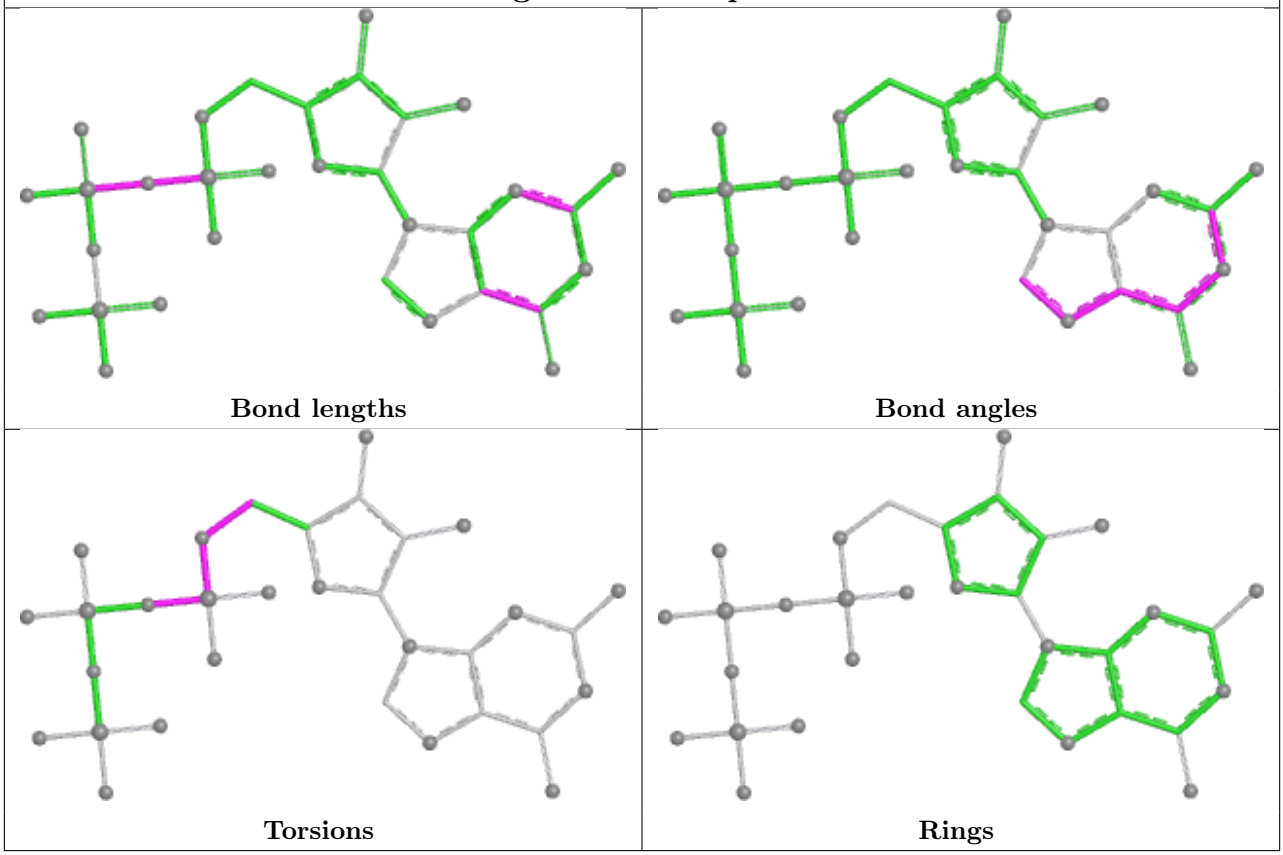
Ligand GTP F3 501



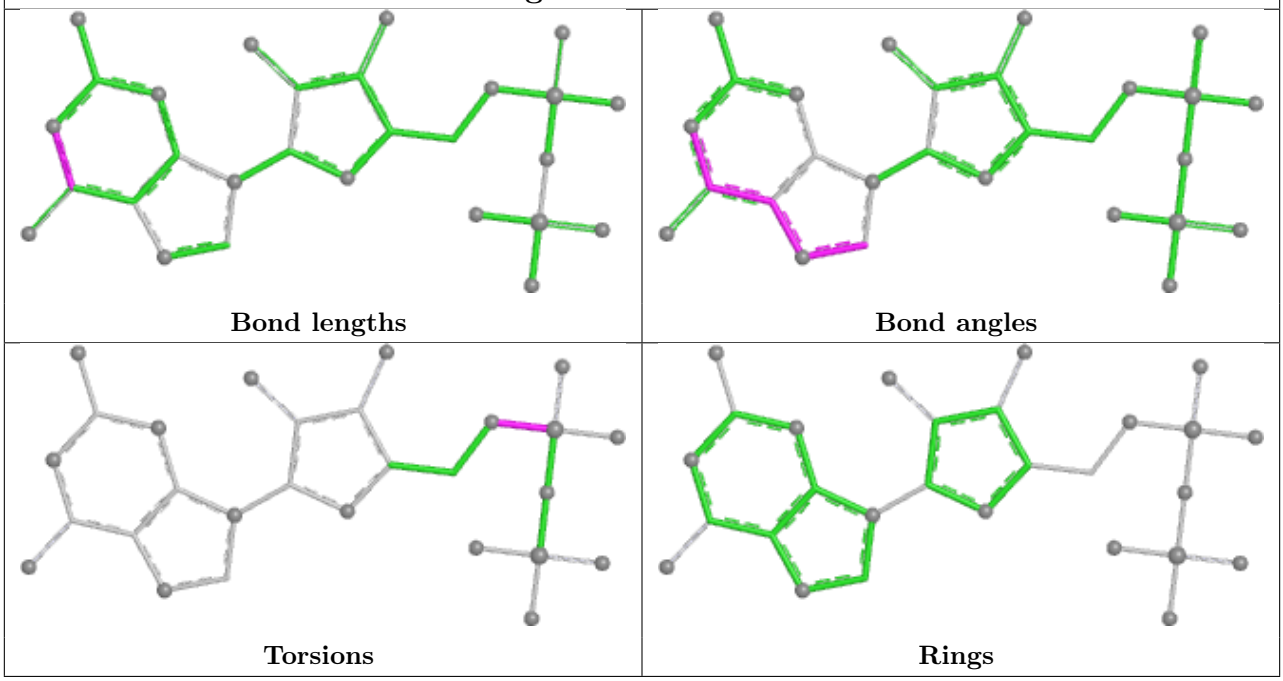
Ligand GTP f 602



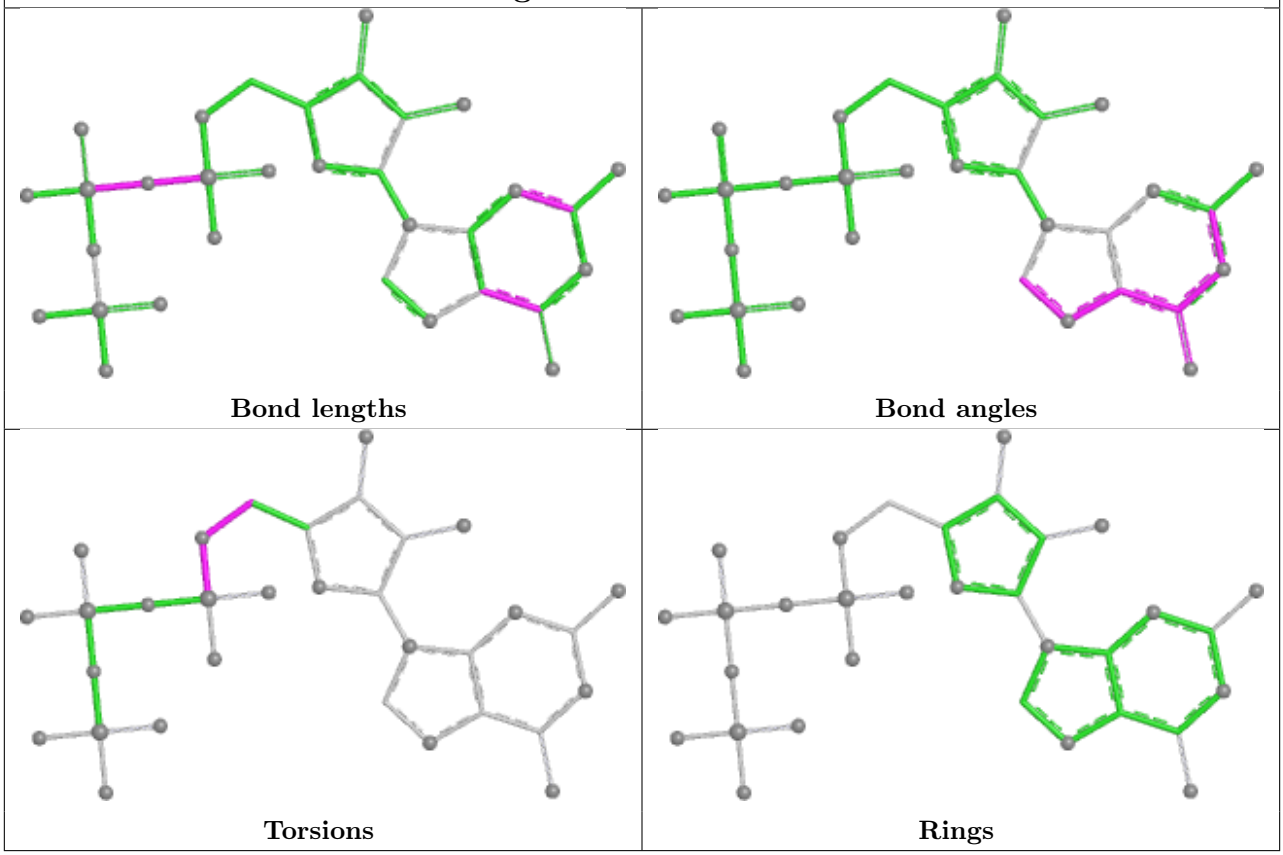
Ligand GTP Gq 501



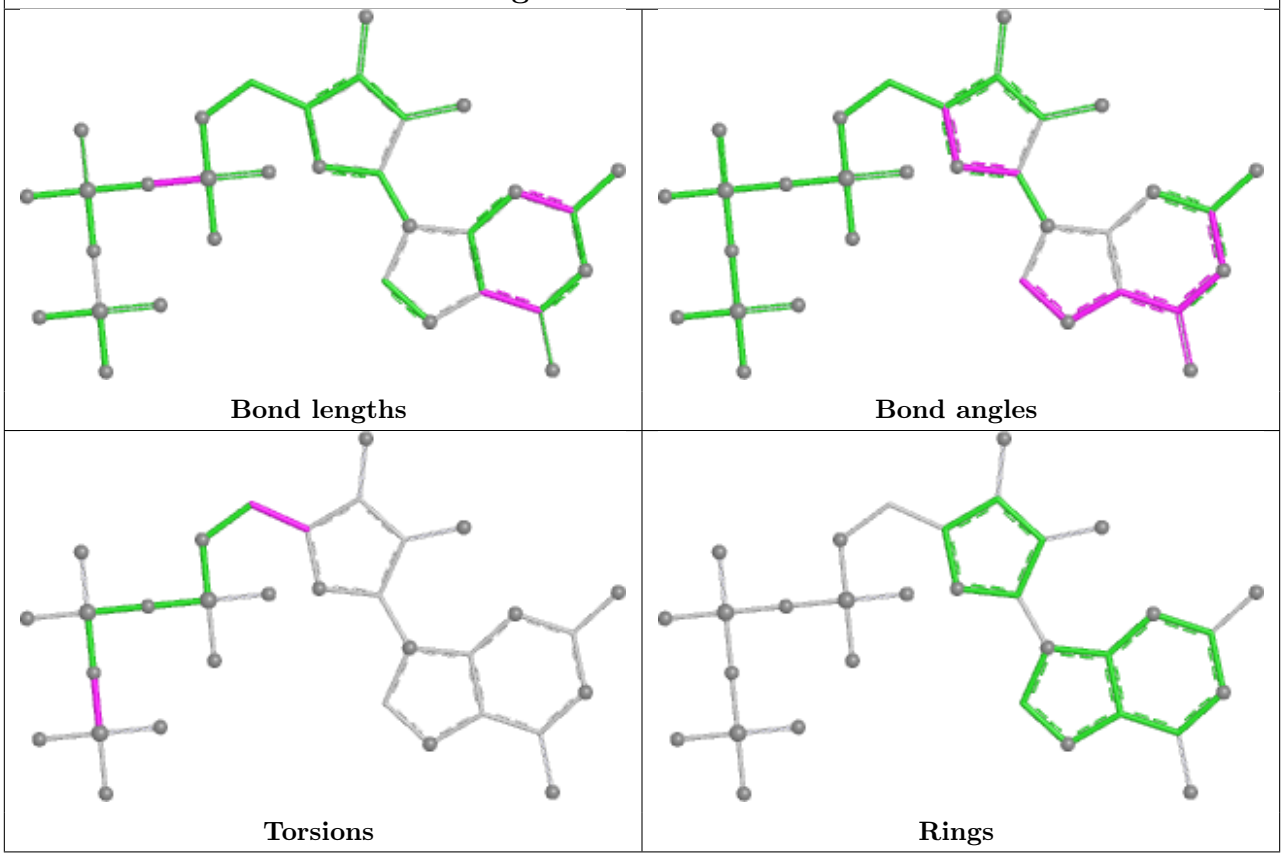
Ligand GDP n 501



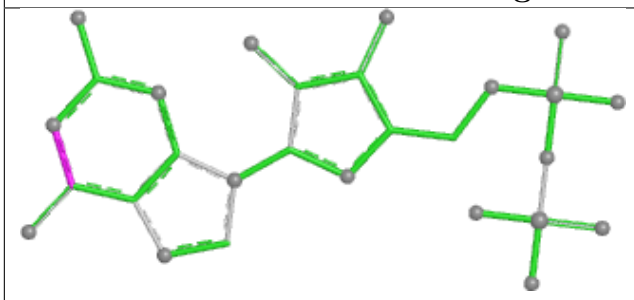
Ligand GTP Go 501



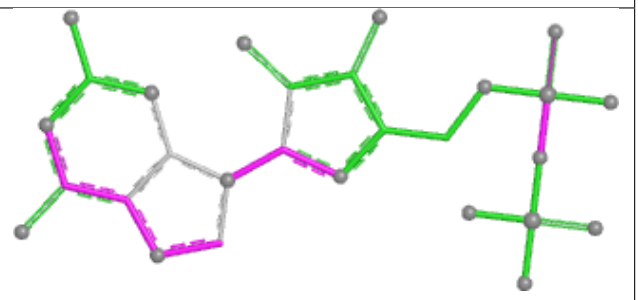
Ligand GTP Aw 602



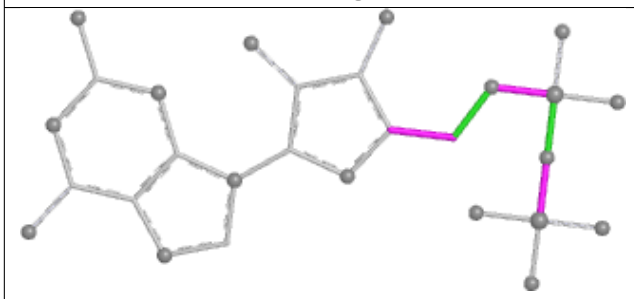
Ligand GDP Dc 501



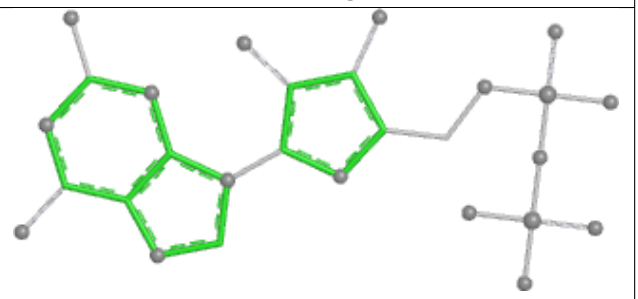
Bond lengths



Bond angles

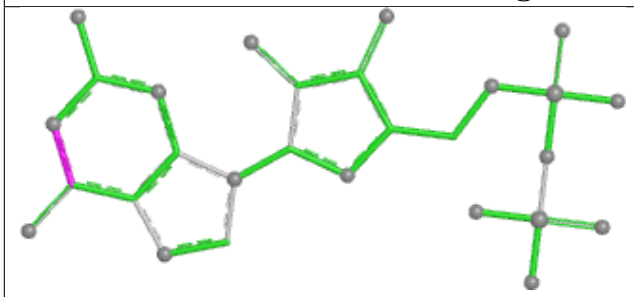


Torsions

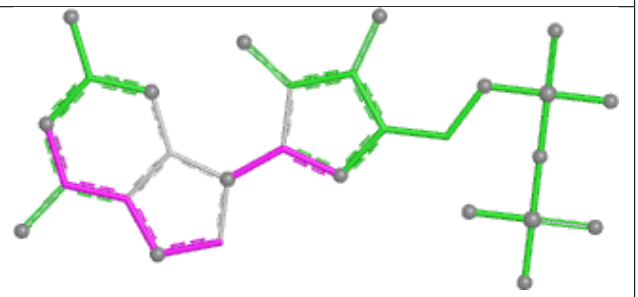


Rings

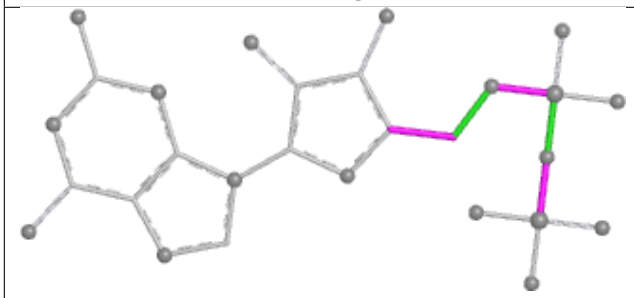
Ligand GDP FJ 501



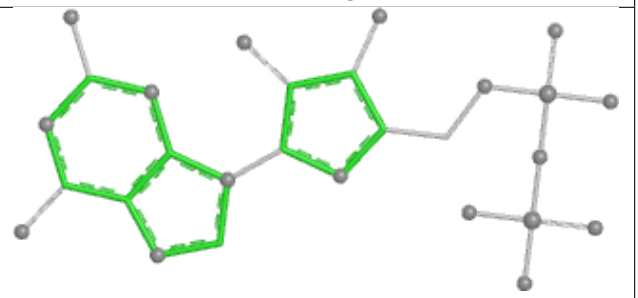
Bond lengths



Bond angles

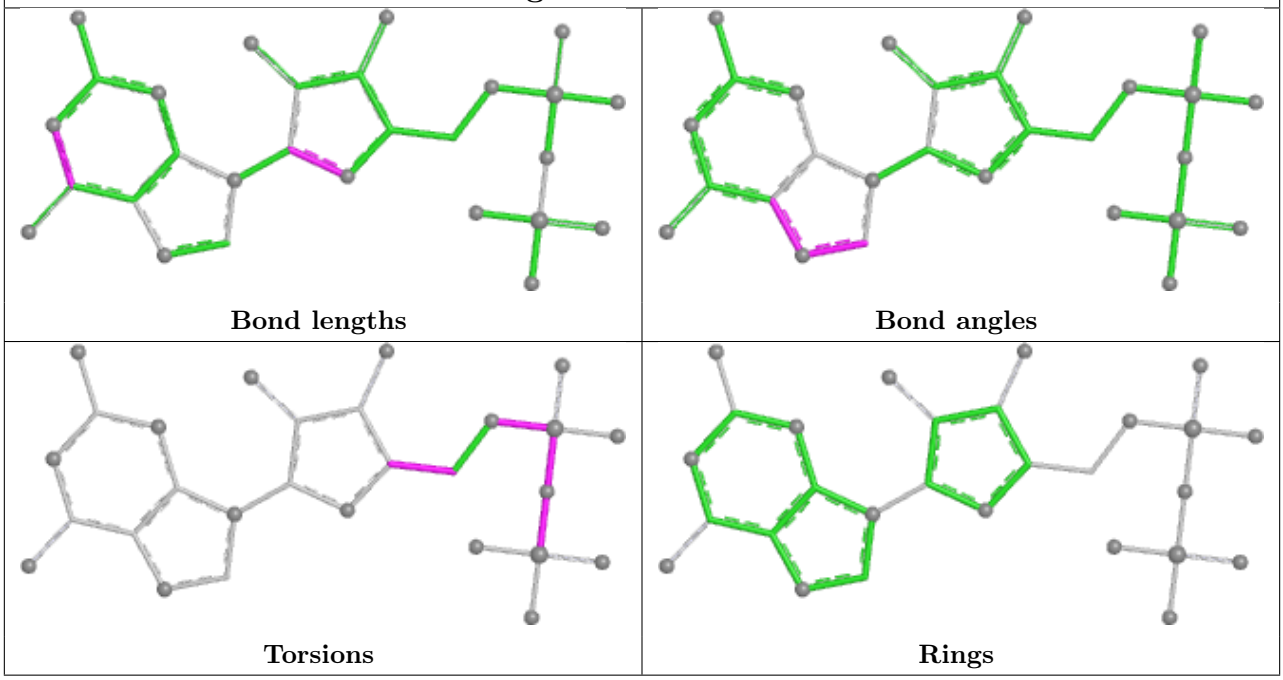


Torsions

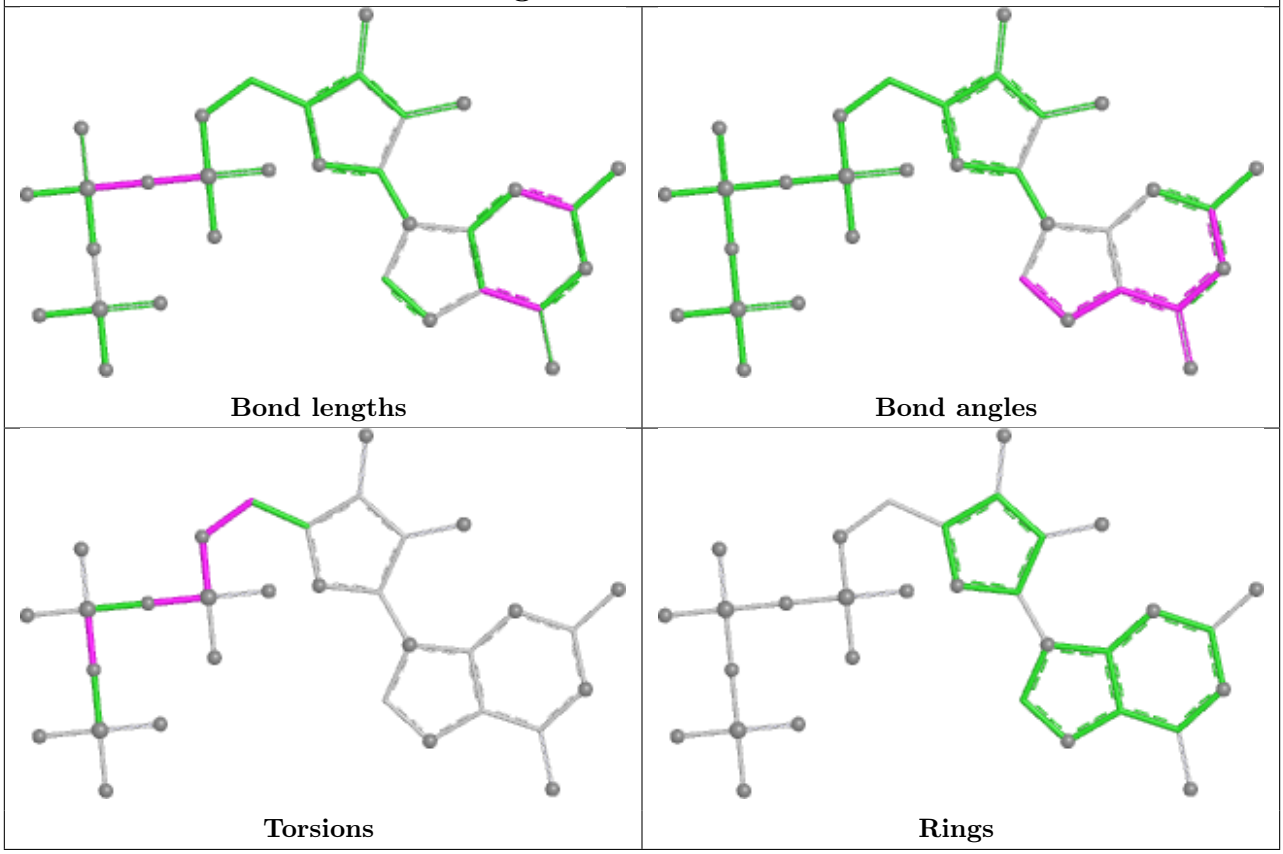


Rings

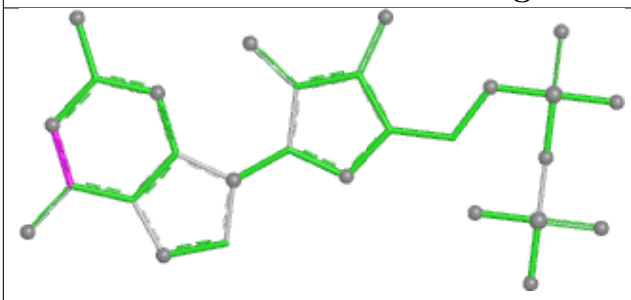
Ligand GDP 0 501



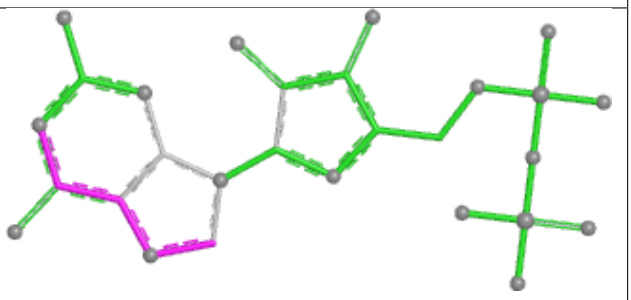
Ligand GTP GJ 501



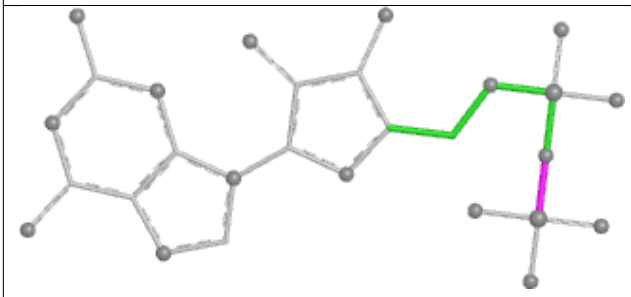
Ligand GDP Ac 501



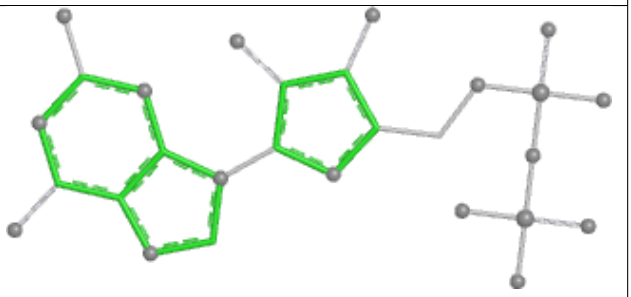
Bond lengths



Bond angles

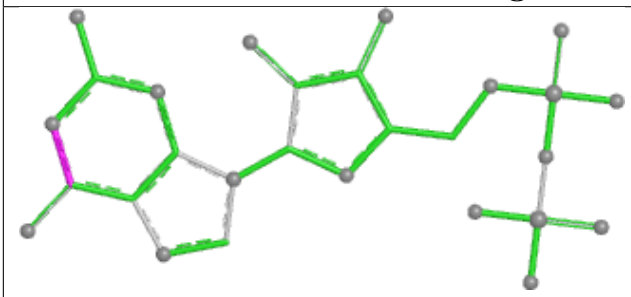


Torsions

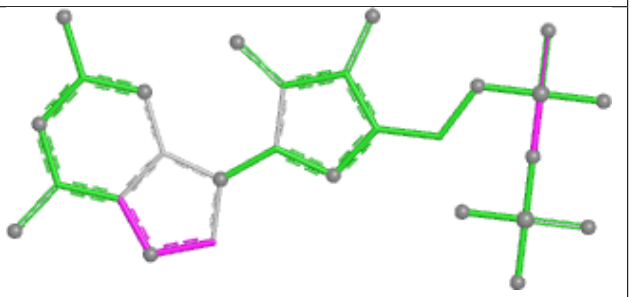


Rings

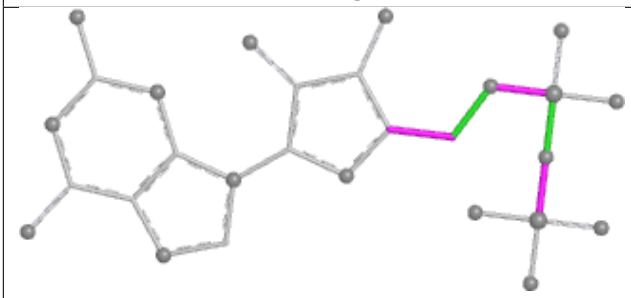
Ligand GDP DT 501



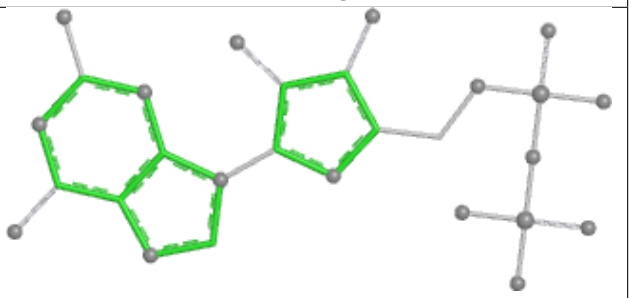
Bond lengths



Bond angles

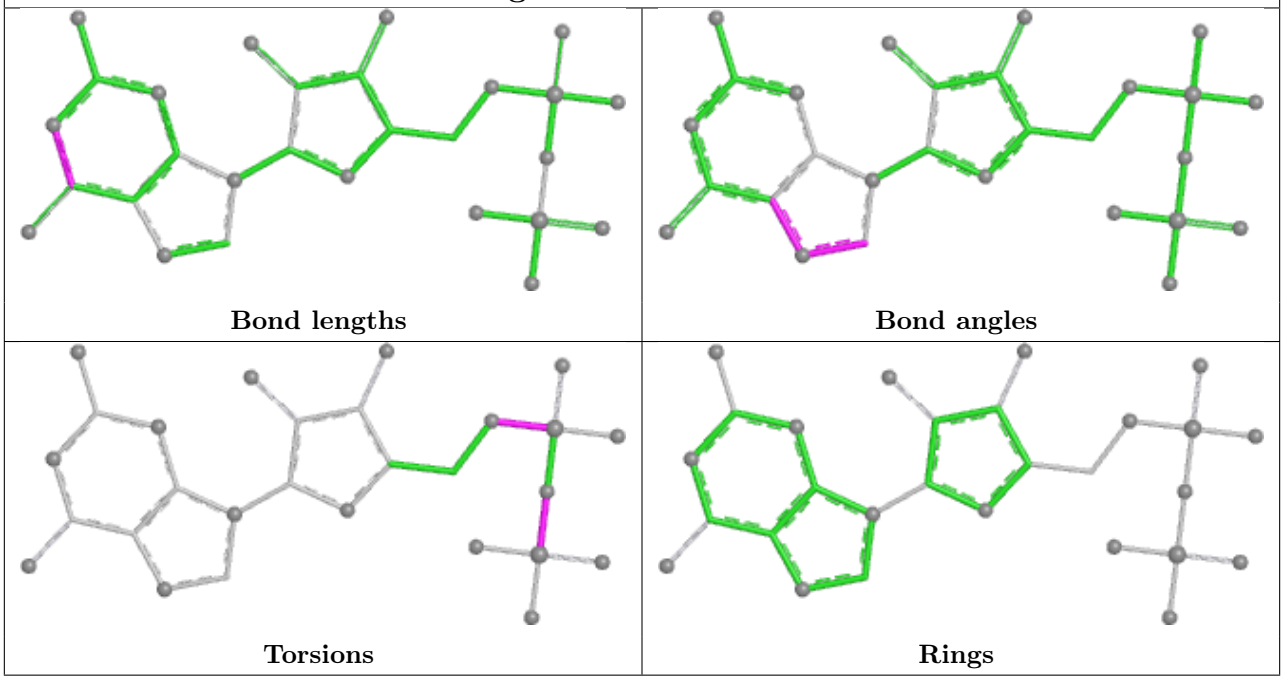


Torsions

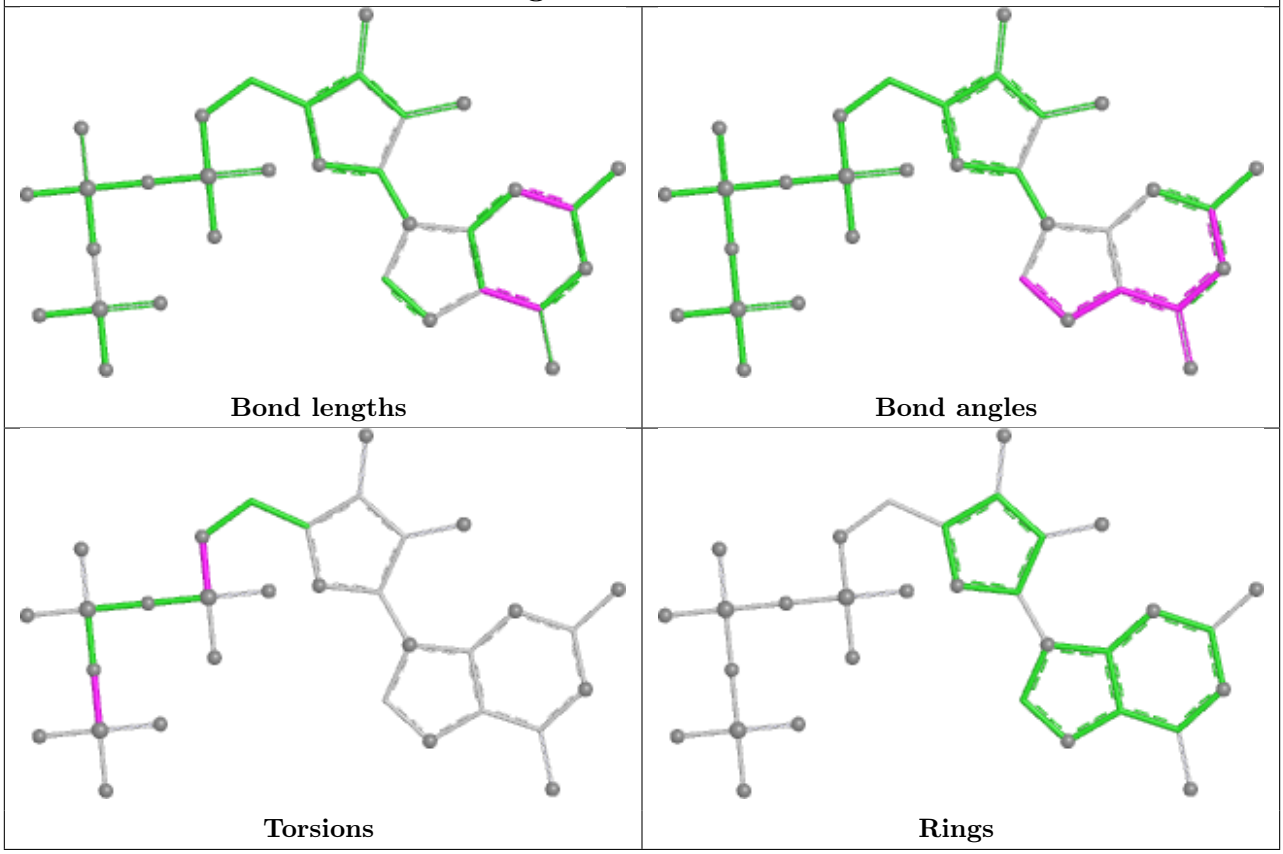


Rings

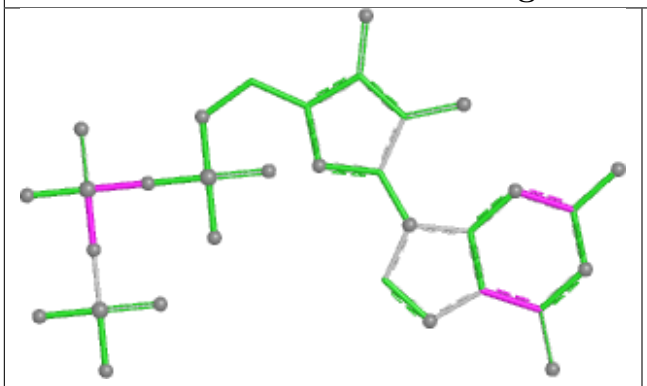
Ligand GDP BG 501



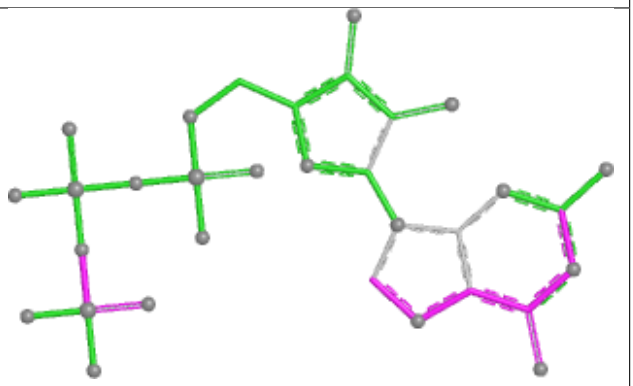
Ligand GTP x 501



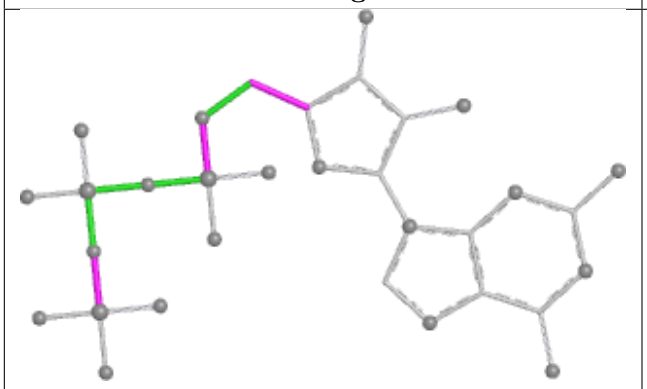
Ligand GTP W 602



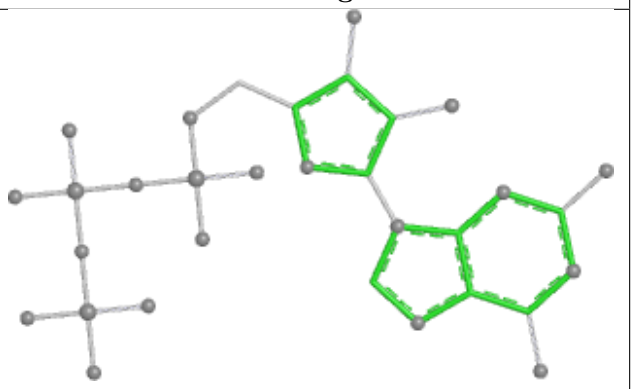
Bond lengths



Bond angles

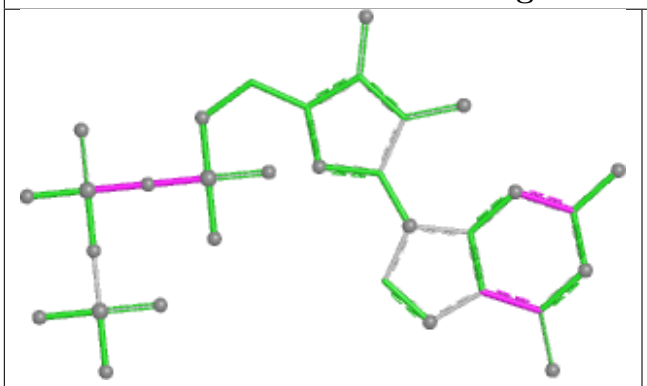


Torsions

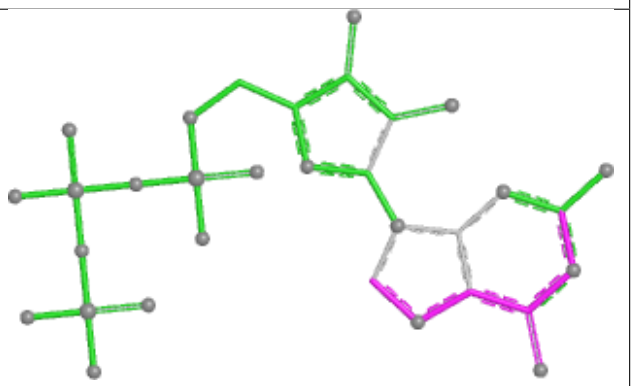


Rings

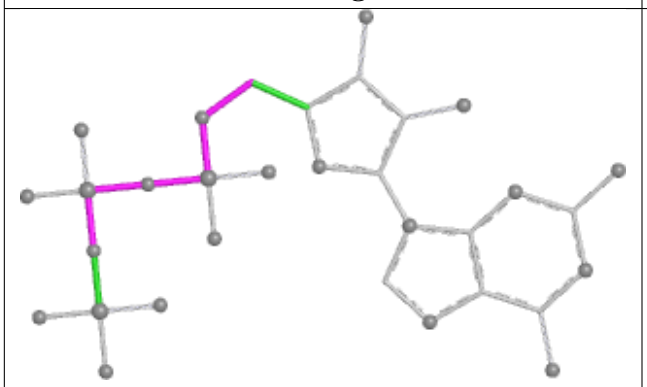
Ligand GTP F8 501



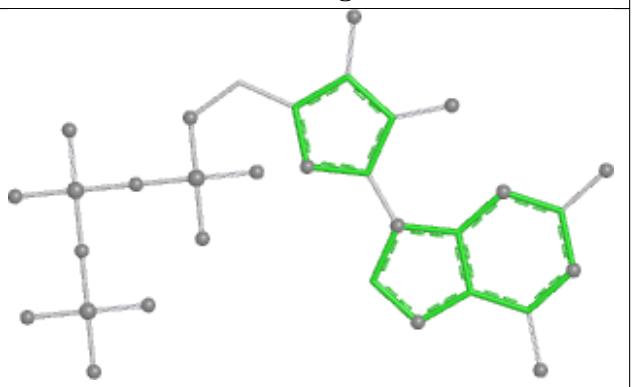
Bond lengths



Bond angles

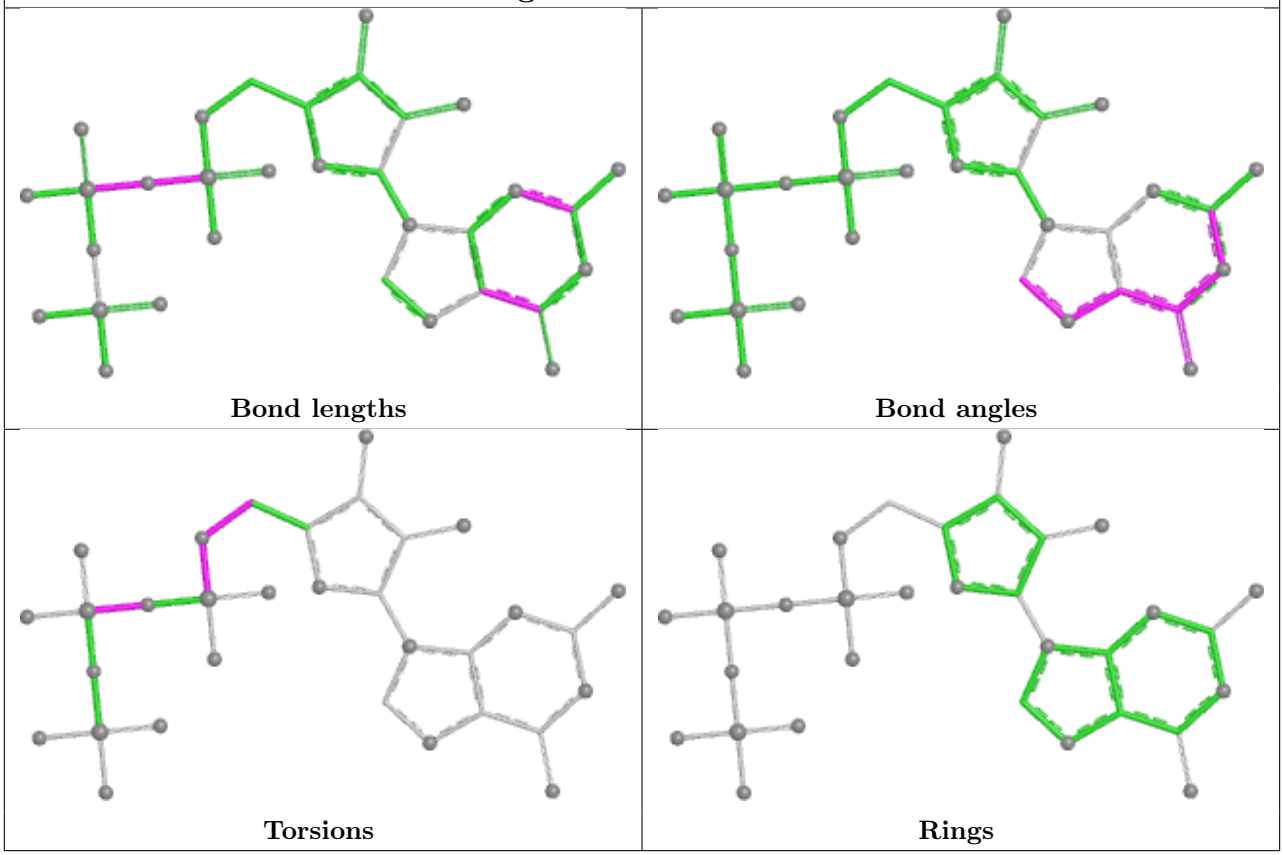


Torsions

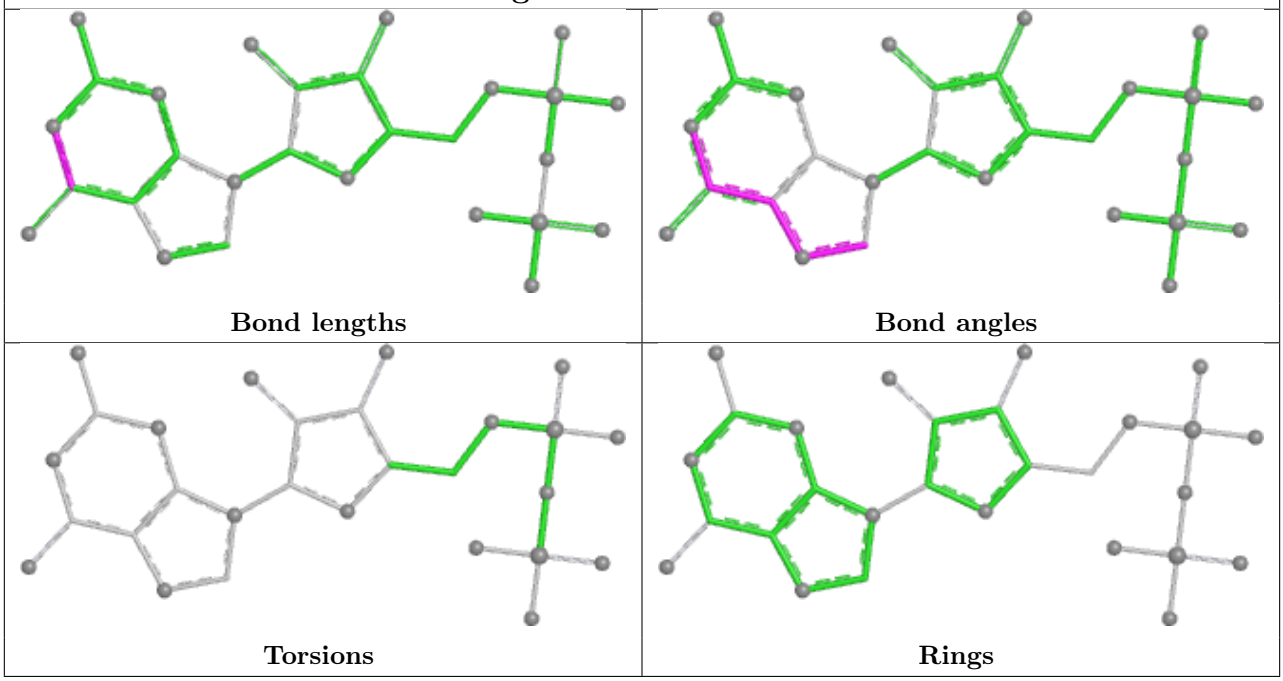


Rings

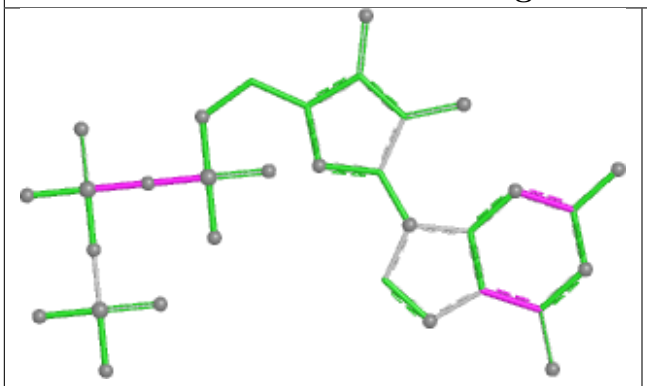
Ligand GTP Es 501



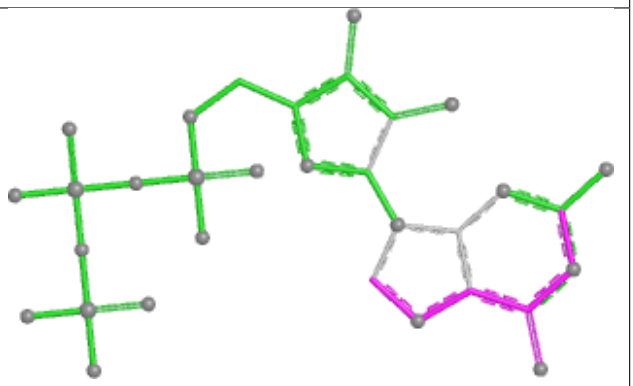
Ligand GDP Au 602



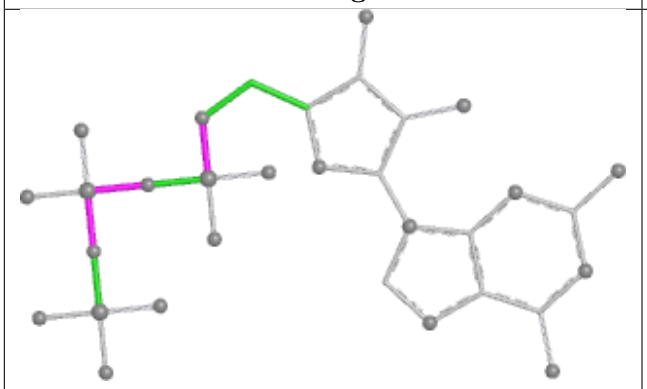
Ligand GTP B1 602



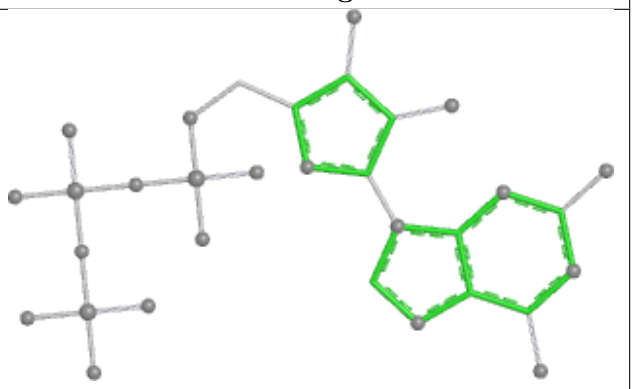
Bond lengths



Bond angles

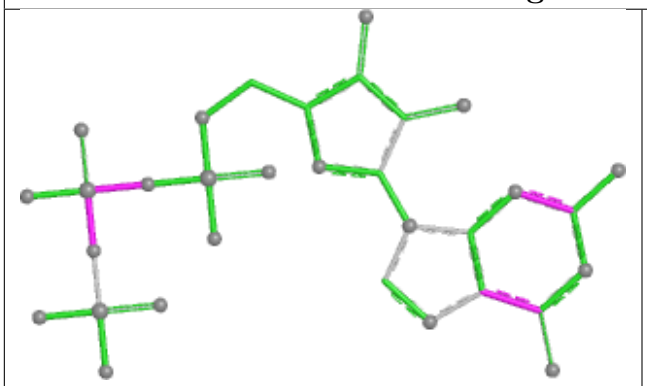


Torsions

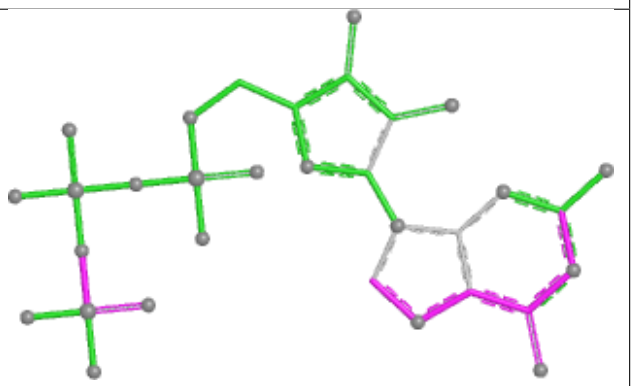


Rings

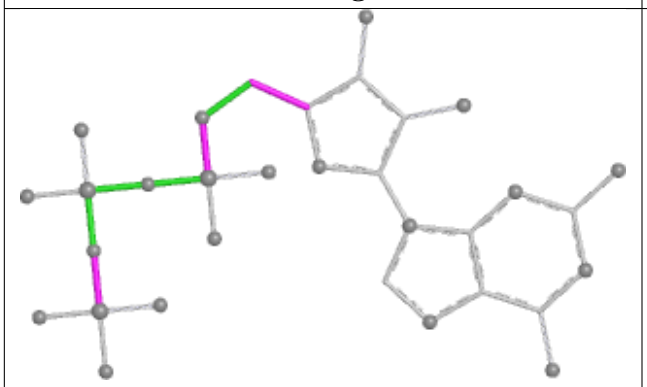
Ligand GTP h 602



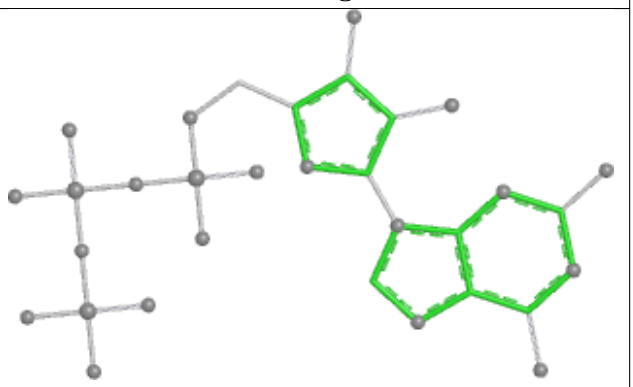
Bond lengths



Bond angles

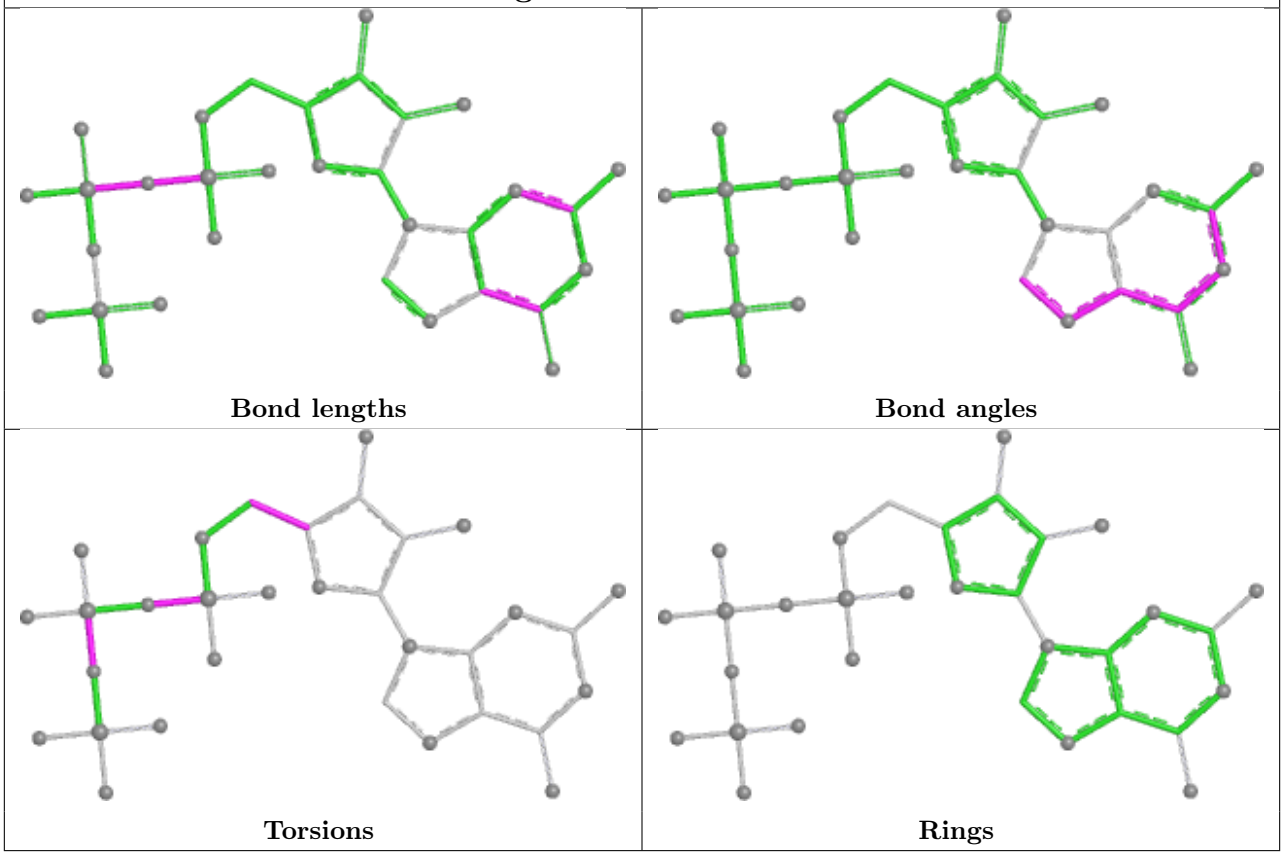


Torsions

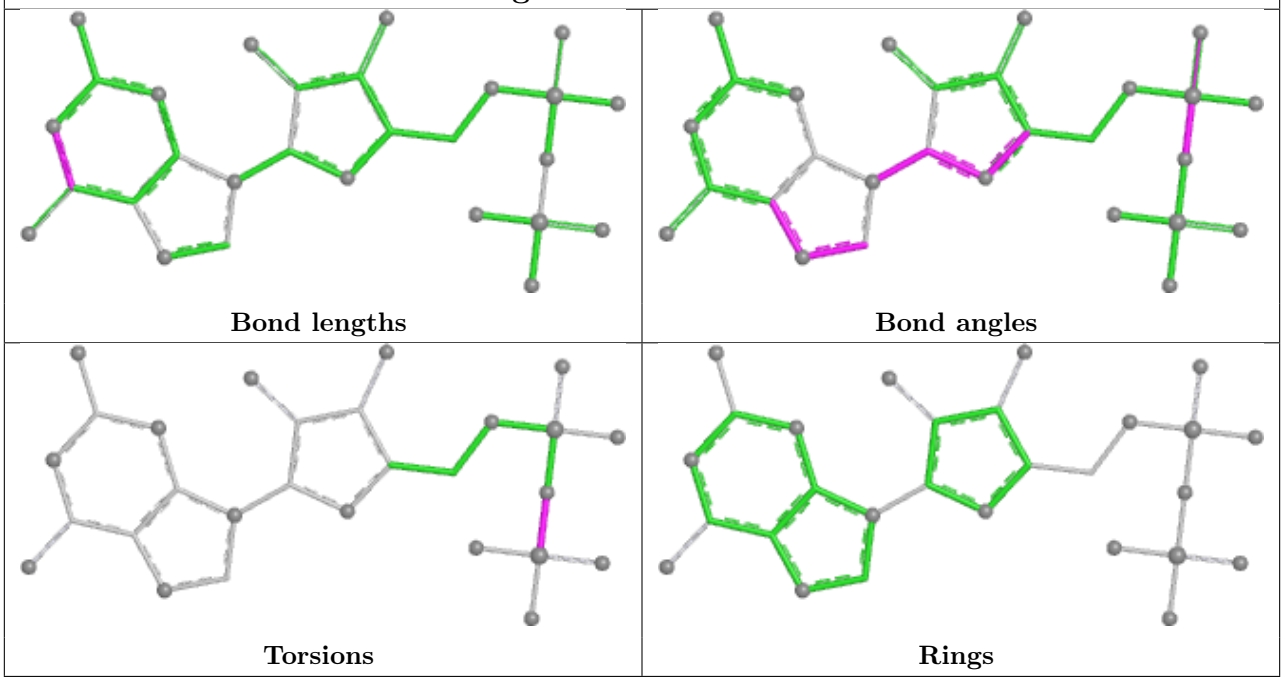


Rings

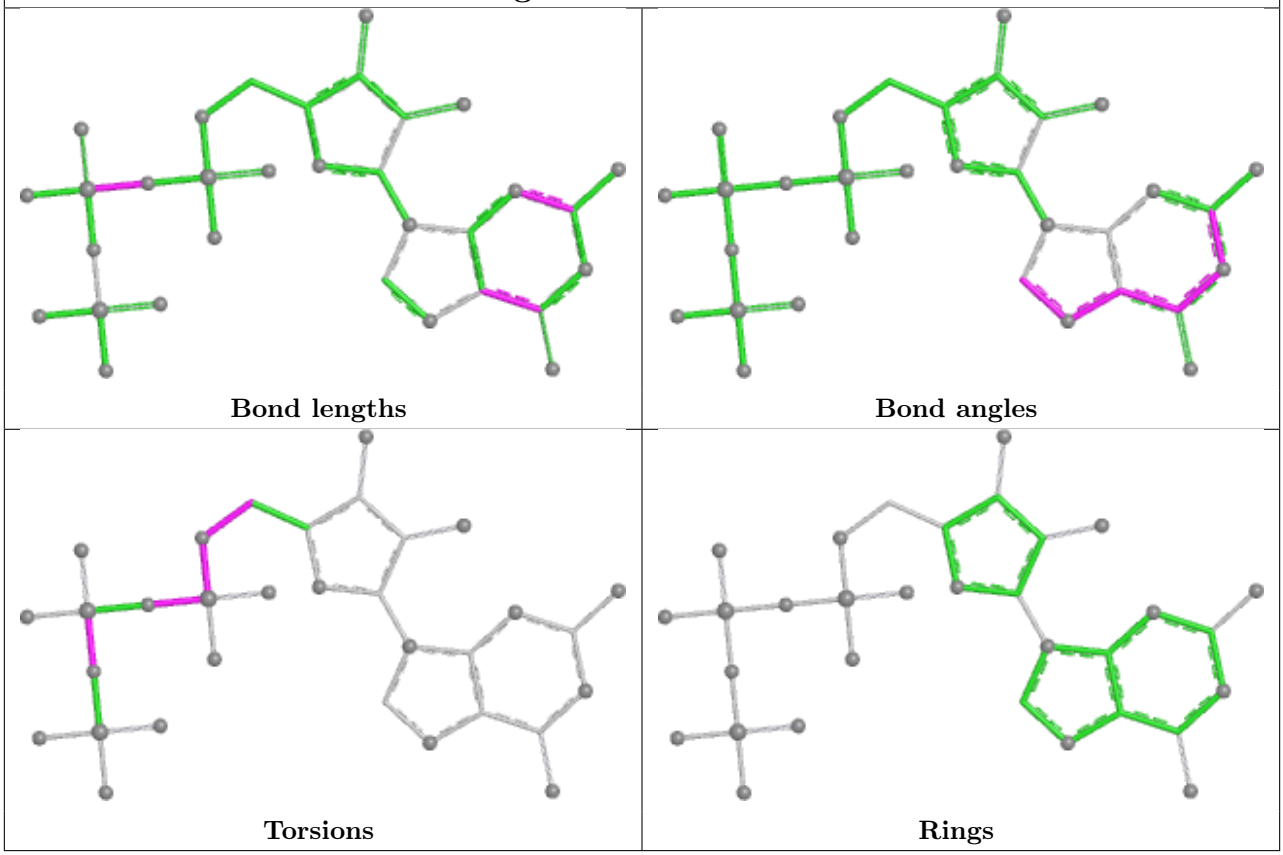
Ligand GTP B8 602



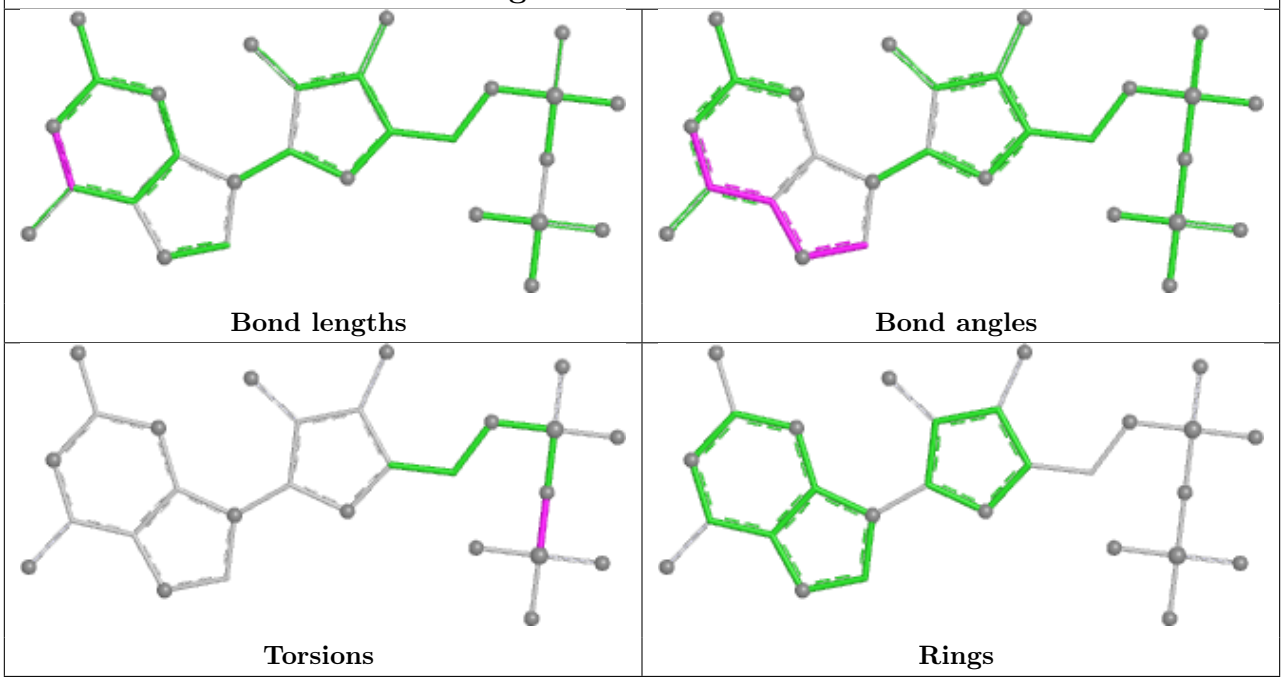
Ligand GDP Dv 501



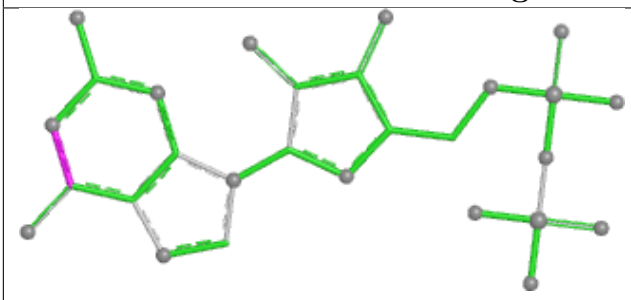
Ligand GTP A8 501



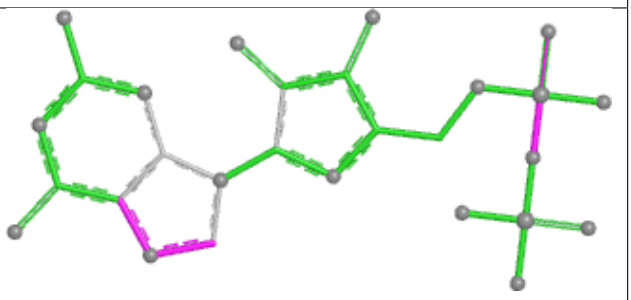
Ligand GDP AB 501



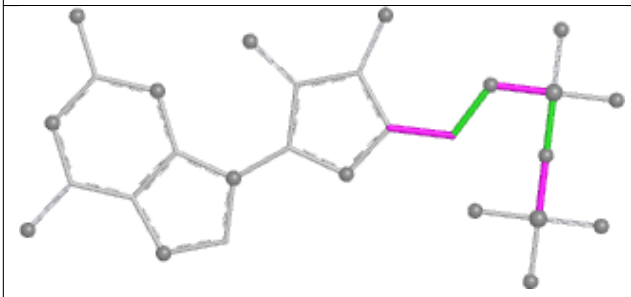
Ligand GDP Dk 501



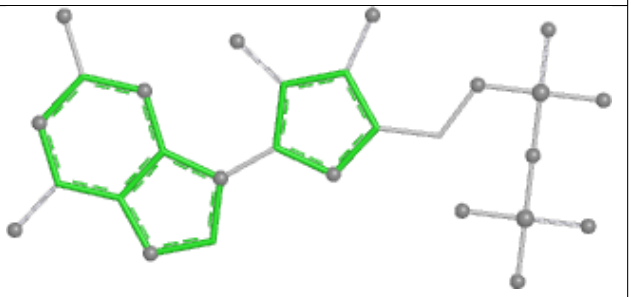
Bond lengths



Bond angles

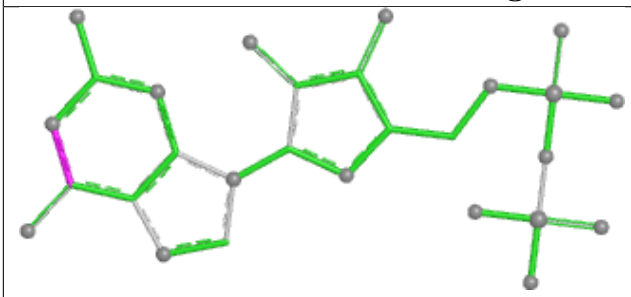


Torsions

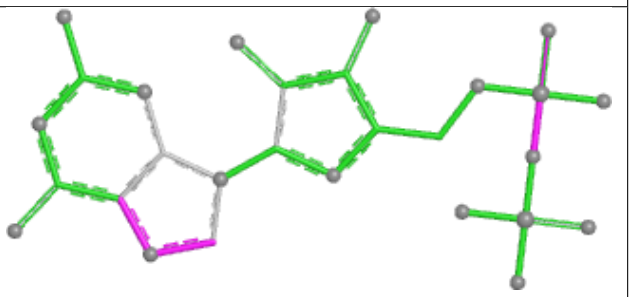


Rings

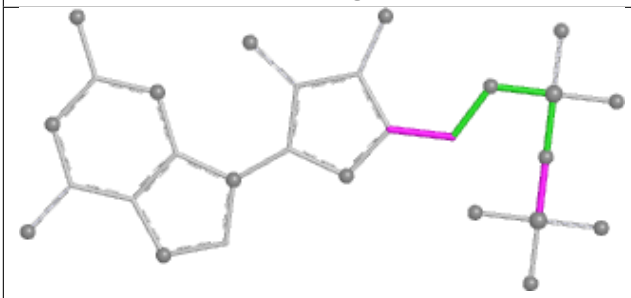
Ligand GDP GH 501



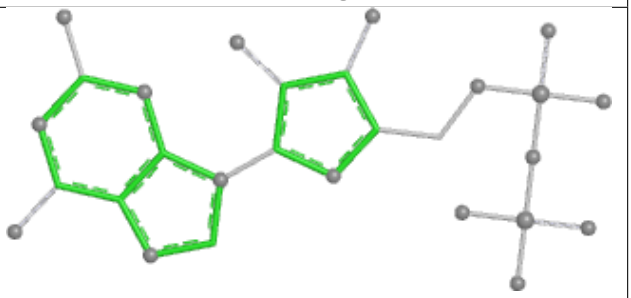
Bond lengths



Bond angles

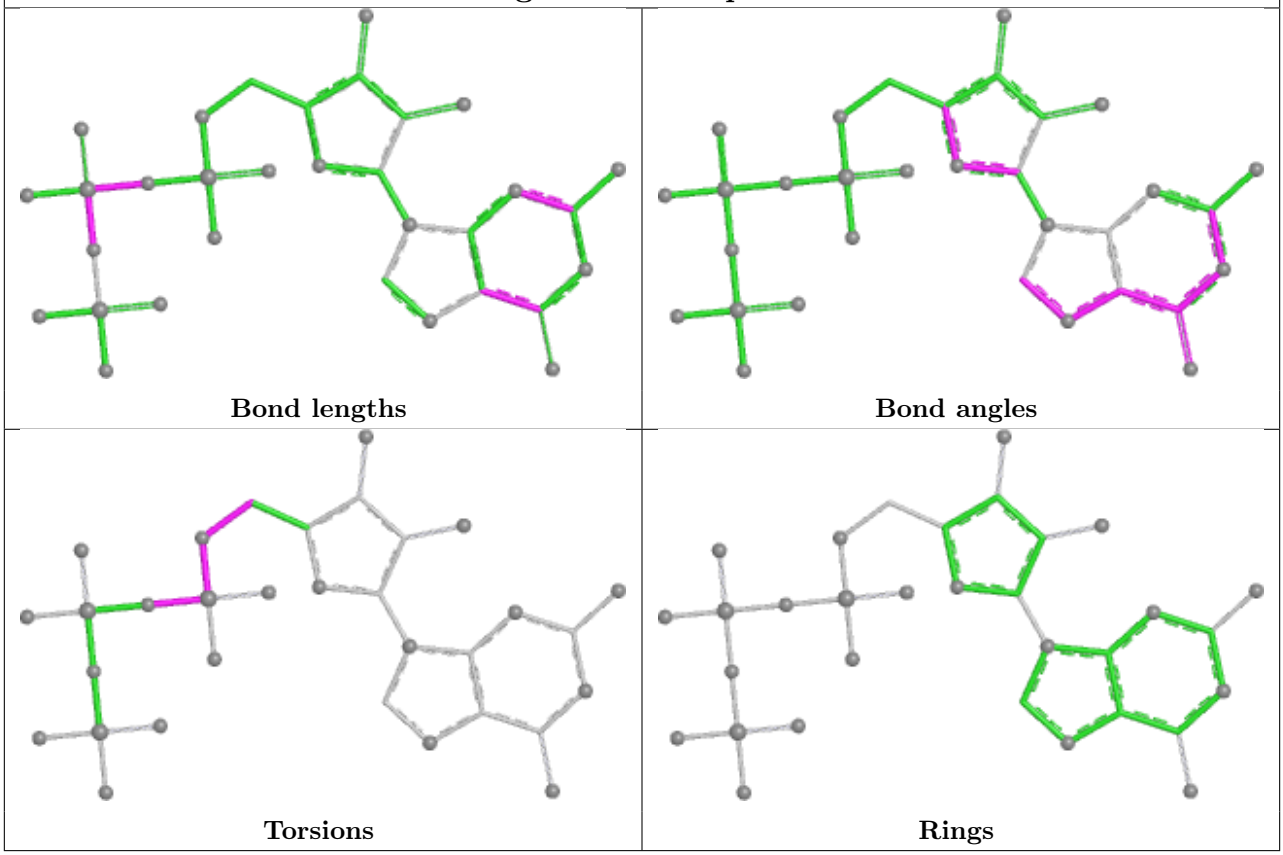


Torsions

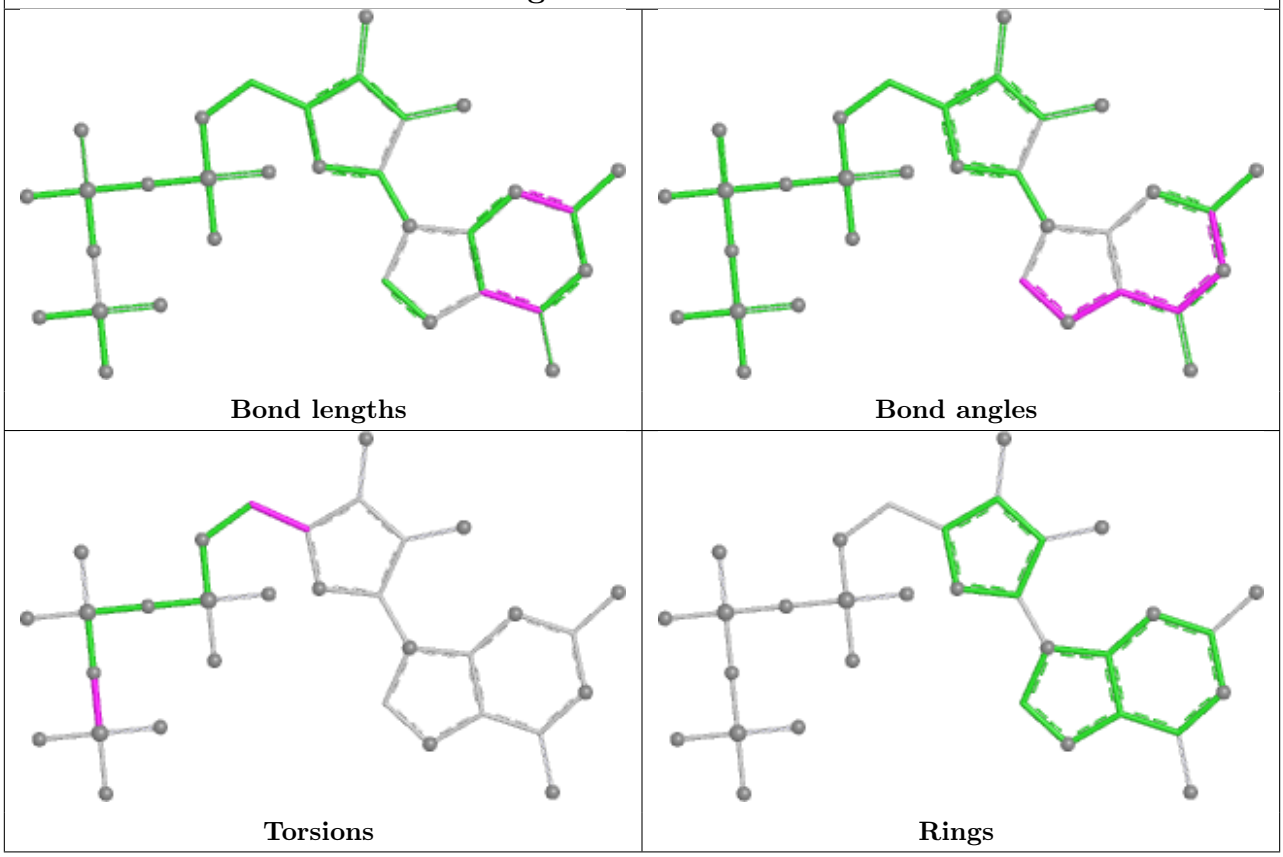


Rings

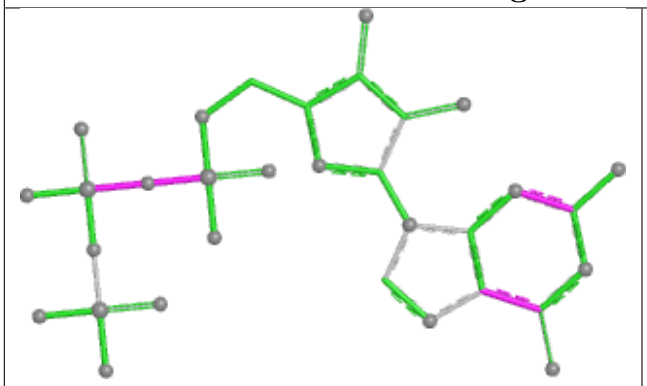
Ligand GTP Eq 501



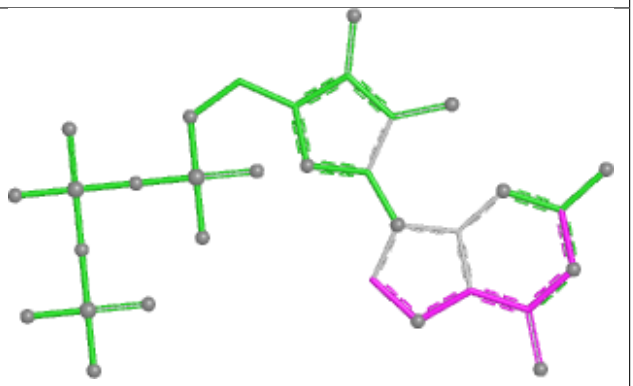
Ligand GTP 1 602



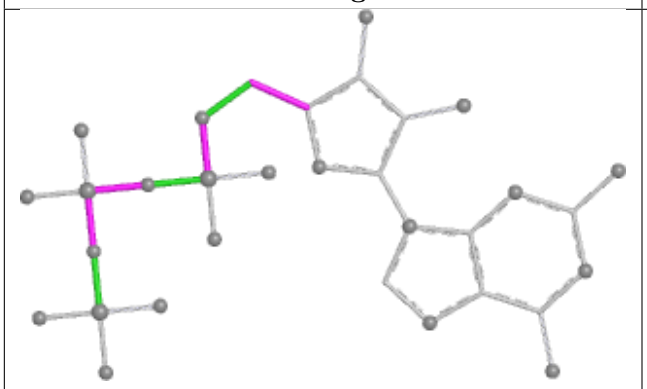
Ligand GTP BN 602



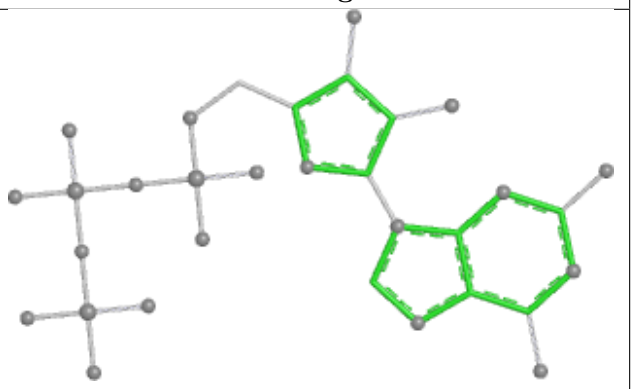
Bond lengths



Bond angles

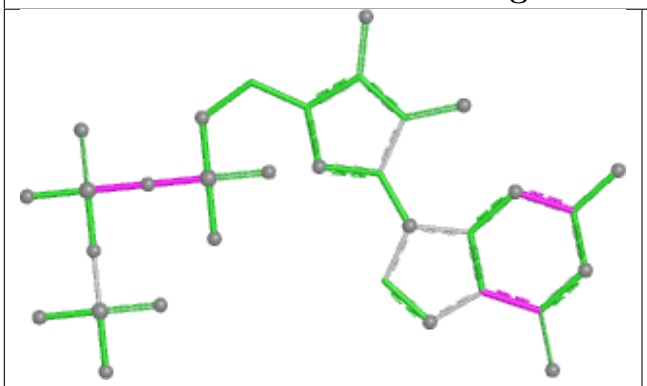


Torsions

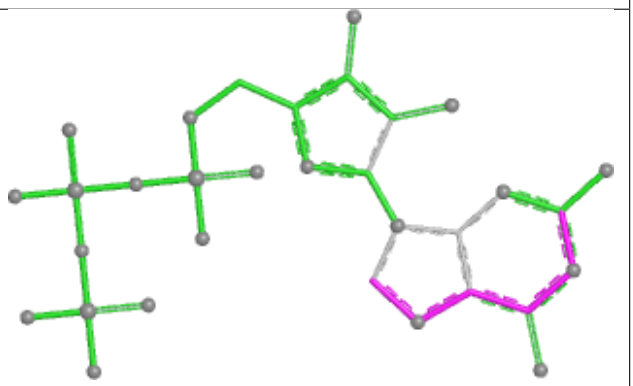


Rings

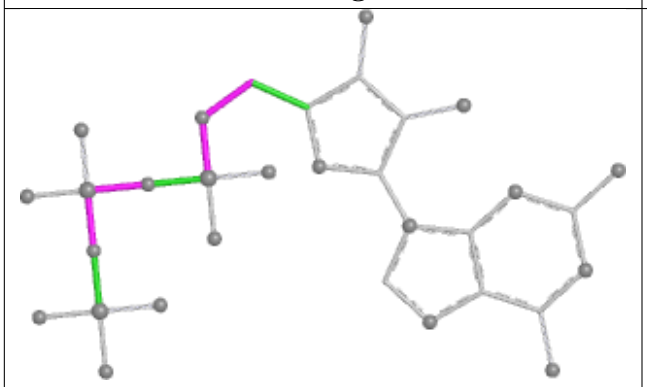
Ligand GTP Em 501



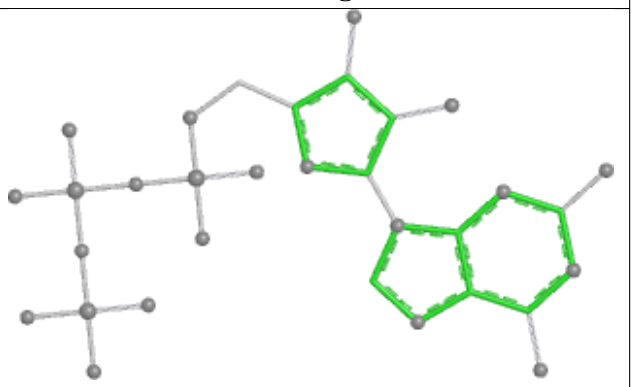
Bond lengths



Bond angles

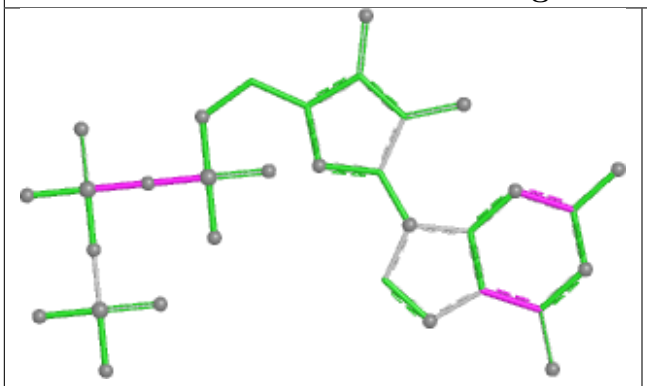


Torsions

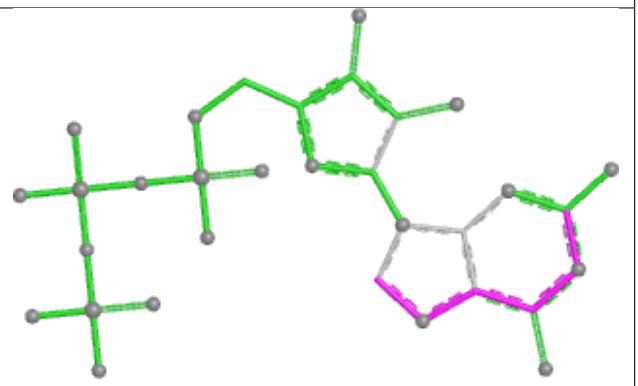


Rings

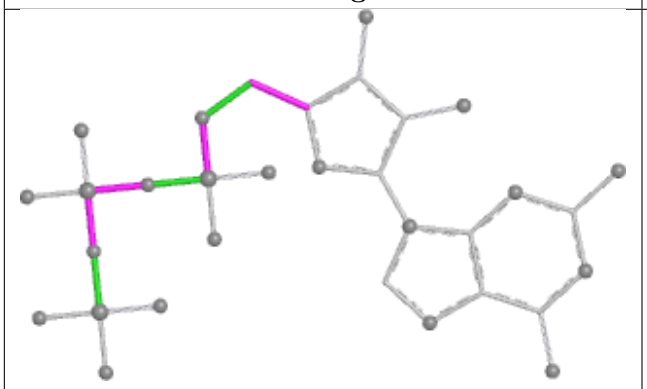
Ligand GTP i 602



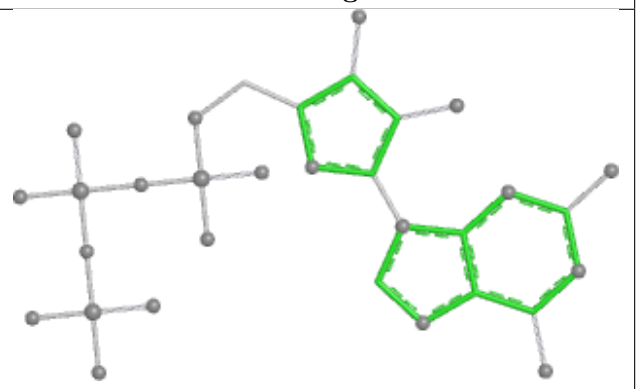
Bond lengths



Bond angles

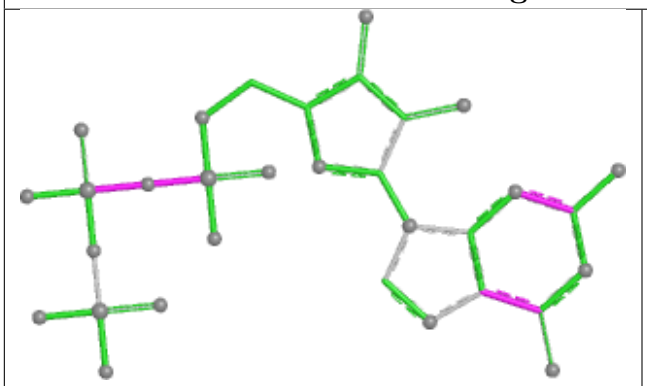


Torsions

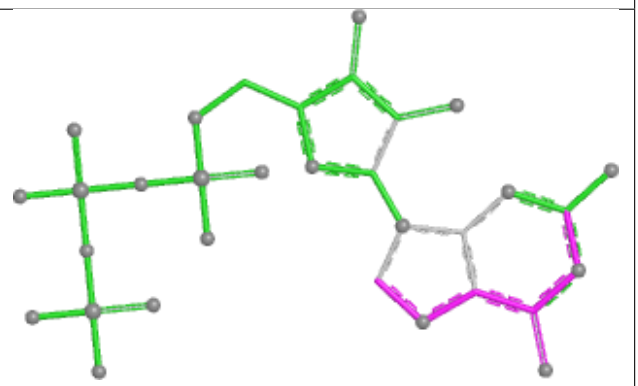


Rings

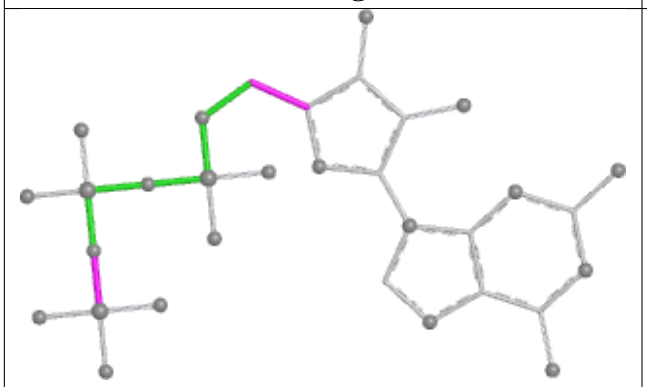
Ligand GTP BK 602



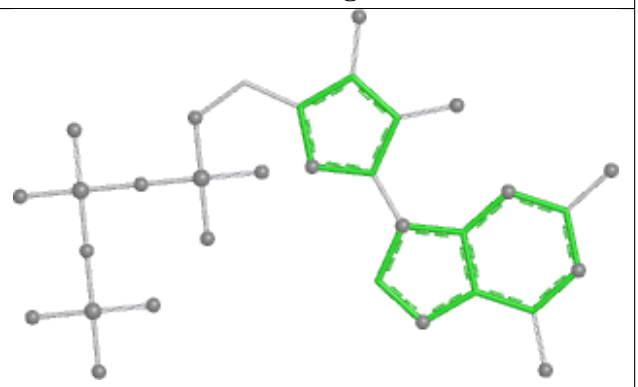
Bond lengths



Bond angles

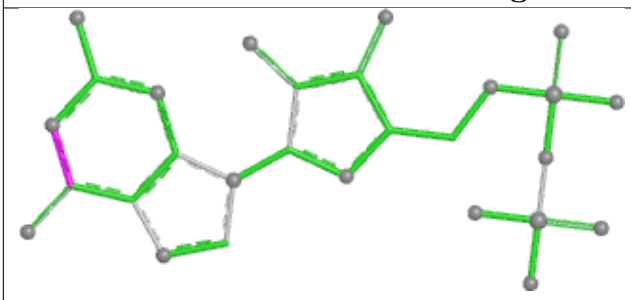


Torsions

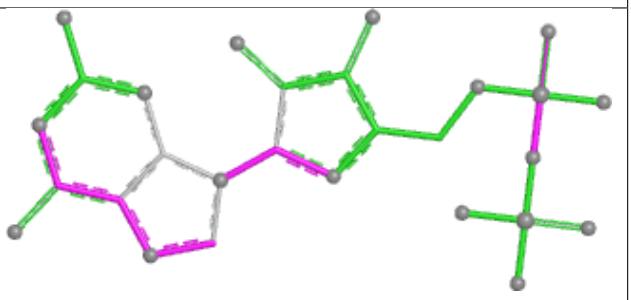


Rings

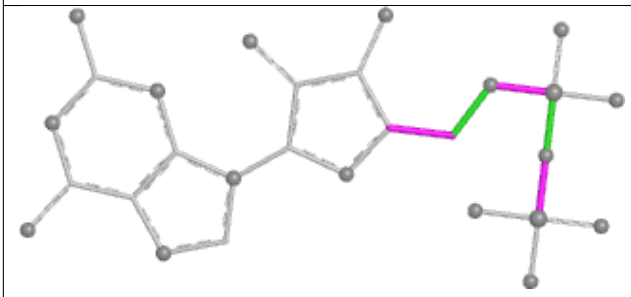
Ligand GDP DL 501



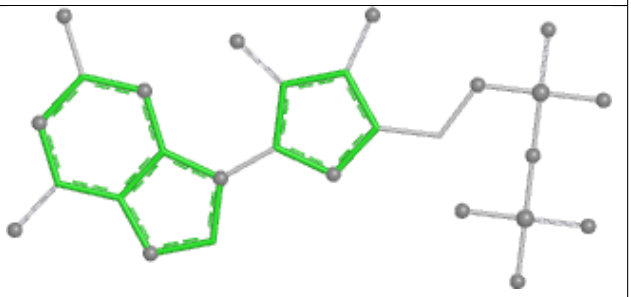
Bond lengths



Bond angles

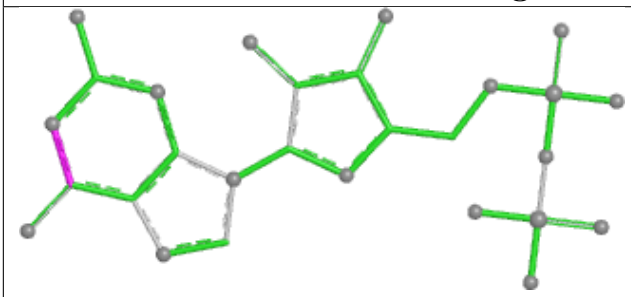


Torsions

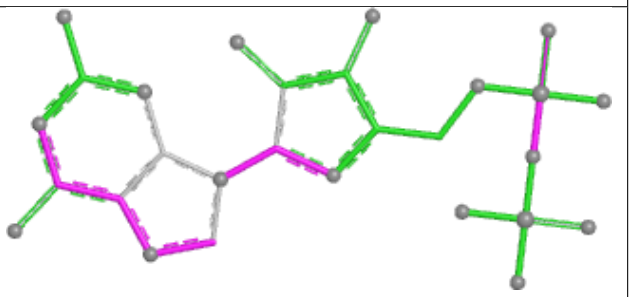


Rings

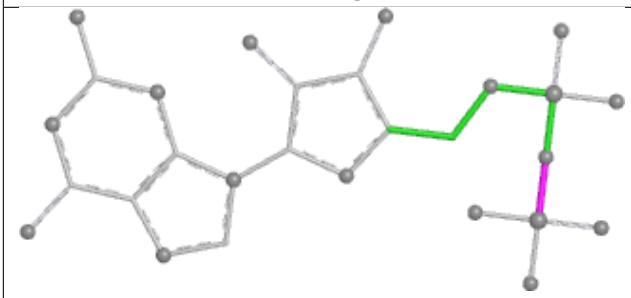
Ligand GDP FE 501



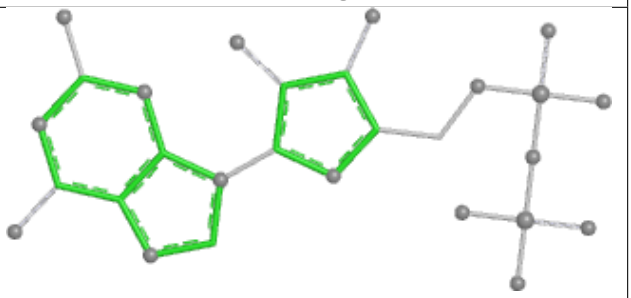
Bond lengths



Bond angles

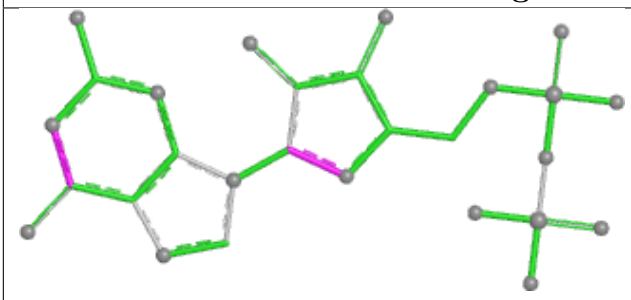


Torsions

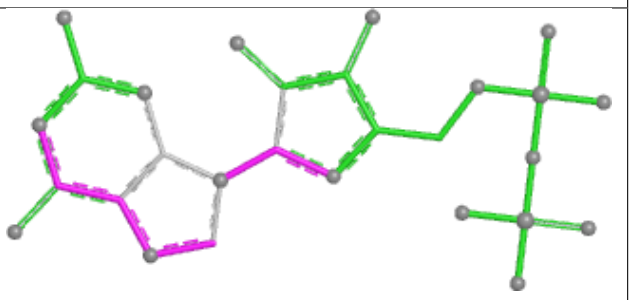


Rings

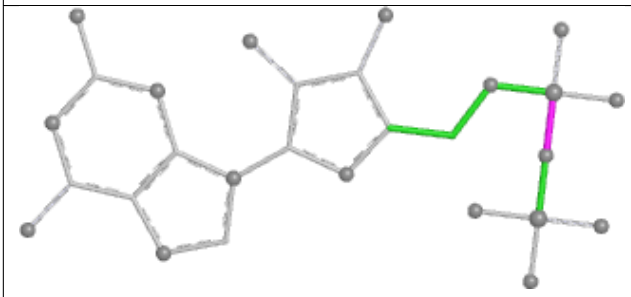
Ligand GDP A3 501



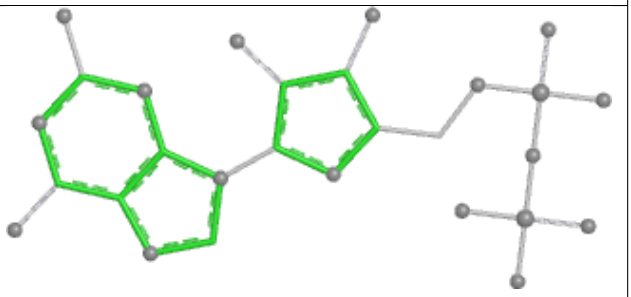
Bond lengths



Bond angles

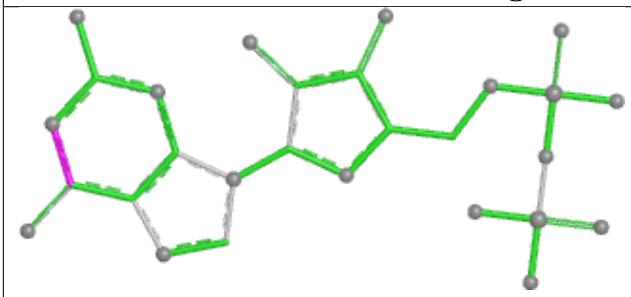


Torsions

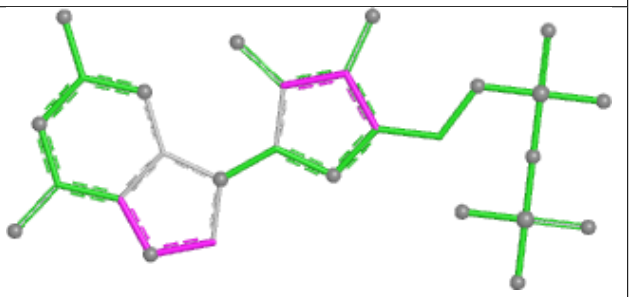


Rings

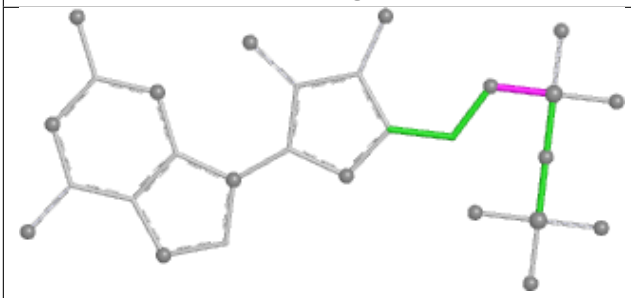
Ligand GDP AA 501



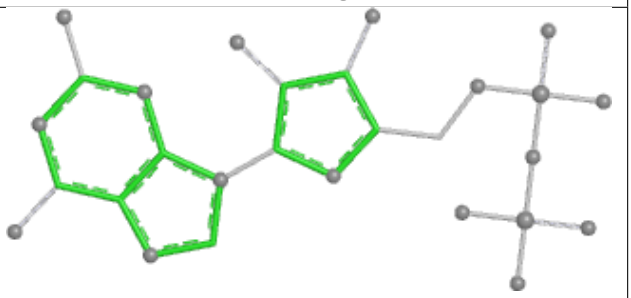
Bond lengths



Bond angles

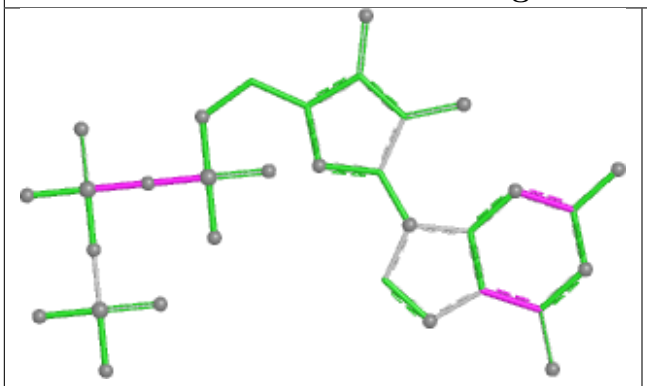


Torsions

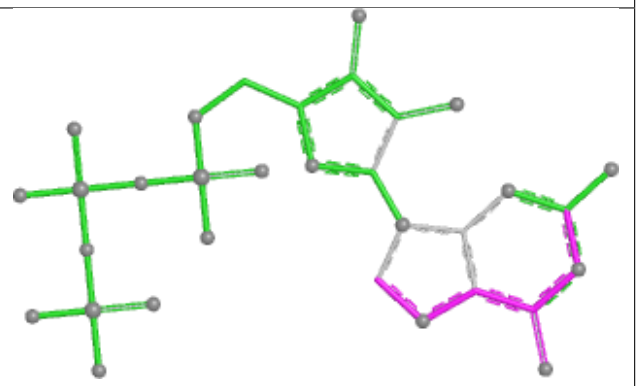


Rings

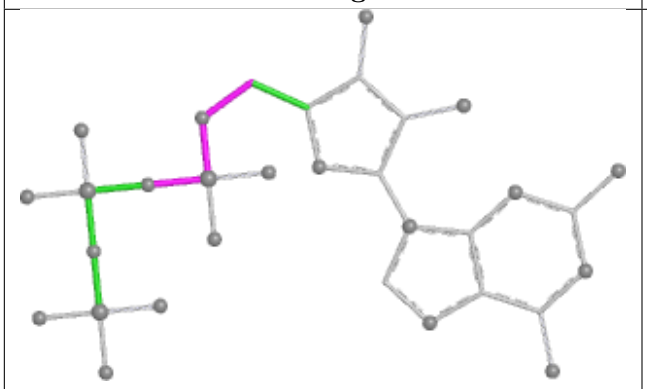
Ligand GTP FX 501



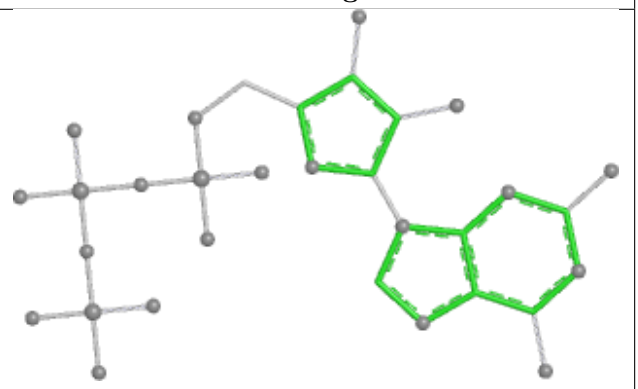
Bond lengths



Bond angles

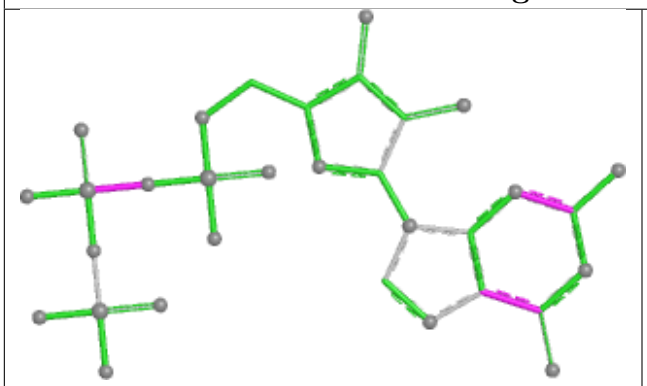


Torsions

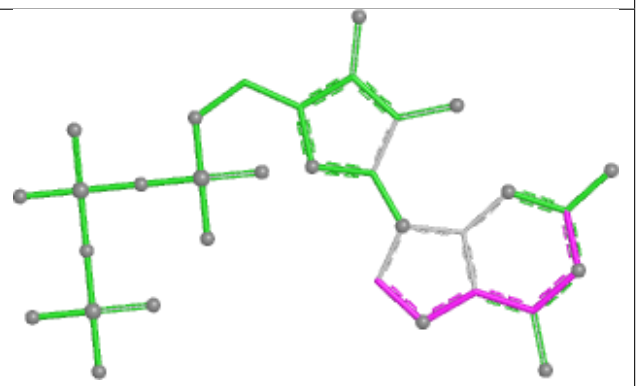


Rings

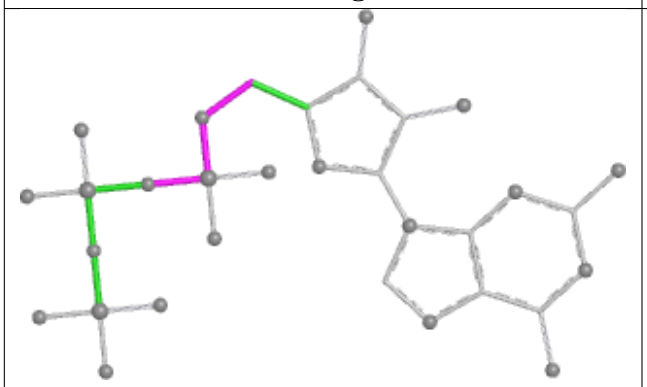
Ligand GTP FV 602



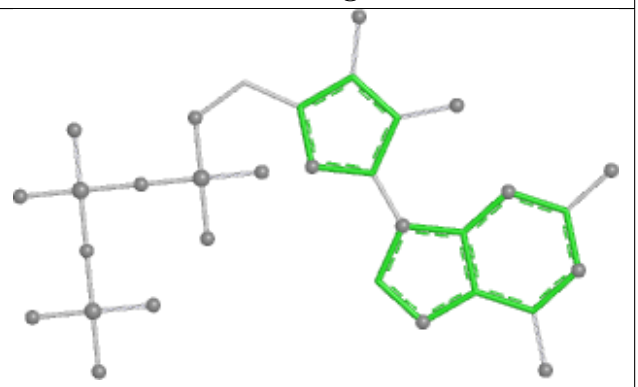
Bond lengths



Bond angles

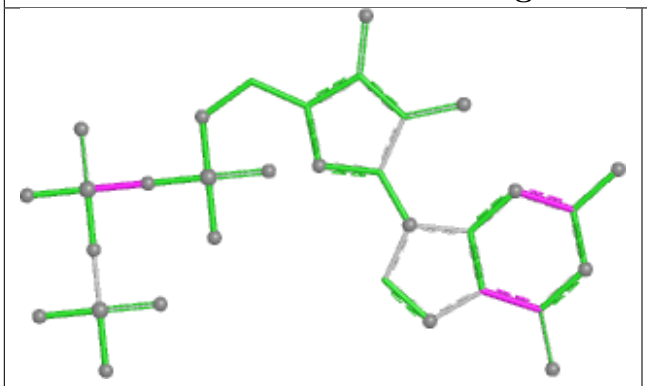


Torsions

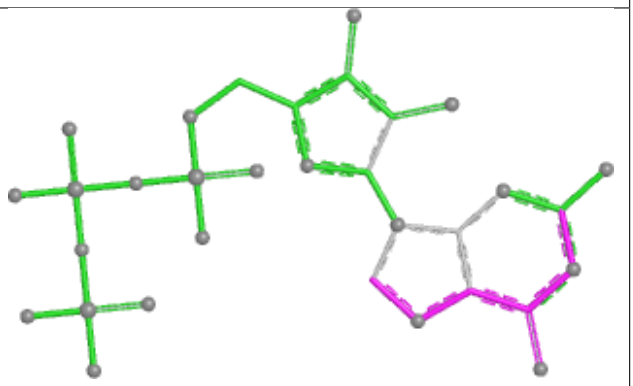


Rings

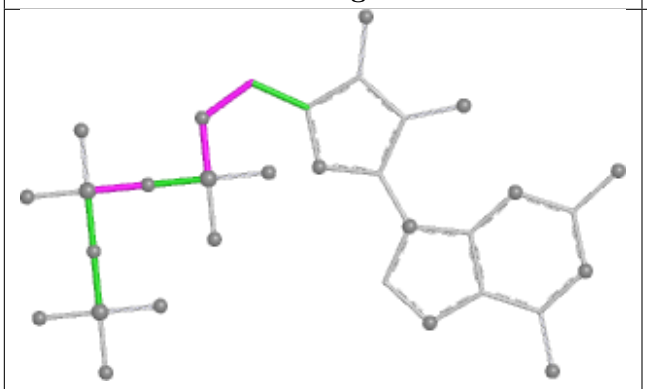
Ligand GTP Eh 501



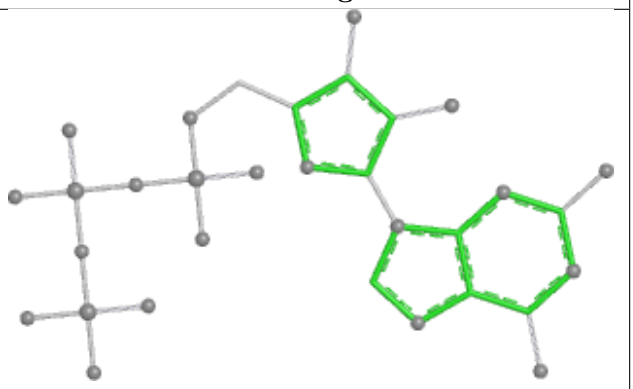
Bond lengths



Bond angles

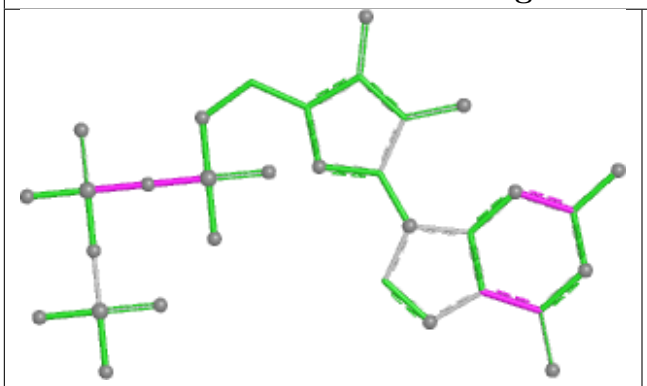


Torsions

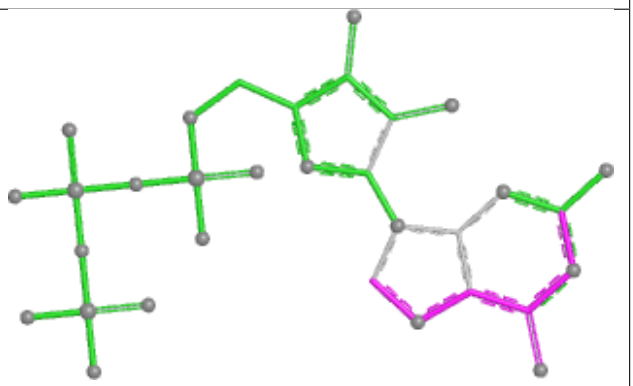


Rings

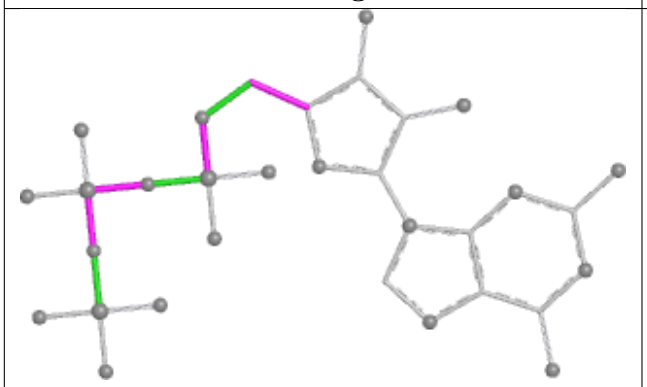
Ligand GTP B2 602



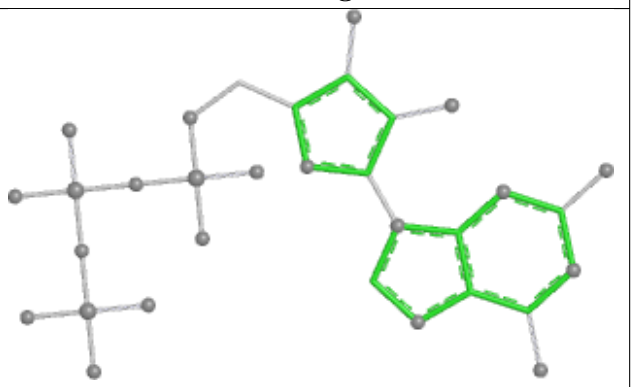
Bond lengths



Bond angles

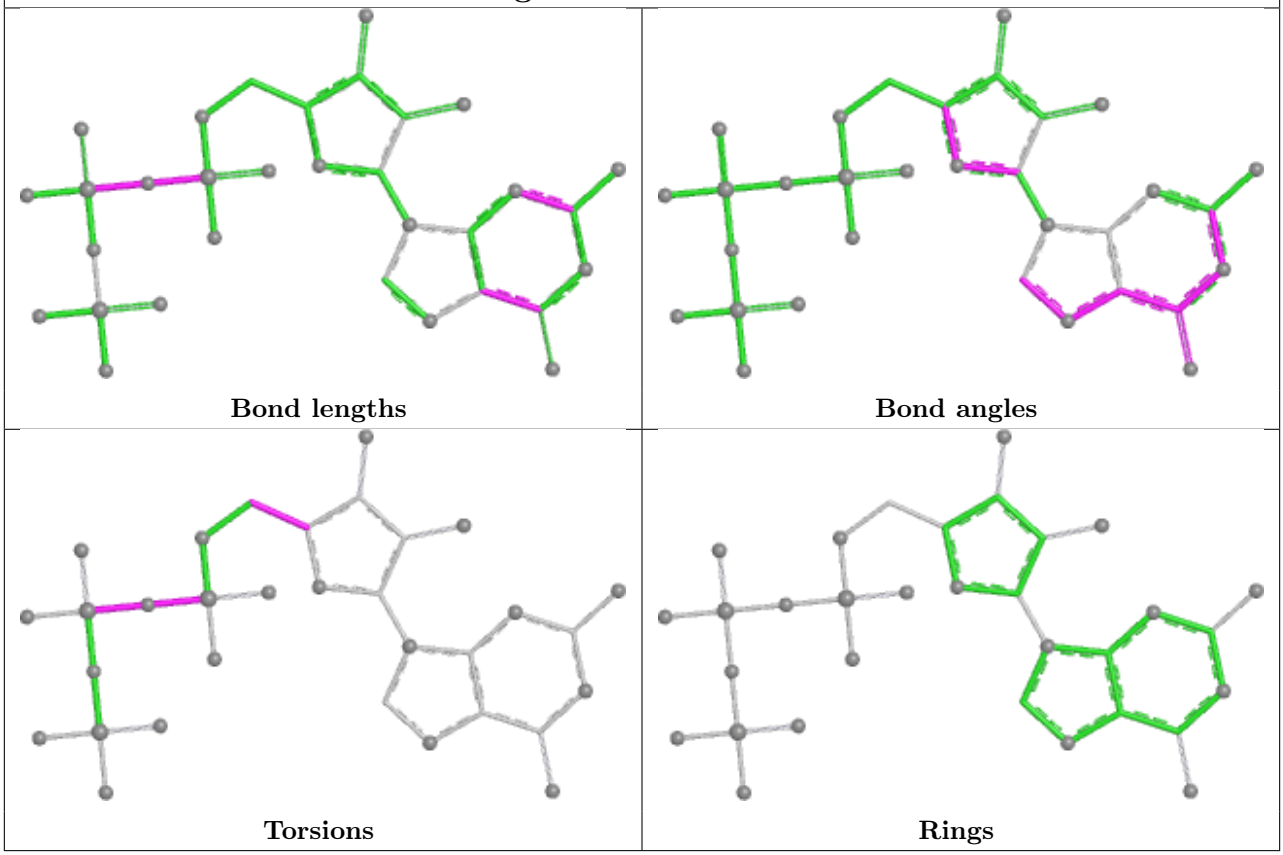


Torsions

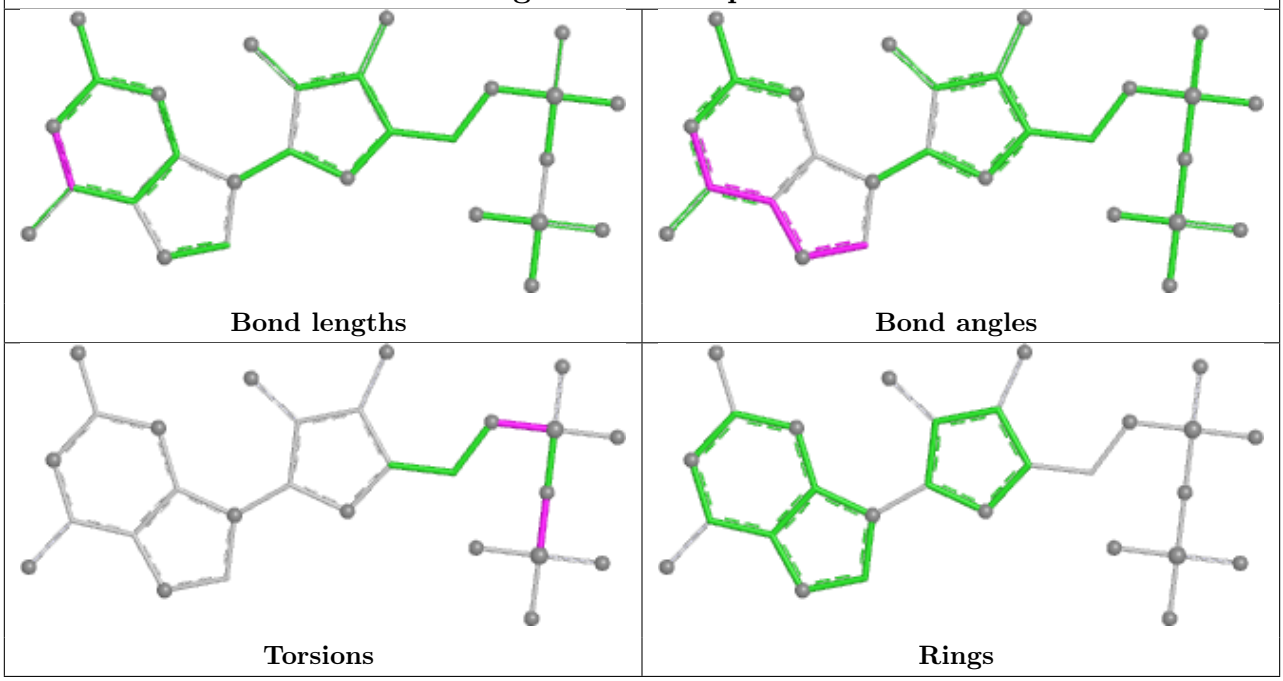


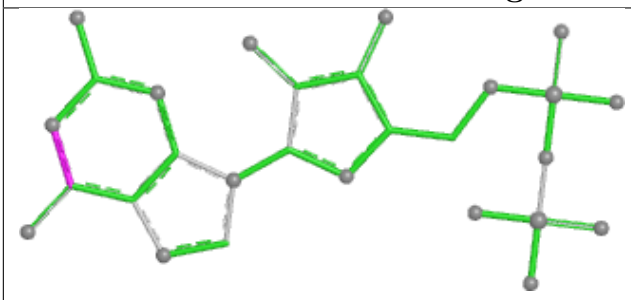
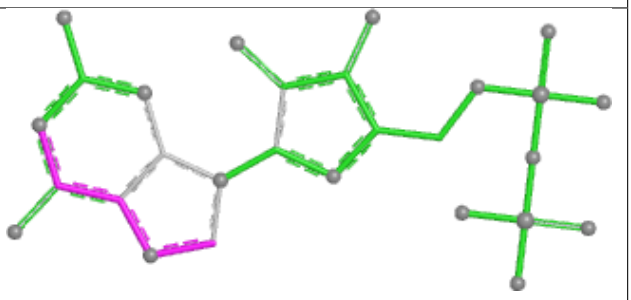
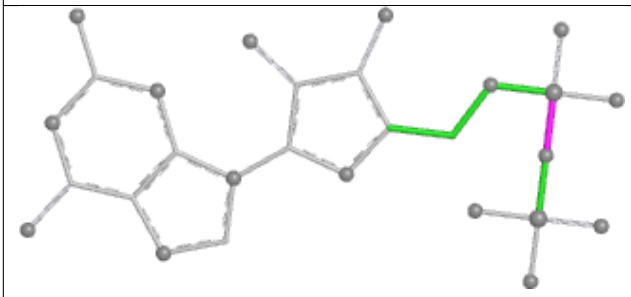
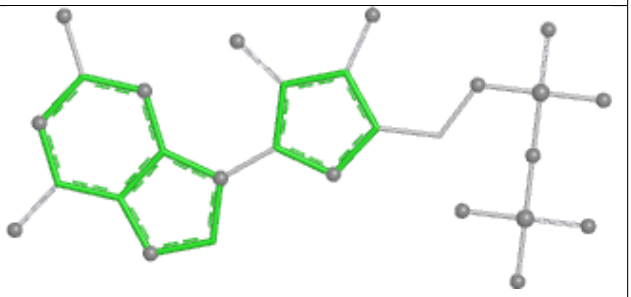
Rings

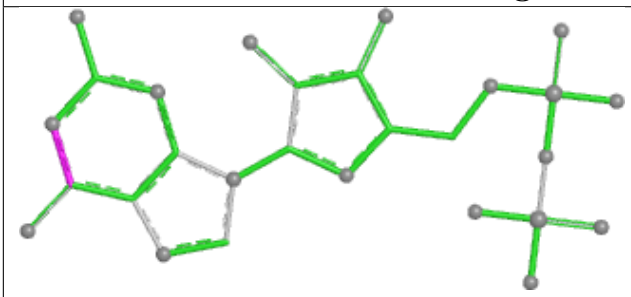
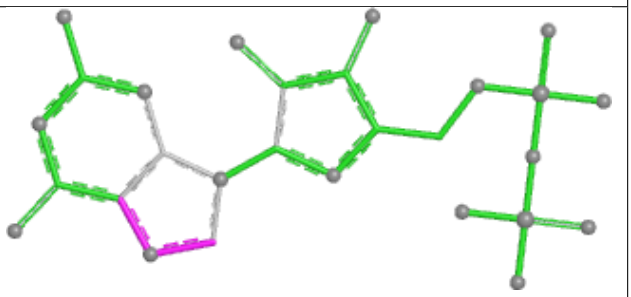
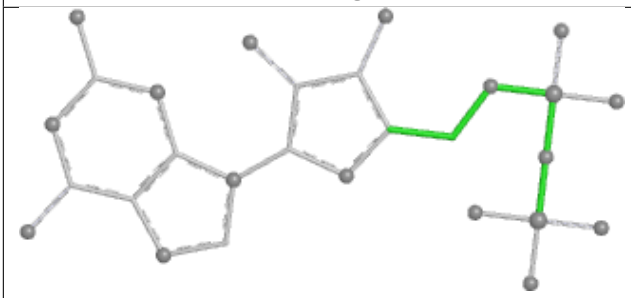
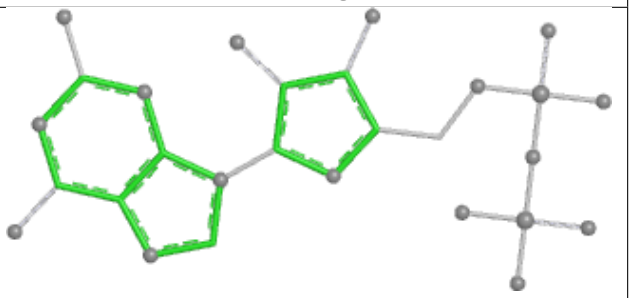
Ligand GTP Bx 602



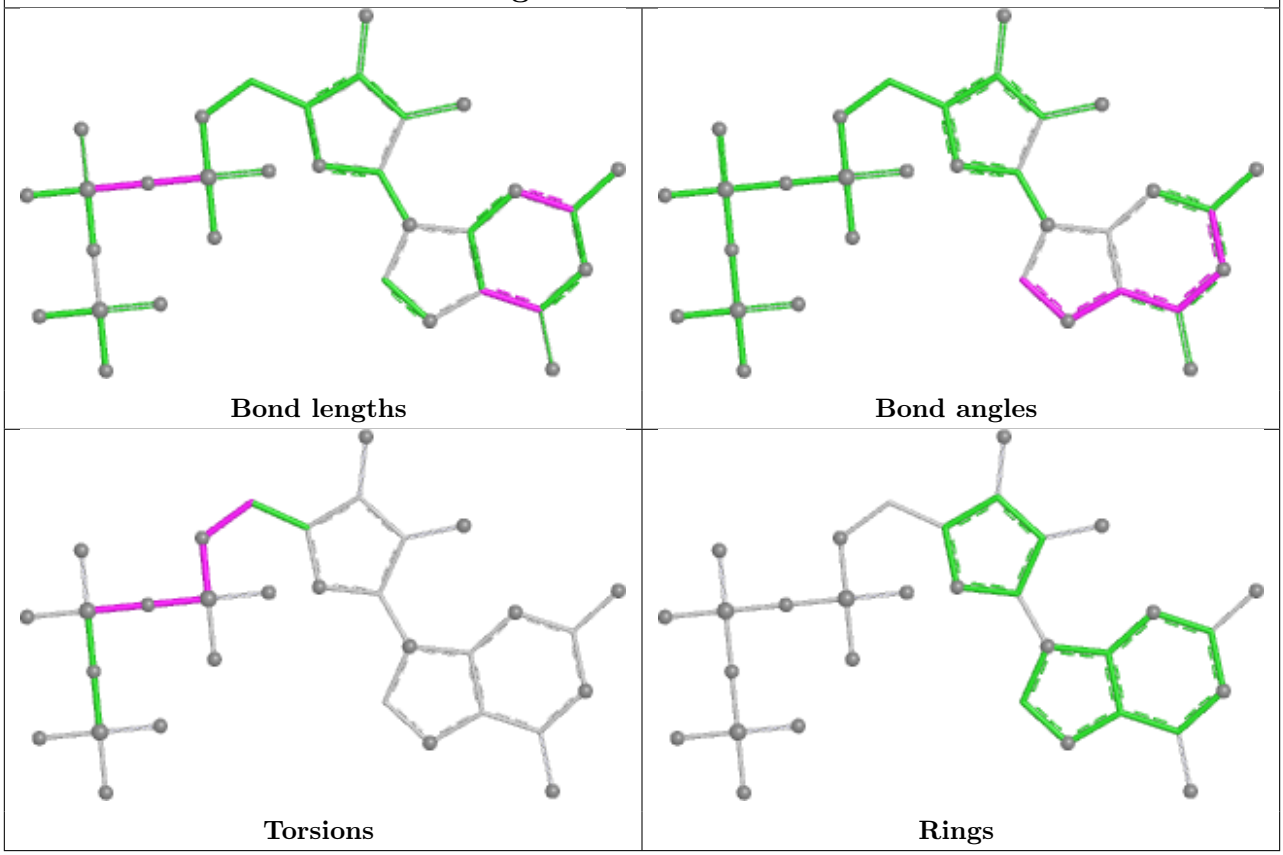
Ligand GDP Bq 602



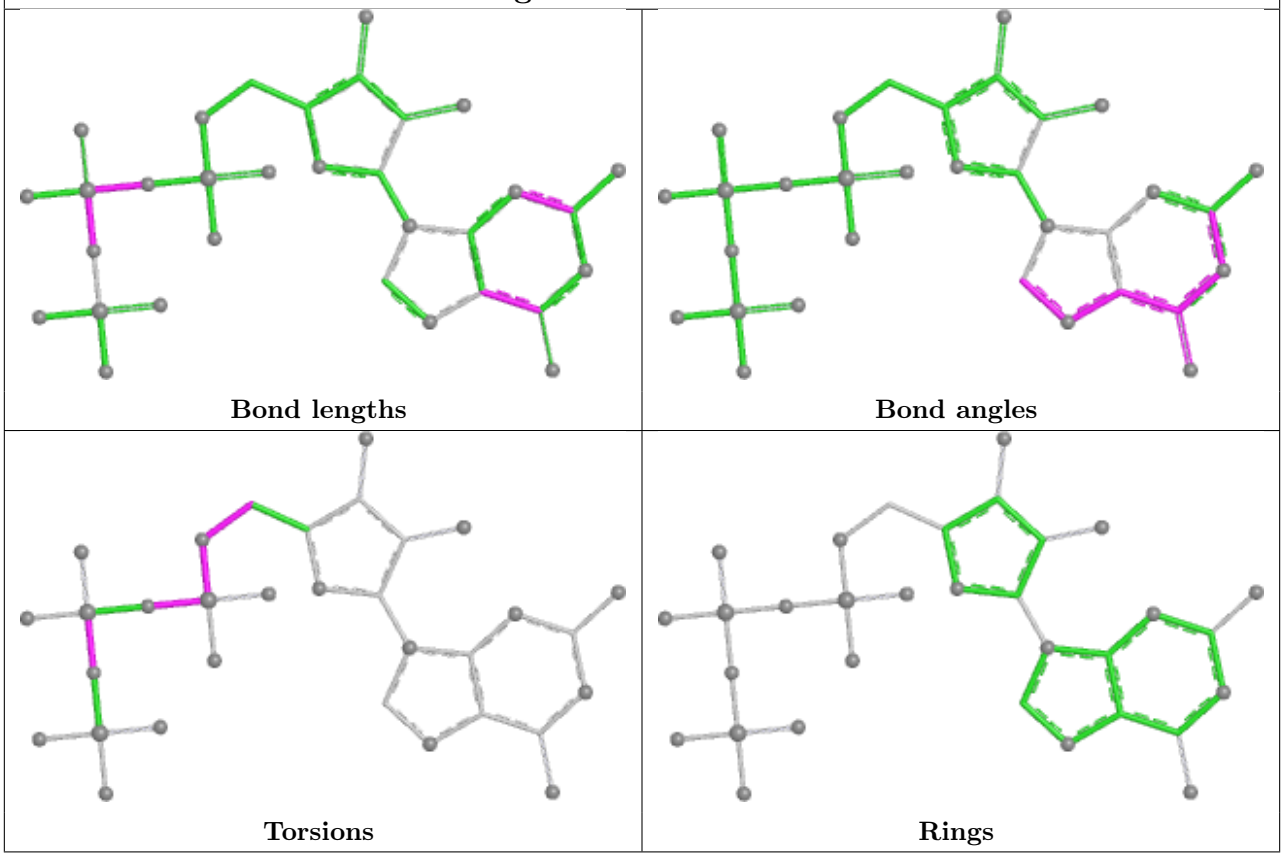
Ligand GDP Am 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP Ds 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

