Full wwPDB EM Validation Report ⓘ

Apr 7, 2026 – 02:55 AM UTC

PDB ID	:	9Y6S / pdb_00009y6s
EMDB ID	:	EMD-72629
Title	:	96-nm repeat of the Leishmania tarentolae doublet microtubule
Authors	:	Doran, M.H.; Brown, A.
Deposited on	:	2025-09-09
Resolution	:	3.70 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	NOT EXECUTED
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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 168 unique types of molecules in this entry. The entry contains 3422719 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
1	A	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	AB	419	Total 3283	C 2056	N 560	O 636	S 31	0	0
1	AD	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	AF	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	AH	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	AJ	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	AL	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	AN	419	Total 3283	C 2056	N 560	O 636	S 31	0	0
1	B	418	Total 3270	C 2039	N 564	O 637	S 30	0	0
1	BD	430	Total 3370	C 2106	N 579	O 653	S 32	0	0
1	BF	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	BH	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	BJ	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	BL	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	BN	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	CA	424	Total 3319	C 2076	N 568	O 643	S 32	0	0
1	CC	430	Total 3370	C 2106	N 579	O 653	S 32	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CE	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CG	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CI	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CK	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CM	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DA	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DC	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DE	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DG	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DI	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DK	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DM	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	E	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EB	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	ED	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EF	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EH	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EJ	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	F	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	FD	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FJ	429	Total	C	N	O	S	0	0
			3361	2100	578	652	31		
1	FL	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	G	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GD	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	GF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GJ	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	GL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	H	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HD	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	I	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	IB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	ID	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JA	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JC	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JE	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JG	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JI	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JK	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JM	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	KA	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	KC	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KE	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KG	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KI	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KK	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KM	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LA	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LC	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LE	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LG	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LI	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LK	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LM	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	M	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MD	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	ML	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	N	420	Total	C	N	O	S	0	0
			3290	2060	561	638	31		
1	NB	420	Total	C	N	O	S	0	0
			3290	2060	561	638	31		
1	ND	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	NF	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	NH	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	NJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	NL	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OB	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	OD	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OF	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OH	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OJ	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OL	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	P	401	Total	C	N	O	S	0	0
			3123	1946	540	609	28		
1	PB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PD	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PH	426	Total	C	N	O	S	0	0
			3342	2089	575	647	31		
1	PJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	QA	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QC	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QE	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	QG	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QI	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QK	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	RA	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	RC	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	RE	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RG	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RI	426	Total	C	N	O	S	0	0
			3342	2088	575	648	31		
1	RK	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	S	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SB	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SD	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SF	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SH	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	SJ	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	T	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	TB	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	TD	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	TF	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	TH	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	TJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	TL	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	U	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UB	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UD	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UF	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UH	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UJ	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	UL	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	V	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	VB	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	VD	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	VF	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	VH	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	VJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	VL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	W	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WB	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WD	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WF	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	WH	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WJ	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WL	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	AP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AZ	419	Total	C	N	O	S	0	0
			3283	2056	560	636	31		
1	BP	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	BR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CO	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CQ	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CS	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CY	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DQ	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	DS	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DY	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	EN	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	EP	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	ER	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	ET	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EV	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FV	429	Total	C	N	O	S	0	0
			3361	2100	578	652	31		
1	FX	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	GN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GP	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	GR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GV	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	GX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	HV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JQ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JS	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JY	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	KO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KQ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KS	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KY	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LQ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LS	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LY	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MZ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PT	426	Total	C	N	O	S	0	0
			3342	2089	575	647	31		
1	PV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	QM	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QO	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QQ	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	QS	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QU	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	QW	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	RM	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	RQ	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RS	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RU	426	Total	C	N	O	S	0	0
			3342	2088	575	648	31		
1	RW	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	SL	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SN	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SP	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SR	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	ST	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	SV	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	TN	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	TP	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	TR	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	TT	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	TV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	TX	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	UN	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UP	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UR	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UT	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UV	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	UX	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	VN	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	VP	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	VR	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	VT	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	VV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	VX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	WN	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WP	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WR	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	WT	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WV	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	WX	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	NN	420	Total	C	N	O	S	0	0
			3290	2060	561	638	31		
1	NP	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	NR	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	NT	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	NV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	NX	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	ON	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	OP	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OR	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OT	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OV	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OX	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	AC	433	Total	C	N	O	S	0	0
			3353	2117	570	643	23		
2	AE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AG	433	Total	C	N	O	S	0	0
			3352	2116	571	642	23		
2	AI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AK	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BA	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	BE	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	BG	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	BK	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	C	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CB	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CD	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CF	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	CH	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CJ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CL	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	D	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DB	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DD	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DF	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	DH	430	Total	C	N	O	S	0	0
			3328	2102	567	636	23		
2	DJ	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DL	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	EA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	EC	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	EE	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	EG	433	Total	C	N	O	S	0	0
			3351	2114	570	644	23		
2	EI	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	EK	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FA	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	FC	434	Total	C	N	O	S	0	0
			3360	2119	571	647	23		
2	FE	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	FG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	FI	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	FK	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	GA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GC	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GE	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	GG	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HC	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	HG	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	HI	431	Total	C	N	O	S	0	0
			3336	2106	568	639	23		
2	HK	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	HM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IC	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	IE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	II	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	J	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	JB	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	JD	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JF	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JH	432	Total	C	N	O	S	0	0
			3342	2110	569	640	23		
2	JJ	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	JL	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	JN	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	K	434	Total	C	N	O	S	0	0
			3358	2119	572	643	24		
2	KB	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KD	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	KF	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KH	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	KJ	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	KL	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KN	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LB	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	LD	429	Total	C	N	O	S	0	0
			3322	2097	566	637	22		
2	LF	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LH	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LJ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LL	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LN	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	MA	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	MC	437	Total	C	N	O	S	0	0
			3379	2133	575	647	24		
2	ME	436	Total	C	N	O	S	0	0
			3368	2124	573	647	24		
2	MG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MK	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MM	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	NA	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NC	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NK	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	NM	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	OA	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	OC	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	OE	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	OG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	OI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	OK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	OM	433	Total	C	N	O	S	0	0
			3352	2115	570	644	23		
2	PA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	PC	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PE	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	PI	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PK	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	PM	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	Q	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	QB	429	Total	C	N	O	S	0	0
			3323	2100	566	634	23		
2	QD	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	QF	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	QH	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	QJ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	QL	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	R	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	RB	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RD	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RF	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RH	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	RJ	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	RL	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SA	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	SC	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SE	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	SI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	SK	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	TA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TC	428	Total	C	N	O	S	0	0
			3314	2093	565	634	22		
2	TE	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	TI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TK	433	Total	C	N	O	S	0	0
			3353	2117	570	643	23		
2	UA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UC	429	Total	C	N	O	S	0	0
			3322	2097	566	637	22		
2	UE	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	UG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	UI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	UK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	VA	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VC	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VE	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VI	432	Total	C	N	O	S	0	0
			3342	2109	569	641	23		
2	VK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	VM	434	Total	C	N	O	S	0	0
			3360	2119	571	647	23		
2	WA	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WC	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WK	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WM	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AO	433	Total	C	N	O	S	0	0
			3353	2117	570	643	23		
2	AQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AS	433	Total	C	N	O	S	0	0
			3352	2116	571	642	23		
2	AU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AW	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AY	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BO	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BQ	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	BS	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	BW	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	BY	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	CN	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CP	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CR	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	CT	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CV	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CX	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	DN	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DP	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DR	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	DT	430	Total	C	N	O	S	0	0
			3328	2102	567	636	23		
2	DV	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DX	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	EM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	EO	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	EQ	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	ES	433	Total	C	N	O	S	0	0
			3351	2114	570	644	23		
2	EU	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	EW	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	FM	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	FO	434	Total	C	N	O	S	0	0
			3360	2119	571	647	23		
2	FQ	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	FS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	FU	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	FW	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	GM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GO	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GQ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	GS	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HO	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	HS	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	HU	431	Total	C	N	O	S	0	0
			3336	2106	568	639	23		
2	HW	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	HY	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IO	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	IQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IY	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JP	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JR	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JT	432	Total	C	N	O	S	0	0
			3342	2110	569	640	23		
2	JV	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	JX	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	JZ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KP	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	KR	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KT	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	KV	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	KX	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	KZ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LP	429	Total	C	N	O	S	0	0
			3322	2097	566	637	22		
2	LR	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LT	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LV	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LX	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LZ	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	MO	437	Total	C	N	O	S	0	0
			3379	2133	575	647	24		
2	MQ	436	Total	C	N	O	S	0	0
			3368	2124	573	647	24		
2	MS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MW	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MY	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	PO	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PQ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	PU	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PW	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	PY	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	QN	429	Total	C	N	O	S	0	0
			3323	2100	566	634	23		
2	QP	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	QR	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	QT	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	QV	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	QX	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	RN	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RP	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RR	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RT	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	RV	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	RX	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SM	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	SO	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SQ	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	SU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	SW	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	TM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TO	428	Total	C	N	O	S	0	0
			3314	2093	565	634	22		
2	TQ	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	TU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	TW	433	Total	C	N	O	S	0	0
			3353	2117	570	643	23		
2	UM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	UO	429	Total	C	N	O	S	0	0
			3322	2097	566	637	22		
2	UQ	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	US	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	UU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	UW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	VO	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VQ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VU	432	Total	C	N	O	S	0	0
			3342	2109	569	641	23		
2	VW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	VY	434	Total	C	N	O	S	0	0
			3360	2119	571	647	23		
2	WO	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WW	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WY	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NO	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	NS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NW	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NY	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	OO	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	OQ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	OS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	OU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	OW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	OY	433	Total	C	N	O	S	0	0
			3352	2115	570	644	23		