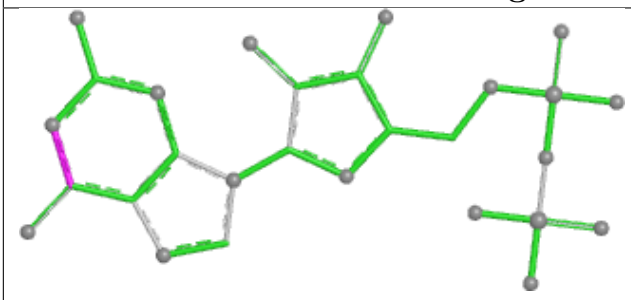
Ligand GTP FU 501



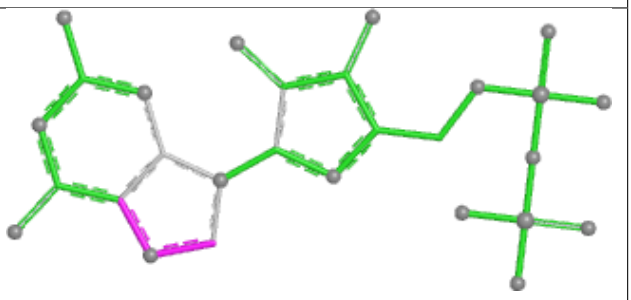
Ligand GTP FZ 501



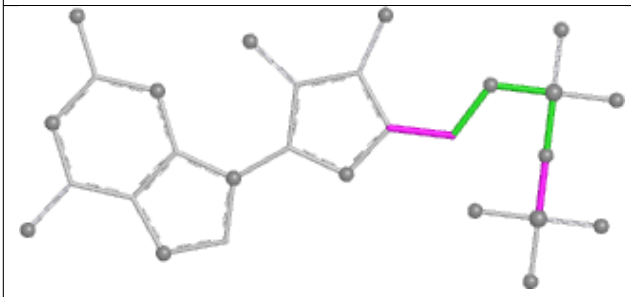
Ligand GDP BC 501



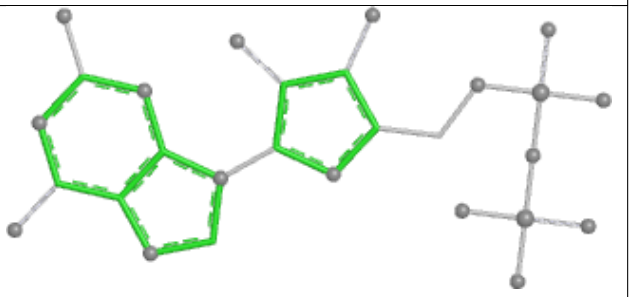
Bond lengths



Bond angles

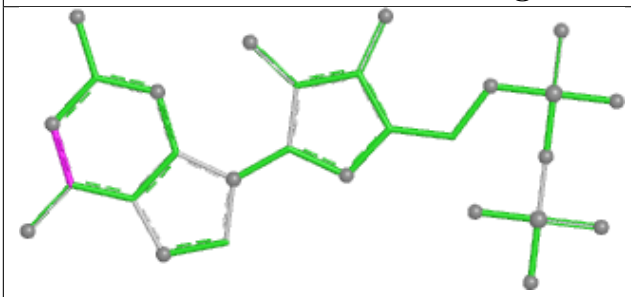


Torsions

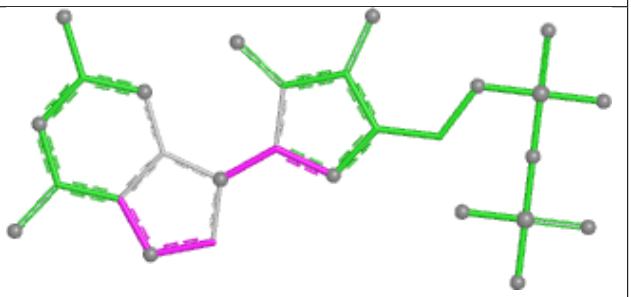


Rings

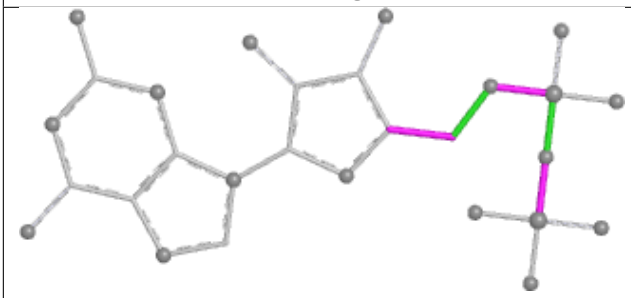
Ligand GDP Fx 501



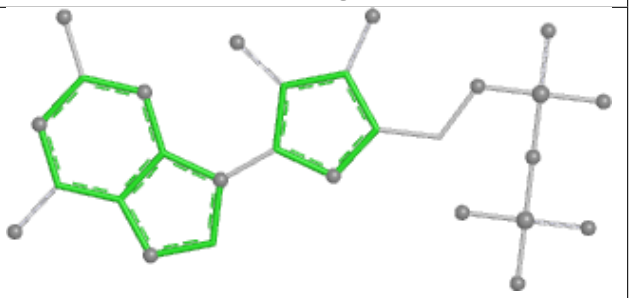
Bond lengths



Bond angles

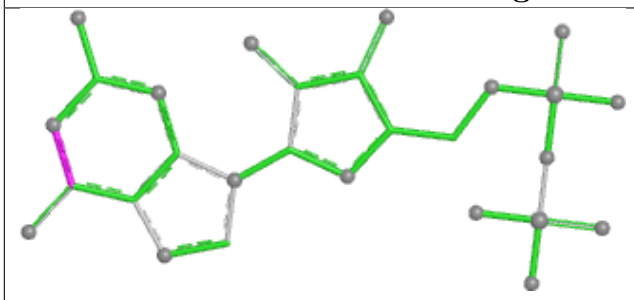


Torsions

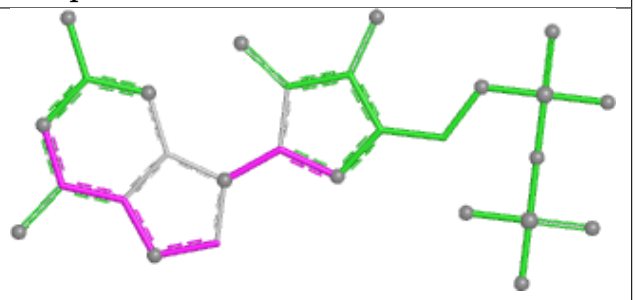


Rings

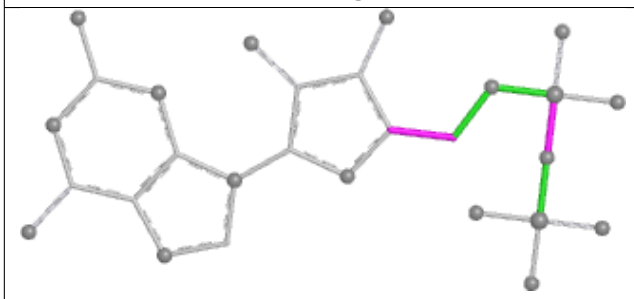
Ligand GDP Bp 501



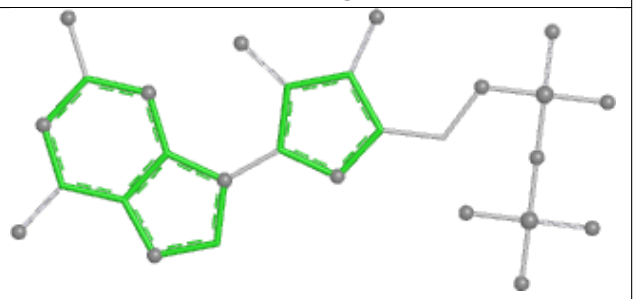
Bond lengths



Bond angles

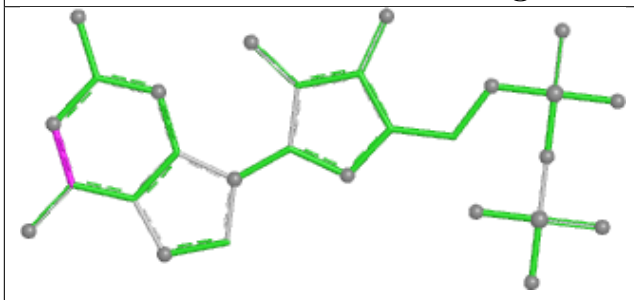


Torsions

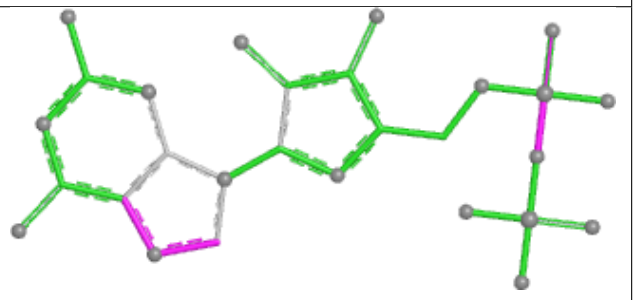


Rings

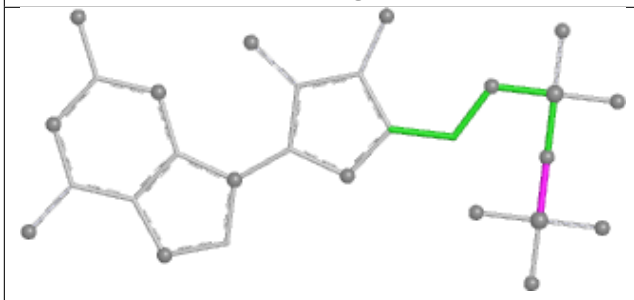
Ligand GDP FC 501



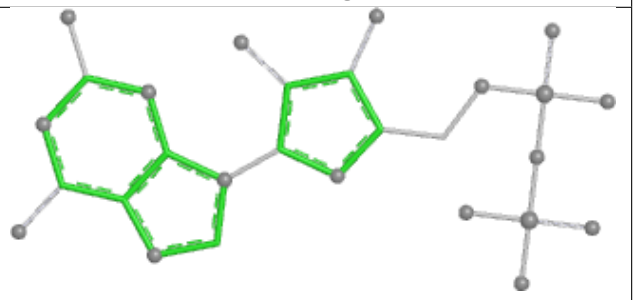
Bond lengths



Bond angles

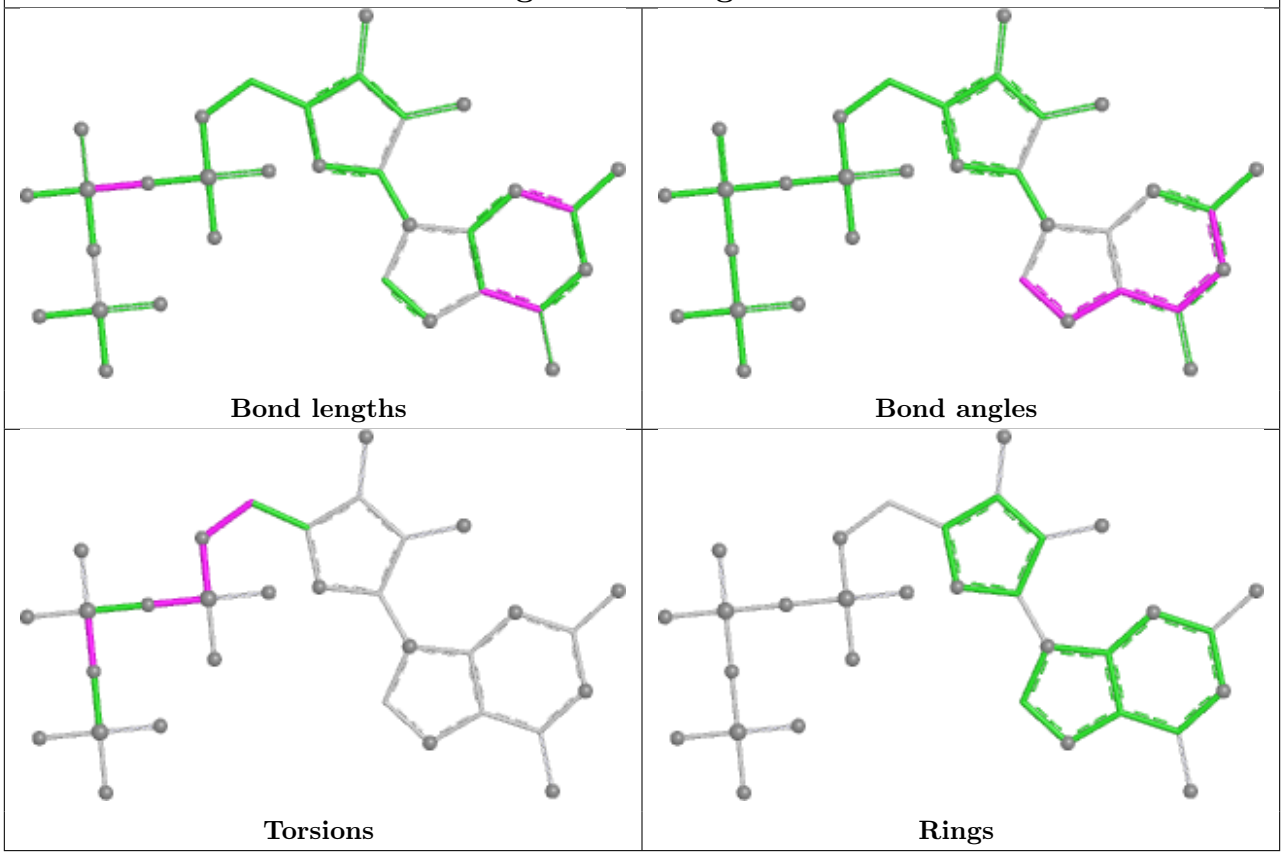


Torsions

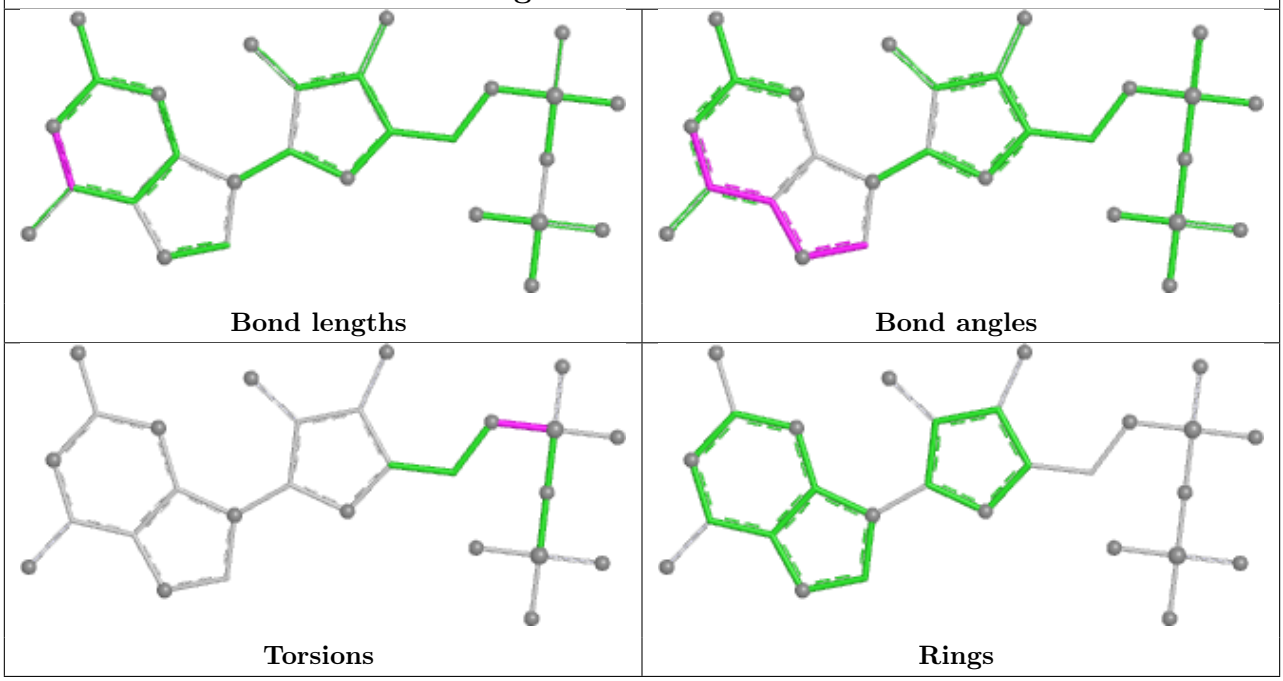


Rings

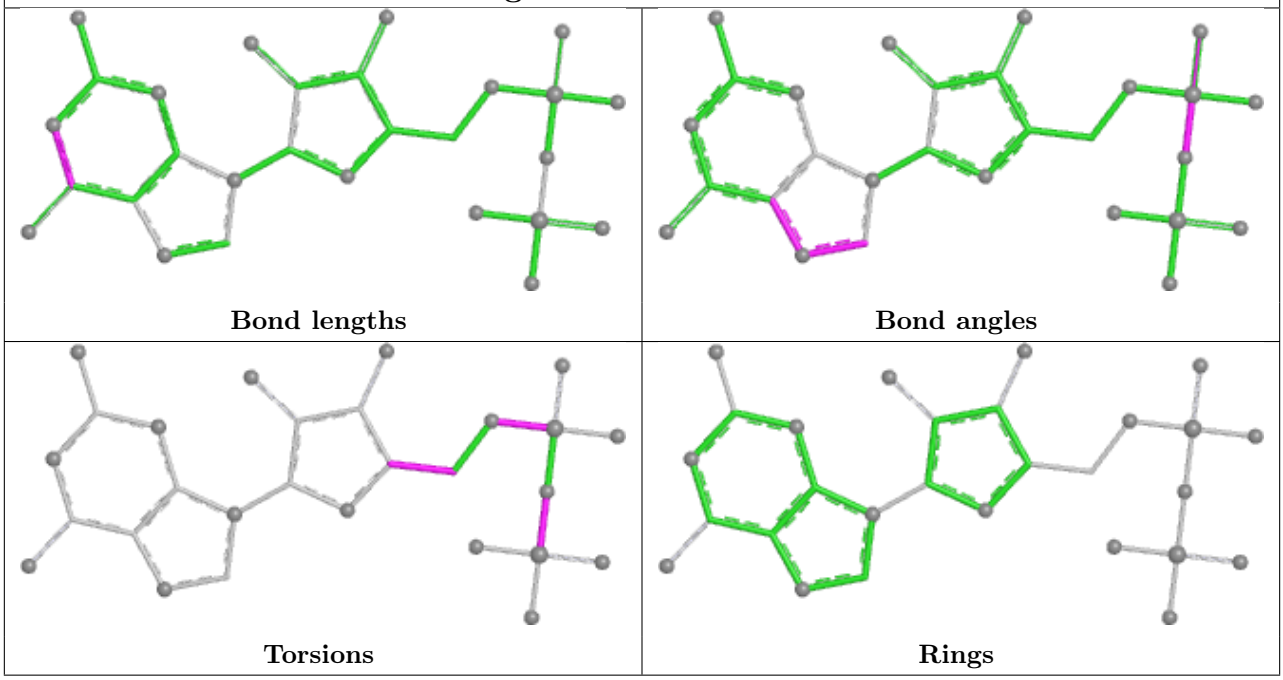
Ligand GTP Eg 501



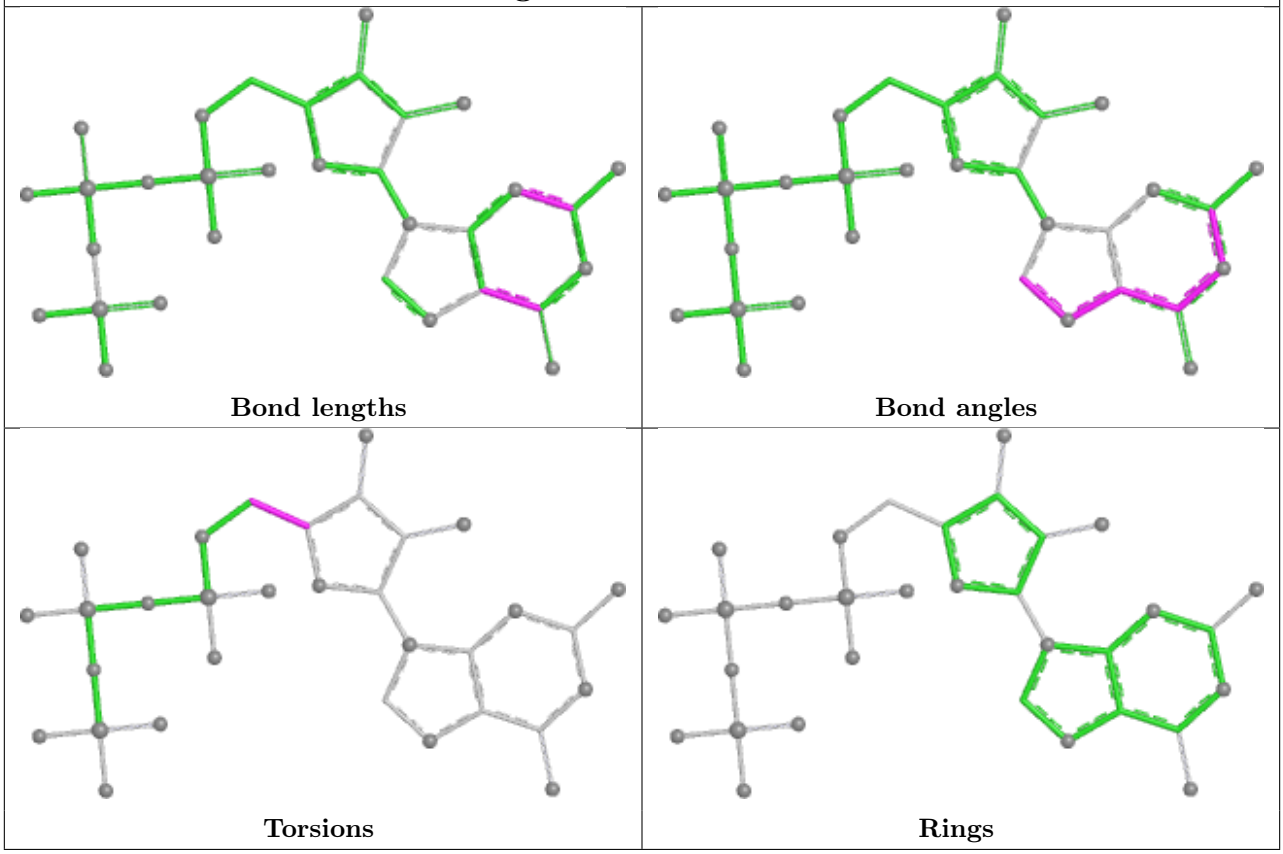
Ligand GDP Ba 501



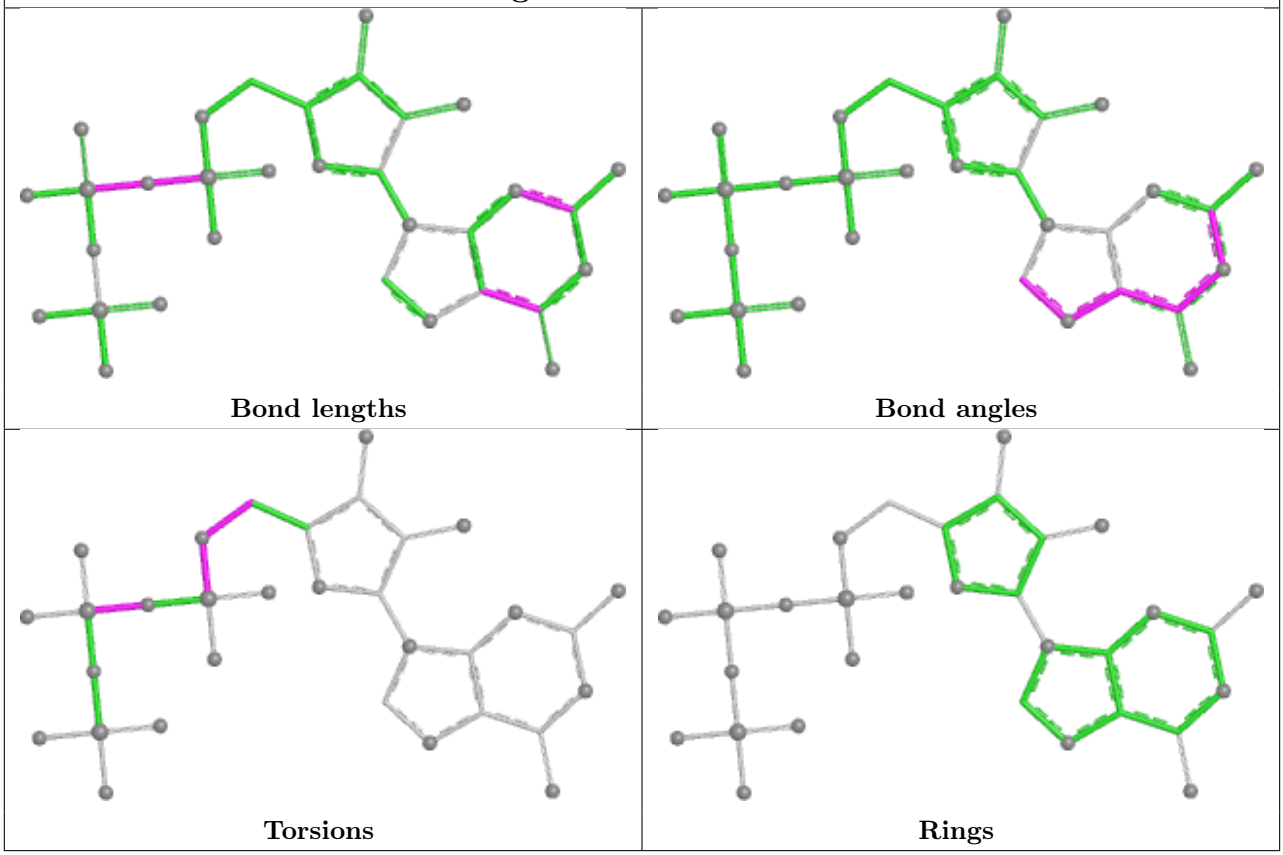
Ligand GDP DM 501



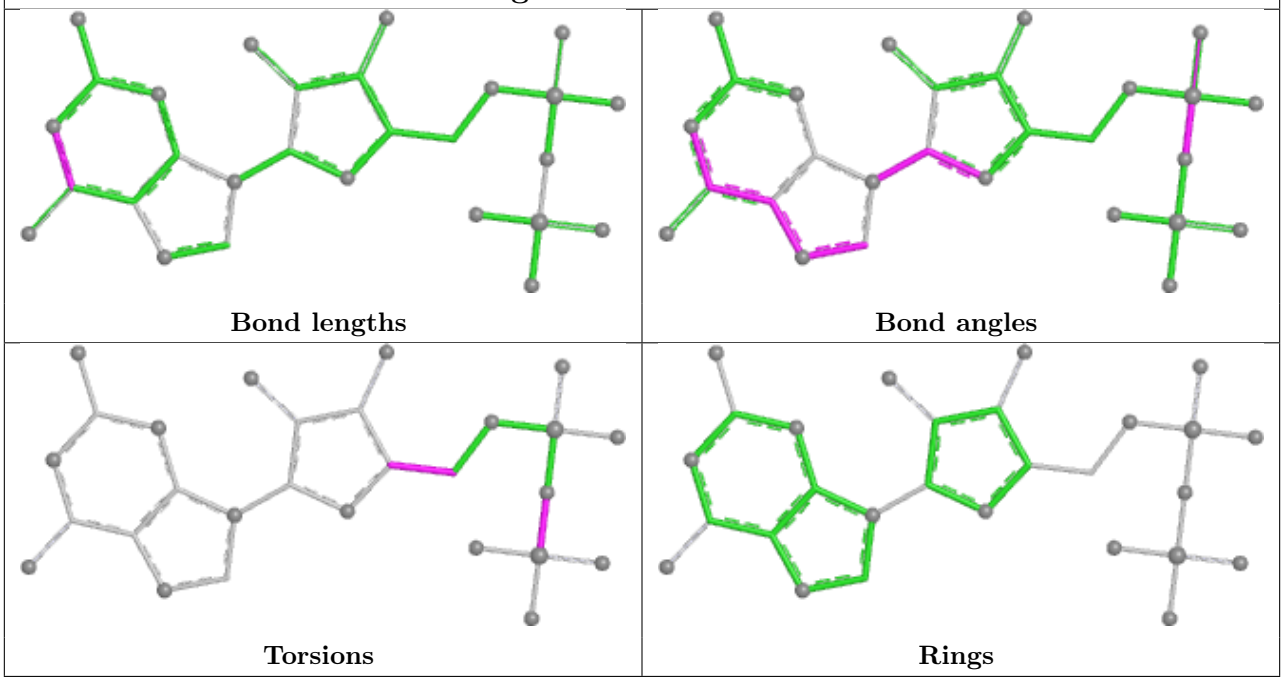
Ligand GTP Bv 602



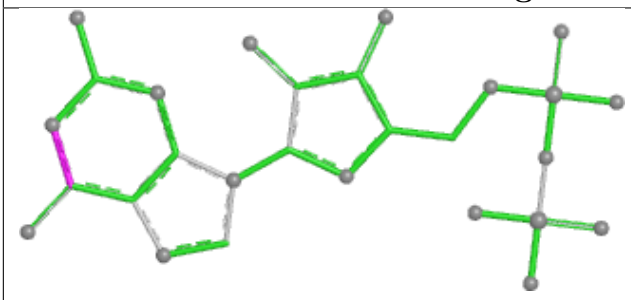
Ligand GTP BP 602



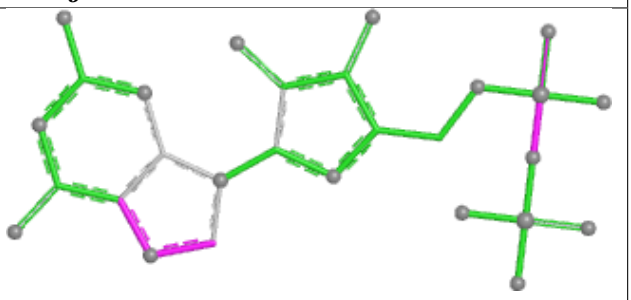
Ligand GDP EP 501



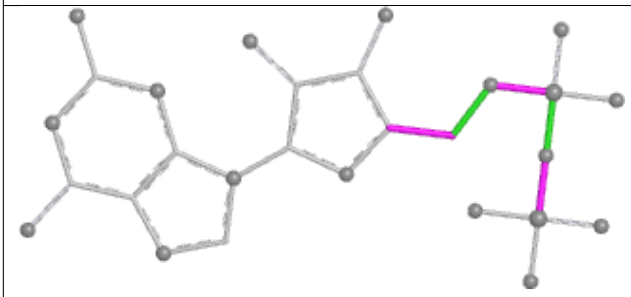
Ligand GDP Dj 501



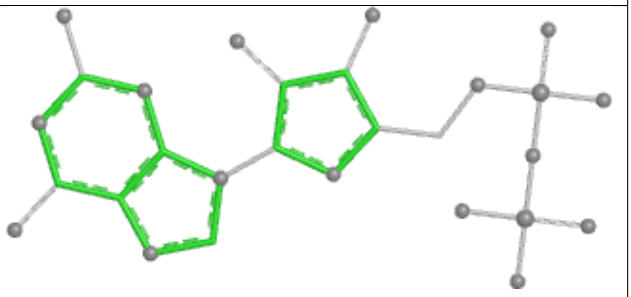
Bond lengths



Bond angles

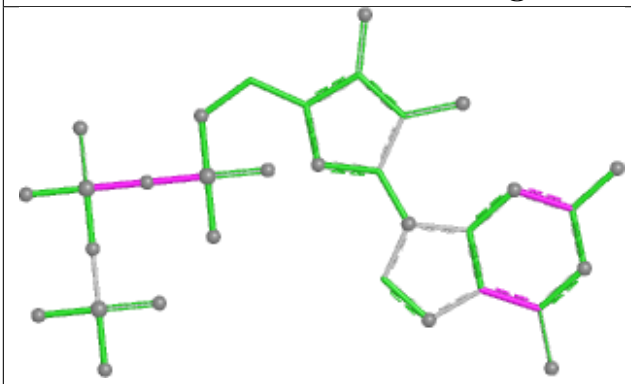


Torsions

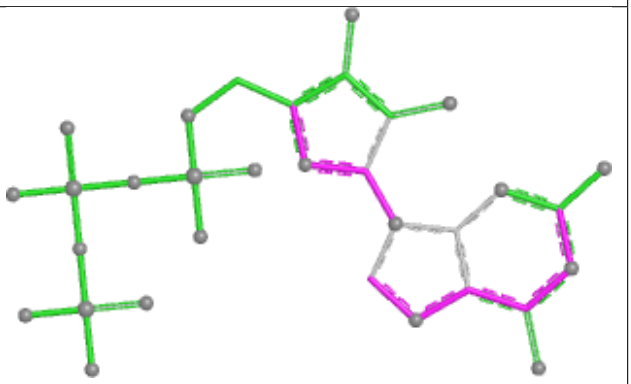


Rings

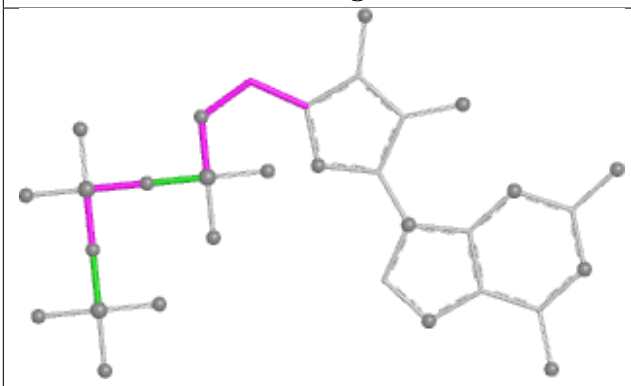
Ligand GTP GR 501



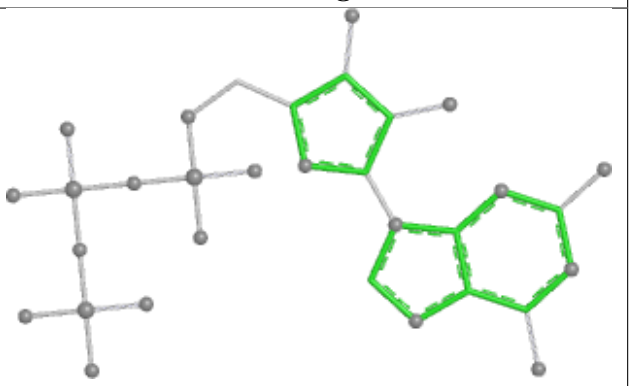
Bond lengths



Bond angles

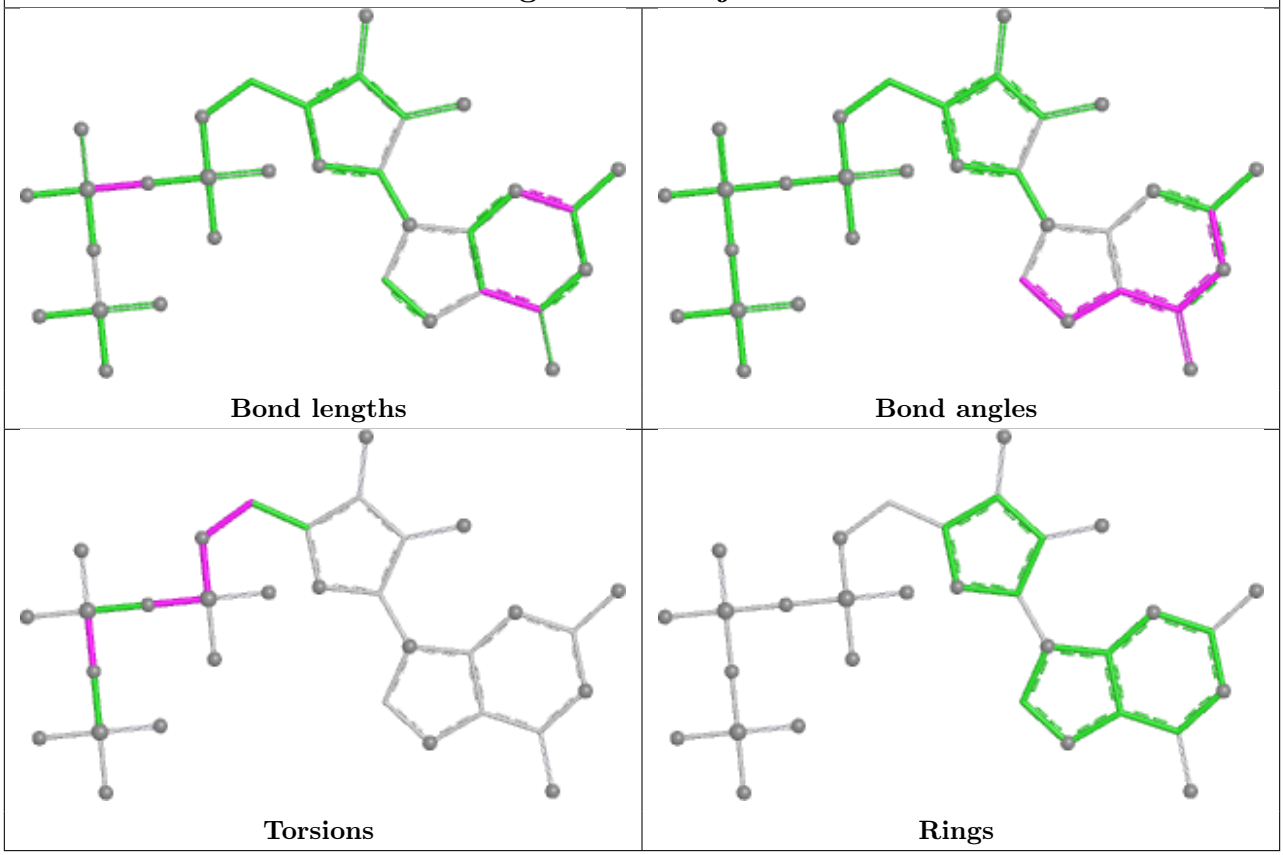


Torsions

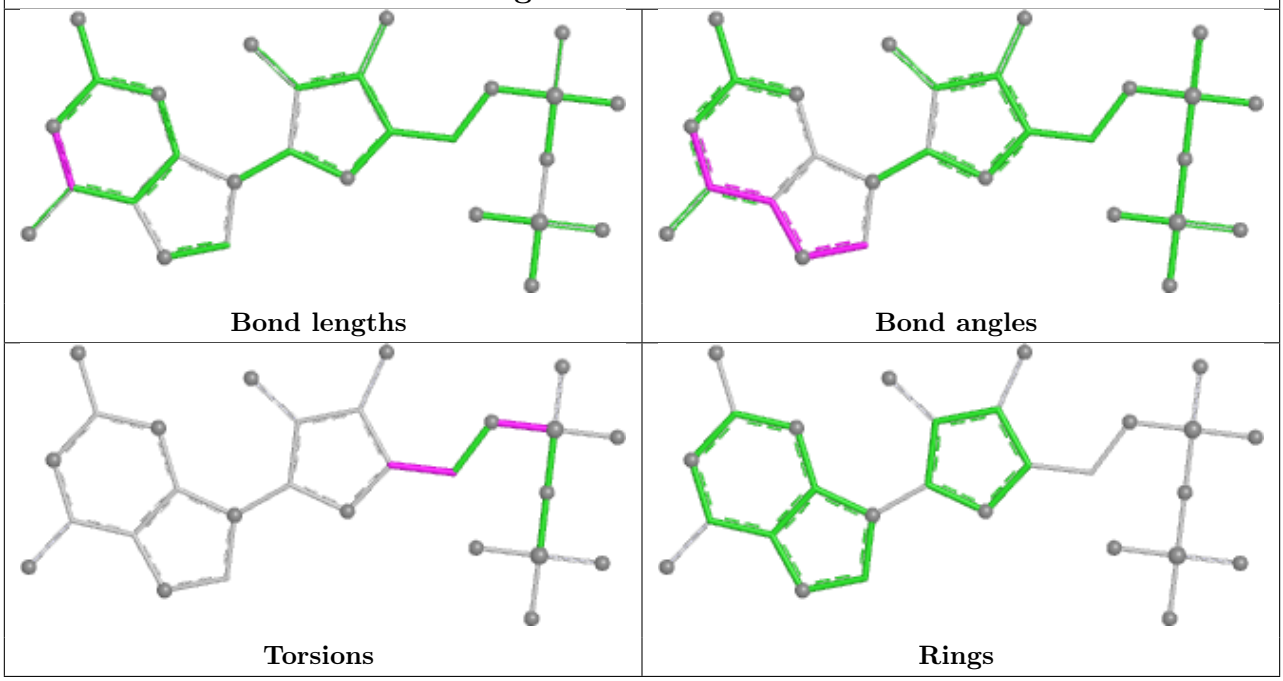


Rings

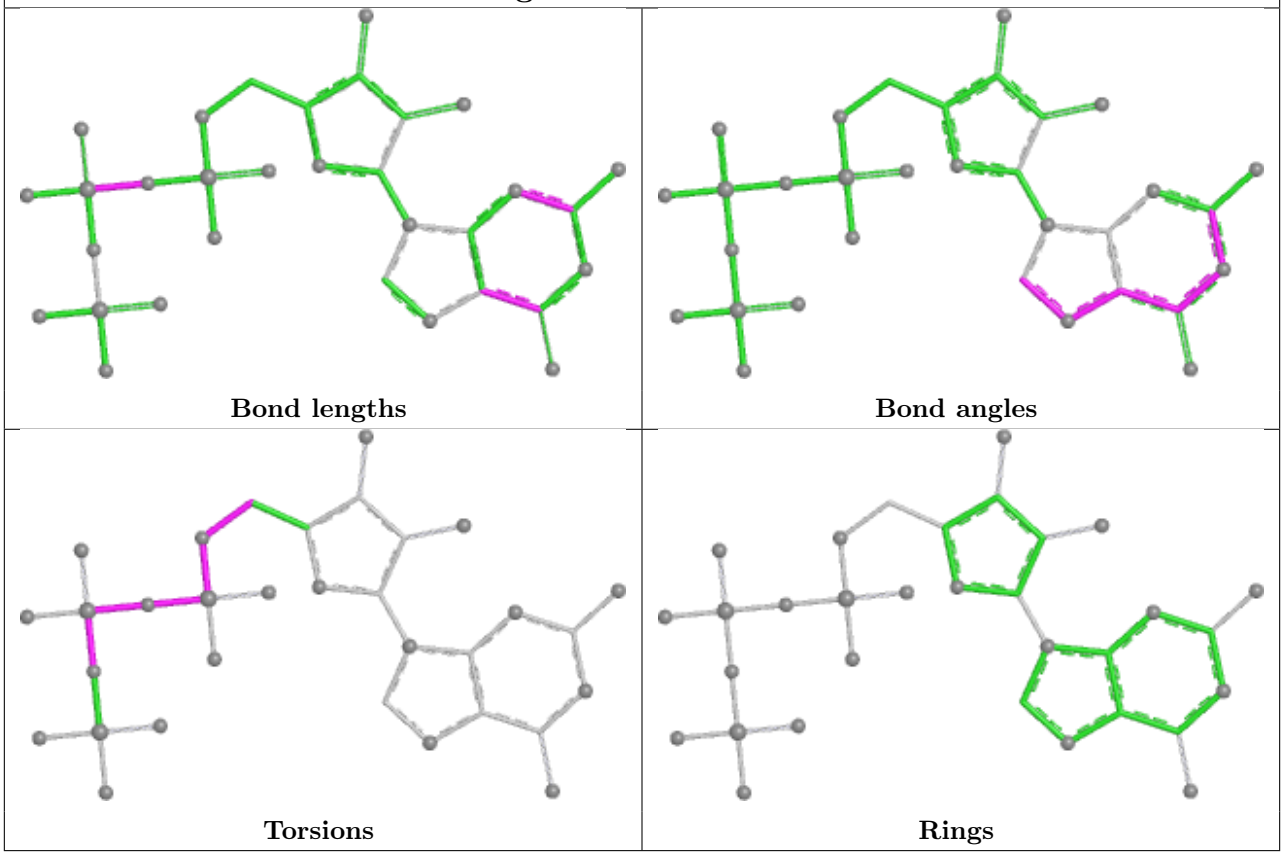
Ligand GTP Ej 501



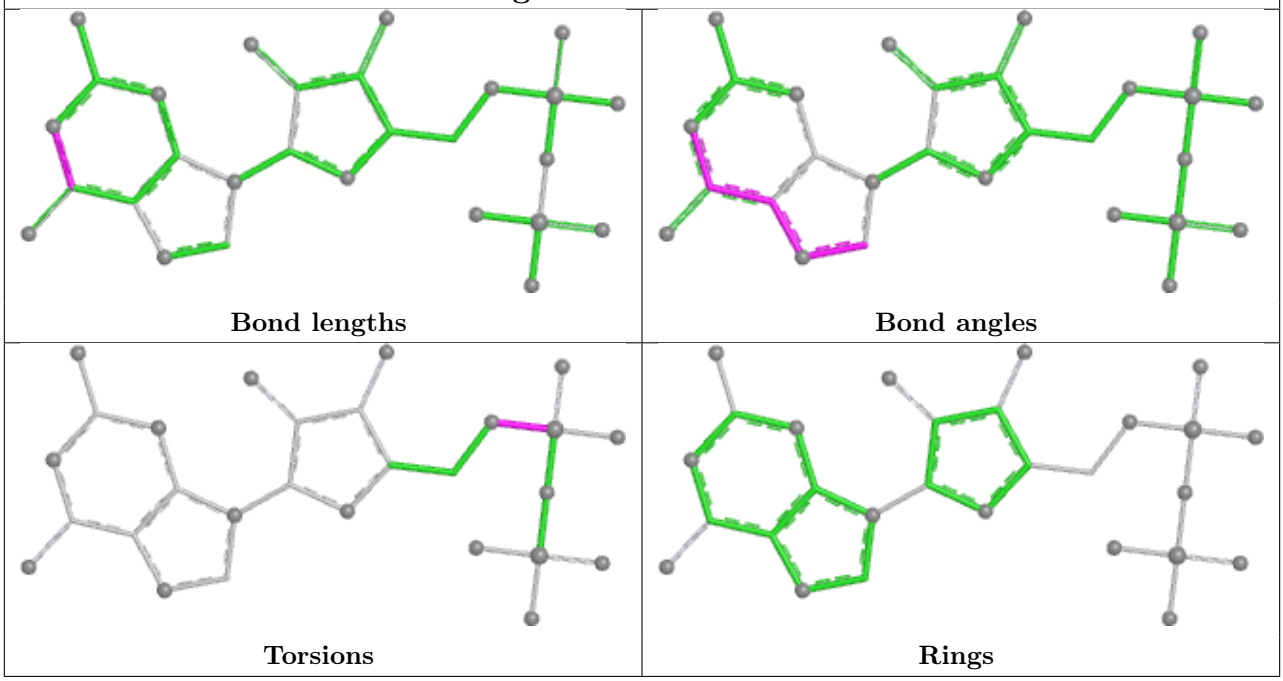
Ligand GDP Dr 501



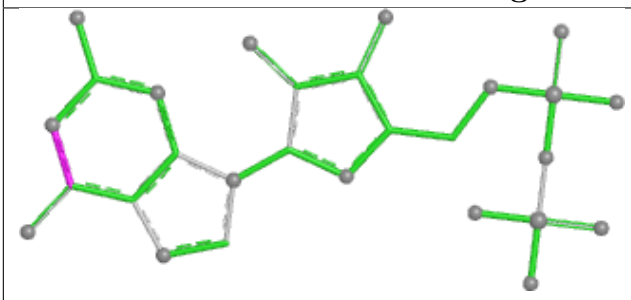
Ligand GTP Gt 501



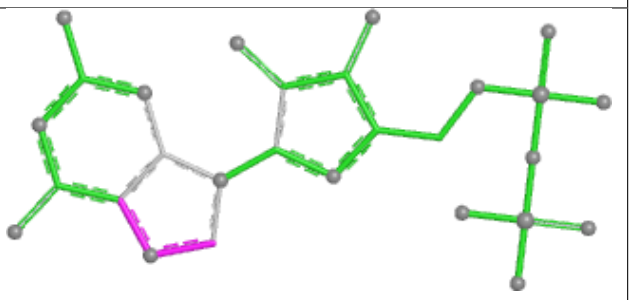
Ligand GDP Bb 501



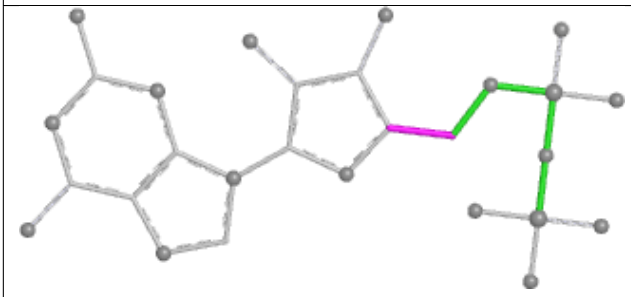
Ligand GDP FB 501



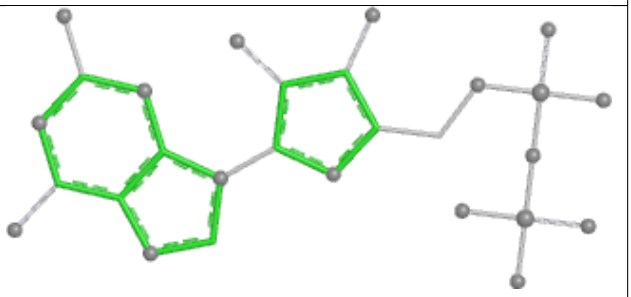
Bond lengths



Bond angles

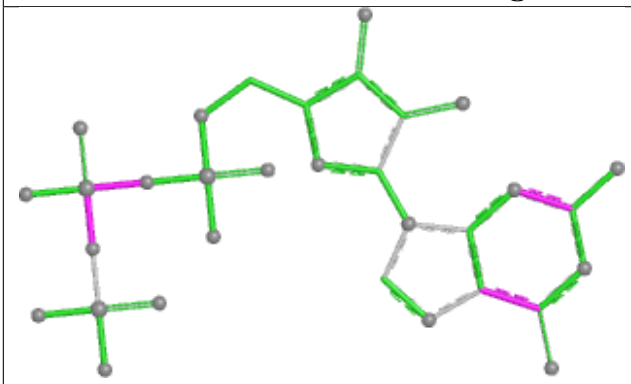


Torsions

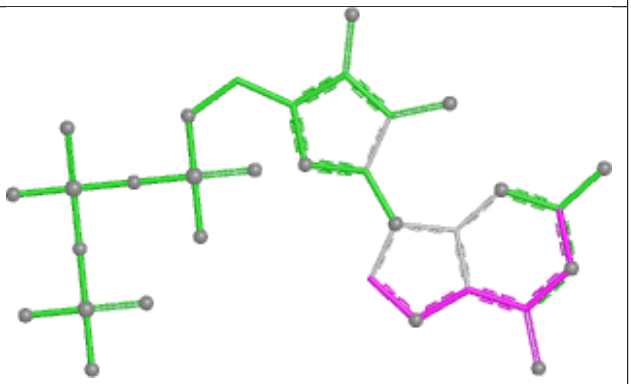


Rings

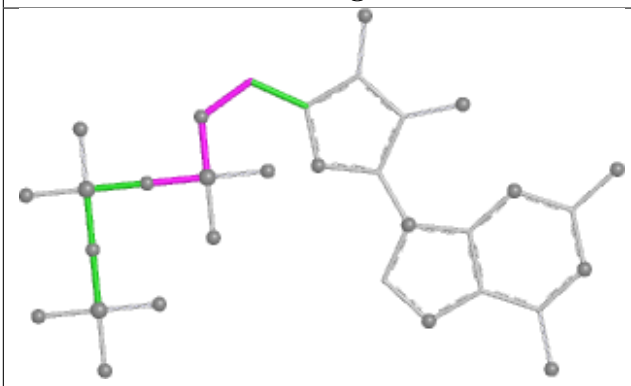
Ligand GTP GB 501



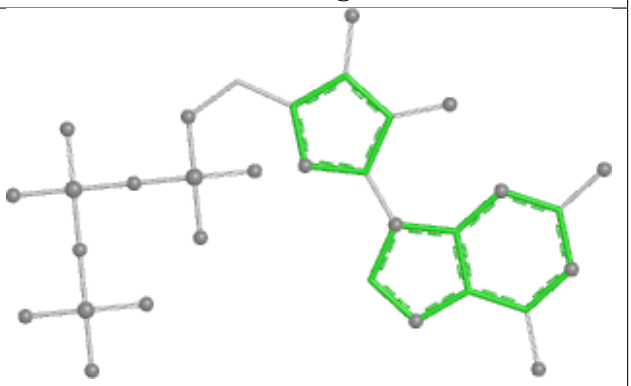
Bond lengths



Bond angles

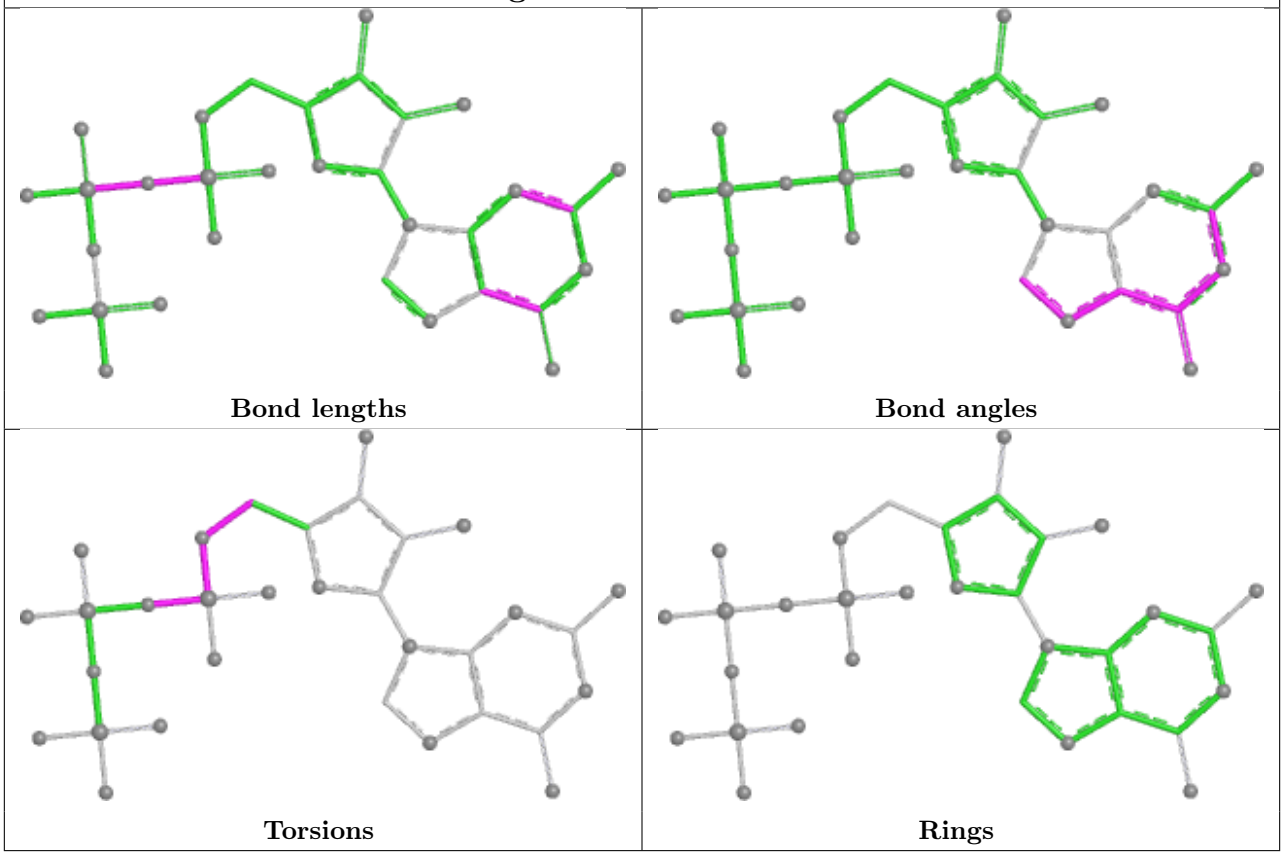


Torsions

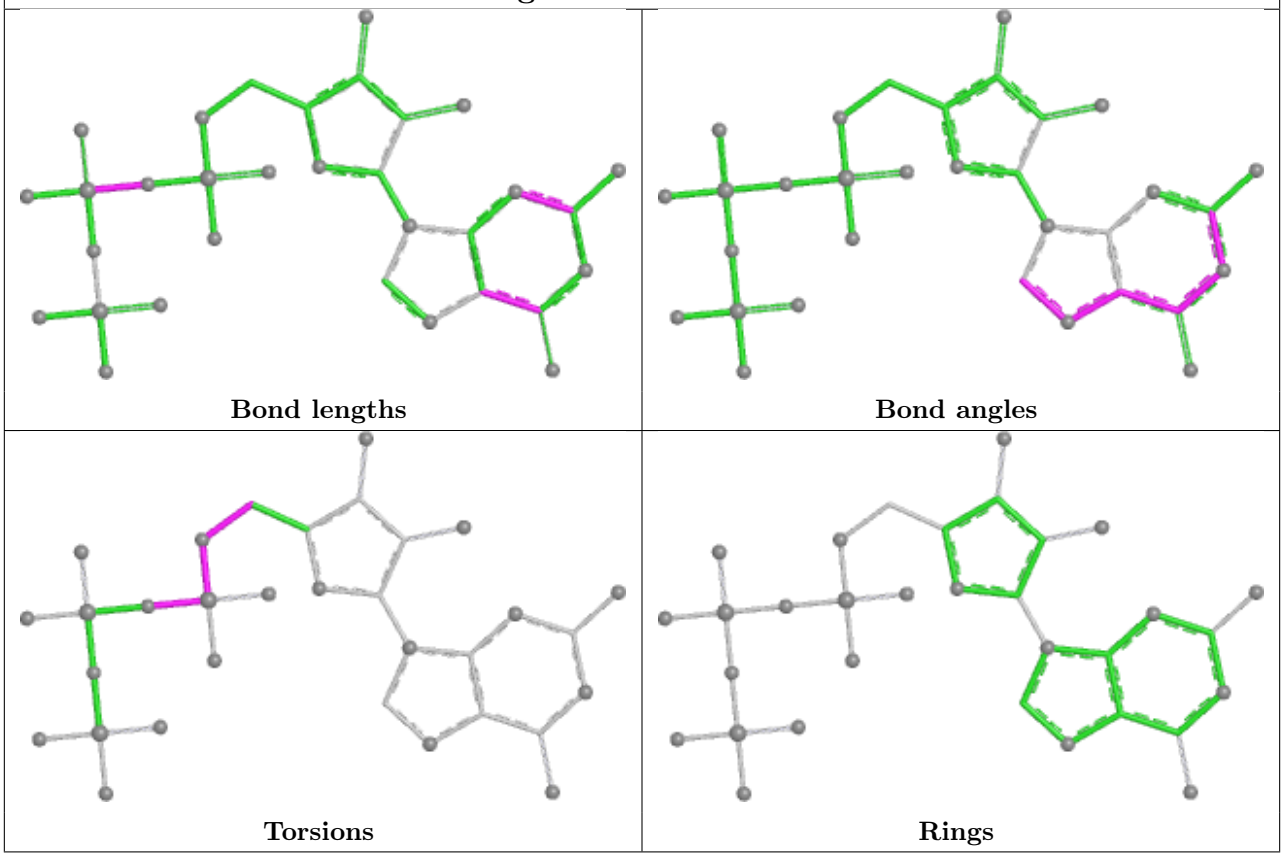


Rings

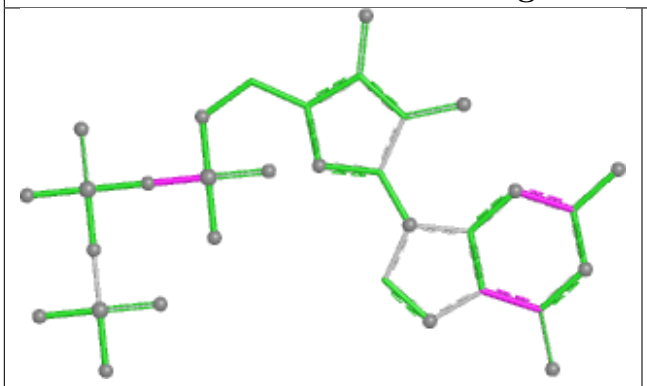
Ligand GTP GK 501



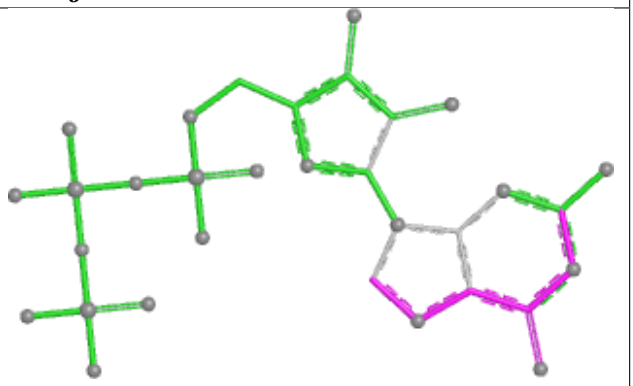
Ligand GTP Er 501



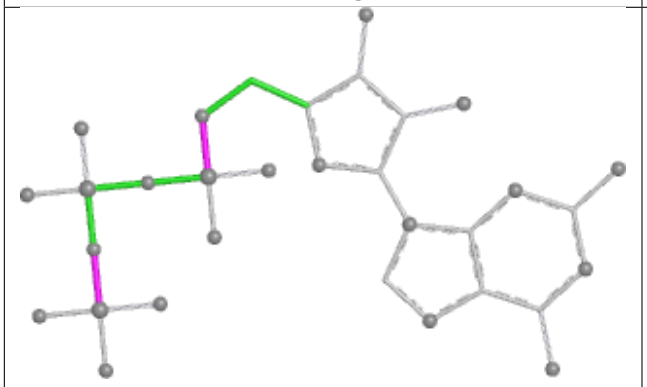
Ligand GTP Aj 501



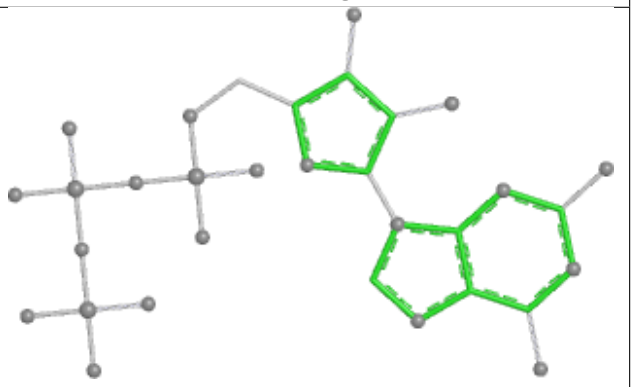
Bond lengths



Bond angles

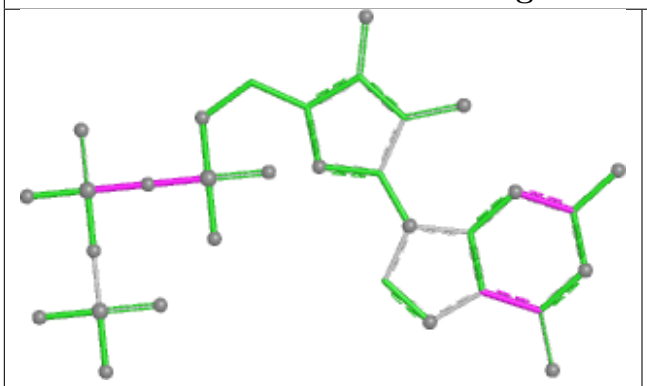


Torsions

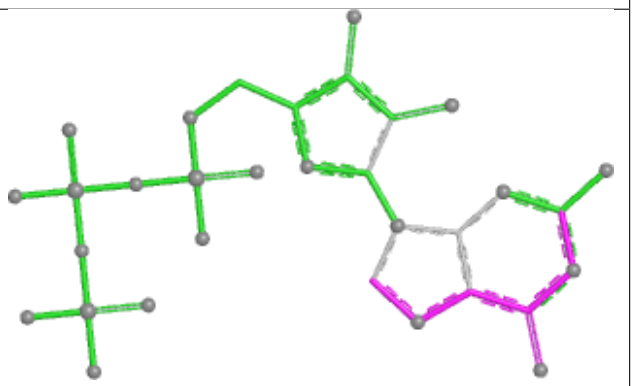


Rings

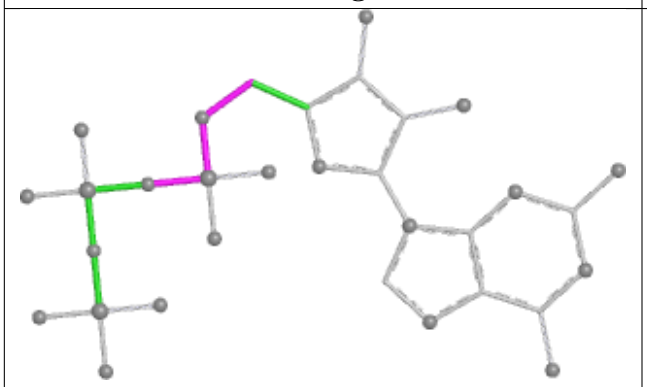
Ligand GTP GI 501



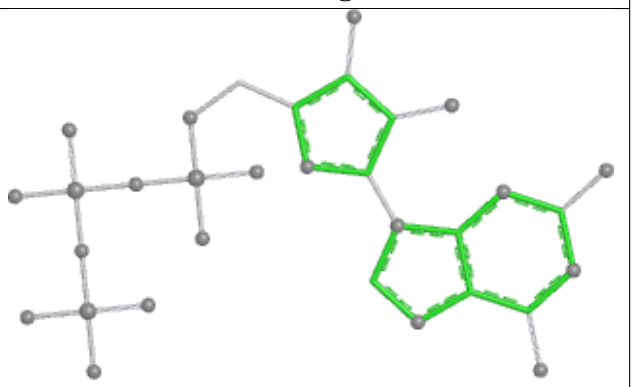
Bond lengths



Bond angles

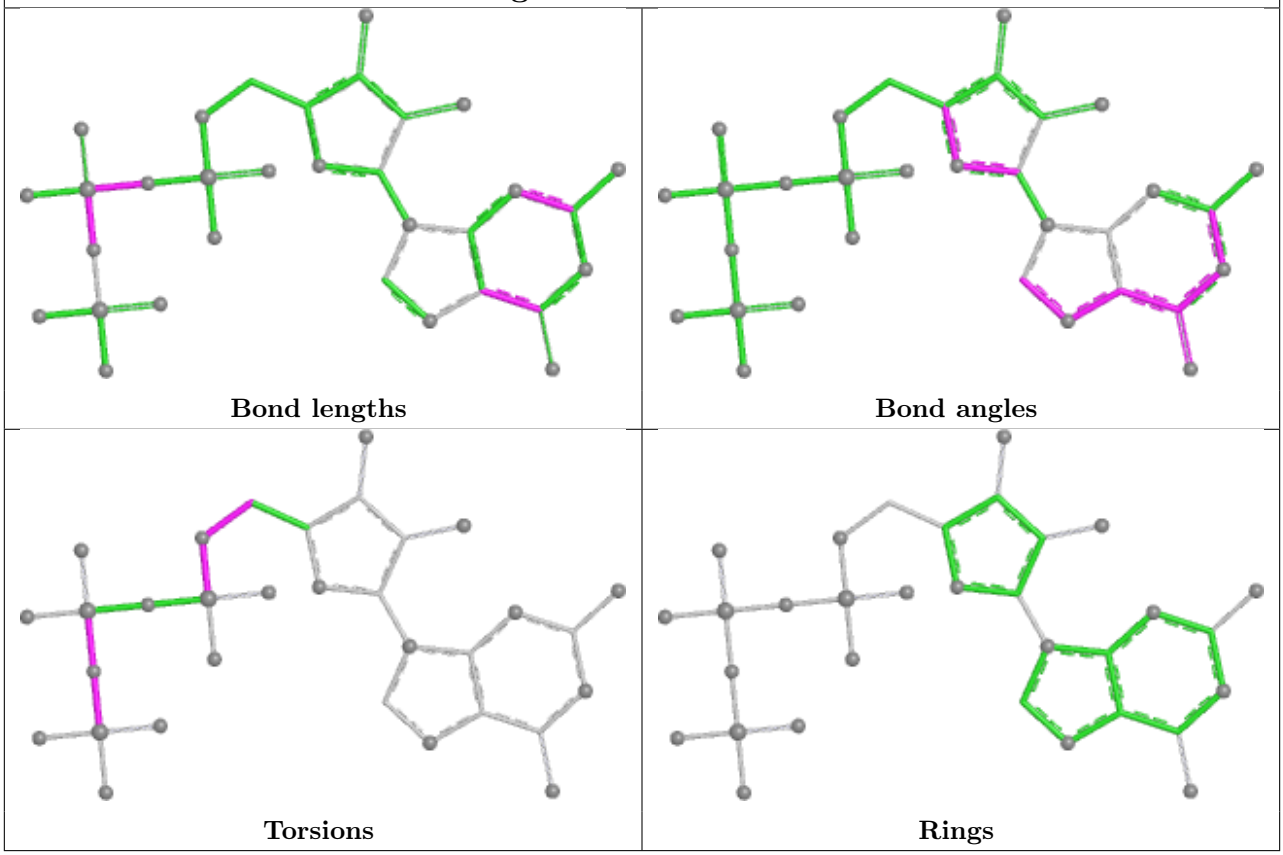


Torsions

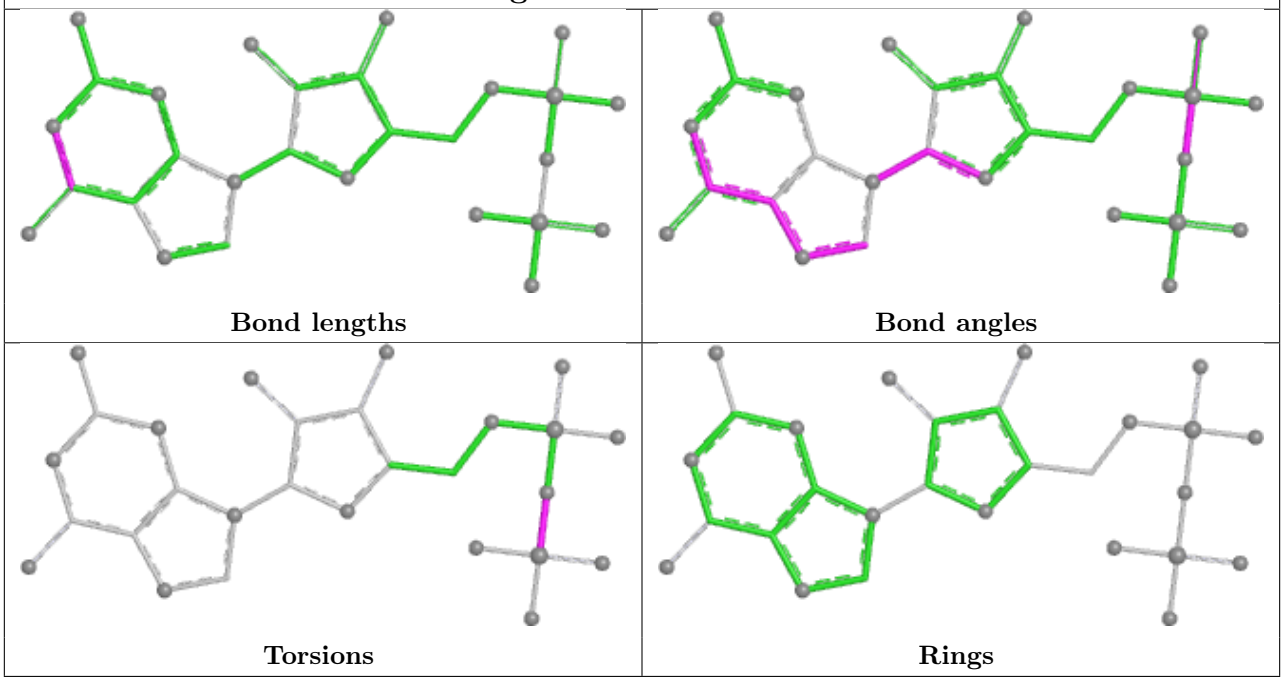


Rings

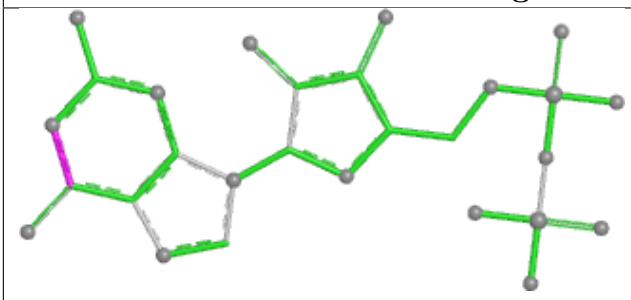
Ligand GTP CB 602



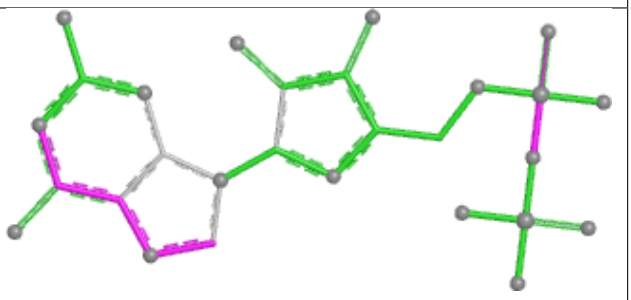
Ligand GDP EV 501



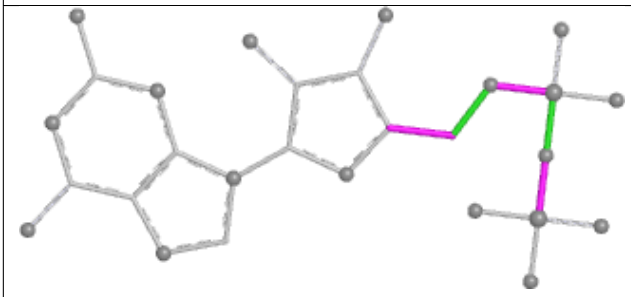
Ligand GDP Da 501



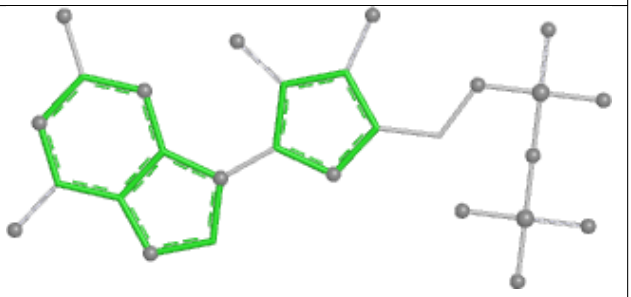
Bond lengths



Bond angles

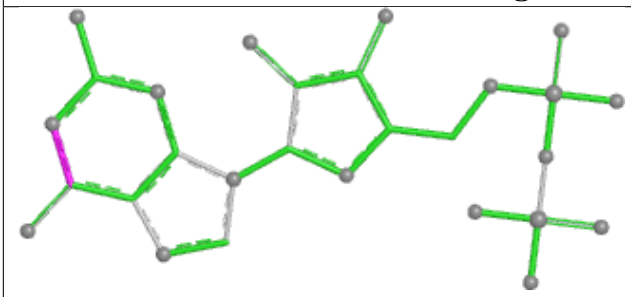


Torsions

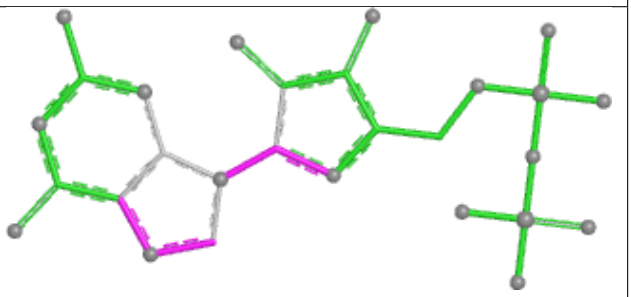


Rings

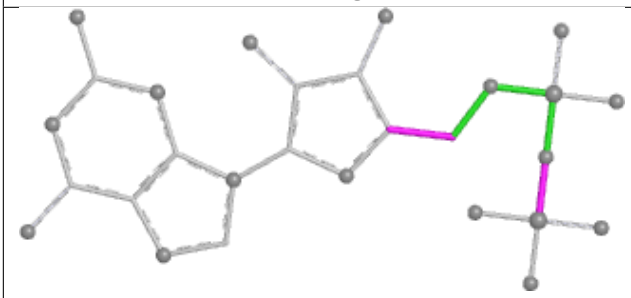
Ligand GDP ES 501



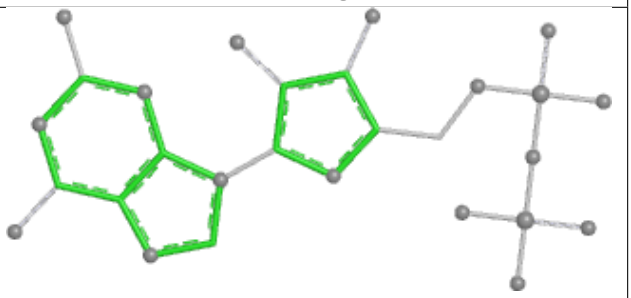
Bond lengths



Bond angles

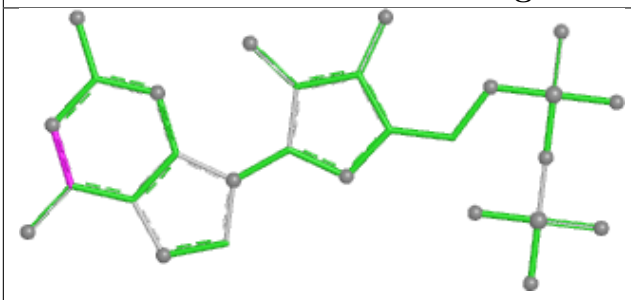


Torsions

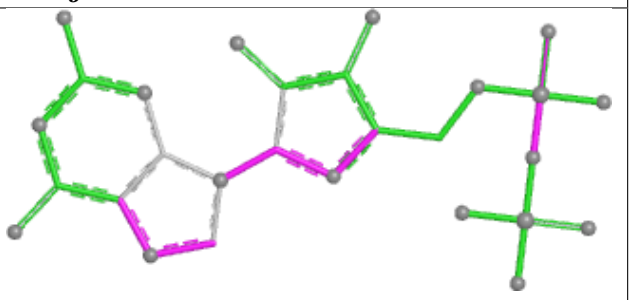


Rings

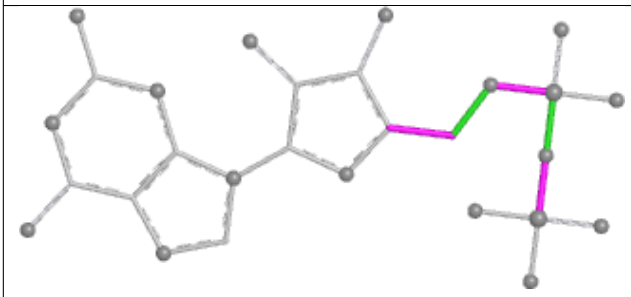
Ligand GDP Gj 501



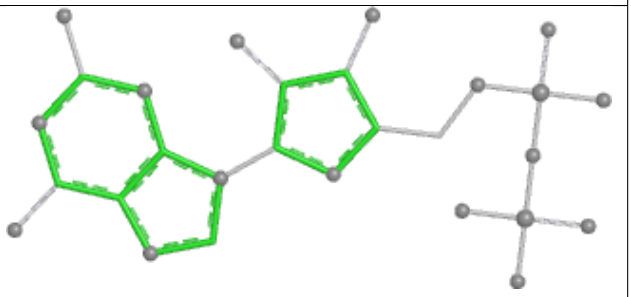
Bond lengths



Bond angles

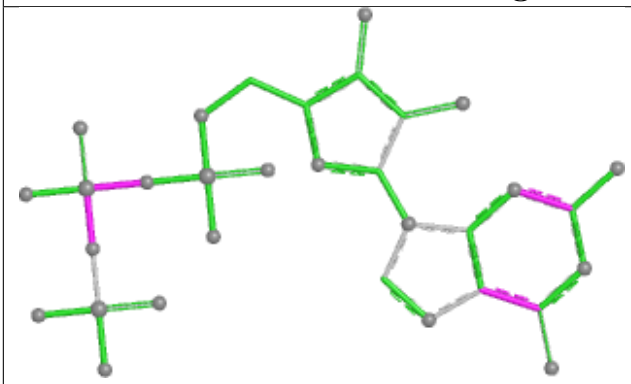


Torsions

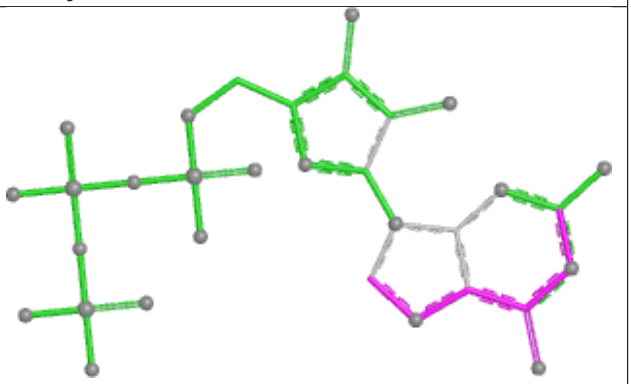


Rings

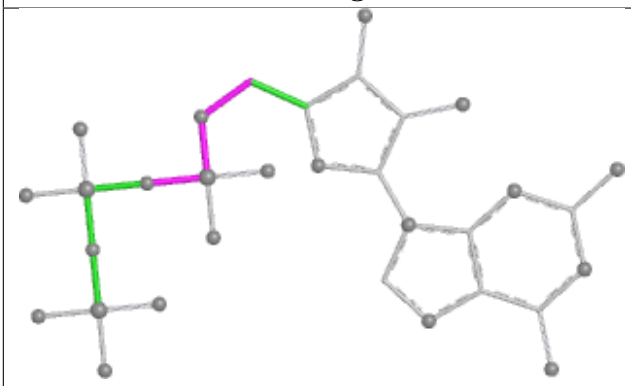
Ligand GTP Gy 501



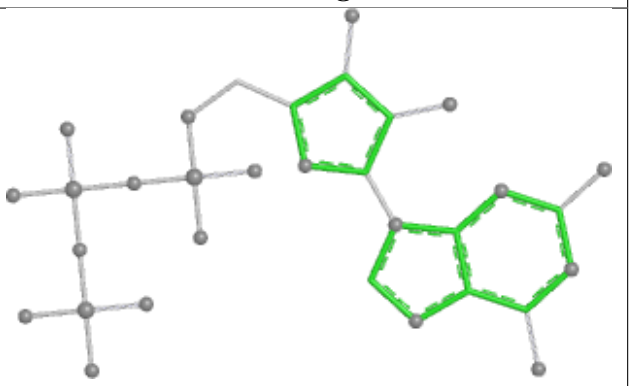
Bond lengths



Bond angles

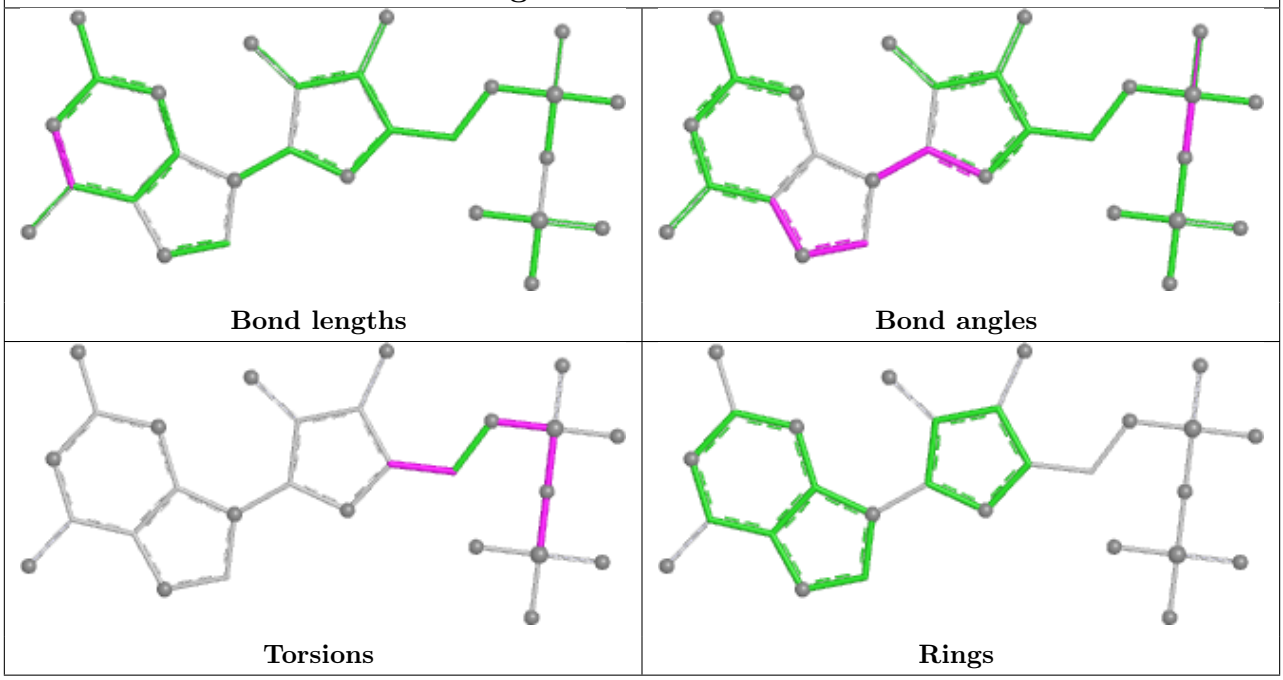


Torsions

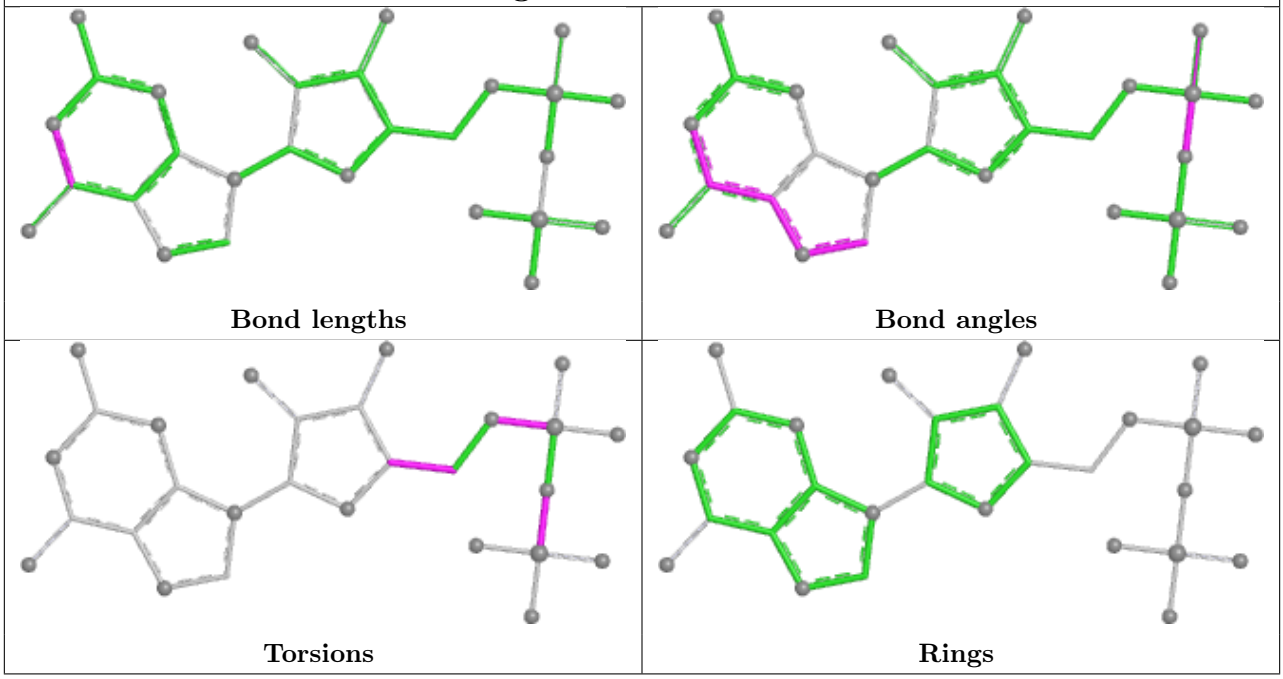


Rings

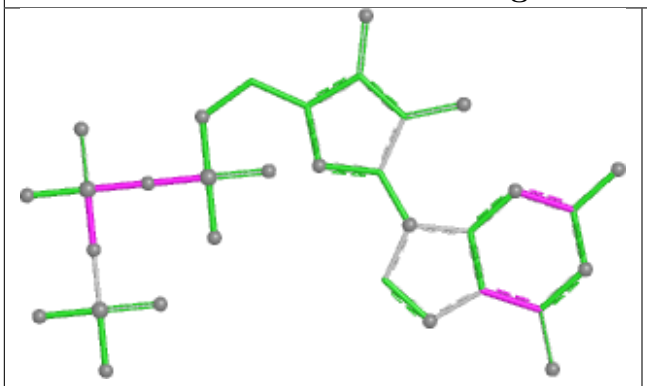
Ligand GDP FK 501



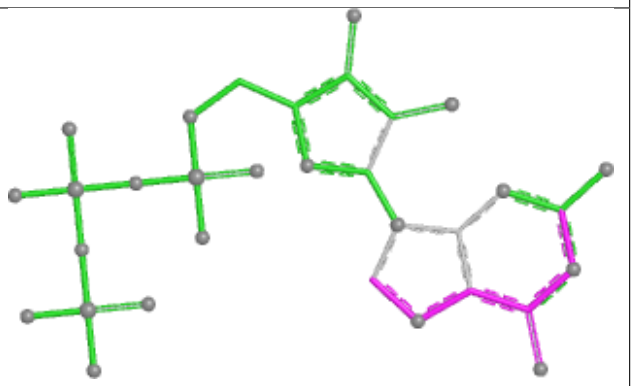
Ligand GDP Fw 501



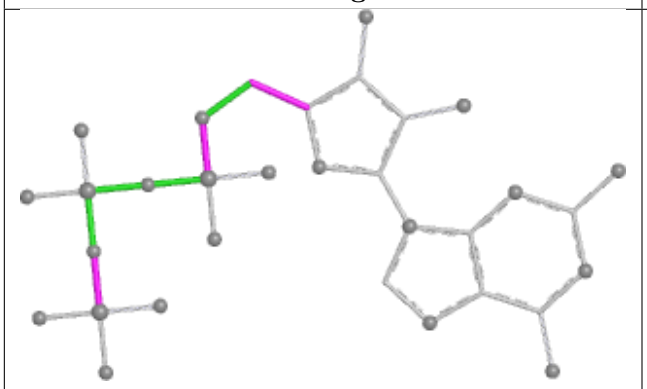
Ligand GTP BR 501



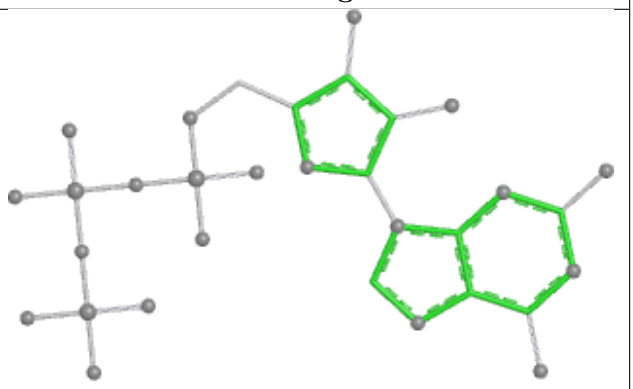
Bond lengths



Bond angles

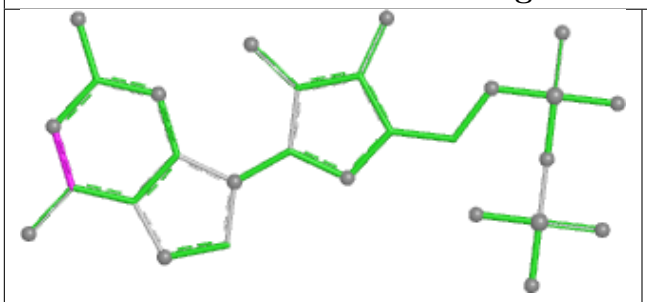


Torsions

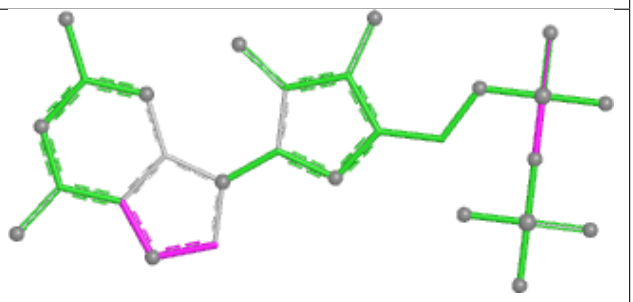


Rings

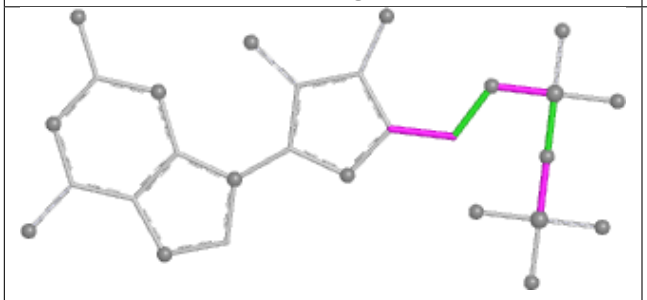
Ligand GDP Ea 501



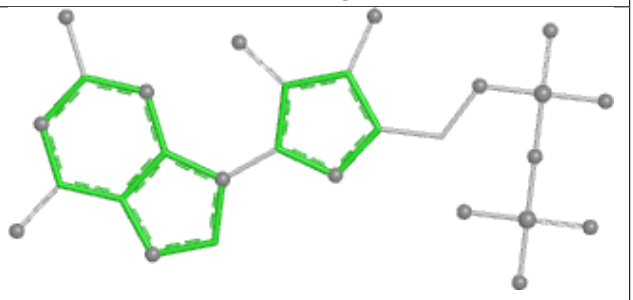
Bond lengths



Bond angles

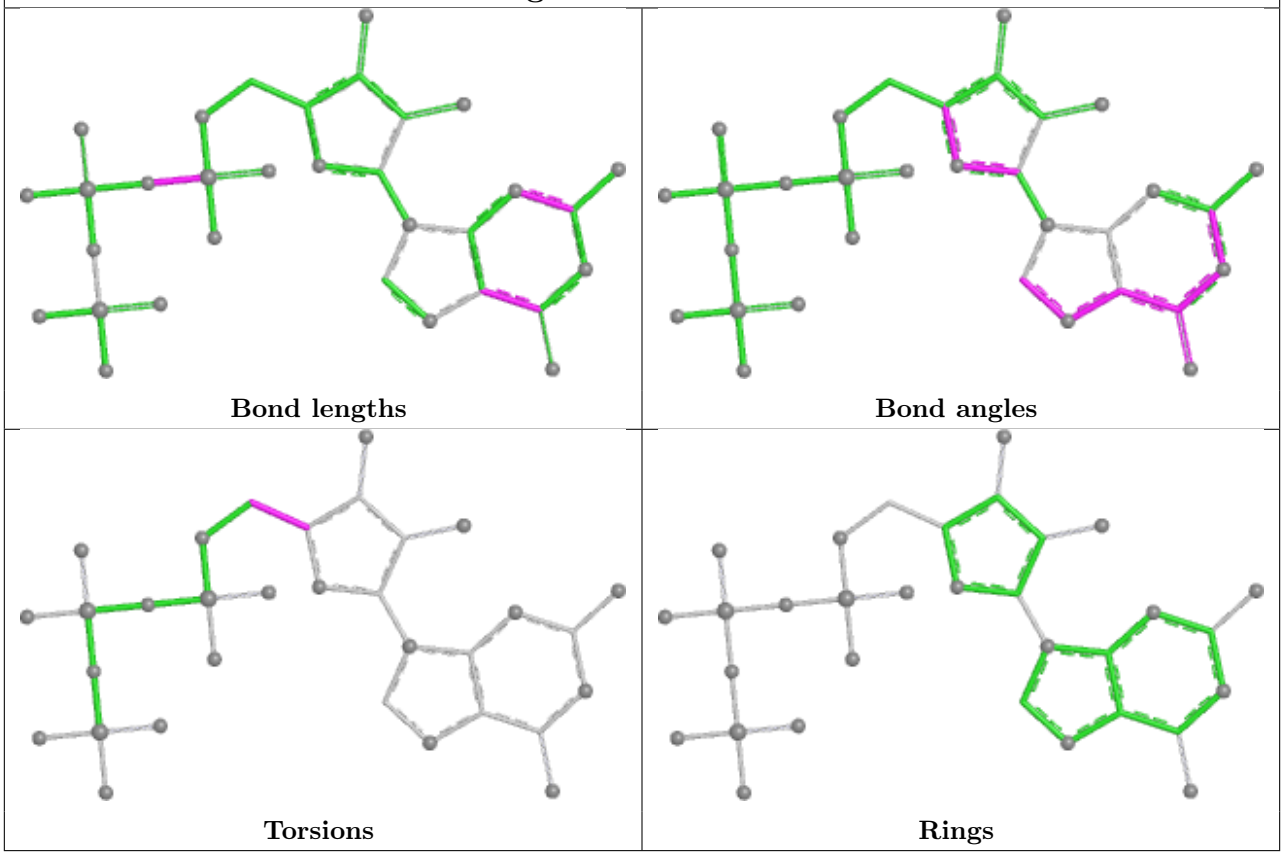


Torsions

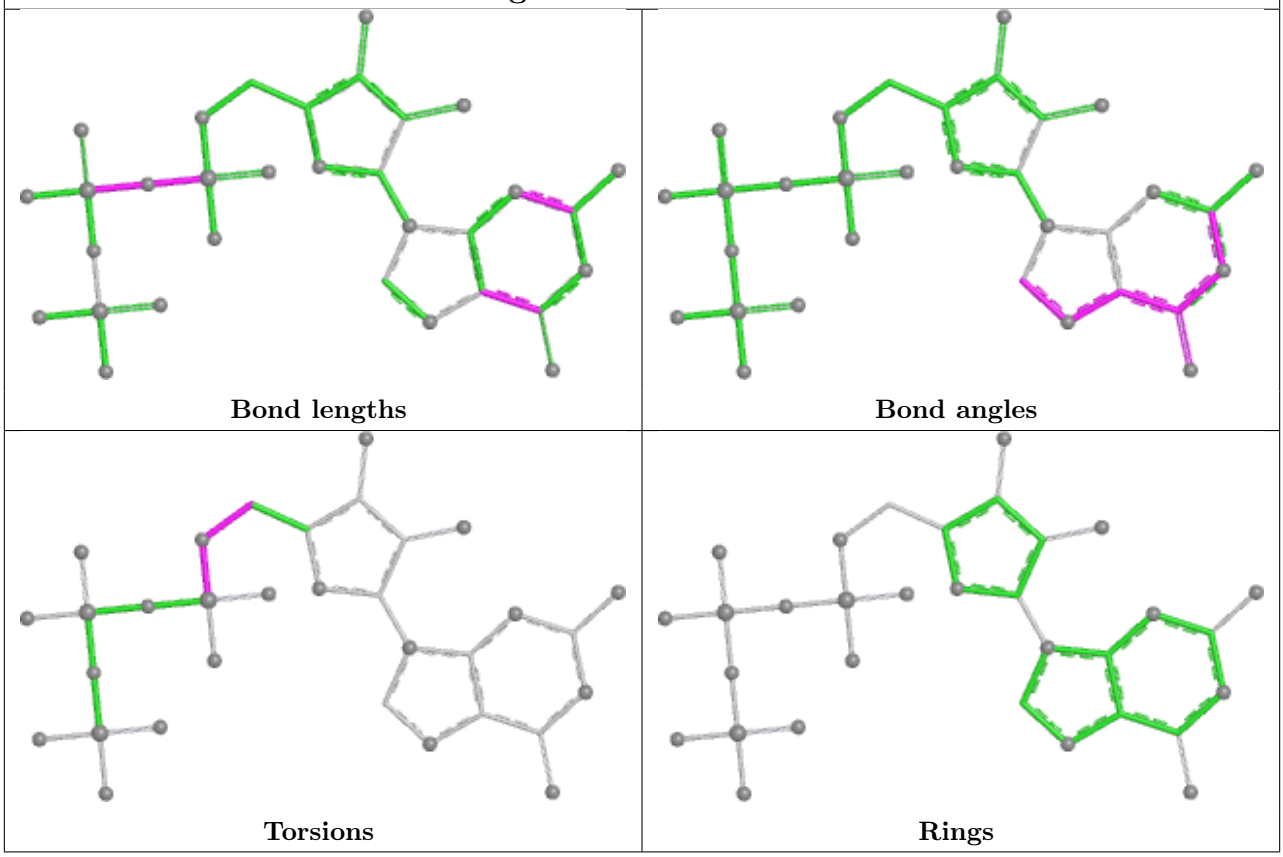


Rings

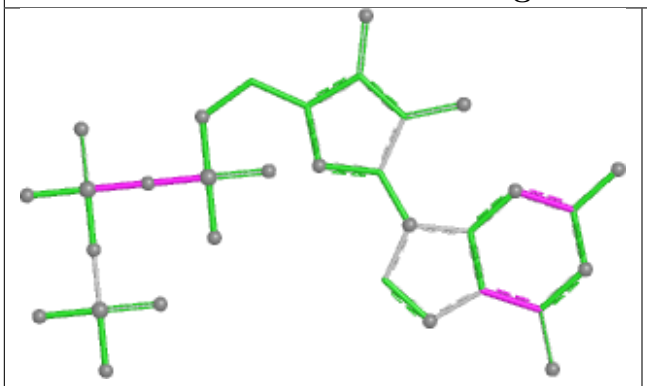
Ligand GTP d 602



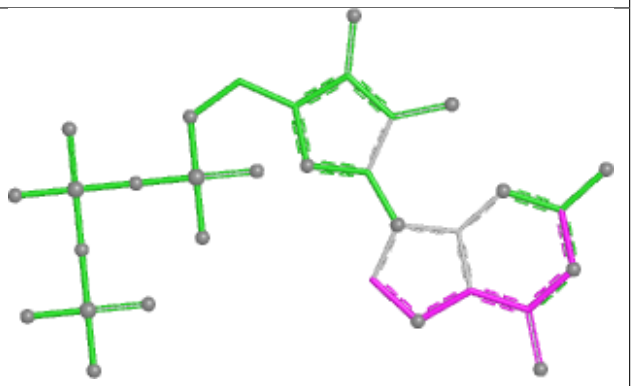
Ligand GTP GA 501



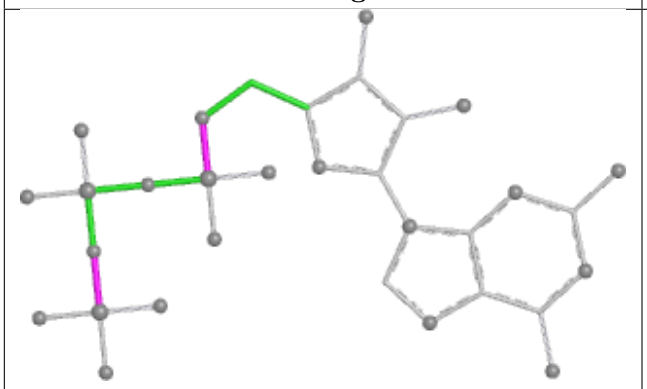
Ligand GTP Ax 602



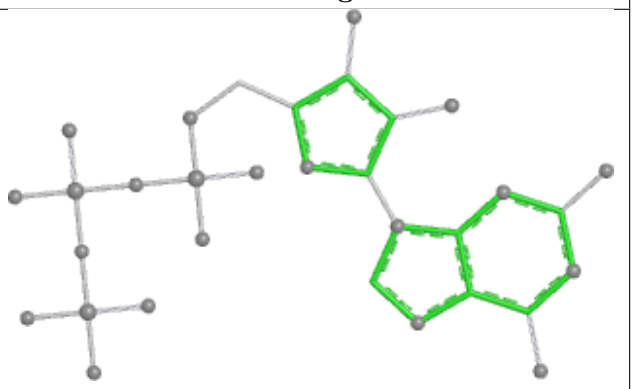
Bond lengths



Bond angles

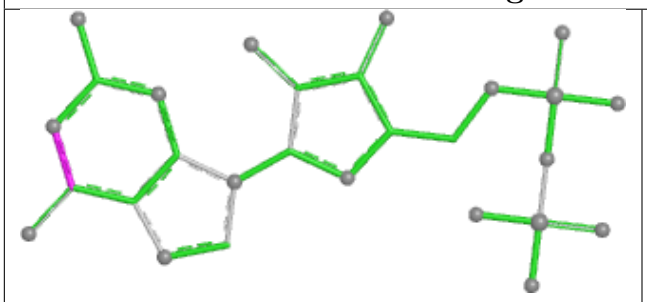


Torsions

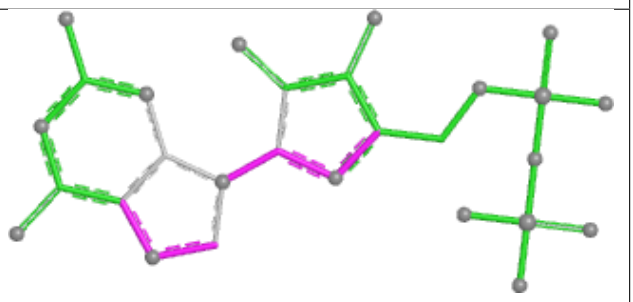


Rings

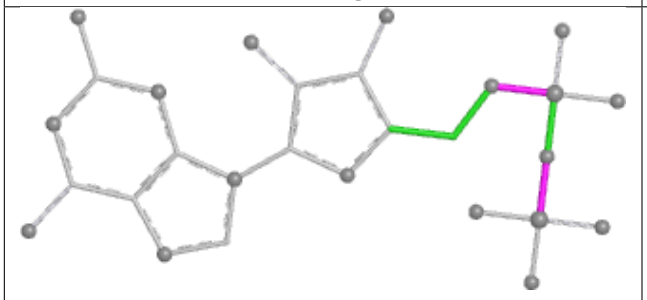
Ligand GDP Gm 501



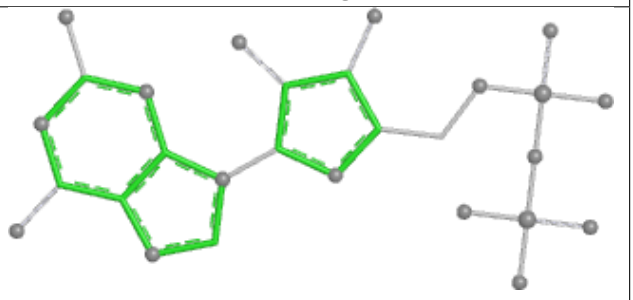
Bond lengths



Bond angles

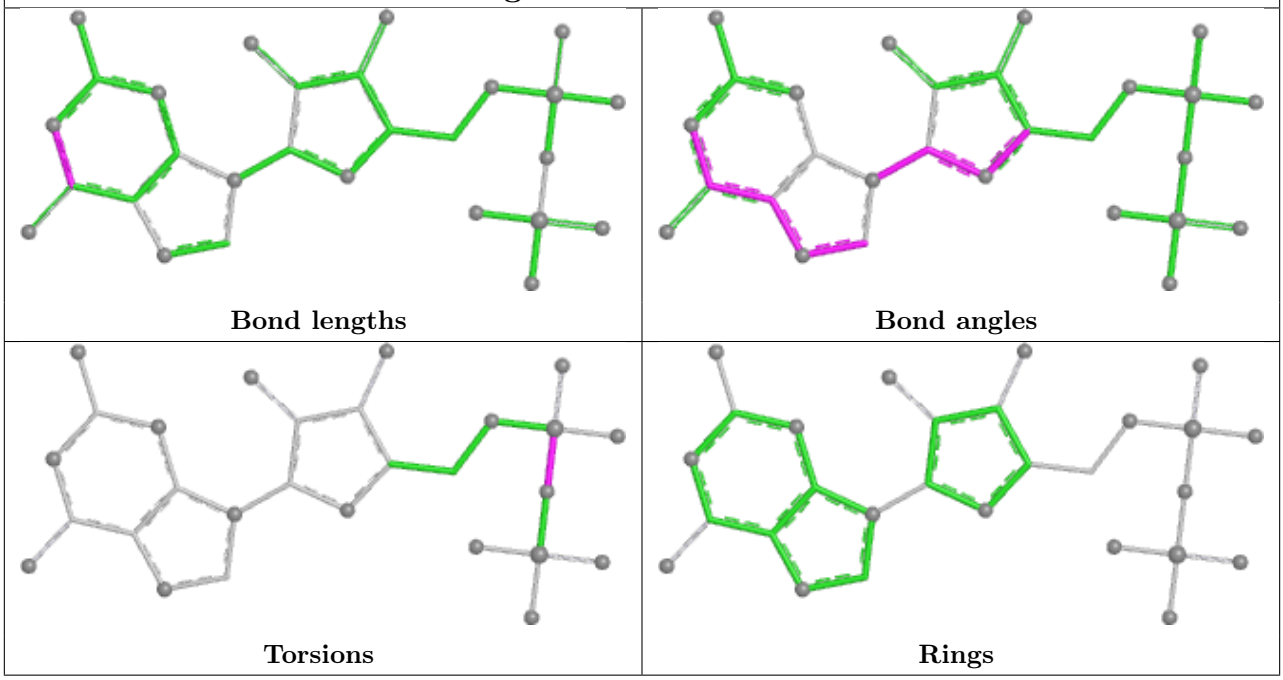


Torsions

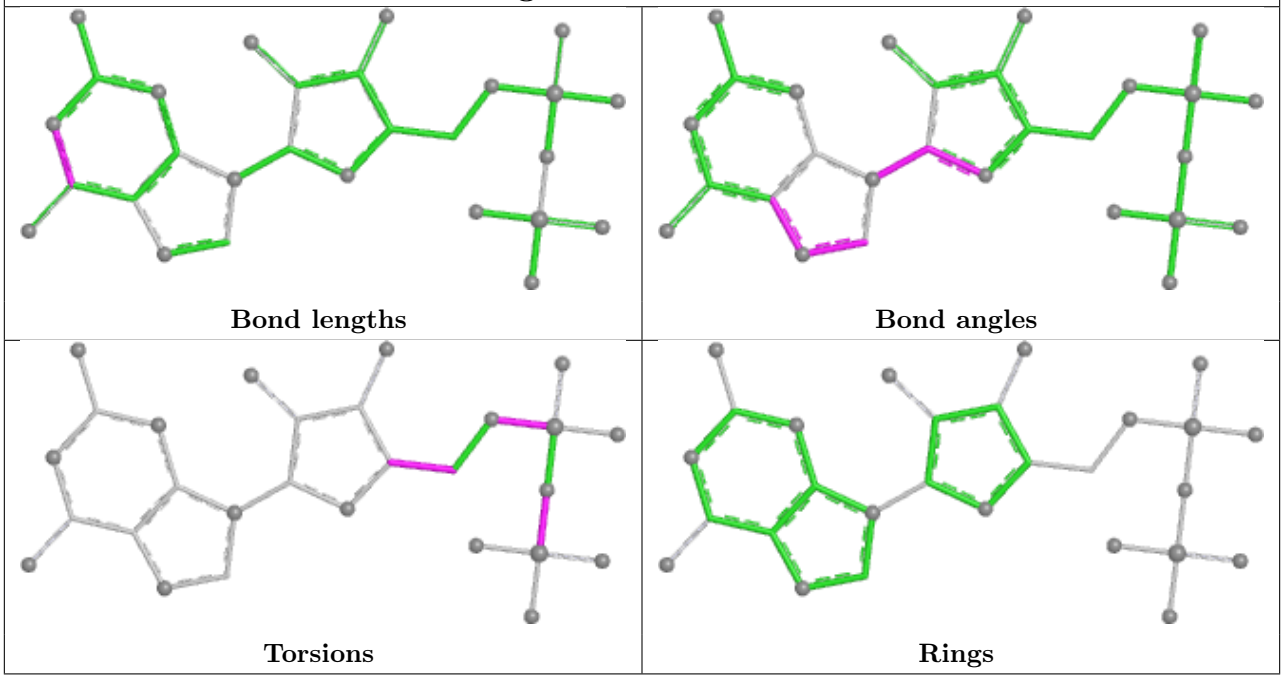


Rings

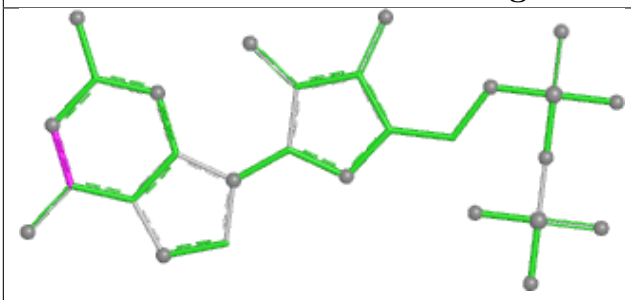
Ligand GDP BW 501



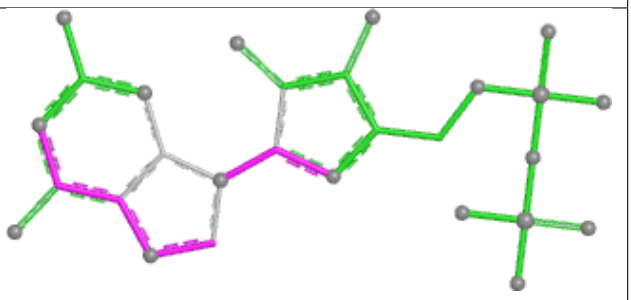
Ligand GDP Fz 501



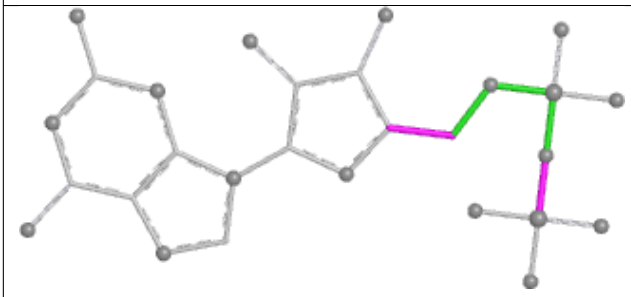
Ligand GDP ER 501



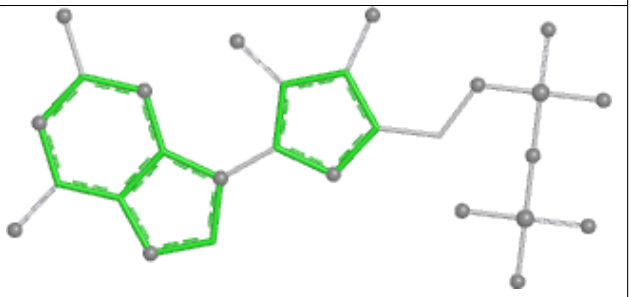
Bond lengths



Bond angles

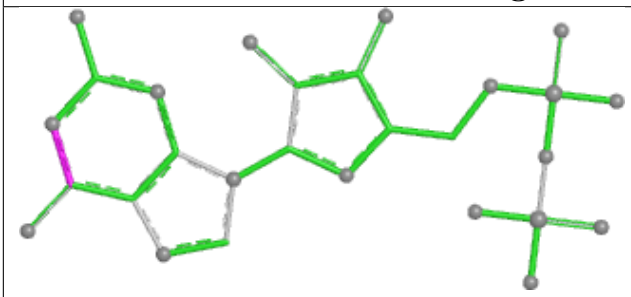


Torsions

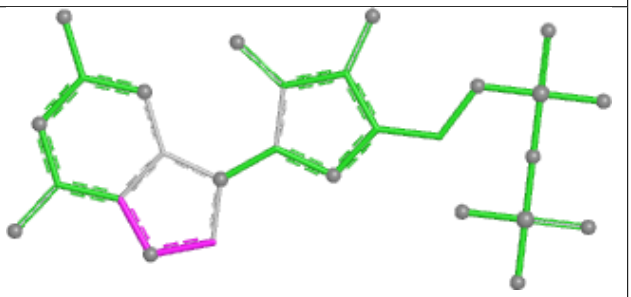


Rings

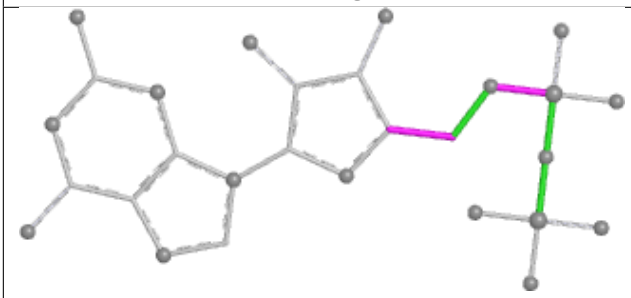
Ligand GDP AF 501



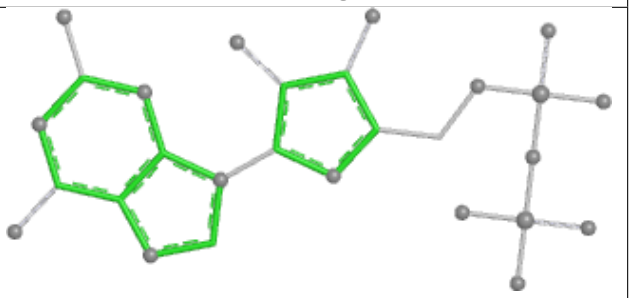
Bond lengths



Bond angles

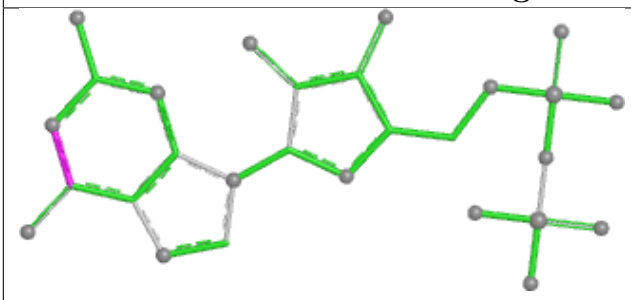


Torsions

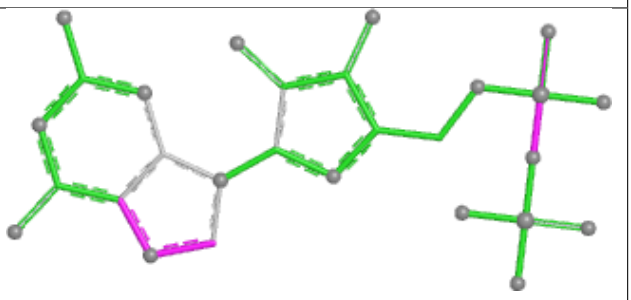


Rings

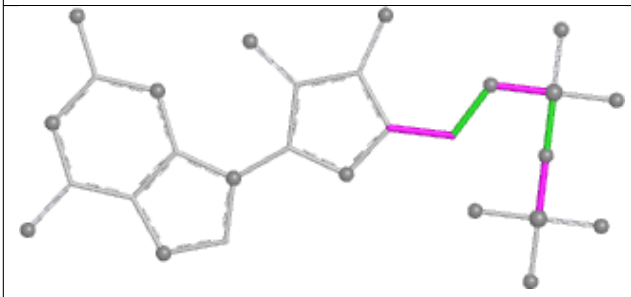
Ligand GDP Ed 501



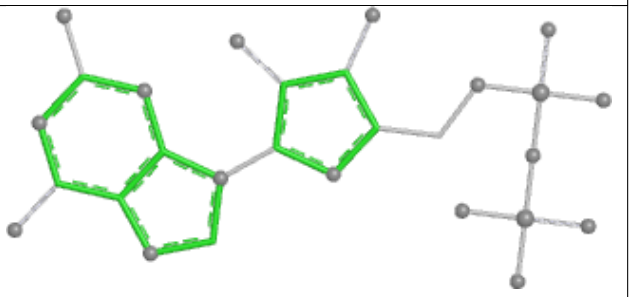
Bond lengths



Bond angles

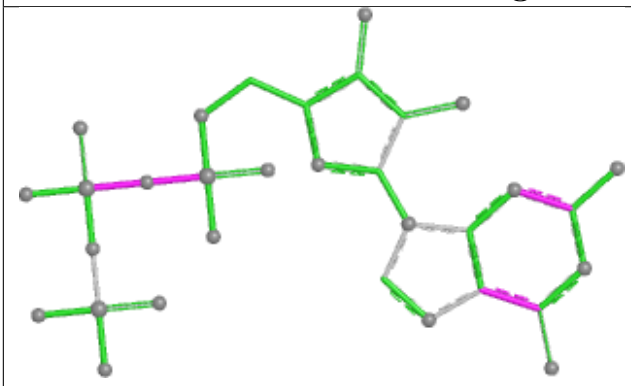


Torsions

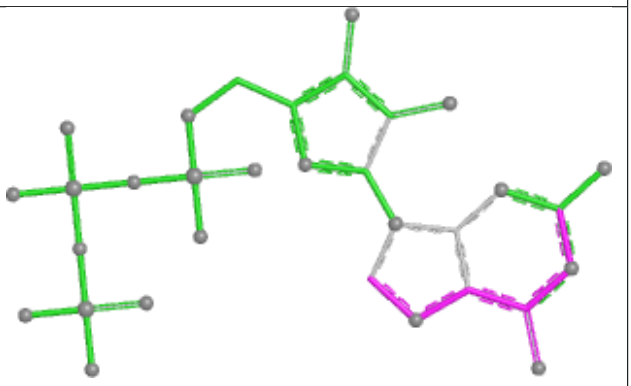


Rings

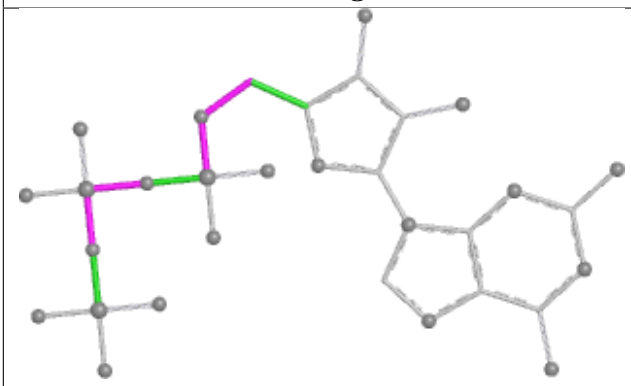
Ligand GTP Gu 501



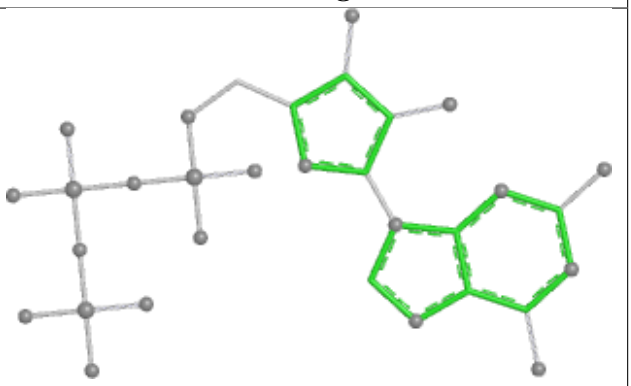
Bond lengths



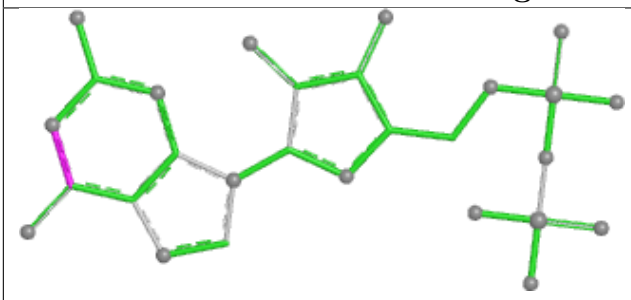
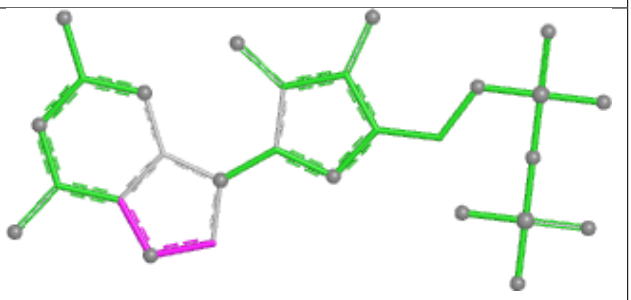
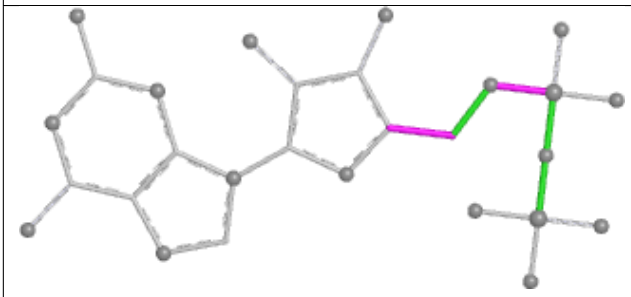
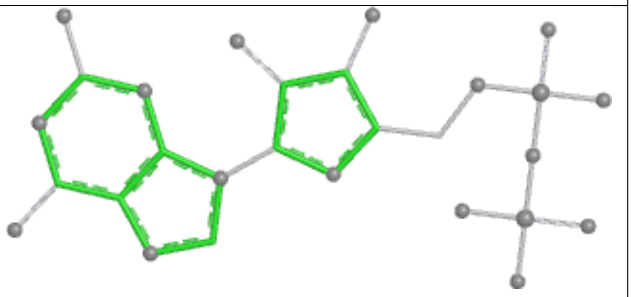
Bond angles

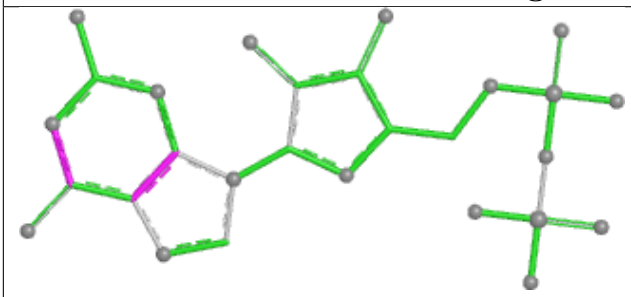
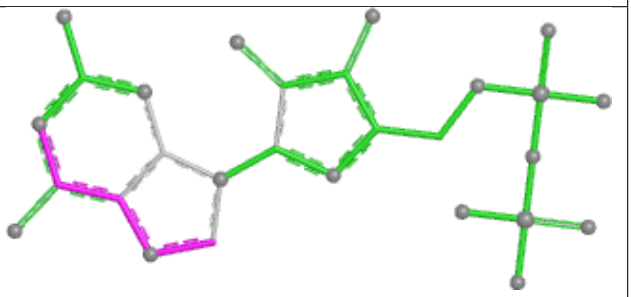
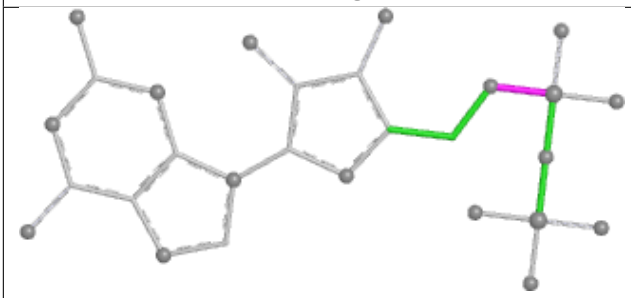
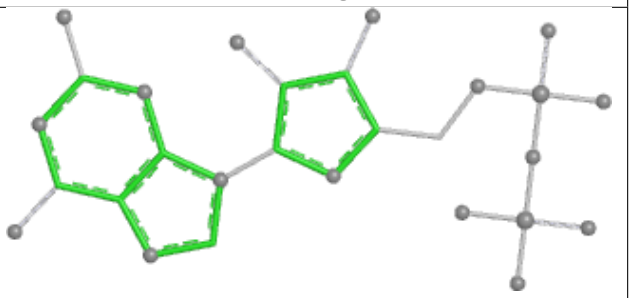


Torsions

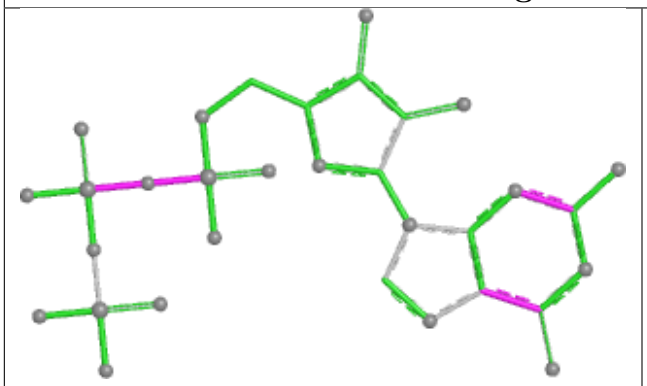


Rings

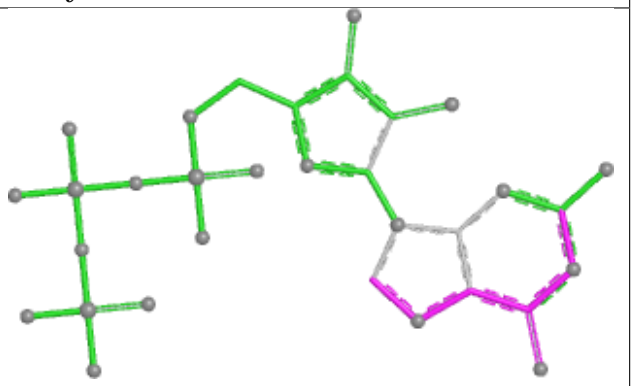
Ligand GDP As 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP r 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

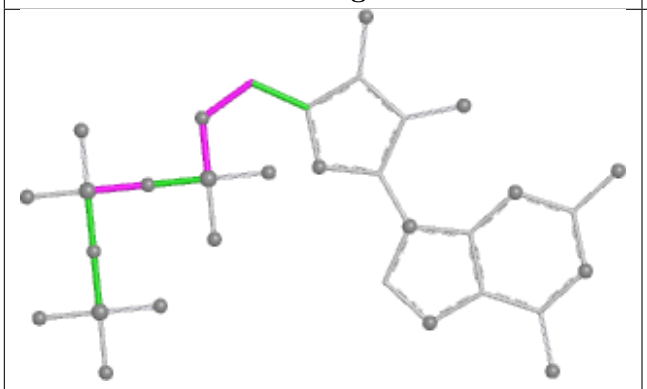
Ligand GTP Ay 602



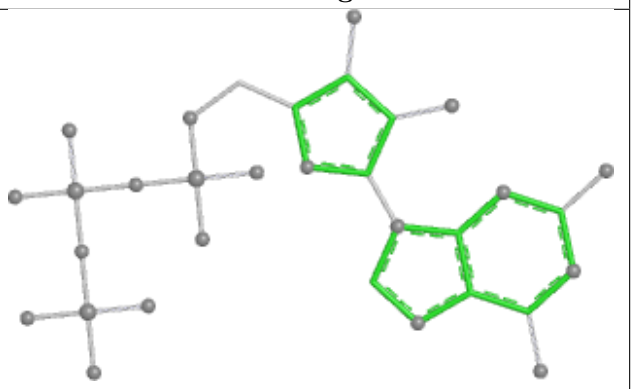
Bond lengths



Bond angles

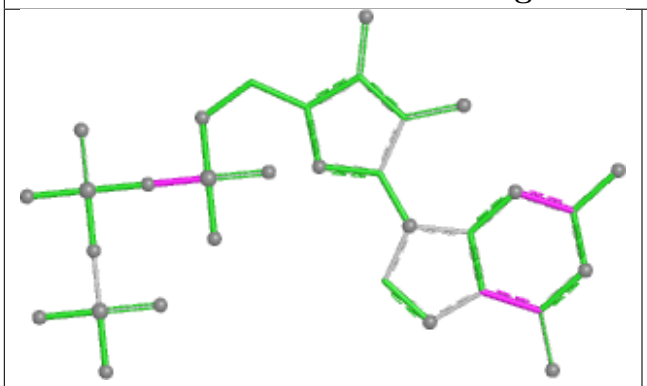


Torsions

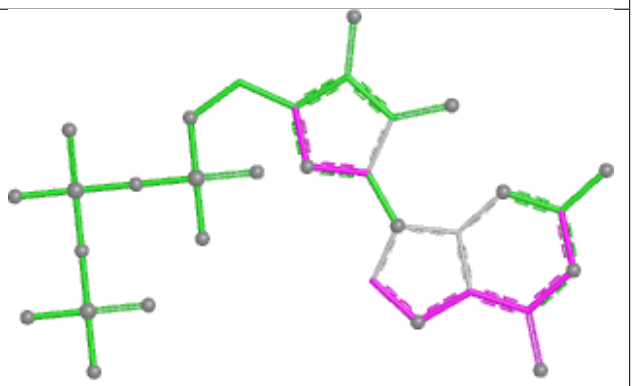


Rings

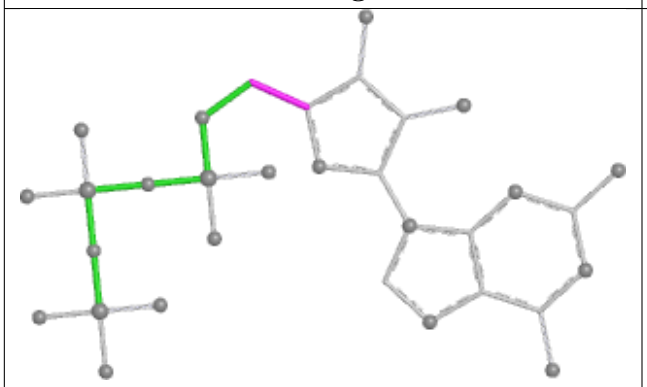
Ligand GTP BJ 602



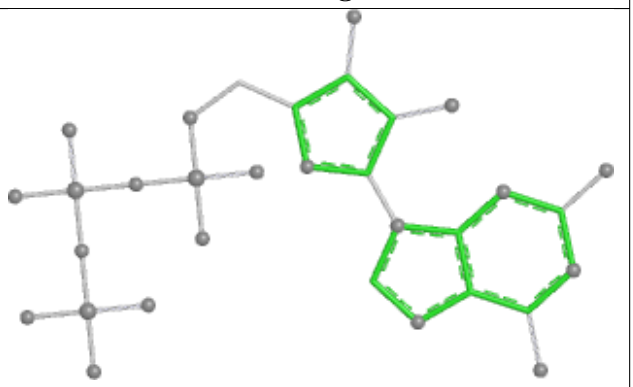
Bond lengths



Bond angles

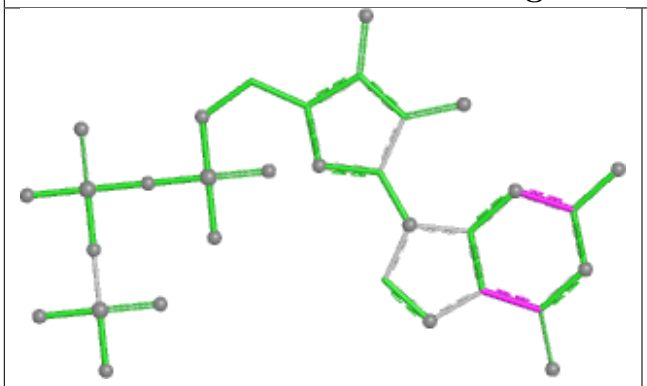


Torsions

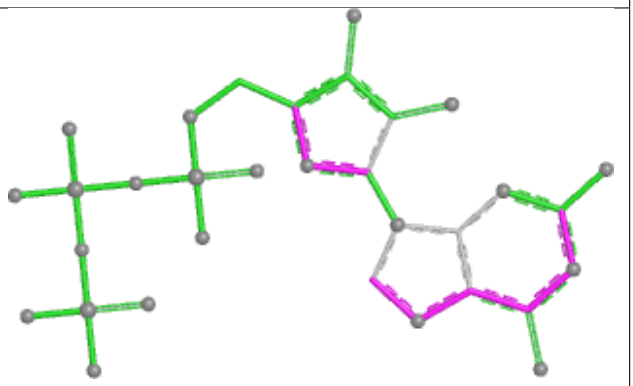


Rings

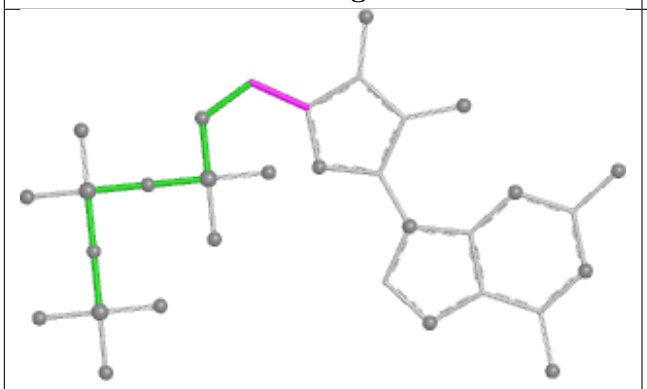
Ligand GTP Z 602



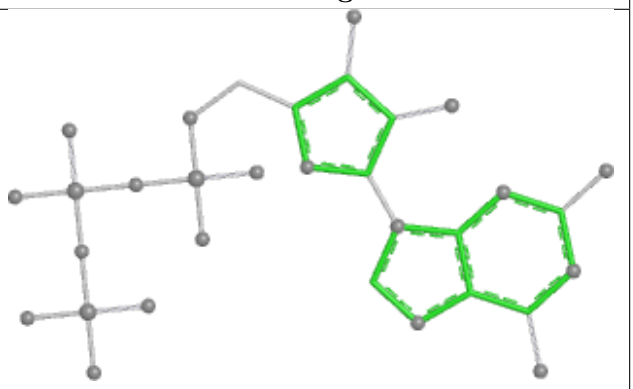
Bond lengths



Bond angles

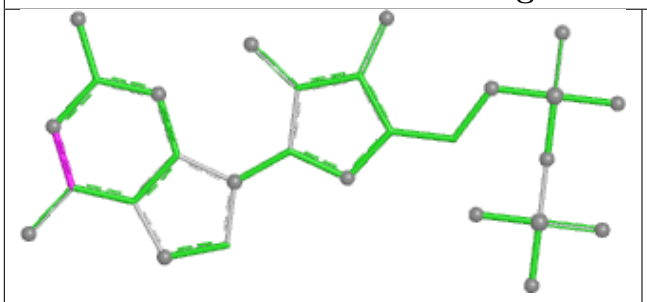


Torsions

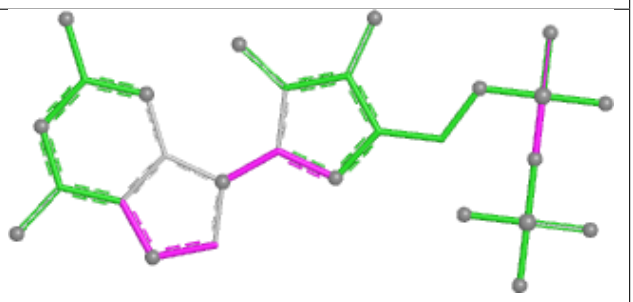


Rings

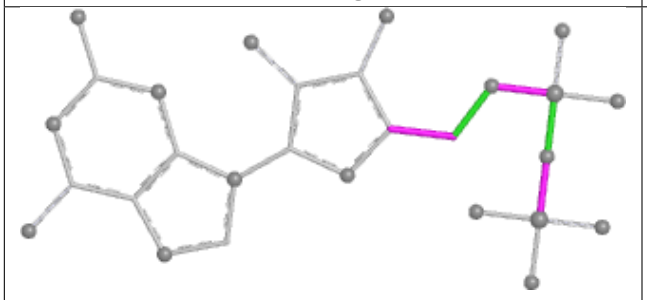
Ligand GDP Di 501



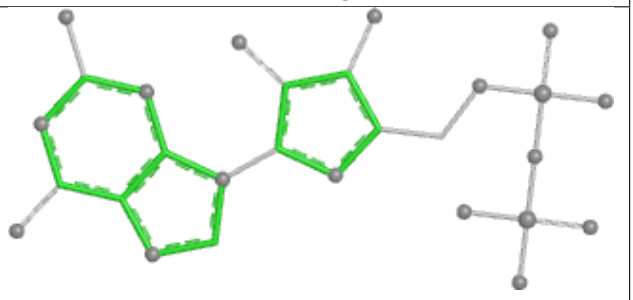
Bond lengths



Bond angles

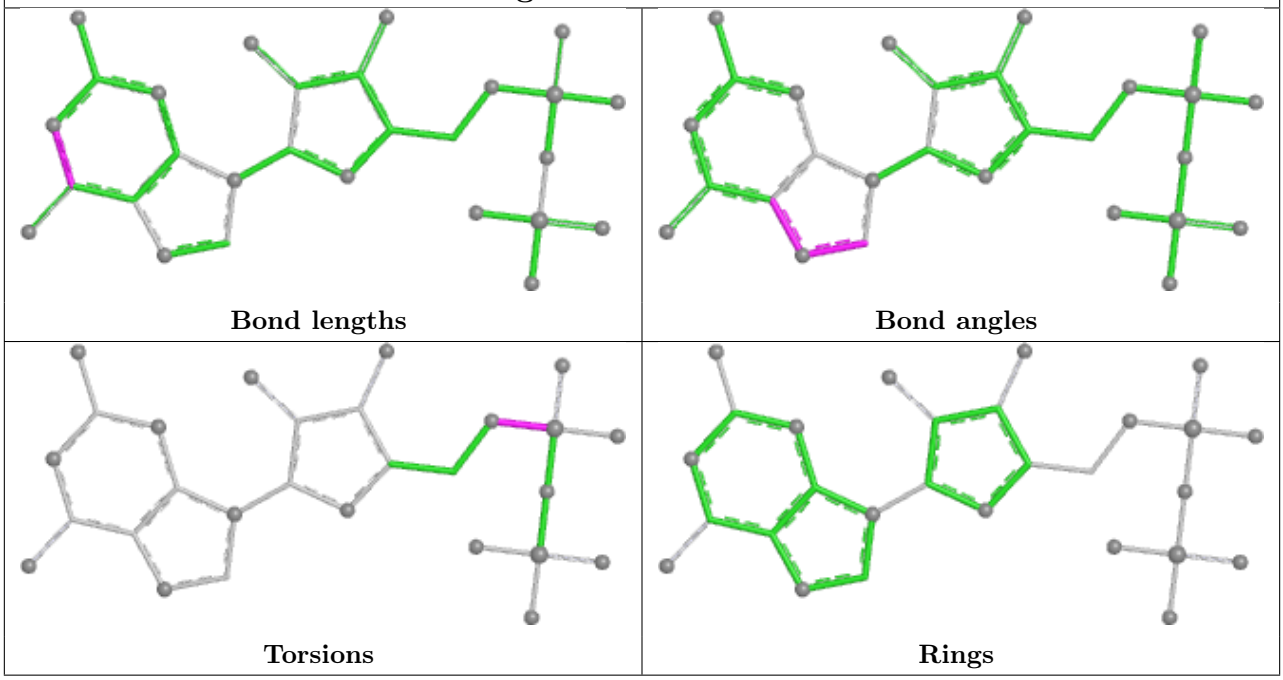


Torsions

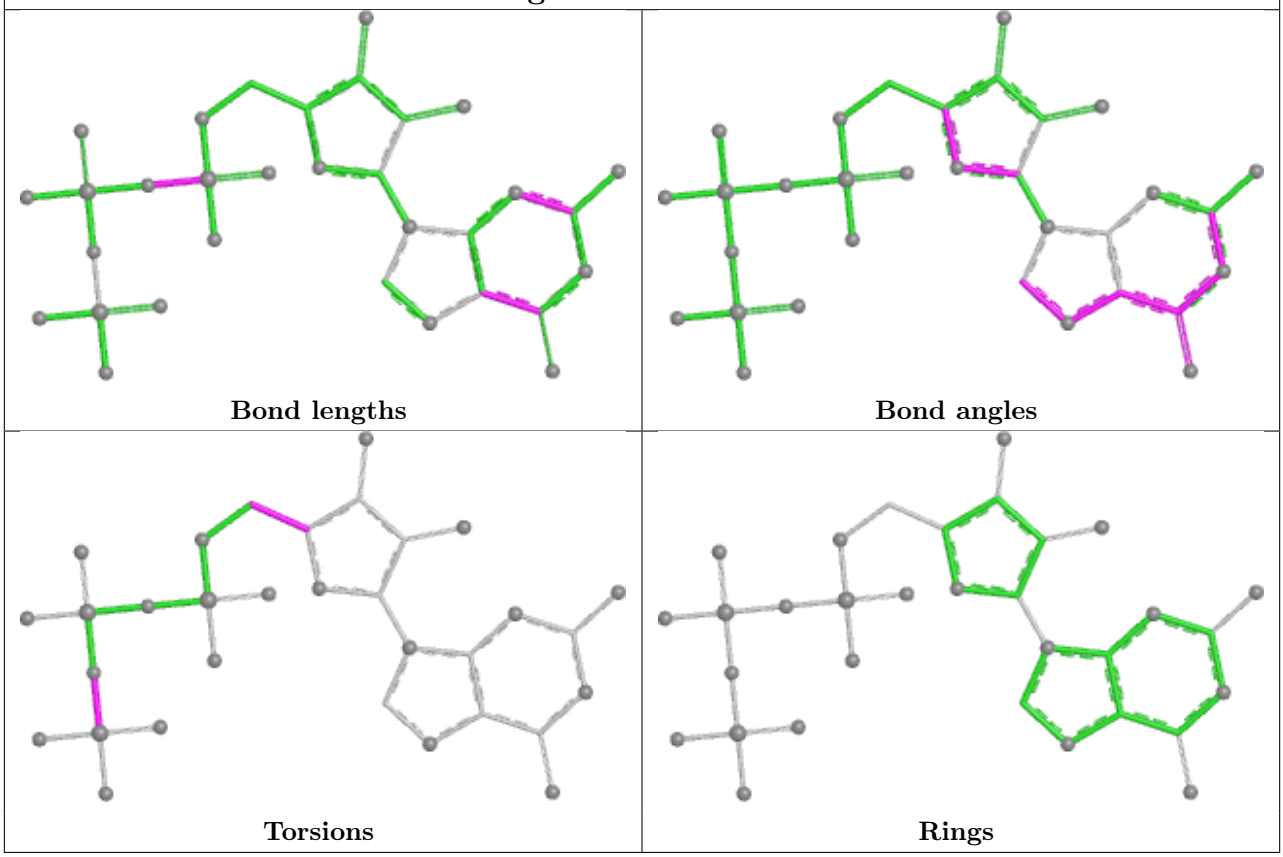


Rings

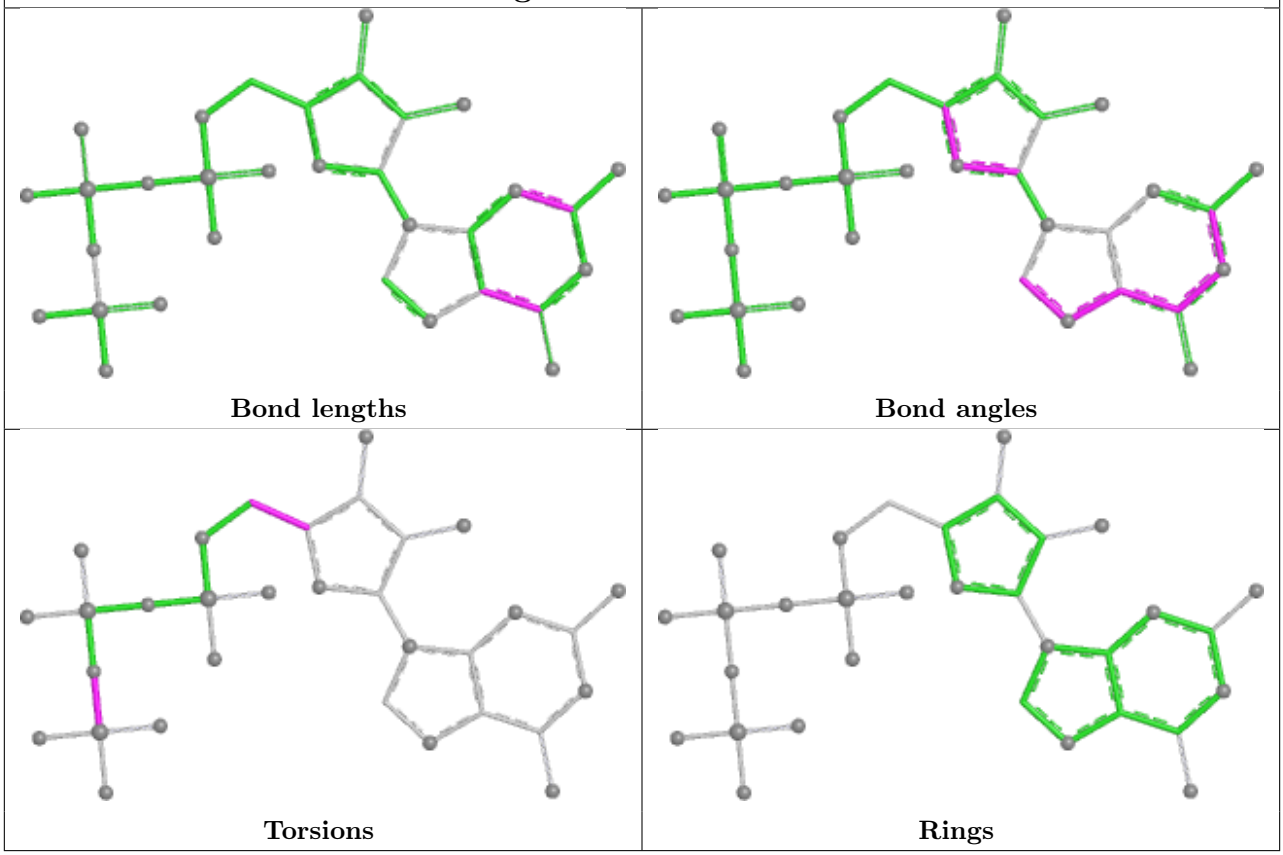
Ligand GDP Af 501



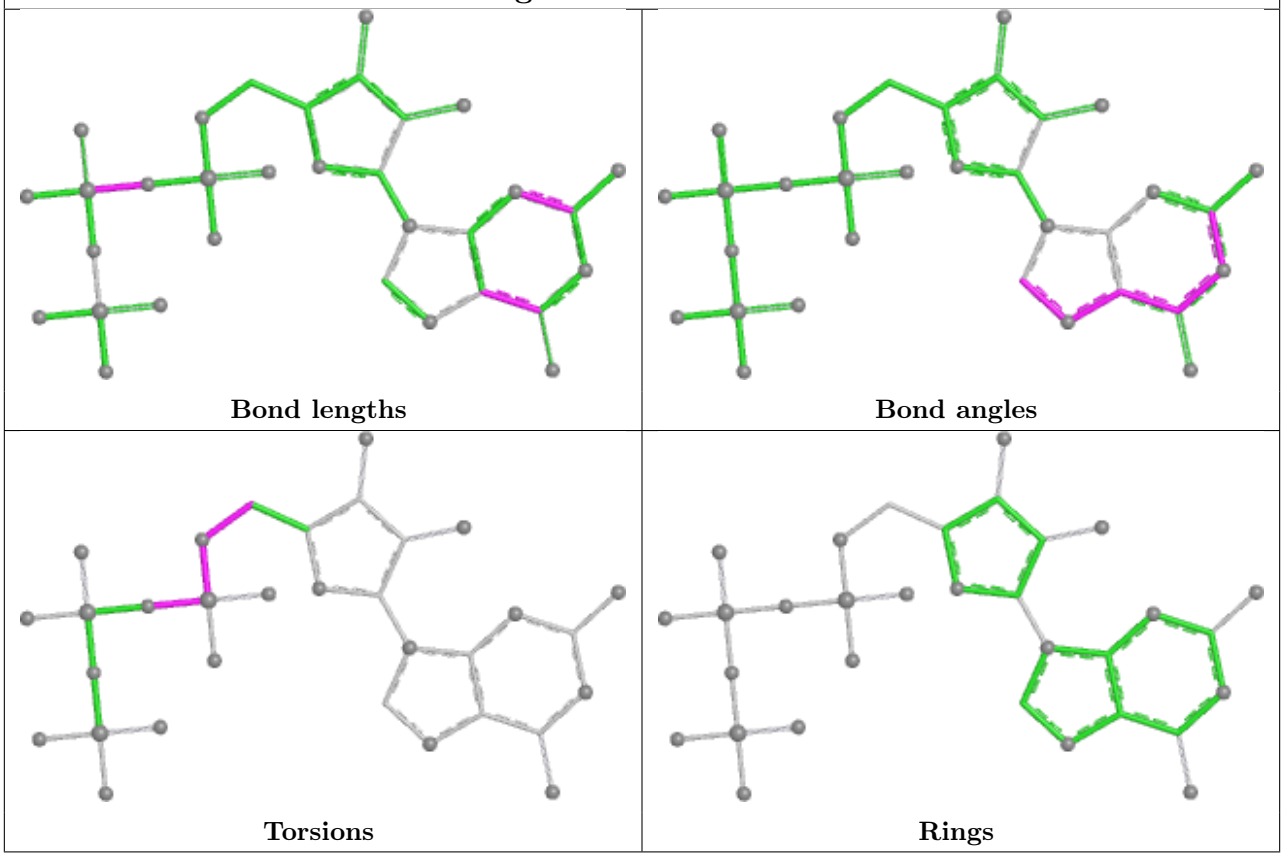
Ligand GTP 6 602



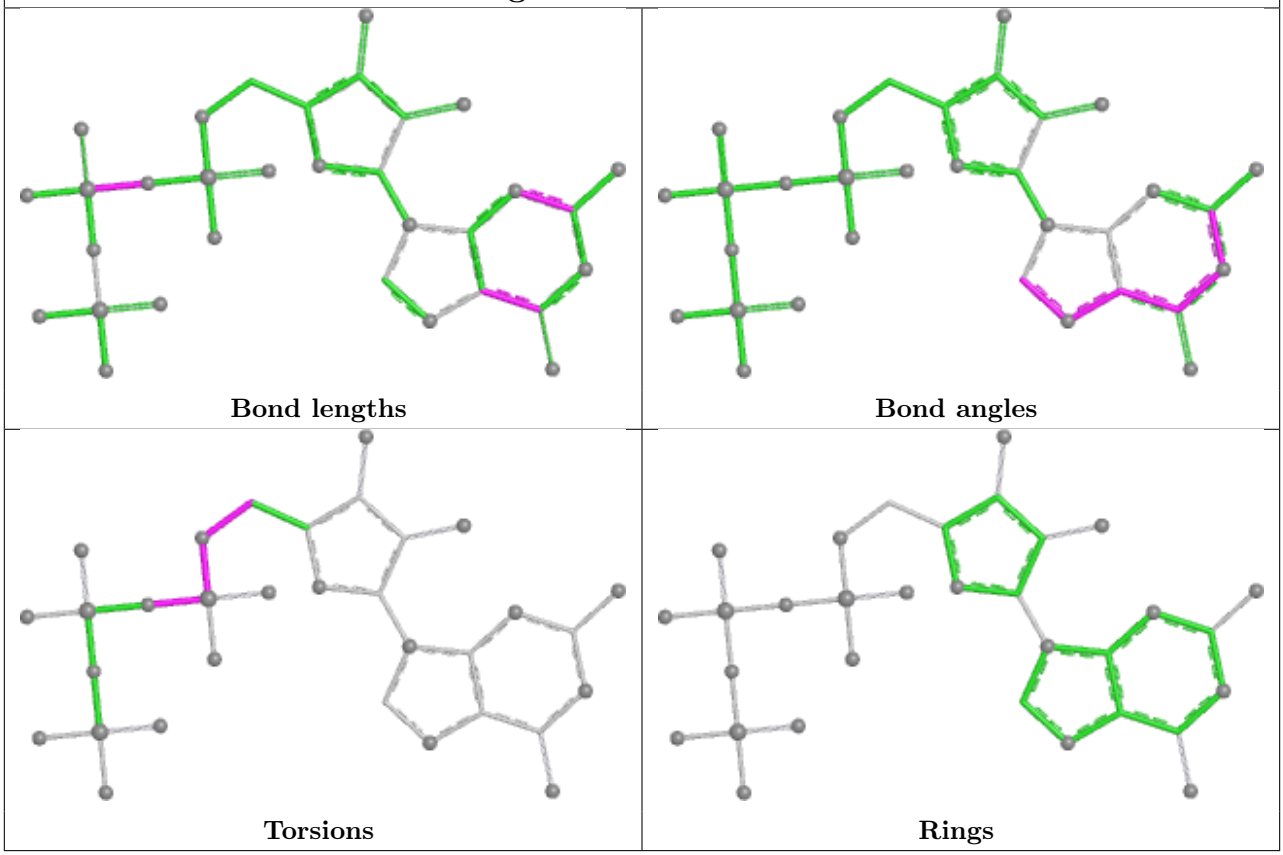
Ligand GTP A2 602



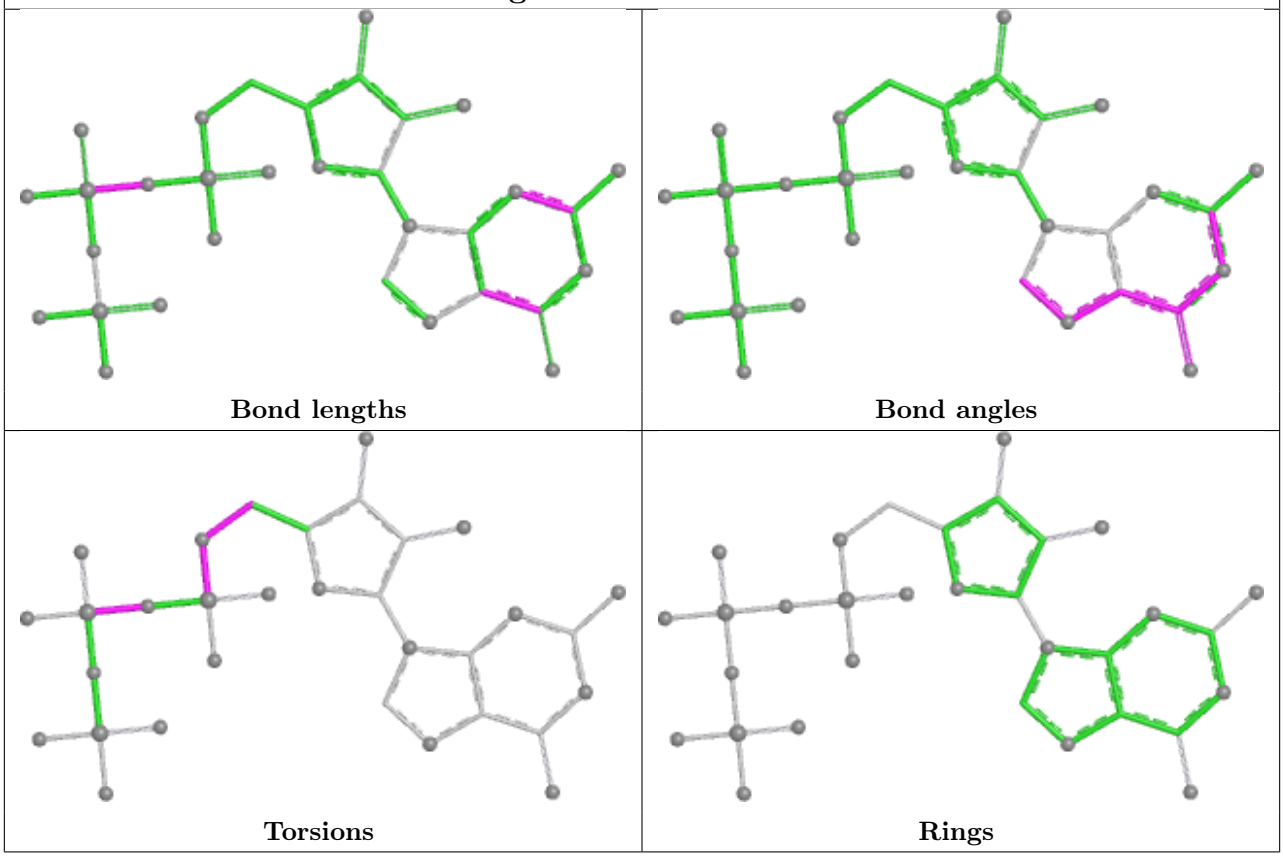
Ligand GTP Eu 501



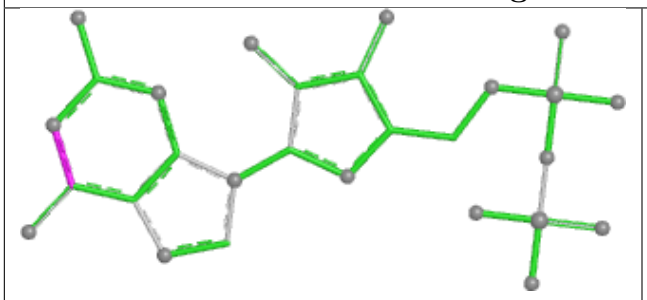
Ligand GTP GG 501



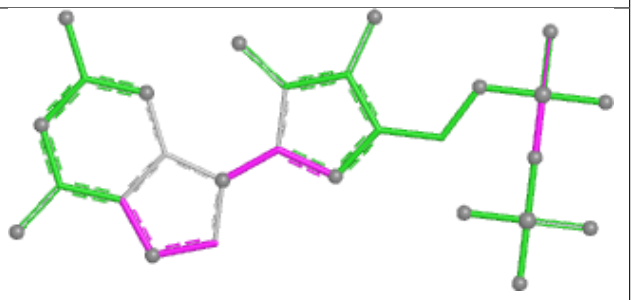
Ligand GTP GO 602



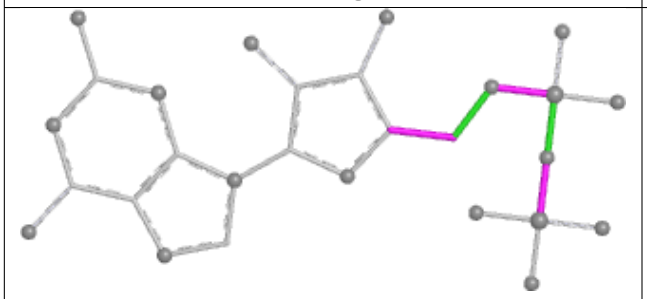
Ligand GDP EY 501



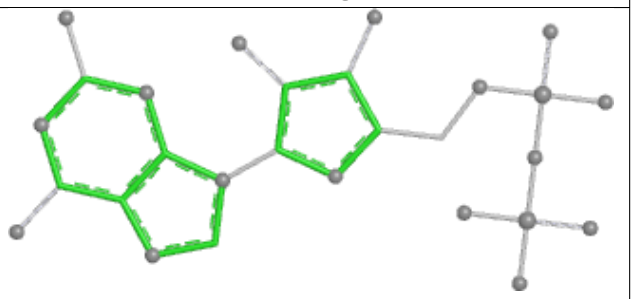
Bond lengths



Bond angles

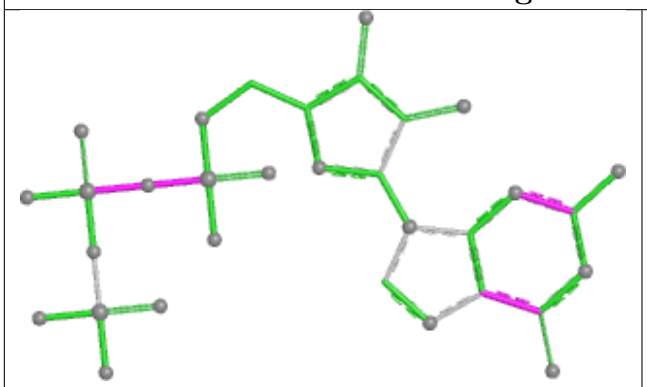


Torsions

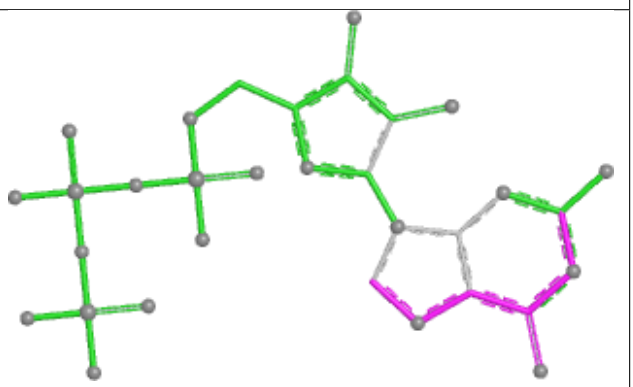


Rings

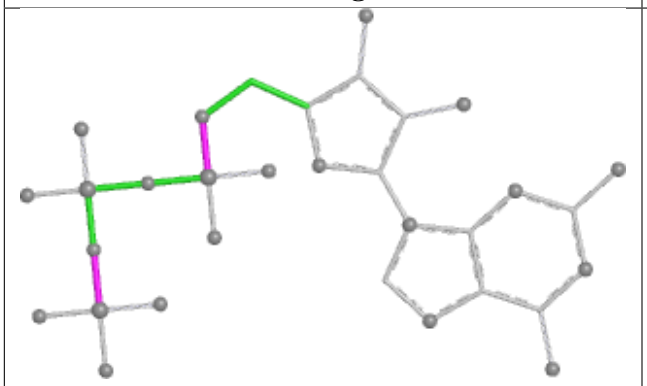
Ligand GTP B0 501



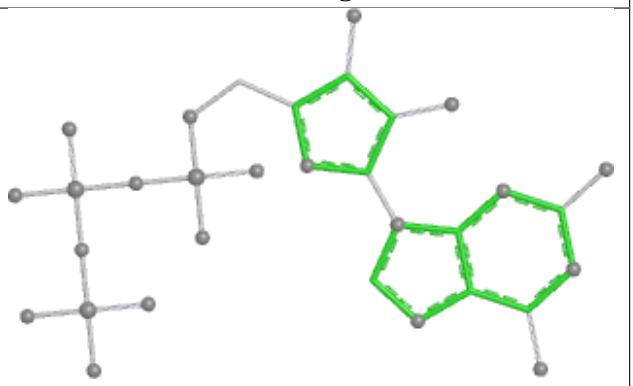
Bond lengths



Bond angles

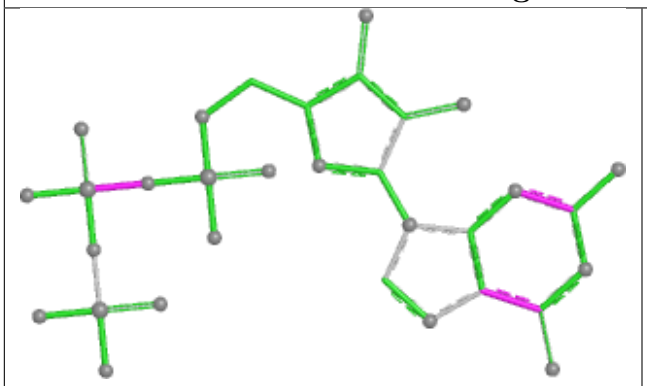


Torsions

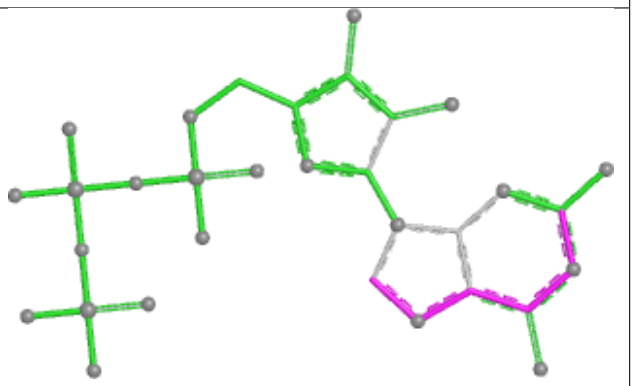


Rings

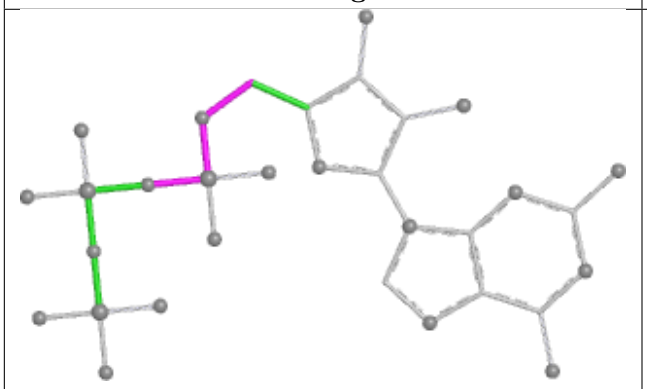
Ligand GTP Gn 501



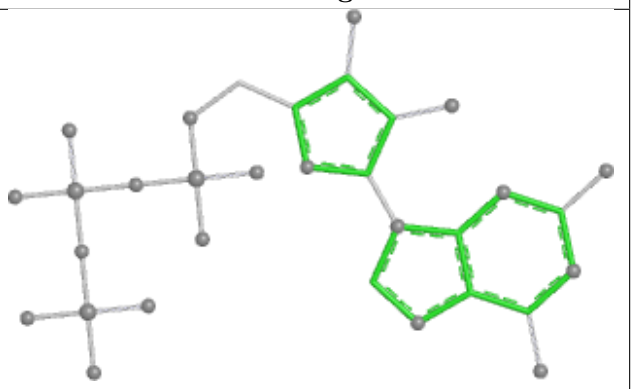
Bond lengths



Bond angles

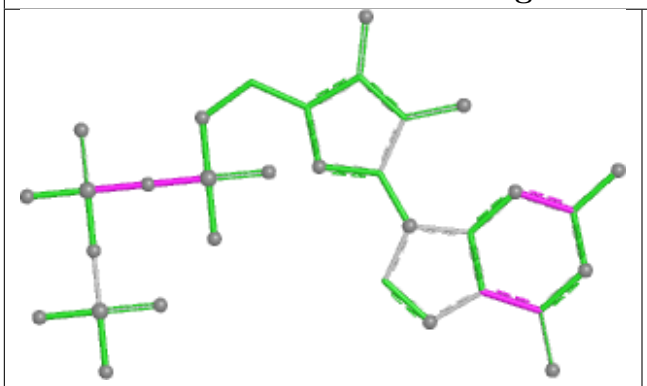


Torsions

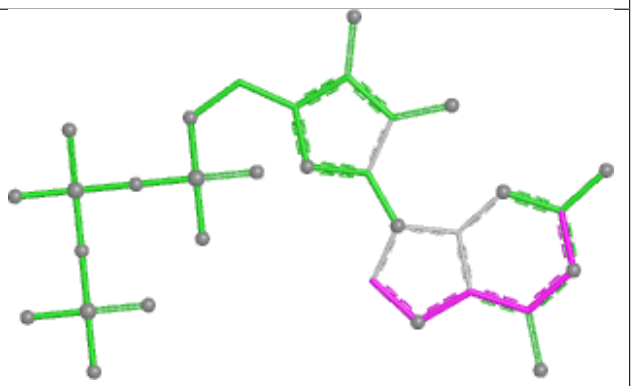


Rings

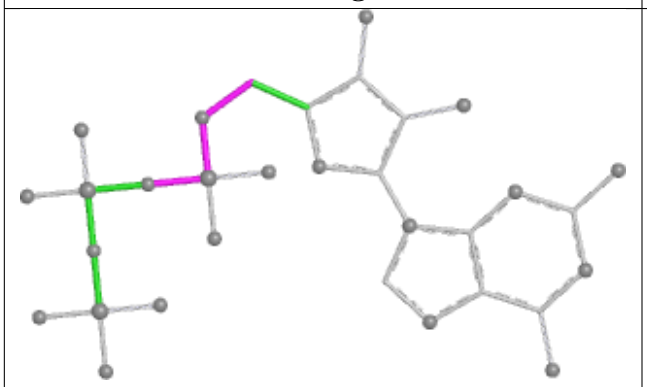
Ligand GTP En 501



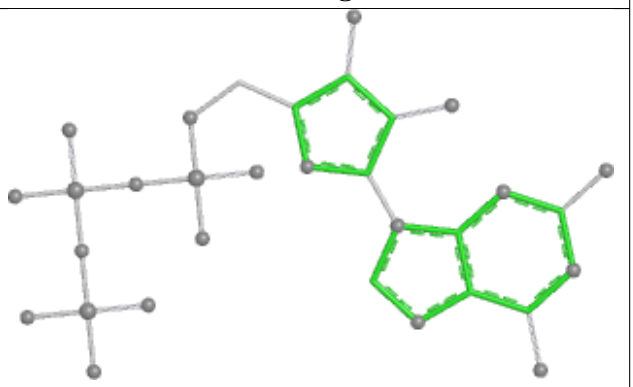
Bond lengths



Bond angles

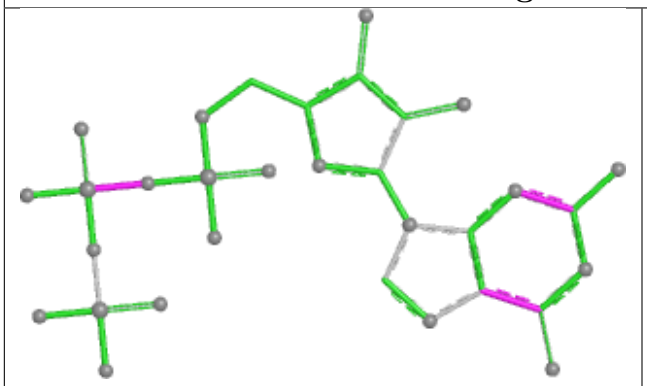


Torsions

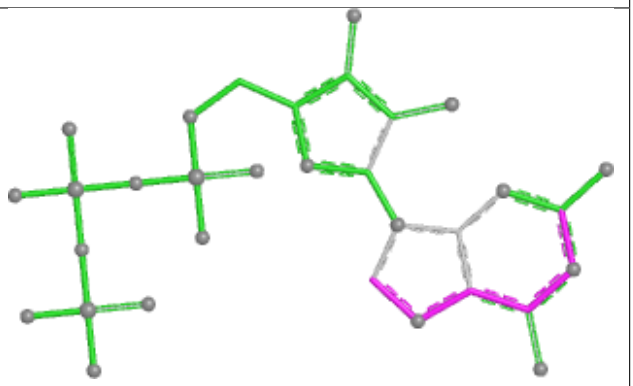


Rings

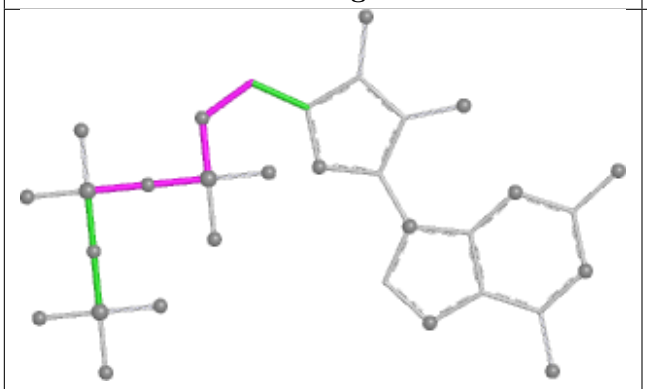
Ligand GTP E4 501



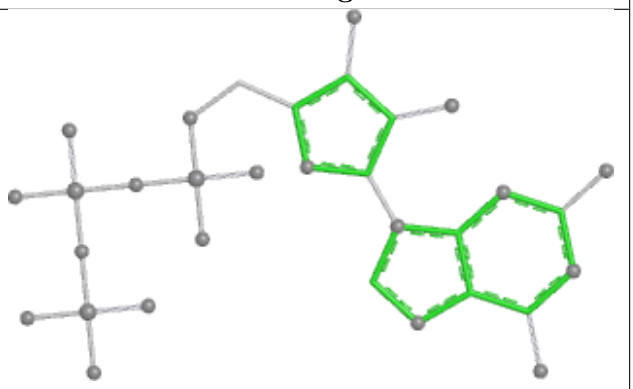
Bond lengths



Bond angles

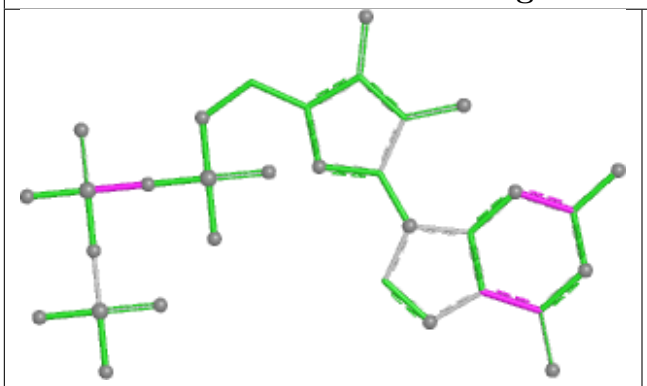


Torsions

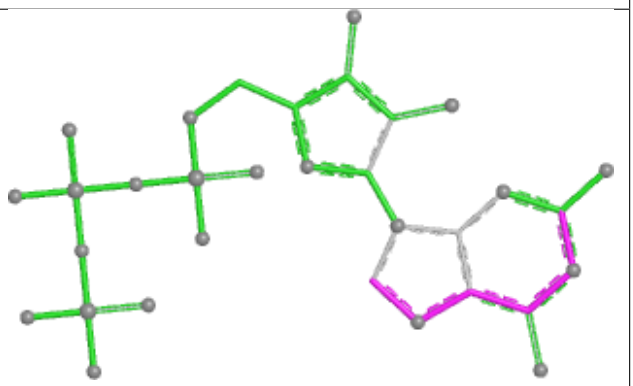


Rings

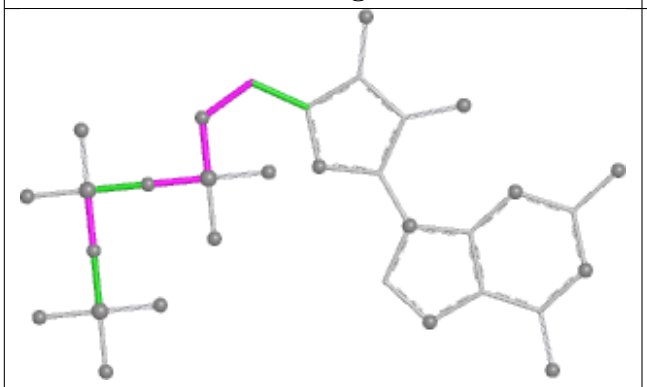
Ligand GTP F0 501



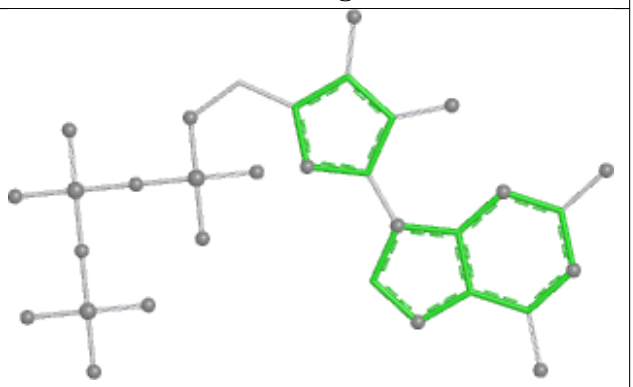
Bond lengths



Bond angles

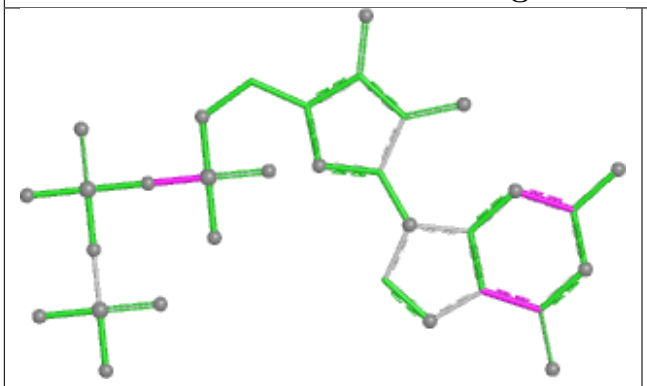


Torsions

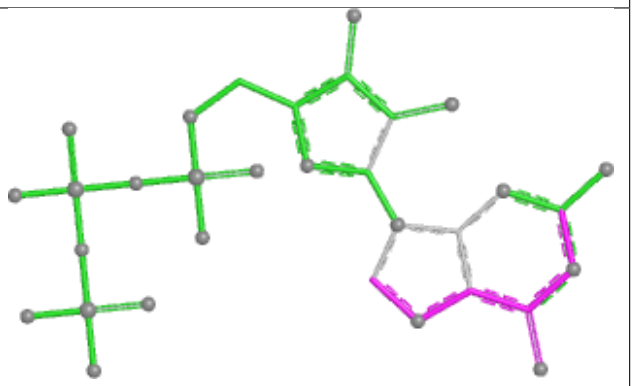


Rings

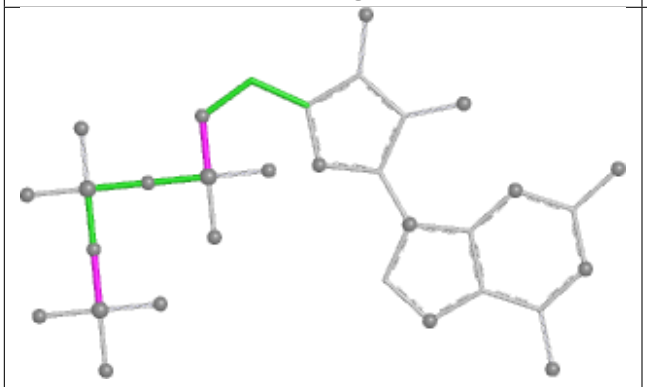
Ligand GTP BT 501



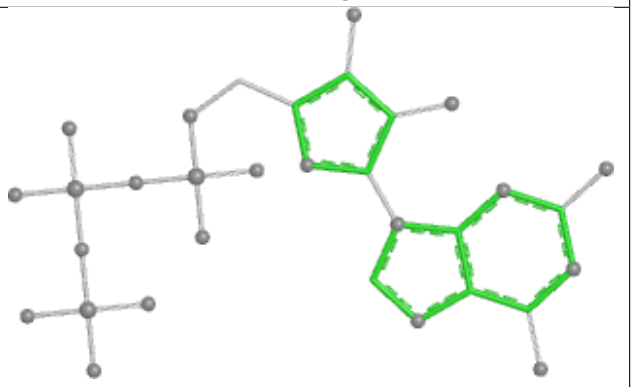
Bond lengths



Bond angles

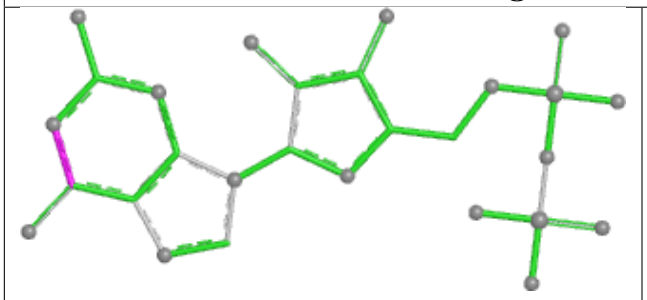


Torsions

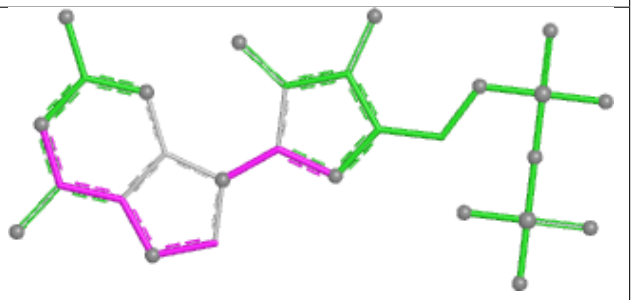


Rings

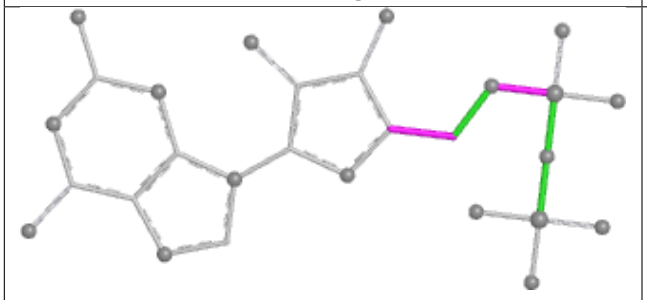
Ligand GDP AX 501



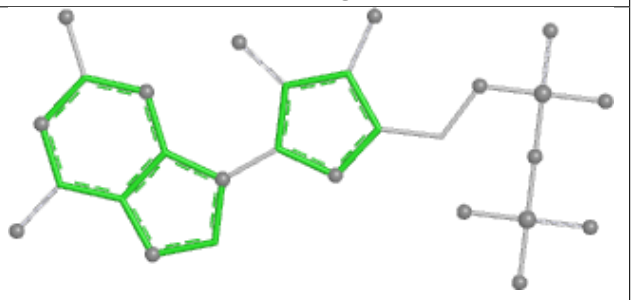
Bond lengths



Bond angles

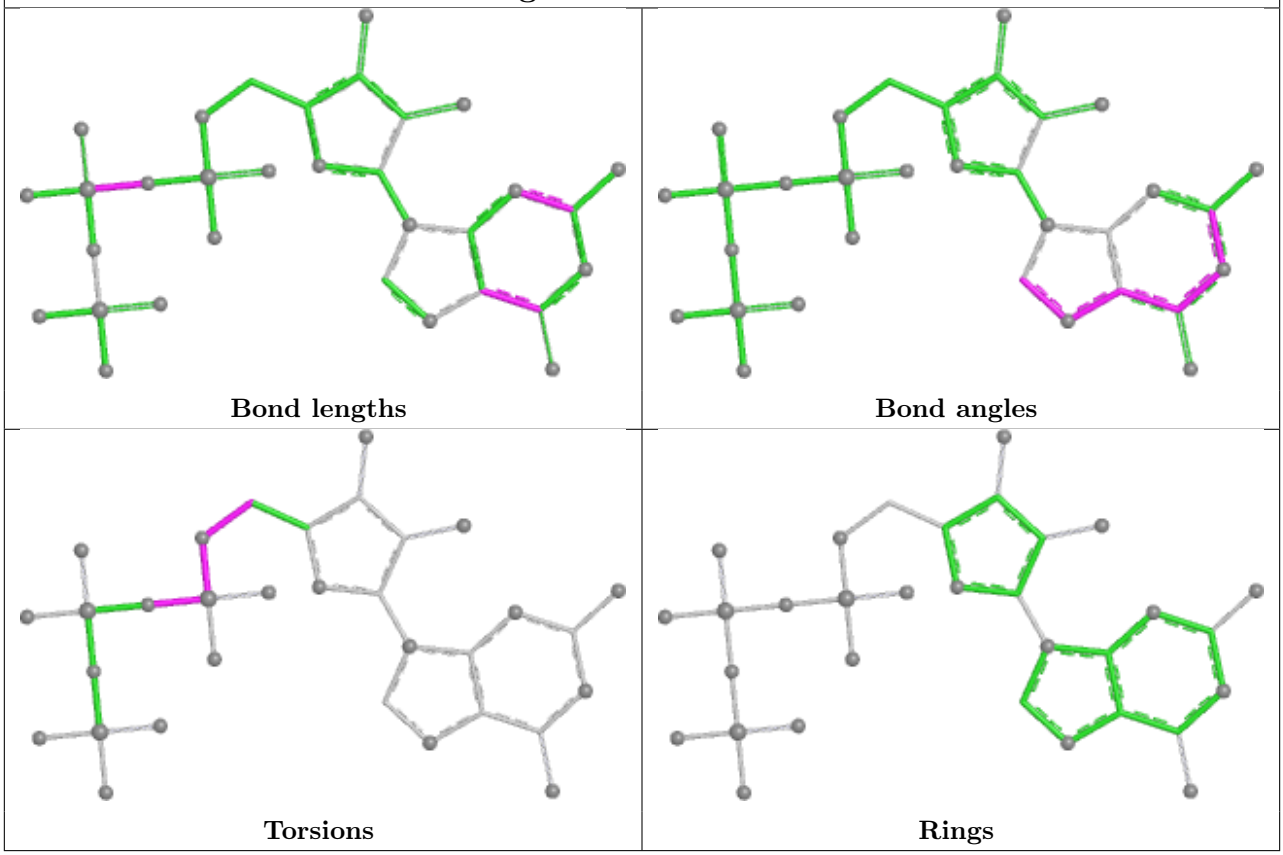


Torsions

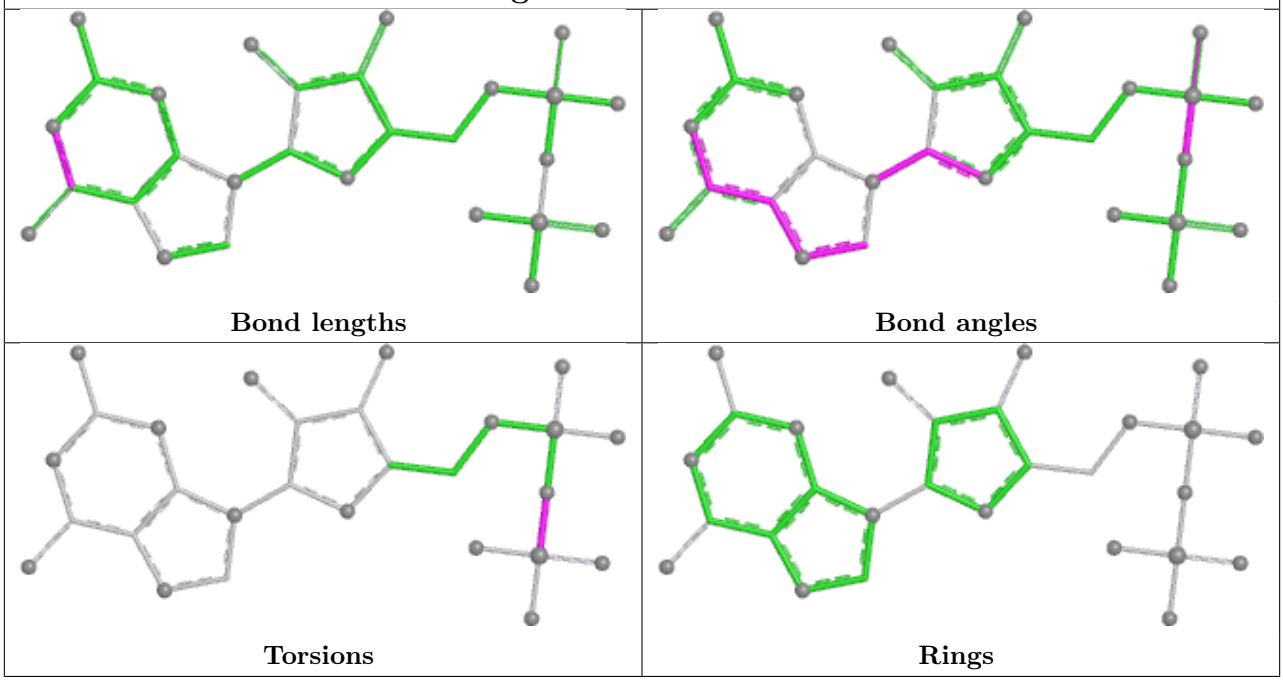


Rings

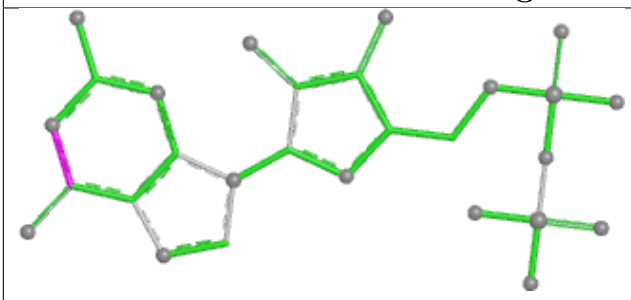
Ligand GTP Fc 501



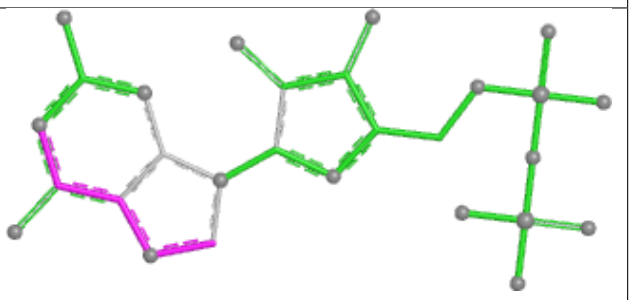
Ligand GDP Gd 501



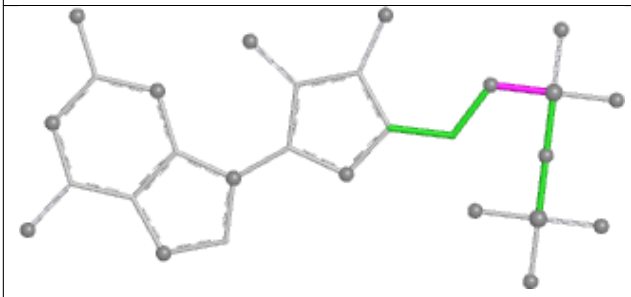
Ligand GDP Bf 501



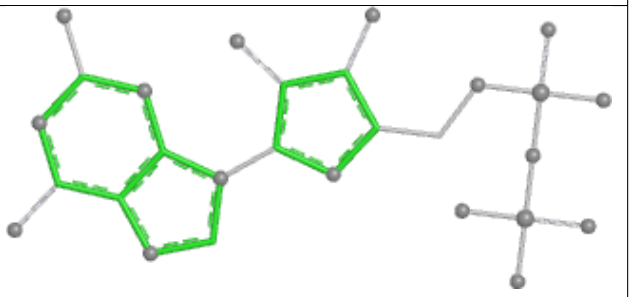
Bond lengths



Bond angles

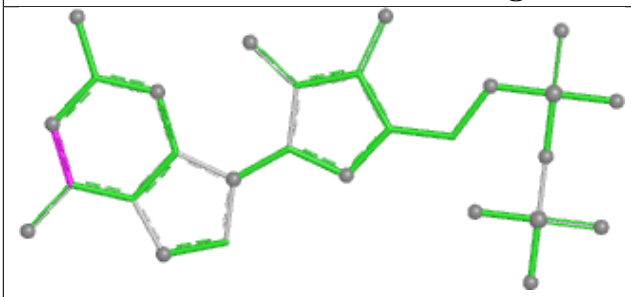


Torsions

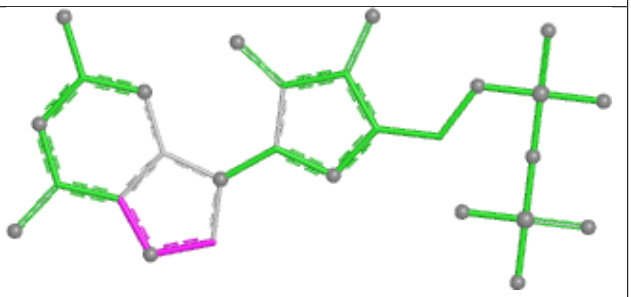


Rings

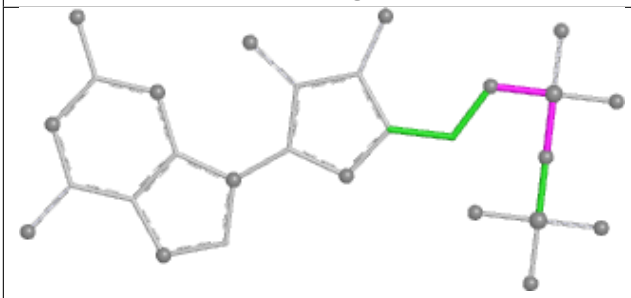
Ligand GDP AG 501



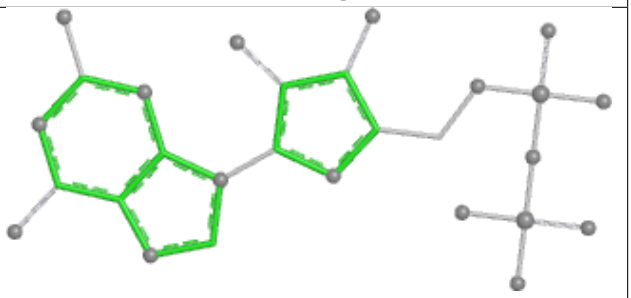
Bond lengths



Bond angles

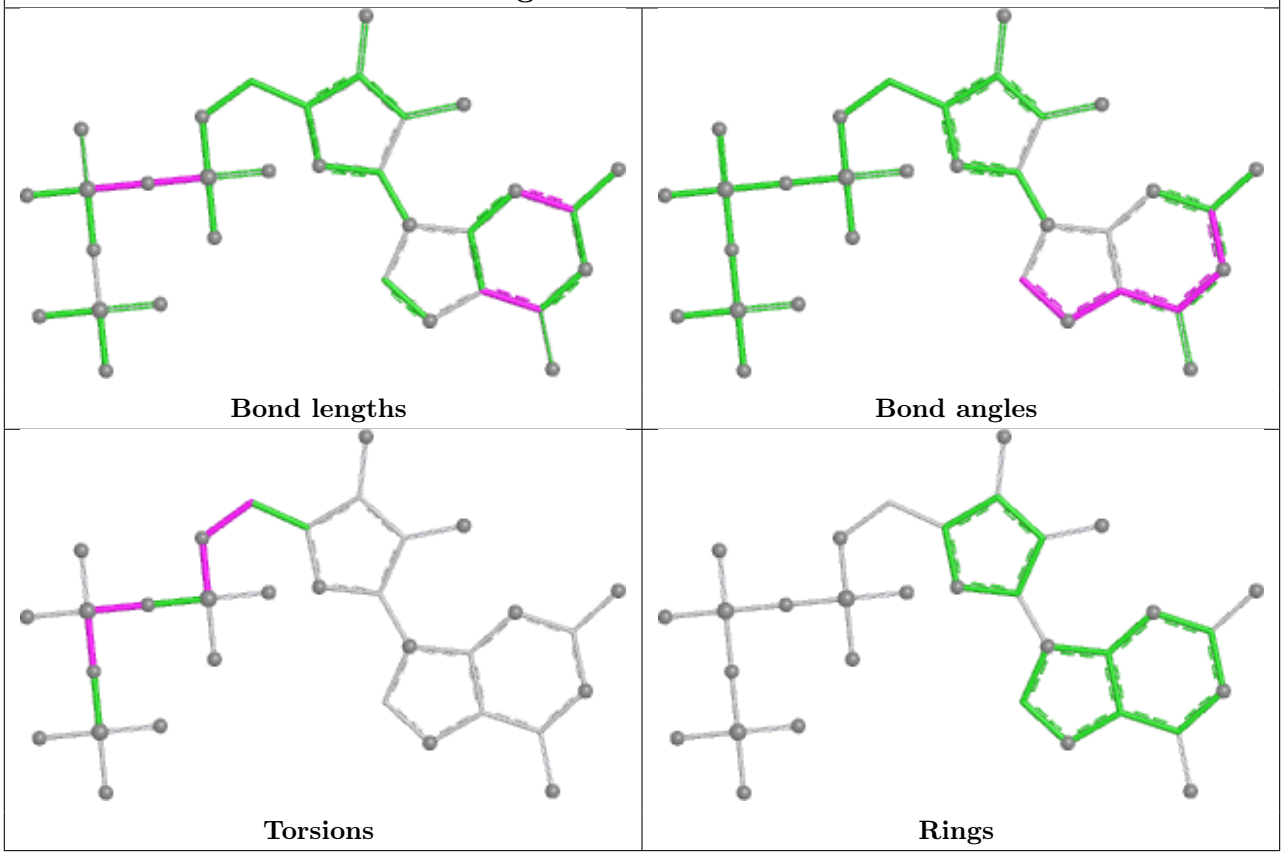


Torsions

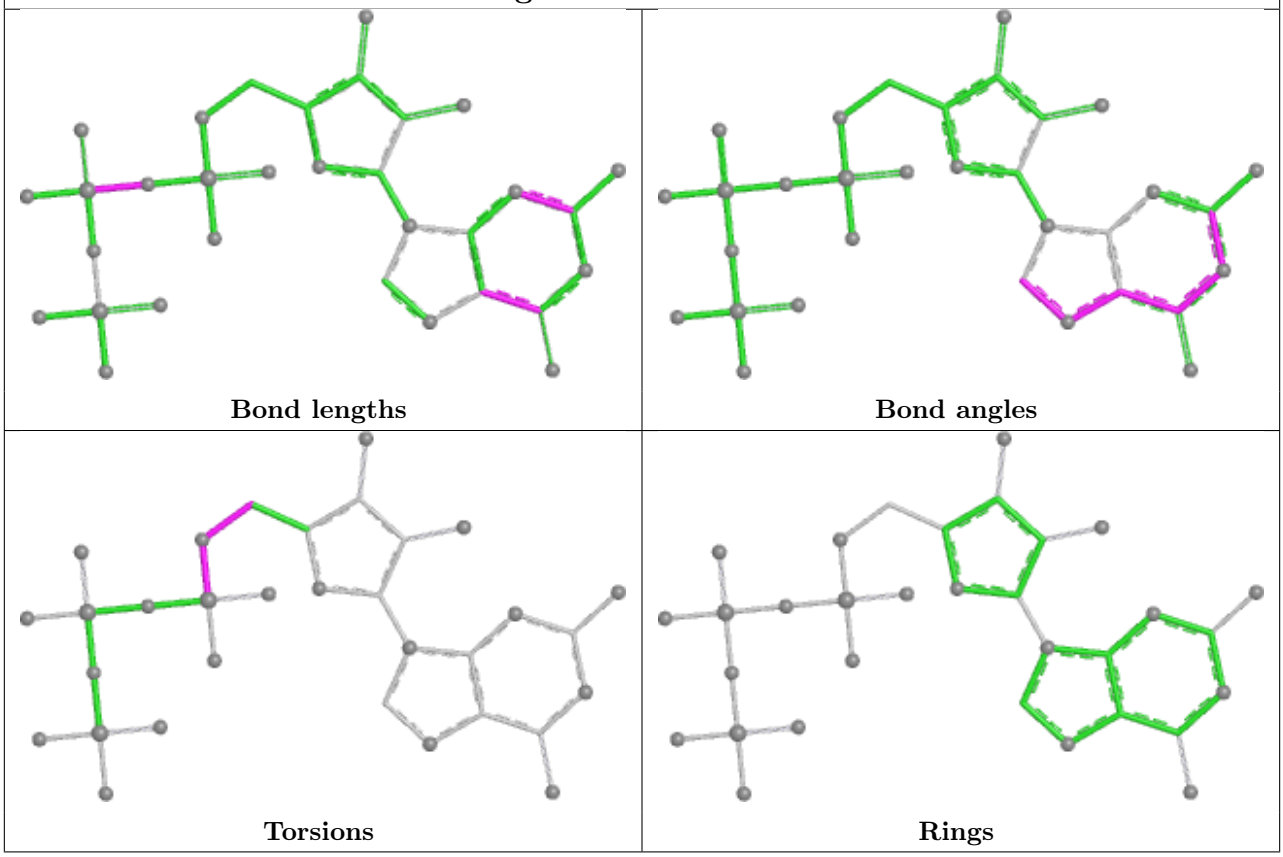


Rings

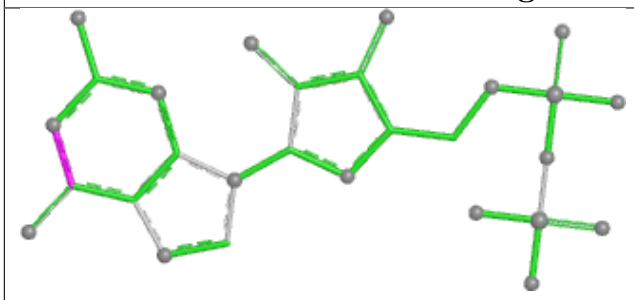
Ligand GTP Ee 501



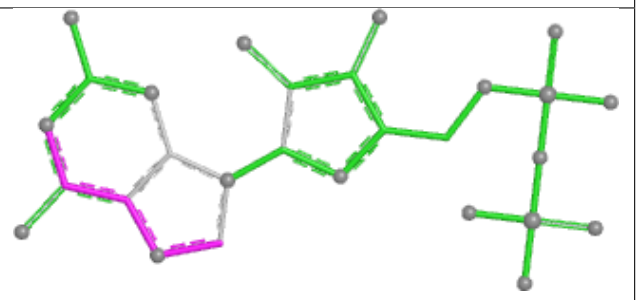
Ligand GTP B4 602



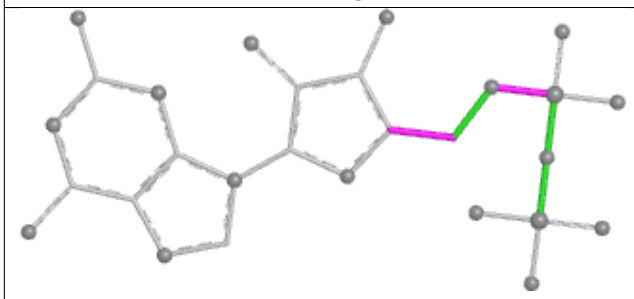
Ligand GDP Bi 501



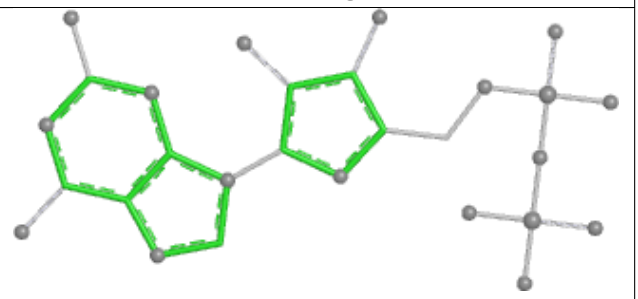