- Molecule 3 is a protein called CFAP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XA	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XB	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XC	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XD	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XE	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XF	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XG	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XH	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	XI	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XJ	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XK	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XL	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		

- Molecule 4 is a protein called PACRGA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	XM	259	Total	C	N	O	S	0	0
			2045	1307	360	370	8		
4	XO	260	Total	C	N	O	S	0	0
			2053	1311	361	373	8		
4	XQ	260	Total	C	N	O	S	0	0
			2053	1311	361	373	8		
4	XR	260	Total	C	N	O	S	0	0
			2056	1313	364	371	8		
4	XT	260	Total	C	N	O	S	0	0
			2053	1311	361	373	8		
4	XV	260	Total	C	N	O	S	0	0
			2053	1311	361	373	8		
4	XW	260	Total	C	N	O	S	0	0
			2056	1313	364	371	8		

- Molecule 5 is a protein called PACRGB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	XN	269	Total	C	N	O	S	0	0
			2116	1359	366	384	7		
5	XP	269	Total	C	N	O	S	0	0
			2116	1359	366	384	7		
5	XS	269	Total	C	N	O	S	0	0
			2116	1359	366	384	7		
5	XU	269	Total	C	N	O	S	0	0
			2116	1359	366	384	7		

- Molecule 6 is a protein called CCDC81.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0A	257	Total	C	N	O	S	0	0
			2004	1261	359	371	13		
6	0	257	Total	C	N	O	S	0	0
			2004	1261	359	371	13		
6	0B	257	Total	C	N	O	S	0	0
			2004	1261	359	371	13		

- Molecule 7 is a protein called CFAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0C	121	Total	C	N	O	S	0	0
			935	584	159	188	4		
7	0D	354	Total	C	N	O	S	0	0
			2723	1683	492	537	11		
7	0E	354	Total	C	N	O	S	0	0
			2723	1683	492	537	11		

- Molecule 8 is a protein called CFAP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	0F	176	Total	C	N	O	S	0	0
			1439	859	288	280	12		
8	0I	285	Total	C	N	O	S	0	0
			2369	1421	471	459	18		
8	0H	349	Total	C	N	O	S	0	0
			2955	1772	596	570	17		
8	0K	28	Total	C	N	O		0	0
			229	146	41	42			
8	9A	226	Total	C	N	O	S	0	0
			1906	1147	379	373	7		
8	0G	444	Total	C	N	O	S	0	0
			3711	2221	751	718	21		
8	0J	449	Total	C	N	O	S	0	0
			3757	2255	754	727	21		

- Molecule 9 is a protein called CFAP52.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0L	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	0M	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0N	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	0O	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	0P	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	0Q	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	9B	310	Total	C	N	O	S	0	0
			2357	1482	416	445	14		

- Molecule 10 is a protein called CFAP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	0R	309	Total	C	N	O	S	0	0
			2628	1579	535	501	13		
10	0T	221	Total	C	N	O	S	0	0
			1874	1148	360	359	7		
10	0S	460	Total	C	N	O	S	0	0
			3908	2370	779	743	16		

- Molecule 11 is a protein called CFAP67A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	0U	333	Total	C	N	O	S	0	0
			2570	1621	437	495	17		
11	0V	333	Total	C	N	O	S	0	0
			2570	1621	437	495	17		

- Molecule 12 is a protein called CFAP67B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	0W	339	Total	C	N	O	S	0	0
			2595	1647	427	501	20		
12	0X	339	Total	C	N	O	S	0	0
			2595	1647	427	501	20		

- Molecule 13 is a protein called CFAP106A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	0Y	233	Total	C	N	O	S	0	0
			1836	1152	334	345	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
13	0Z	235	Total	C	N	O	S	0	0
			1849	1160	337	347	5		
13	0a	233	Total	C	N	O	S	0	0
			1836	1152	334	345	5		
13	0b	235	Total	C	N	O	S	0	0
			1849	1160	337	347	5		

- Molecule 14 is a protein called CFAP106B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0c	237	Total	C	N	O	S	0	0
			1929	1221	337	362	9		
14	0d	265	Total	C	N	O	S	0	0
			2150	1359	378	404	9		
14	0e	265	Total	C	N	O	S	0	0
			2150	1359	378	404	9		

- Molecule 15 is a protein called CFAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	0f	160	Total	C	N	O	S	0	0
			1257	783	222	241	11		
15	0g	160	Total	C	N	O	S	0	0
			1257	783	222	241	11		
15	0h	30	Total	C	N	O	S	0	0
			218	137	34	46	1		

- Molecule 16 is a protein called CFAP115.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	0i	180	Total	C	N	O	S	0	0
			1463	930	264	263	6		
16	0j	688	Total	C	N	O	S	0	0
			5411	3423	987	975	26		
16	0l	640	Total	C	N	O	S	0	0
			5045	3192	918	914	21		
16	0k	710	Total	C	N	O	S	0	0
			5599	3537	1026	1009	27		

- Molecule 17 is a protein called CFAP127.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	0m	142	Total C N O S 1155 704 220 227 4	0	0
17	0n	406	Total C N O S 3388 2054 668 654 12	0	0
17	0o	406	Total C N O S 3388 2054 668 654 12	0	0
17	9C	20	Total C N O 171 107 35 29	0	0

- Molecule 18 is a protein called CFAP141.

Mol	Chain	Residues	Atoms	AltConf	Trace
18	0p	108	Total C N O S 906 557 177 169 3	0	0
18	0q	108	Total C N O S 906 557 177 169 3	0	0

- Molecule 19 is a protein called CFAP143.

Mol	Chain	Residues	Atoms	AltConf	Trace
19	0r	254	Total C N O S 2033 1246 376 396 15	0	0
19	0s	254	Total C N O S 2033 1246 376 396 15	0	0

- Molecule 20 is a protein called CFAP161.

Mol	Chain	Residues	Atoms	AltConf	Trace
20	0t	262	Total C N O S 2062 1298 358 388 18	0	0
20	0u	227	Total C N O S 1769 1117 306 330 16	0	0
20	9D	227	Total C N O S 1769 1117 306 330 16	0	0

- Molecule 21 is a protein called CFAP210.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	0w	449	Total C N O S 3715 2242 741 724 8	0	0
21	0v	73	Total C N O 582 351 115 116	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0y	111	Total	C	N	O	S	0	0
			906	556	175	172	3		
21	0x	490	Total	C	N	O	S	0	0
			4059	2455	802	792	10		

- Molecule 22 is a protein called DMIP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0z	143	Total	C	N	O	S	0	0
			1160	716	220	219	5		
22	1w	180	Total	C	N	O	S	0	0
			1481	915	278	281	7		
22	1x	206	Total	C	N	O	S	0	0
			1680	1031	322	315	12		
22	2A	143	Total	C	N	O	S	0	0
			1157	715	220	217	5		
22	1y	180	Total	C	N	O	S	0	0
			1481	915	278	281	7		
22	1z	206	Total	C	N	O	S	0	0
			1680	1031	322	315	12		

- Molecule 23 is a protein called RIB43.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1A	270	Total	C	N	O	S	0	0
			2286	1390	449	436	11		
23	1D	54	Total	C	N	O	S	0	0
			464	285	91	85	3		
23	1E	362	Total	C	N	O	S	0	0
			3050	1855	590	590	15		
23	1C	195	Total	C	N	O	S	0	0
			1667	1015	321	322	9		
23	1G	74	Total	C	N	O	S	0	0
			635	387	120	124	4		
23	1F	362	Total	C	N	O	S	0	0
			3050	1855	590	590	15		
23	1B	348	Total	C	N	O	S	0	0
			2953	1796	574	568	15		

- Molecule 24 is a protein called RIB72A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1H	588	Total 4698	C 2967	N 812	O 900	S 19	0	0
24	1I	659	Total 5276	C 3326	N 920	O 1003	S 27	0	0
24	1J	670	Total 5356	C 3372	N 940	O 1018	S 26	0	0
24	1K	588	Total 4697	C 2966	N 812	O 900	S 19	0	0
24	1L	659	Total 5276	C 3326	N 920	O 1003	S 27	0	0
24	1M	670	Total 5356	C 3372	N 940	O 1018	S 26	0	0
24	1N	588	Total 4697	C 2966	N 812	O 900	S 19	0	0

- Molecule 25 is a protein called RIB72B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1O	710	Total 5751	C 3614	N 1021	O 1096	S 20	0	0
25	1P	710	Total 5751	C 3614	N 1021	O 1096	S 20	0	0

- Molecule 26 is a protein called RIB72C.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1Q	655	Total 5263	C 3323	N 927	O 988	S 25	0	0
26	1R	655	Total 5263	C 3323	N 927	O 988	S 25	0	0

- Molecule 27 is a protein called RIB72D.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1S	726	Total 5834	C 3696	N 1029	O 1076	S 33	0	0
27	1T	726	Total 5834	C 3696	N 1029	O 1076	S 33	0	0
27	9E	222	Total 1787	C 1125	N 315	O 335	S 12	0	0

- Molecule 28 is a protein called STOP family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1U	120	Total	C	N	O	S	0	0
			942	594	162	181	5		
28	1V	168	Total	C	N	O	S	0	0
			1313	823	230	250	10		
28	1X	120	Total	C	N	O	S	0	0
			942	594	162	181	5		
28	1a	57	Total	C	N	O	S	0	0
			446	279	80	84	3		
28	1b	168	Total	C	N	O	S	0	0
			1313	823	230	250	10		
28	1d	120	Total	C	N	O	S	0	0
			942	594	162	181	5		
28	1e	168	Total	C	N	O	S	0	0
			1313	823	230	250	10		
28	1g	120	Total	C	N	O	S	0	0
			942	594	162	181	5		
28	4V	62	Total	C	N	O	S	0	0
			486	305	86	91	4		
28	1W	48	Total	C	N	O	S	0	0
			371	229	68	69	5		
28	1Z	169	Total	C	N	O	S	0	0
			1325	829	237	252	7		
28	1c	168	Total	C	N	O	S	0	0
			1313	823	230	250	10		
28	9F	35	Total	C	N	O	S	0	0
			263	162	50	46	5		
28	1f	48	Total	C	N	O	S	0	0
			371	229	68	69	5		
28	1i	155	Total	C	N	O	S	0	0
			1218	767	214	230	7		
28	4X	188	Total	C	N	O	S	0	0
			1474	927	255	283	9		
28	4W	222	Total	C	N	O	S	0	0
			1742	1095	304	332	11		
28	1Y	241	Total	C	N	O	S	0	0
			1893	1188	334	360	11		
28	1h	229	Total	C	N	O	S	0	0
			1798	1132	313	342	11		