Bond lengths



Bond angles

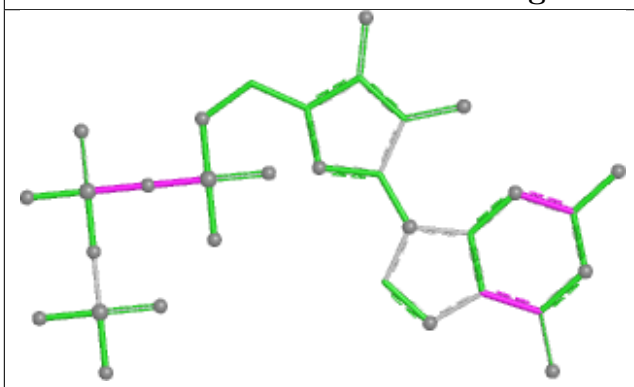


Torsions

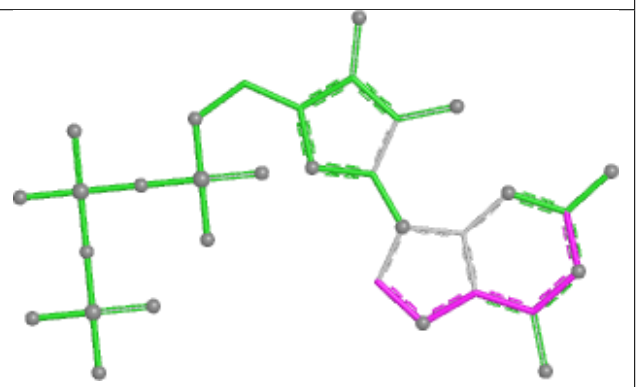


Rings

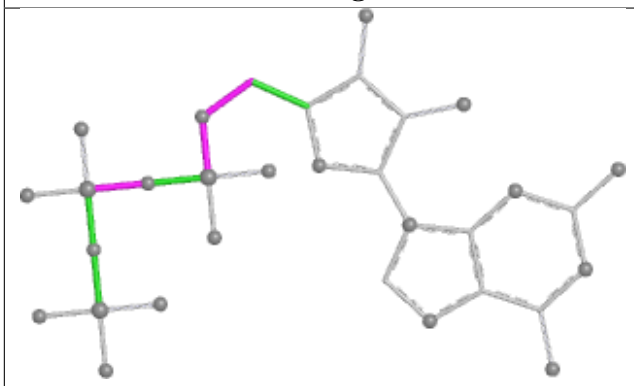
Ligand GTP e 602



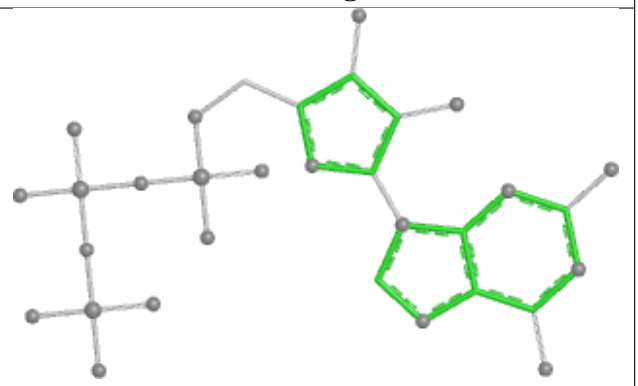
Bond lengths



Bond angles

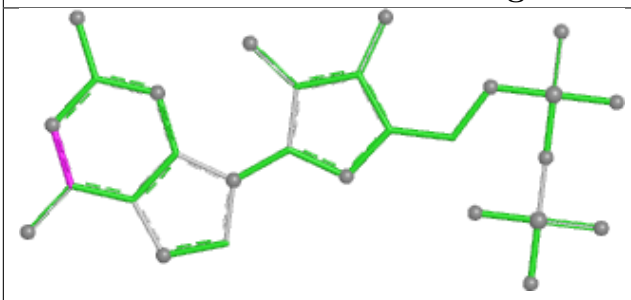


Torsions

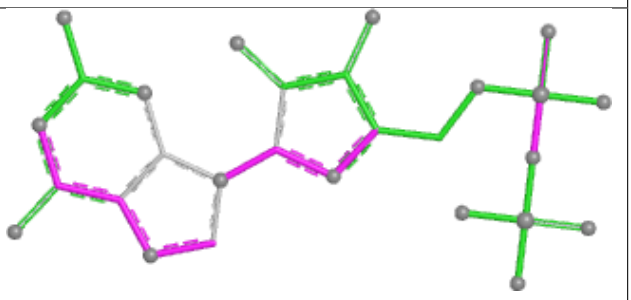


Rings

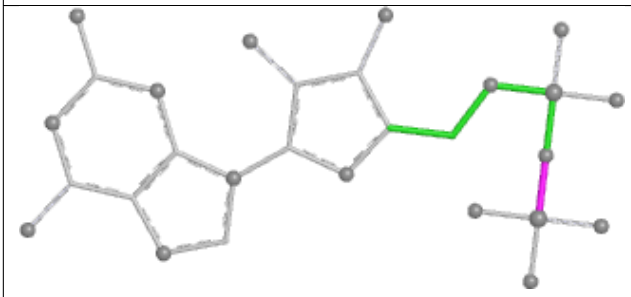
Ligand GDP DR 501



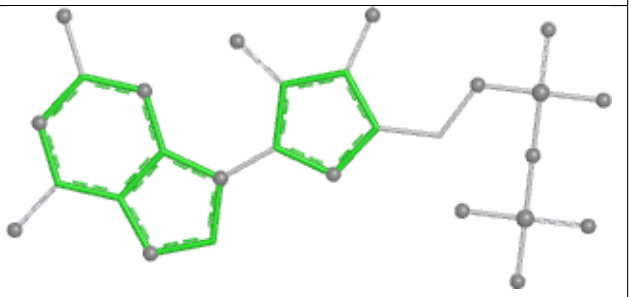
Bond lengths



Bond angles

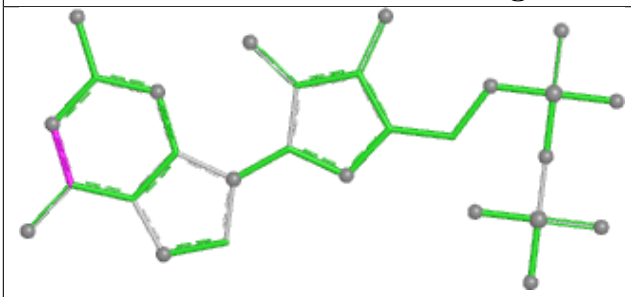


Torsions

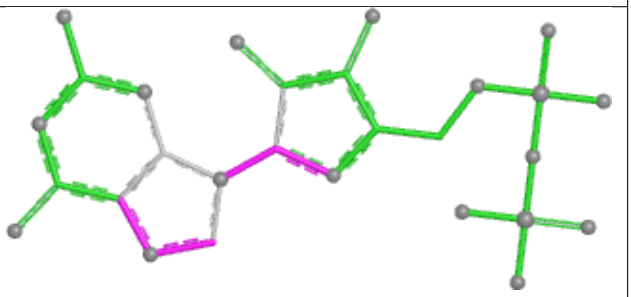


Rings

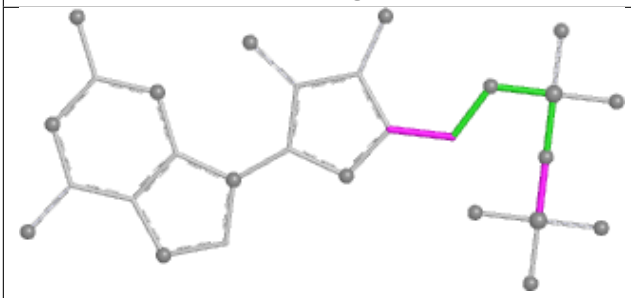
Ligand GDP GZ 501



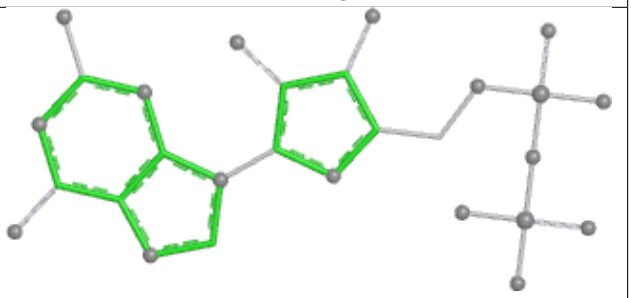
Bond lengths



Bond angles

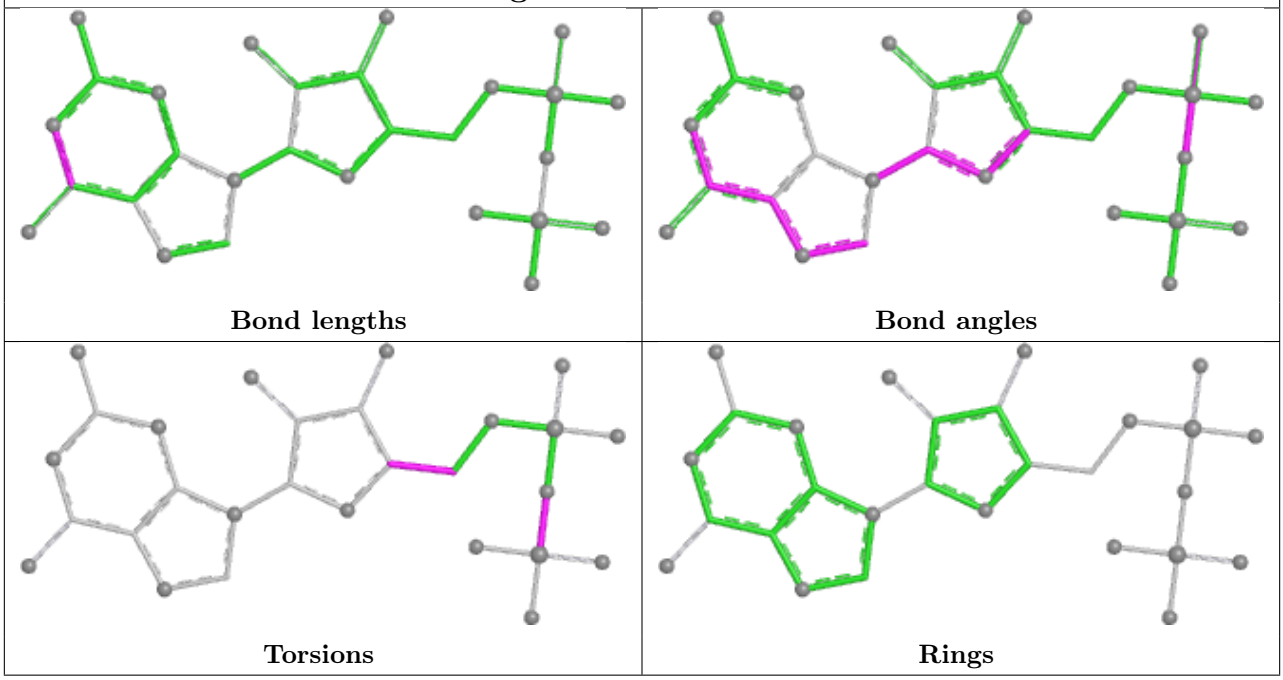


Torsions

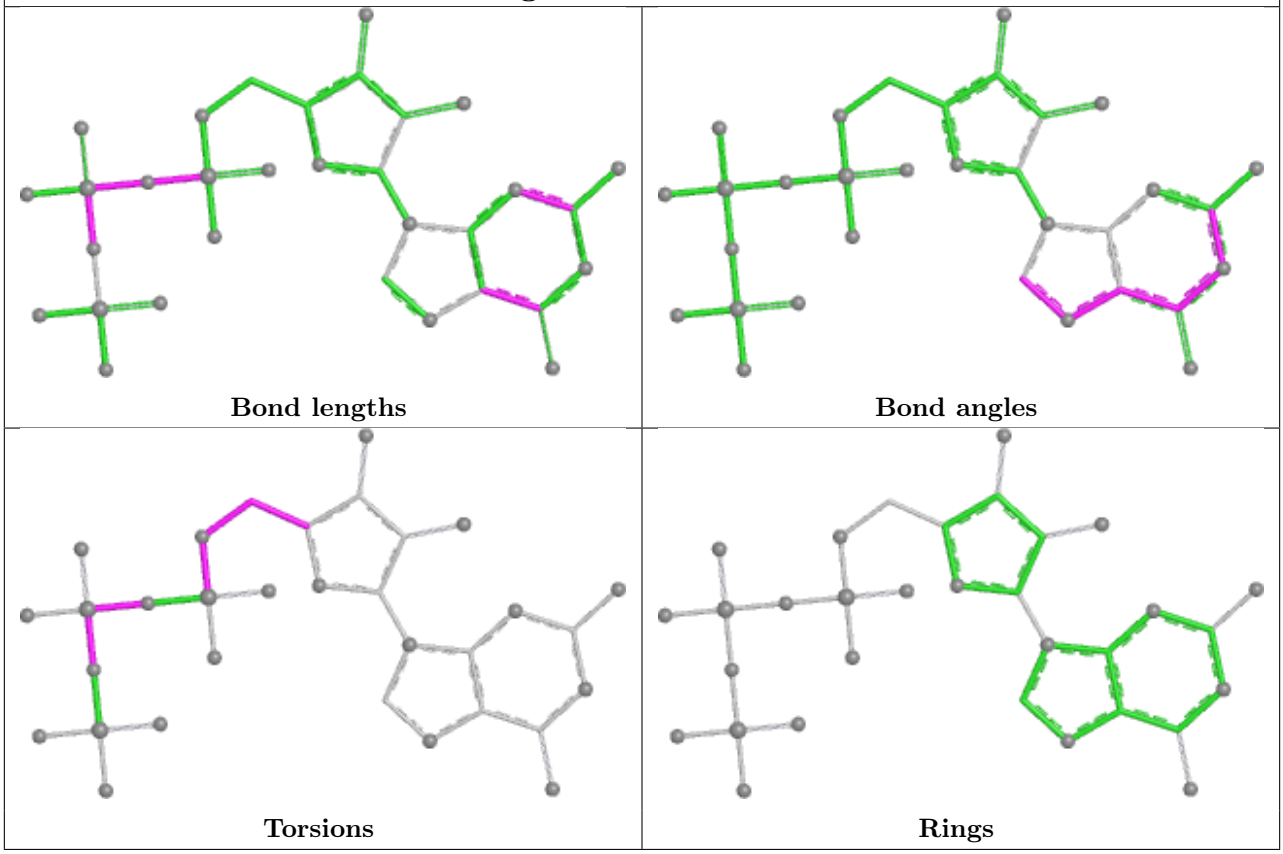


Rings

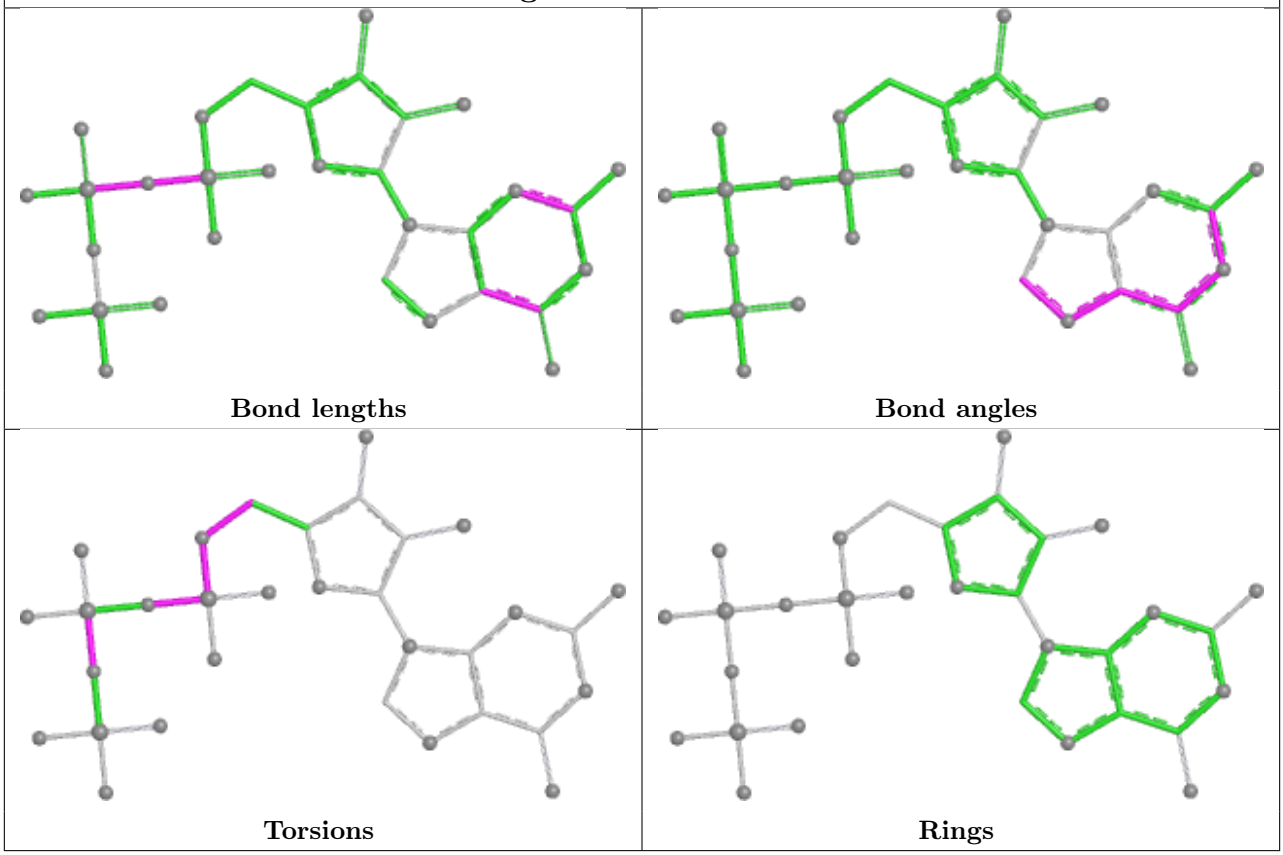
Ligand GDP EO 501



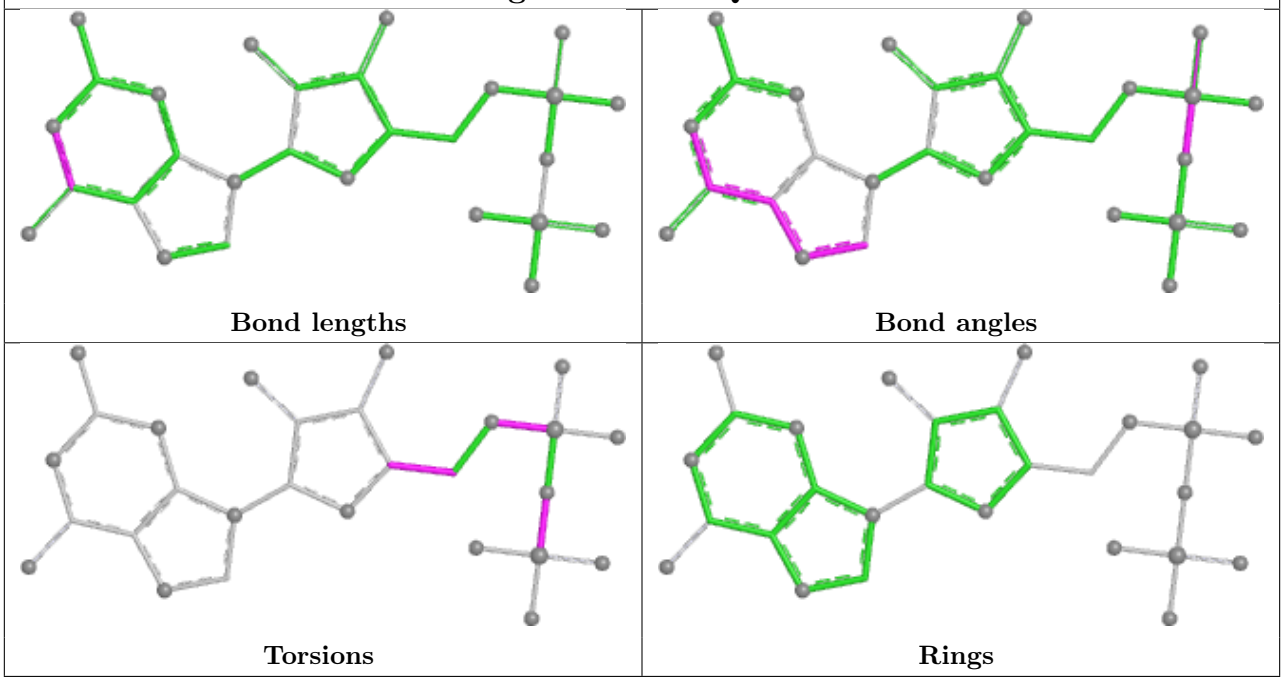
Ligand GTP Ei 501



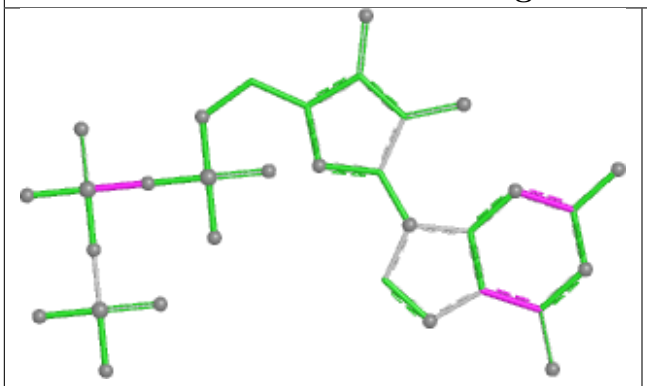
Ligand GTP El 501



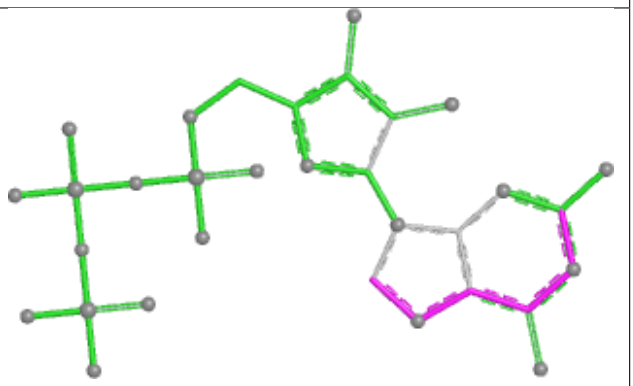
Ligand GDP DQ 501



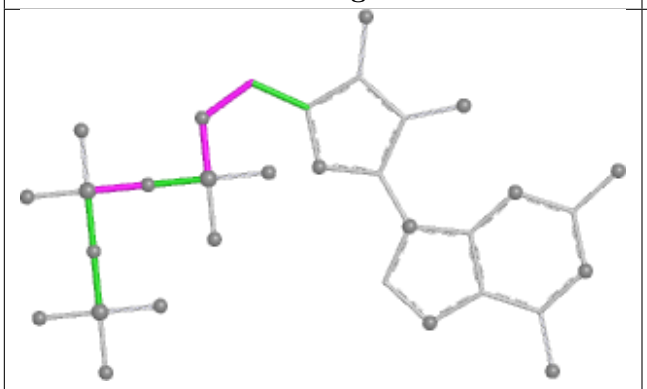
Ligand GTP B3 602



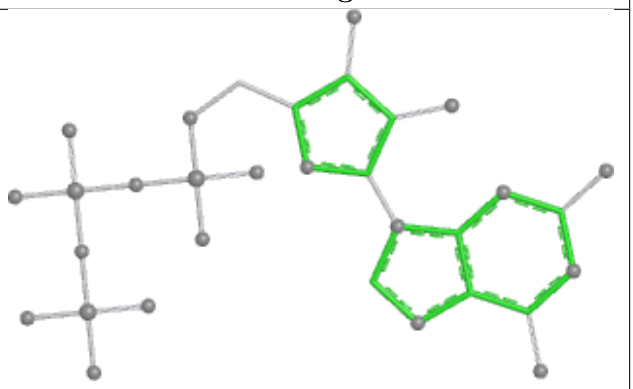
Bond lengths



Bond angles

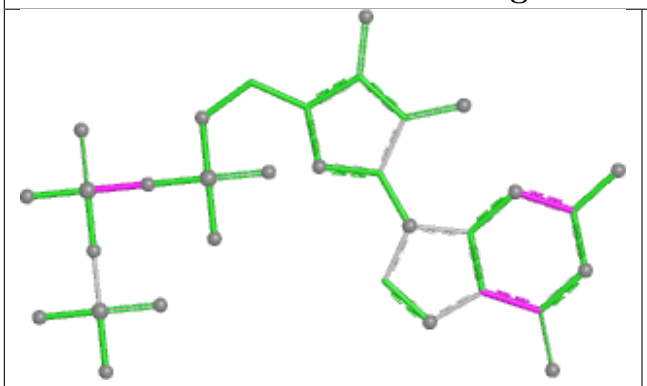


Torsions

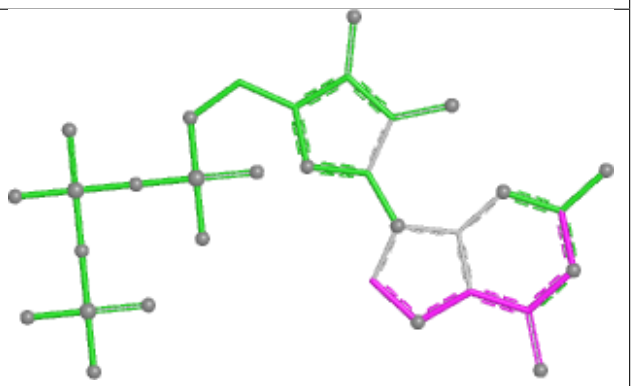


Rings

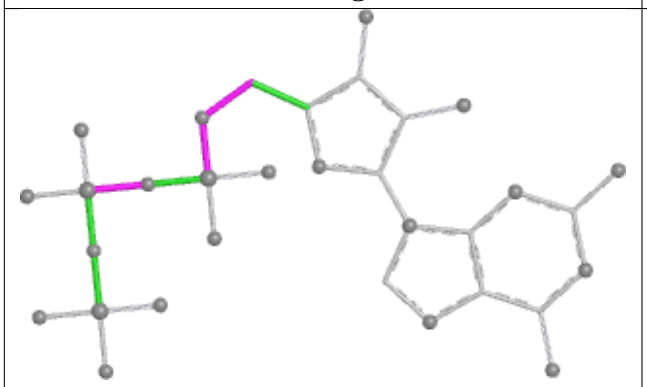
Ligand GTP BO 602



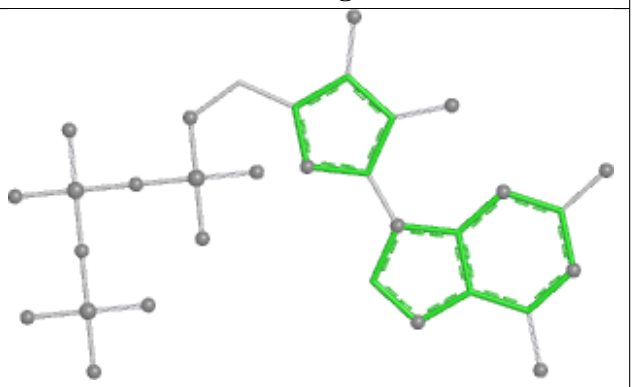
Bond lengths



Bond angles

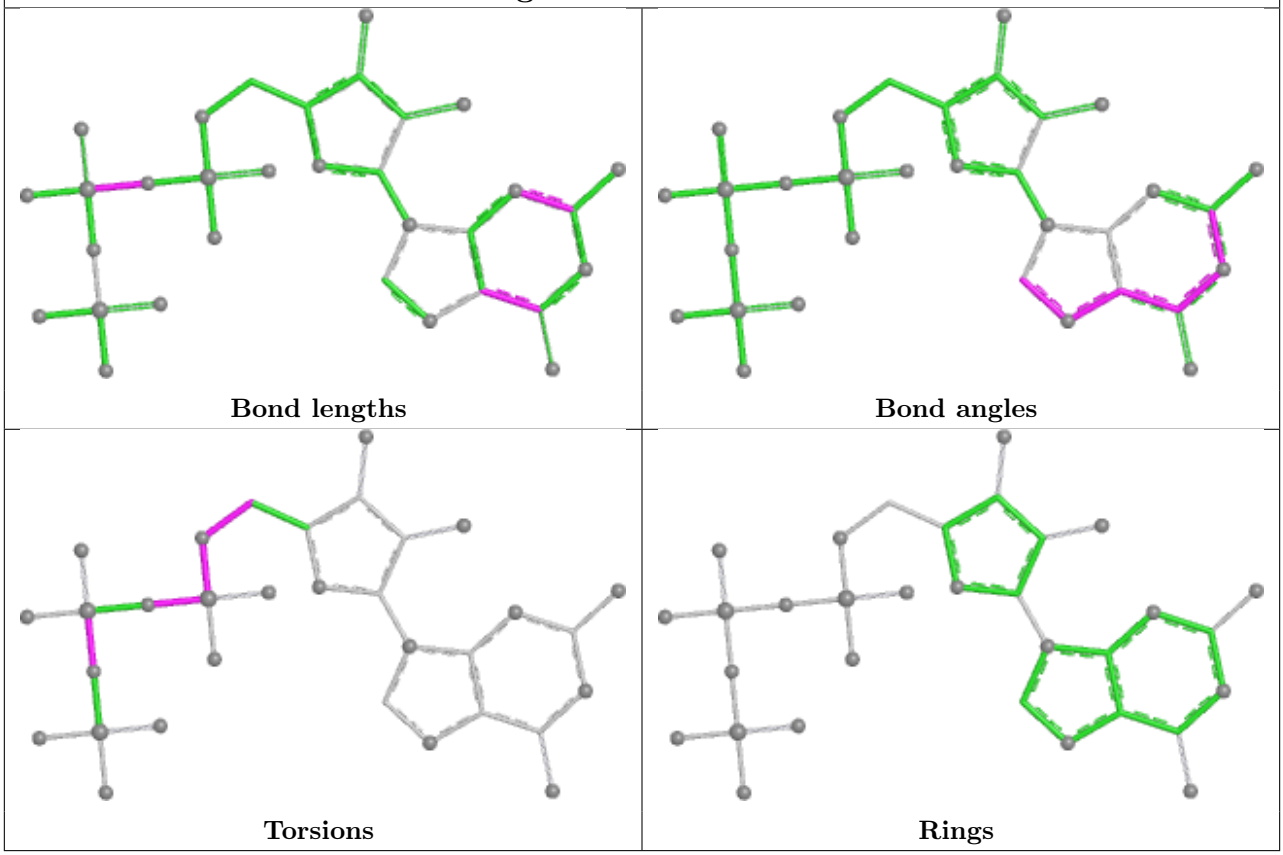


Torsions

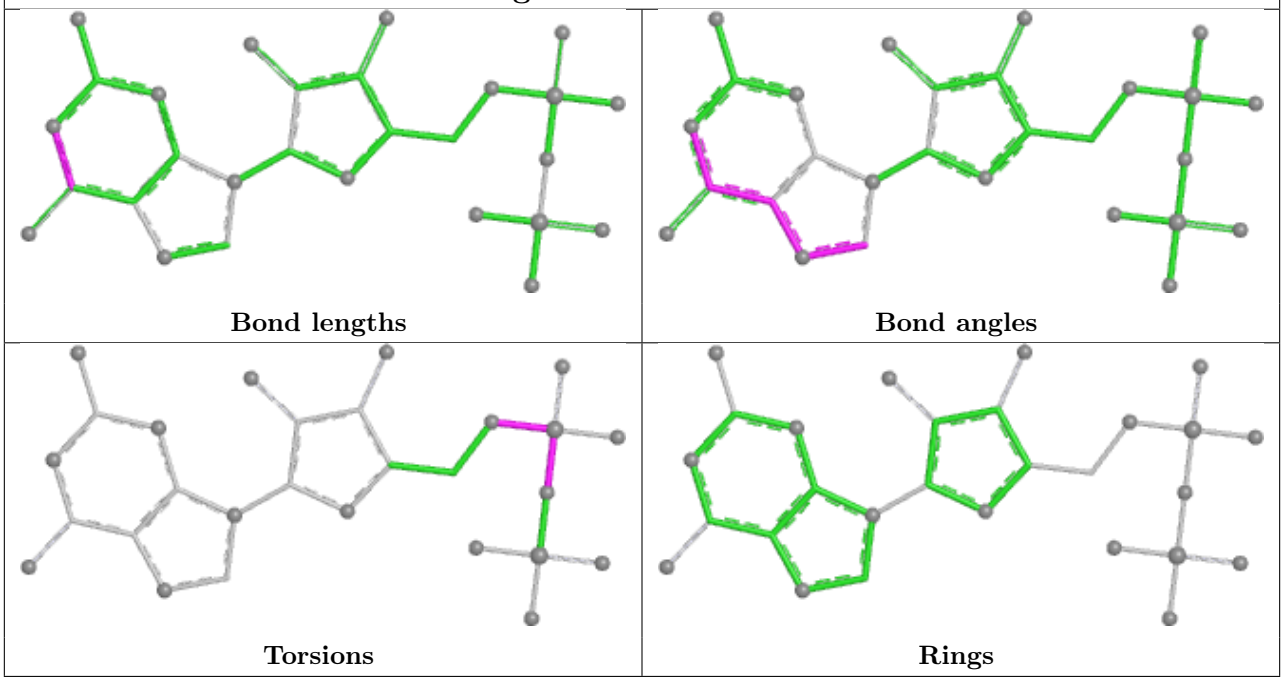


Rings

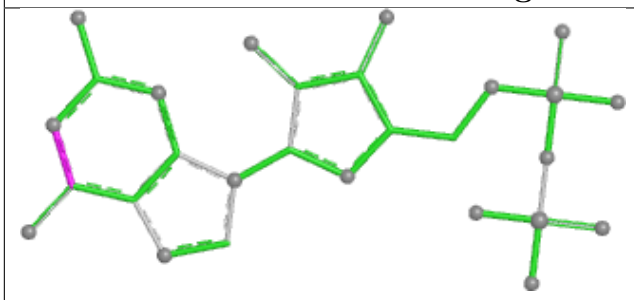
Ligand GTP F9 501



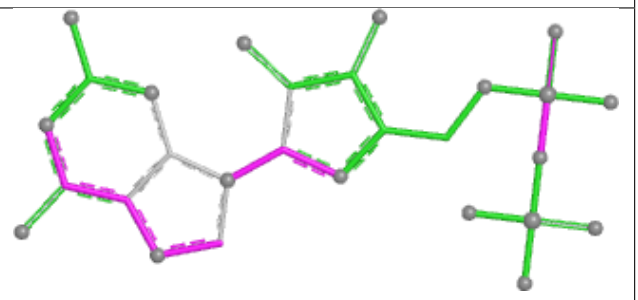
Ligand GDP A0 501



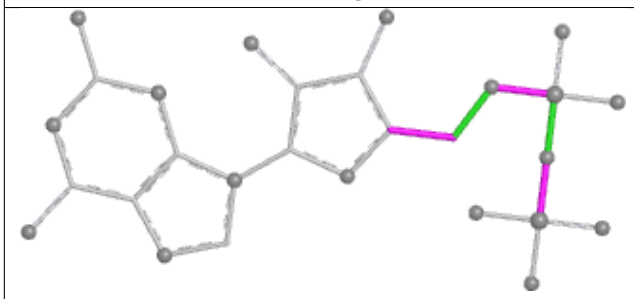
Ligand GDP E0 501



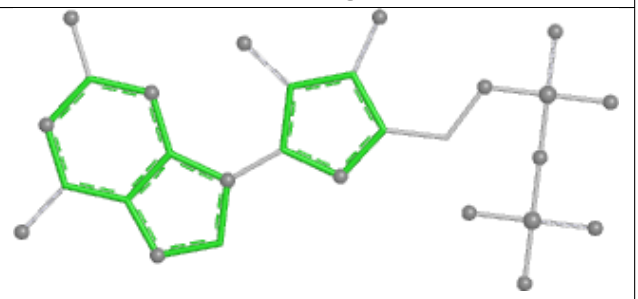
Bond lengths



Bond angles

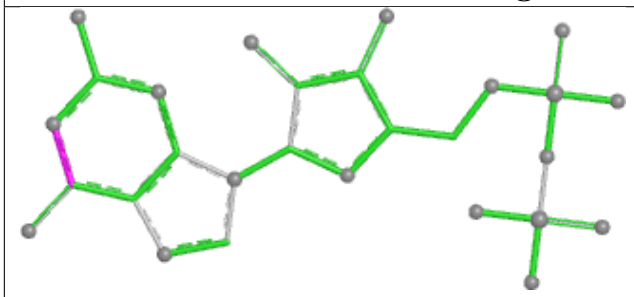


Torsions

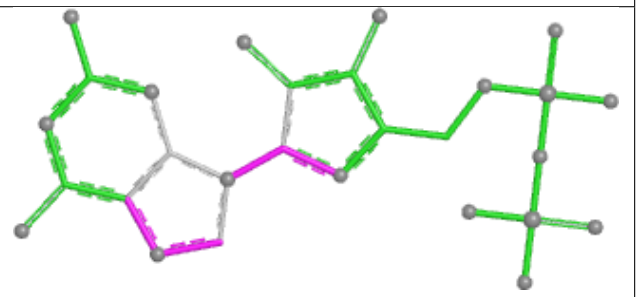


Rings

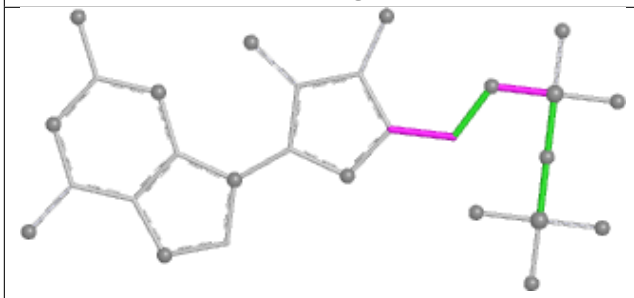
Ligand GDP At 501



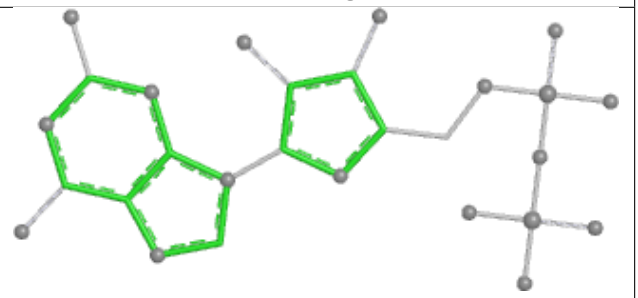
Bond lengths



Bond angles

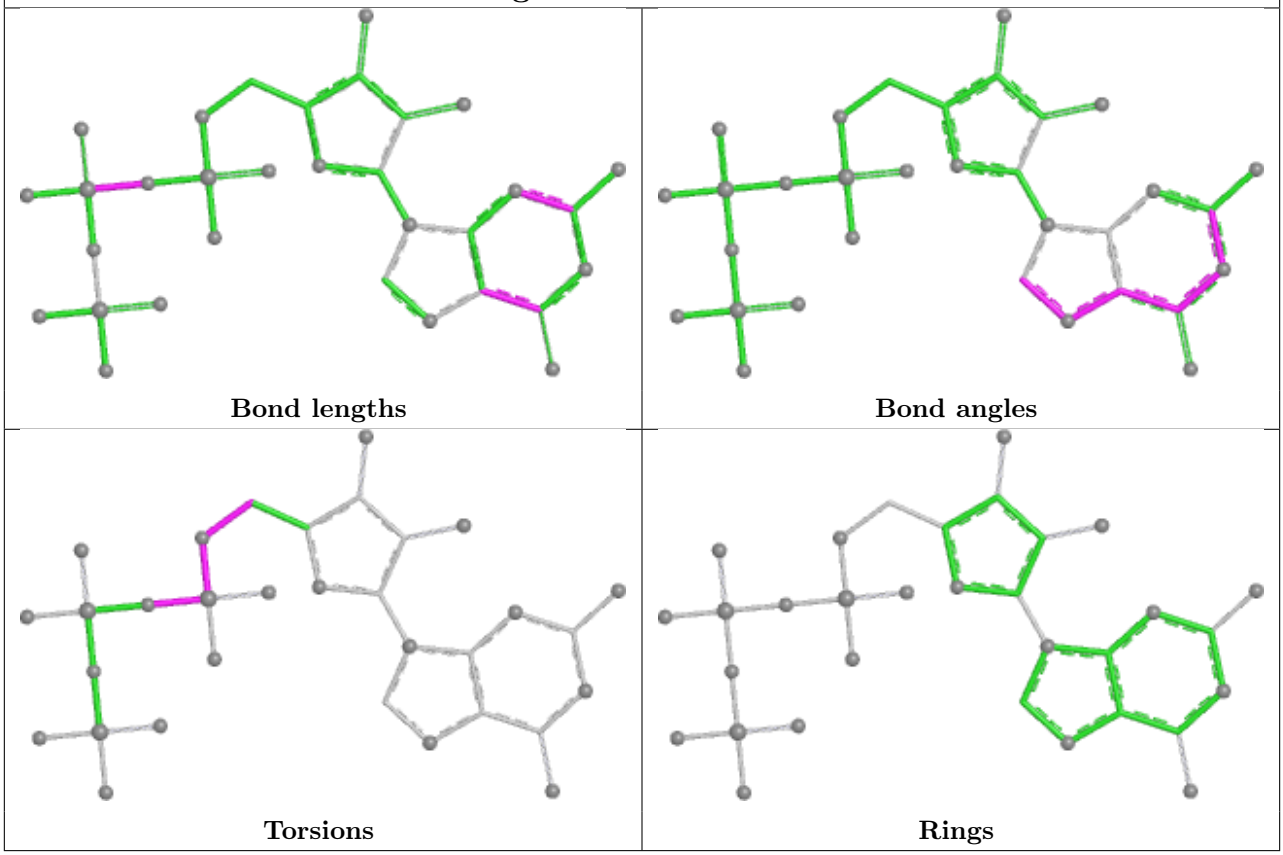


Torsions

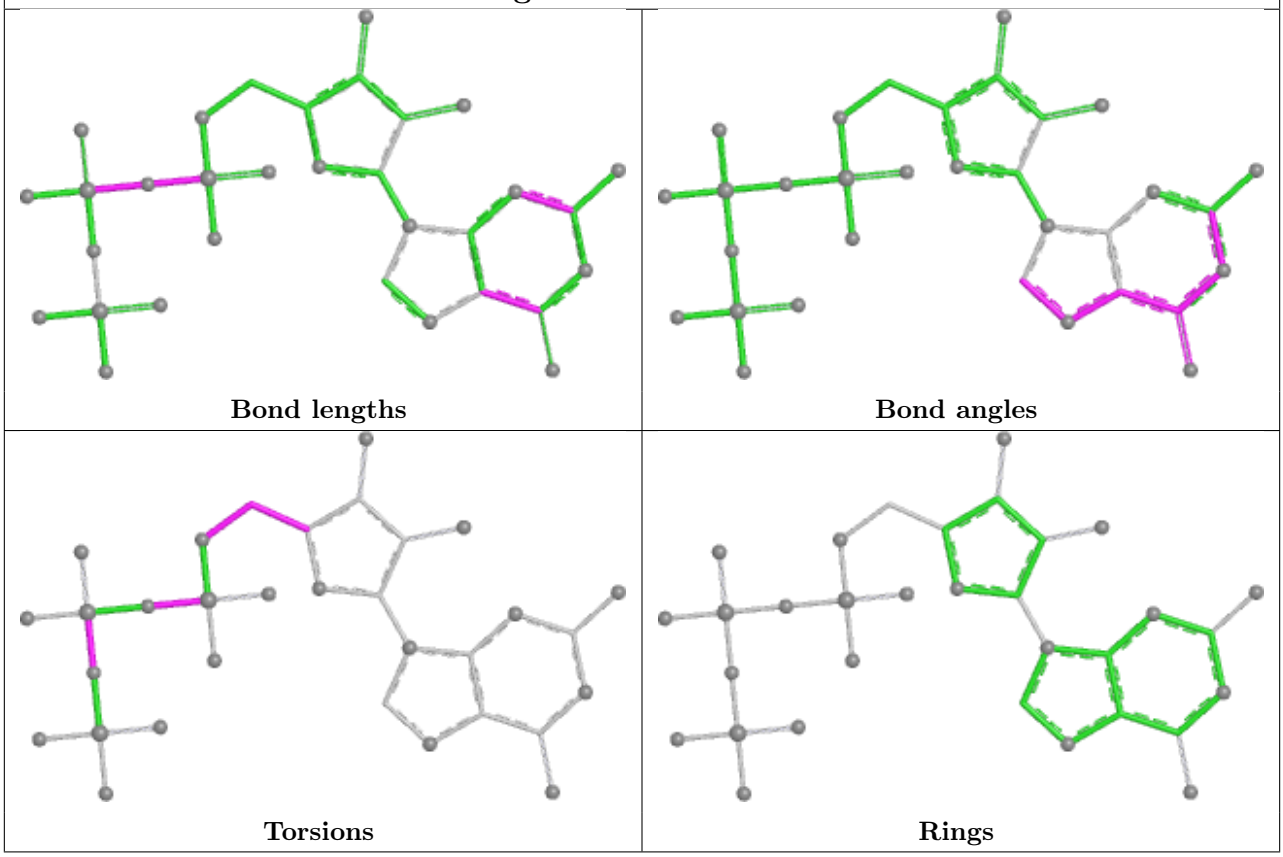


Rings

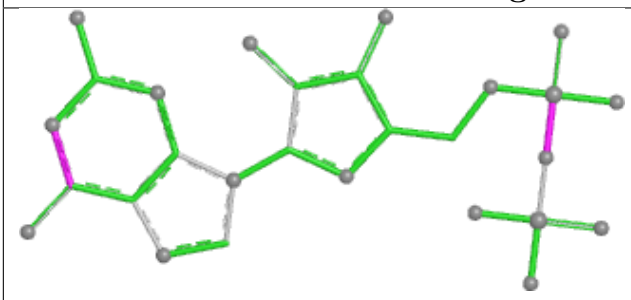
Ligand GTP FO 501



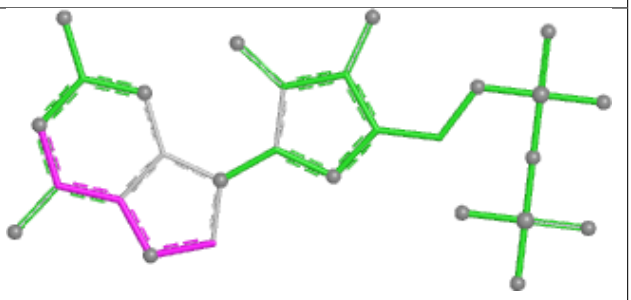
Ligand GTP Ak 602



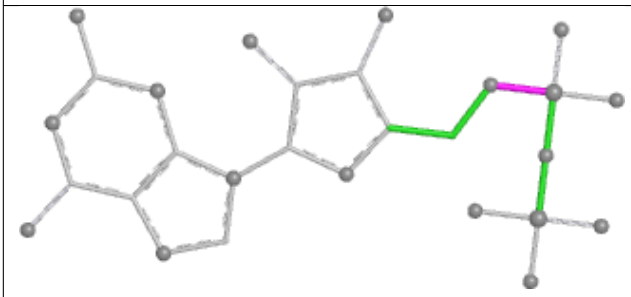
Ligand GDP AV 602



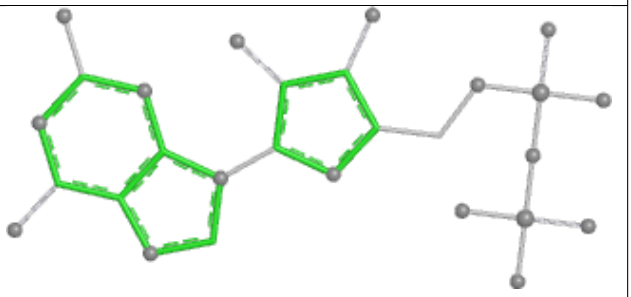
Bond lengths



Bond angles

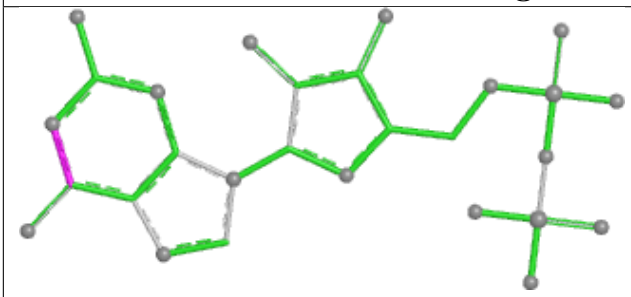


Torsions

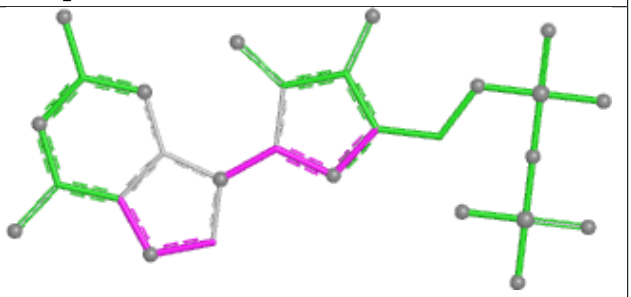


Rings

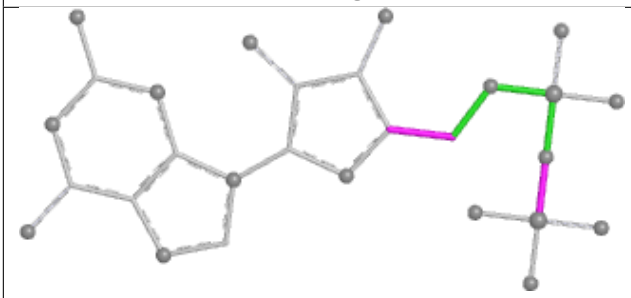
Ligand GDP Fp 501



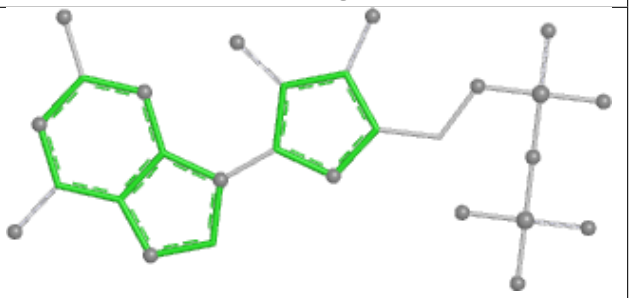
Bond lengths



Bond angles

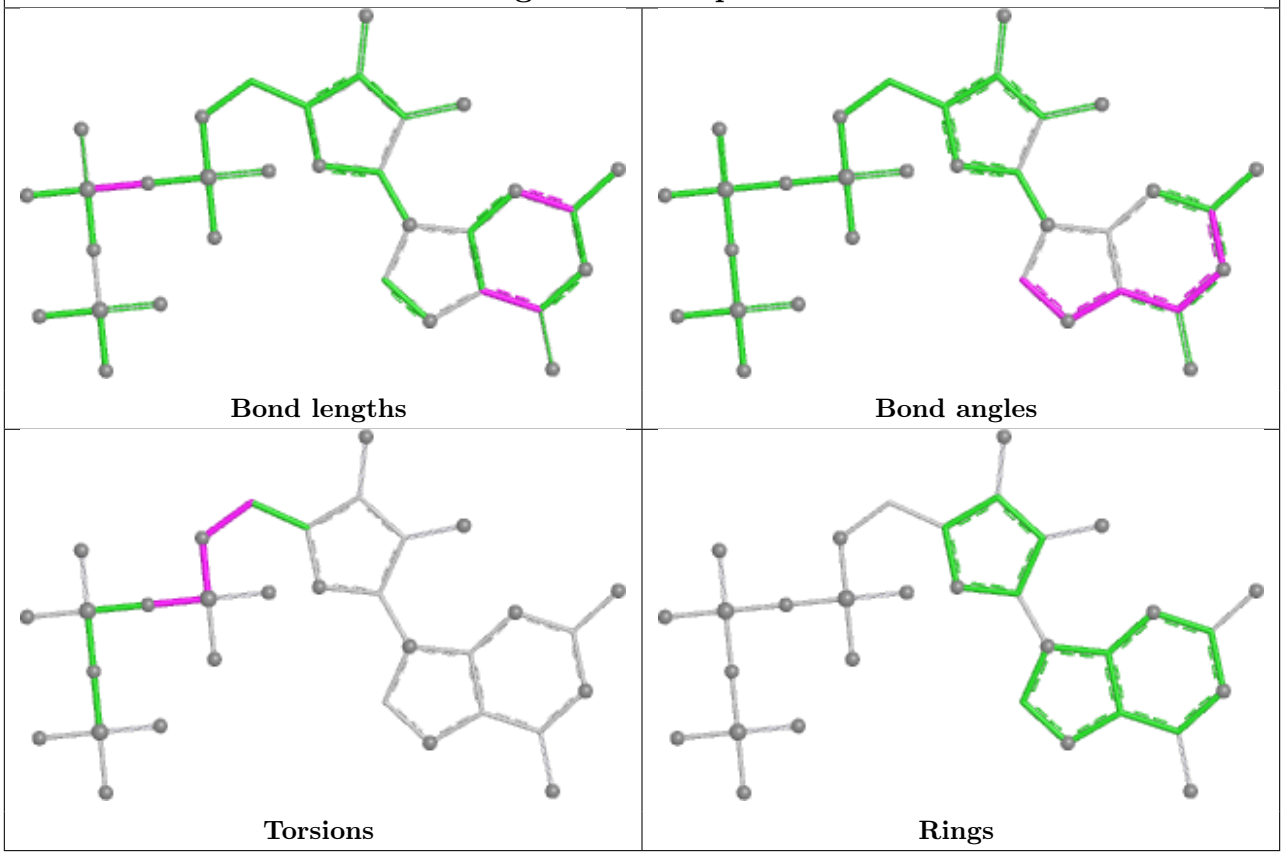


Torsions

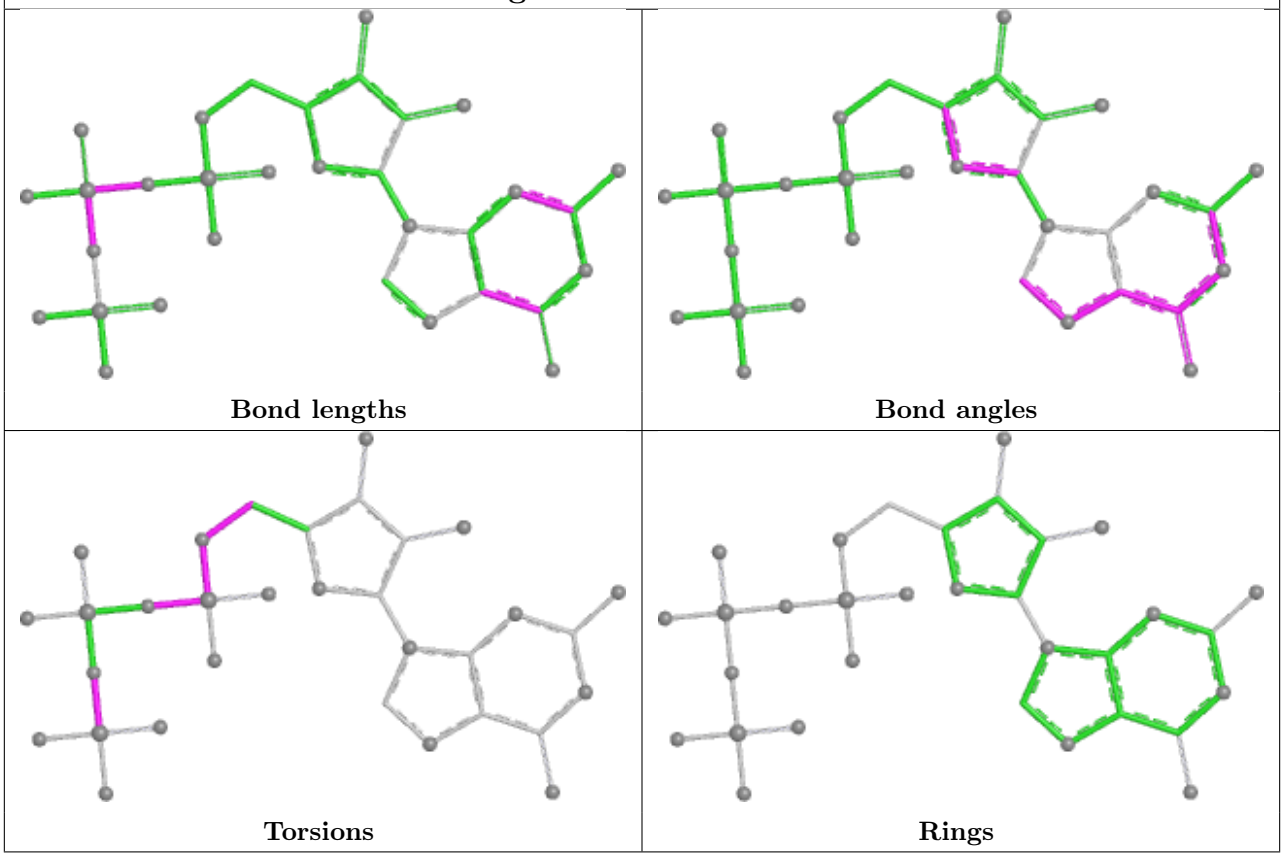


Rings

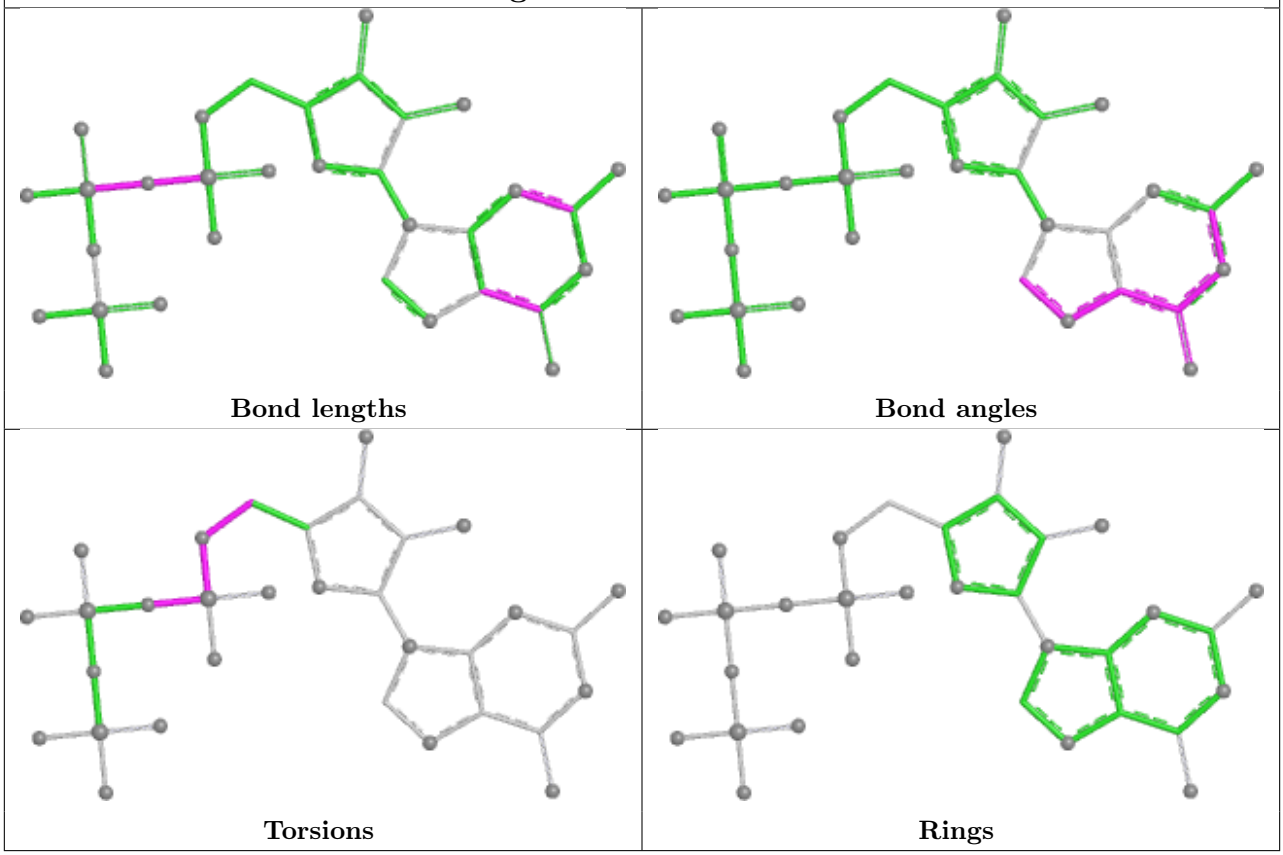
Ligand GTP Ep 501



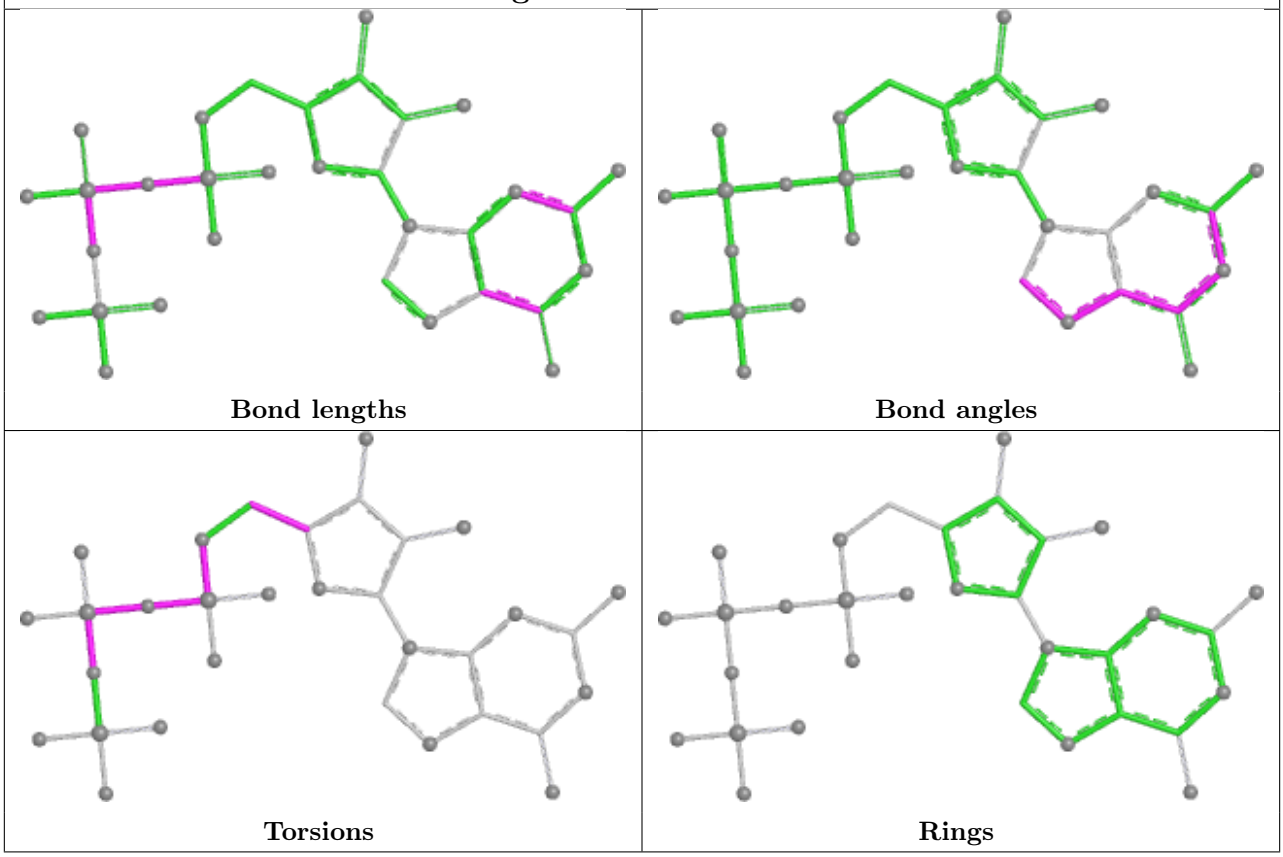
Ligand GTP GN 501



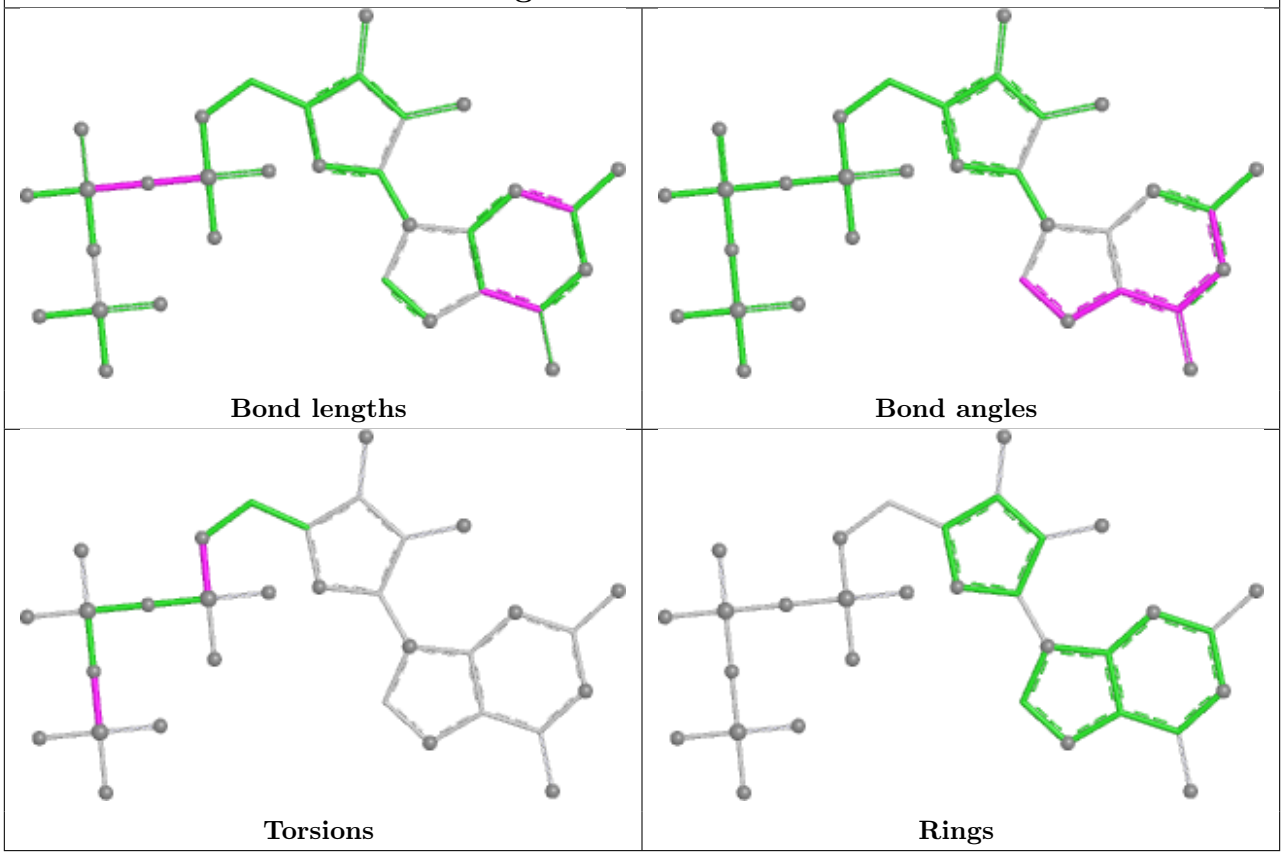
Ligand GTP Gw 501



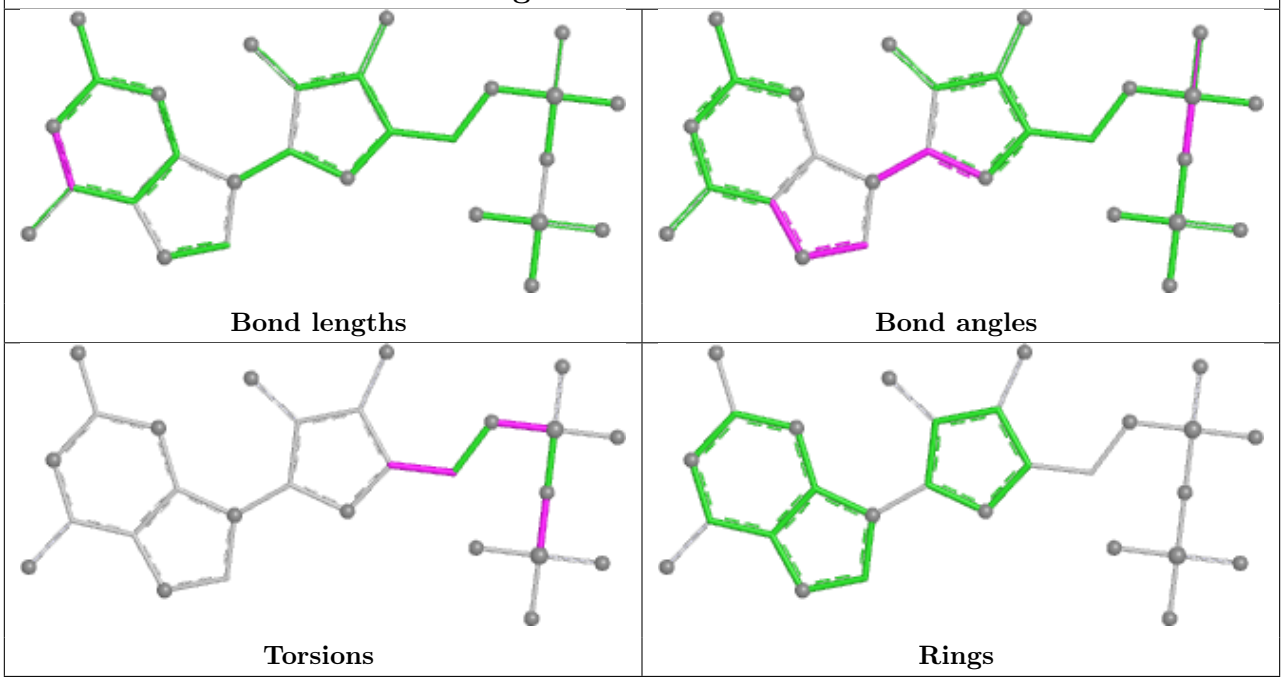
Ligand GTP Ew 501



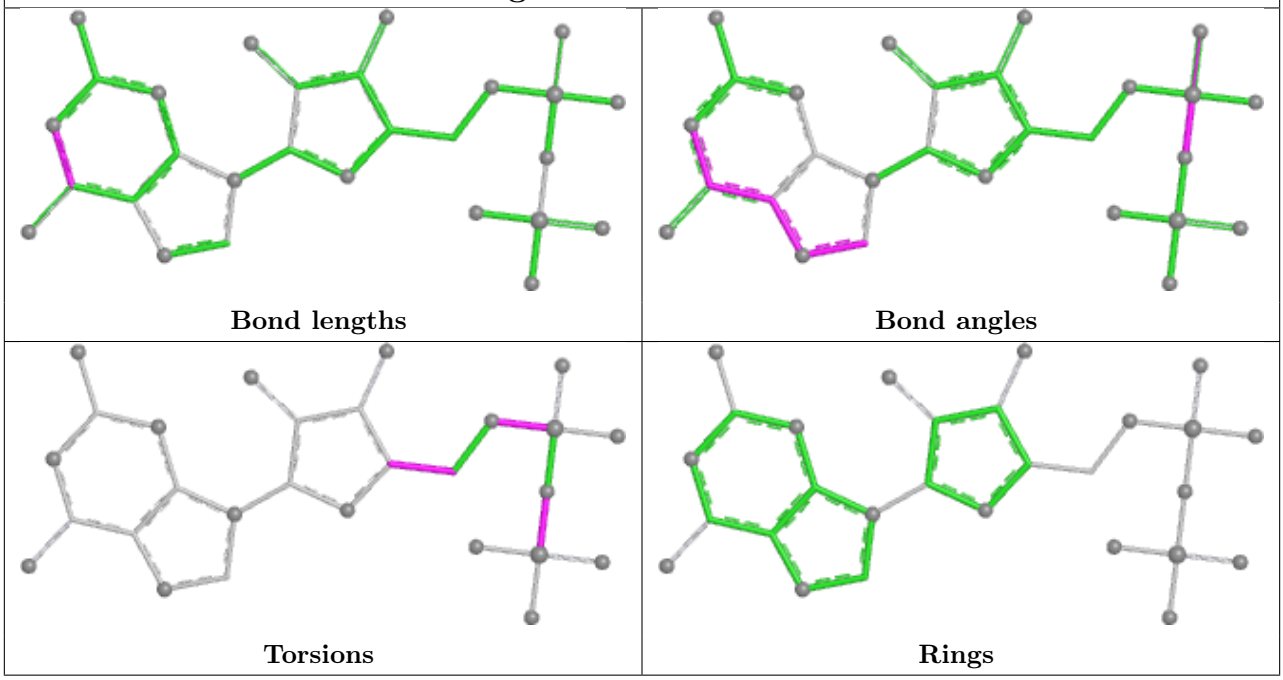
Ligand GTP B7 501



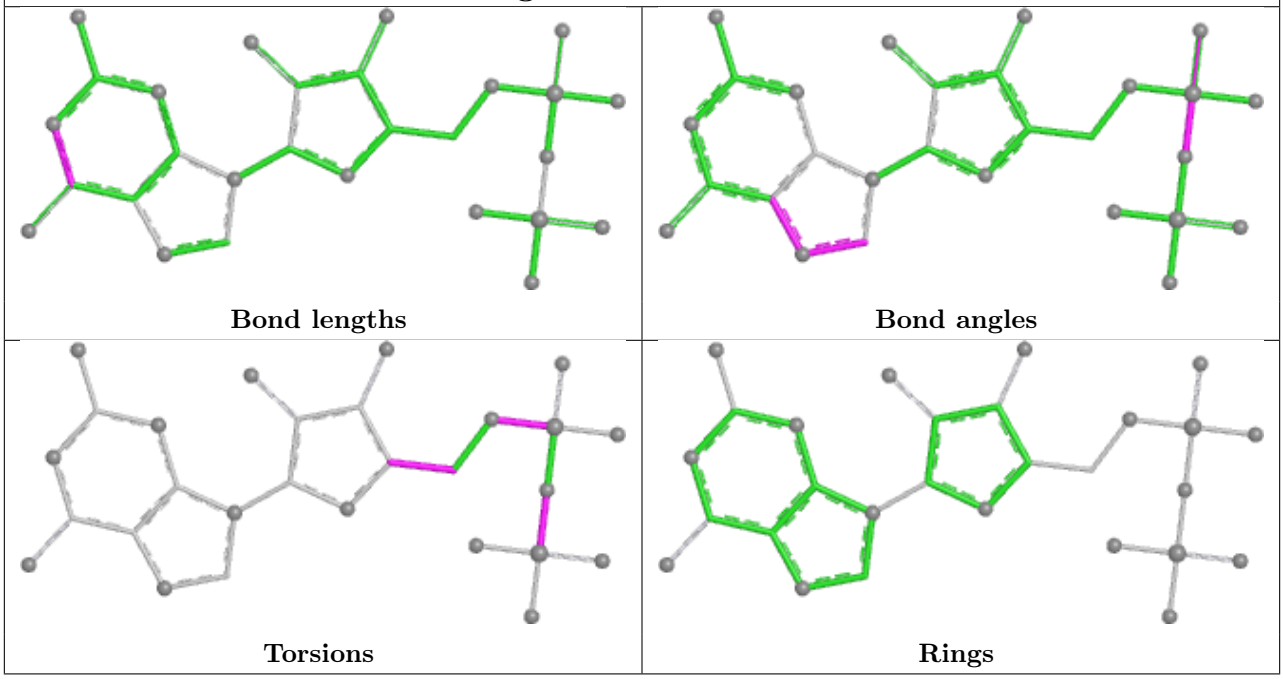
Ligand GDP EL 501



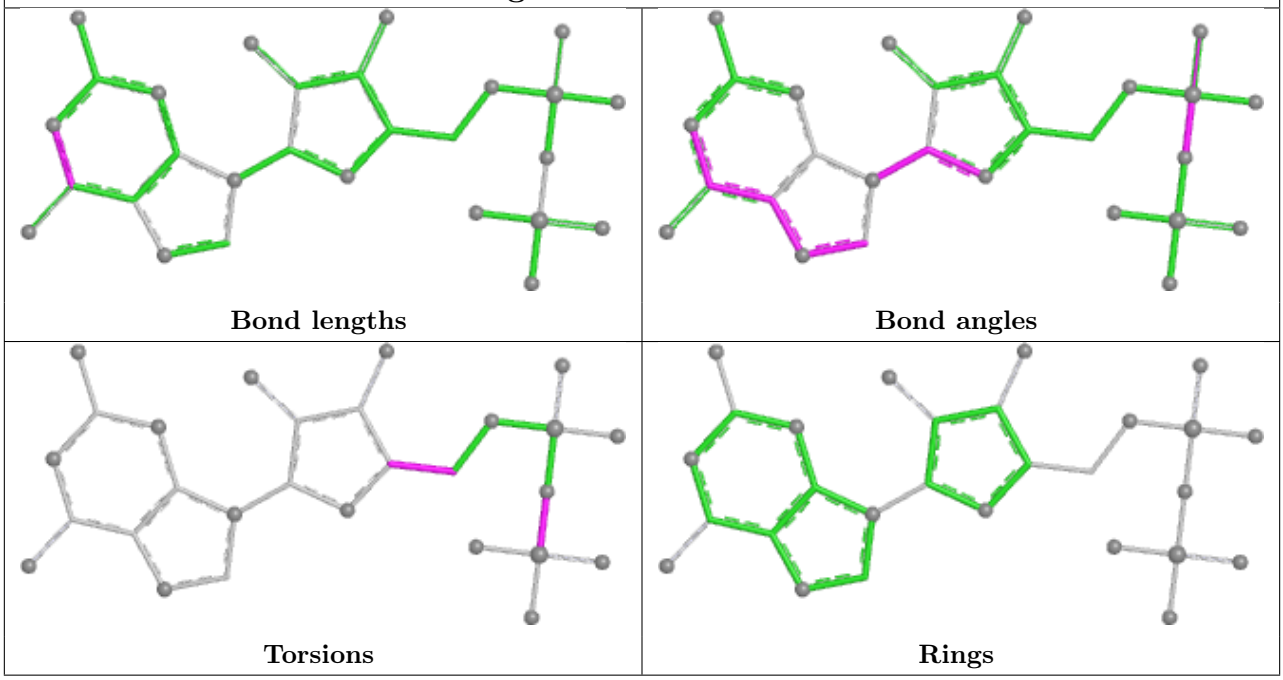
Ligand GDP DV 501



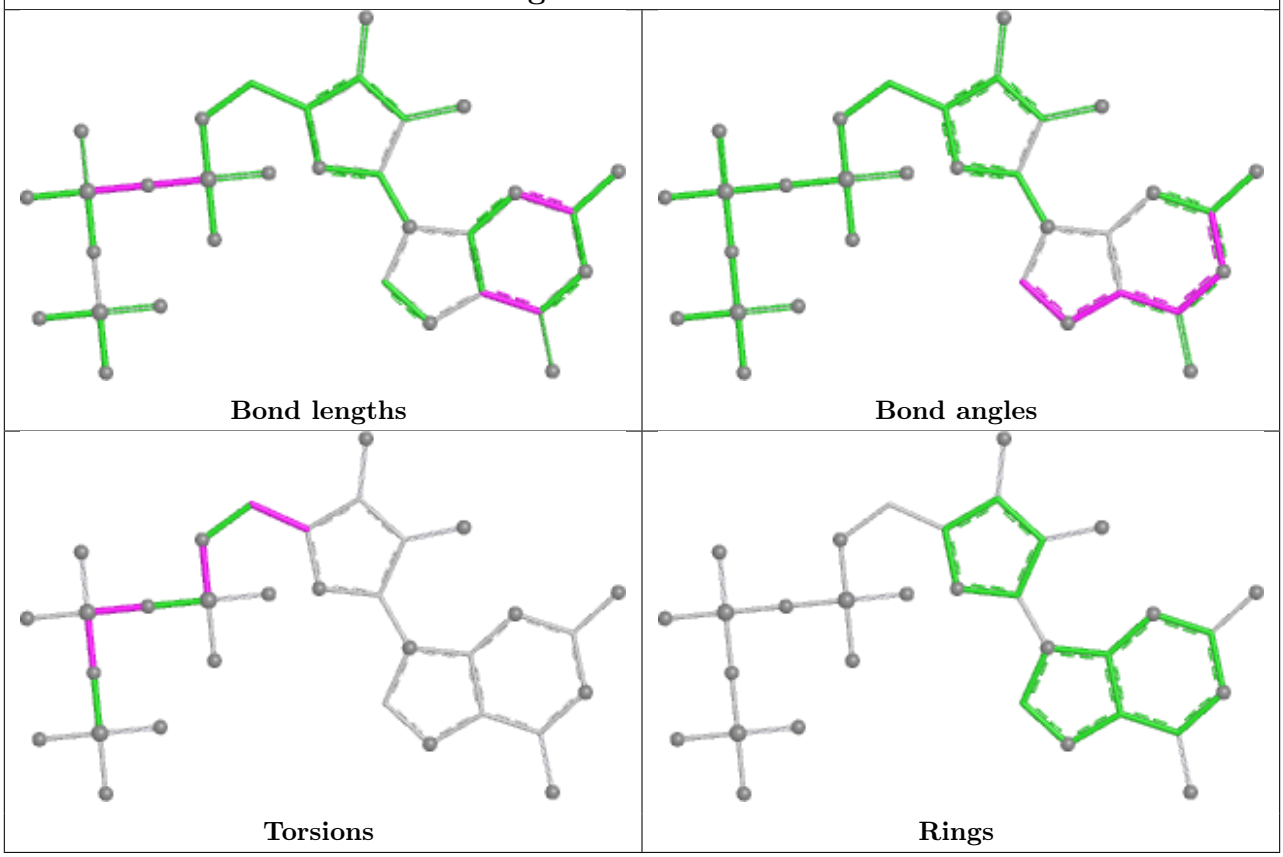
Ligand GDP Ft 501



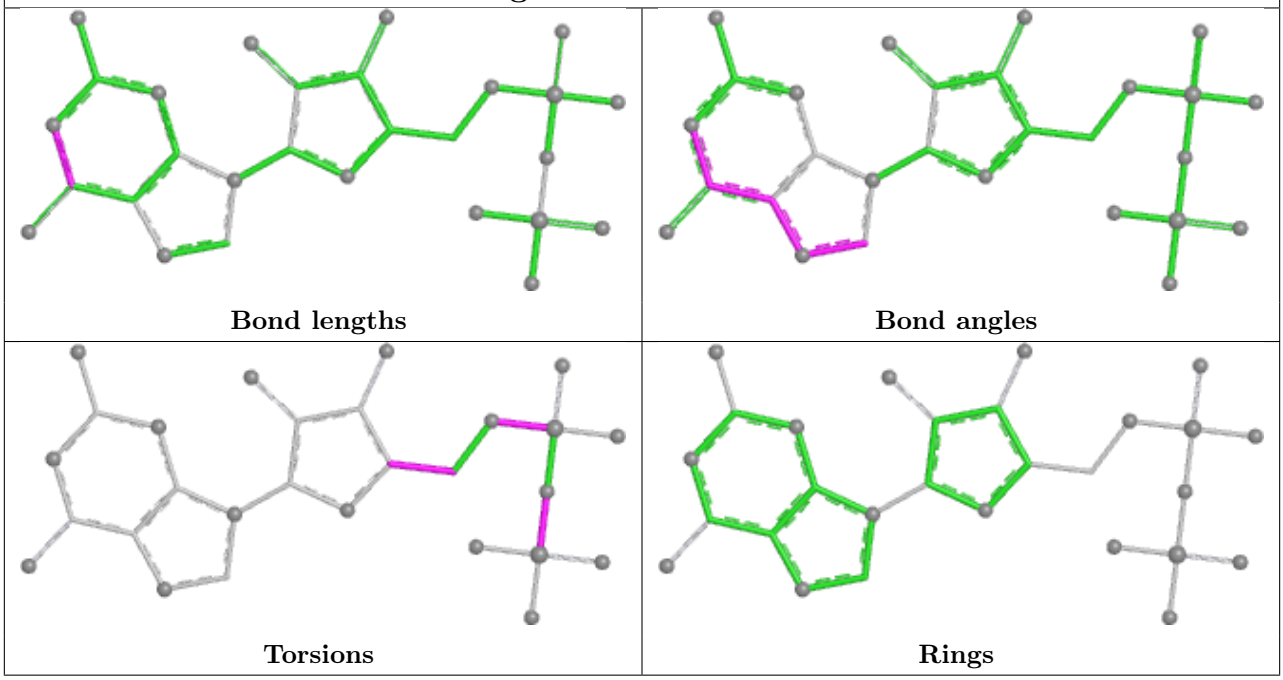
Ligand GDP GY 501



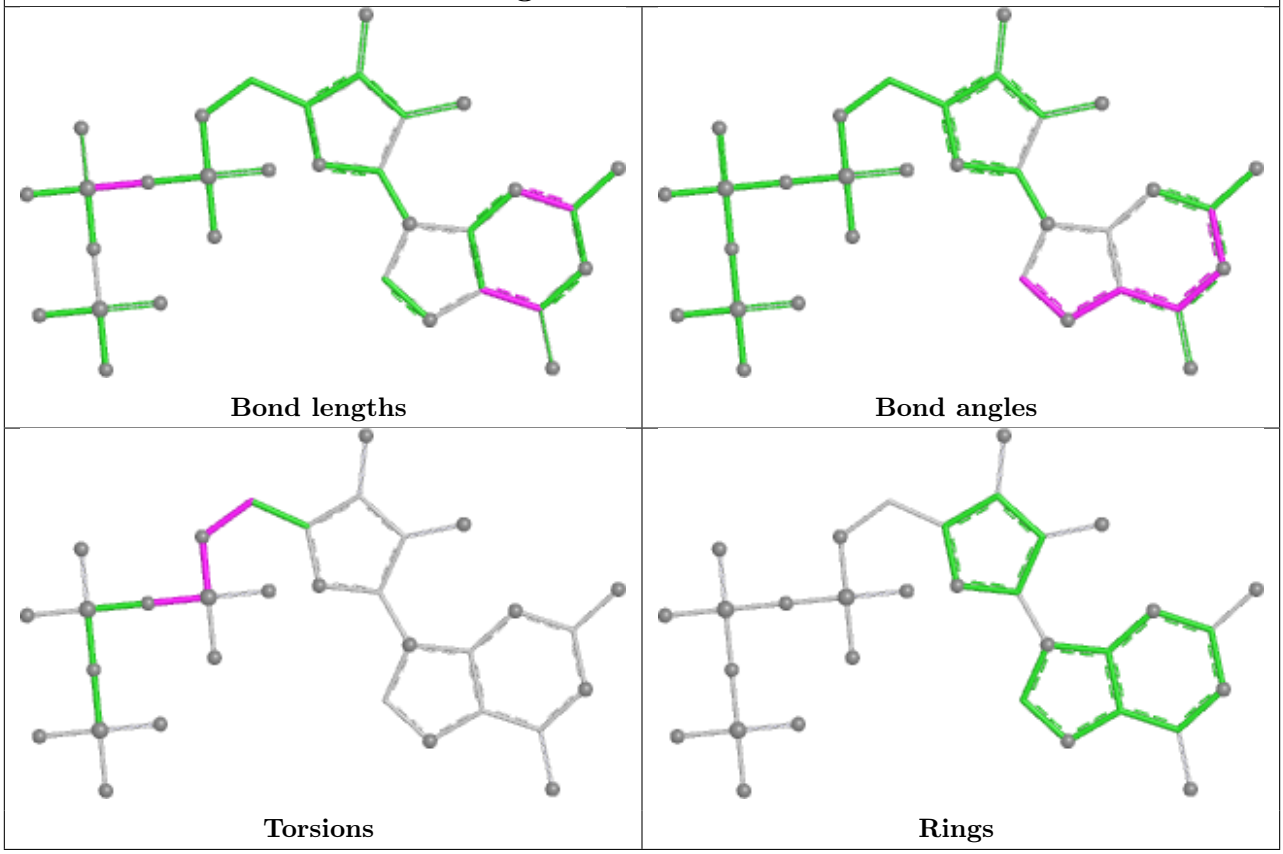
Ligand GTP a 602



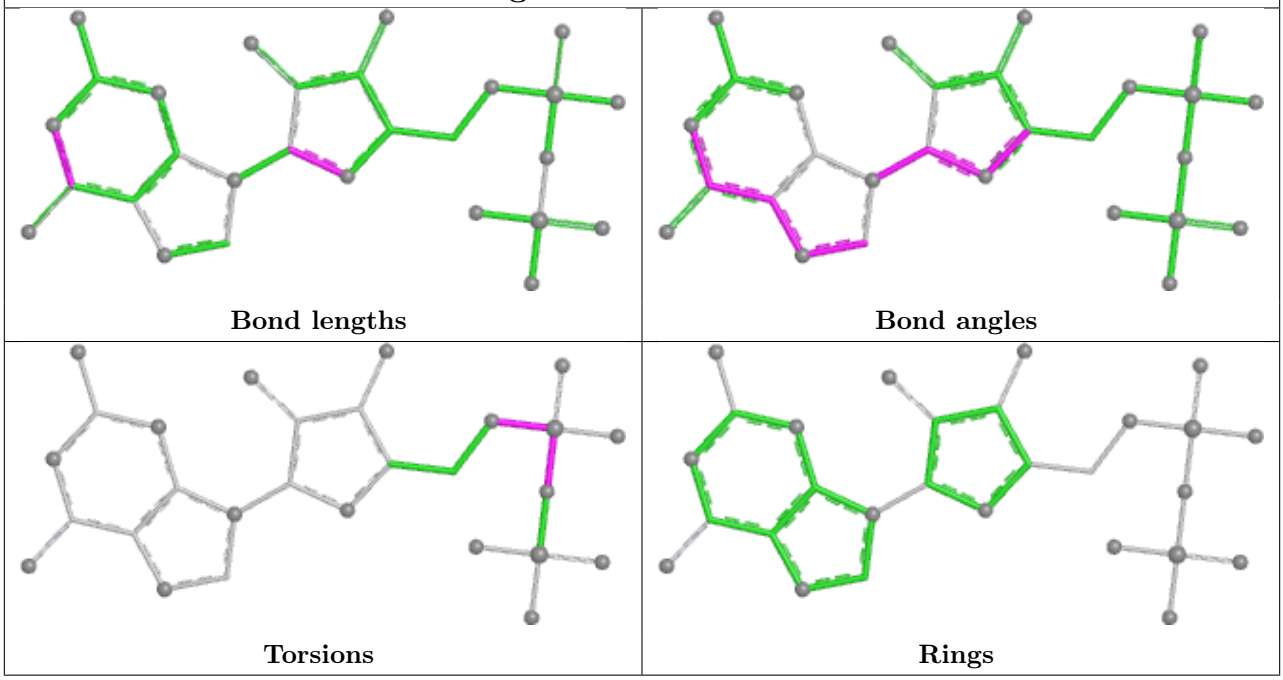
Ligand GDP BB 501



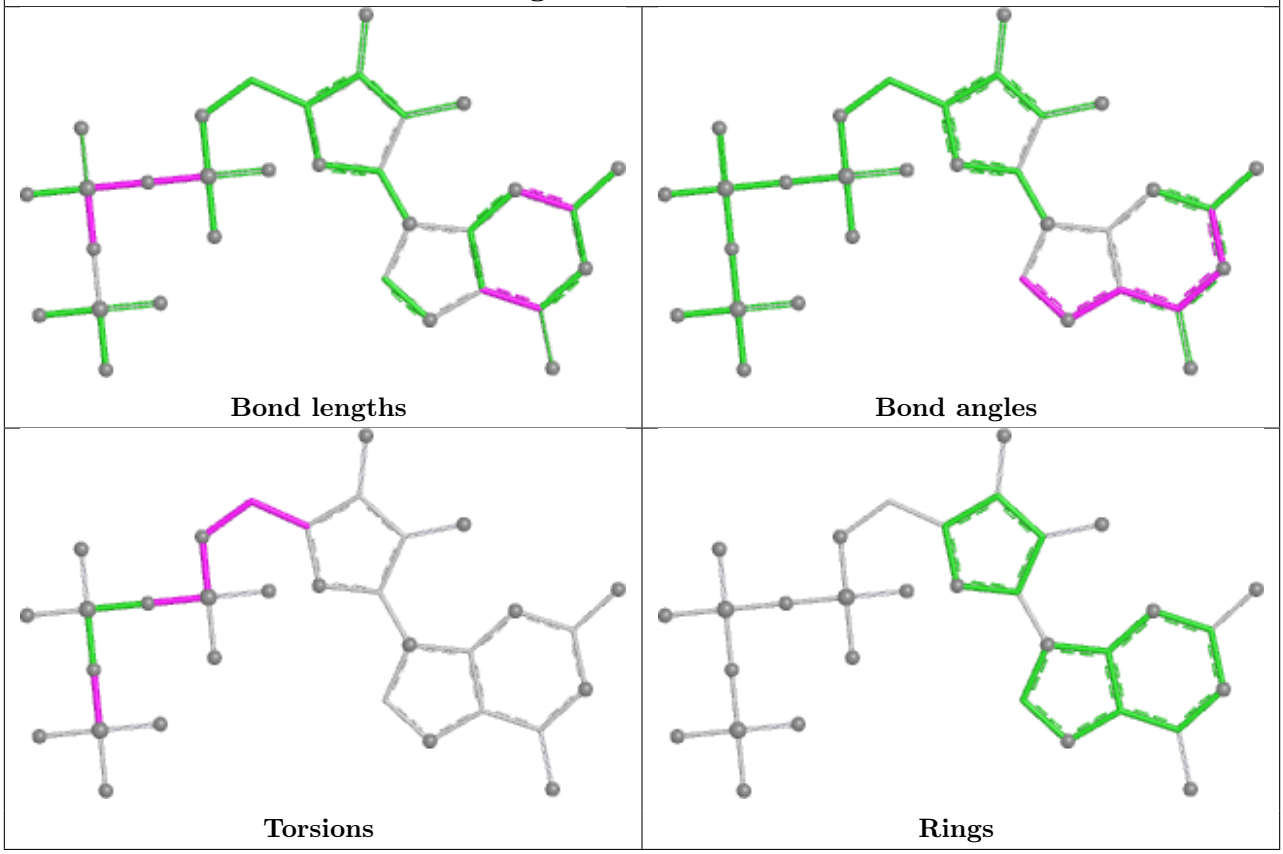
Ligand GTP Bc 501



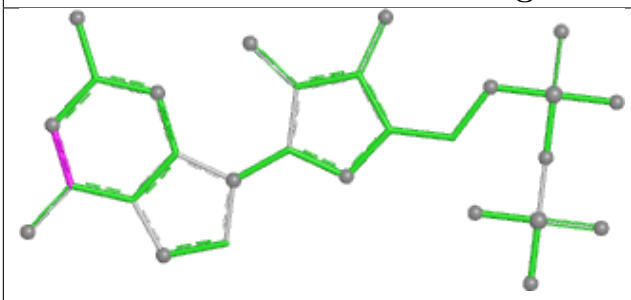
Ligand GDP AC 501



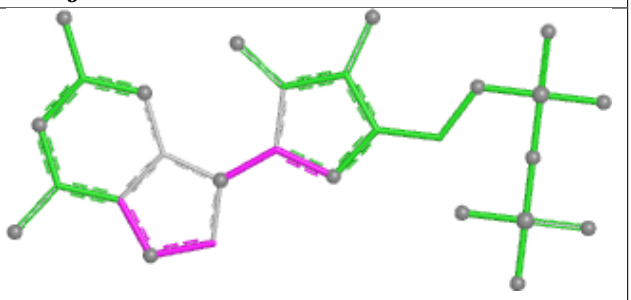
Ligand GTP c 602



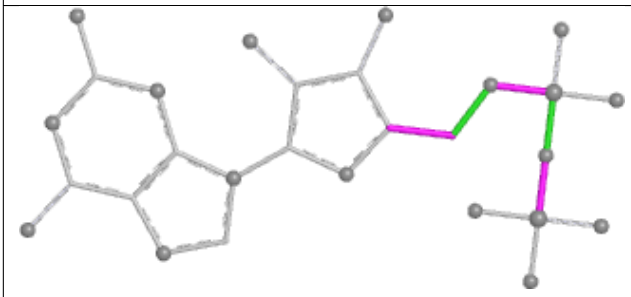
Ligand GDP Bj 501



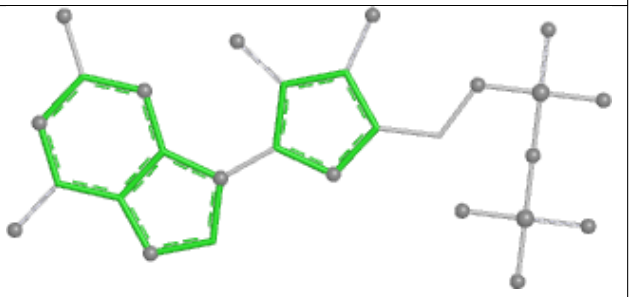
Bond lengths



Bond angles

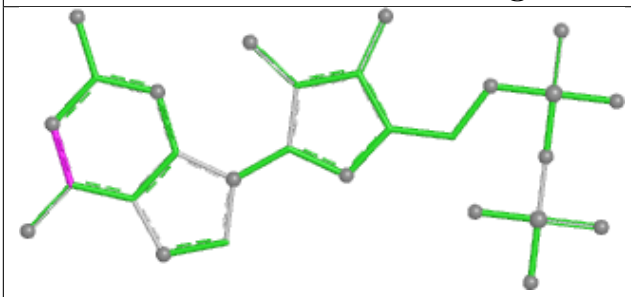


Torsions

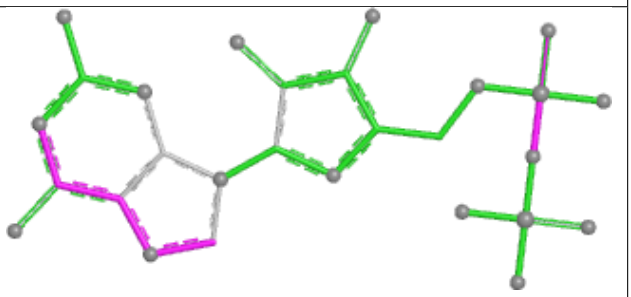


Rings

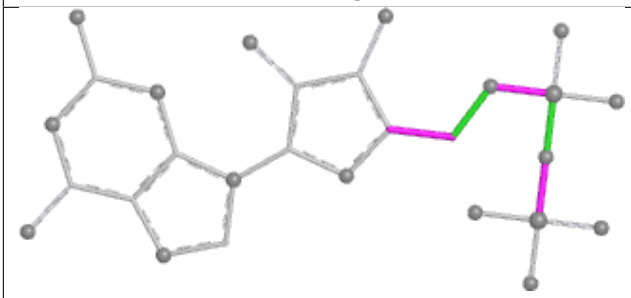
Ligand GDP EU 501



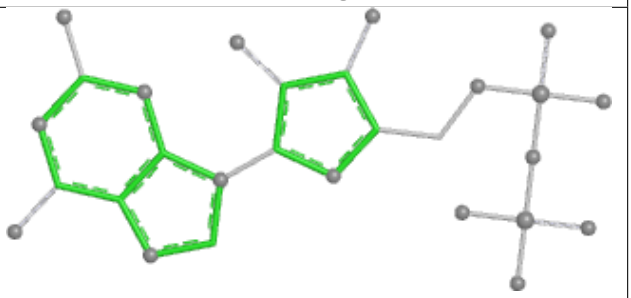
Bond lengths



Bond angles

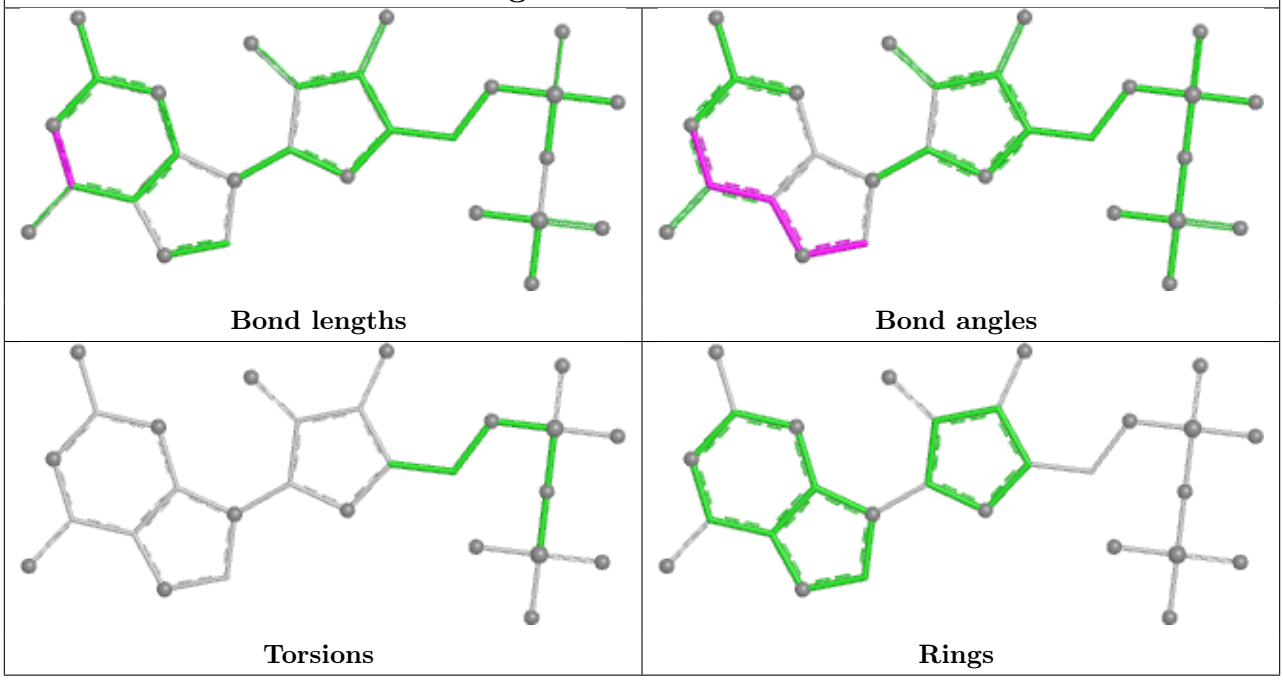