There are 342 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1U	52	LEU	ILE	conflict	UNP A0A504XB09
1U	83	GLU	ASP	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1U	86	GLN	LYS	conflict	UNP A0A504XB09
1U	128	ALA	THR	conflict	UNP A0A504XB09
1U	139	ARG	PRO	conflict	UNP A0A504XB09
1U	171	THR	ALA	conflict	UNP A0A504XB09
1U	186	ASN	SER	conflict	UNP A0A504XB09
1U	192	PRO	GLN	conflict	UNP A0A504XB09
1U	206	THR	VAL	conflict	UNP A0A504XB09
1U	207	LYS	GLN	conflict	UNP A0A504XB09
1U	209	ILE	VAL	conflict	UNP A0A504XB09
1U	220	ALA	THR	conflict	UNP A0A504XB09
1U	221	SER	VAL	conflict	UNP A0A504XB09
1U	223	SER	GLU	conflict	UNP A0A504XB09
1U	230	VAL	MET	conflict	UNP A0A504XB09
1U	239	THR	ALA	conflict	UNP A0A504XB09
1U	243	ILE	THR	conflict	UNP A0A504XB09
1U	252	ILE	LEU	conflict	UNP A0A504XB09
1V	52	LEU	ILE	conflict	UNP A0A504XB09
1V	83	GLU	ASP	conflict	UNP A0A504XB09
1V	86	GLN	LYS	conflict	UNP A0A504XB09
1V	128	ALA	THR	conflict	UNP A0A504XB09
1V	139	ARG	PRO	conflict	UNP A0A504XB09
1V	171	THR	ALA	conflict	UNP A0A504XB09
1V	186	ASN	SER	conflict	UNP A0A504XB09
1V	192	PRO	GLN	conflict	UNP A0A504XB09
1V	206	THR	VAL	conflict	UNP A0A504XB09
1V	207	LYS	GLN	conflict	UNP A0A504XB09
1V	209	ILE	VAL	conflict	UNP A0A504XB09
1V	220	ALA	THR	conflict	UNP A0A504XB09
1V	221	SER	VAL	conflict	UNP A0A504XB09
1V	223	SER	GLU	conflict	UNP A0A504XB09
1V	230	VAL	MET	conflict	UNP A0A504XB09
1V	239	THR	ALA	conflict	UNP A0A504XB09
1V	243	ILE	THR	conflict	UNP A0A504XB09
1V	252	ILE	LEU	conflict	UNP A0A504XB09
1X	52	LEU	ILE	conflict	UNP A0A504XB09
1X	83	GLU	ASP	conflict	UNP A0A504XB09
1X	86	GLN	LYS	conflict	UNP A0A504XB09
1X	128	ALA	THR	conflict	UNP A0A504XB09
1X	139	ARG	PRO	conflict	UNP A0A504XB09
1X	171	THR	ALA	conflict	UNP A0A504XB09
1X	186	ASN	SER	conflict	UNP A0A504XB09
1X	192	PRO	GLN	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1X	206	THR	VAL	conflict	UNP A0A504XB09
1X	207	LYS	GLN	conflict	UNP A0A504XB09
1X	209	ILE	VAL	conflict	UNP A0A504XB09
1X	220	ALA	THR	conflict	UNP A0A504XB09
1X	221	SER	VAL	conflict	UNP A0A504XB09
1X	223	SER	GLU	conflict	UNP A0A504XB09
1X	230	VAL	MET	conflict	UNP A0A504XB09
1X	239	THR	ALA	conflict	UNP A0A504XB09
1X	243	ILE	THR	conflict	UNP A0A504XB09
1X	252	ILE	LEU	conflict	UNP A0A504XB09
1a	52	LEU	ILE	conflict	UNP A0A504XB09
1a	83	GLU	ASP	conflict	UNP A0A504XB09
1a	86	GLN	LYS	conflict	UNP A0A504XB09
1a	128	ALA	THR	conflict	UNP A0A504XB09
1a	139	ARG	PRO	conflict	UNP A0A504XB09
1a	171	THR	ALA	conflict	UNP A0A504XB09
1a	186	ASN	SER	conflict	UNP A0A504XB09
1a	192	PRO	GLN	conflict	UNP A0A504XB09
1a	206	THR	VAL	conflict	UNP A0A504XB09
1a	207	LYS	GLN	conflict	UNP A0A504XB09
1a	209	ILE	VAL	conflict	UNP A0A504XB09
1a	220	ALA	THR	conflict	UNP A0A504XB09
1a	221	SER	VAL	conflict	UNP A0A504XB09
1a	223	SER	GLU	conflict	UNP A0A504XB09
1a	230	VAL	MET	conflict	UNP A0A504XB09
1a	239	THR	ALA	conflict	UNP A0A504XB09
1a	243	ILE	THR	conflict	UNP A0A504XB09
1a	252	ILE	LEU	conflict	UNP A0A504XB09
1b	52	LEU	ILE	conflict	UNP A0A504XB09
1b	83	GLU	ASP	conflict	UNP A0A504XB09
1b	86	GLN	LYS	conflict	UNP A0A504XB09
1b	128	ALA	THR	conflict	UNP A0A504XB09
1b	139	ARG	PRO	conflict	UNP A0A504XB09
1b	171	THR	ALA	conflict	UNP A0A504XB09
1b	186	ASN	SER	conflict	UNP A0A504XB09
1b	192	PRO	GLN	conflict	UNP A0A504XB09
1b	206	THR	VAL	conflict	UNP A0A504XB09
1b	207	LYS	GLN	conflict	UNP A0A504XB09
1b	209	ILE	VAL	conflict	UNP A0A504XB09
1b	220	ALA	THR	conflict	UNP A0A504XB09
1b	221	SER	VAL	conflict	UNP A0A504XB09
1b	223	SER	GLU	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1b	230	VAL	MET	conflict	UNP A0A504XB09
1b	239	THR	ALA	conflict	UNP A0A504XB09
1b	243	ILE	THR	conflict	UNP A0A504XB09
1b	252	ILE	LEU	conflict	UNP A0A504XB09
1d	52	LEU	ILE	conflict	UNP A0A504XB09
1d	83	GLU	ASP	conflict	UNP A0A504XB09
1d	86	GLN	LYS	conflict	UNP A0A504XB09
1d	128	ALA	THR	conflict	UNP A0A504XB09
1d	139	ARG	PRO	conflict	UNP A0A504XB09
1d	171	THR	ALA	conflict	UNP A0A504XB09
1d	186	ASN	SER	conflict	UNP A0A504XB09
1d	192	PRO	GLN	conflict	UNP A0A504XB09
1d	206	THR	VAL	conflict	UNP A0A504XB09
1d	207	LYS	GLN	conflict	UNP A0A504XB09
1d	209	ILE	VAL	conflict	UNP A0A504XB09
1d	220	ALA	THR	conflict	UNP A0A504XB09
1d	221	SER	VAL	conflict	UNP A0A504XB09
1d	223	SER	GLU	conflict	UNP A0A504XB09
1d	230	VAL	MET	conflict	UNP A0A504XB09
1d	239	THR	ALA	conflict	UNP A0A504XB09
1d	243	ILE	THR	conflict	UNP A0A504XB09
1d	252	ILE	LEU	conflict	UNP A0A504XB09
1e	52	LEU	ILE	conflict	UNP A0A504XB09
1e	83	GLU	ASP	conflict	UNP A0A504XB09
1e	86	GLN	LYS	conflict	UNP A0A504XB09
1e	128	ALA	THR	conflict	UNP A0A504XB09
1e	139	ARG	PRO	conflict	UNP A0A504XB09
1e	171	THR	ALA	conflict	UNP A0A504XB09
1e	186	ASN	SER	conflict	UNP A0A504XB09
1e	192	PRO	GLN	conflict	UNP A0A504XB09
1e	206	THR	VAL	conflict	UNP A0A504XB09
1e	207	LYS	GLN	conflict	UNP A0A504XB09
1e	209	ILE	VAL	conflict	UNP A0A504XB09
1e	220	ALA	THR	conflict	UNP A0A504XB09
1e	221	SER	VAL	conflict	UNP A0A504XB09
1e	223	SER	GLU	conflict	UNP A0A504XB09
1e	230	VAL	MET	conflict	UNP A0A504XB09
1e	239	THR	ALA	conflict	UNP A0A504XB09
1e	243	ILE	THR	conflict	UNP A0A504XB09
1e	252	ILE	LEU	conflict	UNP A0A504XB09
1g	52	LEU	ILE	conflict	UNP A0A504XB09
1g	83	GLU	ASP	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1g	86	GLN	LYS	conflict	UNP A0A504XB09
1g	128	ALA	THR	conflict	UNP A0A504XB09
1g	139	ARG	PRO	conflict	UNP A0A504XB09
1g	171	THR	ALA	conflict	UNP A0A504XB09
1g	186	ASN	SER	conflict	UNP A0A504XB09
1g	192	PRO	GLN	conflict	UNP A0A504XB09
1g	206	THR	VAL	conflict	UNP A0A504XB09
1g	207	LYS	GLN	conflict	UNP A0A504XB09
1g	209	ILE	VAL	conflict	UNP A0A504XB09
1g	220	ALA	THR	conflict	UNP A0A504XB09
1g	221	SER	VAL	conflict	UNP A0A504XB09
1g	223	SER	GLU	conflict	UNP A0A504XB09
1g	230	VAL	MET	conflict	UNP A0A504XB09
1g	239	THR	ALA	conflict	UNP A0A504XB09
1g	243	ILE	THR	conflict	UNP A0A504XB09
1g	252	ILE	LEU	conflict	UNP A0A504XB09
4V	52	LEU	ILE	conflict	UNP A0A504XB09
4V	83	GLU	ASP	conflict	UNP A0A504XB09
4V	86	GLN	LYS	conflict	UNP A0A504XB09
4V	128	ALA	THR	conflict	UNP A0A504XB09
4V	139	ARG	PRO	conflict	UNP A0A504XB09
4V	171	THR	ALA	conflict	UNP A0A504XB09
4V	186	ASN	SER	conflict	UNP A0A504XB09
4V	192	PRO	GLN	conflict	UNP A0A504XB09
4V	206	THR	VAL	conflict	UNP A0A504XB09
4V	207	LYS	GLN	conflict	UNP A0A504XB09
4V	209	ILE	VAL	conflict	UNP A0A504XB09
4V	220	ALA	THR	conflict	UNP A0A504XB09
4V	221	SER	VAL	conflict	UNP A0A504XB09
4V	223	SER	GLU	conflict	UNP A0A504XB09
4V	230	VAL	MET	conflict	UNP A0A504XB09
4V	239	THR	ALA	conflict	UNP A0A504XB09
4V	243	ILE	THR	conflict	UNP A0A504XB09
4V	252	ILE	LEU	conflict	UNP A0A504XB09
1W	52	LEU	ILE	conflict	UNP A0A504XB09
1W	83	GLU	ASP	conflict	UNP A0A504XB09
1W	86	GLN	LYS	conflict	UNP A0A504XB09
1W	128	ALA	THR	conflict	UNP A0A504XB09
1W	139	ARG	PRO	conflict	UNP A0A504XB09
1W	171	THR	ALA	conflict	UNP A0A504XB09
1W	186	ASN	SER	conflict	UNP A0A504XB09
1W	192	PRO	GLN	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1W	206	THR	VAL	conflict	UNP A0A504XB09
1W	207	LYS	GLN	conflict	UNP A0A504XB09
1W	209	ILE	VAL	conflict	UNP A0A504XB09
1W	220	ALA	THR	conflict	UNP A0A504XB09
1W	221	SER	VAL	conflict	UNP A0A504XB09
1W	223	SER	GLU	conflict	UNP A0A504XB09
1W	230	VAL	MET	conflict	UNP A0A504XB09
1W	239	THR	ALA	conflict	UNP A0A504XB09
1W	243	ILE	THR	conflict	UNP A0A504XB09
1W	252	ILE	LEU	conflict	UNP A0A504XB09
1Z	52	LEU	ILE	conflict	UNP A0A504XB09
1Z	83	GLU	ASP	conflict	UNP A0A504XB09
1Z	86	GLN	LYS	conflict	UNP A0A504XB09
1Z	128	ALA	THR	conflict	UNP A0A504XB09
1Z	139	ARG	PRO	conflict	UNP A0A504XB09
1Z	171	THR	ALA	conflict	UNP A0A504XB09
1Z	186	ASN	SER	conflict	UNP A0A504XB09
1Z	192	PRO	GLN	conflict	UNP A0A504XB09
1Z	206	THR	VAL	conflict	UNP A0A504XB09
1Z	207	LYS	GLN	conflict	UNP A0A504XB09
1Z	209	ILE	VAL	conflict	UNP A0A504XB09
1Z	220	ALA	THR	conflict	UNP A0A504XB09
1Z	221	SER	VAL	conflict	UNP A0A504XB09
1Z	223	SER	GLU	conflict	UNP A0A504XB09
1Z	230	VAL	MET	conflict	UNP A0A504XB09
1Z	239	THR	ALA	conflict	UNP A0A504XB09
1Z	243	ILE	THR	conflict	UNP A0A504XB09
1Z	252	ILE	LEU	conflict	UNP A0A504XB09
1c	52	LEU	ILE	conflict	UNP A0A504XB09
1c	83	GLU	ASP	conflict	UNP A0A504XB09
1c	86	GLN	LYS	conflict	UNP A0A504XB09
1c	128	ALA	THR	conflict	UNP A0A504XB09
1c	139	ARG	PRO	conflict	UNP A0A504XB09
1c	171	THR	ALA	conflict	UNP A0A504XB09
1c	186	ASN	SER	conflict	UNP A0A504XB09
1c	192	PRO	GLN	conflict	UNP A0A504XB09
1c	206	THR	VAL	conflict	UNP A0A504XB09
1c	207	LYS	GLN	conflict	UNP A0A504XB09
1c	209	ILE	VAL	conflict	UNP A0A504XB09
1c	220	ALA	THR	conflict	UNP A0A504XB09
1c	221	SER	VAL	conflict	UNP A0A504XB09
1c	223	SER	GLU	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1c	230	VAL	MET	conflict	UNP A0A504XB09
1c	239	THR	ALA	conflict	UNP A0A504XB09
1c	243	ILE	THR	conflict	UNP A0A504XB09
1c	252	ILE	LEU	conflict	UNP A0A504XB09
9F	52	LEU	ILE	conflict	UNP A0A504XB09
9F	83	GLU	ASP	conflict	UNP A0A504XB09
9F	86	GLN	LYS	conflict	UNP A0A504XB09
9F	128	ALA	THR	conflict	UNP A0A504XB09
9F	139	ARG	PRO	conflict	UNP A0A504XB09
9F	171	THR	ALA	conflict	UNP A0A504XB09
9F	186	ASN	SER	conflict	UNP A0A504XB09
9F	192	PRO	GLN	conflict	UNP A0A504XB09
9F	206	THR	VAL	conflict	UNP A0A504XB09
9F	207	LYS	GLN	conflict	UNP A0A504XB09
9F	209	ILE	VAL	conflict	UNP A0A504XB09
9F	220	ALA	THR	conflict	UNP A0A504XB09
9F	221	SER	VAL	conflict	UNP A0A504XB09
9F	223	SER	GLU	conflict	UNP A0A504XB09
9F	230	VAL	MET	conflict	UNP A0A504XB09
9F	239	THR	ALA	conflict	UNP A0A504XB09
9F	243	ILE	THR	conflict	UNP A0A504XB09
9F	252	ILE	LEU	conflict	UNP A0A504XB09
1f	52	LEU	ILE	conflict	UNP A0A504XB09
1f	83	GLU	ASP	conflict	UNP A0A504XB09
1f	86	GLN	LYS	conflict	UNP A0A504XB09
1f	128	ALA	THR	conflict	UNP A0A504XB09
1f	139	ARG	PRO	conflict	UNP A0A504XB09
1f	171	THR	ALA	conflict	UNP A0A504XB09
1f	186	ASN	SER	conflict	UNP A0A504XB09
1f	192	PRO	GLN	conflict	UNP A0A504XB09
1f	206	THR	VAL	conflict	UNP A0A504XB09
1f	207	LYS	GLN	conflict	UNP A0A504XB09
1f	209	ILE	VAL	conflict	UNP A0A504XB09
1f	220	ALA	THR	conflict	UNP A0A504XB09
1f	221	SER	VAL	conflict	UNP A0A504XB09
1f	223	SER	GLU	conflict	UNP A0A504XB09
1f	230	VAL	MET	conflict	UNP A0A504XB09
1f	239	THR	ALA	conflict	UNP A0A504XB09
1f	243	ILE	THR	conflict	UNP A0A504XB09
1f	252	ILE	LEU	conflict	UNP A0A504XB09
1i	52	LEU	ILE	conflict	UNP A0A504XB09
1i	83	GLU	ASP	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1i	86	GLN	LYS	conflict	UNP A0A504XB09
1i	128	ALA	THR	conflict	UNP A0A504XB09
1i	139	ARG	PRO	conflict	UNP A0A504XB09
1i	171	THR	ALA	conflict	UNP A0A504XB09
1i	186	ASN	SER	conflict	UNP A0A504XB09
1i	192	PRO	GLN	conflict	UNP A0A504XB09
1i	206	THR	VAL	conflict	UNP A0A504XB09
1i	207	LYS	GLN	conflict	UNP A0A504XB09
1i	209	ILE	VAL	conflict	UNP A0A504XB09
1i	220	ALA	THR	conflict	UNP A0A504XB09
1i	221	SER	VAL	conflict	UNP A0A504XB09
1i	223	SER	GLU	conflict	UNP A0A504XB09
1i	230	VAL	MET	conflict	UNP A0A504XB09
1i	239	THR	ALA	conflict	UNP A0A504XB09
1i	243	ILE	THR	conflict	UNP A0A504XB09
1i	252	ILE	LEU	conflict	UNP A0A504XB09
4X	52	LEU	ILE	conflict	UNP A0A504XB09
4X	83	GLU	ASP	conflict	UNP A0A504XB09
4X	86	GLN	LYS	conflict	UNP A0A504XB09
4X	128	ALA	THR	conflict	UNP A0A504XB09
4X	139	ARG	PRO	conflict	UNP A0A504XB09
4X	171	THR	ALA	conflict	UNP A0A504XB09
4X	186	ASN	SER	conflict	UNP A0A504XB09
4X	192	PRO	GLN	conflict	UNP A0A504XB09
4X	206	THR	VAL	conflict	UNP A0A504XB09
4X	207	LYS	GLN	conflict	UNP A0A504XB09
4X	209	ILE	VAL	conflict	UNP A0A504XB09
4X	220	ALA	THR	conflict	UNP A0A504XB09
4X	221	SER	VAL	conflict	UNP A0A504XB09
4X	223	SER	GLU	conflict	UNP A0A504XB09
4X	230	VAL	MET	conflict	UNP A0A504XB09
4X	239	THR	ALA	conflict	UNP A0A504XB09
4X	243	ILE	THR	conflict	UNP A0A504XB09
4X	252	ILE	LEU	conflict	UNP A0A504XB09
4W	52	LEU	ILE	conflict	UNP A0A504XB09
4W	83	GLU	ASP	conflict	UNP A0A504XB09
4W	86	GLN	LYS	conflict	UNP A0A504XB09
4W	128	ALA	THR	conflict	UNP A0A504XB09
4W	139	ARG	PRO	conflict	UNP A0A504XB09
4W	171	THR	ALA	conflict	UNP A0A504XB09
4W	186	ASN	SER	conflict	UNP A0A504XB09
4W	192	PRO	GLN	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
4W	206	THR	VAL	conflict	UNP A0A504XB09
4W	207	LYS	GLN	conflict	UNP A0A504XB09
4W	209	ILE	VAL	conflict	UNP A0A504XB09
4W	220	ALA	THR	conflict	UNP A0A504XB09
4W	221	SER	VAL	conflict	UNP A0A504XB09
4W	223	SER	GLU	conflict	UNP A0A504XB09
4W	230	VAL	MET	conflict	UNP A0A504XB09
4W	239	THR	ALA	conflict	UNP A0A504XB09
4W	243	ILE	THR	conflict	UNP A0A504XB09
4W	252	ILE	LEU	conflict	UNP A0A504XB09
1Y	52	LEU	ILE	conflict	UNP A0A504XB09
1Y	83	GLU	ASP	conflict	UNP A0A504XB09
1Y	86	GLN	LYS	conflict	UNP A0A504XB09
1Y	128	ALA	THR	conflict	UNP A0A504XB09
1Y	139	ARG	PRO	conflict	UNP A0A504XB09
1Y	171	THR	ALA	conflict	UNP A0A504XB09
1Y	186	ASN	SER	conflict	UNP A0A504XB09
1Y	192	PRO	GLN	conflict	UNP A0A504XB09
1Y	206	THR	VAL	conflict	UNP A0A504XB09
1Y	207	LYS	GLN	conflict	UNP A0A504XB09
1Y	209	ILE	VAL	conflict	UNP A0A504XB09
1Y	220	ALA	THR	conflict	UNP A0A504XB09
1Y	221	SER	VAL	conflict	UNP A0A504XB09
1Y	223	SER	GLU	conflict	UNP A0A504XB09
1Y	230	VAL	MET	conflict	UNP A0A504XB09
1Y	239	THR	ALA	conflict	UNP A0A504XB09
1Y	243	ILE	THR	conflict	UNP A0A504XB09
1Y	252	ILE	LEU	conflict	UNP A0A504XB09
1h	52	LEU	ILE	conflict	UNP A0A504XB09
1h	83	GLU	ASP	conflict	UNP A0A504XB09
1h	86	GLN	LYS	conflict	UNP A0A504XB09
1h	128	ALA	THR	conflict	UNP A0A504XB09
1h	139	ARG	PRO	conflict	UNP A0A504XB09
1h	171	THR	ALA	conflict	UNP A0A504XB09
1h	186	ASN	SER	conflict	UNP A0A504XB09
1h	192	PRO	GLN	conflict	UNP A0A504XB09
1h	206	THR	VAL	conflict	UNP A0A504XB09
1h	207	LYS	GLN	conflict	UNP A0A504XB09
1h	209	ILE	VAL	conflict	UNP A0A504XB09
1h	220	ALA	THR	conflict	UNP A0A504XB09
1h	221	SER	VAL	conflict	UNP A0A504XB09
1h	223	SER	GLU	conflict	UNP A0A504XB09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1h	230	VAL	MET	conflict	UNP A0A504XB09
1h	239	THR	ALA	conflict	UNP A0A504XB09
1h	243	ILE	THR	conflict	UNP A0A504XB09
1h	252	ILE	LEU	conflict	UNP A0A504XB09