Torsions

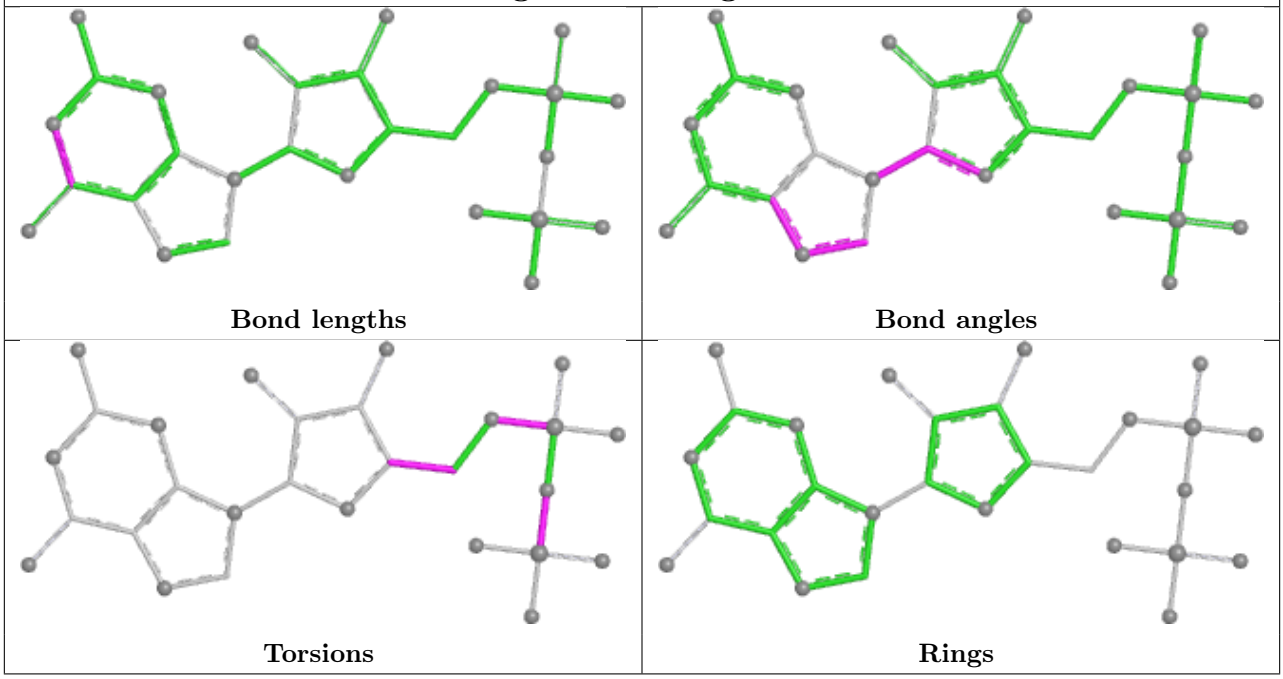


Rings

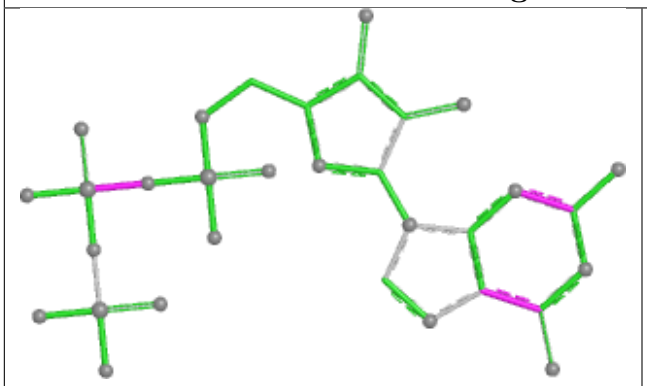
Ligand GDP Dw 501



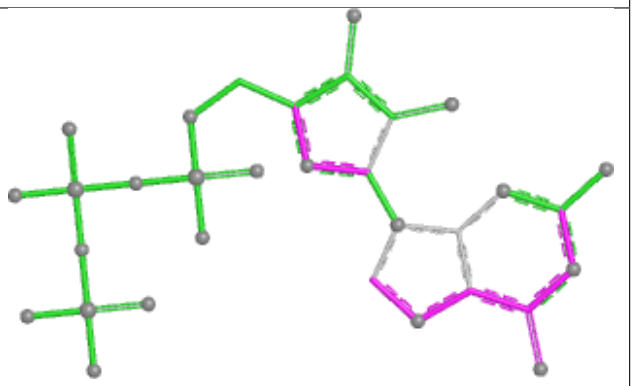
Ligand GDP Gg 501



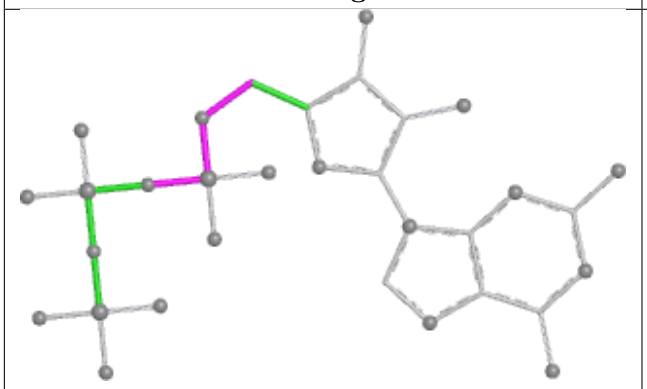
Ligand GTP BV 602



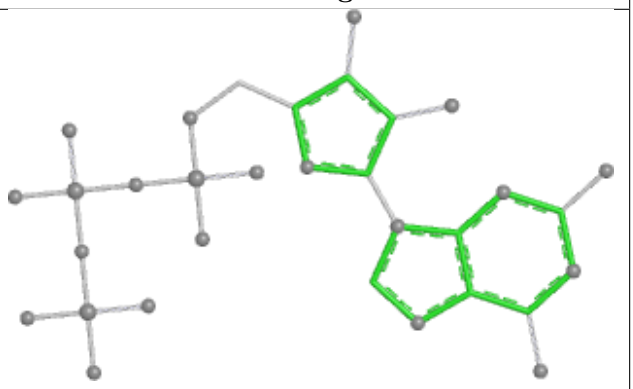
Bond lengths



Bond angles

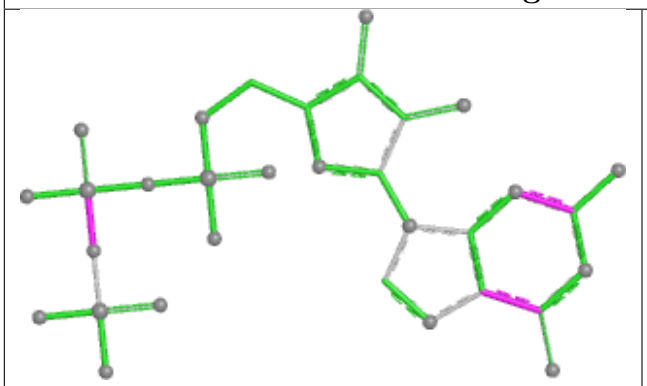


Torsions

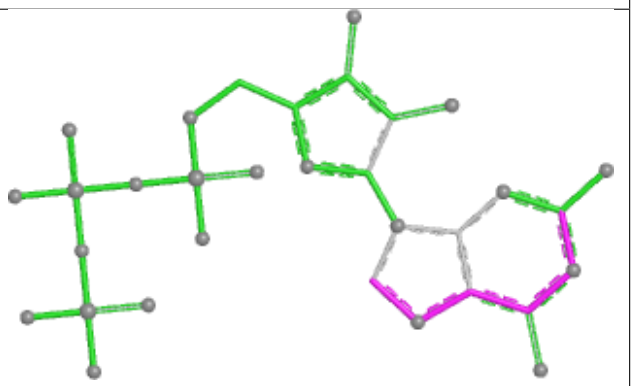


Rings

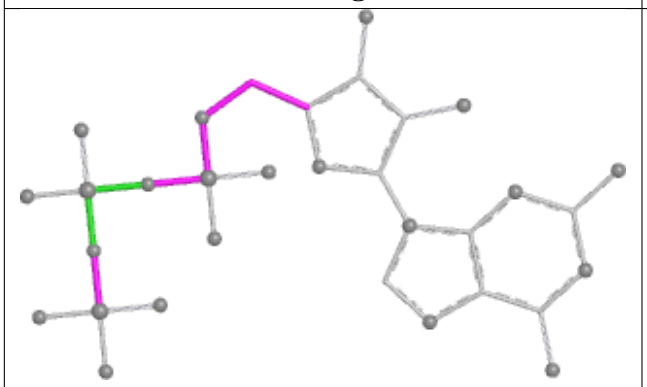
Ligand GTP Y 602



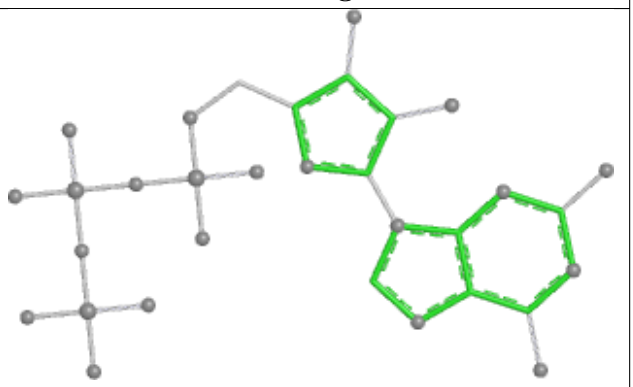
Bond lengths



Bond angles

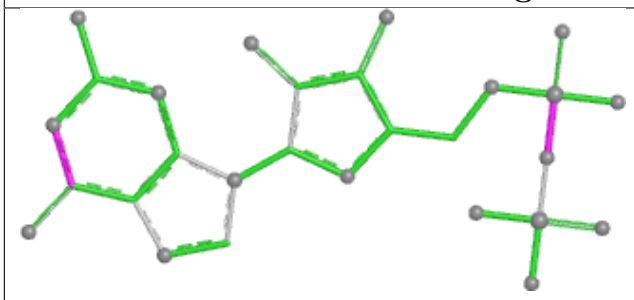


Torsions

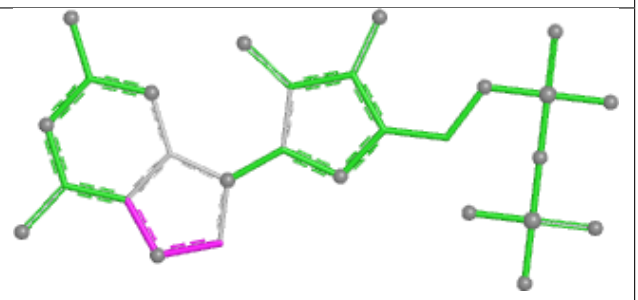


Rings

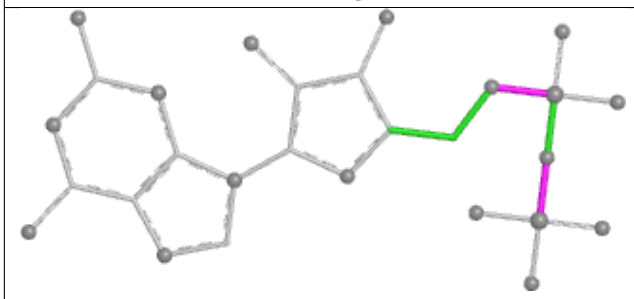
Ligand GDP Ar 501



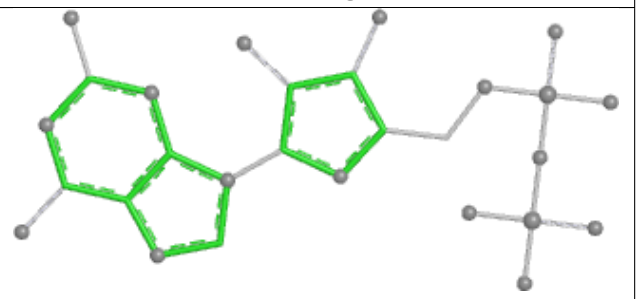
Bond lengths



Bond angles

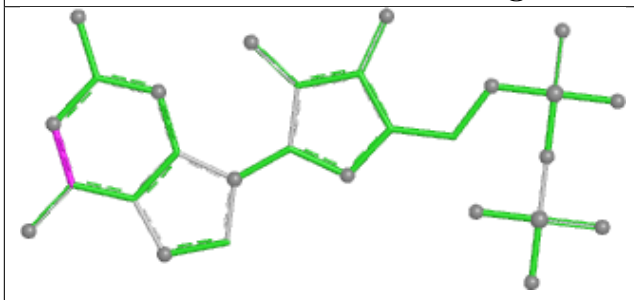


Torsions

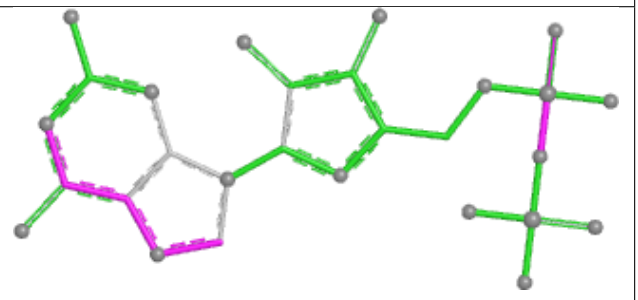


Rings

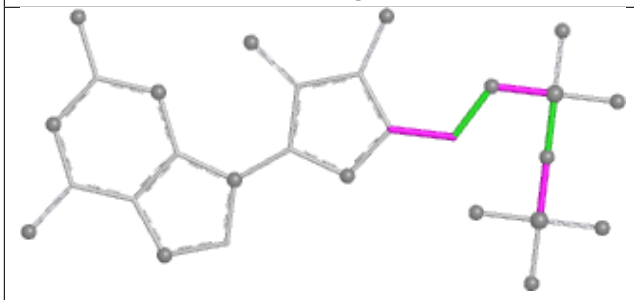
Ligand GDP DN 501



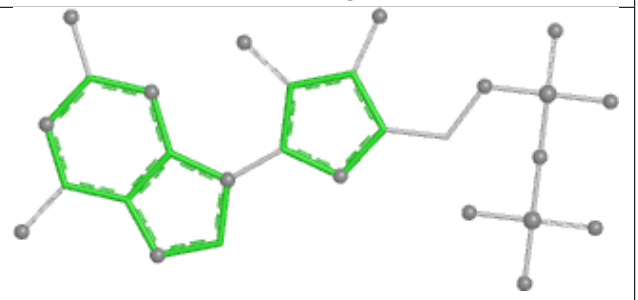
Bond lengths



Bond angles

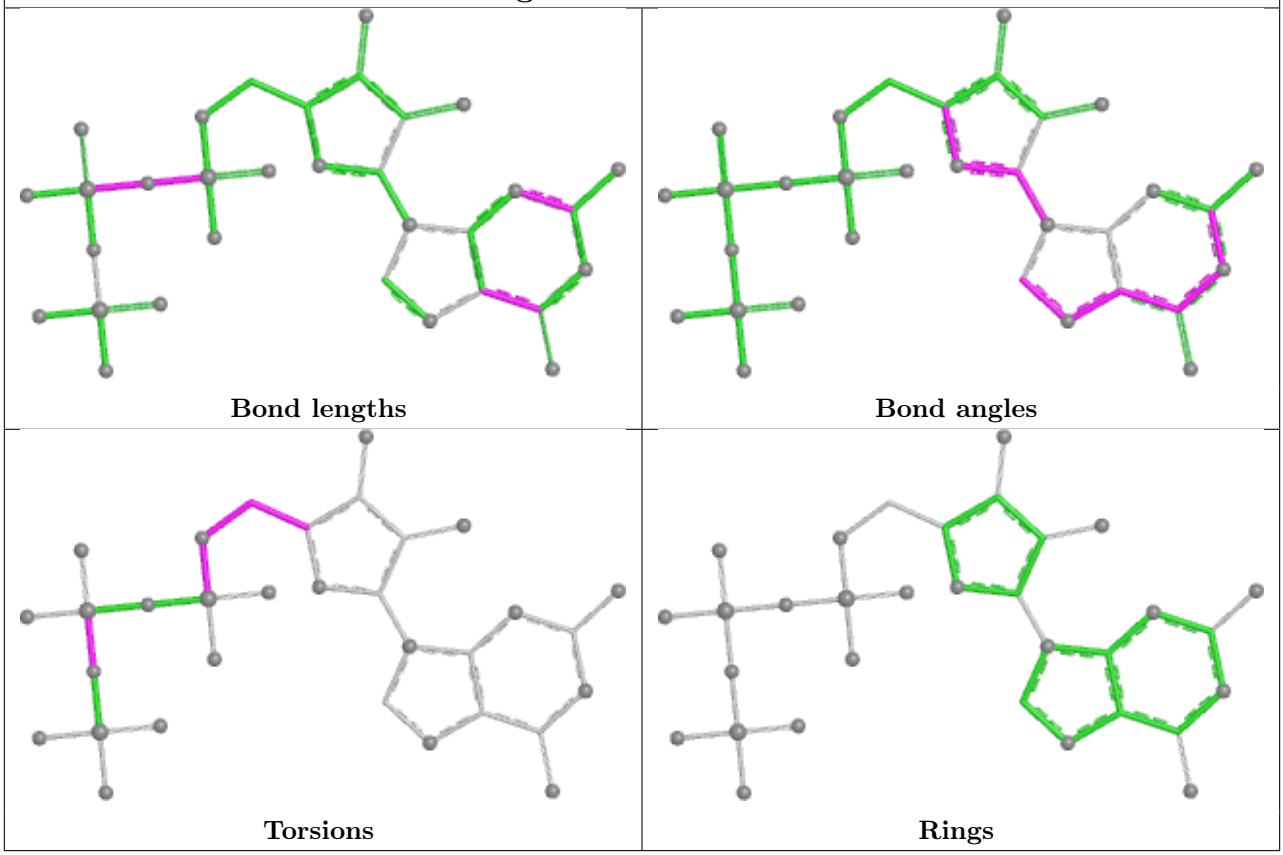


Torsions

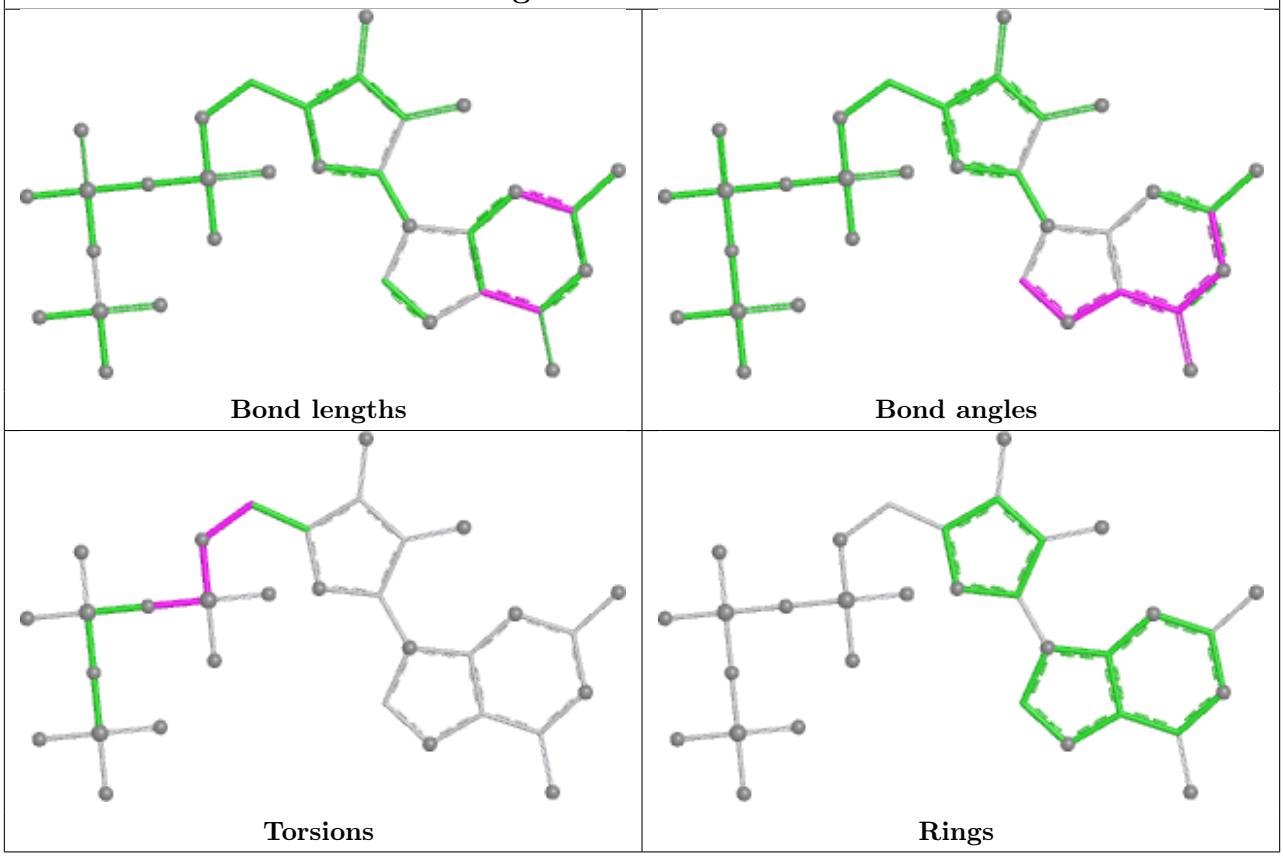


Rings

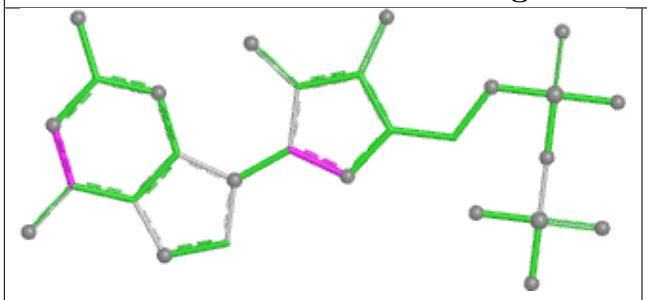
Ligand GTP E6 602



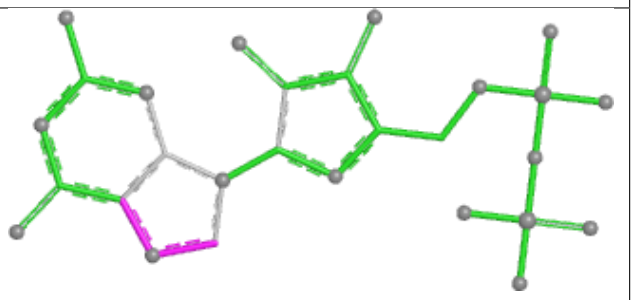
Ligand GTP GS 501



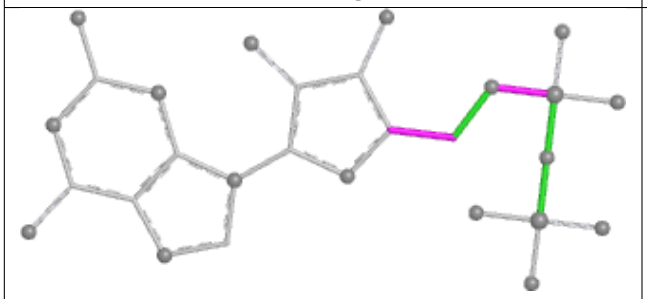
Ligand GDP AT 501



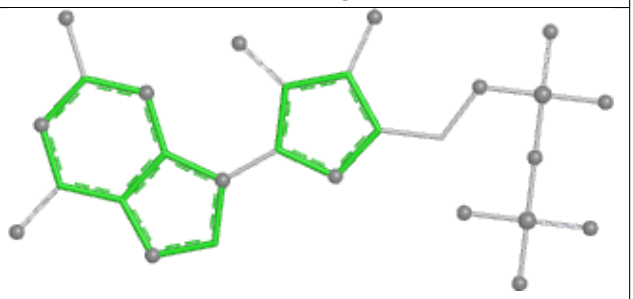
Bond lengths



Bond angles

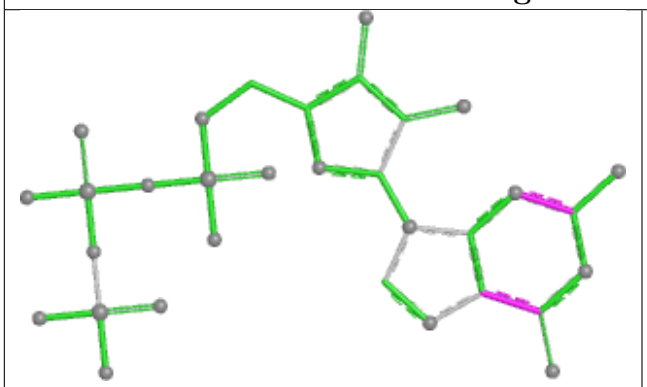


Torsions

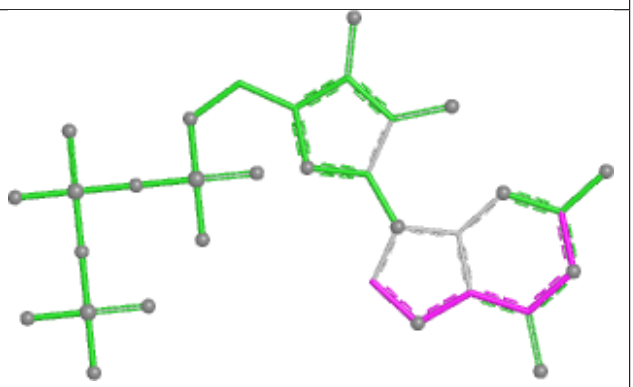


Rings

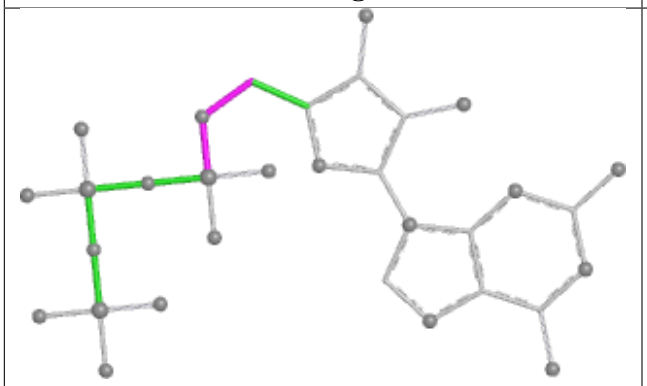
Ligand GTP G6 501



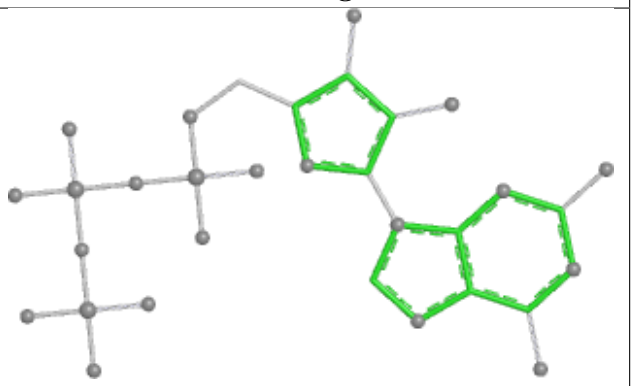
Bond lengths



Bond angles

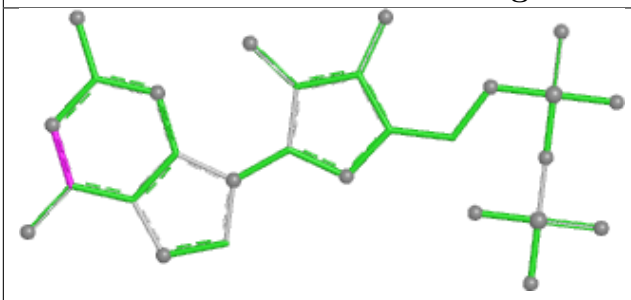


Torsions

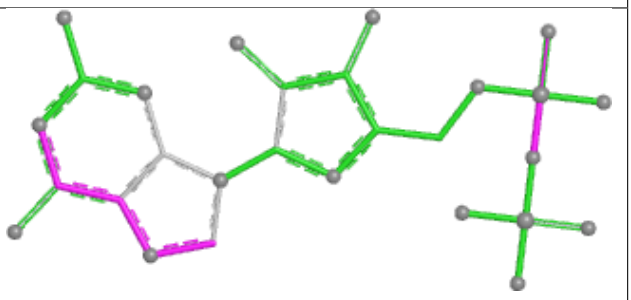


Rings

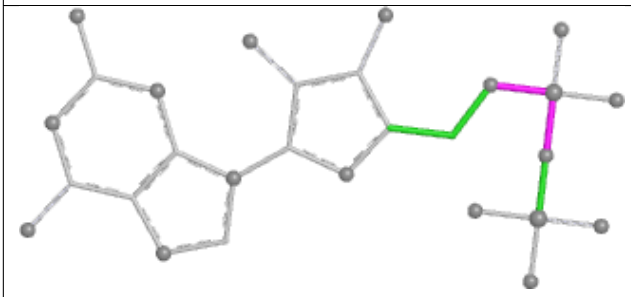
Ligand GDP AS 502



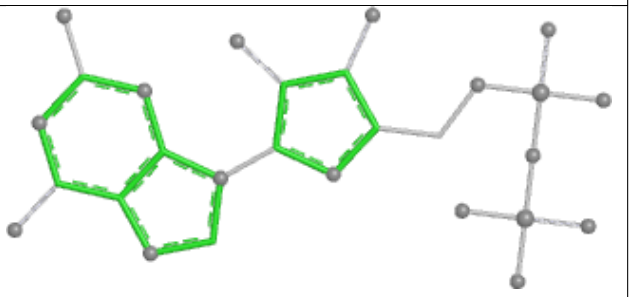
Bond lengths



Bond angles

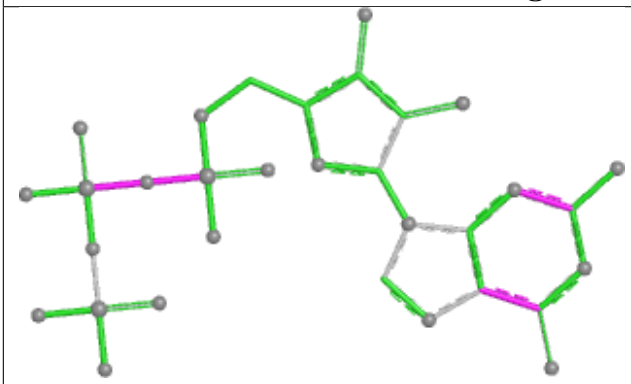


Torsions

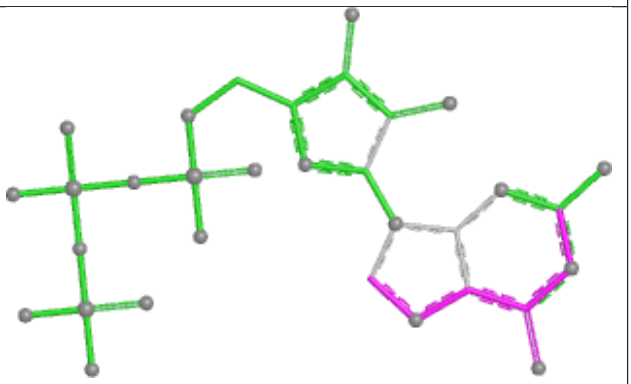


Rings

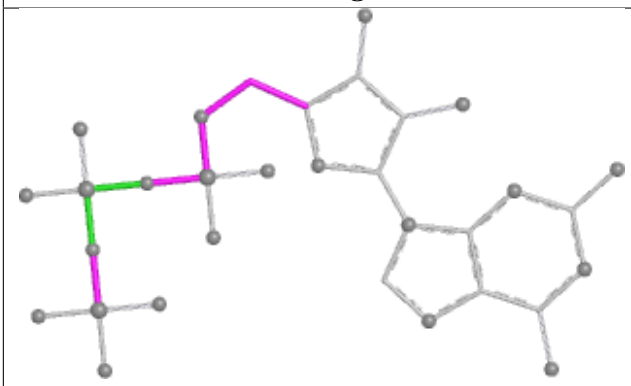
Ligand GTP o 501



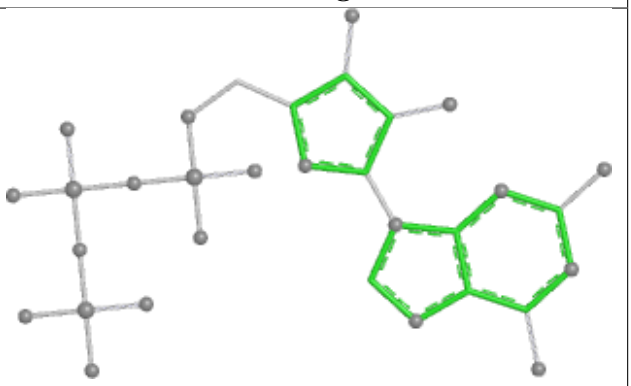
Bond lengths



Bond angles

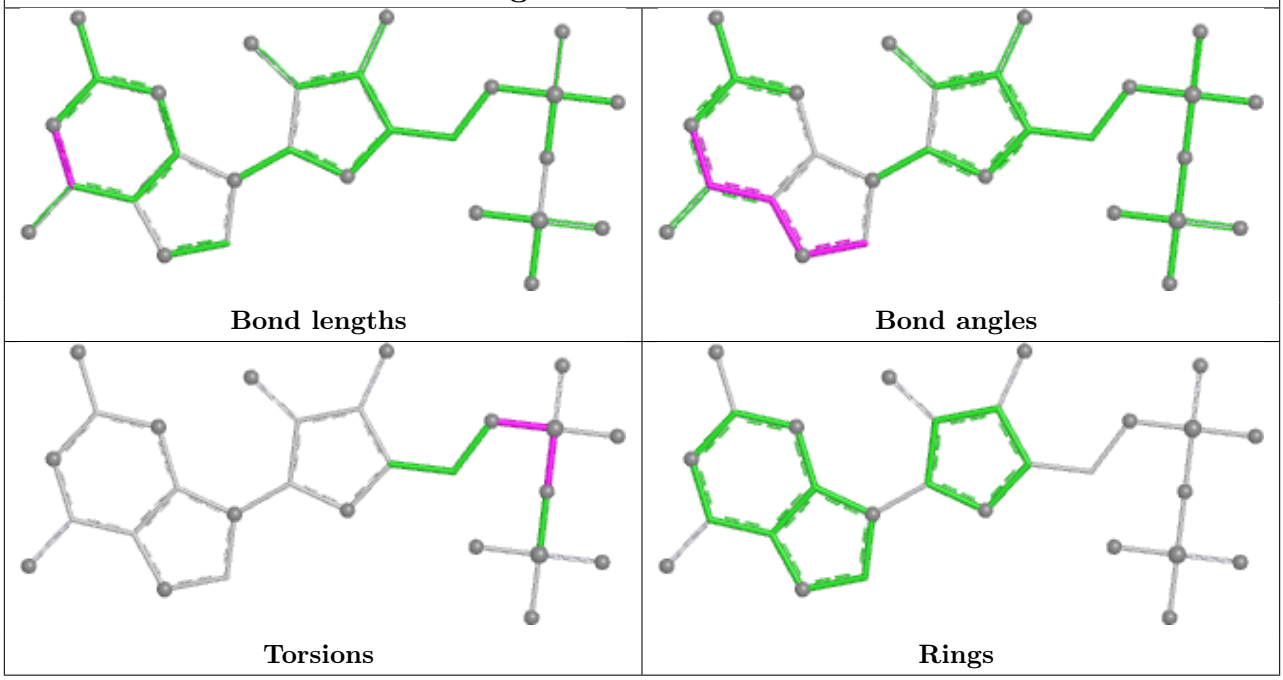


Torsions

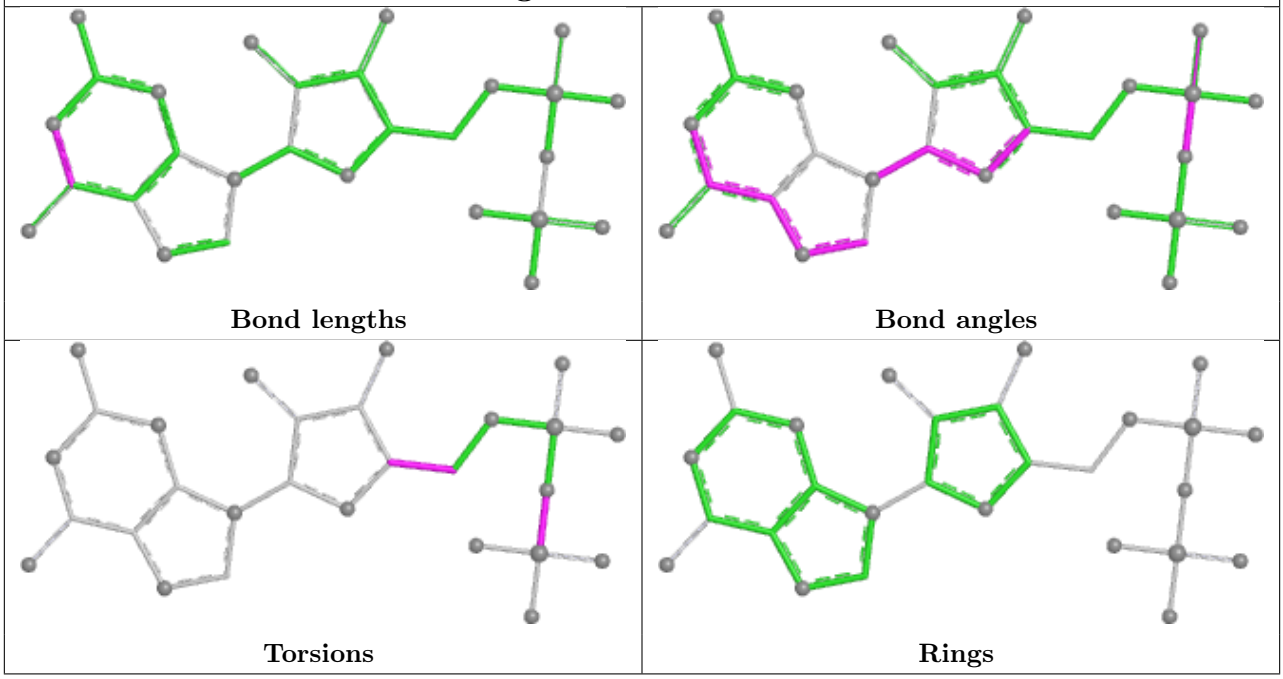


Rings

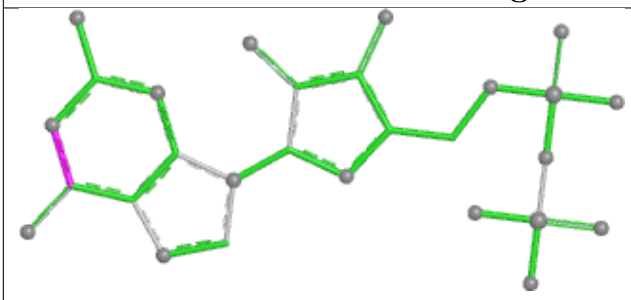
Ligand GDP AE 501



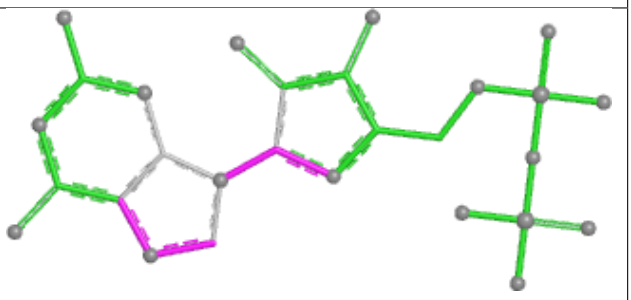
Ligand GDP Gf 501



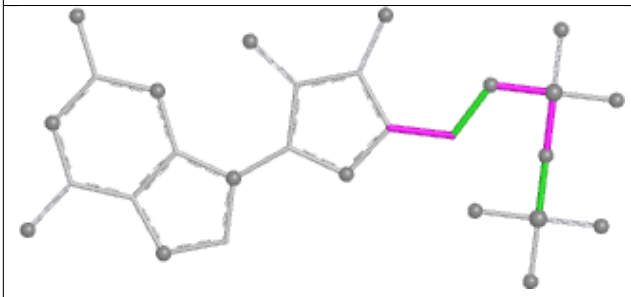
Ligand GDP BF 501



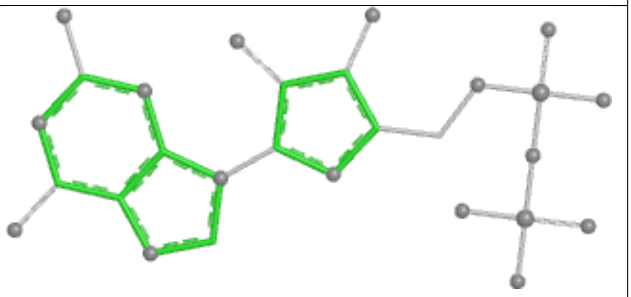
Bond lengths



Bond angles

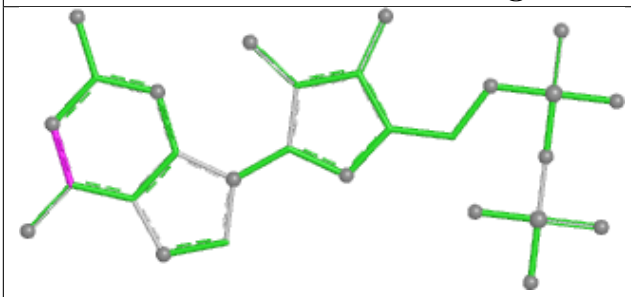


Torsions

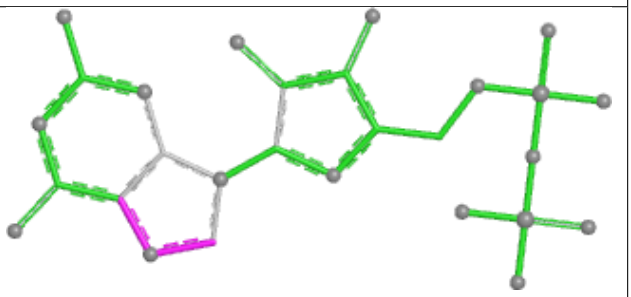


Rings

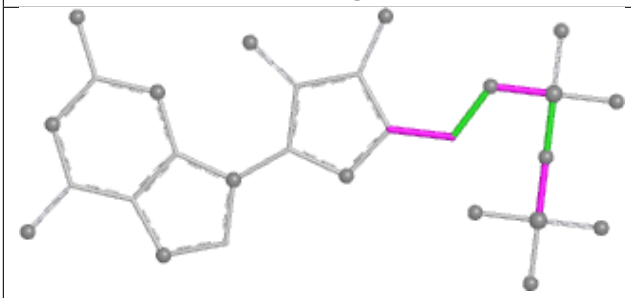
Ligand GDP AR 501



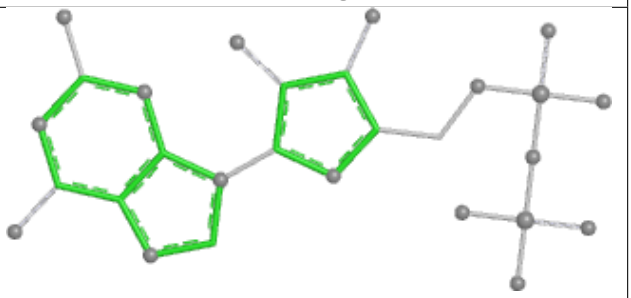
Bond lengths



Bond angles

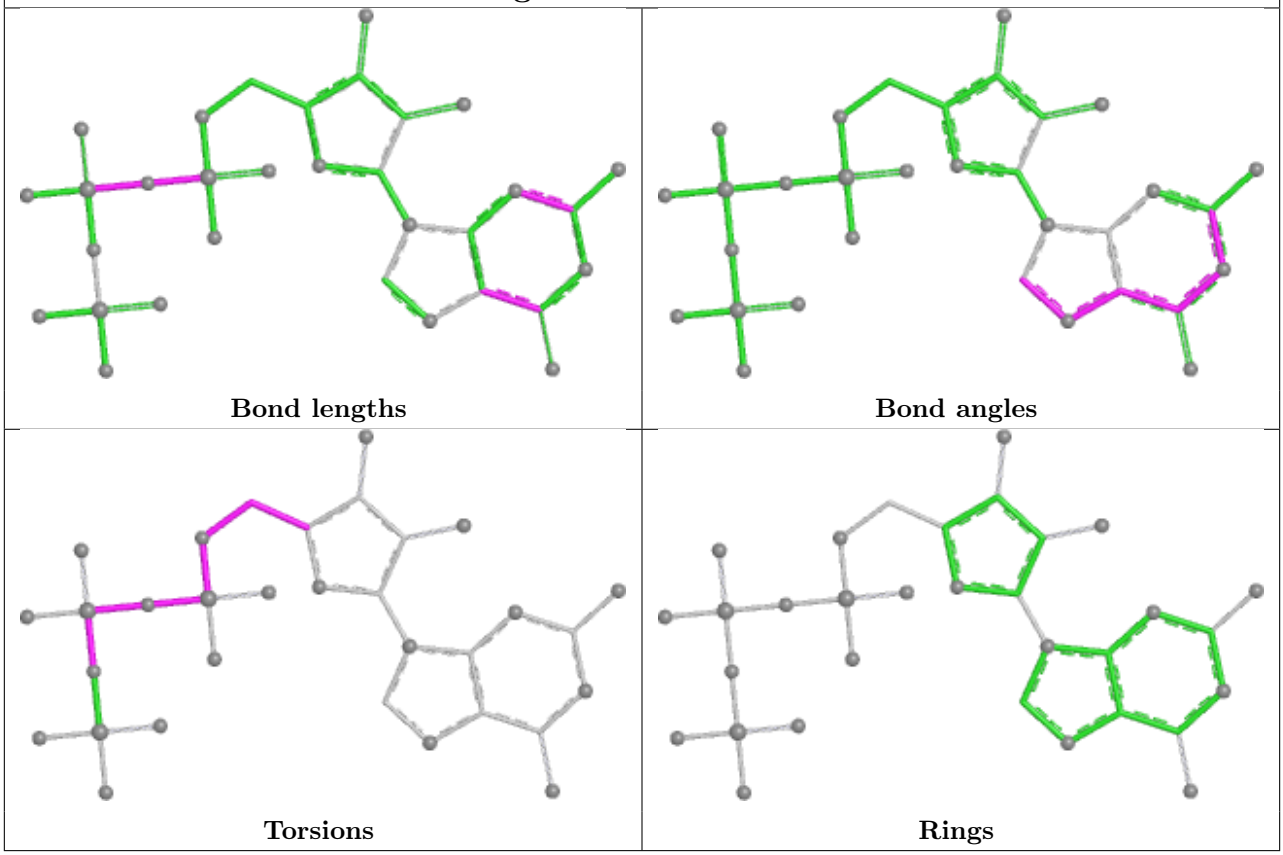


Torsions

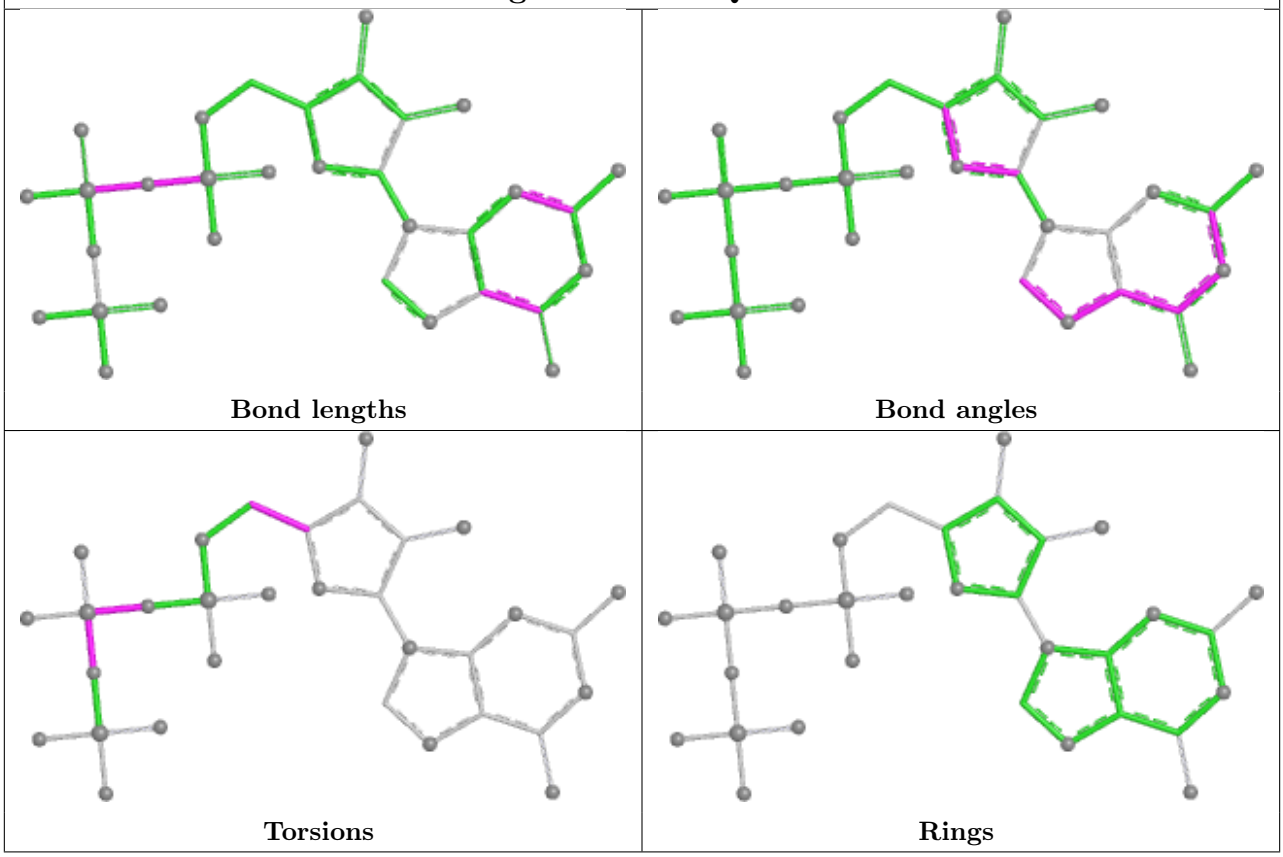


Rings

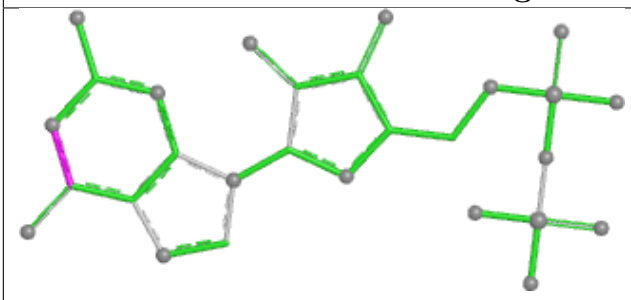
Ligand GTP G4 602



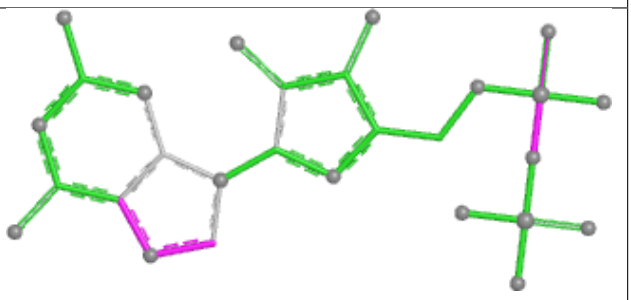
Ligand GTP GQ 602



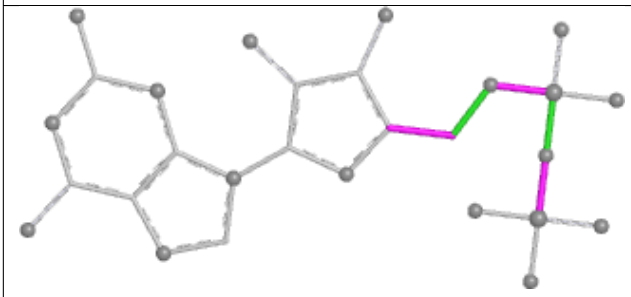
Ligand GDP F4 501



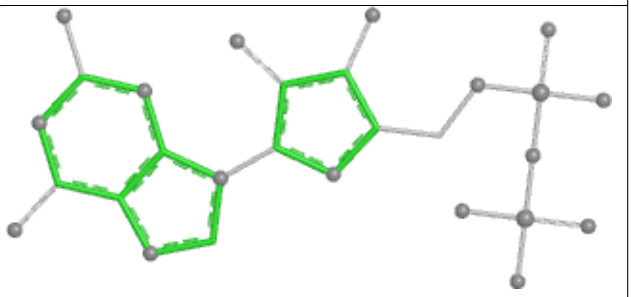
Bond lengths



Bond angles

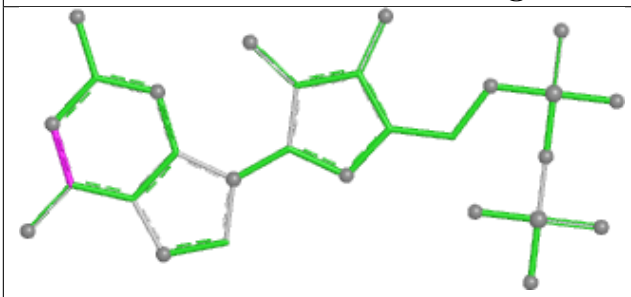


Torsions

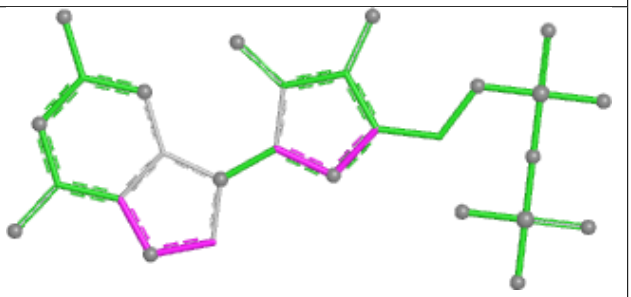


Rings

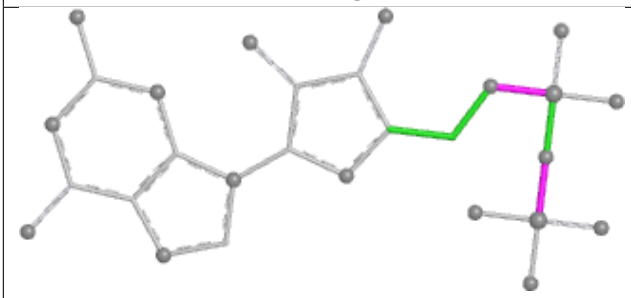
Ligand GDP BH 501



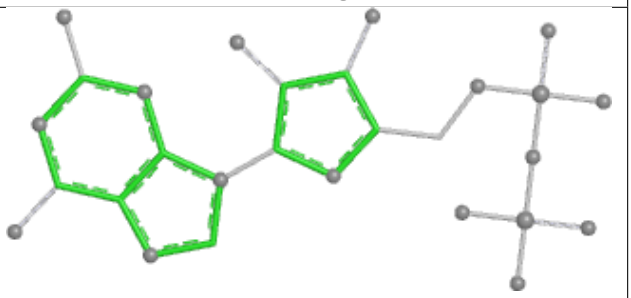
Bond lengths



Bond angles

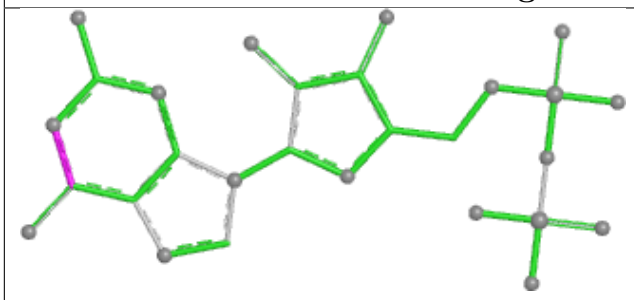


Torsions

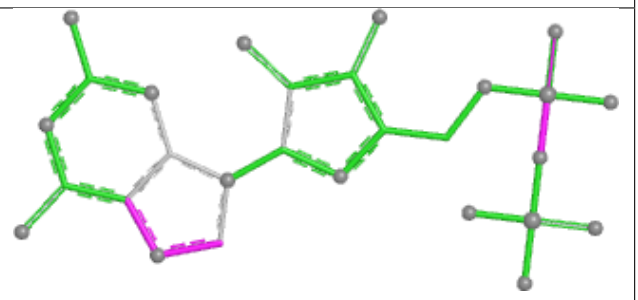


Rings

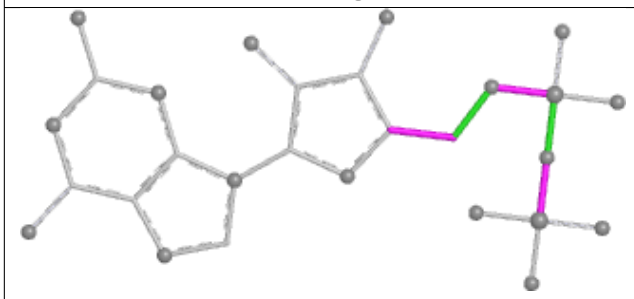
Ligand GDP Ef 501



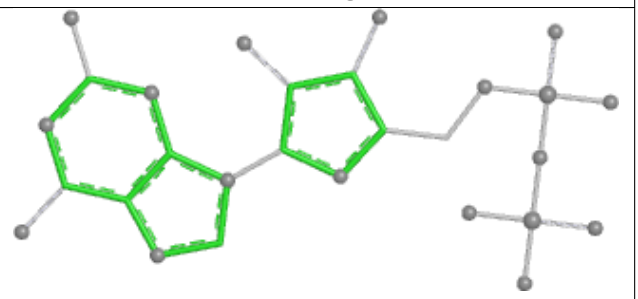
Bond lengths



Bond angles

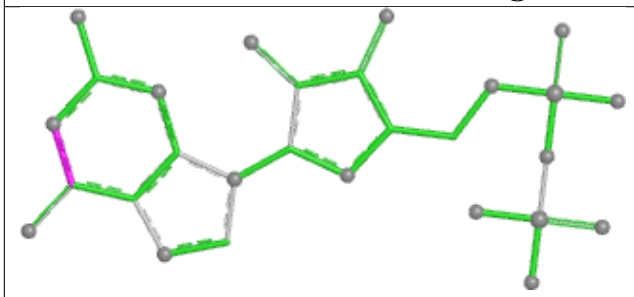


Torsions

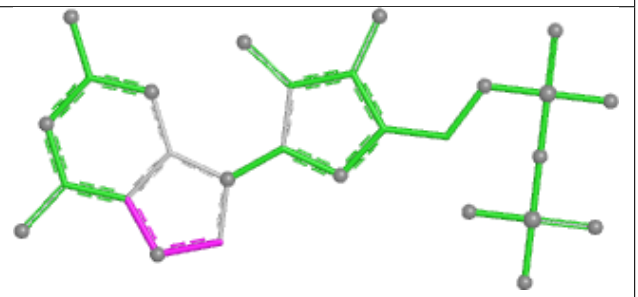


Rings

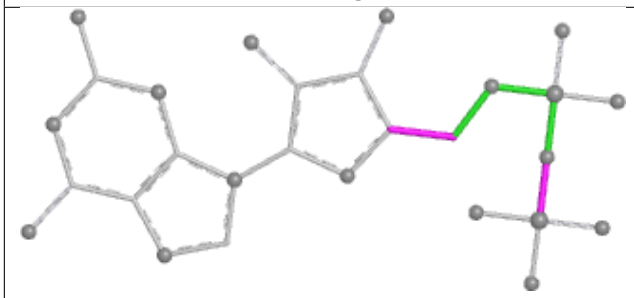
Ligand GDP DX 501



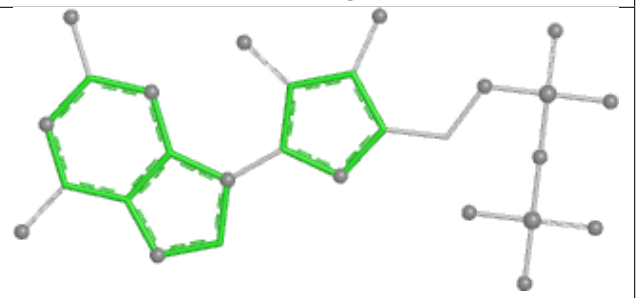
Bond lengths



Bond angles

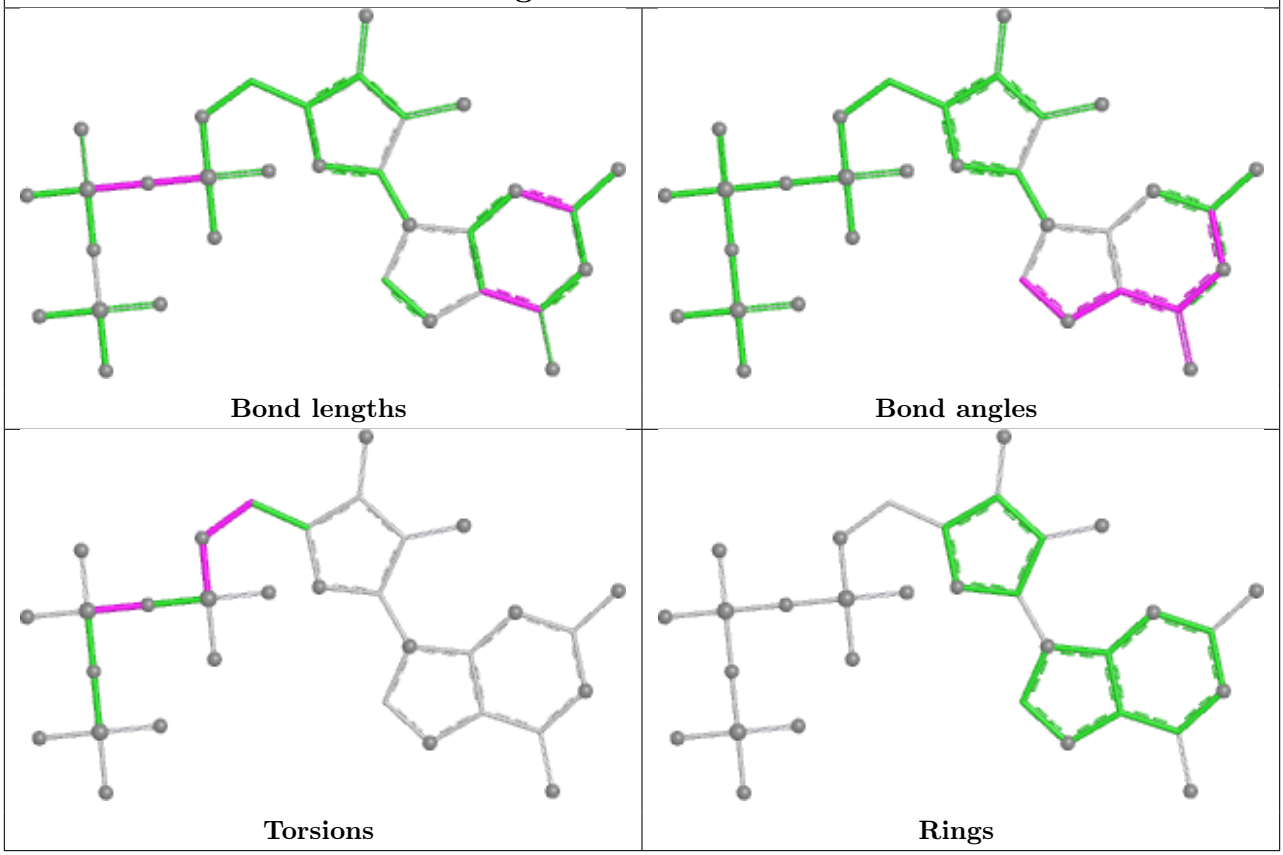


Torsions

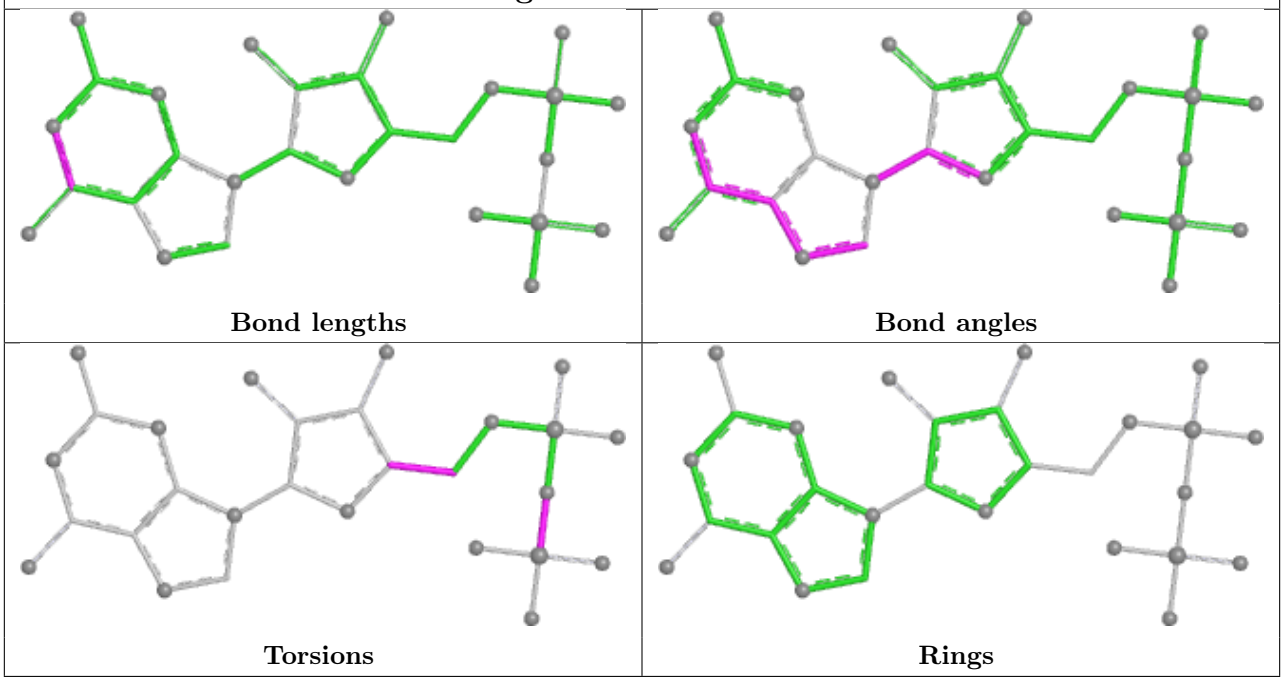


Rings

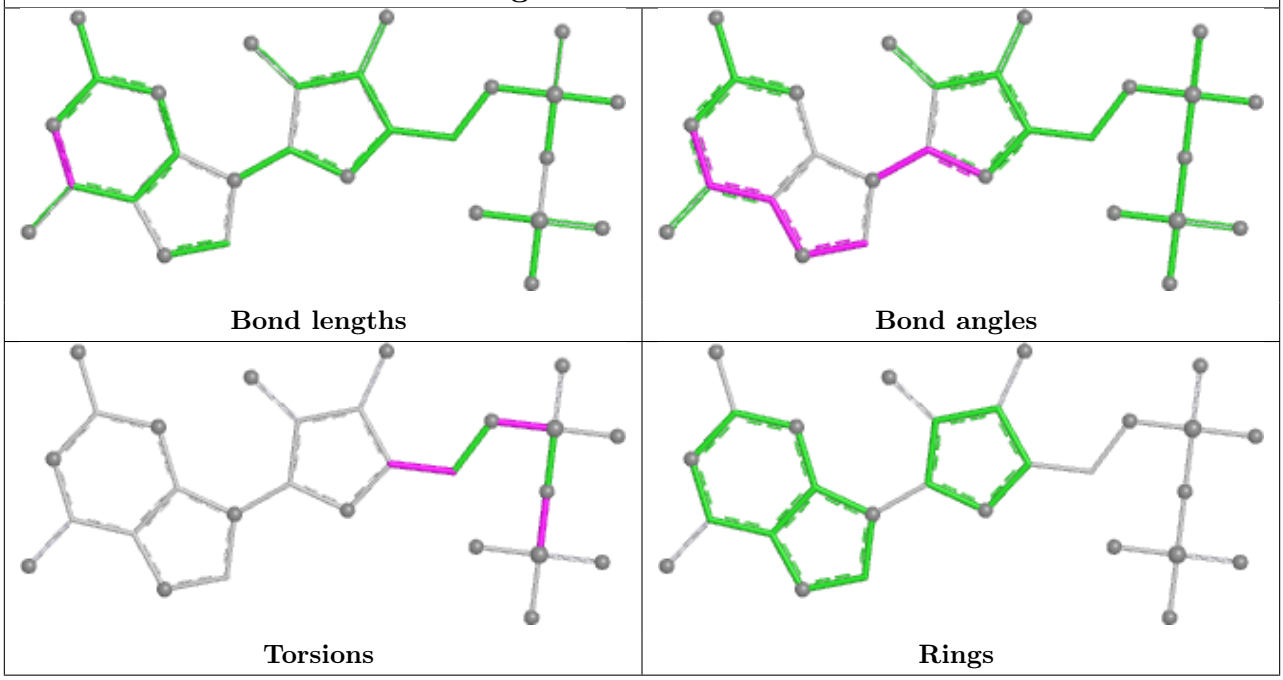
Ligand GTP B9 602



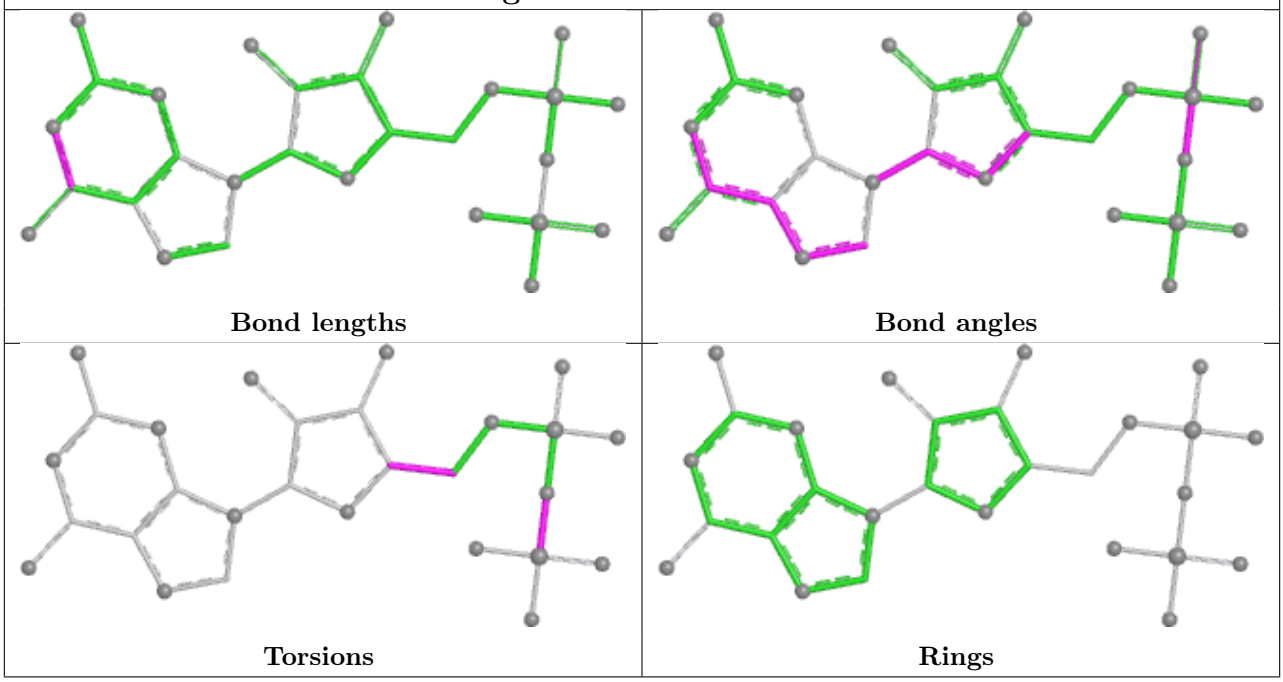
Ligand GDP Fn 501



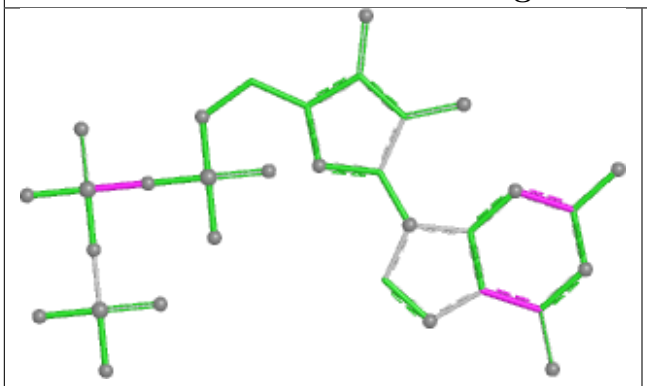