- Molecule 29 is a protein called DMIP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1j	113	Total	C	N	O	S	0	0
			909	584	153	168	4		
29	1k	103	Total	C	N	O	S	0	0
			801	502	140	157	2		
29	1l	113	Total	C	N	O	S	0	0
			909	584	153	168	4		
29	1m	103	Total	C	N	O	S	0	0
			801	502	140	157	2		
29	1n	113	Total	C	N	O	S	0	0
			909	584	153	168	4		
29	9G	53	Total	C	N	O	S	0	0
			420	268	72	78	2		

- Molecule 30 is a protein called DMIP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1o	128	Total	C	N	O	S	0	0
			1035	645	193	192	5		
30	1p	128	Total	C	N	O	S	0	0
			1035	645	193	192	5		

- Molecule 31 is a protein called DMIP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1q	214	Total	C	N	O	S	0	0
			1679	1025	322	321	11		
31	1r	106	Total	C	N	O	S	0	0
			868	532	166	165	5		
31	1s	183	Total	C	N	O	S	0	0
			1446	884	273	277	12		
31	1t	214	Total	C	N	O	S	0	0
			1679	1025	322	321	11		
31	1u	106	Total	C	N	O	S	0	0
			868	532	166	165	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1v	183	Total	C	N	O	S	0	0
			1446	884	273	277	12		
31	9H	75	Total	C	N	O	S	0	0
			618	372	125	116	5		

- Molecule 32 is a protein called DMIP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2B	251	Total	C	N	O	S	0	0
			1977	1231	357	377	12		
32	2C	230	Total	C	N	O	S	0	0
			1814	1130	329	344	11		
32	2D	251	Total	C	N	O	S	0	0
			1977	1231	357	377	12		
32	2E	230	Total	C	N	O	S	0	0
			1814	1130	329	344	11		

- Molecule 33 is a protein called DMIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2F	284	Total	C	N	O	S	0	0
			2253	1411	411	418	13		
33	2G	283	Total	C	N	O	S	0	0
			2245	1407	409	416	13		
33	2H	288	Total	C	N	O	S	0	0
			2281	1428	416	424	13		
33	2I	243	Total	C	N	O	S	0	0
			1937	1208	355	363	11		
33	2J	283	Total	C	N	O	S	0	0
			2245	1407	409	416	13		
33	2K	288	Total	C	N	O	S	0	0
			2281	1428	416	424	13		
33	9I	243	Total	C	N	O	S	0	0
			1937	1208	355	363	11		

- Molecule 34 is a protein called DMIP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2L	172	Total	C	N	O	S	0	0
			1433	904	254	269	6		
34	2M	172	Total	C	N	O	S	0	0
			1433	904	254	269	6		

- Molecule 35 is a protein called DMIP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2N	135	Total	C	N	O	S	0	0
			1103	698	208	194	3		
35	2P	161	Total	C	N	O	S	0	0
			1324	827	251	240	6		
35	2O	274	Total	C	N	O	S	0	0
			2235	1404	420	402	9		

- Molecule 36 is a protein called DMIP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2Q	291	Total	C	N	O	S	0	0
			2320	1483	394	429	14		
36	2R	291	Total	C	N	O	S	0	0
			2320	1483	394	429	14		

- Molecule 37 is a protein called DMIP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2S	237	Total	C	N	O	S	0	0
			1798	1126	317	340	15		

- Molecule 38 is a protein called DMIP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2U	229	Total	C	N	O	S	0	0
			1807	1111	329	355	12		
38	2V	109	Total	C	N	O	S	0	0
			870	530	167	169	4		
38	2W	109	Total	C	N	O	S	0	0
			870	530	167	169	4		

- Molecule 39 is a protein called DMIP13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	2X	227	Total	C	N	O	S	0	0
			1774	1081	355	328	10		
39	2Y	227	Total	C	N	O	S	0	0
			1774	1081	355	328	10		

- Molecule 40 is a protein called DMIP14.

Mol	Chain	Residues	Atoms	AltConf	Trace
40	2Z	283	Total C N O S 2258 1427 412 414 5	0	0
40	2a	283	Total C N O S 2258 1427 412 414 5	0	0

- Molecule 41 is a protein called DMIP15.

Mol	Chain	Residues	Atoms	AltConf	Trace
41	2b	121	Total C N O S 1006 613 195 194 4	0	0
41	2e	325	Total C N O S 2735 1649 546 526 14	0	0
41	2h	237	Total C N O S 1978 1187 396 385 10	0	0
41	2k	167	Total C N O S 1369 834 266 262 7	0	0
41	2n	42	Total C N O 361 219 72 70	0	0
41	2o	287	Total C N O S 2453 1473 490 478 12	0	0
41	2d	245	Total C N O S 2092 1254 418 408 12	0	0
41	2f	325	Total C N O S 2735 1649 546 526 14	0	0
41	2g	52	Total C N O S 454 275 89 88 2	0	0
41	2j	149	Total C N O S 1301 776 266 252 7	0	0
41	2m	264	Total C N O S 2228 1338 445 432 13	0	0
41	2p	287	Total C N O S 2453 1473 490 478 12	0	0
41	2q	49	Total C N O S 425 257 86 80 2	0	0
41	2c	306	Total C N O S 2599 1565 519 502 13	0	0
41	2i	309	Total C N O S 2615 1574 523 505 13	0	0
41	2l	325	Total C N O S 2735 1649 546 526 14	0	0

- Molecule 42 is a protein called DMIP16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	2r	315	Total	C	N	O	S	0	0
			2473	1564	439	460	10		
42	2s	315	Total	C	N	O	S	0	0
			2473	1564	439	460	10		

- Molecule 43 is a protein called DMIP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	2t	214	Total	C	N	O	S	0	0
			1713	1075	302	324	12		
43	2u	214	Total	C	N	O	S	0	0
			1713	1075	302	324	12		

- Molecule 44 is a protein called DMIP18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2v	280	Total	C	N	O	S	0	0
			2264	1438	391	425	10		
44	2w	412	Total	C	N	O	S	0	0
			3291	2082	565	629	15		
44	2x	412	Total	C	N	O	S	0	0
			3291	2082	565	629	15		

- Molecule 45 is a protein called DMIP19.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2y	287	Total	C	N	O	S	0	0
			2316	1424	424	460	8		
45	3A	187	Total	C	N	O	S	0	0
			1435	890	257	287	1		
45	2z	409	Total	C	N	O	S	0	0
			3258	2010	596	644	8		

- Molecule 46 is a protein called DMIP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3B	418	Total	C	N	O	S	0	0
			3308	2069	596	631	12		
46	3C	418	Total	C	N	O	S	0	0
			3308	2069	596	631	12		

- Molecule 47 is a protein called DMIP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3D	412	Total	C	N	O	S	0	0
			3212	1986	586	628	12		
47	3E	412	Total	C	N	O	S	0	0
			3212	1986	586	628	12		

- Molecule 48 is a protein called DMIP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3I	80	Total	C	N	O	S	0	0
			640	400	114	122	4		
48	3F	155	Total	C	N	O	S	0	0
			1254	777	240	230	7		
48	3G	90	Total	C	N	O	S	0	0
			733	456	139	134	4		
48	3H	103	Total	C	N	O	S	0	0
			832	516	161	151	4		
48	3M	29	Total	C	N	O	S	0	0
			247	155	44	45	3		
48	3L	29	Total	C	N	O	S	0	0
			247	155	44	45	3		
48	9J	80	Total	C	N	O	S	0	0
			640	400	114	122	4		
48	3J	90	Total	C	N	O	S	0	0
			733	456	139	134	4		
48	3K	103	Total	C	N	O	S	0	0
			832	516	161	151	4		
48	3O	29	Total	C	N	O	S	0	0
			247	155	44	45	3		
48	3N	29	Total	C	N	O	S	0	0
			247	155	44	45	3		

- Molecule 49 is a protein called DMIP23.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3P	256	Total	C	N	O	S	0	0
			2002	1260	351	380	11		
49	3Q	490	Total	C	N	O	S	0	0
			3825	2406	666	735	18		
49	3R	490	Total	C	N	O	S	0	0
			3825	2406	666	735	18		

- Molecule 50 is a protein called DMIP24.

Mol	Chain	Residues	Atoms	AltConf	Trace
50	3S	25	Total C N O S 182 109 36 33 4	0	0
50	X1	39	Total C N O 304 183 58 63	0	0
50	3T	64	Total C N O S 486 292 94 96 4	0	0

- Molecule 51 is a protein called DMIP25.

Mol	Chain	Residues	Atoms	AltConf	Trace
51	3U	140	Total C N O S 1074 681 186 203 4	0	0
51	3V	140	Total C N O S 1074 681 186 203 4	0	0

- Molecule 52 is a protein called DMIP26.

Mol	Chain	Residues	Atoms	AltConf	Trace
52	3X	202	Total C N O S 1650 1025 305 309 11	0	0
52	3W	153	Total C N O S 1264 786 231 239 8	0	0
52	3Y	49	Total C N O S 386 239 74 70 3	0	0

- Molecule 53 is a protein called DMIP27.

Mol	Chain	Residues	Atoms	AltConf	Trace
53	3Z	181	Total C N O S 1405 862 264 271 8	0	0
53	3a	87	Total C N O S 712 442 130 136 4	0	0
53	4Y	181	Total C N O S 1403 860 264 271 8	0	0

- Molecule 54 is a protein called ArcMAP2.

Mol	Chain	Residues	Atoms	AltConf	Trace
54	3b	136	Total C N O S 1126 695 204 223 4	0	0
54	3c	136	Total C N O S 1126 695 204 223 4	0	0

- Molecule 55 is a protein called ArcMAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3d	148	Total	C	N	O	S	0	0
			1240	765	229	240	6		
55	3e	148	Total	C	N	O	S	0	0
			1240	765	229	240	6		

- Molecule 56 is a protein called ArcMAP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3f	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3g	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3h	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3i	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3j	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3k	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3l	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		

- Molecule 57 is a protein called ArcMAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	3m	144	Total	C	N	O	S	0	0
			1216	745	236	231	4		
57	3n	144	Total	C	N	O	S	0	0
			1216	745	236	231	4		

- Molecule 58 is a protein called CFAP96.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	3o	55	Total	C	N	O	S	0	0
			459	293	79	85	2		
58	3p	161	Total	C	N	O	S	0	0
			1276	821	220	233	2		
58	4O	175	Total	C	N	O	S	0	0
			1399	899	245	253	2		
58	4a	154	Total	C	N	O	S	0	0
			1233	796	213	223	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
58	3q	148	Total C N O S 1159 744 201 212 2	0	0
58	4Q	69	Total C N O S 529 346 84 98 1	0	0
58	4c	69	Total C N O S 529 346 84 98 1	0	0
58	4P	215	Total C N O S 1707 1103 290 311 3	0	0
58	4b	194	Total C N O S 1541 1000 258 281 2	0	0

- Molecule 59 is a protein called CFAP97.

Mol	Chain	Residues	Atoms	AltConf	Trace
59	3r	130	Total C N O S 1098 668 221 205 4	0	0
59	3s	130	Total C N O S 1098 668 221 205 4	0	0
59	3t	130	Total C N O S 1098 668 221 205 4	0	0
59	3u	130	Total C N O S 1098 668 221 205 4	0	0
59	3v	63	Total C N O S 533 326 105 98 4	0	0

- Molecule 60 is a protein called DMAP1.

Mol	Chain	Residues	Atoms	AltConf	Trace
60	3w	166	Total C N O S 1362 872 235 249 6	0	0
60	3y	126	Total C N O S 985 625 178 181 1	0	0
60	3x	267	Total C N O S 2165 1380 381 397 7	0	0

- Molecule 61 is a protein called DMAP2.

Mol	Chain	Residues	Atoms	AltConf	Trace
61	4A	29	Total C N O S 229 142 43 43 1	0	0
61	4B	201	Total C N O S 1584 1003 275 302 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4C	201	Total	C	N	O	S	0	0
			1584	1003	275	302	4		

- Molecule 62 is a protein called distal DC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	5B	393	Total	C	N	O	S	0	0
			3140	1922	594	613	11		
62	5C	393	Total	C	N	O	S	0	0
			3140	1922	594	613	11		
62	5D	393	Total	C	N	O	S	0	0
			3140	1922	594	613	11		
62	5E	168	Total	C	N	O	S	0	0
			1348	828	258	257	5		
62	5A	225	Total	C	N	O	S	0	0
			1792	1094	336	356	6		

- Molecule 63 is a protein called ODAD1 central coiled coil region domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5G	444	Total	C	N	O	S	0	0
			3594	2191	674	710	19		
63	5H	444	Total	C	N	O	S	0	0
			3594	2191	674	710	19		
63	5I	444	Total	C	N	O	S	0	0
			3594	2191	674	710	19		
63	5J	185	Total	C	N	O	S	0	0
			1541	942	295	296	8		
63	5F	259	Total	C	N	O	S	0	0
			2053	1249	379	414	11		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5G	273	PHE	SER	conflict	UNP A0A640KPU2
5H	273	PHE	SER	conflict	UNP A0A640KPU2
5I	273	PHE	SER	conflict	UNP A0A640KPU2
5J	273	PHE	SER	conflict	UNP A0A640KPU2
5F	273	PHE	SER	conflict	UNP A0A640KPU2

- Molecule 64 is a protein called ODA dDC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	5K	384	Total	C	N	O	S	0	0
			3128	1989	546	572	21		
64	5L	384	Total	C	N	O	S	0	0
			3128	1989	546	572	21		
64	5M	384	Total	C	N	O	S	0	0
			3128	1989	546	572	21		
64	5N	384	Total	C	N	O	S	0	0
			3128	1989	546	572	21		

- Molecule 65 is a protein called DC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	5O	107	Total	C	N	O	S	0	0
			809	523	130	152	4		
65	5P	107	Total	C	N	O	S	0	0
			809	523	130	152	4		
65	5Q	107	Total	C	N	O	S	0	0
			809	523	130	152	4		
65	5R	107	Total	C	N	O	S	0	0
			809	523	130	152	4		

- Molecule 66 is a protein called DC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	5S	92	Total	C	N	O	S	0	0
			749	470	137	133	9		
66	5T	92	Total	C	N	O	S	0	0
			749	470	137	133	9		
66	5U	92	Total	C	N	O	S	0	0
			749	470	137	133	9		
66	5V	92	Total	C	N	O	S	0	0
			749	470	137	133	9		

- Molecule 67 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	5X	4565	Total	C	N	O	S	0	0
			36792	23377	6358	6859	198		
67	5W	3144	Total	C	N	O	S	0	0
			25199	16022	4339	4693	145		
67	5Y	4565	Total	C	N	O	S	0	0
			36794	23378	6359	6859	198		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
67	5Z	4565	Total 36793	C 23378	N 6358	O 6859	S 198	0	0
67	5a	1201	Total 9781	C 6190	N 1721	O 1827	S 43	0	0

- Molecule 68 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	5c	4178	Total 33422	C 21212	N 5674	O 6353	S 183	0	0
68	5b	2730	Total 21827	C 13877	N 3716	O 4102	S 132	0	0
68	5d	4178	Total 33422	C 21212	N 5674	O 6353	S 183	0	0
68	5e	4178	Total 33422	C 21212	N 5674	O 6353	S 183	0	0
68	5f	1240	Total 9901	C 6257	N 1666	O 1934	S 44	0	0