Ligand GDP AL 501



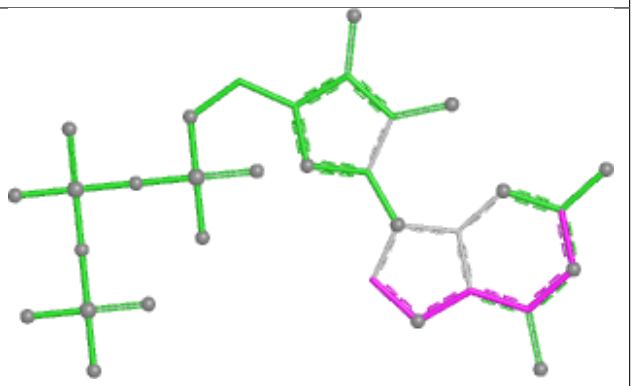
Ligand GDP GW 501



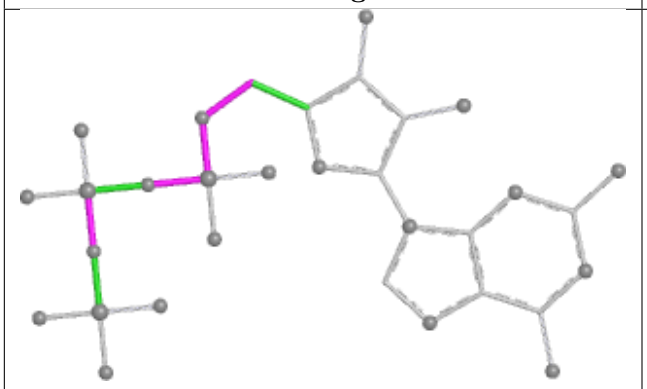
Ligand GTP Bd 501



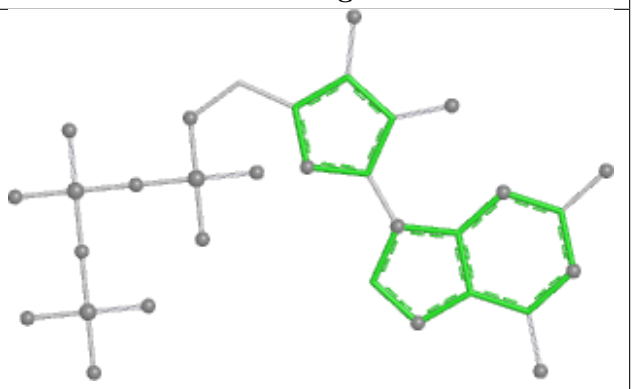
Bond lengths



Bond angles

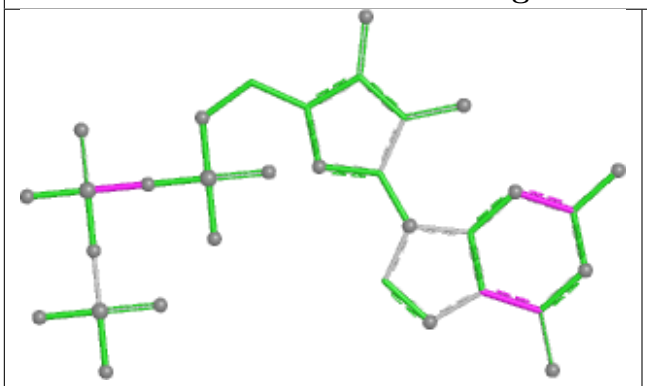


Torsions

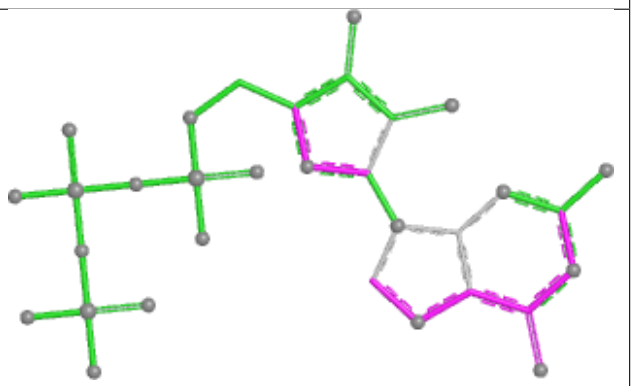


Rings

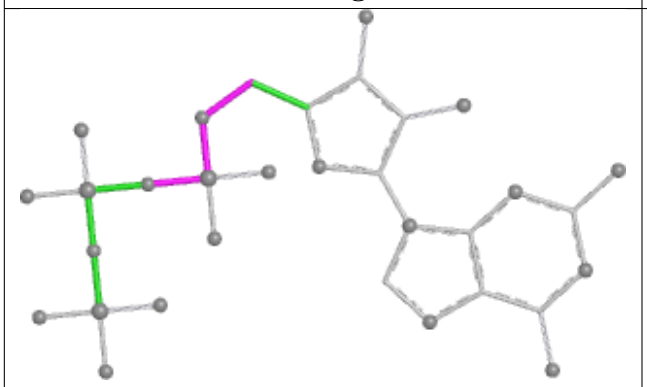
Ligand GTP FY 501



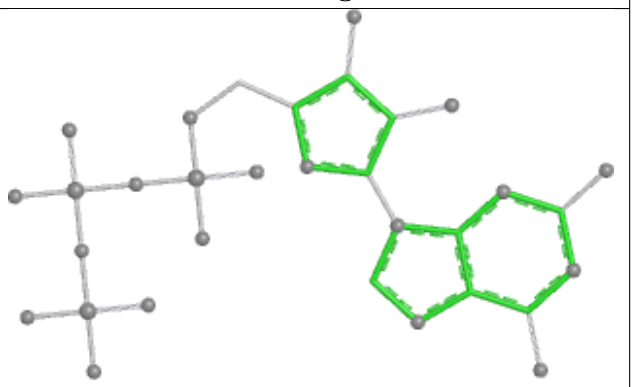
Bond lengths



Bond angles

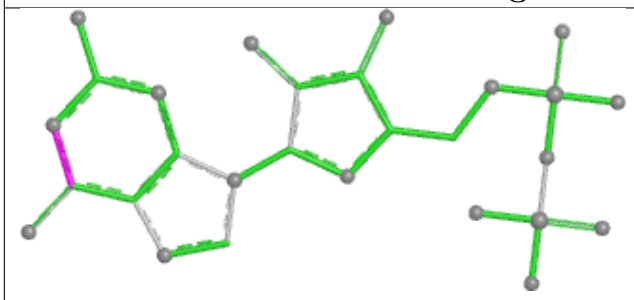


Torsions

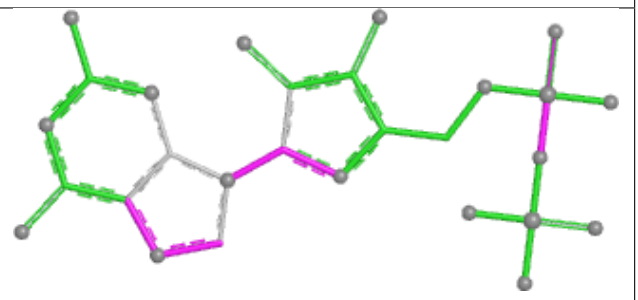


Rings

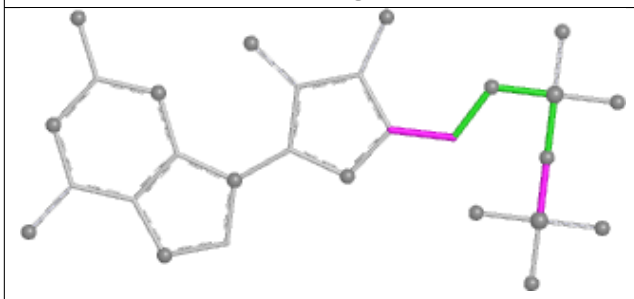
Ligand GDP DP 501



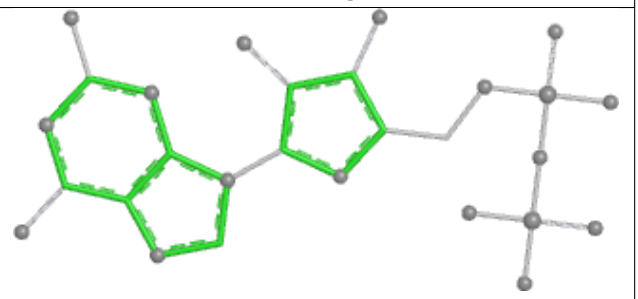
Bond lengths



Bond angles

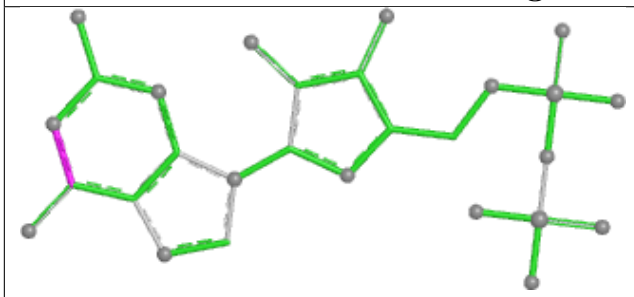


Torsions

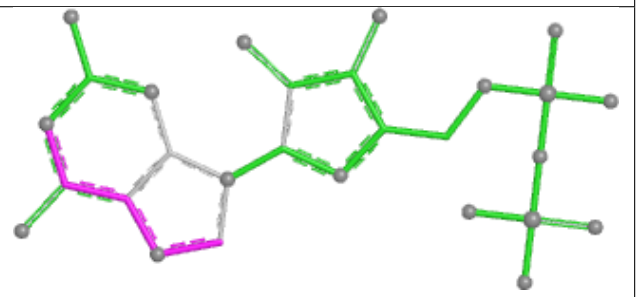


Rings

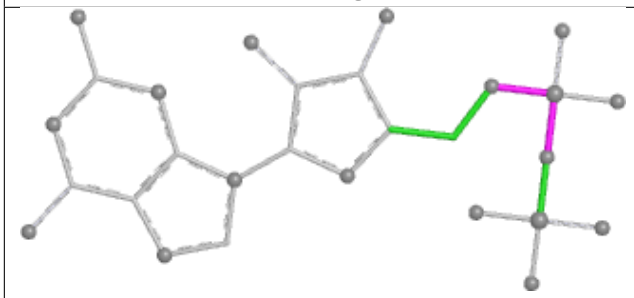
Ligand GDP 8 501



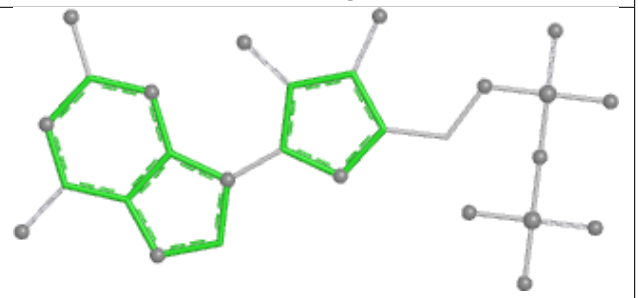
Bond lengths



Bond angles

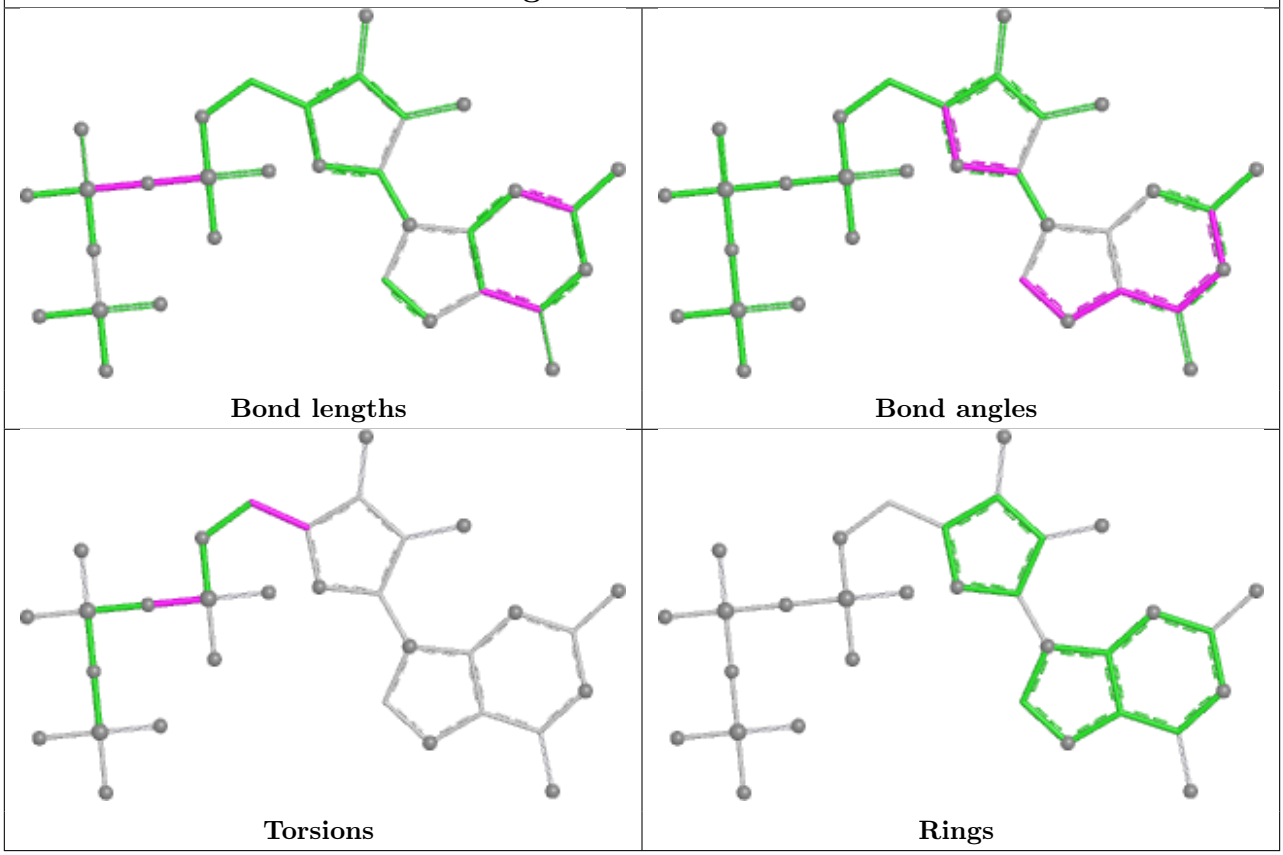


Torsions

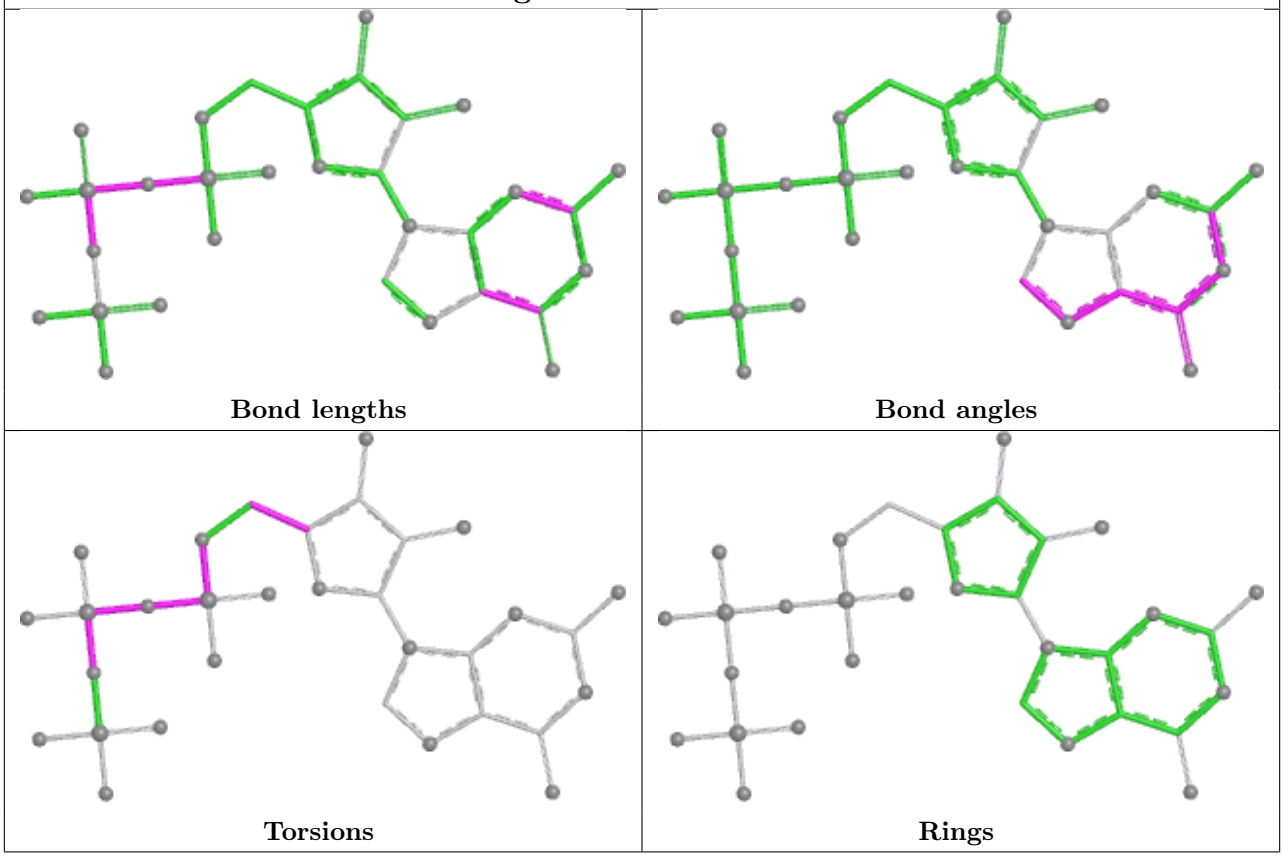


Rings

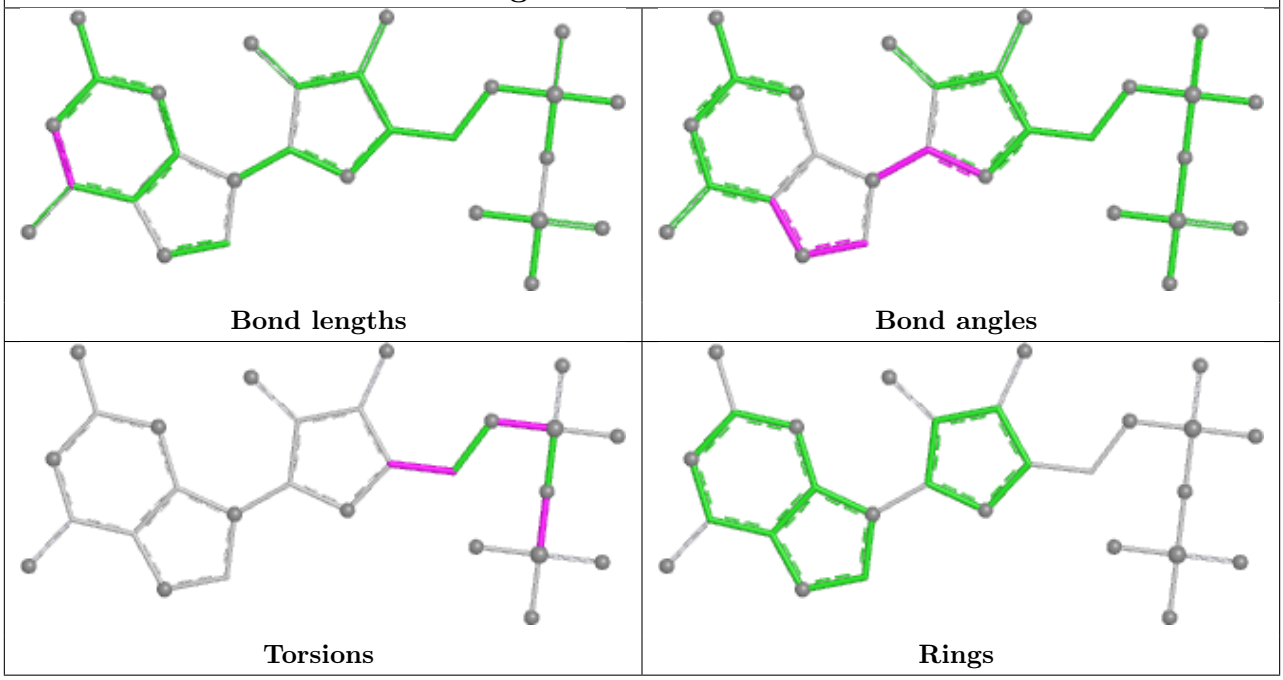
Ligand GTP V 602



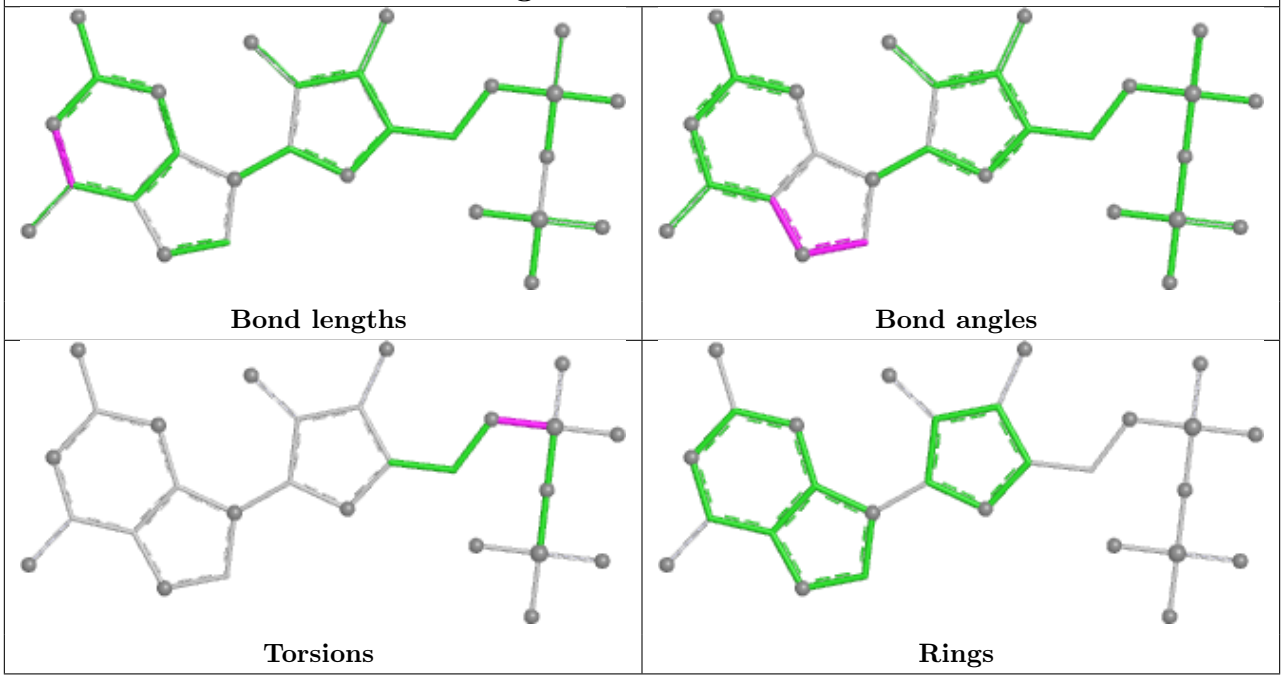
Ligand GTP G3 602



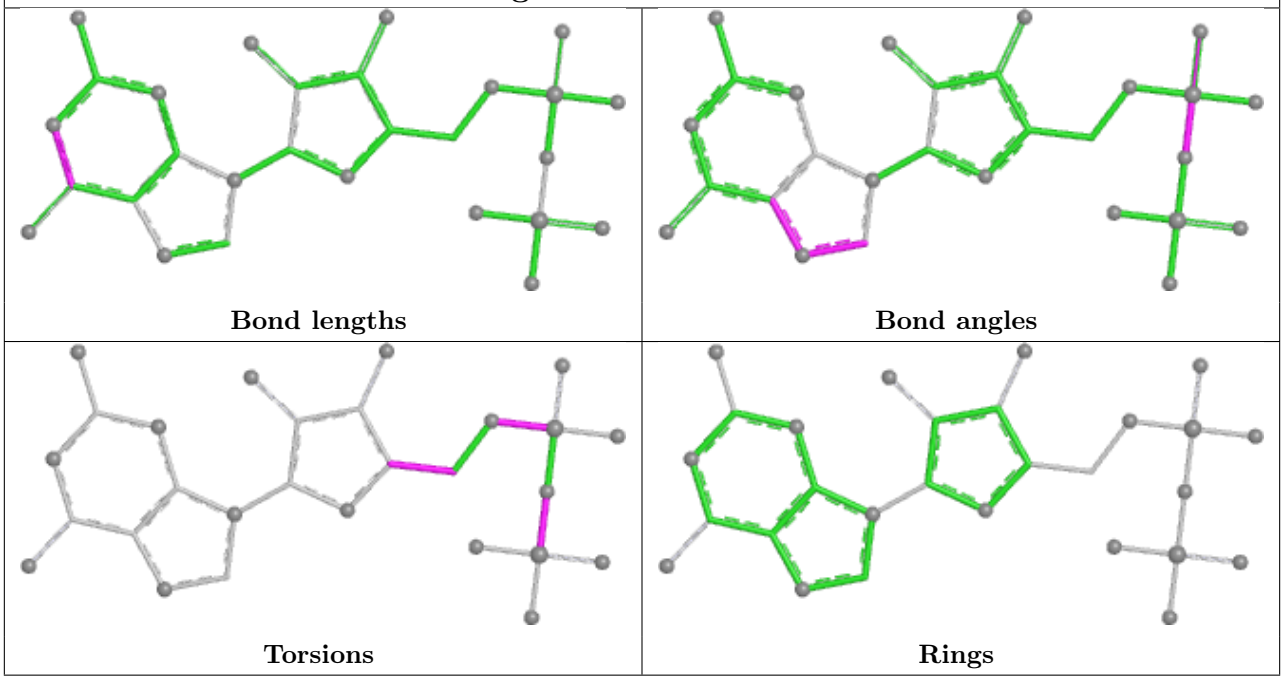
Ligand GDP FH 501



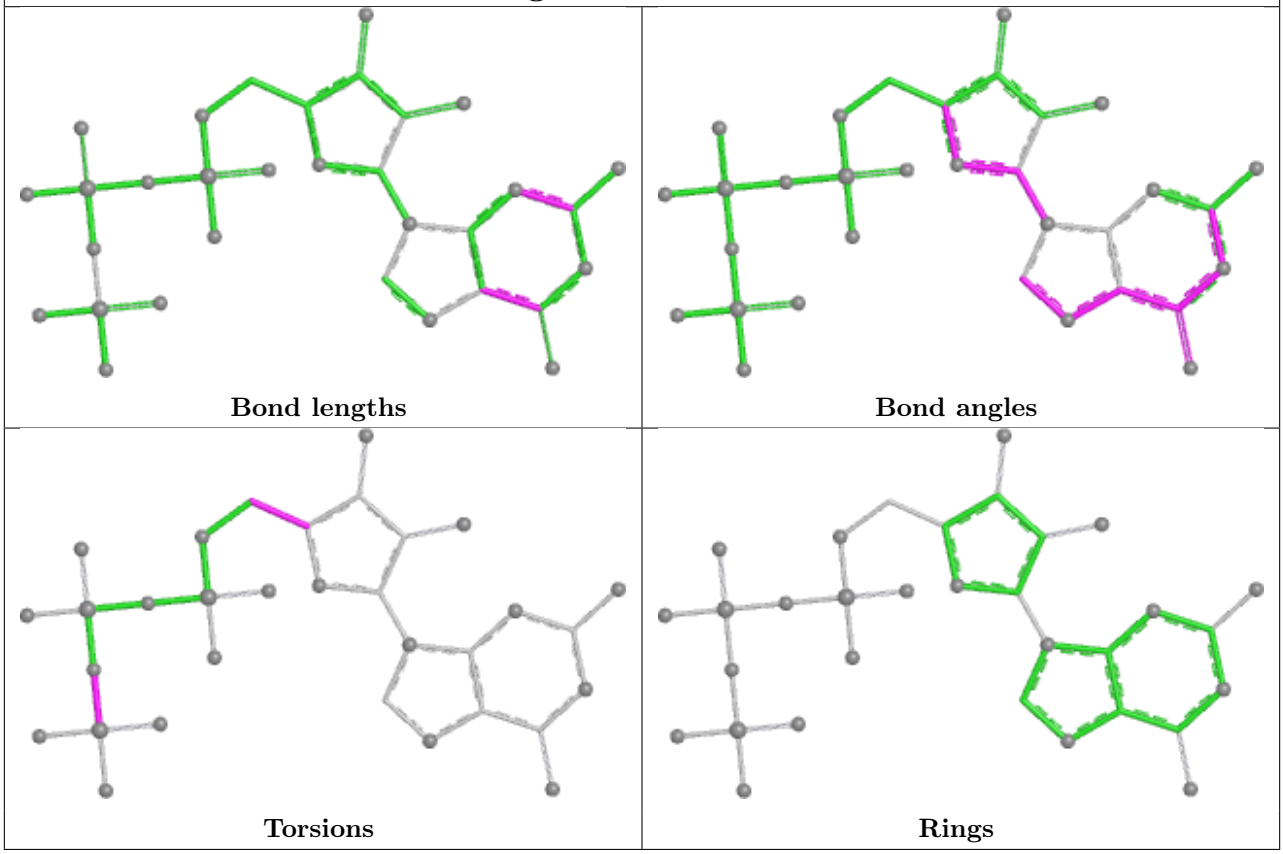
Ligand GDP Bt 501



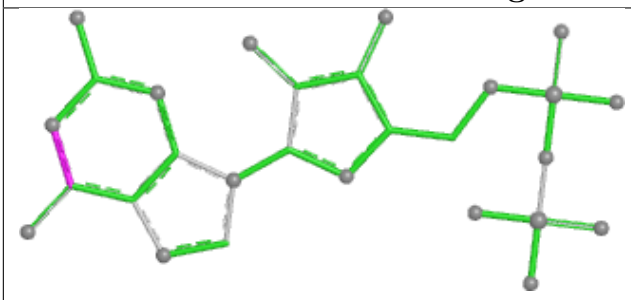
Ligand GDP Db 501



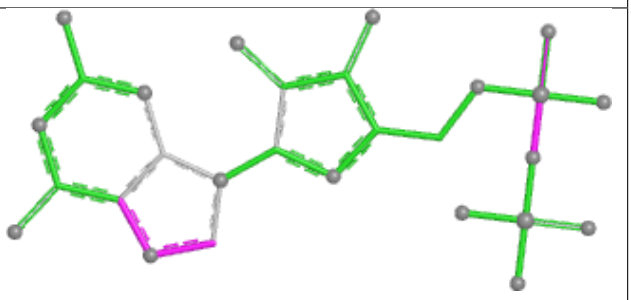
Ligand GTP 4 602



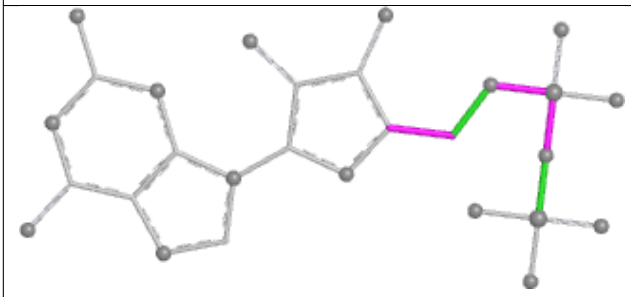
Ligand GDP BD 501



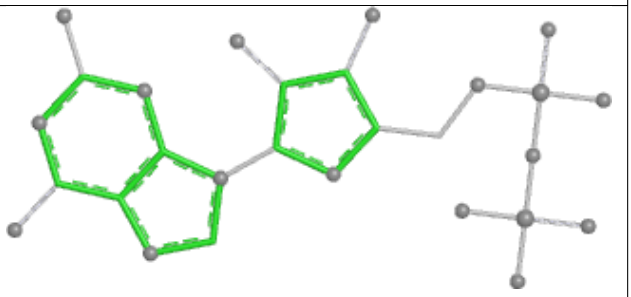
Bond lengths



Bond angles

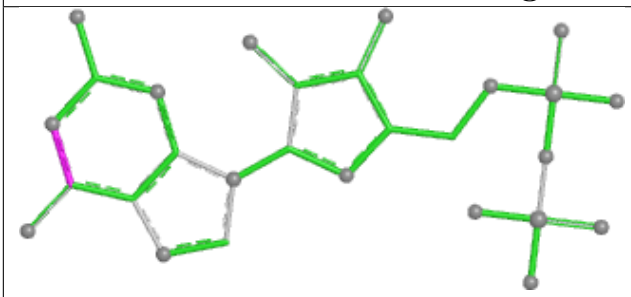


Torsions

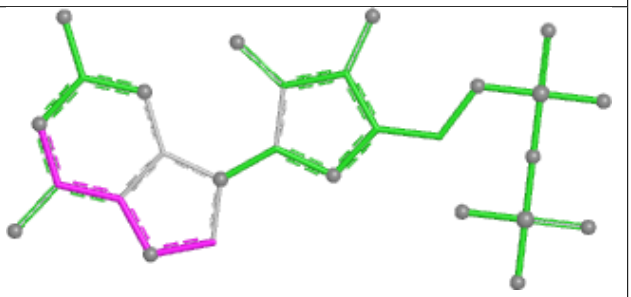


Rings

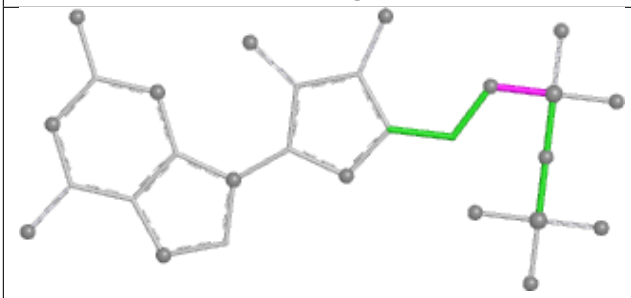
Ligand GDP O 501



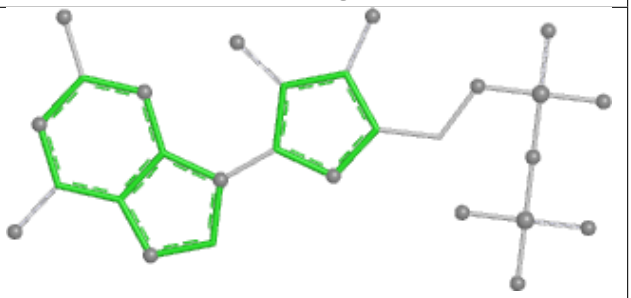
Bond lengths



Bond angles

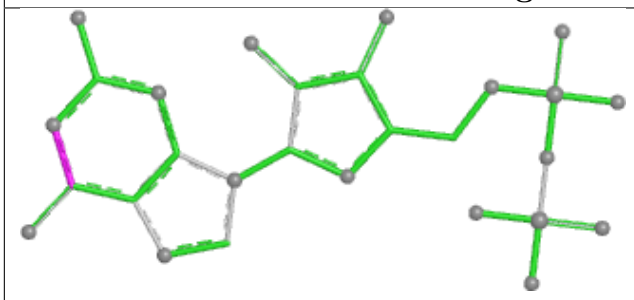


Torsions

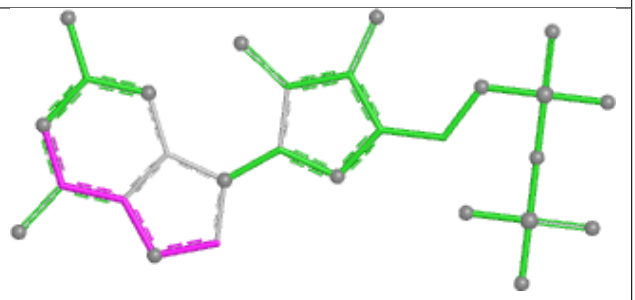


Rings

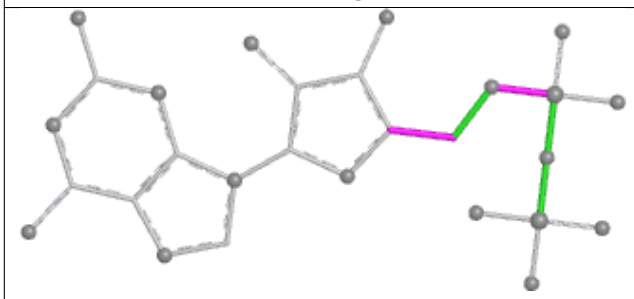
Ligand GDP Bs 501



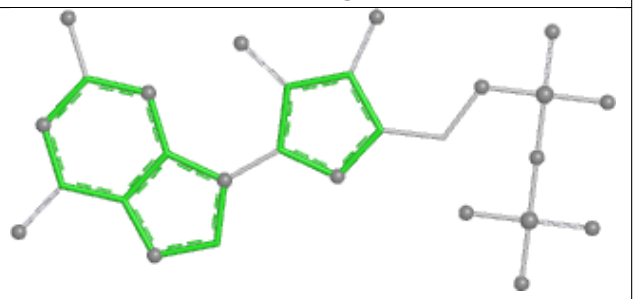
Bond lengths



Bond angles

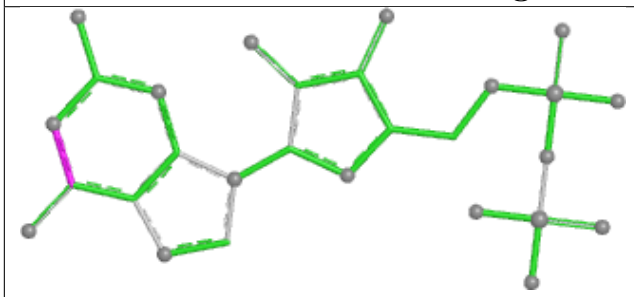


Torsions

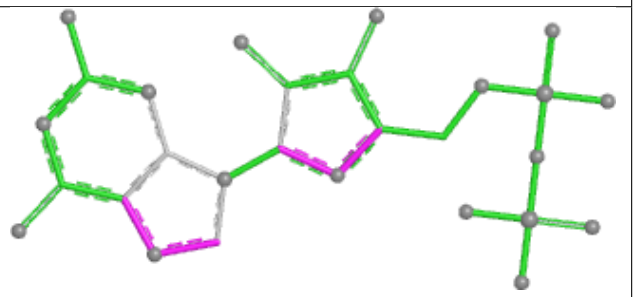


Rings

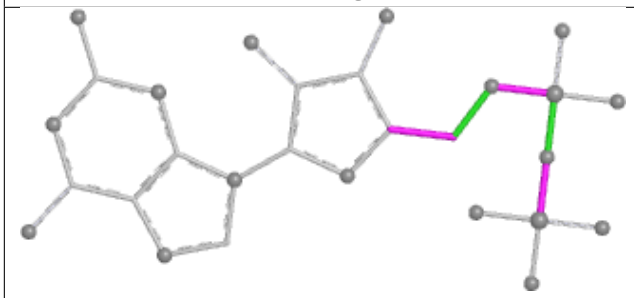
Ligand GDP Ad 501



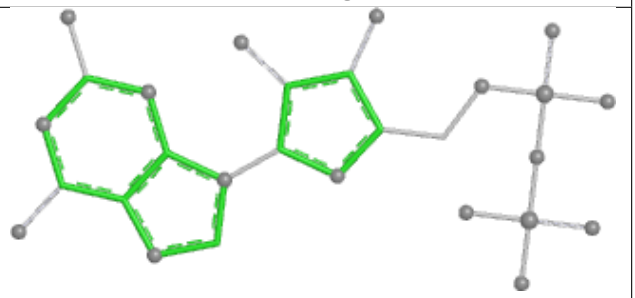
Bond lengths



Bond angles

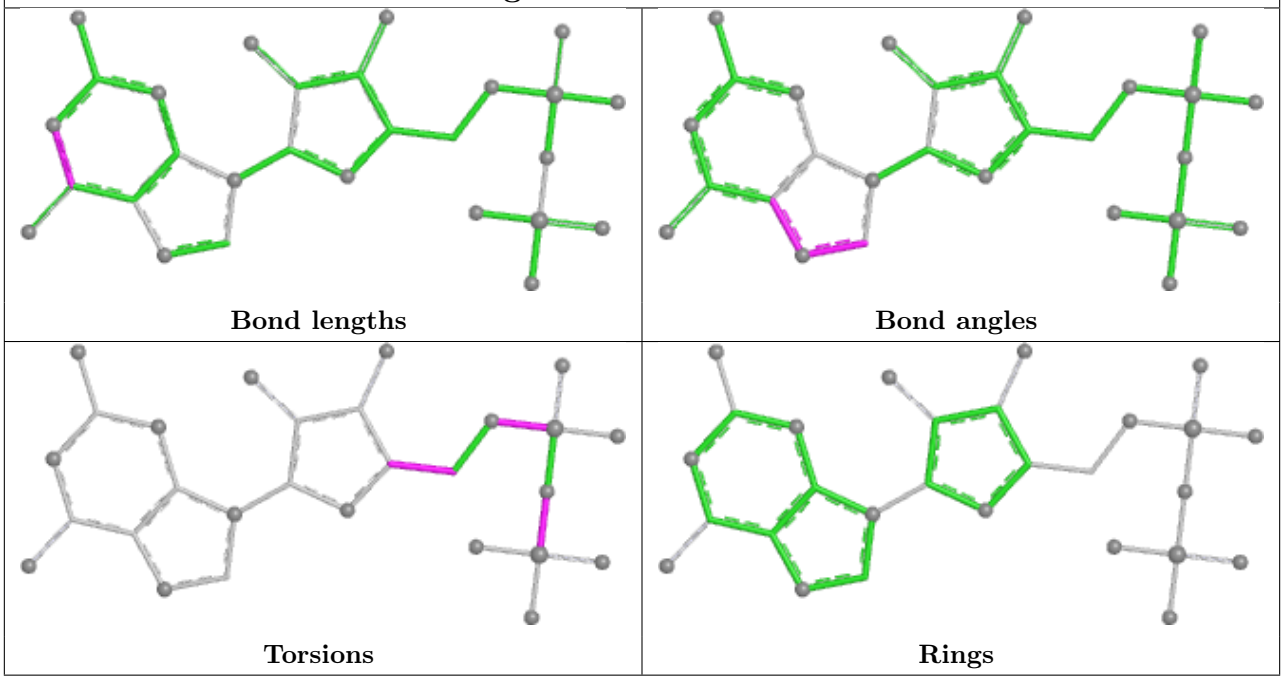


Torsions

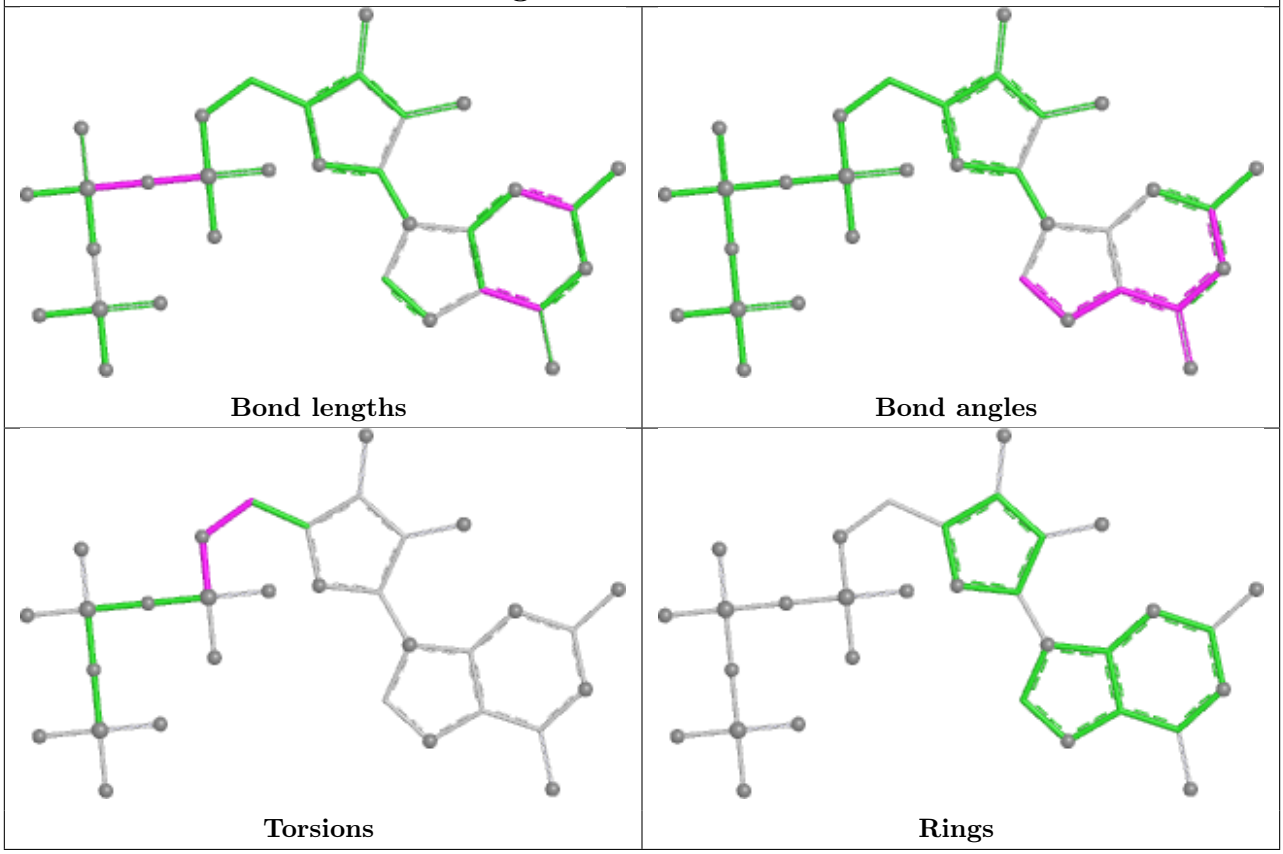


Rings

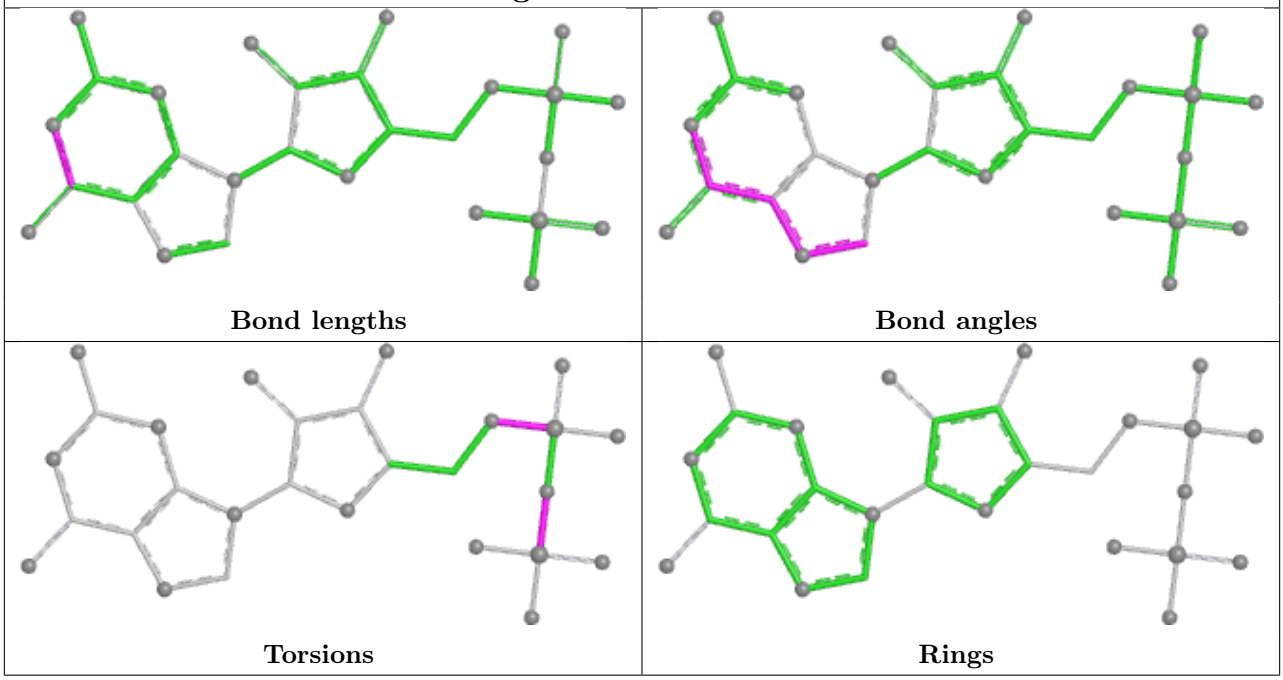
Ligand GDP DW 501



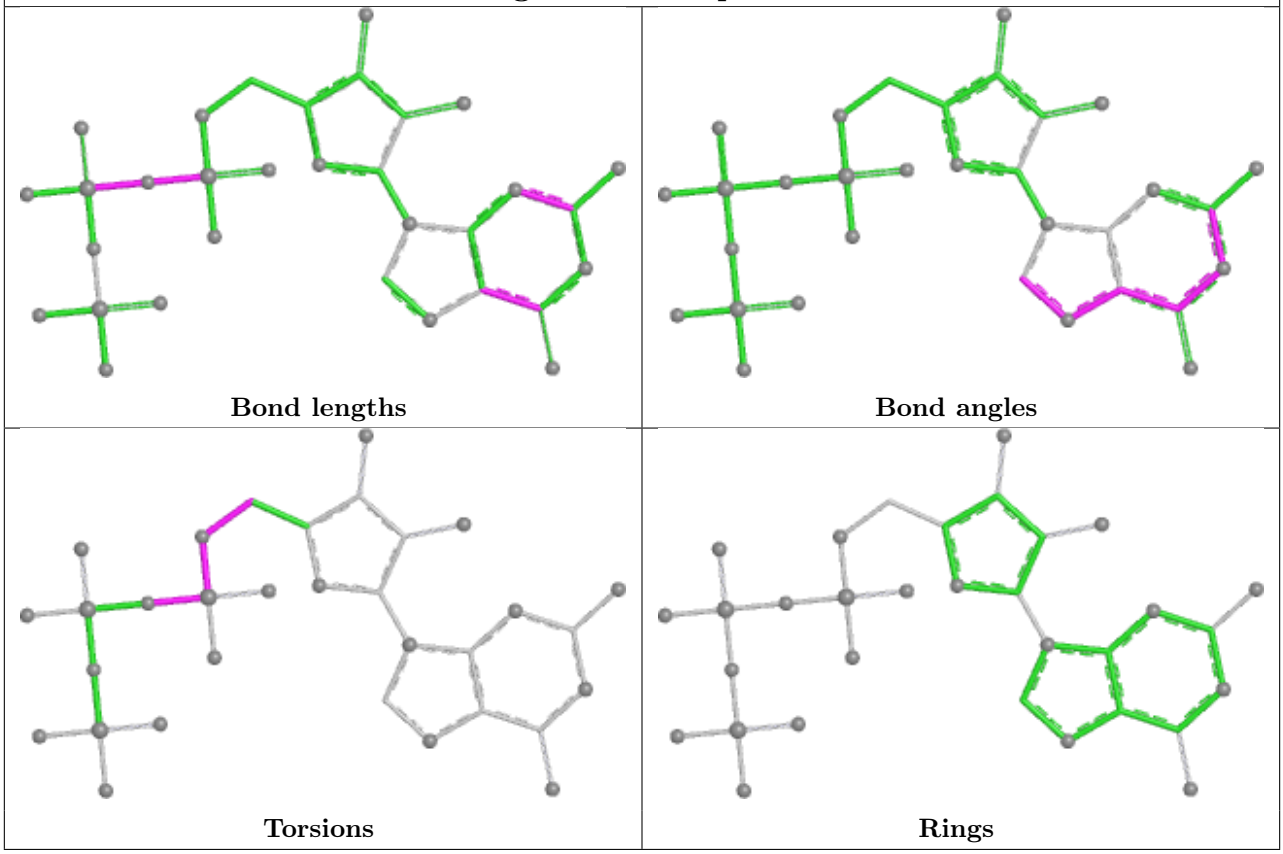
Ligand GTP GL 501



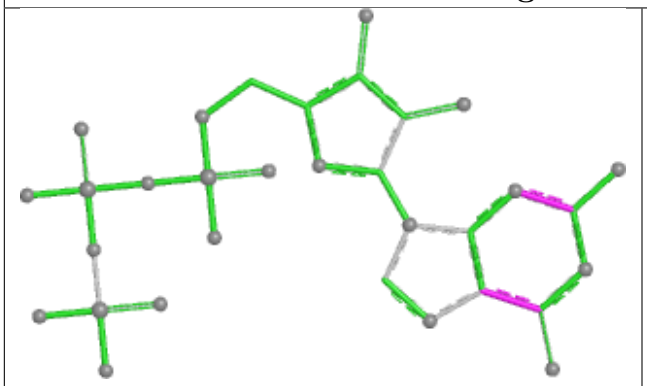
Ligand GDP Bh 501



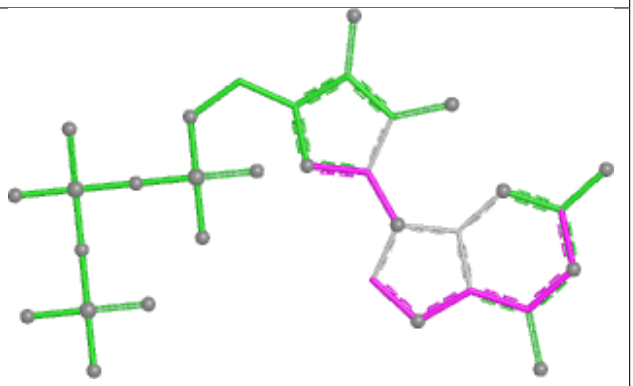
Ligand GTP Gp 501



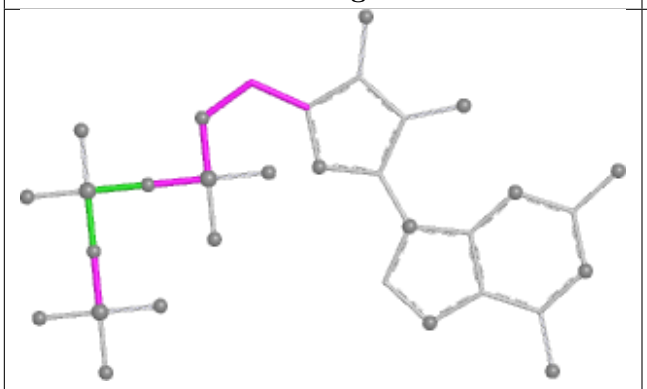
Ligand GTP BI 602



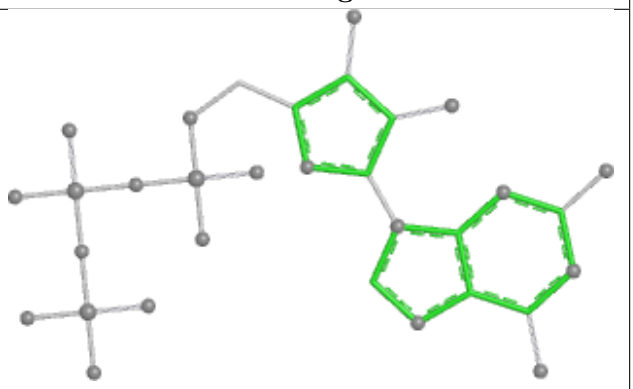
Bond lengths



Bond angles

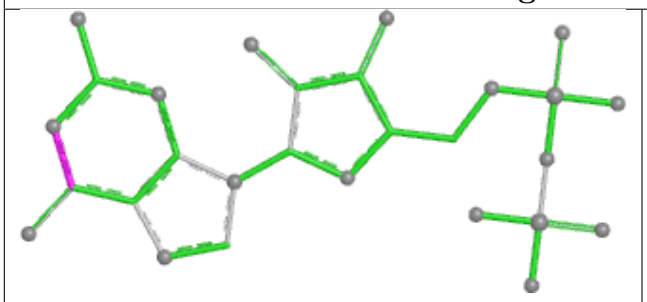


Torsions

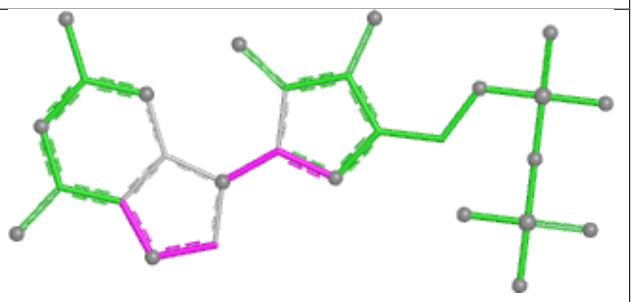


Rings

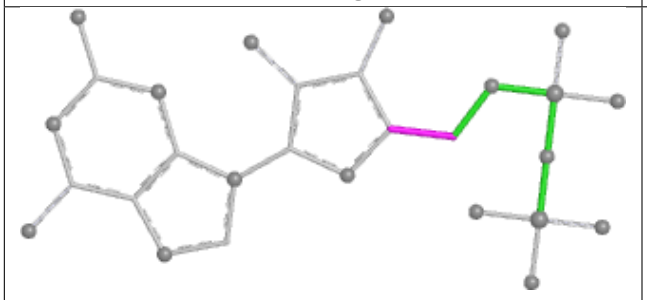
Ligand GDP Fr 501



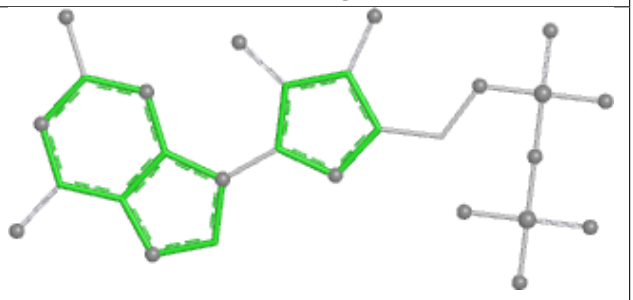
Bond lengths



Bond angles

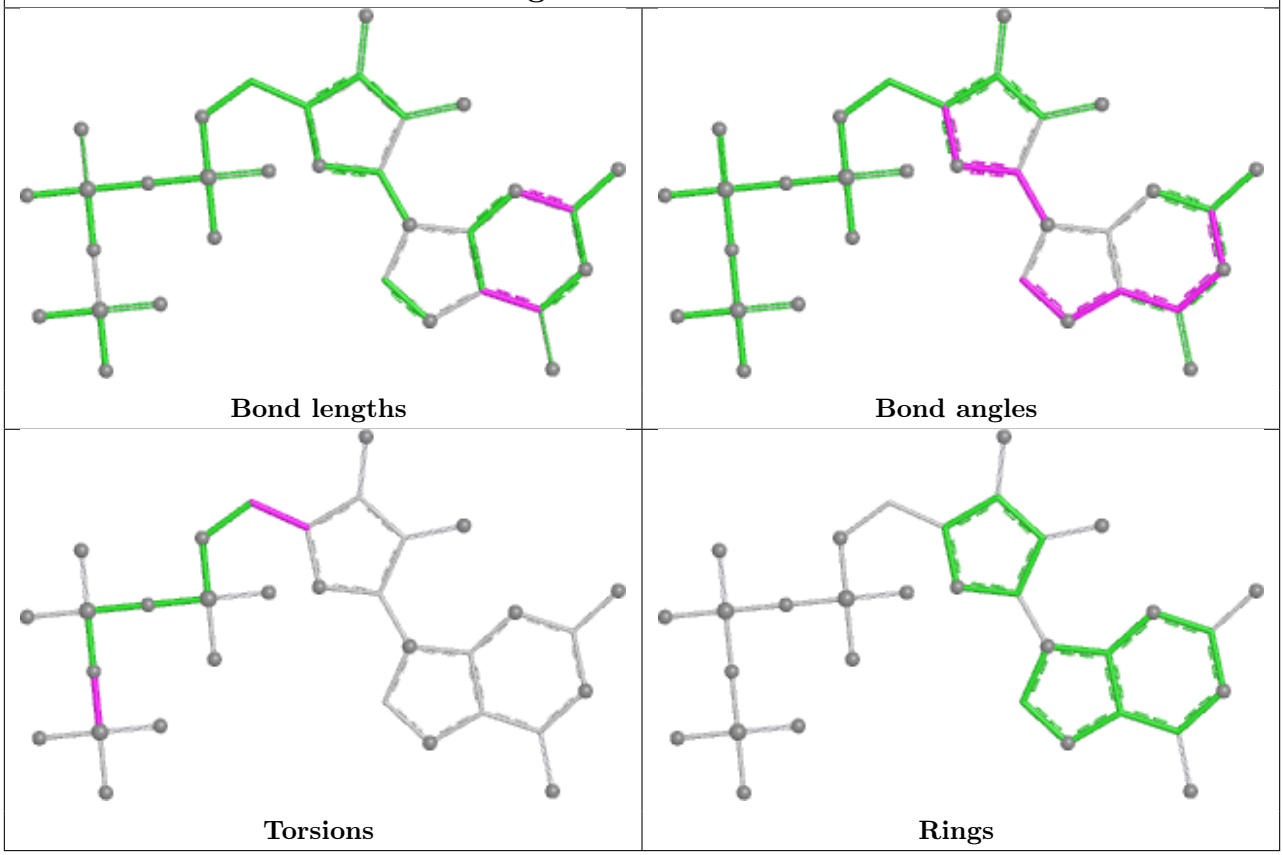


Torsions

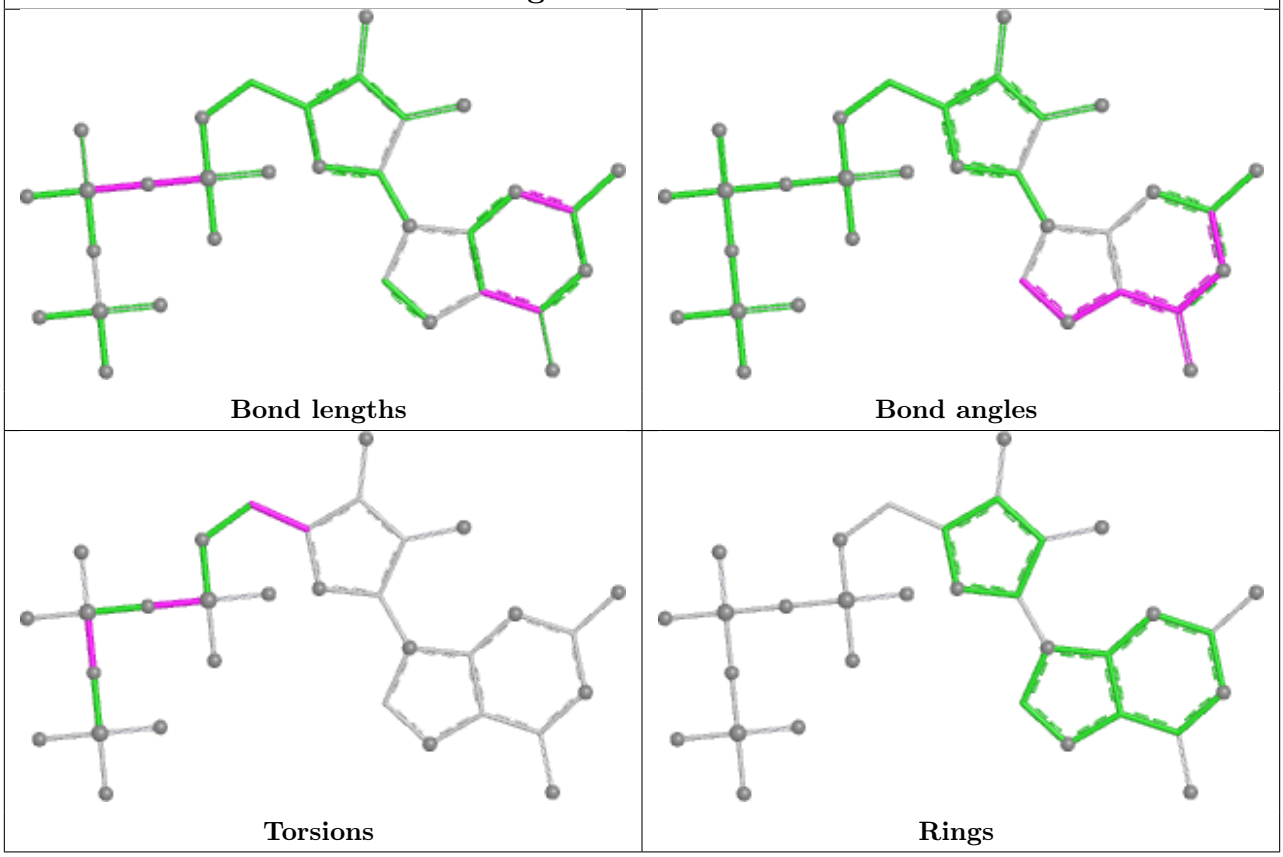


Rings

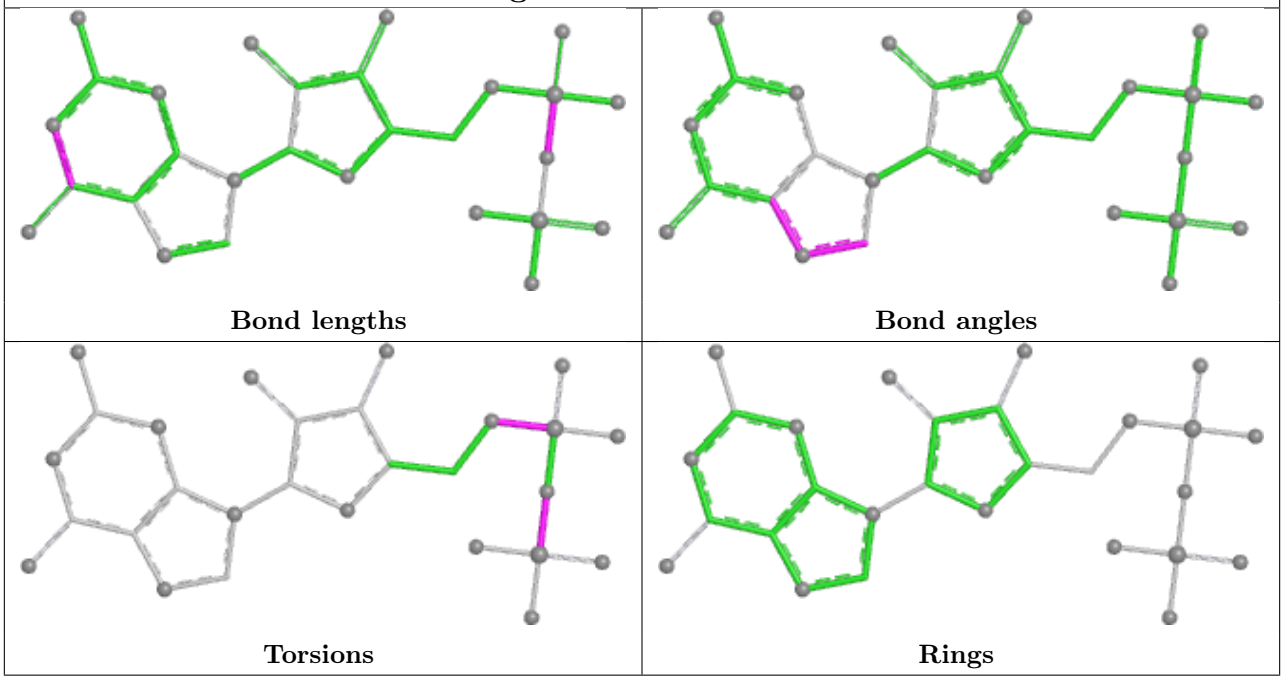
Ligand GTP 2 602



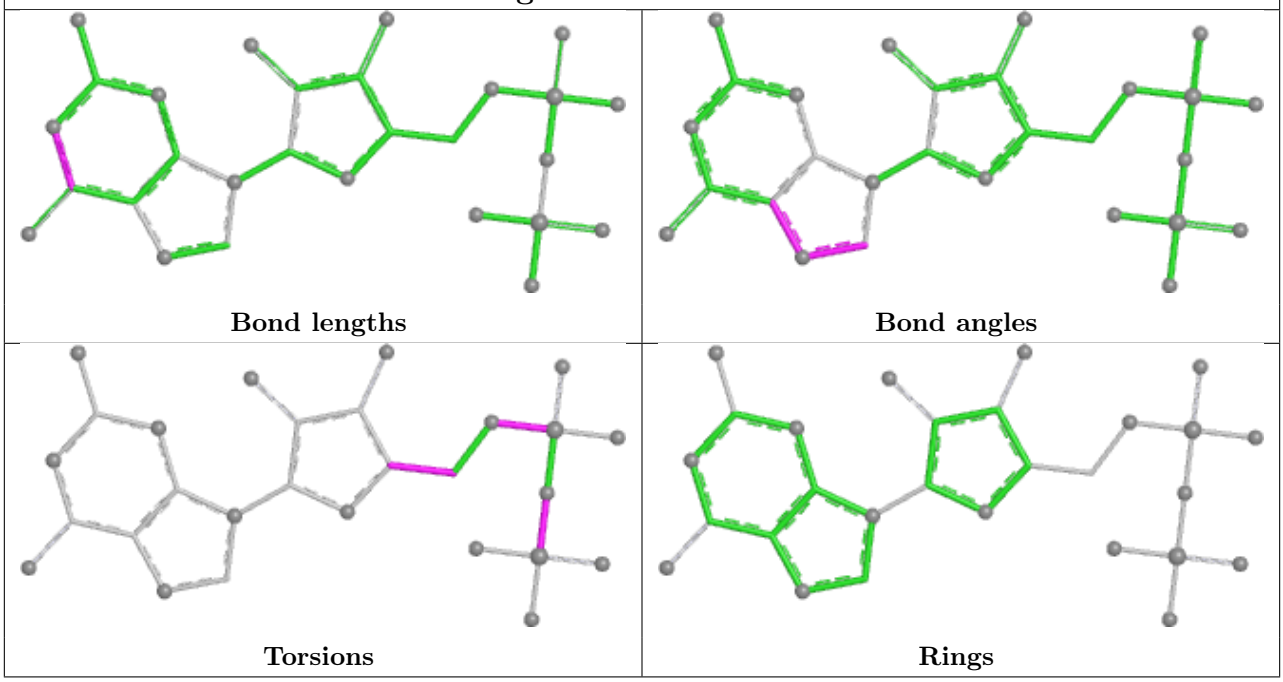
Ligand GTP v 602



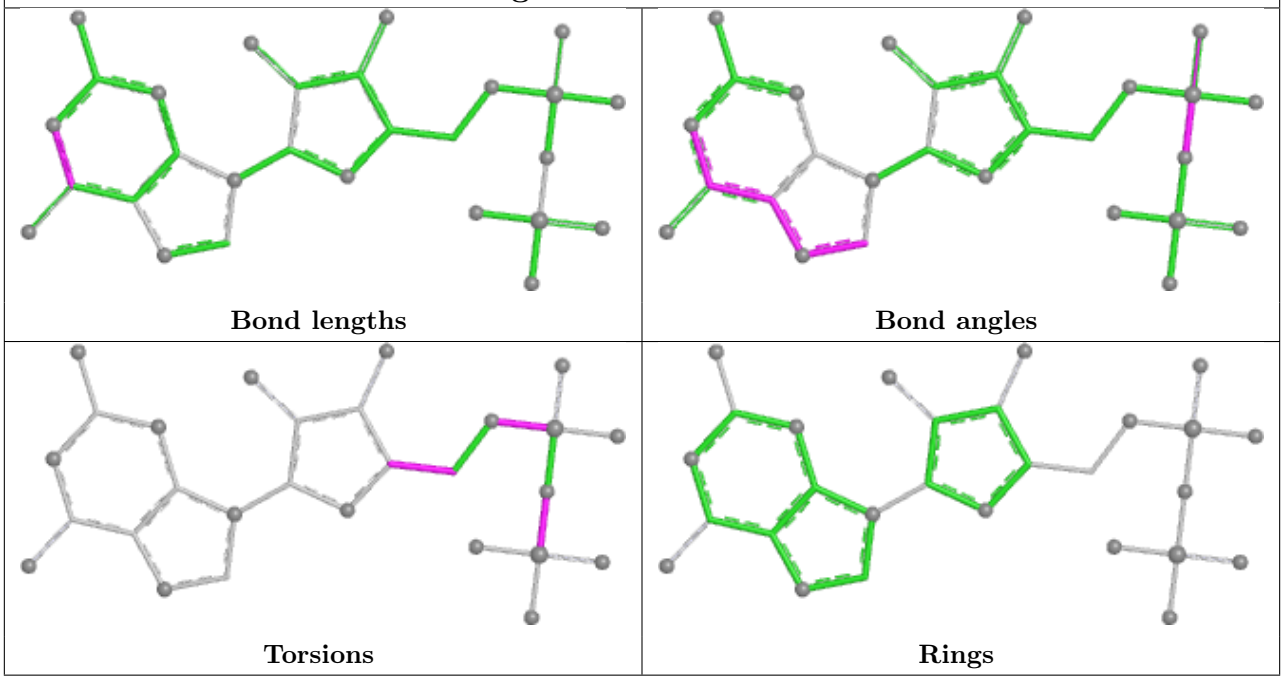
Ligand GDP AY 501



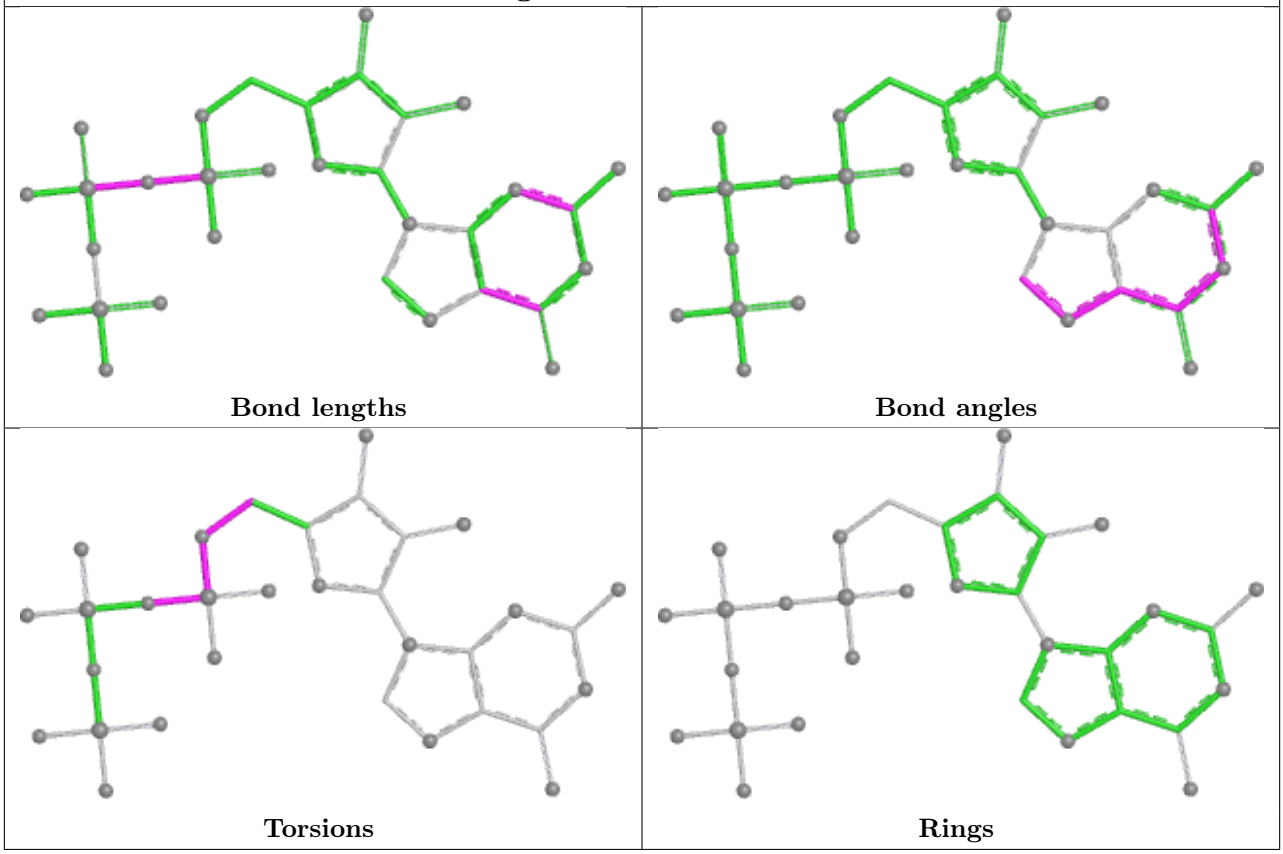
Ligand GDP Gi 501



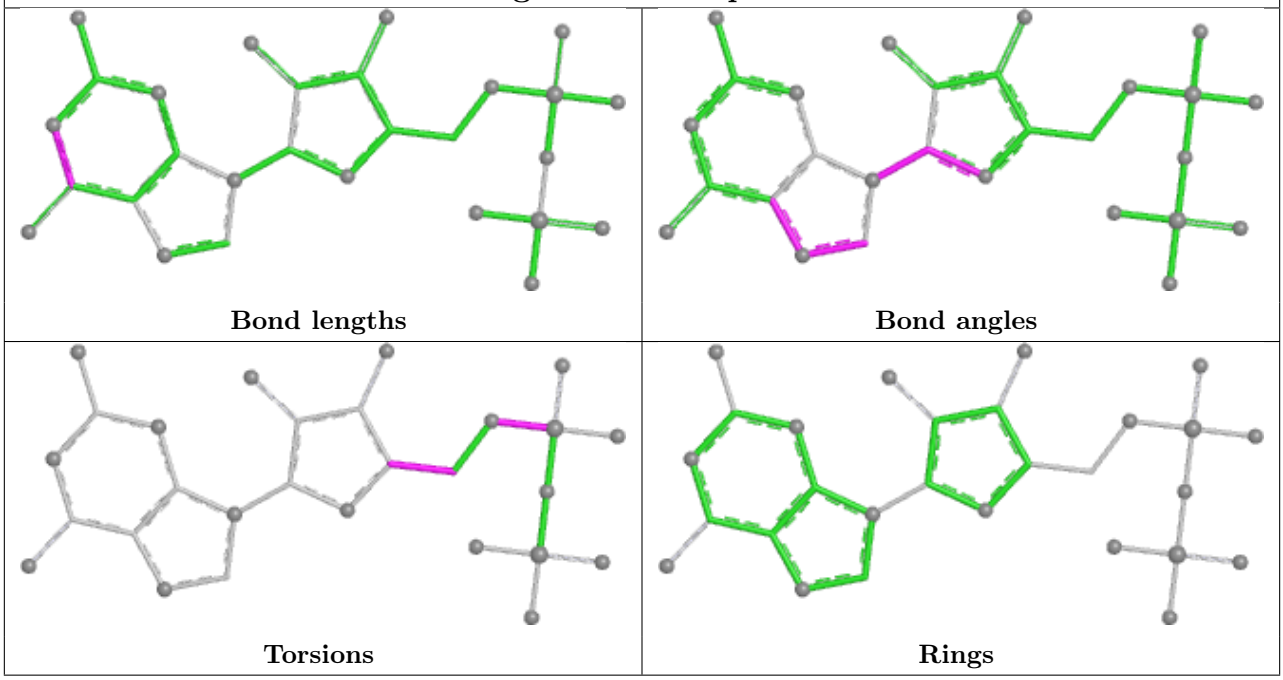
Ligand GDP DS 501



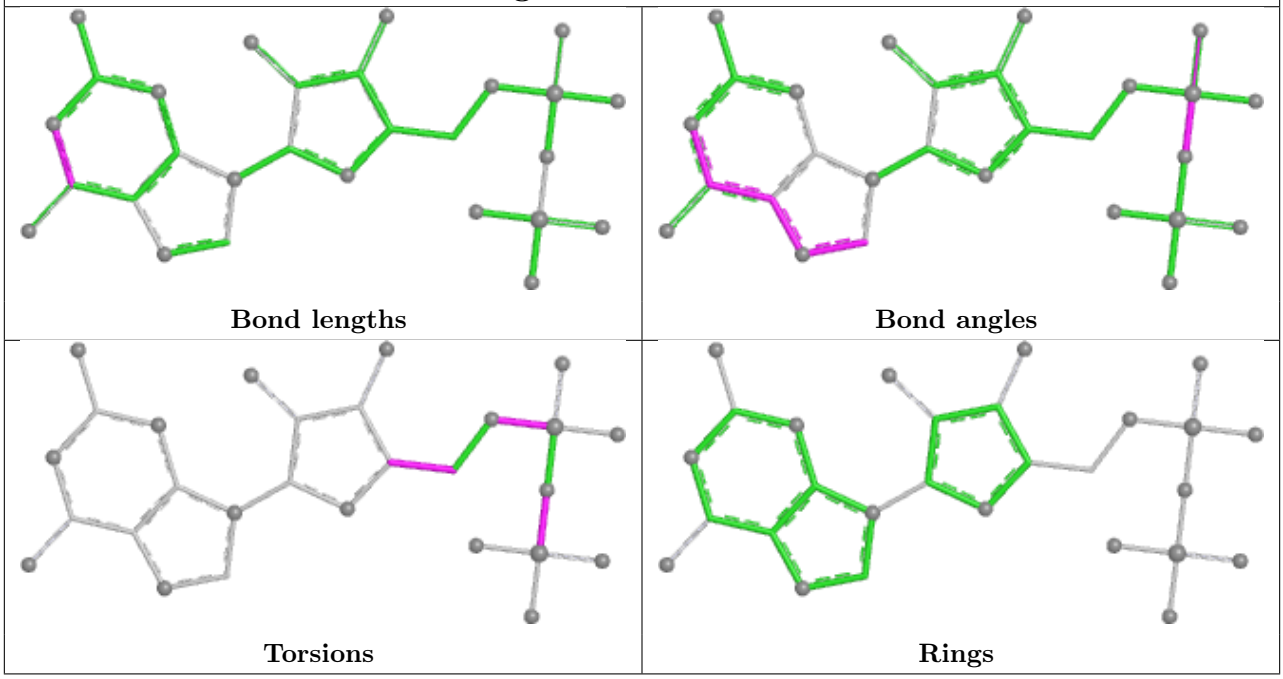
Ligand GTP Gr 501

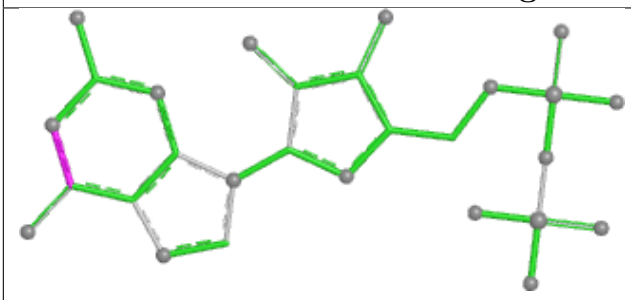
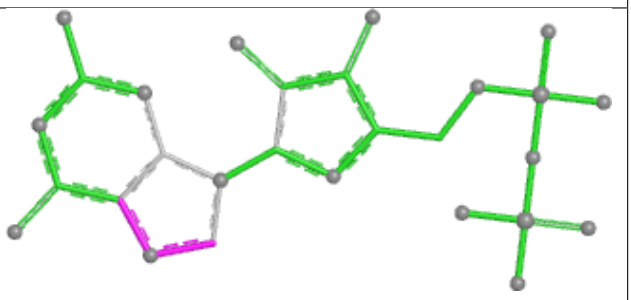
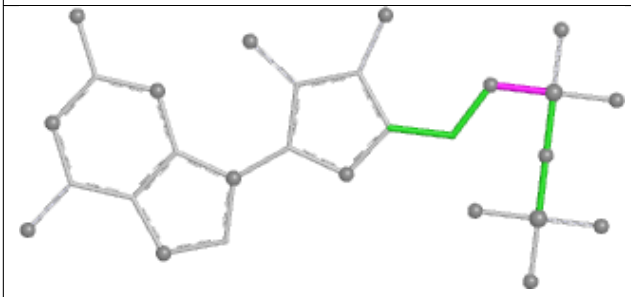
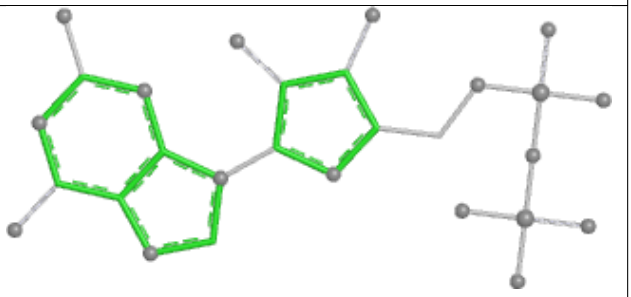


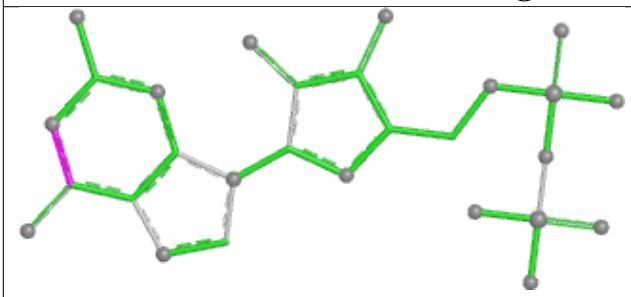
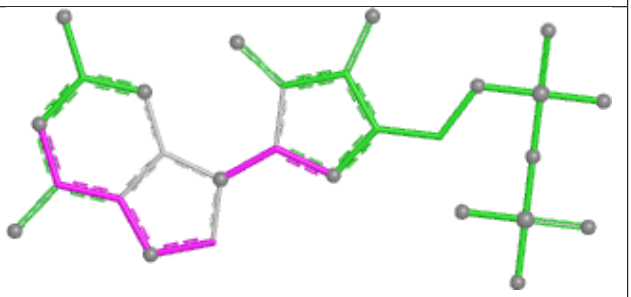
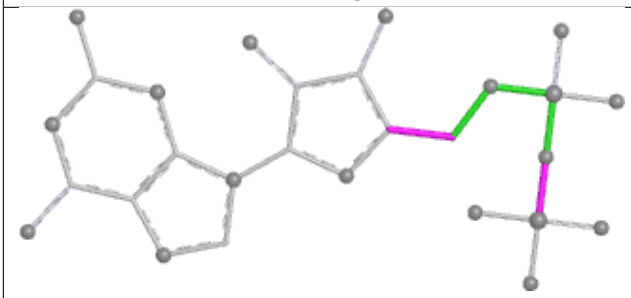
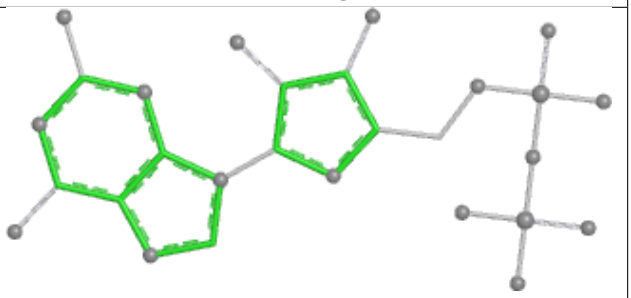
Ligand GDP Aq 501



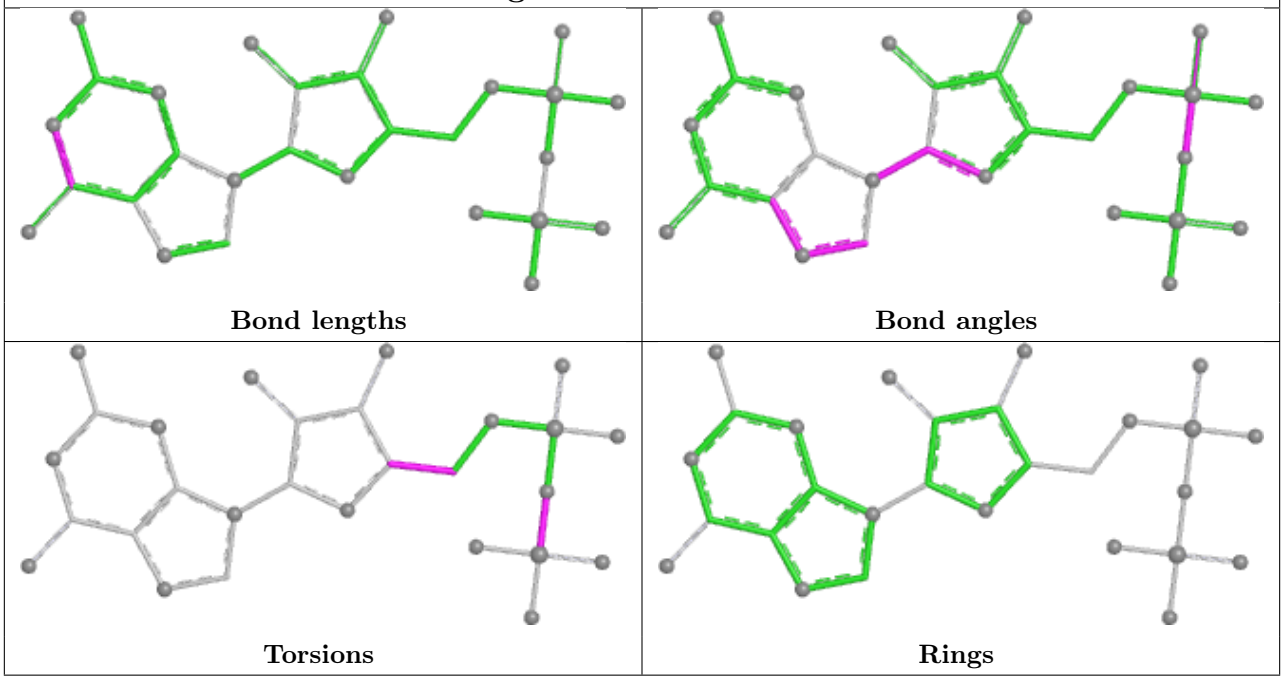
Ligand GDP Gc 501



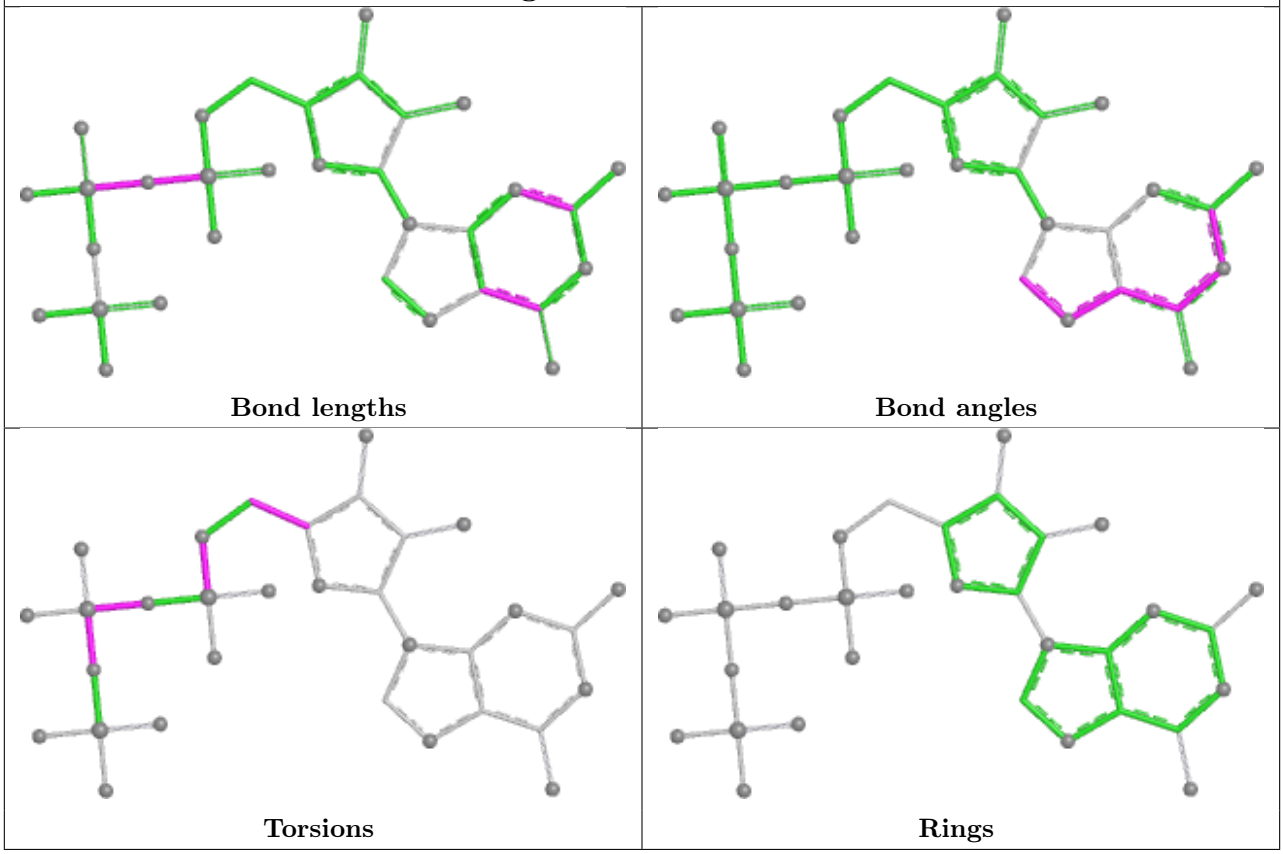
Ligand GDP m 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP Fo 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