- Molecule 69 is a protein called Dynein intermediate-chain-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	5g	565	Total 4413	C 2802	N 751	O 830	S 30	0	0
69	5h	565	Total 4413	C 2802	N 751	O 830	S 30	0	0
69	5i	565	Total 4413	C 2802	N 751	O 830	S 30	0	0
69	5j	565	Total 4413	C 2802	N 751	O 830	S 30	0	0

- Molecule 70 is a protein called Dynein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	5k	596	Total 4766	C 2990	N 832	O 918	S 26	0	0
70	5l	596	Total 4766	C 2990	N 832	O 918	S 26	0	0
70	5m	596	Total 4766	C 2990	N 832	O 918	S 26	0	0
70	5n	596	Total 4766	C 2990	N 832	O 918	S 26	0	0

- Molecule 71 is a protein called Dynein axonemal light chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	5o	208	Total	C	N	O	S	0	0
			1661	1047	292	312	10		
71	5p	208	Total	C	N	O	S	0	0
			1661	1047	292	312	10		
71	5q	208	Total	C	N	O	S	0	0
			1661	1047	292	312	10		
71	5r	208	Total	C	N	O	S	0	0
			1661	1047	292	312	10		

- Molecule 72 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	5s	202	Total	C	N	O	S	0	0
			1576	1004	271	292	9		
72	5t	202	Total	C	N	O	S	0	0
			1576	1004	271	292	9		
72	5u	202	Total	C	N	O	S	0	0
			1576	1004	271	292	9		
72	5v	202	Total	C	N	O	S	0	0
			1576	1004	271	292	9		

- Molecule 73 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	5w	112	Total	C	N	O	S	0	0
			867	544	152	166	5		
73	5x	112	Total	C	N	O	S	0	0
			867	544	152	166	5		
73	5y	112	Total	C	N	O	S	0	0
			867	544	152	166	5		
73	5z	112	Total	C	N	O	S	0	0
			867	544	152	166	5		

- Molecule 74 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	6A	97	Total	C	N	O	S	0	0
			771	481	137	148	5		
74	6B	97	Total	C	N	O	S	0	0
			771	481	137	148	5		
74	6C	97	Total	C	N	O	S	0	0
			771	481	137	148	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
74	6D	97	Total 771	C 481	N 137	O 148	S 5	0	0

- Molecule 75 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	6E	99	Total 824	C 532	N 133	O 151	S 8	0	0
75	6F	99	Total 824	C 532	N 133	O 151	S 8	0	0
75	6G	99	Total 824	C 532	N 133	O 151	S 8	0	0
75	6H	99	Total 824	C 532	N 133	O 151	S 8	0	0

- Molecule 76 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	6I	90	Total 721	C 466	N 117	O 133	S 5	0	0
76	6J	90	Total 721	C 466	N 117	O 133	S 5	0	0
76	6K	90	Total 721	C 466	N 117	O 133	S 5	0	0
76	6L	90	Total 721	C 466	N 117	O 133	S 5	0	0

- Molecule 77 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	6M	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	6N	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	6O	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	6P	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	7U	88	Total 717	C 463	N 117	O 131	S 6	0	0
77	7V	88	Total 717	C 463	N 117	O 131	S 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
77	7W	83	Total	C	N	O	S	0	0
			677	440	108	123	6		
77	7X	83	Total	C	N	O	S	0	0
			677	440	108	123	6		
77	7S	87	Total	C	N	O	S	0	0
			709	459	115	129	6		
77	7T	77	Total	C	N	O	S	0	0
			632	413	100	113	6		
77	9k	88	Total	C	N	O	S	0	0
			717	463	117	131	6		
77	9l	88	Total	C	N	O	S	0	0
			717	463	117	131	6		
77	9m	83	Total	C	N	O	S	0	0
			677	440	108	123	6		
77	9n	83	Total	C	N	O	S	0	0
			677	440	108	123	6		
77	9i	87	Total	C	N	O	S	0	0
			709	459	115	129	6		
77	9j	77	Total	C	N	O	S	0	0
			632	413	100	113	6		
77	8s	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8t	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8c	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8d	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8e	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8f	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8g	83	Total	C	N	O	S	0	0
			677	440	108	123	6		
77	8h	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8i	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8j	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8k	91	Total	C	N	O	S	0	0
			745	481	121	136	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
77	8l	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8m	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8n	91	Total	C	N	O	S	0	0
			745	481	121	136	7		

- Molecule 78 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	6Q	89	Total	C	N	O	S	0	0
			733	470	126	133	4		
78	6R	89	Total	C	N	O	S	0	0
			733	470	126	133	4		
78	6S	89	Total	C	N	O	S	0	0
			733	470	126	133	4		
78	6T	89	Total	C	N	O	S	0	0
			733	470	126	133	4		

- Molecule 79 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	6U	91	Total	C	N	O	S	0	0
			749	489	119	134	7		
79	6V	91	Total	C	N	O	S	0	0
			749	489	119	134	7		
79	6W	91	Total	C	N	O	S	0	0
			749	489	119	134	7		
79	6X	91	Total	C	N	O	S	0	0
			749	489	119	134	7		

- Molecule 80 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	6Y	96	Total	C	N	O	S	0	0
			767	483	134	146	4		
80	6Z	96	Total	C	N	O	S	0	0
			767	483	134	146	4		
80	6a	96	Total	C	N	O	S	0	0
			767	483	134	146	4		
80	6b	96	Total	C	N	O	S	0	0
			767	483	134	146	4		

- Molecule 81 is a protein called Outer arm dynein-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	6c	100	Total	C	N	O	S	0	0
			795	515	126	150	4		
81	6d	100	Total	C	N	O	S	0	0
			795	515	126	150	4		
81	6e	100	Total	C	N	O	S	0	0
			795	515	126	150	4		
81	6f	100	Total	C	N	O	S	0	0
			795	515	126	150	4		

- Molecule 82 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	6g	113	Total	C	N	O	S	0	0
			913	580	156	171	6		
82	6h	113	Total	C	N	O	S	0	0
			913	580	156	171	6		
82	6i	113	Total	C	N	O	S	0	0
			913	580	156	171	6		
82	6j	113	Total	C	N	O	S	0	0
			913	580	156	171	6		

- Molecule 83 is a protein called IDAa heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	6k	3972	Total	C	N	O	S	0	0
			31758	20128	5481	5984	165		

- Molecule 84 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	6l	371	Total	C	N	O	S	0	0
			2911	1836	495	556	24		
84	7A	361	Total	C	N	O	S	0	0
			2835	1789	480	544	22		

- Molecule 85 is a protein called DLP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	6m	410	Total	C	N	O	S	0	0
			3265	2032	592	633	8		

- Molecule 86 is a protein called Dynein arm light chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	6n	207	Total	C	N	O	S	0	0
			1701	1060	306	330	5		
86	6r	211	Total	C	N	O	S	0	0
			1725	1070	311	338	6		

- Molecule 87 is a protein called Putative dynein heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	6o	3797	Total	C	N	O	S	0	0
			30354	19276	5261	5630	187		

- Molecule 88 is a protein called Actin-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	6p	407	Total	C	N	O	S	0	0
			3087	1937	529	608	13		

- Molecule 89 is a protein called 33 kDa inner dynein arm light chain, axonemal, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	6q	226	Total	C	N	O	S	0	0
			1812	1131	340	337	4		

- Molecule 90 is a protein called Anaphase-promoting complex subunit 5 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	6s	245	Total	C	N	O	S	0	0
			1886	1182	344	345	15		

- Molecule 91 is a protein called Actin-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	9R	302	Total	C	N	O	S	0	0
			2382	1509	413	448	12		

- Molecule 92 is a protein called Centrin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	9S	129	Total	C	N	O	S	0	0
			1052	652	181	213	6		

- Molecule 93 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	9Q	3918	Total	C	N	O	S	0	0
			30600	19344	5306	5780	170		

- Molecule 94 is a protein called ARM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	9T	381	Total	C	N	O	S	0	0
			2975	1859	557	548	11		

- Molecule 95 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	6t	4062	Total	C	N	O	S	0	0
			32279	20527	5507	6050	195		

- Molecule 96 is a protein called Actin-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	6u	392	Total	C	N	O	S	0	0
			3067	1935	536	580	16		

- Molecule 97 is a protein called DLP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	6v	312	Total	C	N	O	S	0	0
			2471	1523	461	475	12		

- Molecule 98 is a protein called Dynein arm light chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	6w	274	Total	C	N	O	S	0	0
			2183	1354	416	409	4		

- Molecule 99 is a protein called TAX-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	6x	326	Total	C	N	O	S	0	0
			2613	1656	458	486	13		

- Molecule 100 is a protein called Tetratricopeptide repeat protein 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
100	6y	383	Total	C	N	O	S	0	0
			3020	1880	539	583	18		

- Molecule 101 is a protein called Roadblock/LAMTOR2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	7Q	96	Total	C	N	O	S	0	0
			734	460	126	144	4		
101	9g	96	Total	C	N	O	S	0	0
			734	460	126	144	4		

- Molecule 102 is a protein called Dynein-associated protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
102	7R	109	Total	C	N	O	S	0	0
			867	546	153	164	4		
102	9h	109	Total	C	N	O	S	0	0
			867	546	153	164	4		

- Molecule 103 is a protein called IC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
103	7N	325	Total	C	N	O	S	0	0
			2566	1645	445	462	14		
103	9c	325	Total	C	N	O	S	0	0
			2566	1645	445	462	14		

- Molecule 104 is a protein called Dynein axonemal intermediate chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	7O	233	Total	C	N	O	S	0	0
			1828	1167	315	337	9		
104	9d	392	Total	C	N	O	S	0	0
			3092	1954	531	590	17		

- Molecule 105 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
105	9M	103	Total	C	N	O	S	0	0
			845	535	144	161	5		
105	9p	103	Total	C	N	O	S	0	0
			845	535	144	161	5		