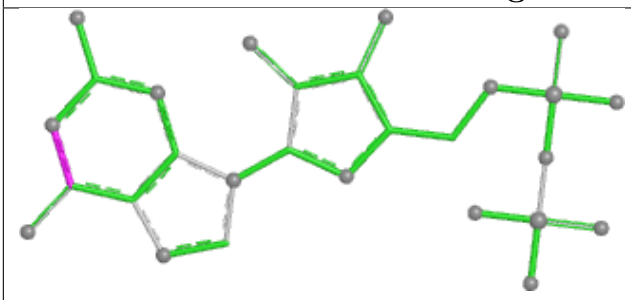
Ligand GDP GV 501



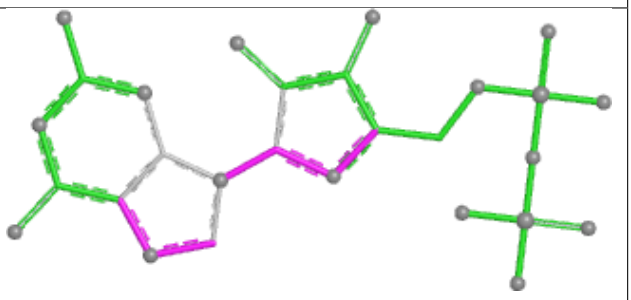
Ligand GTP Fi 501



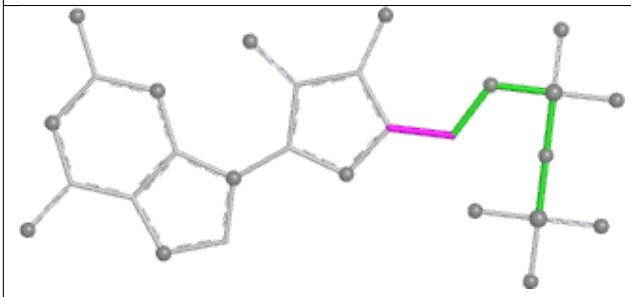
Ligand GDP AU 501



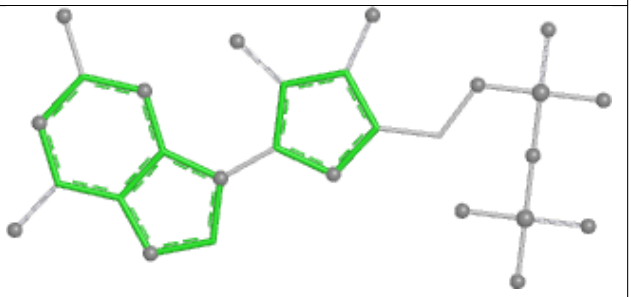
Bond lengths



Bond angles

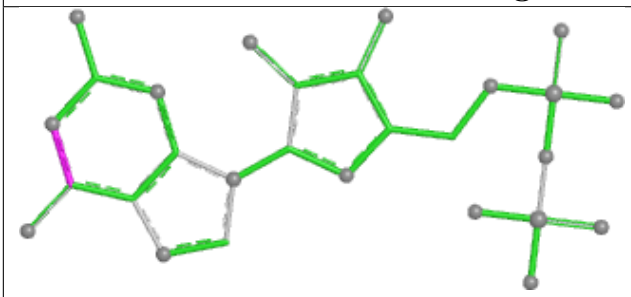


Torsions

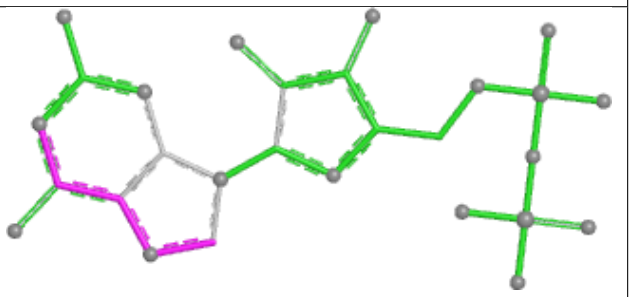


Rings

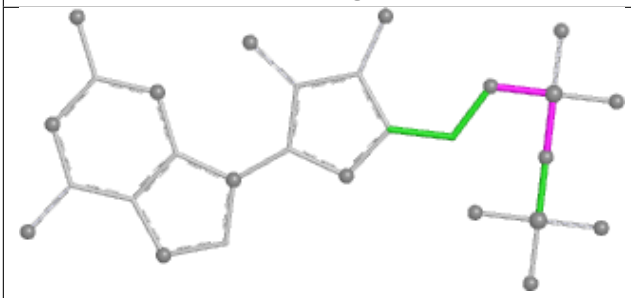
Ligand GDP Be 501



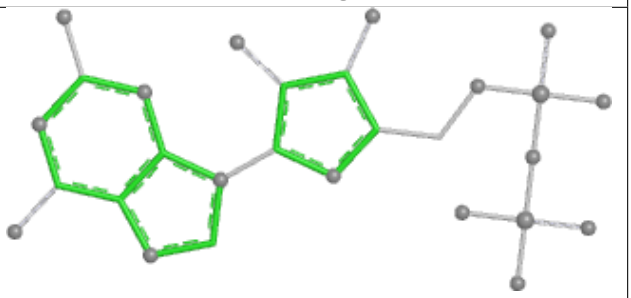
Bond lengths



Bond angles

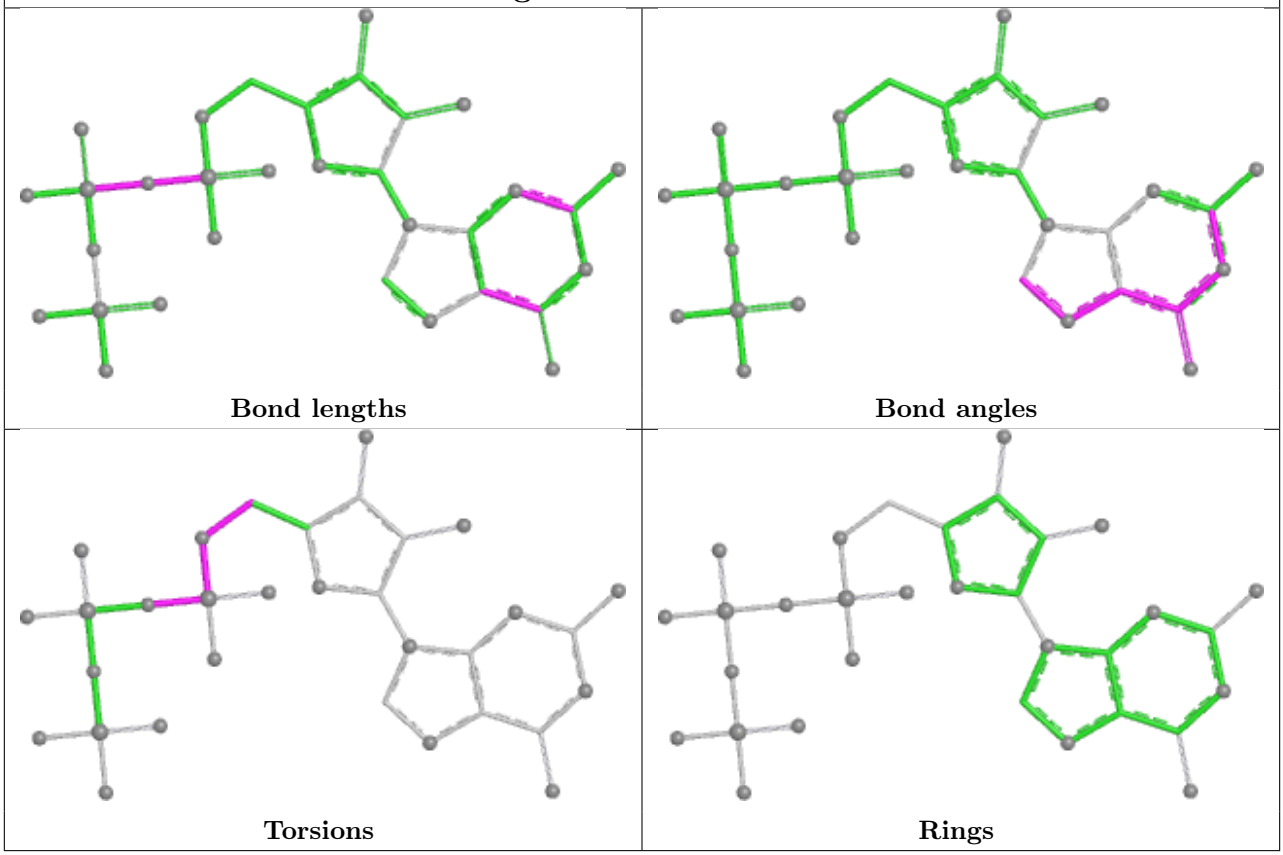


Torsions

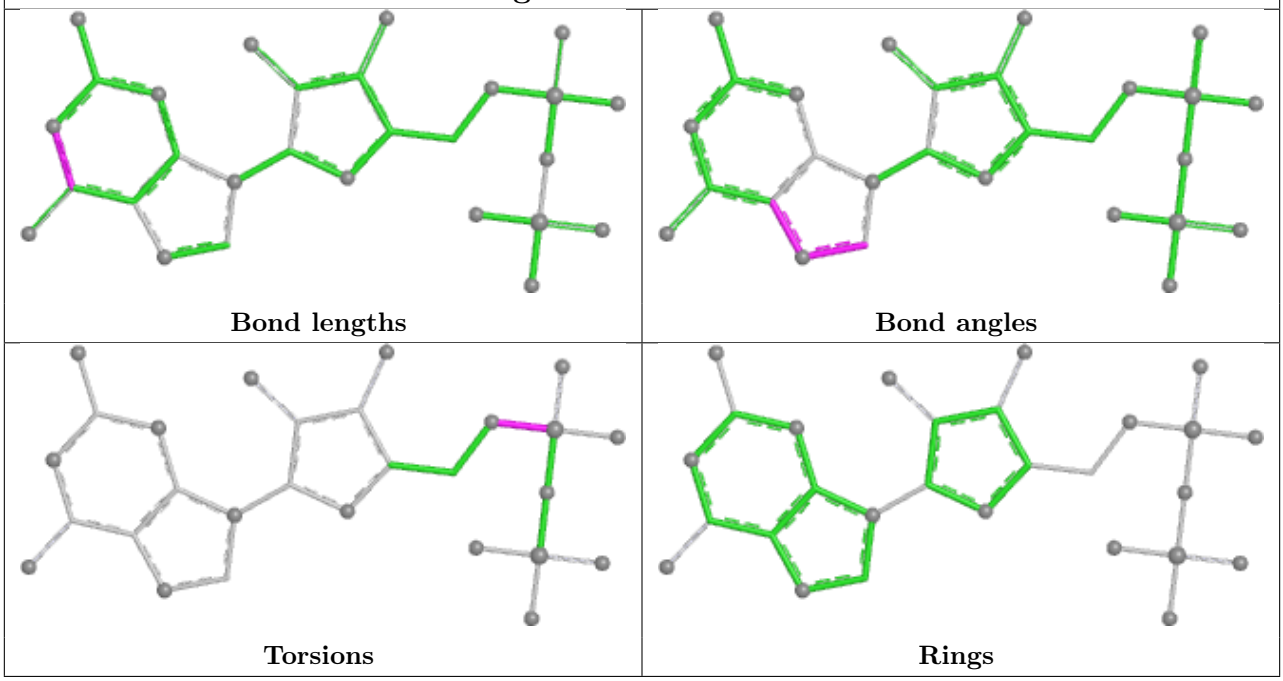


Rings

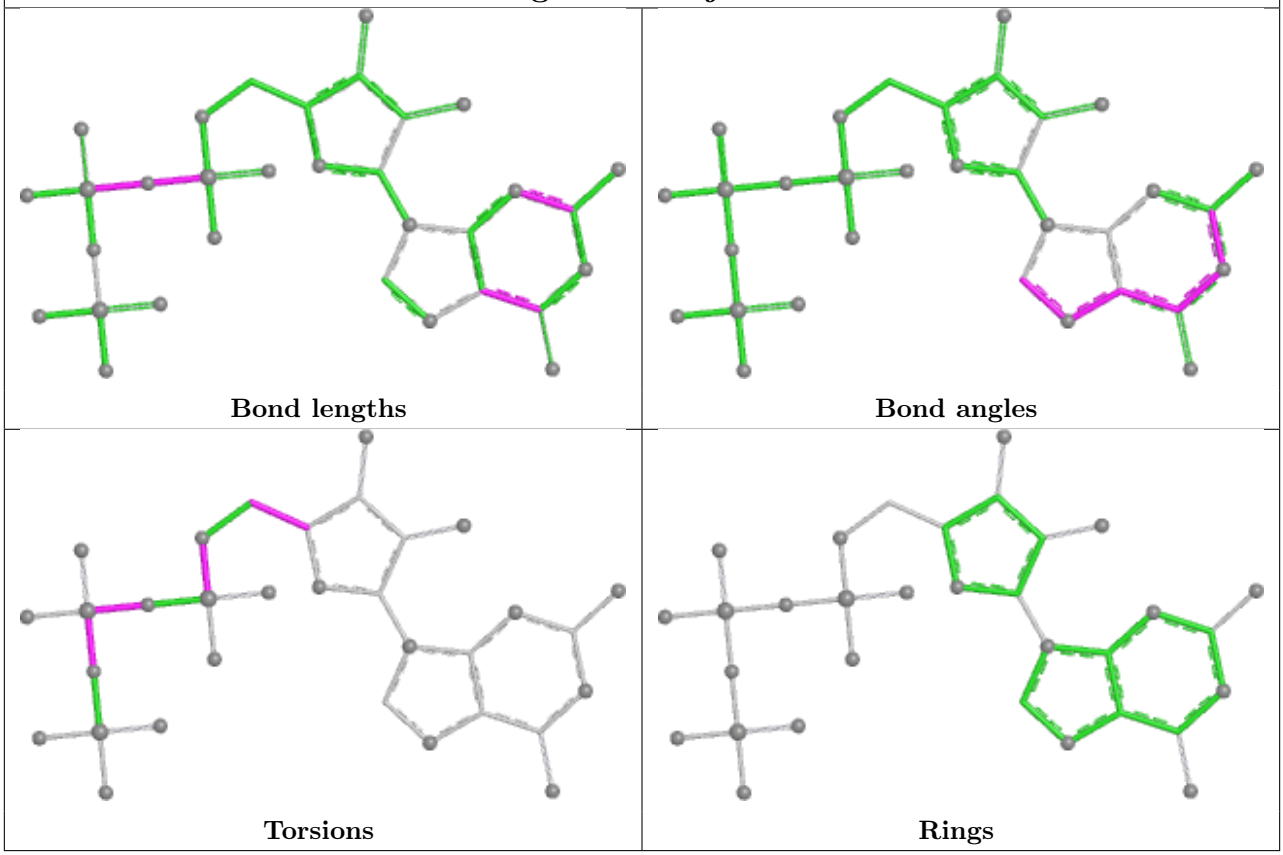
Ligand GTP G1 501



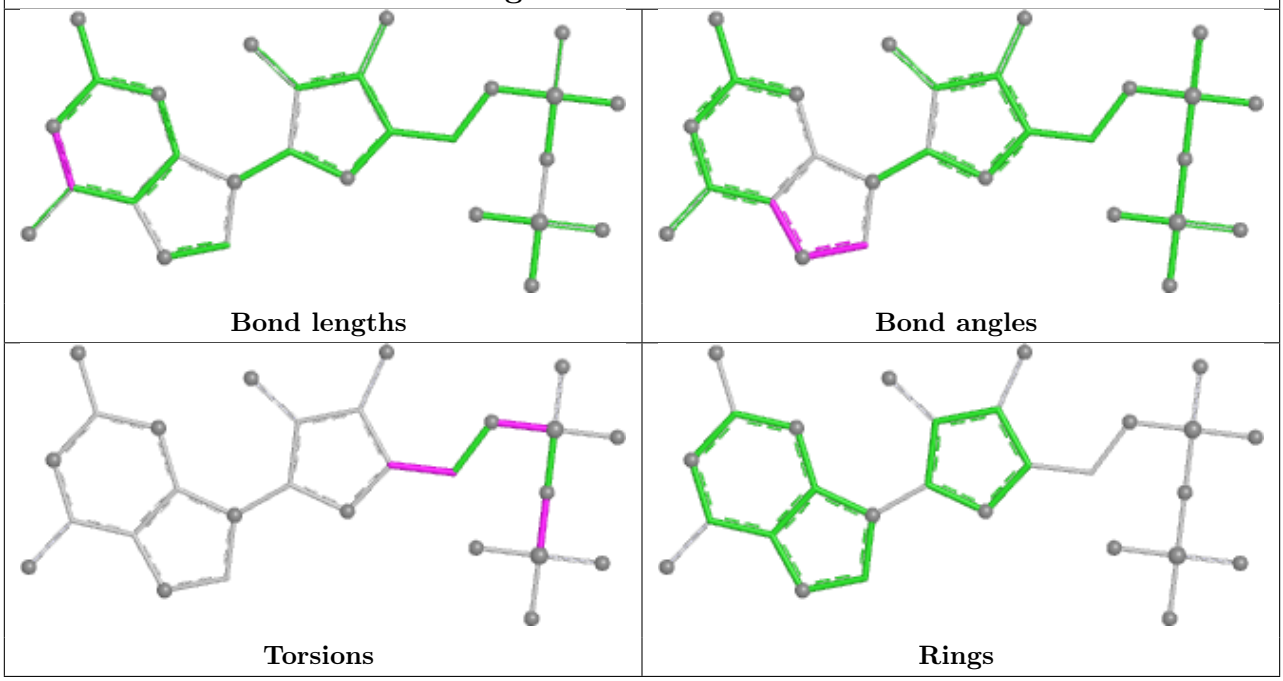
Ligand GDP Ao 501



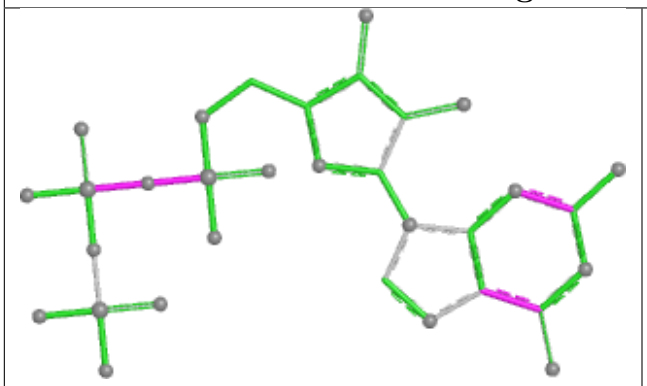
Ligand GTP j 602



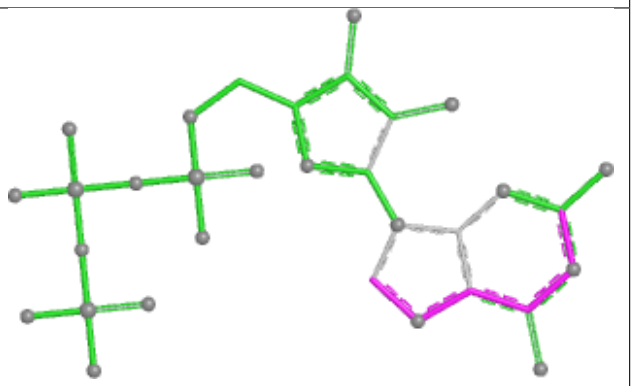
Ligand GDP EW 501



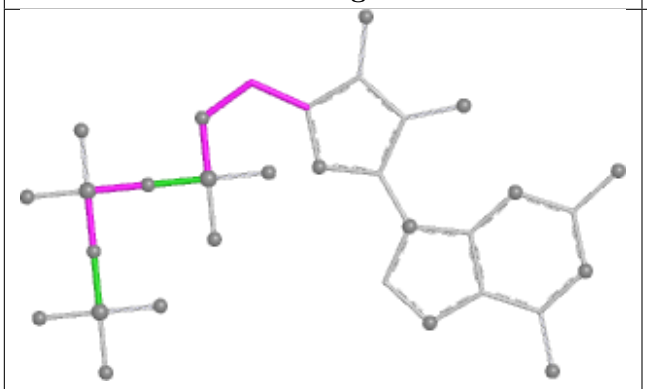
Ligand GTP E2 501



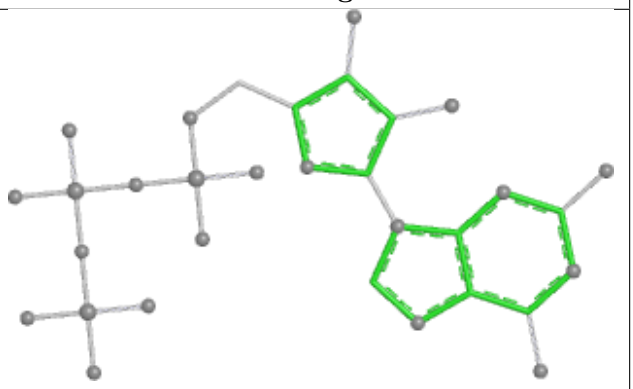
Bond lengths



Bond angles

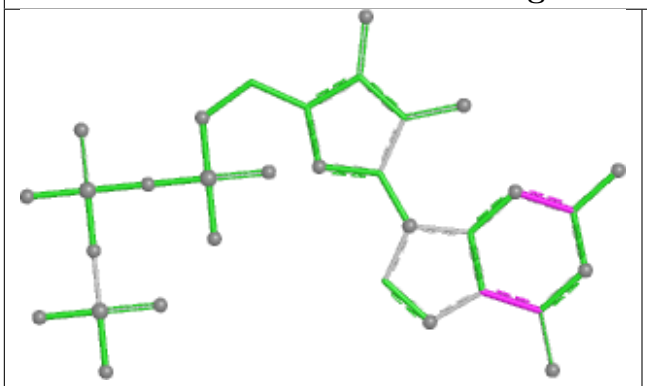


Torsions

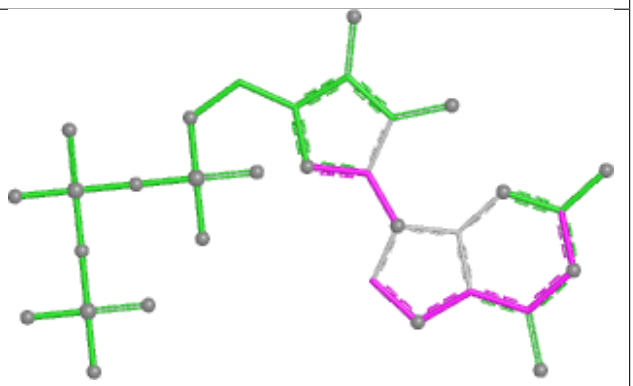


Rings

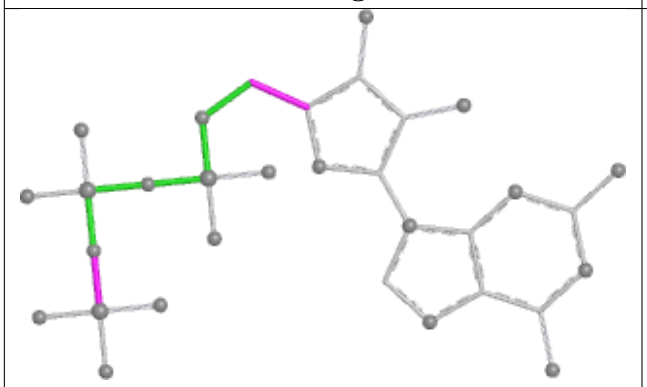
Ligand GTP 3 602



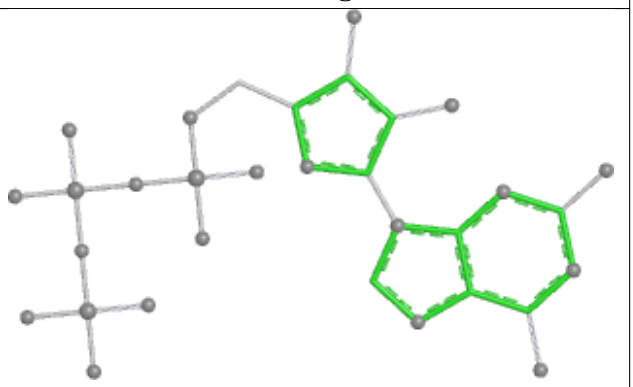
Bond lengths



Bond angles

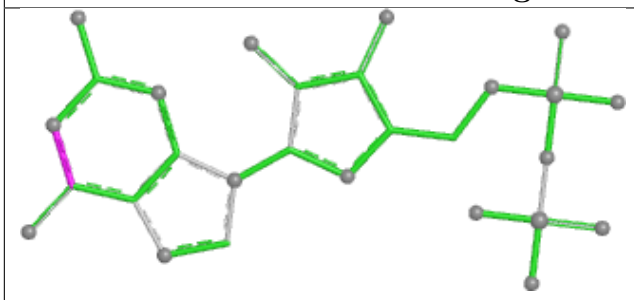


Torsions

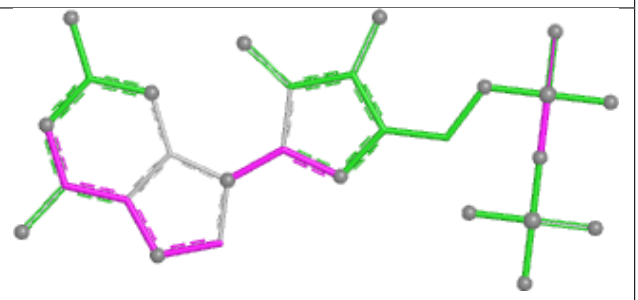


Rings

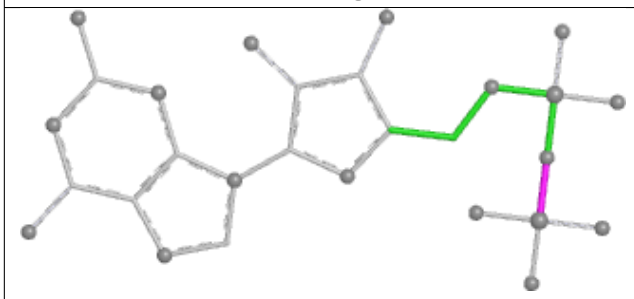
Ligand GDP De 501



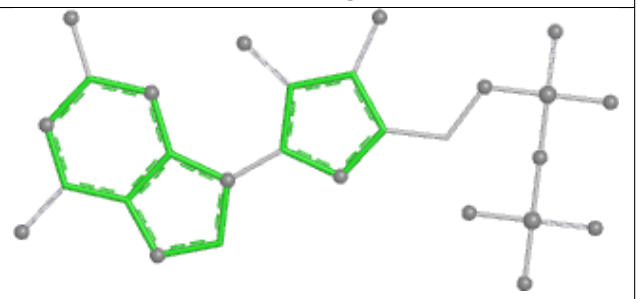
Bond lengths



Bond angles

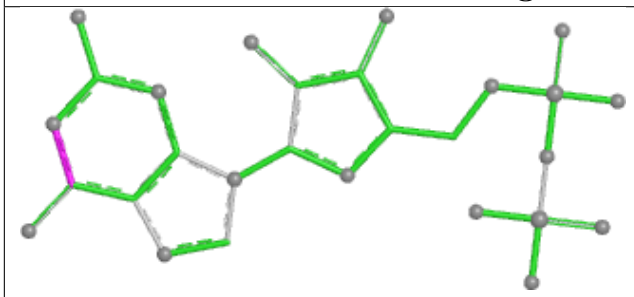


Torsions

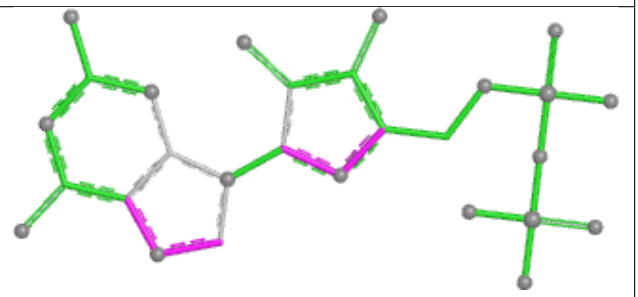


Rings

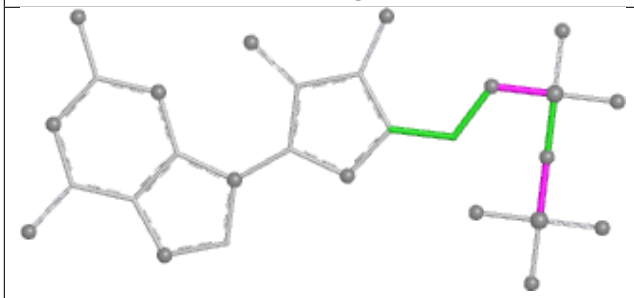
Ligand GDP Ai 501



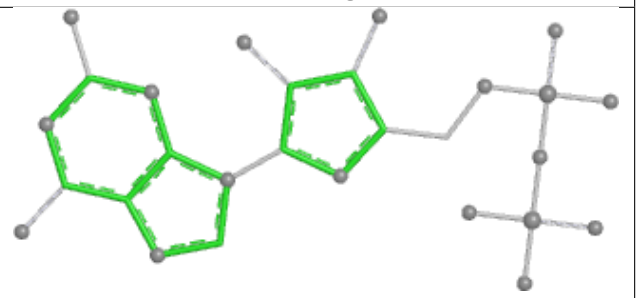
Bond lengths



Bond angles

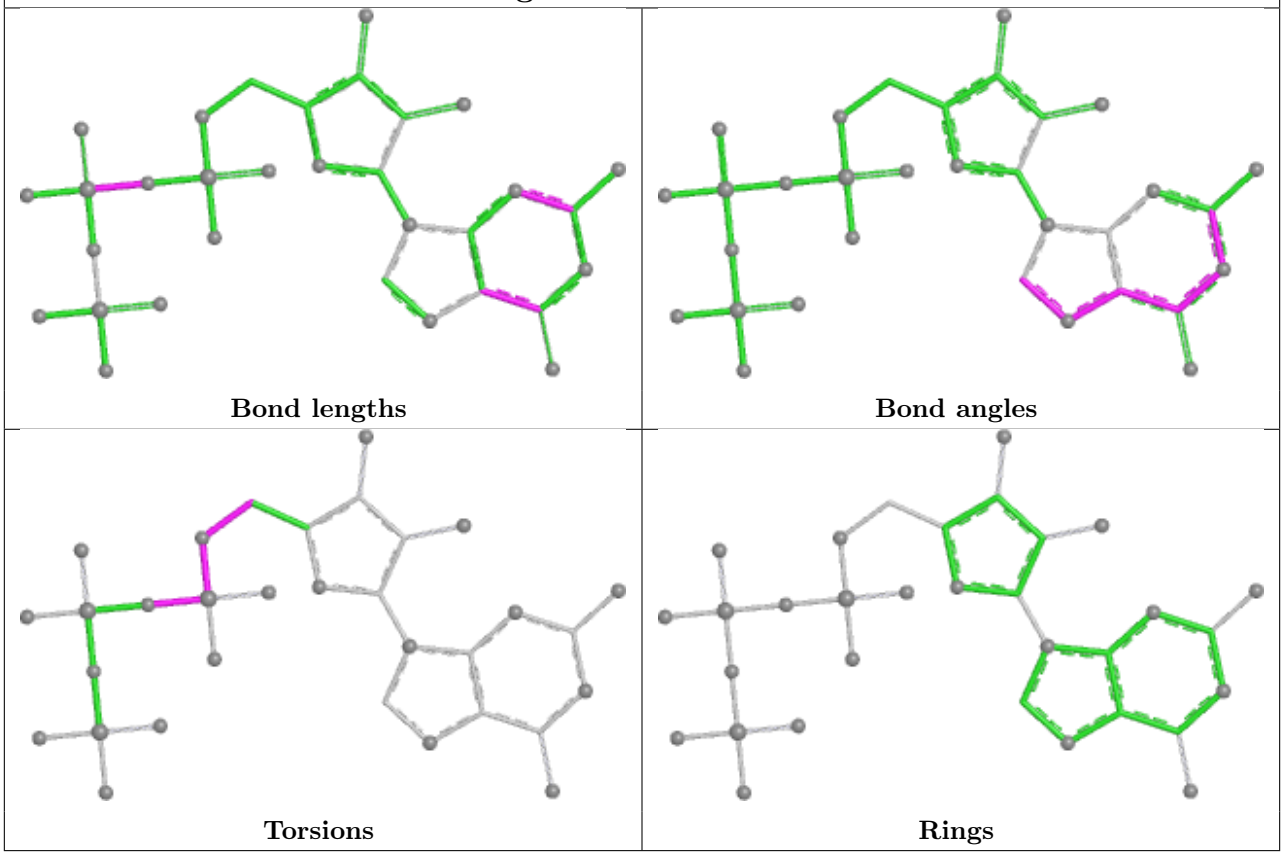


Torsions

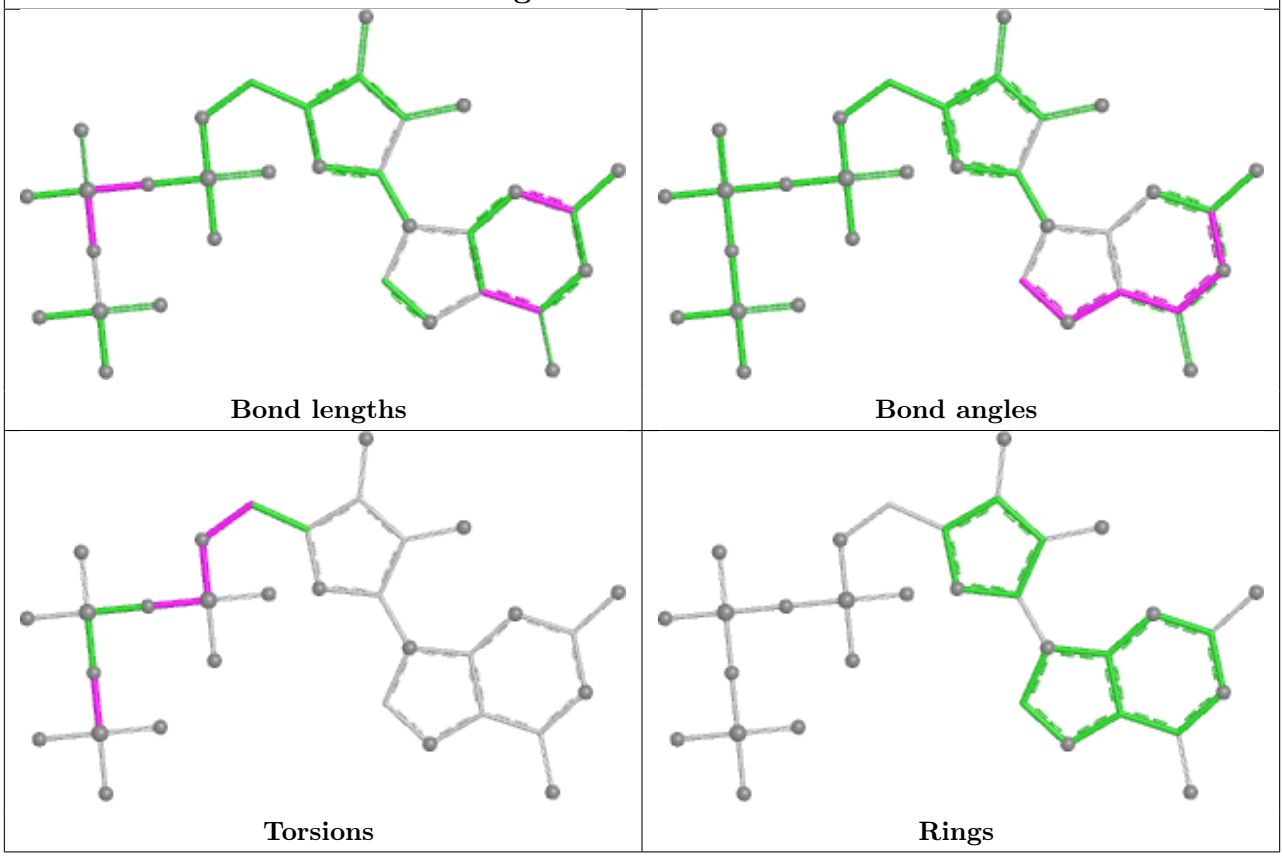


Rings

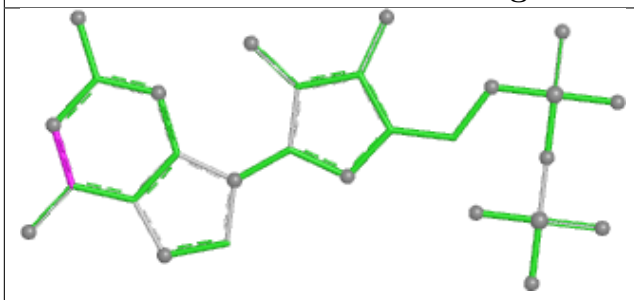
Ligand GTP E8 501



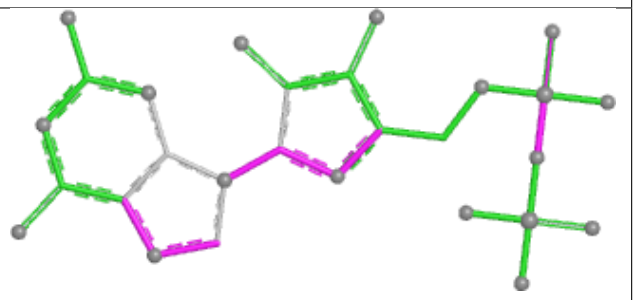
Ligand GTP G2 501



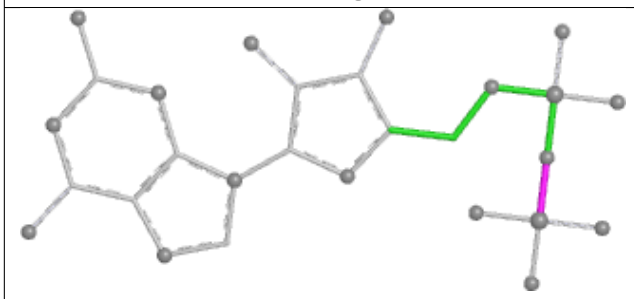
Ligand GDP FN 501



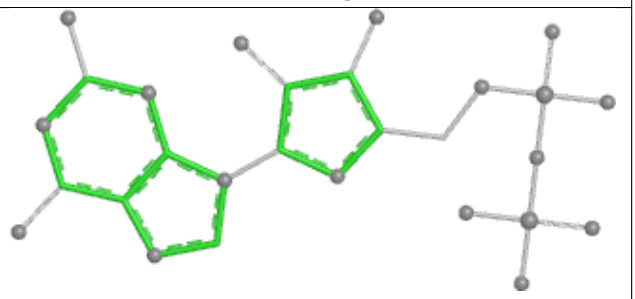
Bond lengths



Bond angles

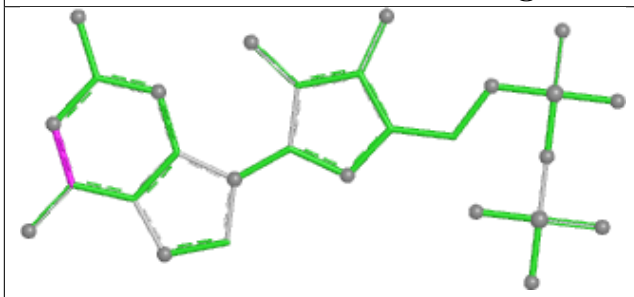


Torsions

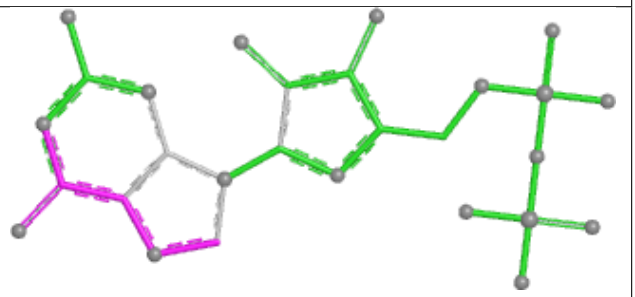


Rings

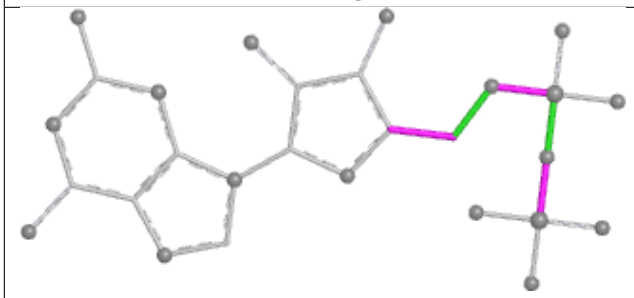
Ligand GDP Bl 602



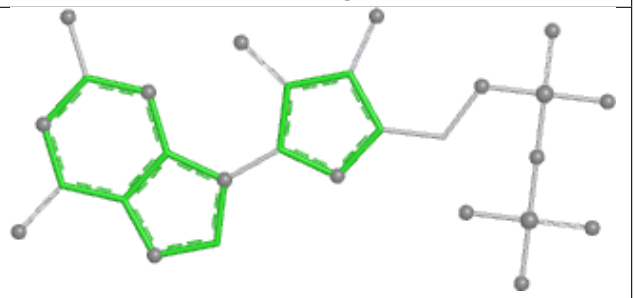
Bond lengths



Bond angles

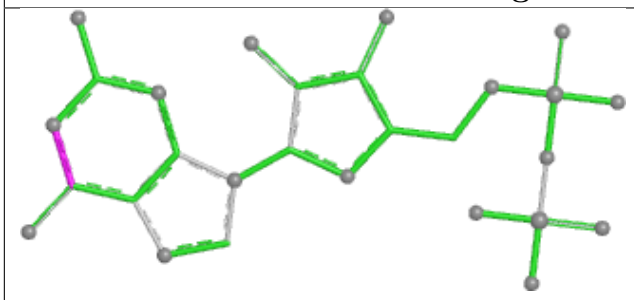


Torsions

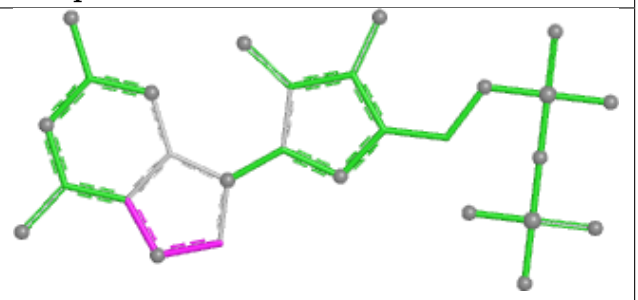


Rings

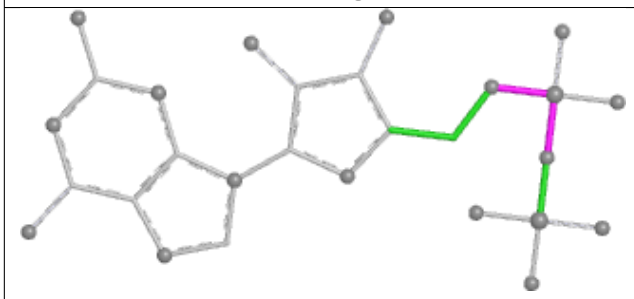
Ligand GDP Ap 501



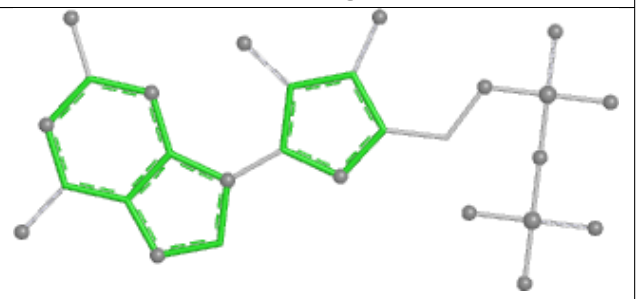
Bond lengths



Bond angles

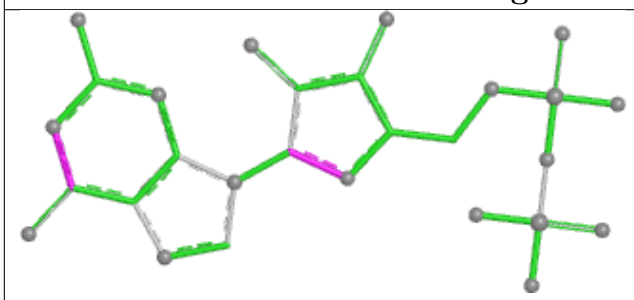


Torsions

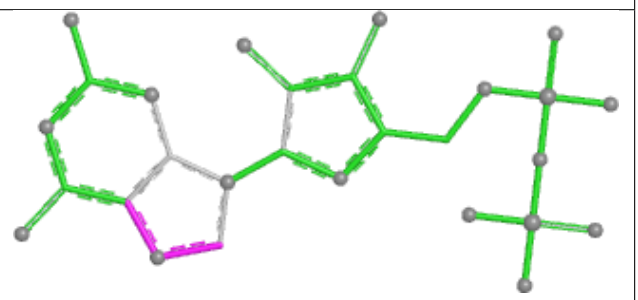


Rings

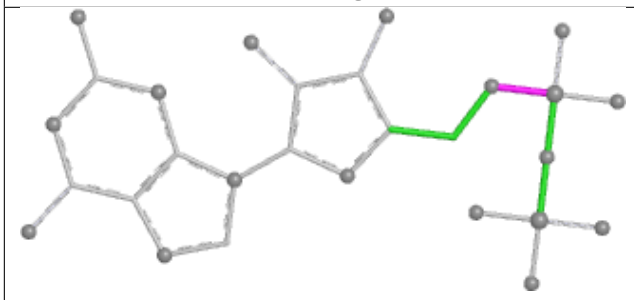
Ligand GDP BE 501



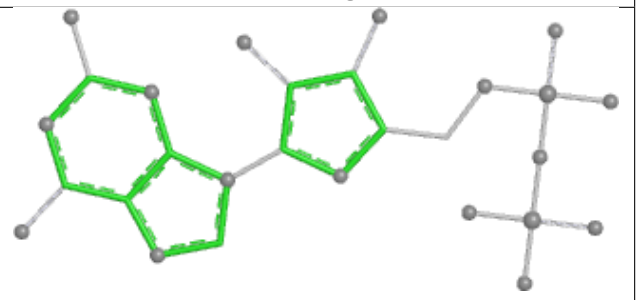
Bond lengths



Bond angles

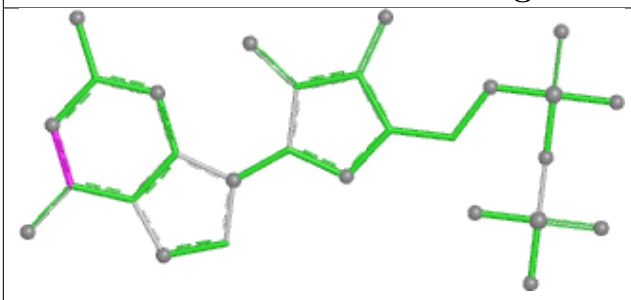


Torsions

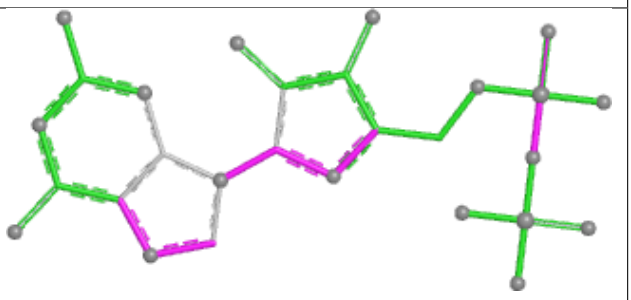


Rings

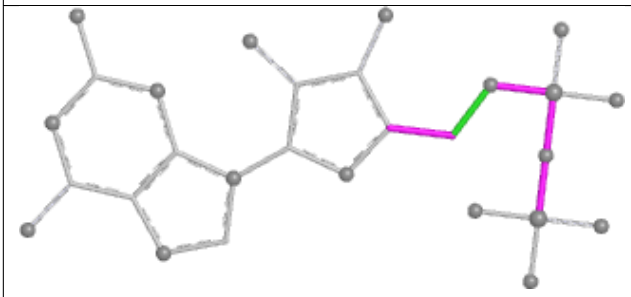
Ligand GDP F1 501



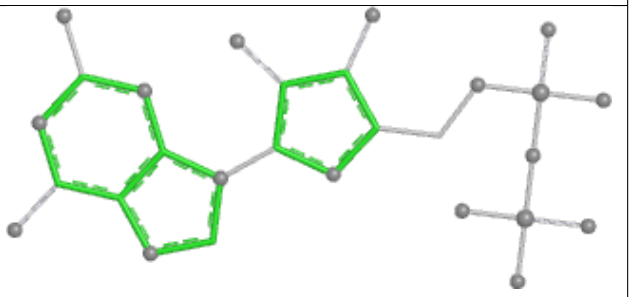
Bond lengths



Bond angles

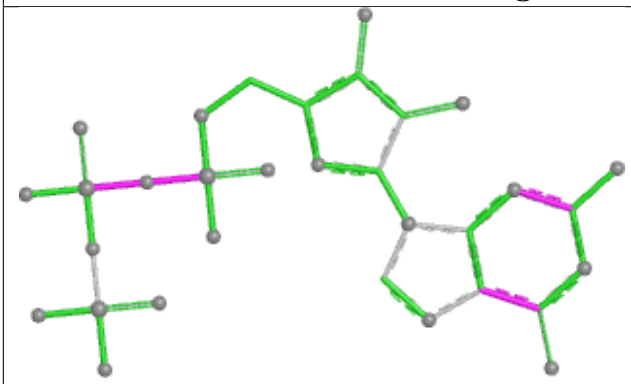


Torsions

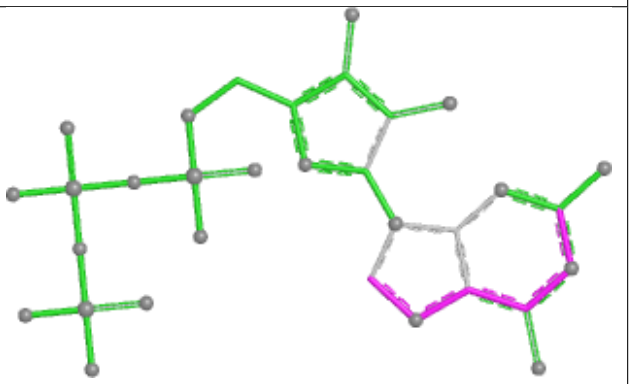


Rings

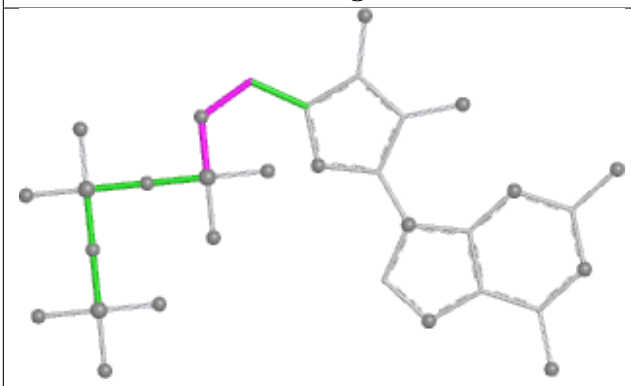
Ligand GTP Gs 501



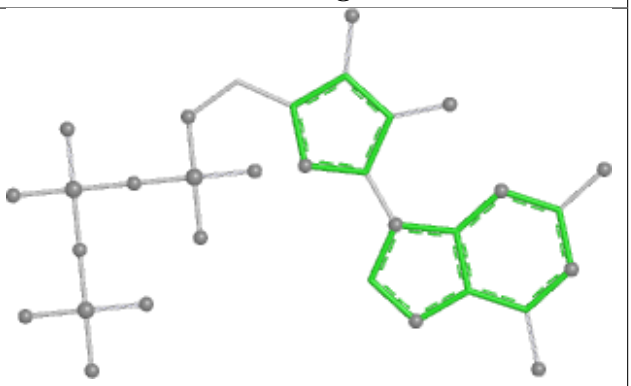
Bond lengths



Bond angles

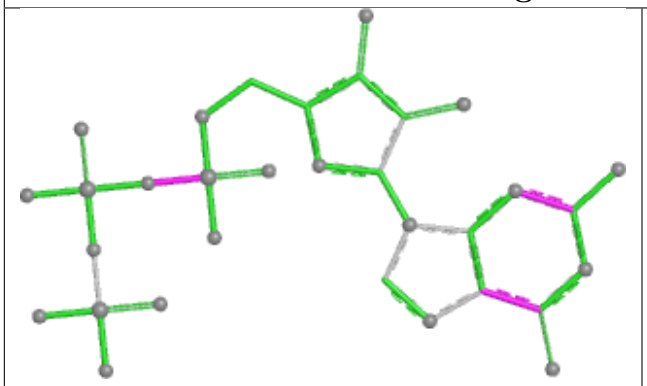


Torsions

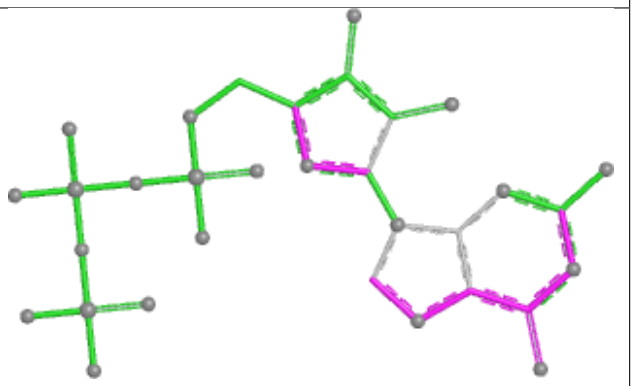


Rings

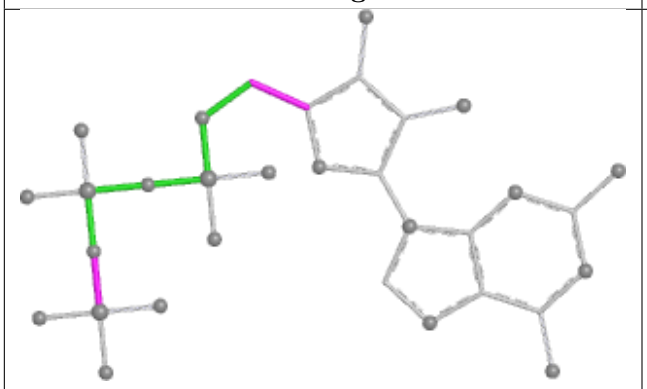
Ligand GTP B5 602



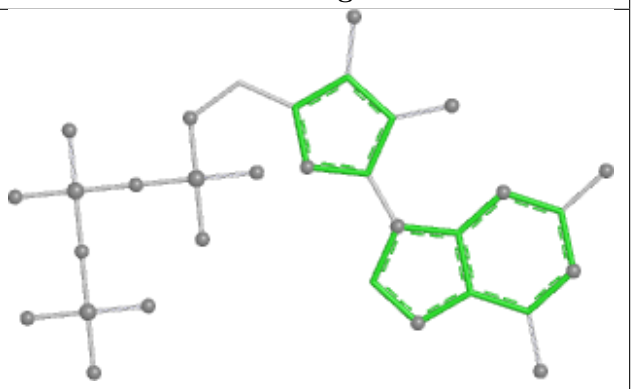
Bond lengths



Bond angles

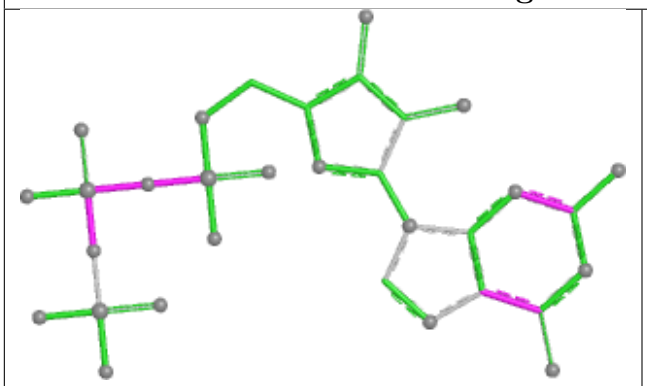


Torsions

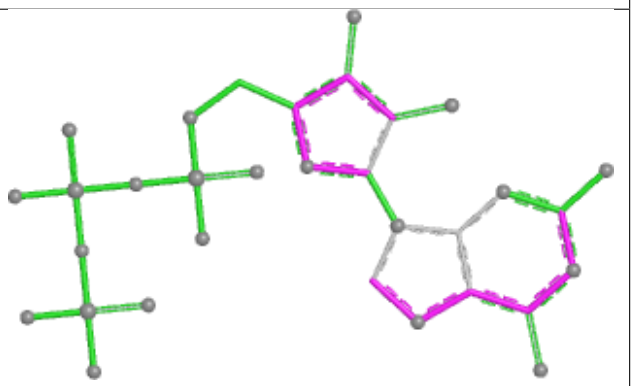


Rings

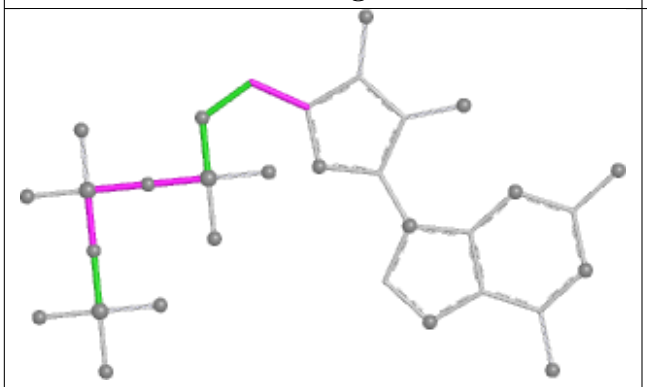
Ligand GTP E5 501



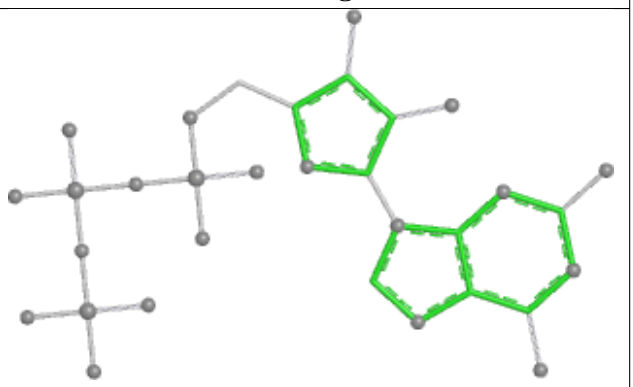
Bond lengths



Bond angles

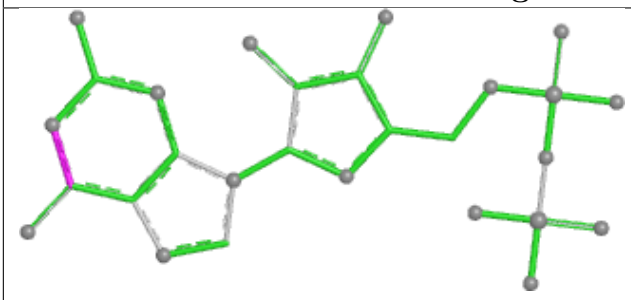


Torsions

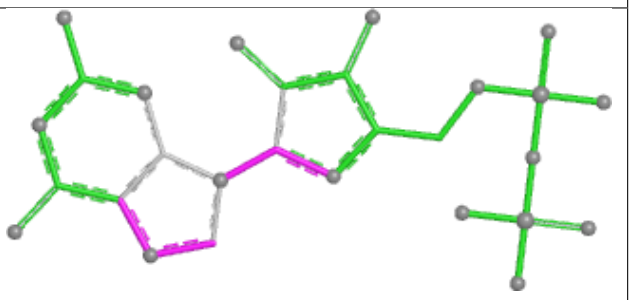


Rings

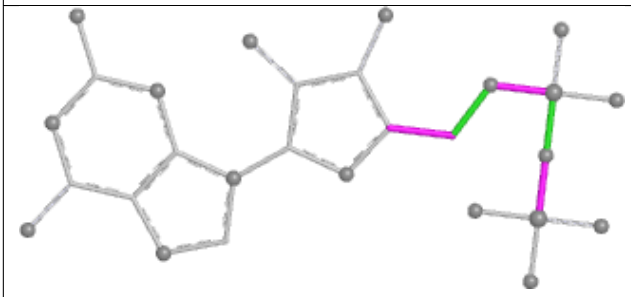
Ligand GDP EZ 501



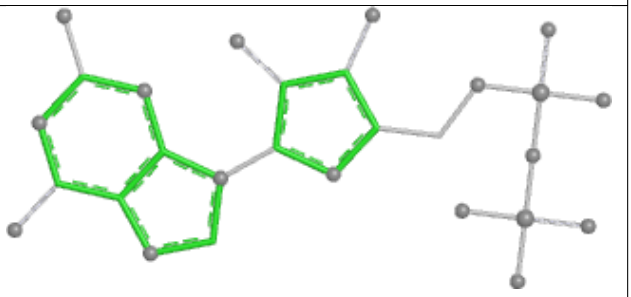
Bond lengths



Bond angles

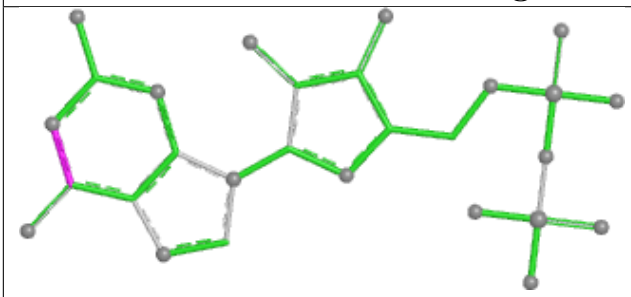


Torsions

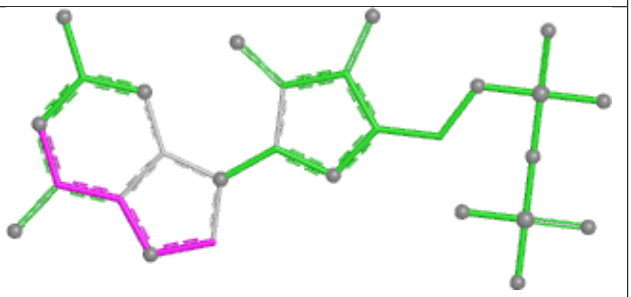


Rings

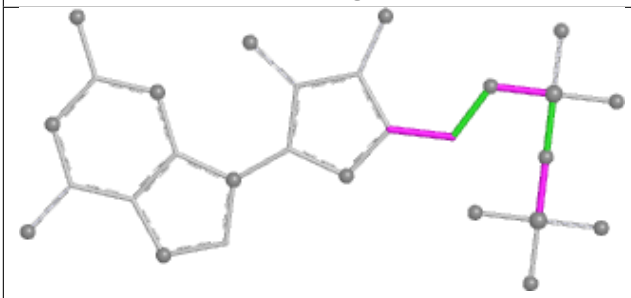
Ligand GDP Aa 501



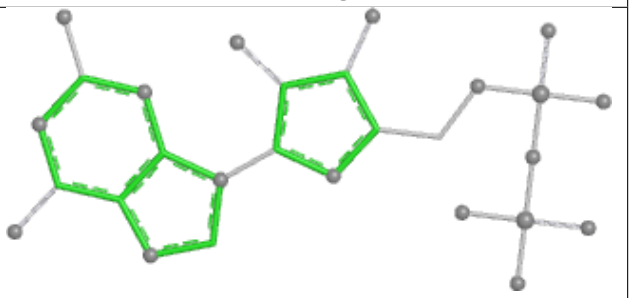
Bond lengths



Bond angles

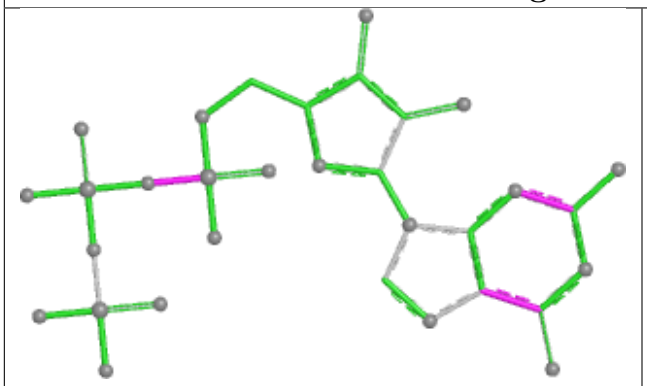


Torsions

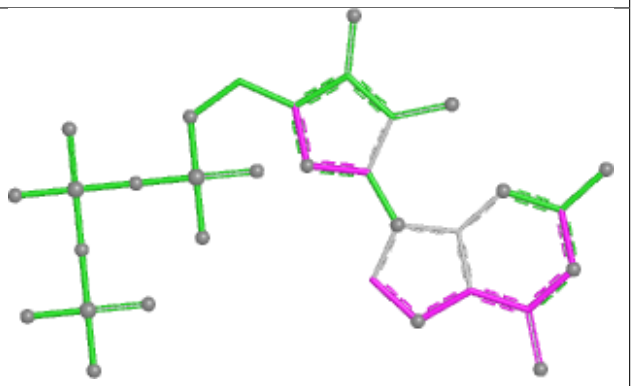


Rings

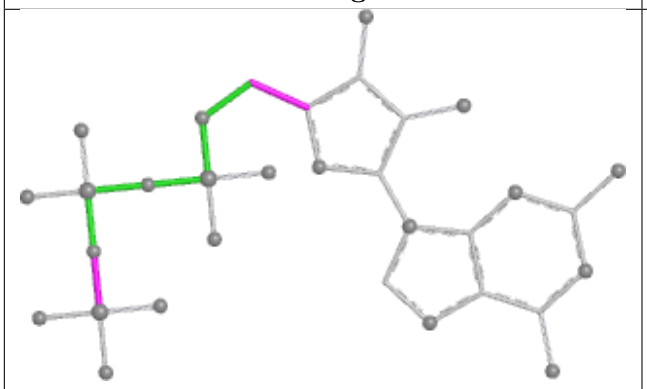
Ligand GTP t 602



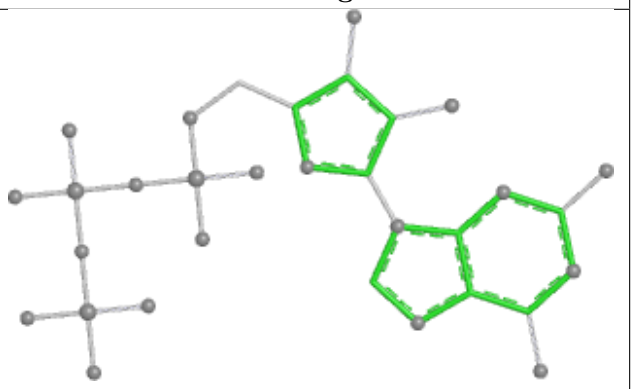
Bond lengths



Bond angles

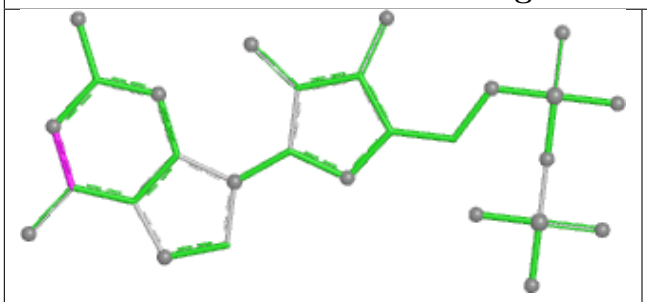


Torsions

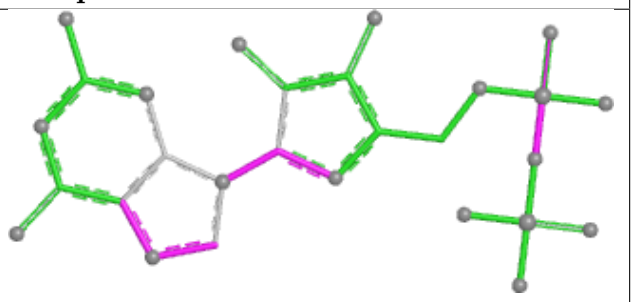


Rings

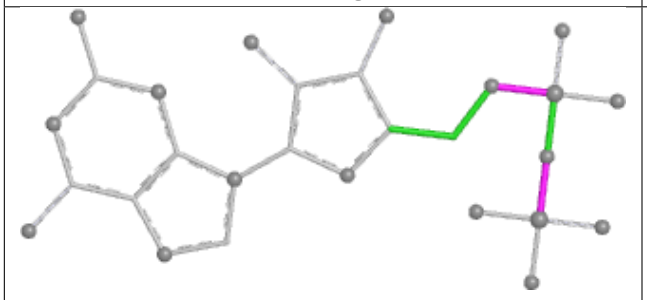
Ligand GDP Fq 501



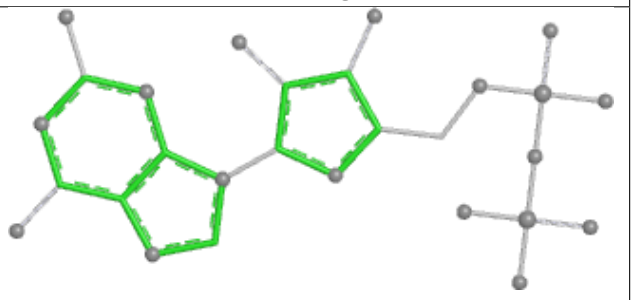
Bond lengths



Bond angles

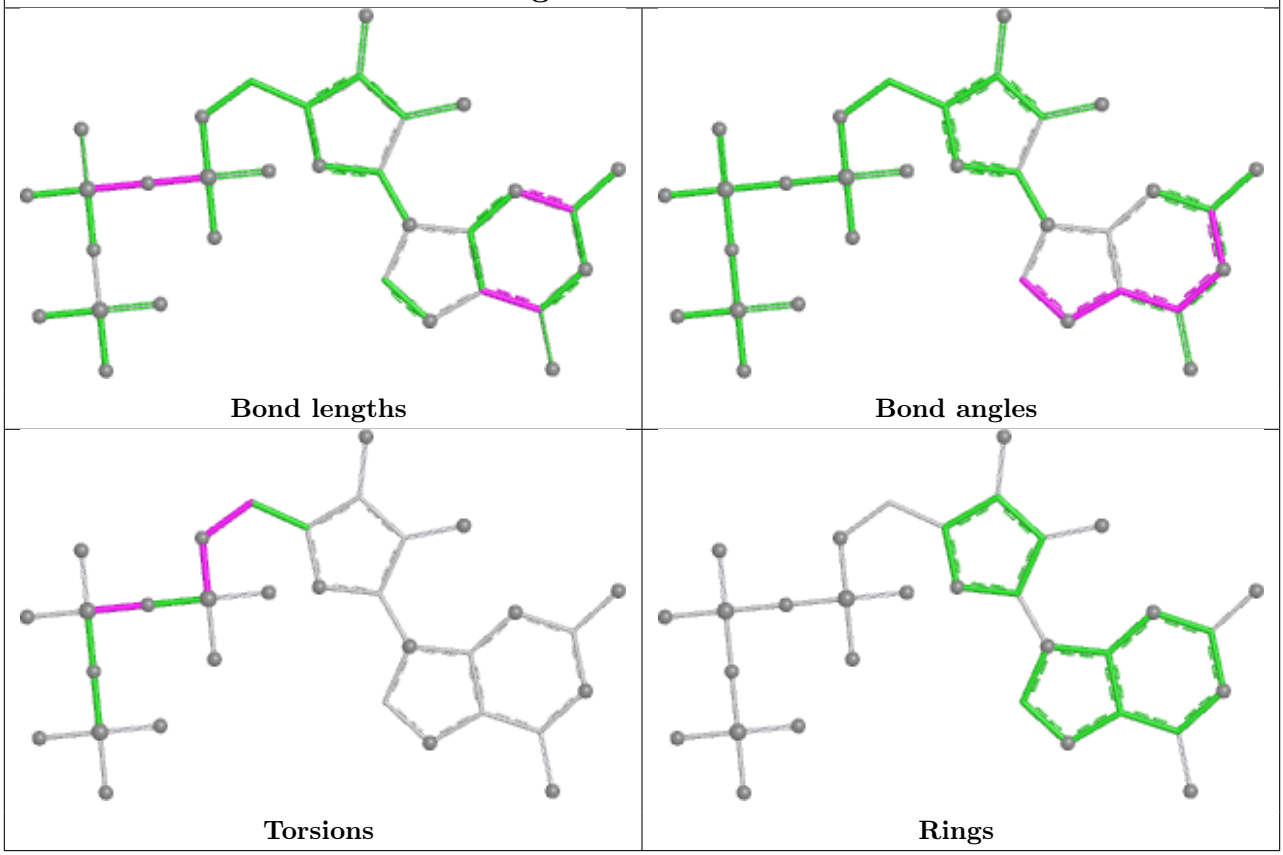


Torsions

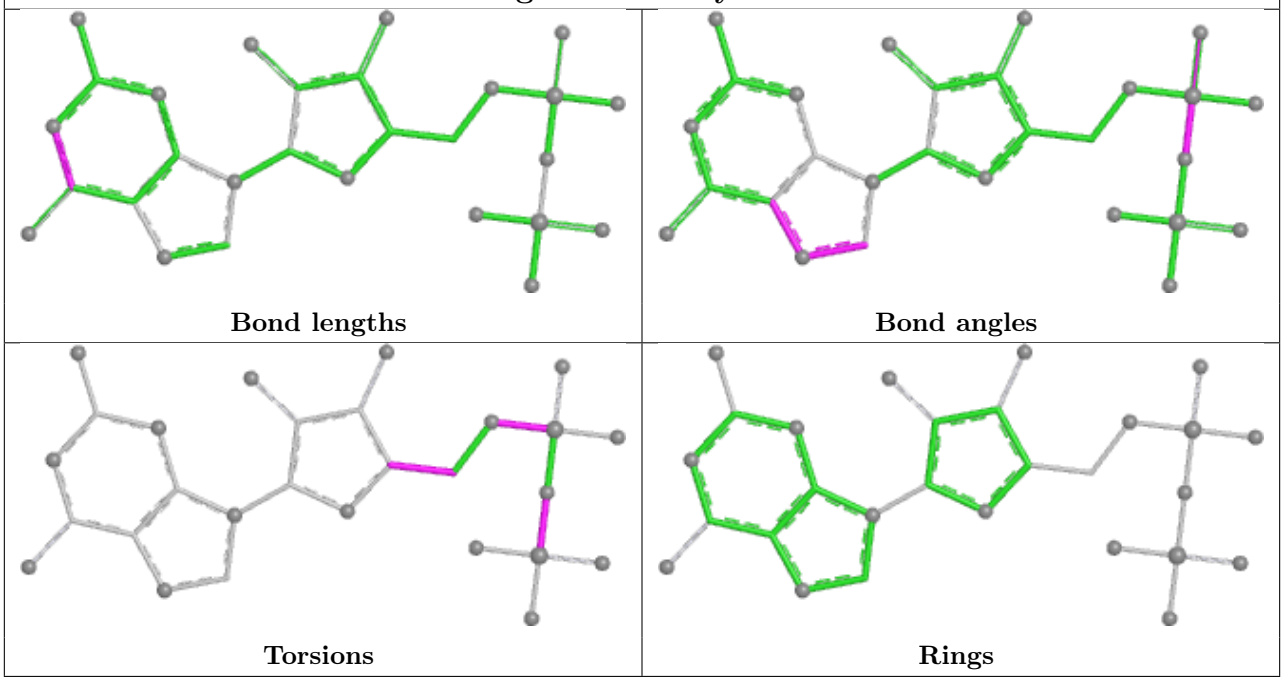


Rings

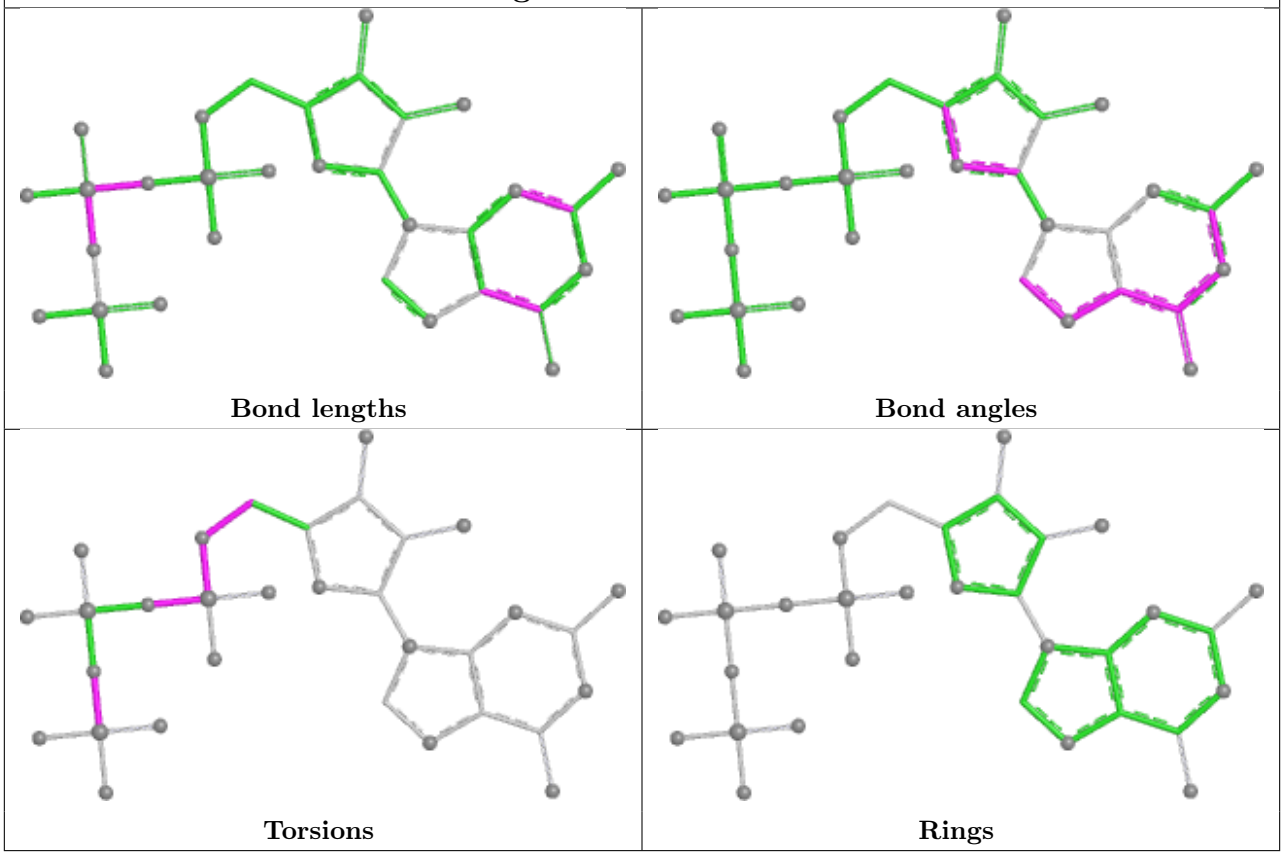
Ligand GTP l 602



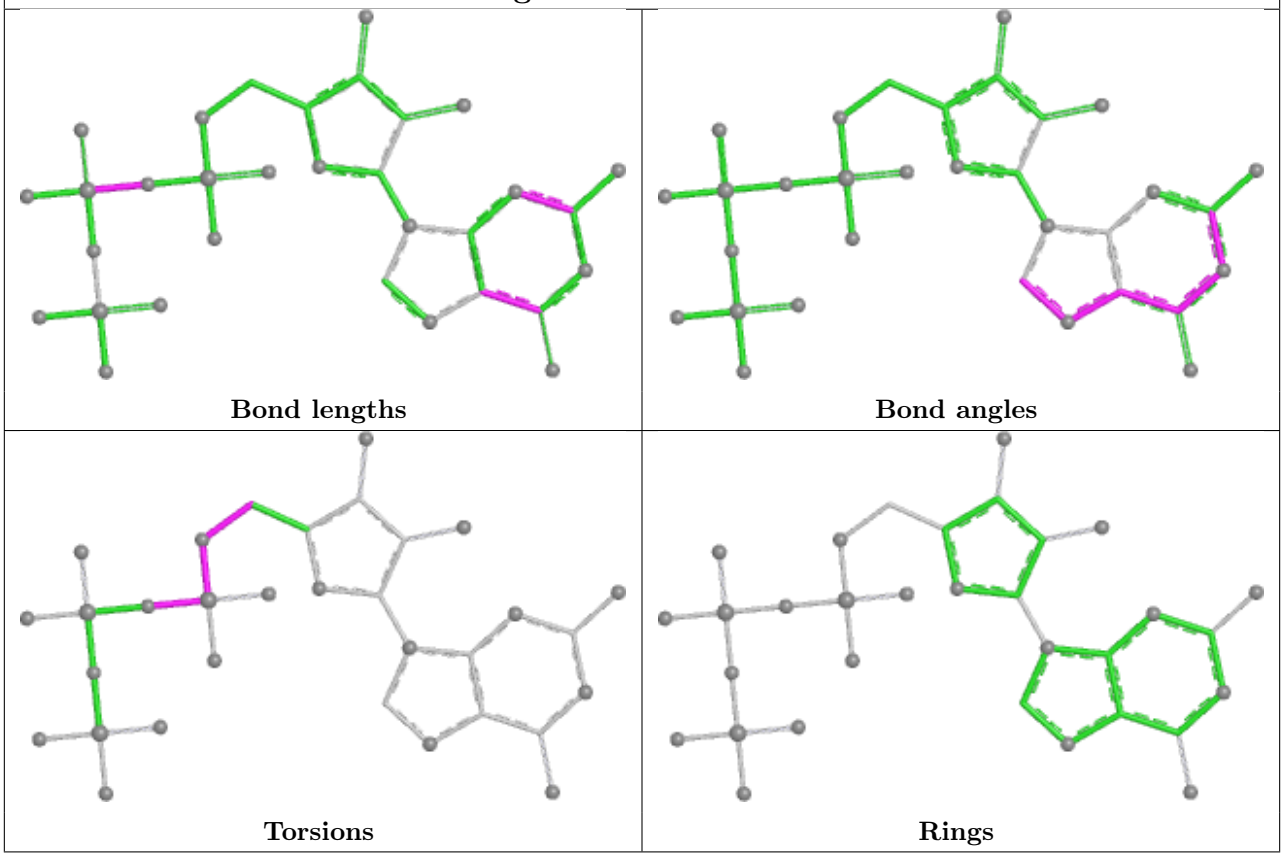
Ligand GDP Fy 501



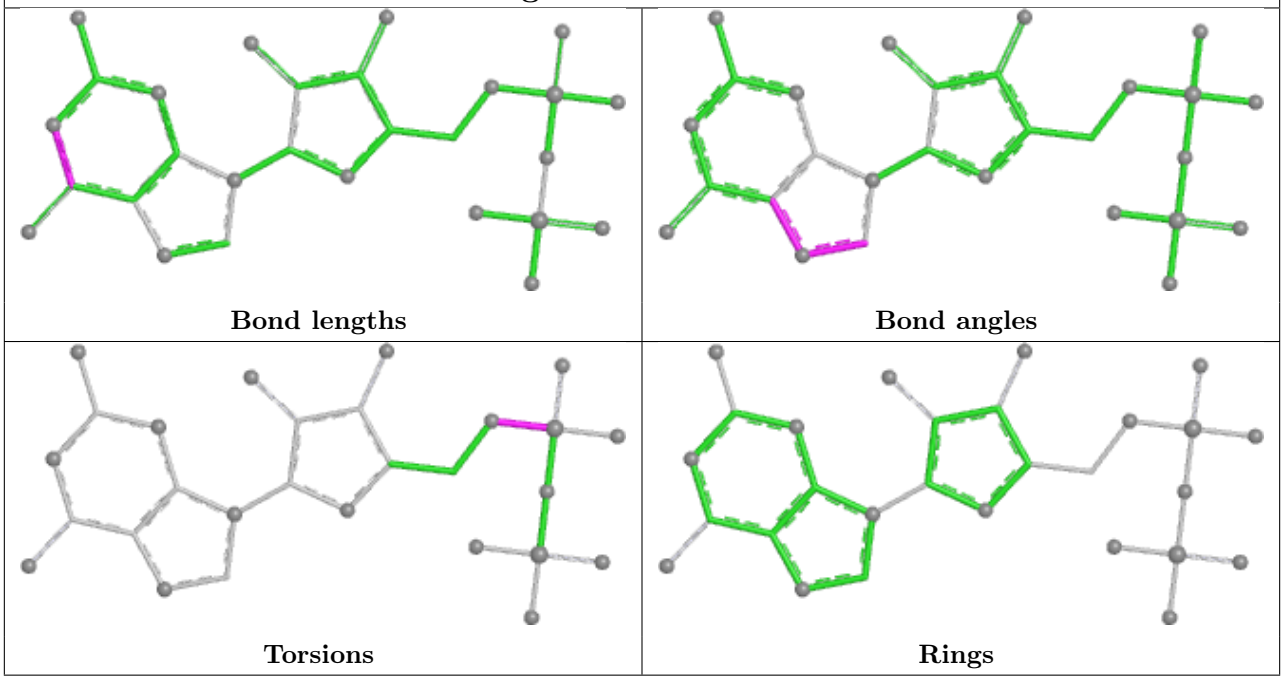
Ligand GTP Gx 501



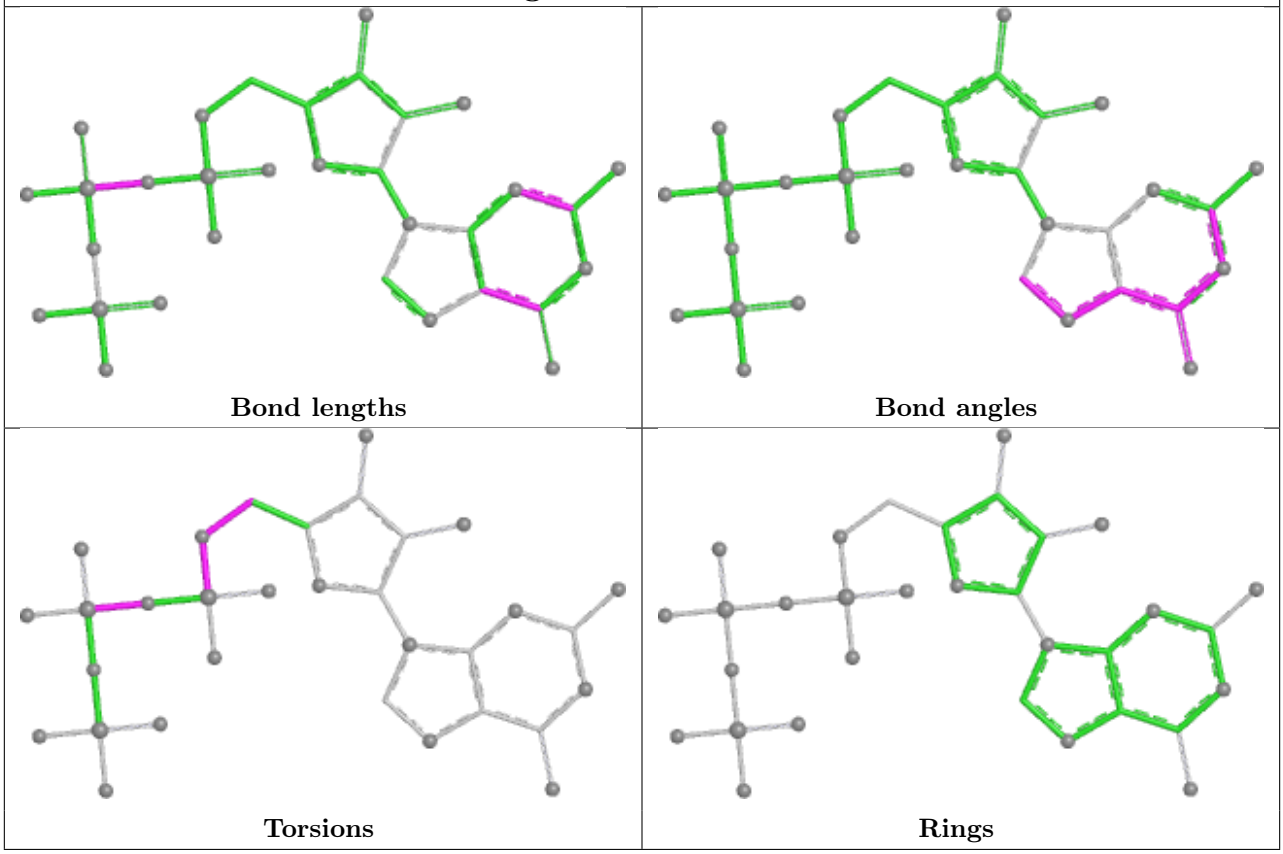
Ligand GTP G5 501



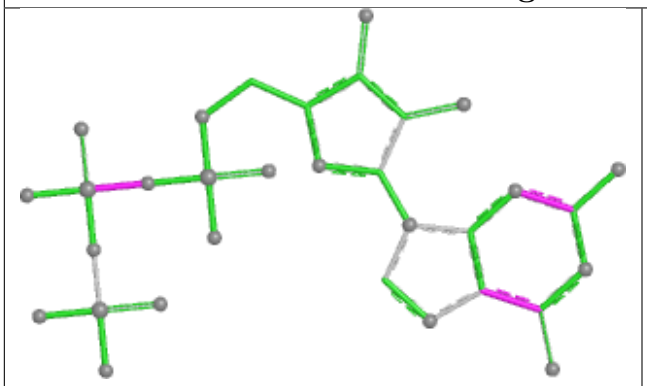
Ligand GDP U 501



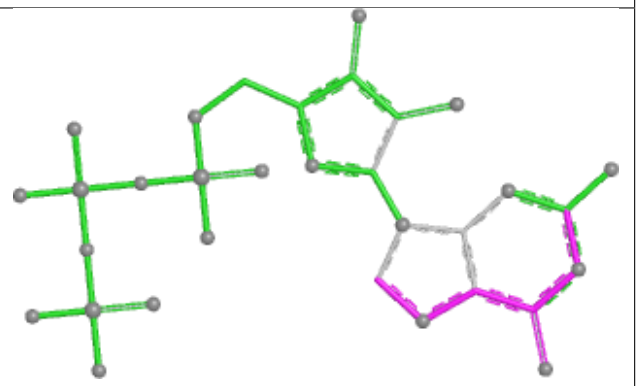
Ligand GTP w 602



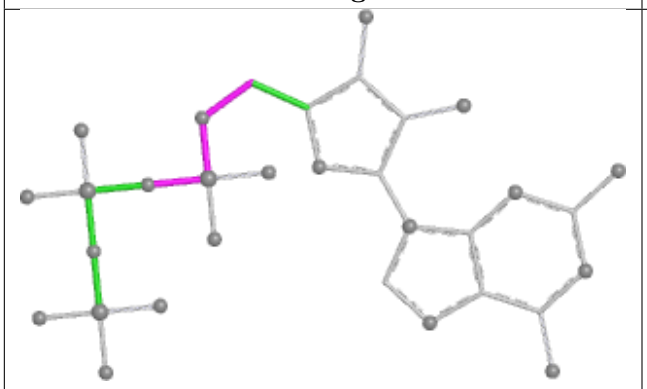
Ligand GTP Fa 501



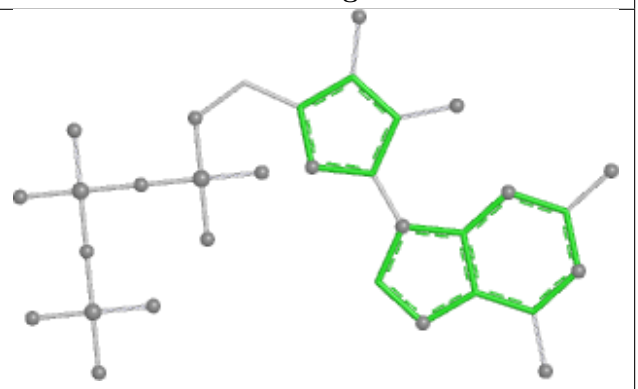
Bond lengths



Bond angles

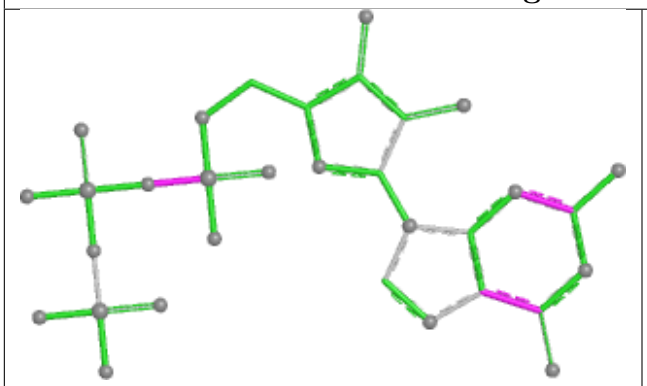


Torsions

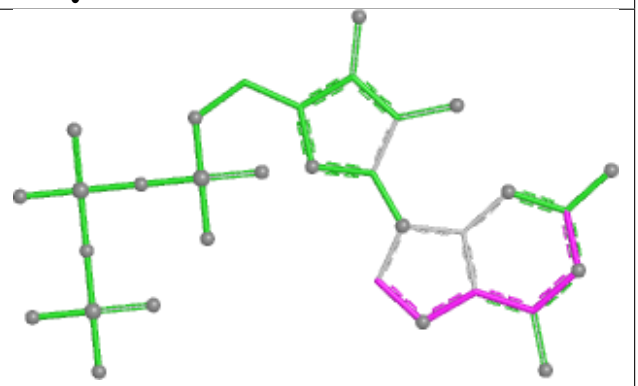


Rings

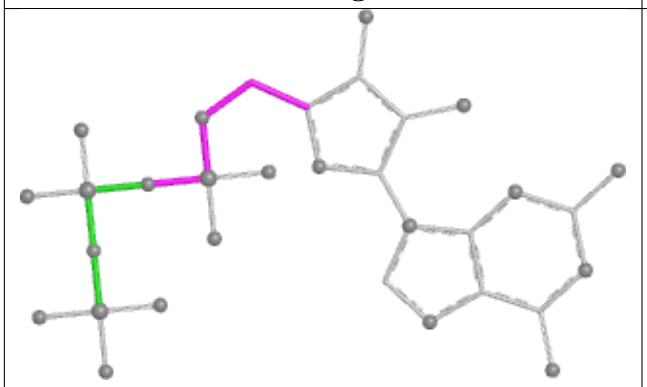
Ligand GTP Q 602



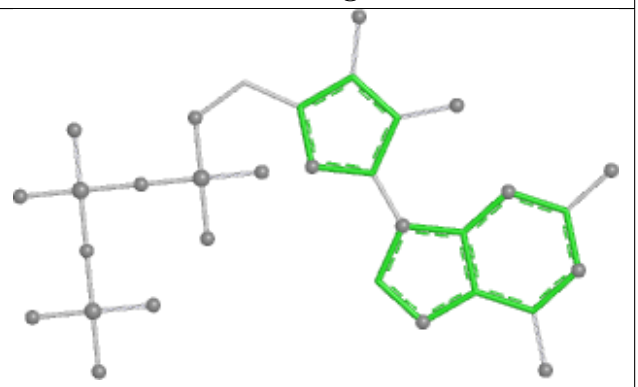
Bond lengths



Bond angles

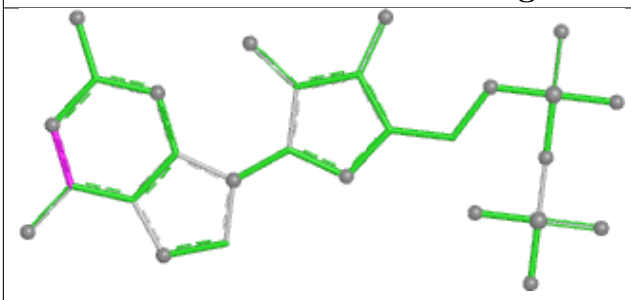


Torsions

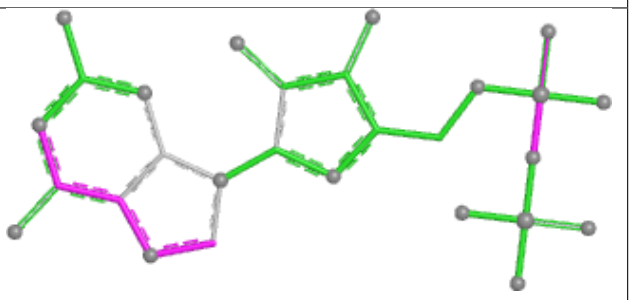


Rings

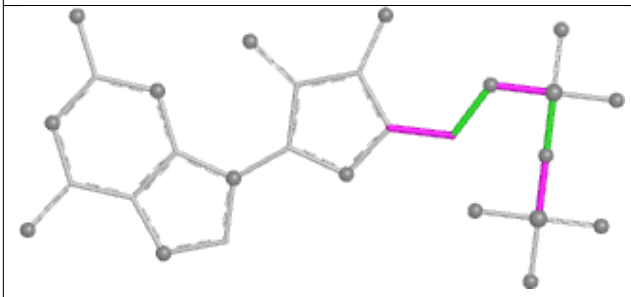
Ligand GDP Fl 501



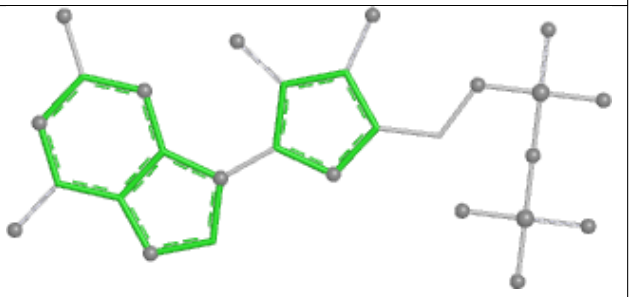
Bond lengths



Bond angles

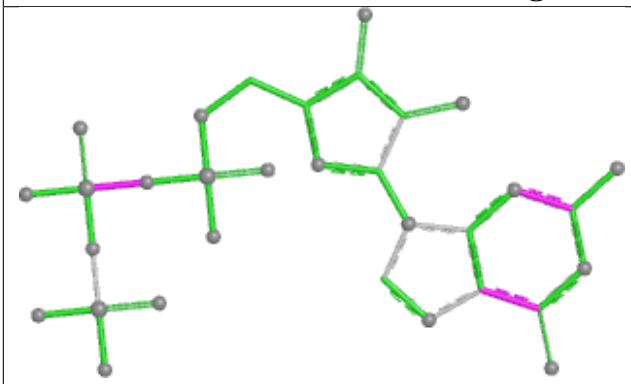


Torsions

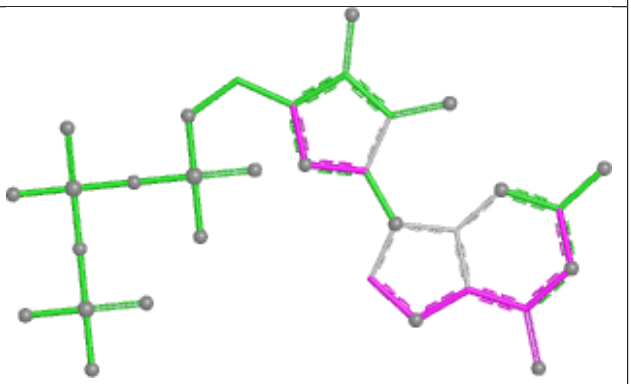


Rings

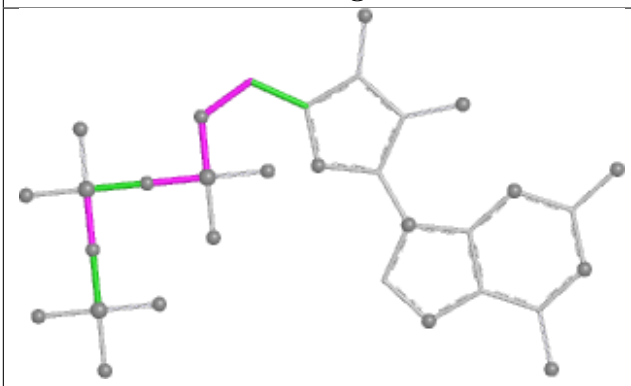
Ligand GTP z 602



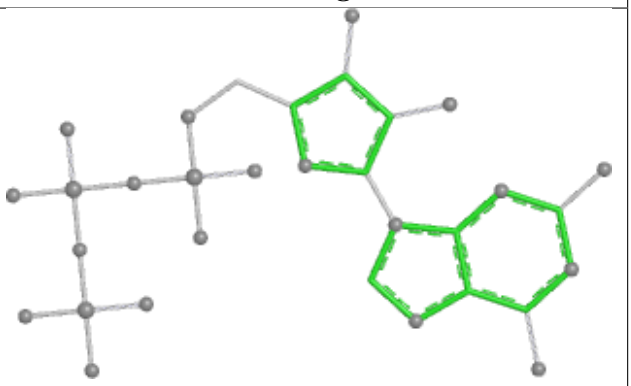
Bond lengths



Bond angles

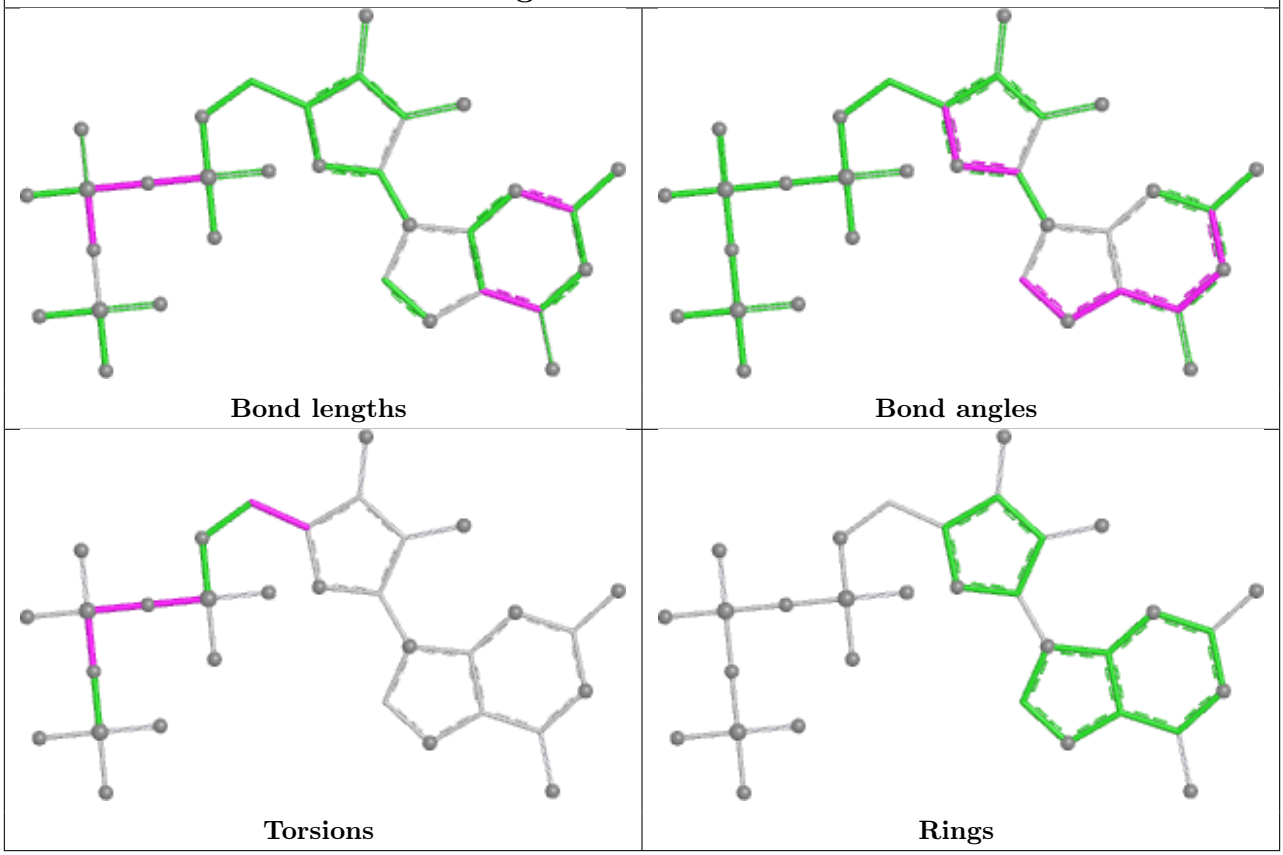


Torsions

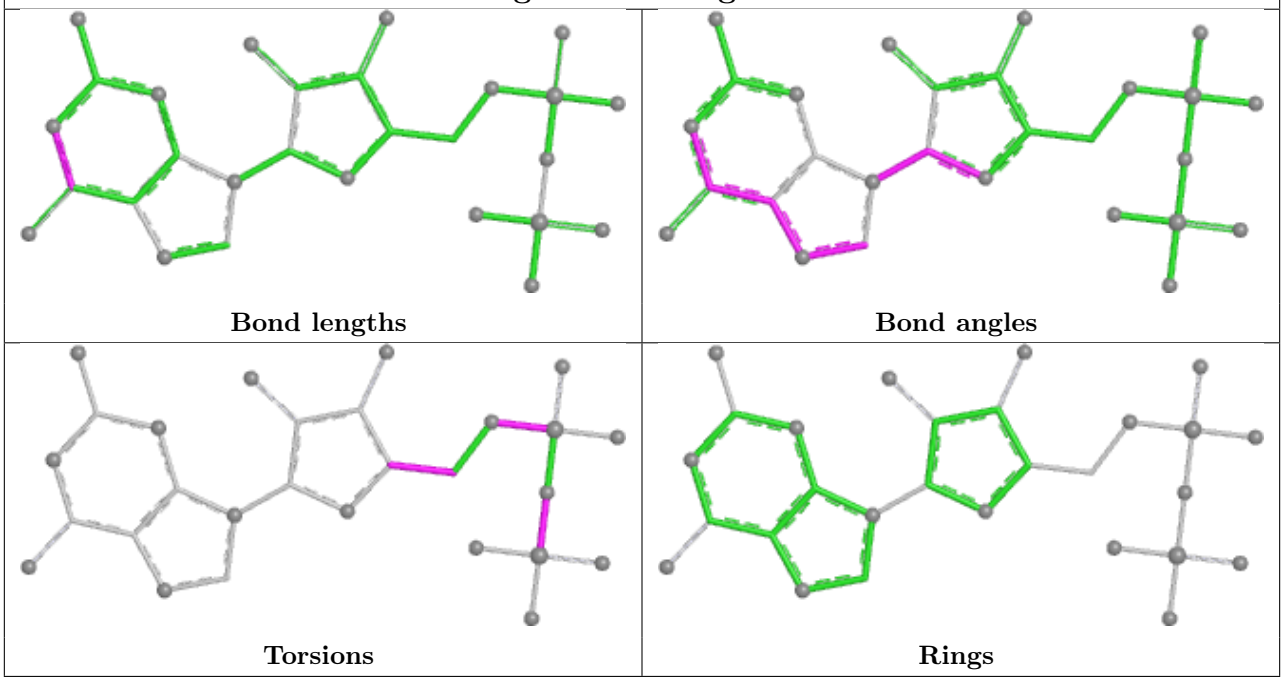


Rings

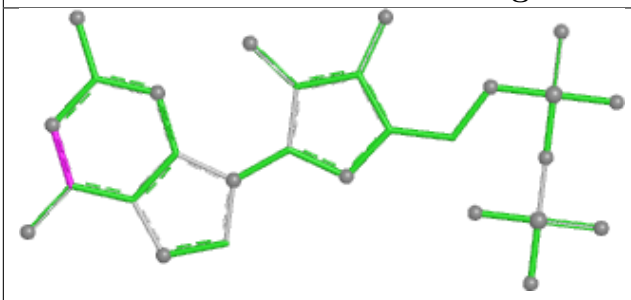
Ligand GTP E1 501



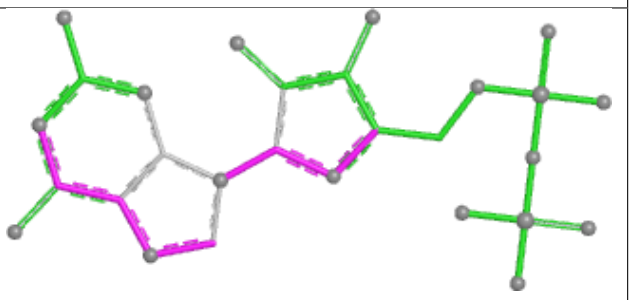
Ligand GDP Bg 501



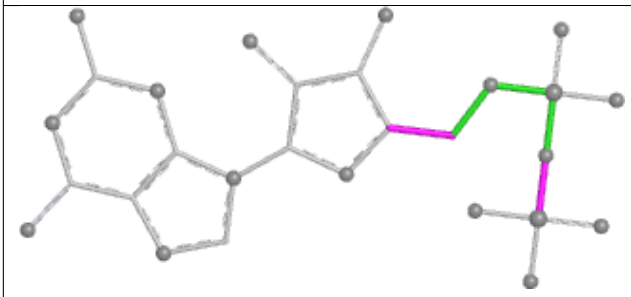
Ligand GDP FA 501



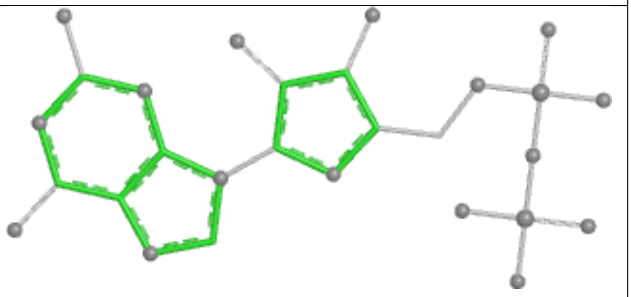
Bond lengths



Bond angles

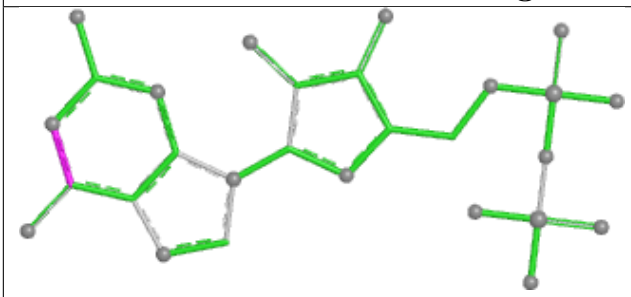


Torsions

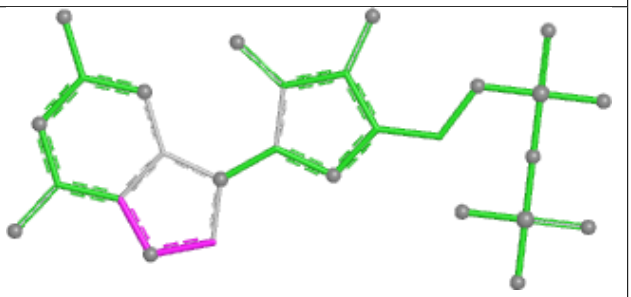


Rings

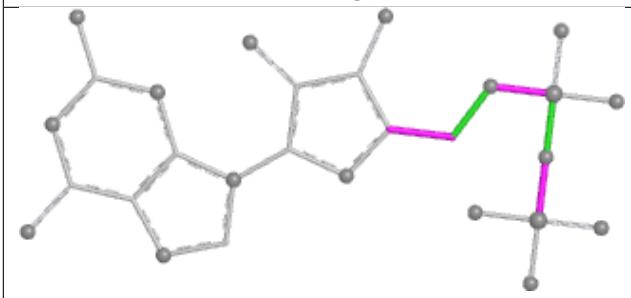
Ligand GDP FI 501



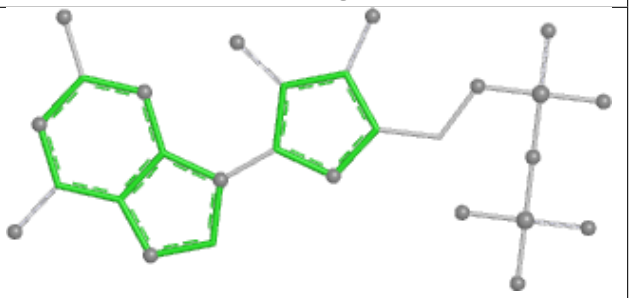
Bond lengths



Bond angles

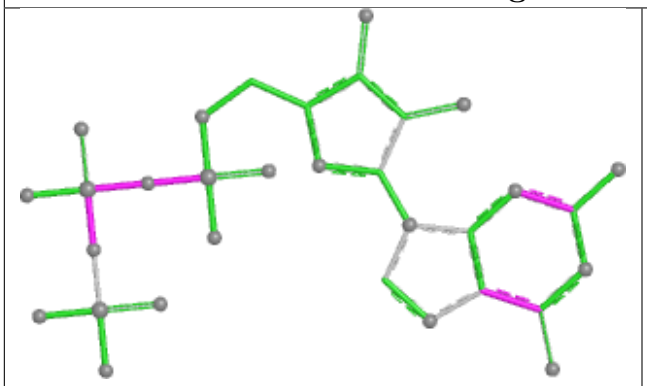


Torsions

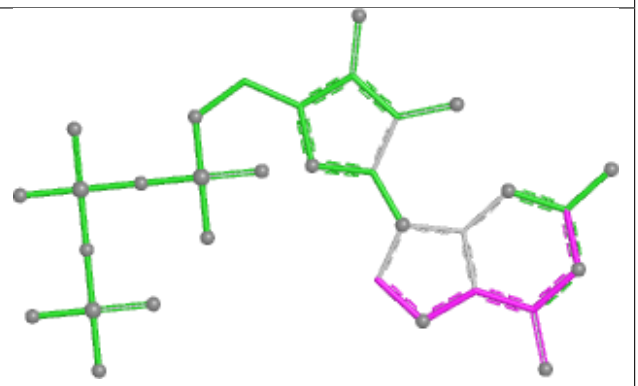


Rings

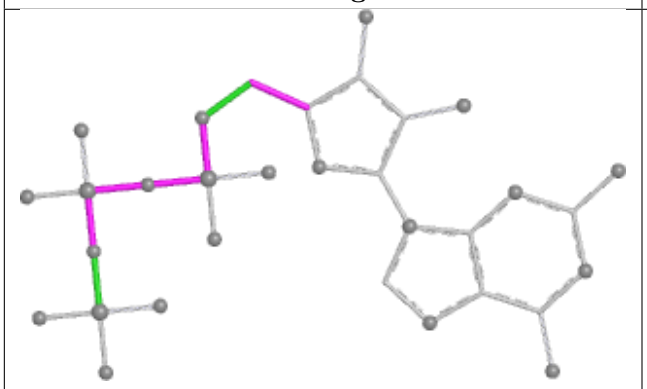
Ligand GTP GD 501



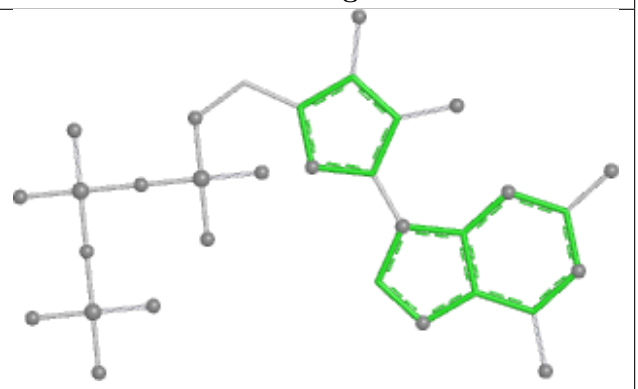
Bond lengths



Bond angles

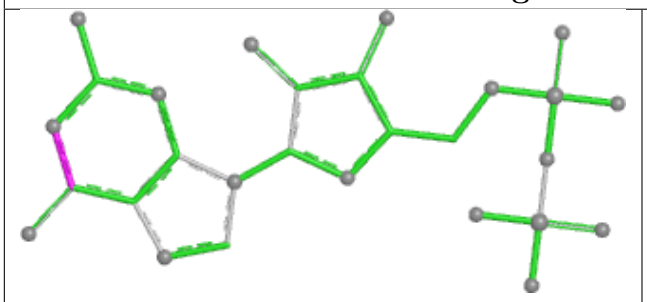


Torsions

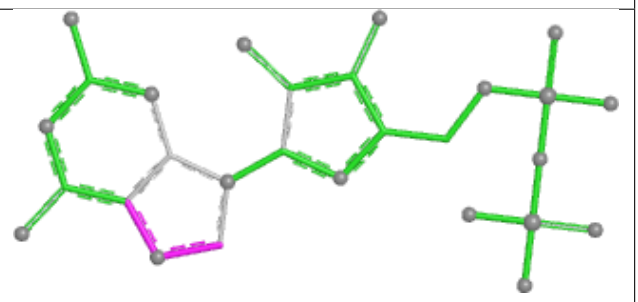


Rings

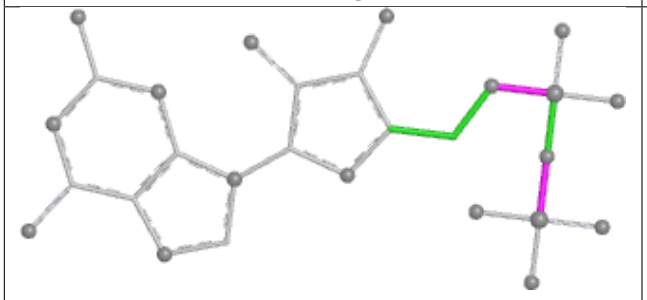
Ligand GDP Ah 602



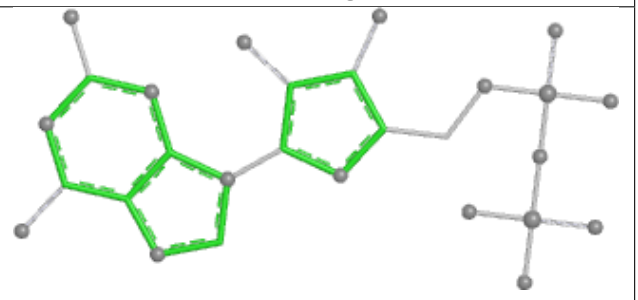
Bond lengths



Bond angles

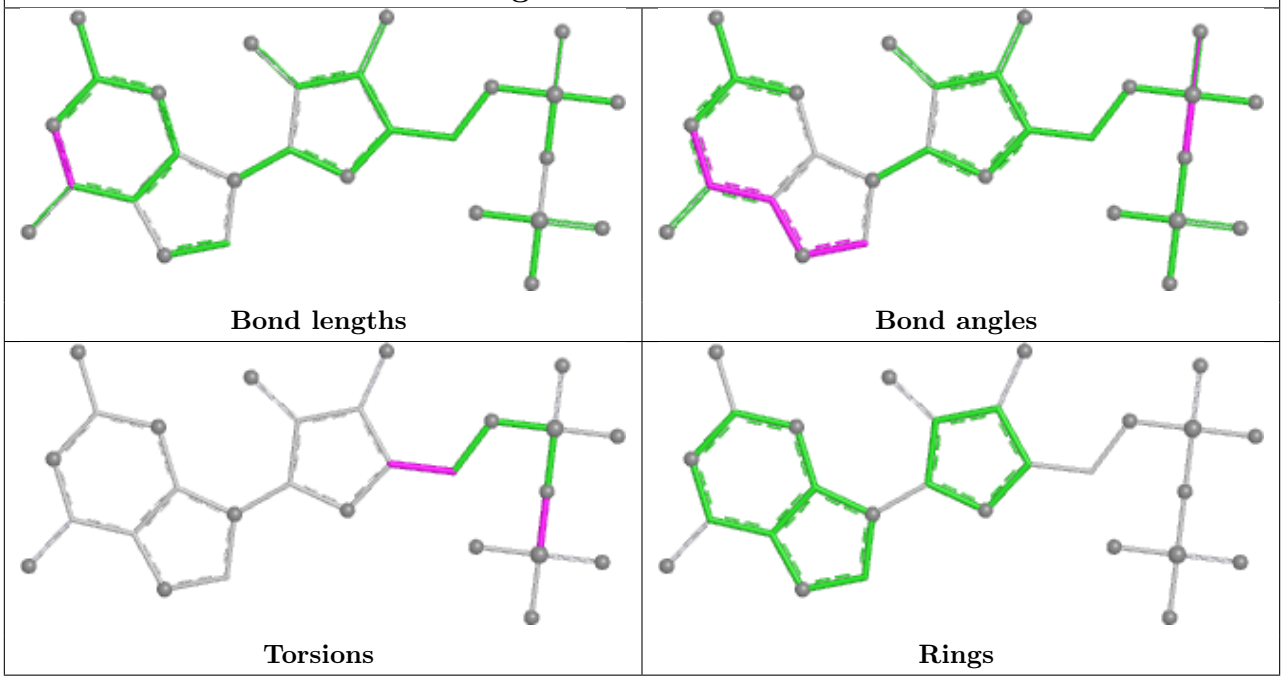


Torsions

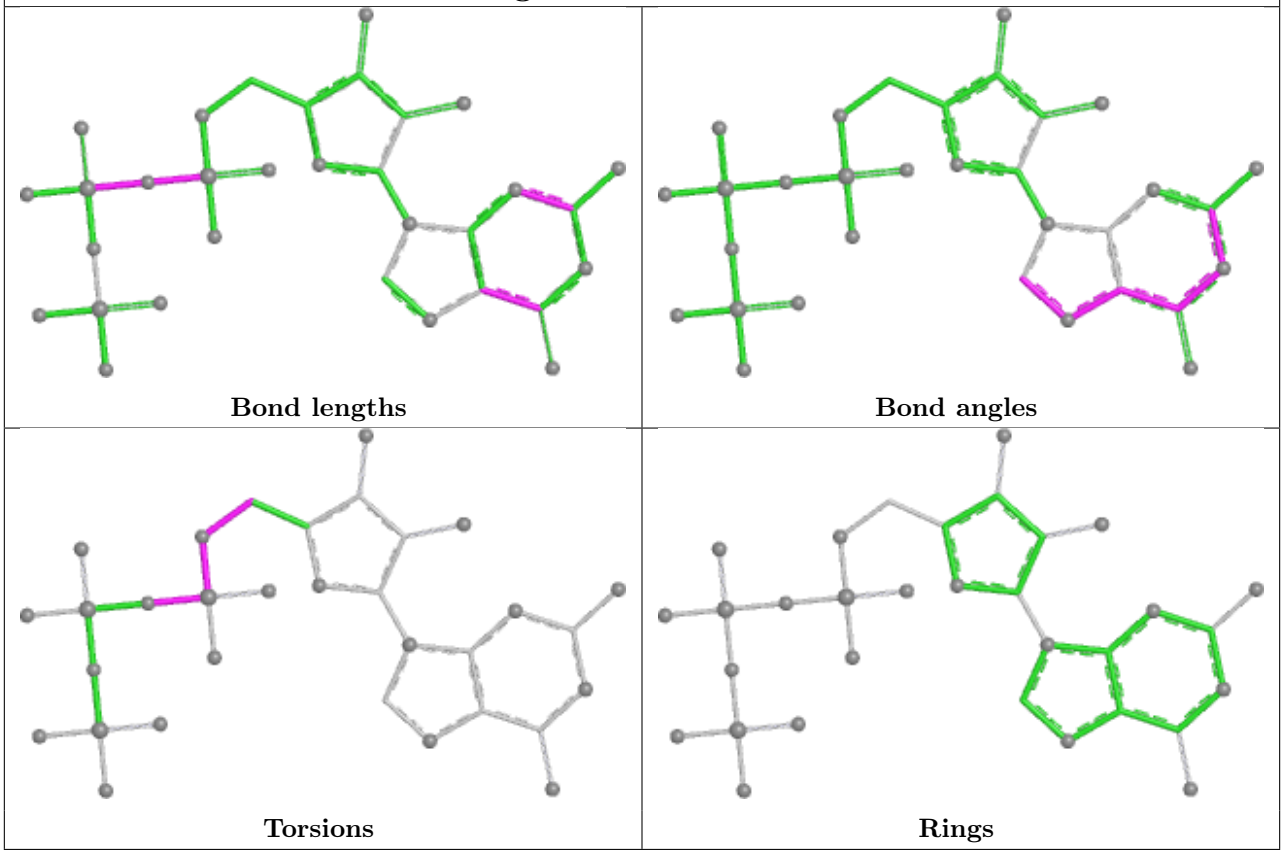


Rings

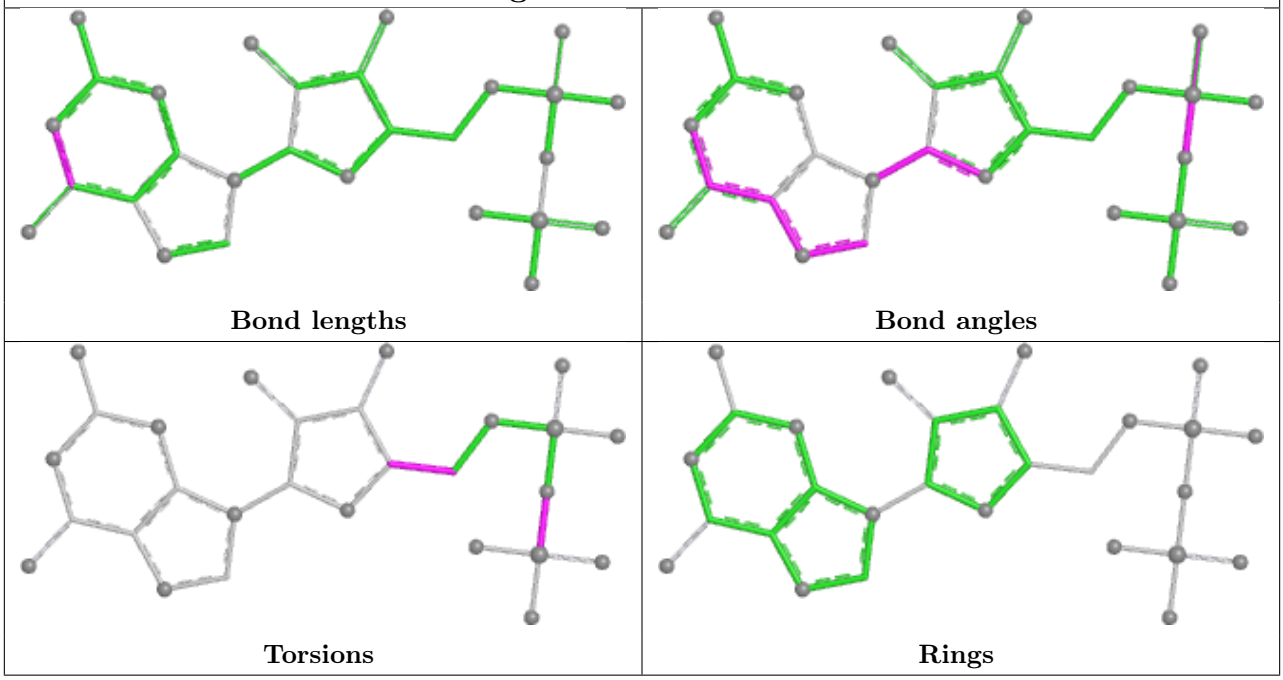
Ligand GDP Dh 501



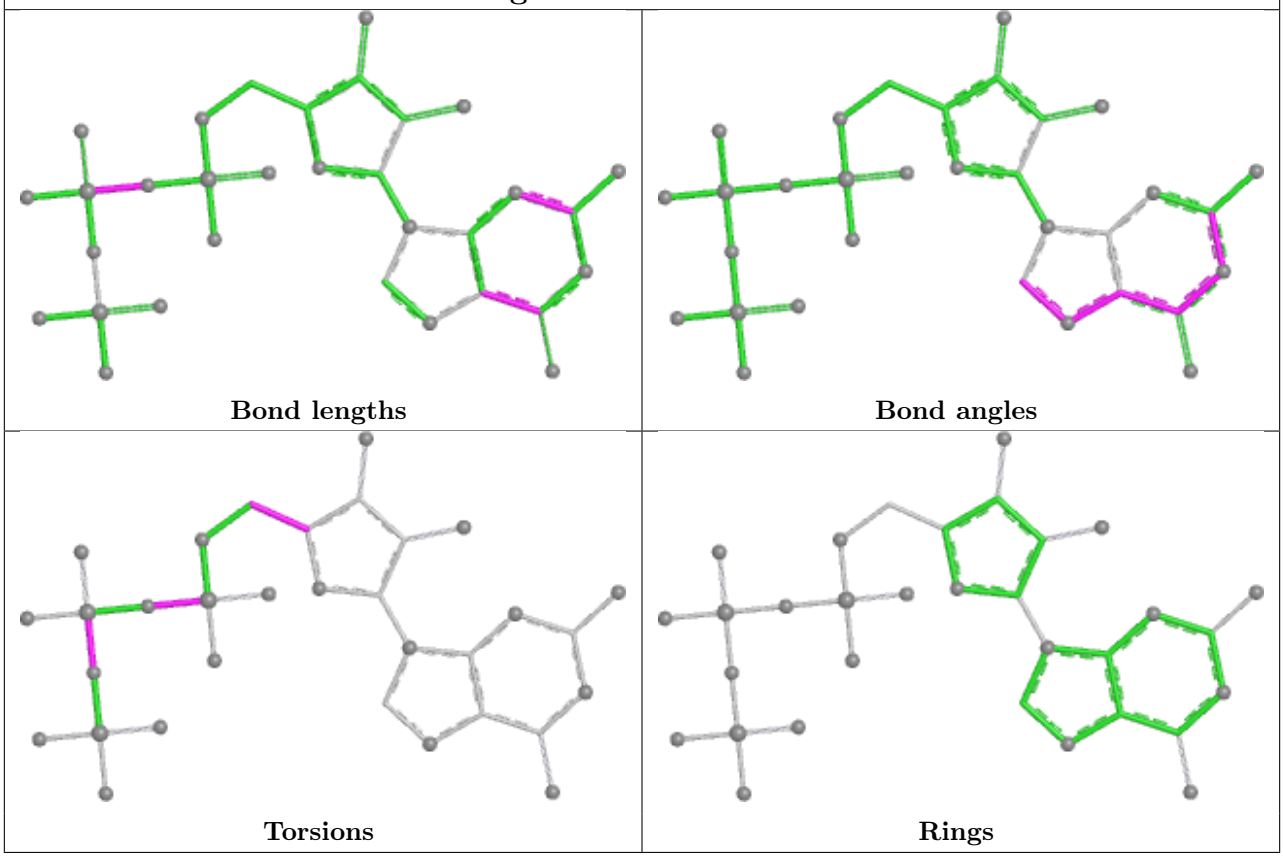
Ligand GTP A4 501



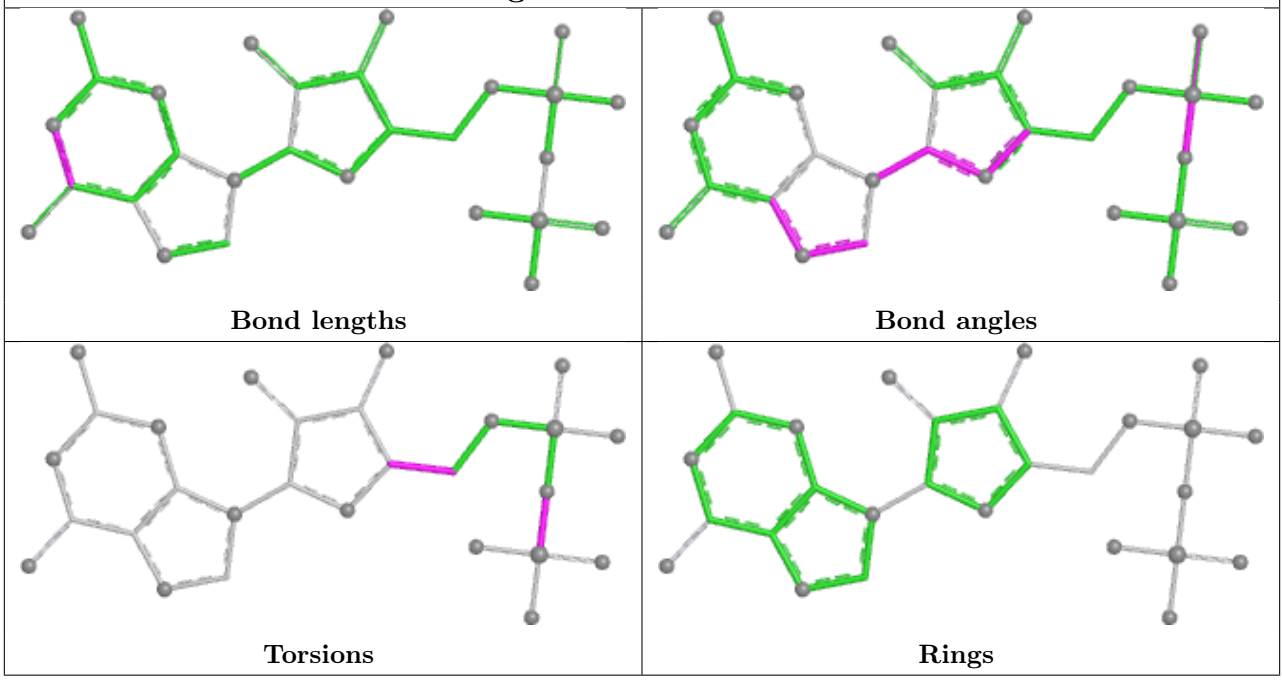
Ligand GDP EN 501



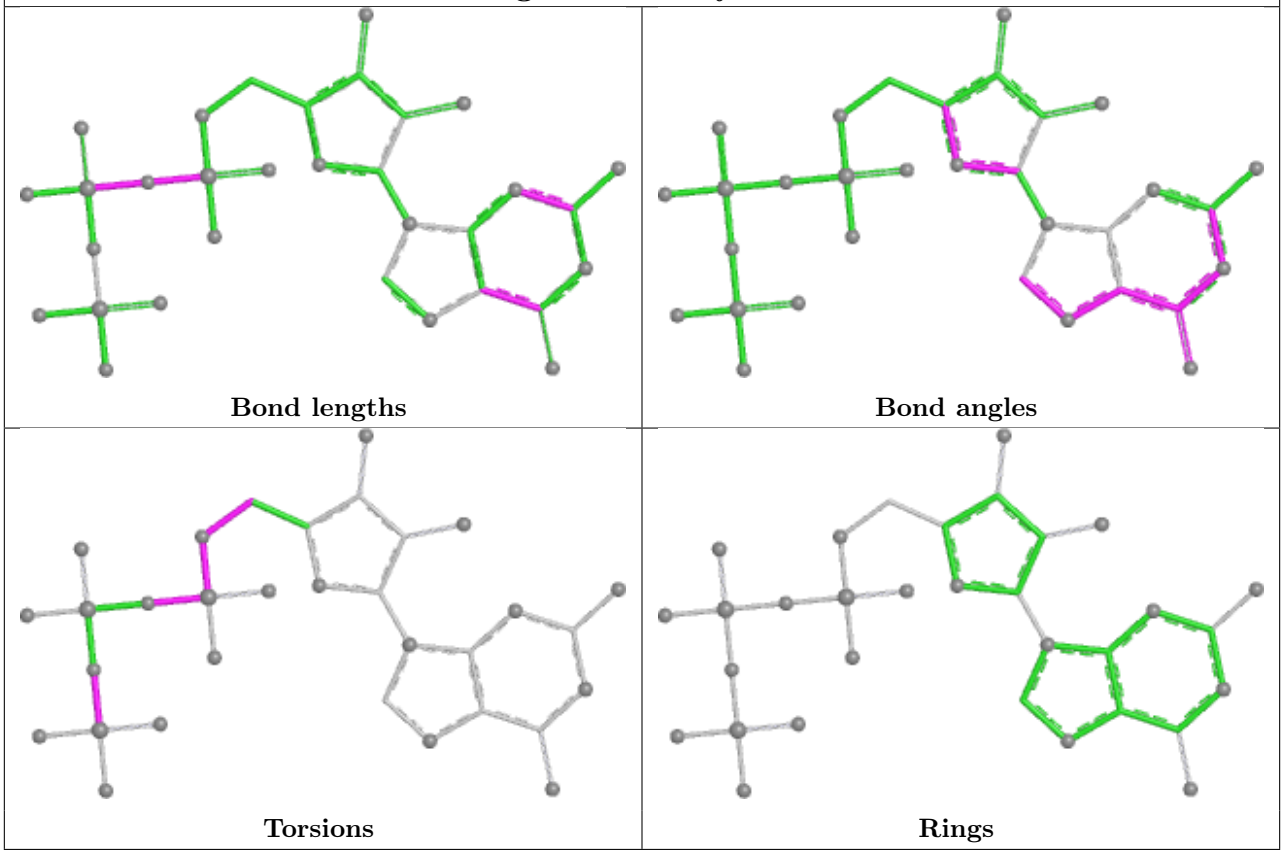
Ligand GTP CA 602



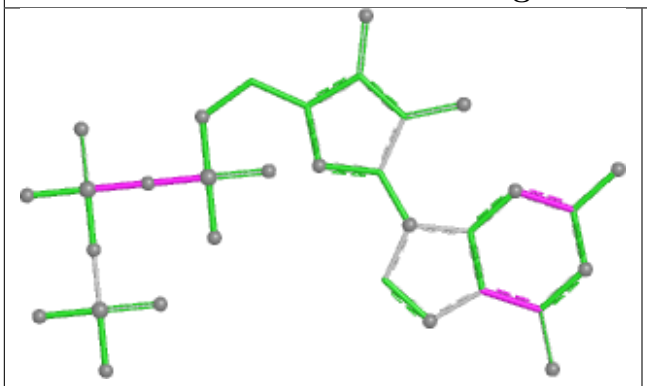
Ligand GDP GU 501



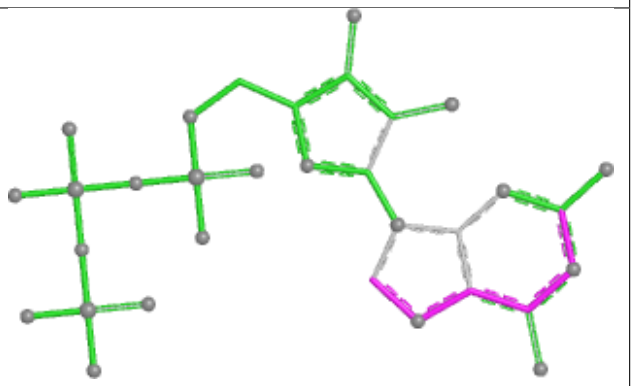
Ligand GTP Ey 602



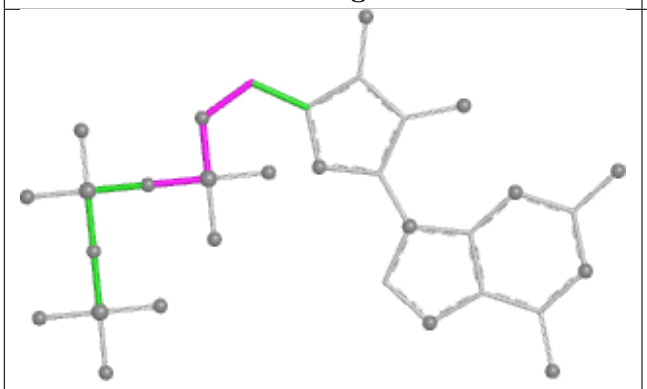
Ligand GTP FP 501



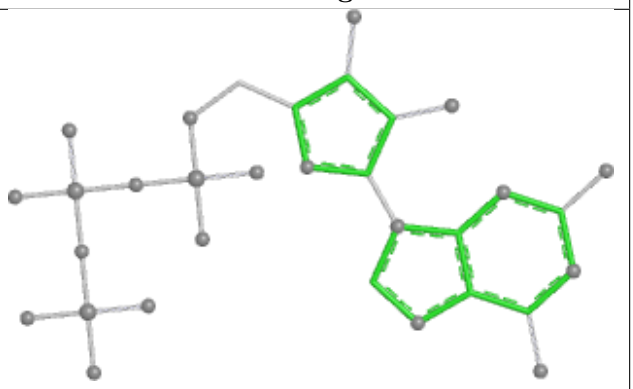
Bond lengths



Bond angles

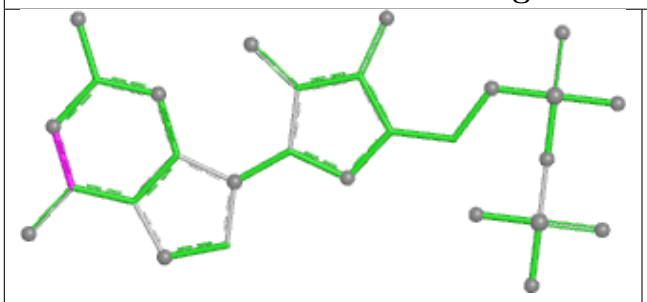


Torsions

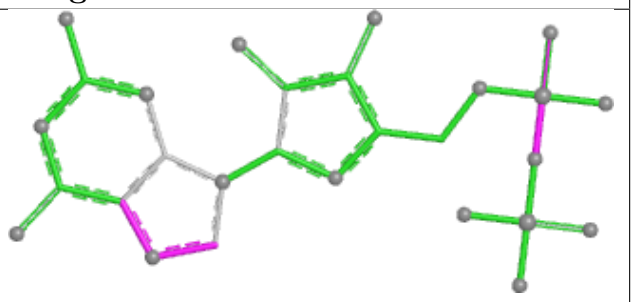


Rings

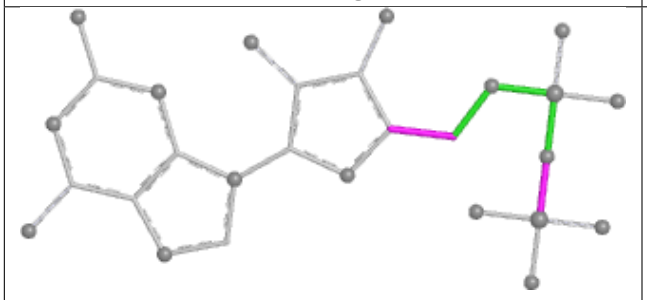
Ligand GDP Dg 501



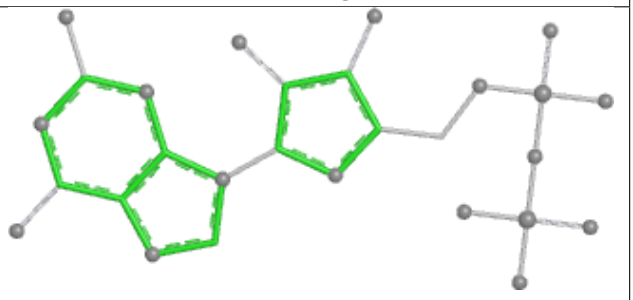
Bond lengths



Bond angles

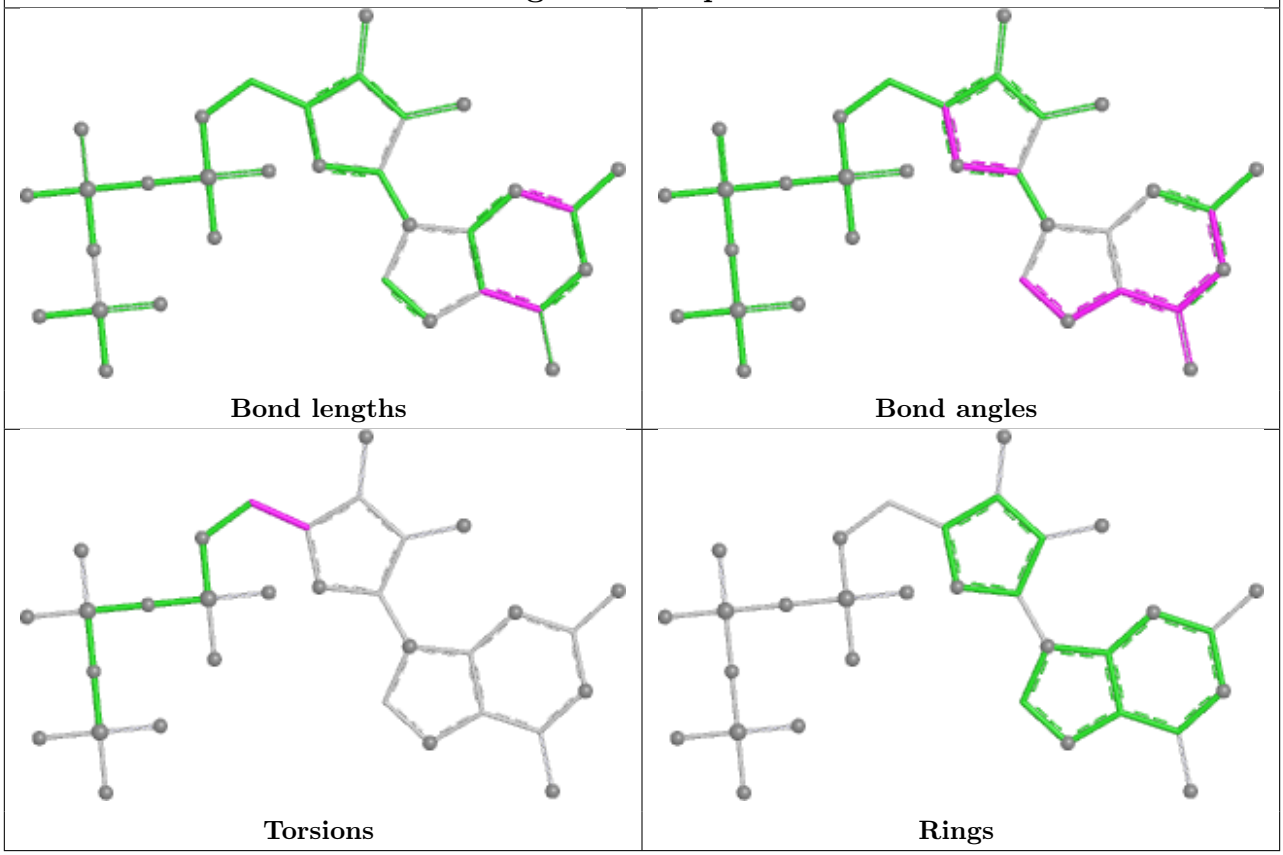


Torsions

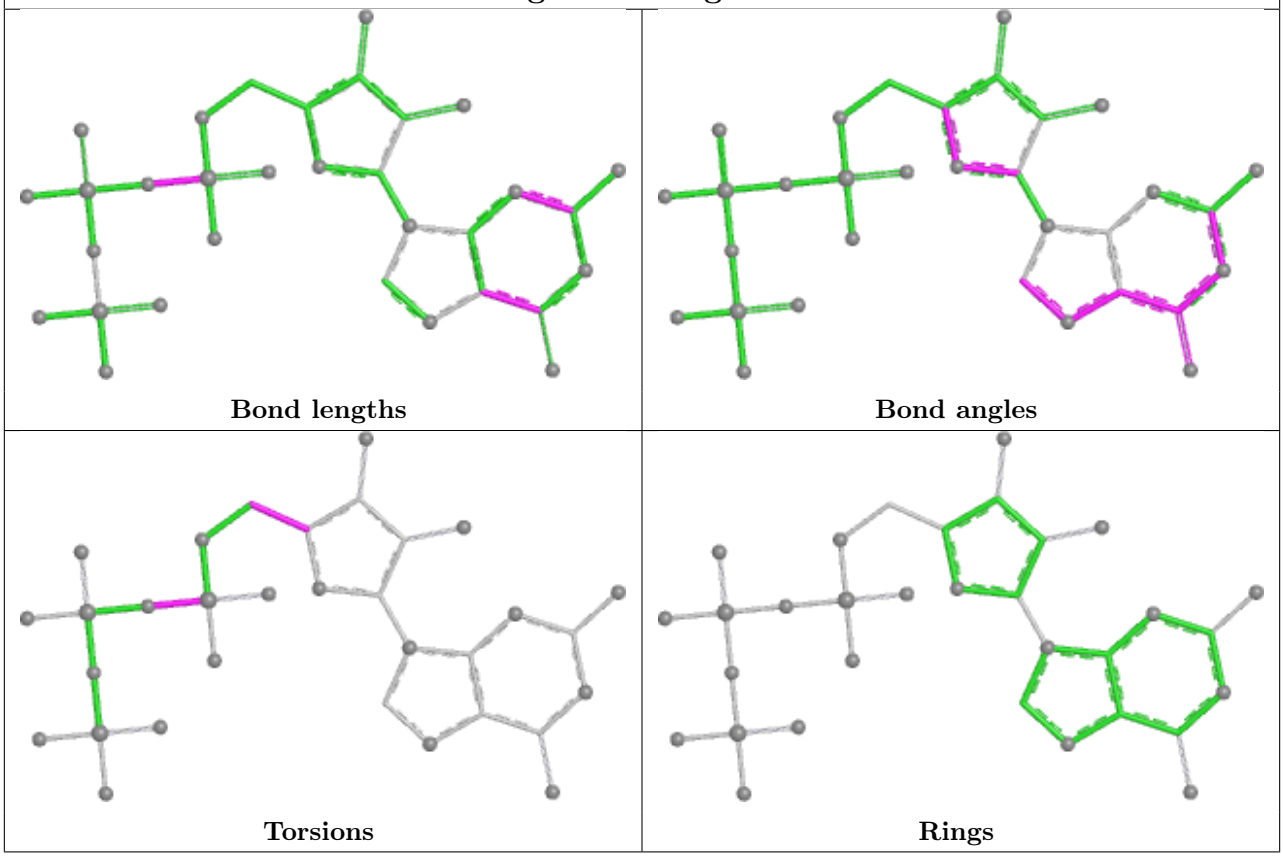


Rings

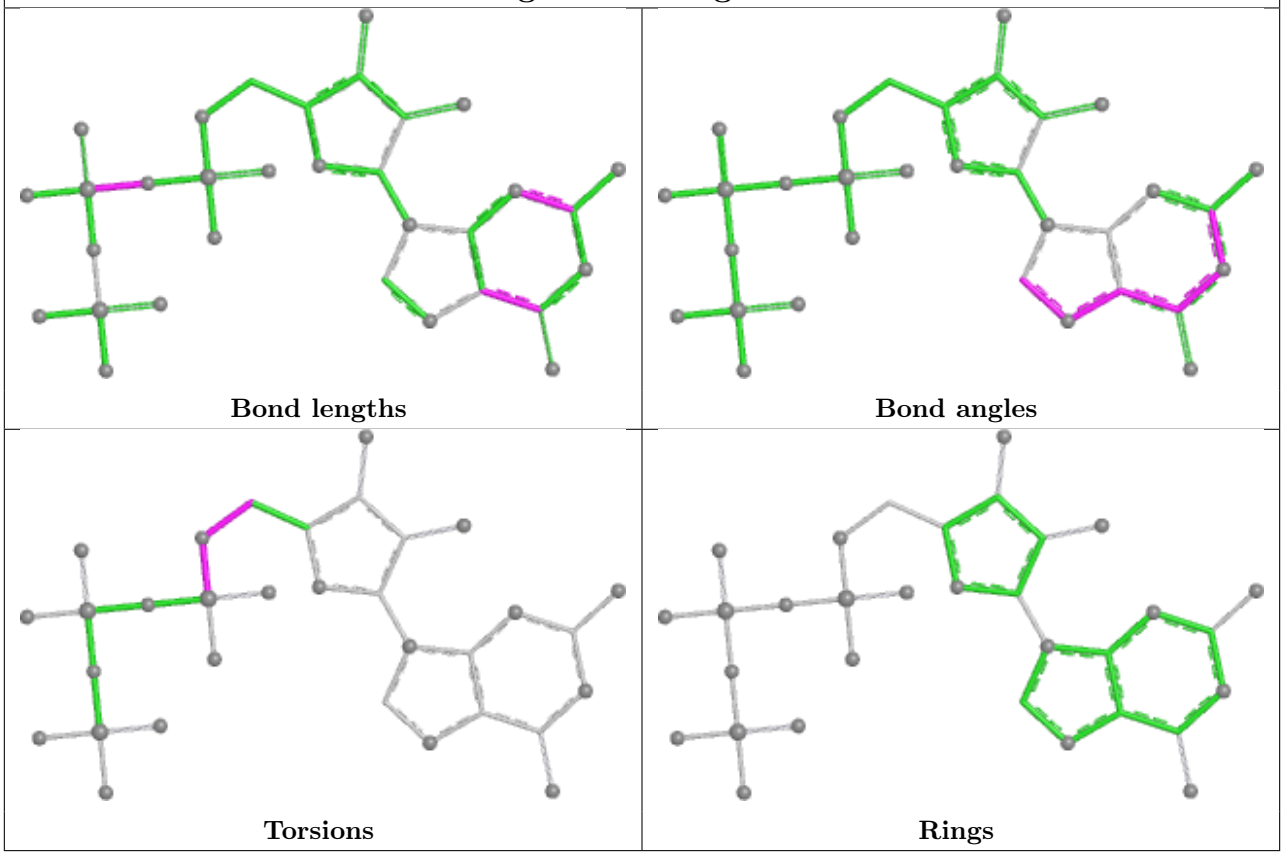
Ligand GTP p 602



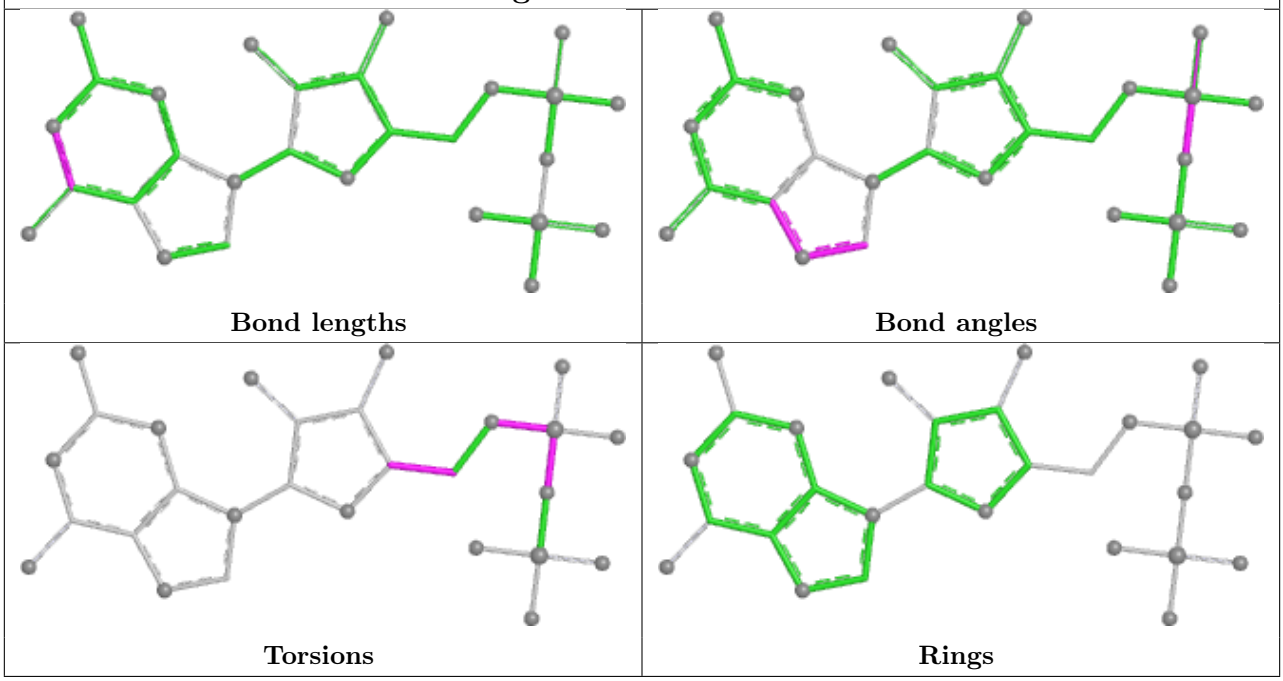
Ligand GTP g 602



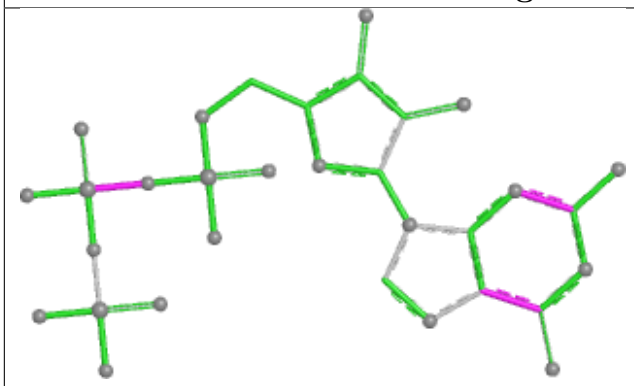
Ligand GTP Fg 501



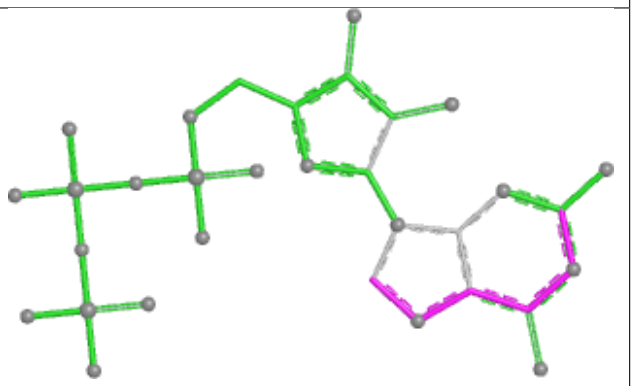
Ligand GDP Bn 501



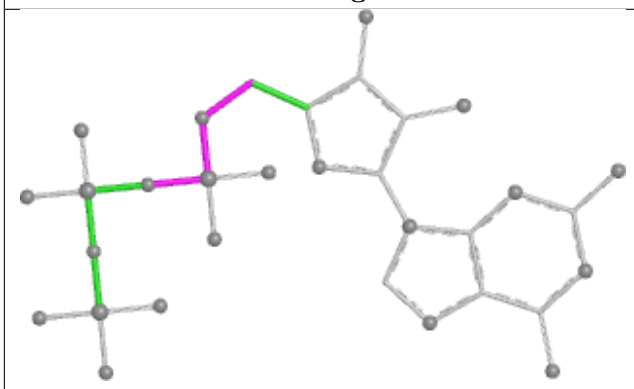
Ligand GTP Eo 501



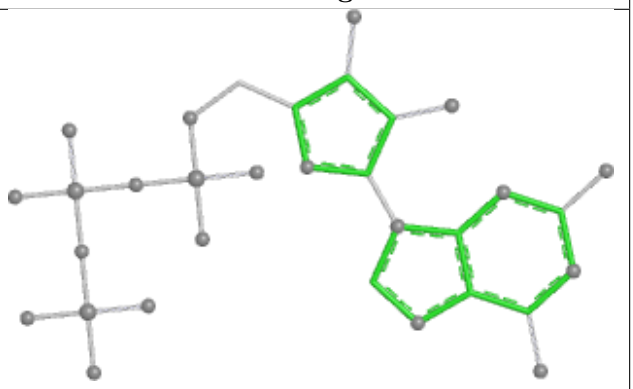
Bond lengths



Bond angles

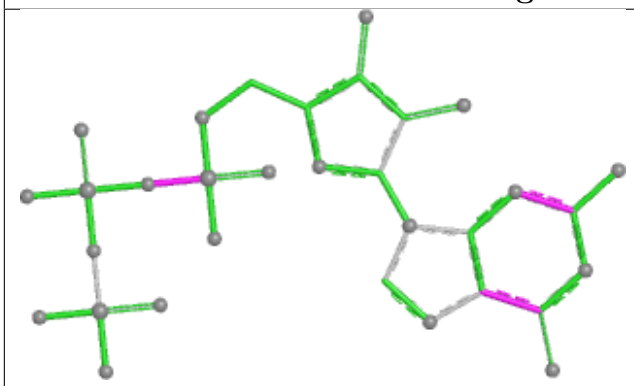


Torsions

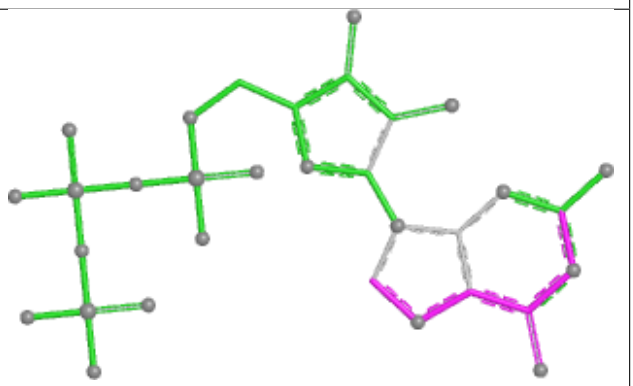


Rings

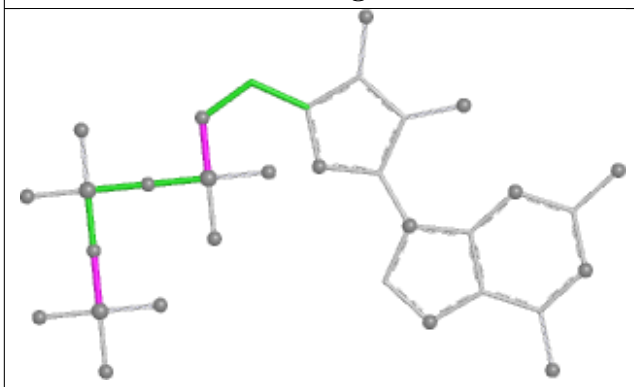
Ligand GTP AI 501



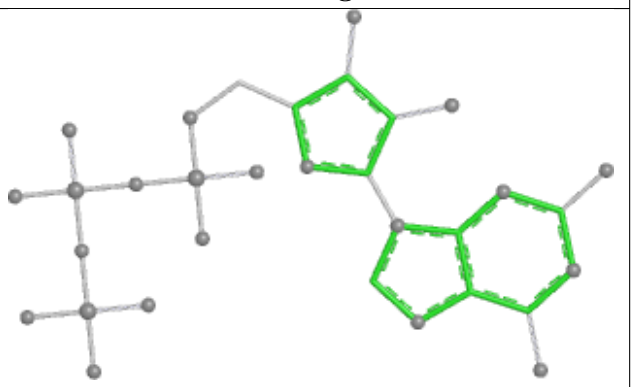
Bond lengths



Bond angles

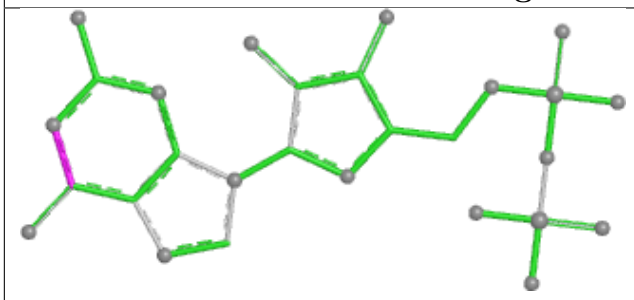


Torsions

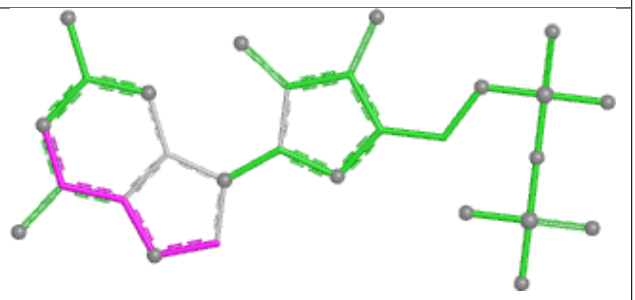


Rings

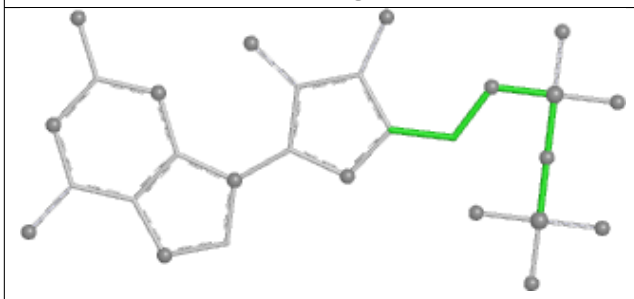
Ligand GDP Dt 501



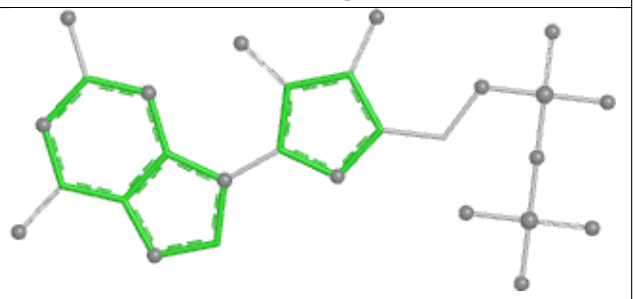
Bond lengths



Bond angles

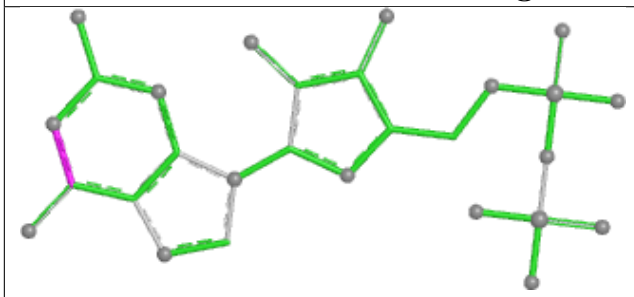


Torsions

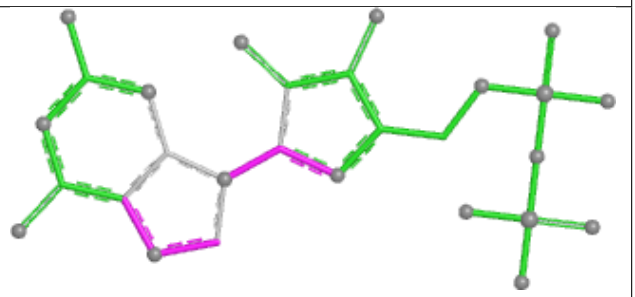


Rings

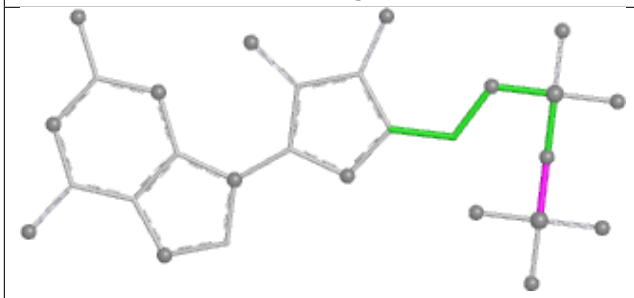
Ligand GDP Fu 501



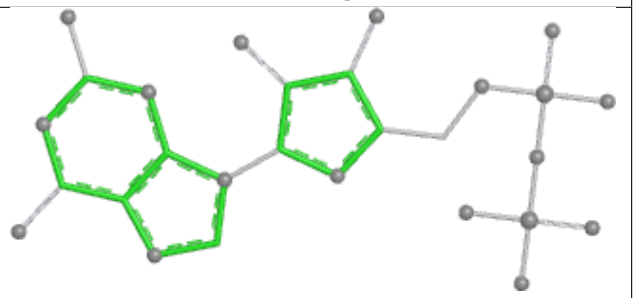
Bond lengths



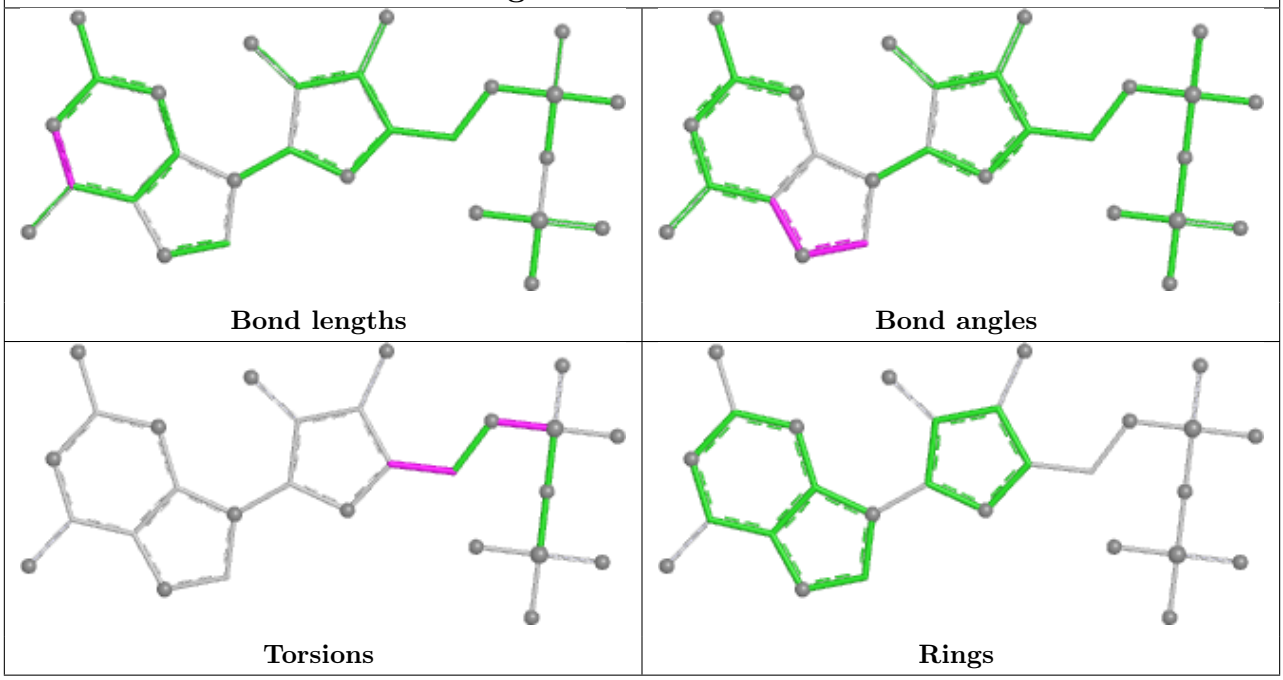
Bond angles



Torsions



Rings

Ligand GDP AH 501	
 Bond lengths	Bond angles
Torsions	Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

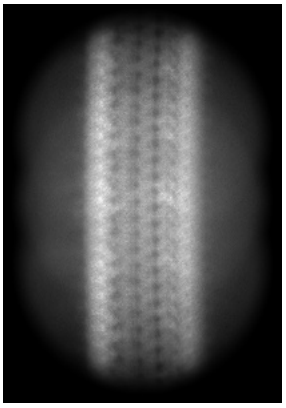
5 Map visualisation (i)

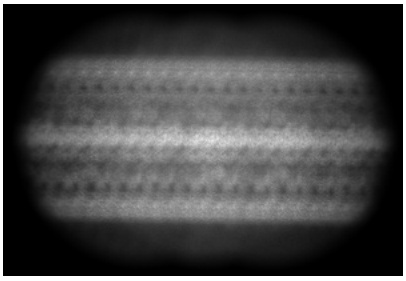
This section contains visualisations of the EMDB entry EMD-46580. These allow visual inspection of the internal detail of the map and identification of artifacts.

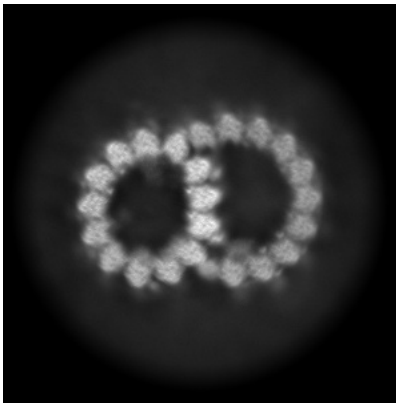
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections (i)

5.1.1 Primary map


X

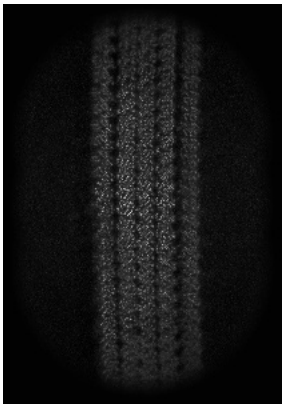

Y

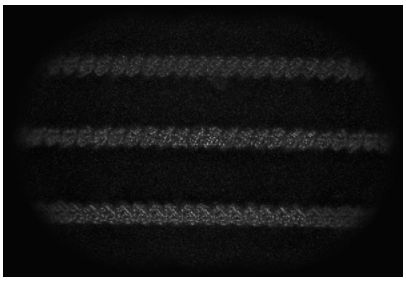

Z

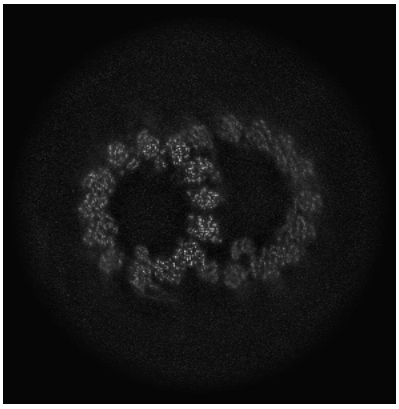
The images above show the map projected in three orthogonal directions.

5.2 Central slices (i)

5.2.1 Primary map


X Index: 326

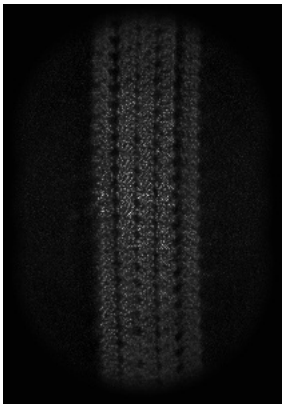

Y Index: 332

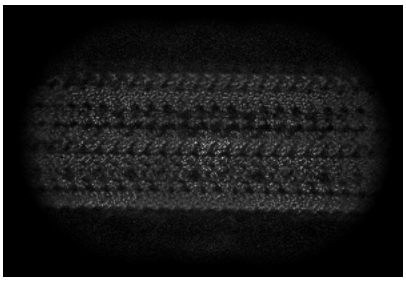

Z Index: 479

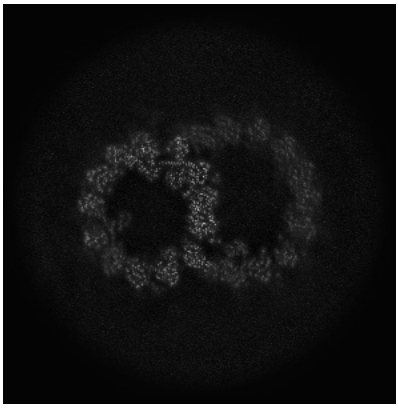
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

5.3.1 Primary map


X Index: 325

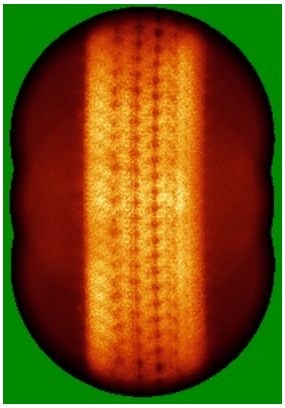

Y Index: 234

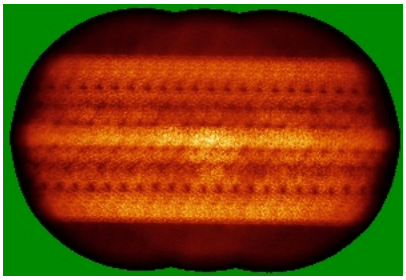

Z Index: 494

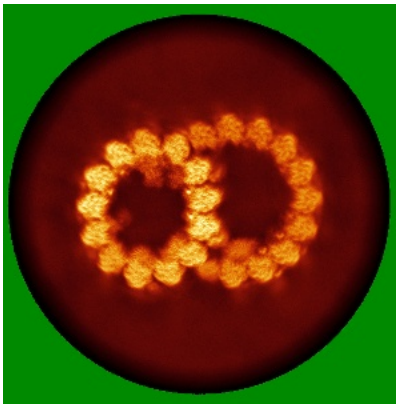
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) (i)

5.4.1 Primary map


X

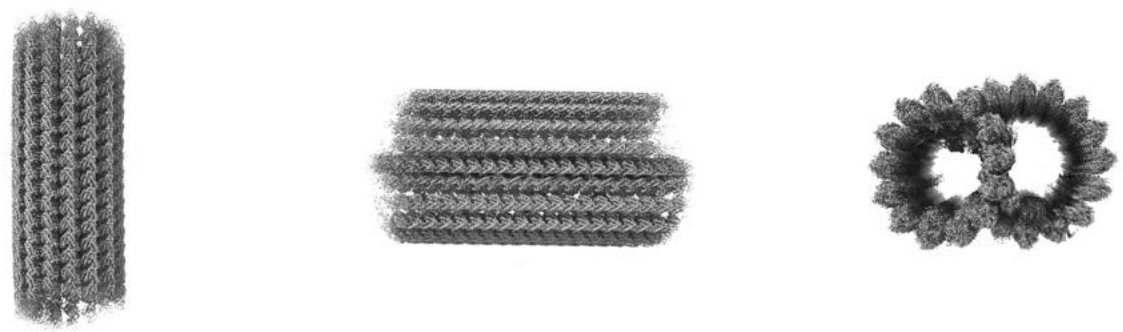

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views (i)

5.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

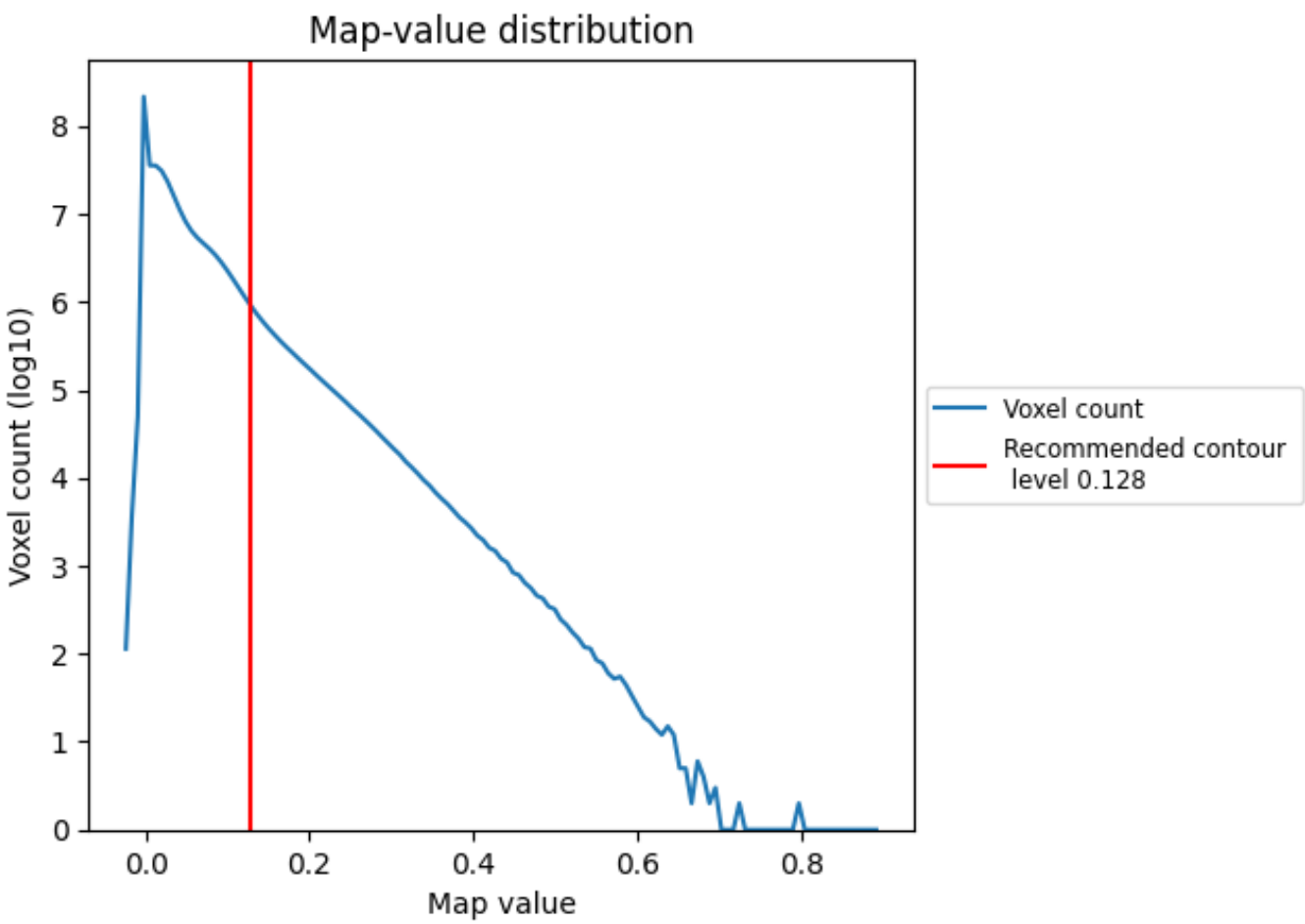
5.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

6 Map analysis (i)

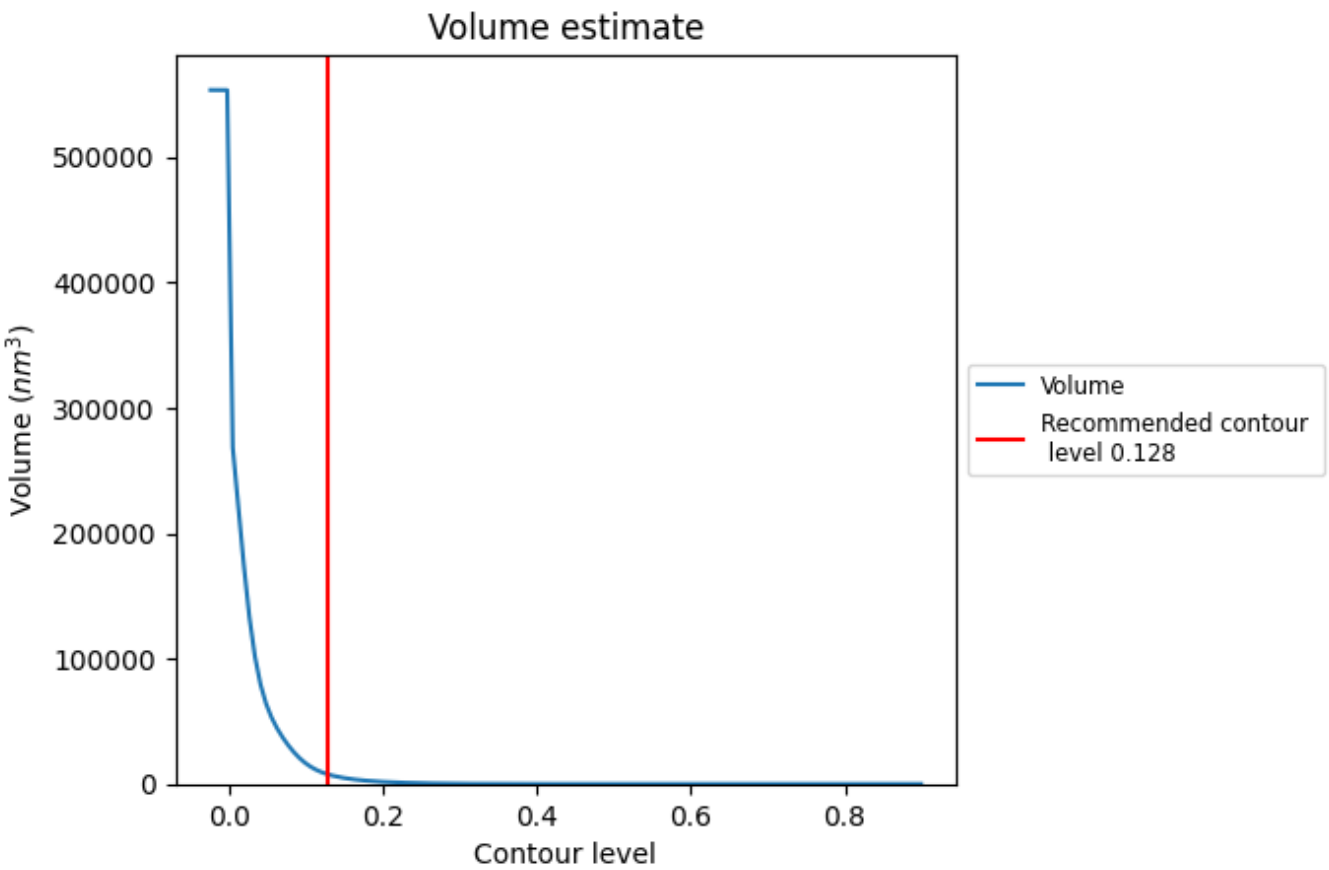
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

6.2 Volume estimate (i)



The volume at the recommended contour level is 7740 nm^3; this corresponds to an approximate mass of 6992 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

6.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

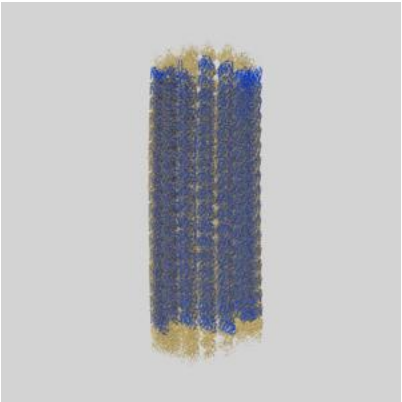
7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

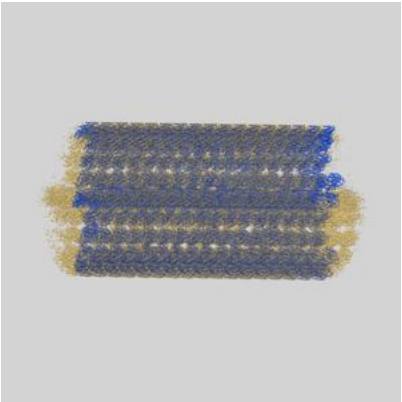
8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-46580 and PDB model 9D5N. Per-residue inclusion information can be found in section ?? on page ??.

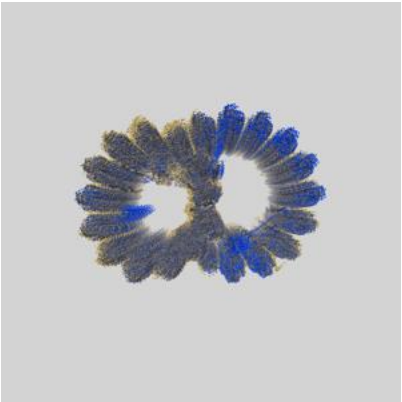
8.1 Map-model overlay (i)



X



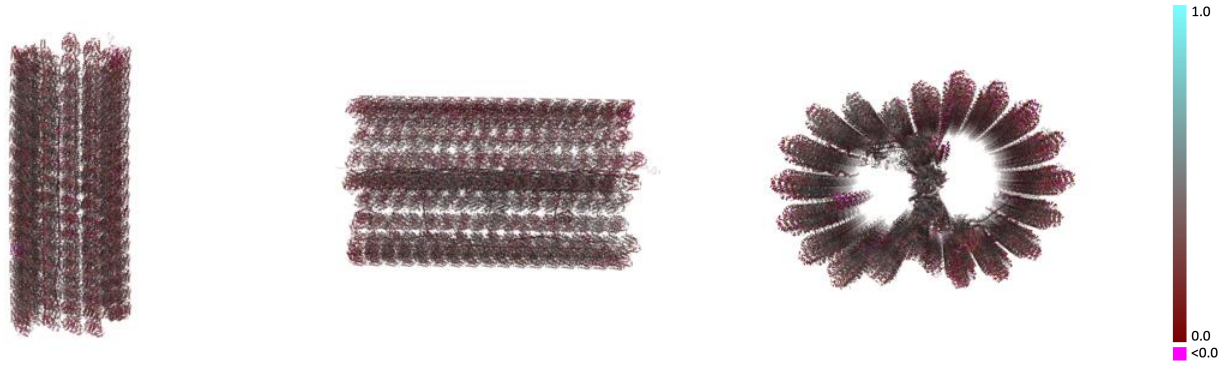
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

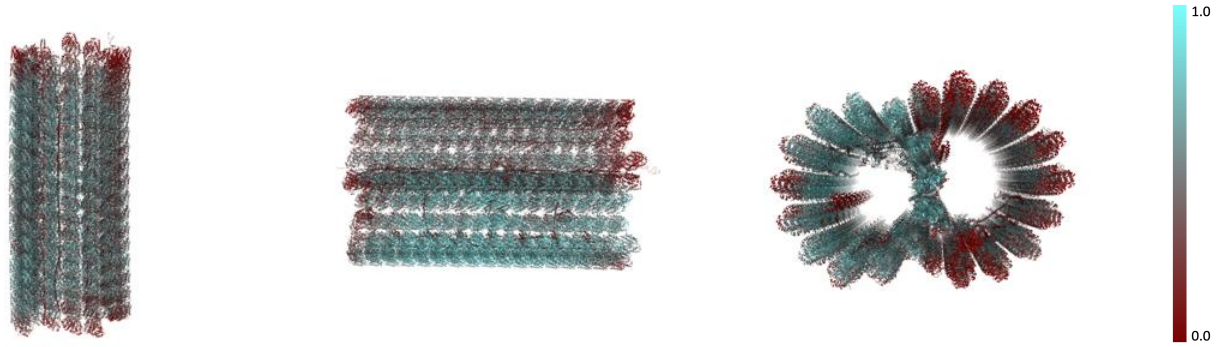
8.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

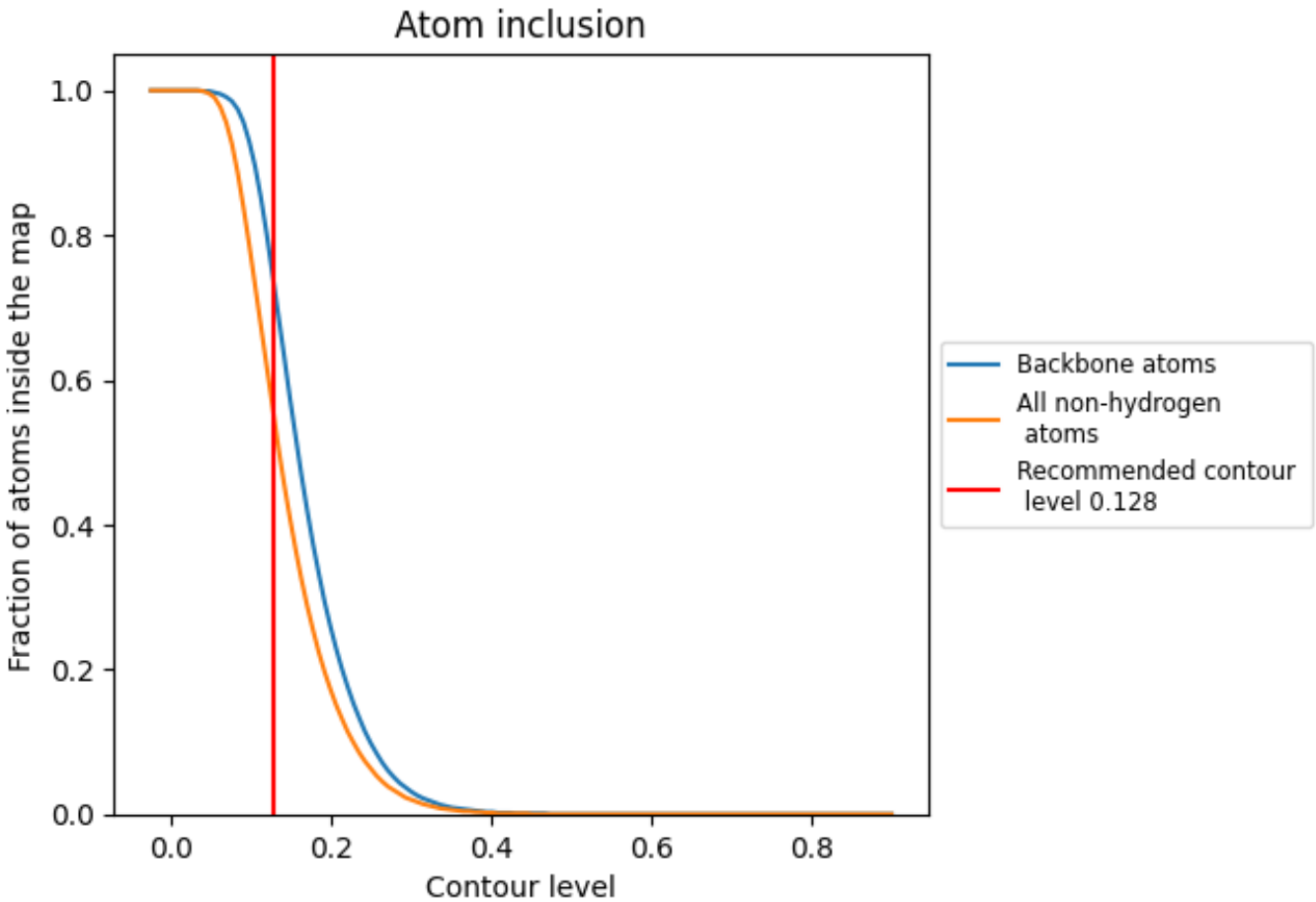
8.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.128).

8.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5560	0.3310
0	0.4340	0.2860
1	0.4530	0.3020
2	0.4420	0.2960
3	0.5040	0.3310
4	0.3290	0.3010
5	0.4640	0.3170
6	0.4580	0.3190
7	0.1970	0.0050
8	0.3830	0.2850
9	0.5300	0.3180
A	0.3480	0.2660
A0	0.1420	0.2460
A1	0.2540	0.2580
A2	0.5190	0.3300
A3	0.4130	0.3060
A4	0.5900	0.3050
A5	0.7260	0.3540
A6	0.6090	0.3110
A7	0.6150	0.3250
A8	0.6670	0.3710
A9	0.2970	0.2630
AA	0.5140	0.3220
AB	0.4410	0.2870
AC	0.4460	0.3360
AD	0.6560	0.3670
AE	0.4410	0.2940
AF	0.5170	0.3170
AG	0.4980	0.3200
AH	0.4390	0.3300
AI	0.4900	0.3090
AJ	0.6270	0.3750
AK	0.4550	0.3190
AL	0.5110	0.3230
AM	0.4310	0.3150

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AN	0.5030	0.3100
AO	0.4860	0.2970
AP	0.6090	0.3460
AQ	0.5020	0.3060
AR	0.6210	0.3510
AS	0.4460	0.3100
AT	0.4670	0.2720
AU	0.5180	0.3160
AV	0.4480	0.2620
AW	0.5410	0.3260
AX	0.5040	0.3060
AY	0.3800	0.2860
AZ	0.4600	0.2880
Aa	0.4590	0.3160
Ab	0.5760	0.3510
Ac	0.4560	0.2900
Ad	0.5830	0.3620
Ae	0.4120	0.3220
Af	0.5040	0.3160
Ag	0.5370	0.3560
Ah	0.4730	0.3150
Ai	0.5600	0.3680
Aj	0.4010	0.3100
Ak	0.2070	0.2820
Al	0.4870	0.3140
Am	0.1100	0.2350
An	0.4130	0.3140
Ao	0.2580	0.2880
Ap	0.2300	0.2840
Aq	0.2390	0.2710
Ar	0.2480	0.2920
As	0.3540	0.2920
At	0.3320	0.2970
Au	0.3200	0.2850
Av	0.1530	0.2710
Aw	0.2120	0.2570
Ax	0.1370	0.2200
Ay	0.3210	0.3050
Az	0.6200	0.3510
B	0.1360	0.1820
B0	0.4720	0.2870
B1	0.5180	0.3380

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B2	0.5950	0.3480
B3	0.5520	0.3450
B4	0.6030	0.3630
B5	0.4740	0.2920
B6	0.3640	0.2700
B7	0.4960	0.2580
B8	0.5130	0.3280
B9	0.5350	0.3410
BA	0.4420	0.2990
BB	0.3430	0.2810
BC	0.3480	0.2710
BD	0.2800	0.2860
BE	0.3700	0.2690
BF	0.5300	0.3320
BG	0.3430	0.2710
BH	0.5810	0.3440
BI	0.4820	0.3230
BJ	0.3740	0.3230
BK	0.1470	0.2140
BL	0.4880	0.3100
BM	0.4570	0.2950
BN	0.6070	0.3550
BO	0.5380	0.3450
BP	0.6300	0.3670
BQ	0.4260	0.3160
BR	0.1840	0.2330
BS	0.6010	0.3670
BT	0.4620	0.3170
BU	0.6300	0.3590
BV	0.3160	0.2890
BW	0.5200	0.3180
BX	0.4710	0.3050
BY	0.5030	0.3060
BZ	0.4680	0.2950
Ba	0.5340	0.3350
Bb	0.4680	0.2930
Bc	0.7630	0.3870
Bd	0.8090	0.4020
Be	0.4680	0.3130
Bf	0.4580	0.2940
Bg	0.4330	0.2680
Bh	0.4410	0.2850

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bi	0.4230	0.2580
Bj	0.4470	0.2850
Bk	0.5280	0.3300
Bl	0.4730	0.2440
Bm	0.5370	0.3400
Bn	0.4160	0.2750
Bo	0.4940	0.2820
Bp	0.5440	0.3250
Bq	0.4880	0.2770
Br	0.5620	0.3300
Bs	0.4760	0.3130
Bt	0.4020	0.2660
Bu	0.4160	0.2780
Bv	0.4390	0.2890
Bw	0.4800	0.2940
Bx	0.3820	0.2760
By	0.4550	0.2690
Bz	0.4970	0.2900
C	0.1080	0.1580
C1	0.4590	0.3760
C2	0.4110	0.3200
C3	0.4910	0.3420
CA	0.6330	0.3660
CB	0.3750	0.2920
CC	0.3330	0.3060
CD	0.1450	0.2080
CE	0.4930	0.3340
CF	0.1610	0.2140
CG	0.3700	0.2540
CH	0.0420	0.2570
CI	0.1940	0.3090
CJ	0.2940	0.2170
CK	0.2000	0.1920
CL	0.1990	0.2300
CM	0.7220	0.4110
CN	0.6110	0.4130
CO	0.3730	0.2910
CP	0.0710	0.2340
CQ	0.4400	0.3610
CR	0.4640	0.3290
CS	0.6320	0.3960
CT	0.3560	0.1970

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CU	0.3020	0.2220
CV	0.4600	0.2370
CW	0.4860	0.2990
CX	0.3350	0.2360
CY	0.4500	0.3290
CZ	0.4350	0.3260
Ca	0.3100	0.2550
Cb	0.2050	0.2220
Cc	0.2550	0.2490
Cd	0.5270	0.3820
Ce	0.4610	0.3560
Cf	0.2210	0.2360
Cg	0.1870	0.2470
Ch	0.3960	0.2410
Ci	0.3920	0.2960
Cj	0.3500	0.2130
Ck	0.3700	0.2930
Cl	0.3250	0.2280
Cm	0.6610	0.3840
Cn	0.5700	0.3670
Co	0.3600	0.2860
Cp	0.3860	0.2830
Cq	0.3770	0.3160
Cr	0.4180	0.2880
Cs	0.4190	0.2750
Ct	0.4540	0.3380
Cu	0.4760	0.3460
Cv	0.5150	0.3580
Cw	0.6290	0.4170
Cx	0.5590	0.3750
Cy	0.5720	0.3700
Cz	0.6080	0.3820
D	0.3930	0.3240
DL	0.7150	0.3520
DM	0.7840	0.3610
DN	0.7860	0.3460
DO	0.7320	0.3620
DP	0.6680	0.3560
DQ	0.5880	0.3140
DR	0.7310	0.3490
DS	0.7120	0.3450
DT	0.7970	0.3560

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DU	0.5800	0.3030
DV	0.6500	0.3380
DW	0.7300	0.3310
DX	0.7610	0.3660
DY	0.4540	0.3040
DZ	0.6680	0.3870
Da	0.6730	0.3740
Db	0.5690	0.3410
Dc	0.4600	0.2540
Dd	0.2700	0.2370
De	0.3860	0.2420
Df	0.8110	0.3510
Dg	0.8050	0.3610
Dh	0.6530	0.3180
Di	0.7850	0.3730
Dj	0.7820	0.3360
Dk	0.8000	0.3520
Dq	0.4020	0.2720
Dr	0.6730	0.3420
Ds	0.7400	0.3610
Dt	0.6110	0.3090
Du	0.6810	0.3680
Dv	0.6380	0.3750
Dw	0.7440	0.3600
Dx	0.8380	0.4150
E	0.5650	0.3690
E0	0.5670	0.2770
E1	0.7290	0.3860
E2	0.7730	0.3910
E3	0.7560	0.3890
E4	0.6710	0.3510
E5	0.7210	0.3740
E6	0.8060	0.4140
E7	0.7940	0.4150
E8	0.7480	0.3770
E9	0.7630	0.3800
EL	0.7070	0.3550
EM	0.7850	0.3720
EN	0.5010	0.3160
EO	0.7150	0.3530
EP	0.7980	0.3620
EQ	0.5730	0.3330

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
ER	0.6100	0.3260
ES	0.6050	0.3770
ET	0.6740	0.3760
EU	0.6070	0.3850
EV	0.6810	0.3820
EW	0.7730	0.3910
EX	0.6500	0.3920
EY	0.7010	0.3820
EZ	0.6510	0.3850
Ea	0.4740	0.3260
Eb	0.7560	0.3860
Ec	0.2940	0.2820
Ed	0.7160	0.3780
Ee	0.7210	0.3500
Ef	0.6300	0.3560
Eg	0.7780	0.3560
Eh	0.6830	0.3230
Ei	0.7650	0.3650
Ej	0.7840	0.3400
Ek	0.7590	0.3830
El	0.7850	0.3460
Em	0.6350	0.3520
En	0.7880	0.3610
Eo	0.7290	0.3500
Ep	0.6220	0.3380
Eq	0.5190	0.2560
Er	0.6340	0.3800
Es	0.5470	0.3020
Et	0.6440	0.3880
Eu	0.6350	0.3630
Ev	0.6250	0.3100
Ew	0.6690	0.3870
Ex	0.7360	0.3920
Ey	0.6550	0.3640
Ez	0.4350	0.3210
F	0.5010	0.3440
F0	0.6500	0.3940
F1	0.7670	0.3890
F2	0.7630	0.3980
F3	0.6420	0.3780
F4	0.7280	0.3850
F5	0.6360	0.3650

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
F6	0.5710	0.3340
F7	0.3790	0.2800
F8	0.5710	0.3320
F9	0.6200	0.3510
FA	0.6900	0.3500
FB	0.7410	0.3820
FC	0.6630	0.3590
FD	0.7800	0.4130
FE	0.6100	0.3560
FF	0.8140	0.4100
FG	0.6760	0.3650
FH	0.8870	0.4470
FI	0.8740	0.4430
FJ	0.8230	0.4120
FK	0.8630	0.4470
FL	0.8140	0.4120
FM	0.5770	0.3090
FN	0.7920	0.3940
FO	0.7650	0.3680
FP	0.6970	0.3780
FQ	0.7670	0.3590
FR	0.7310	0.3710
FS	0.7770	0.3860
FT	0.6850	0.3480
FU	0.6760	0.3580
FV	0.7070	0.3770
FW	0.7500	0.3950
FX	0.5480	0.2830
FY	0.7040	0.3690
FZ	0.6180	0.3390
Fa	0.7000	0.3850
Fb	0.7210	0.3790
Fc	0.6940	0.3860
Fd	0.7940	0.4090
Fe	0.8570	0.4350
Ff	0.8360	0.4250
Fg	0.8370	0.4300
Fh	0.4690	0.3460
Fi	0.5830	0.3710
Fj	0.6160	0.3750
Fk	0.6120	0.3570
Fl	0.6730	0.3700

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Fm	0.1910	0.2280
Fn	0.6900	0.3870
Fo	0.3900	0.2770
Fp	0.6910	0.3830
Fq	0.5520	0.3170
Fr	0.6990	0.3960
Fs	0.6310	0.3750
Ft	0.7100	0.4090
Fu	0.6520	0.3960
Fv	0.7240	0.3740
Fw	0.5850	0.3650
Fx	0.8260	0.4220
Fy	0.7850	0.4100
Fz	0.7480	0.3930
G	0.3330	0.2490
G0	0.6690	0.3530
G1	0.5840	0.3410
G2	0.7780	0.4000
G3	0.7040	0.3790
G4	0.8620	0.4310
G5	0.8400	0.4330
G6	0.8020	0.4210
G7	0.5440	0.2570
G8	0.7370	0.3540
G9	0.6680	0.3670
GA	0.4370	0.2950
GB	0.6750	0.4040
GC	0.4770	0.3360
GD	0.6980	0.3850
GE	0.8110	0.4140
GF	0.7910	0.4080
GG	0.7430	0.3780
GH	0.3670	0.2460
GI	0.4370	0.2980
GJ	0.6010	0.3240
GK	0.6530	0.3310
GL	0.5980	0.3070
GM	0.3620	0.2820
GN	0.5430	0.3230
GO	0.5340	0.3480
GP	0.5620	0.3660
GQ	0.8490	0.4210

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GR	0.8800	0.4370
GS	0.8360	0.4340
GT	0.8340	0.4250
GU	0.8210	0.3630
GV	0.8220	0.3770
GW	0.6380	0.3090
GX	0.7540	0.3590
GY	0.4710	0.2390
GZ	0.5540	0.2700
Ga	0.4610	0.2660
Gb	0.7170	0.3580
Gc	0.5410	0.3240
Gd	0.7340	0.3850
Ge	0.6970	0.3890
Gf	0.7350	0.3800
Gg	0.7910	0.4150
Gh	0.7910	0.4190
Gi	0.8540	0.4220
Gj	0.7450	0.4030
Gk	0.8460	0.4370
Gl	0.7510	0.3570
Gm	0.8390	0.4360
Gn	0.8140	0.3670
Go	0.7020	0.3370
Gp	0.8150	0.3670
Gq	0.7550	0.3240
Gr	0.8100	0.3690
Gs	0.7710	0.3380
Gt	0.7010	0.3370
Gu	0.7830	0.3590
Gv	0.7240	0.3530
Gw	0.5140	0.2480
Gx	0.6120	0.2870
Gy	0.5130	0.2900
Gz	0.7280	0.3740
H	0.6910	0.3860
HA	0.4550	0.3160
HB	0.2310	0.2990
HC	0.0370	0.2370
HD	0.4920	0.3310
I	0.2770	0.1940
M	0.6290	0.3880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
N	0.5230	0.2380
O	0.4340	0.3050
P	0.4870	0.3160
Q	0.4970	0.3110
R	0.4680	0.3200
S	0.4610	0.2760
T	0.4190	0.3040
U	0.3850	0.2710
V	0.4800	0.2950
W	0.4330	0.2350
X	0.4780	0.3260
Y	0.5040	0.3200
Z	0.4200	0.3110
a	0.5760	0.3310
b	0.5430	0.3300
c	0.3110	0.2920
d	0.3600	0.3090
e	0.5680	0.3380
f	0.5560	0.3400
g	0.4800	0.2940
h	0.4340	0.3080
i	0.5810	0.3670
j	0.4400	0.3370
k	0.5830	0.3750
l	0.3600	0.3230
m	0.3860	0.3060
n	0.0390	0.2080
o	0.0330	0.1930
p	0.0810	0.2180
q	0.1210	0.2110
r	0.3620	0.2830
s	0.5240	0.3240
t	0.4590	0.3200
u	0.4970	0.2920
v	0.4580	0.3060
w	0.4440	0.3110
x	0.4550	0.2350
y	0.4170	0.3010
z	0.5240	0.3480