- Molecule 106 is a protein called Dynein-light chain-protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
106	9L	103	Total	C	N	O	S	0	0
			791	498	134	153	6		
106	9o	103	Total	C	N	O	S	0	0
			791	498	134	153	6		

- Molecule 107 is a protein called Ankyrin/TPR repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	7F	296	Total	C	N	O	S	0	0
			2252	1376	409	452	15		
107	9e	296	Total	C	N	O	S	0	0
			2252	1376	409	452	15		

- Molecule 108 is a protein called IC97/Casc1 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	9K	565	Total	C	N	O	S	0	0
			4601	2917	798	866	20		
108	9f	565	Total	C	N	O	S	0	0
			4601	2917	798	866	20		

- Molecule 109 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
109	7G	3724	Total	C	N	O	S	0	0
			29867	18977	5125	5599	166		
109	9a	1431	Total	C	N	O	S	0	0
			11631	7372	2038	2172	49		

- Molecule 110 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
110	7I	3788	Total	C	N	O	S	0	0
			30637	19418	5331	5707	181		
110	9b	1106	Total	C	N	O	S	0	0
			9051	5738	1585	1677	51		

- Molecule 111 is a protein called DUF4200 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
111	9U	81	Total	C	N	O	S	0	0
			616	373	115	122	6		
111	9r	286	Total	C	N	O	S	0	0
			2334	1425	442	451	16		

- Molecule 112 is a protein called DUF4200 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
112	9V	83	Total	C	N	O	S	0	0
			692	428	134	126	4		
112	9s	298	Total	C	N	O	S	0	0
			2453	1506	457	478	12		

- Molecule 113 is a protein called Leucine-rich repeat-containing protein 51.

Mol	Chain	Residues	Atoms					AltConf	Trace
113	9q	442	Total	C	N	O	S	0	0
			3509	2209	633	652	15		

- Molecule 114 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
114	6z	3680	Total	C	N	O	S	0	0
			29150	18419	5041	5528	162		

- Molecule 115 is a protein called Centrin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
115	7B	152	Total	C	N	O	S	0	0
			1202	758	200	237	7		

- Molecule 116 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
116	7C	3636	Total	C	N	O	S	0	0
			28996	18416	4982	5443	155		

- Molecule 117 is a protein called Actin-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
117	7D	419	Total	C	N	O	S	0	0
			3190	1998	563	609	20		

- Molecule 118 is a protein called Centrin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
118	7E	150	Total	C	N	O	S	0	0
			1210	750	209	247	4		

- Molecule 119 is a protein called Dynein regulatory complex protein 1 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
119	8A	452	Total	C	N	O	S	0	0
			3770	2334	704	721	11		

- Molecule 120 is a protein called Cilia- and flagella-associated protein 91.

Mol	Chain	Residues	Atoms					AltConf	Trace
120	8K	214	Total	C	N	O	S	0	0
			1728	1060	340	322	6		

- Molecule 121 is a protein called T-lymphocyte triggering factor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
121	8E	431	Total	C	N	O	S	0	0
			3596	2204	671	704	17		

- Molecule 122 is a protein called T-lymphocyte triggering factor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
122	8D	400	Total	C	N	O	S	0	0
			3394	2103	619	662	10		

- Molecule 123 is a protein called Dynein regulatory complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
123	8B	372	Total	C	N	O	S	0	0
			3062	1883	550	609	20		

- Molecule 124 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
124	8J	778	Total	C	N	O	S	0	0
			6100	3823	1111	1137	29		

- Molecule 125 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
125	8F	456	Total	C	N	O	S	0	0
			3580	2241	648	668	23		

- Molecule 126 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
126	8M	148	Total	C	N	O	S	0	0
			1163	713	186	254	10		
126	8L	148	Total	C	N	O	S	0	0
			1163	713	186	254	10		
126	9N	149	Total	C	N	O	S	0	0
			1173	719	188	256	10		
126	9O	149	Total	C	N	O	S	0	0
			1173	719	188	256	10		

- Molecule 127 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
127	8N	323	Total	C	N	O	S	0	0
			2458	1543	438	462	15		

- Molecule 128 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
128	8O	387	Total	C	N	O	S	0	0
			2870	1778	522	556	14		

- Molecule 129 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
129	8P	99	Total	C	N	O	S	0	0
			814	519	135	157	3		
129	4f	73	Total	C	N	O	S	0	0
			621	396	106	117	2		

- Molecule 130 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
130	8R	337	Total	C	N	O	S	0	0
			2445	1514	433	488	10		

- Molecule 131 is a protein called Transglutaminase-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
131	8G	606	Total	C	N	O	S	0	0
			4902	3115	848	917	22		

- Molecule 132 is a protein called Dynein regulatory complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
132	8C	546	Total	C	N	O	S	0	0
			4418	2757	806	840	15		

- Molecule 133 is a protein called Dynein regulatory complex protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
133	8H	120	Total	C	N	O	S	0	0
			935	565	177	189	4		

- Molecule 134 is a protein called Dynein regulatory complex protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
134	8I	174	Total	C	N	O	S	0	0
			1433	873	278	277	5		

- Molecule 135 is a protein called Cilia- and flagella-associated protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
135	7K	1298	Total	C	N	O	S	0	0
			10069	6250	1827	1919	73		

- Molecule 136 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
136	7L	1476	Total	C	N	O	S	0	0
			11521	7199	2068	2189	65		

- Molecule 137 is a protein called Tudor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
137	7M	252	Total	C	N	O	S	0	0
			1985	1261	325	387	12		

- Molecule 138 is a protein called CFAP253.

Mol	Chain	Residues	Atoms					AltConf	Trace
138	8r	197	Total	C	N	O	S	0	0
			1627	1014	313	297	3		

- Molecule 139 is a protein called Radial spoke protein 3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
139	8u	44	Total	C	N	O	S	0	0
			354	211	74	66	3		
139	8v	40	Total	C	N	O	S	0	0
			330	200	66	60	4		
139	8o	59	Total	C	N	O	S	0	0
			483	299	79	104	1		
139	8p	99	Total	C	N	O	S	0	0
			803	499	136	163	5		

- Molecule 140 is a protein called Kinesin-MORN.

Mol	Chain	Residues	Atoms					AltConf	Trace
140	8a	620	Total	C	N	O	S	0	0
			5006	3129	913	936	28		

- Molecule 141 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
141	8b	366	Total	C	N	O	S	0	0
			2764	1713	496	535	20		

- Molecule 142 is a protein called Cilia- and flagella-associated protein 206.

Mol	Chain	Residues	Atoms					AltConf	Trace
142	8q	560	Total	C	N	O	S	0	0
			4277	2684	757	807	29		

- Molecule 143 is a protein called Cilia- and flagella-associated protein 251.

Mol	Chain	Residues	Atoms					AltConf	Trace
143	8w	1005	Total	C	N	O	S	0	0
			7768	4918	1350	1452	48		

- Molecule 144 is a protein called Coiled-coil domain-containing protein 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
144	4R	359	Total	C	N	O	S	0	0
			2942	1806	541	587	8		
144	4S	282	Total	C	N	O	S	0	0
			2339	1419	439	473	8		

- Molecule 145 is a protein called Coiled-coil domain-containing protein 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
145	4T	430	Total	C	N	O	S	0	0
			3493	2145	643	684	21		
145	4U	276	Total	C	N	O	S	0	0
			2260	1372	421	458	9		

- Molecule 146 is a protein called CCDC113/CCDC96 coiled-coil domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
146	9t	255	Total	C	N	O	S	0	0
			2109	1292	421	388	8		

- Molecule 147 is a protein called Cilia- and flagella-associated protein 263.

Mol	Chain	Residues	Atoms					AltConf	Trace
147	9u	283	Total	C	N	O	S	0	0
			2270	1377	438	444	11		

- Molecule 148 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
148	4D	105	Total	C	N	O	S	0	0
			836	517	167	150	2		

- Molecule 149 is a protein called C2HC/C3H-type domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
149	4E	27	Total	C	N	O	0	0
			216	134	44	38		

- Molecule 150 is a protein called Sperm-tail PG-rich repeat.

Mol	Chain	Residues	Atoms					AltConf	Trace
150	4F	254	Total	C	N	O	S	0	0
			1945	1226	351	361	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
150	4G	83	Total 661	C 420	N 111	O 127	S 3	0	0

- Molecule 151 is a protein called DMAP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
151	4H	45	Total 359	C 223	N 67	O 68	S 1	0	0

- Molecule 152 is a protein called DMAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
152	4I	120	Total 959	C 595	N 194	O 168	S 2	0	0
152	4J	57	Total 456	C 279	N 78	O 94	S 5	0	0

- Molecule 153 is a protein called IJAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
153	4K	50	Total 400	C 245	N 82	O 68	S 5	0	0

- Molecule 154 is a protein called LIM zinc-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
154	4L	128	Total 998	C 614	N 187	O 184	S 13	0	0

- Molecule 155 is a protein called IJAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
155	4M	75	Total 581	C 362	N 105	O 112	S 2	0	0
155	4N	177	Total 1437	C 893	N 277	O 263	S 4	0	0

- Molecule 156 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
156	4d	491	Total	C	N	O	S	0	0
			3737	2317	683	711	26		

- Molecule 157 is a protein called Ribonuclease inhibitor-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
157	4e	507	Total	C	N	O	S	0	0
			3833	2362	721	729	21		

- Molecule 158 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
158	4g	84	Total	C	N	O	S	0	0
			660	408	128	121	3		

- Molecule 159 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
159	9W	919	Total	C	N	O	S	0	0
			7288	4584	1287	1377	40		

- Molecule 160 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
160	9X	971	Total	C	N	O	S	0	0
			7686	4789	1396	1462	39		

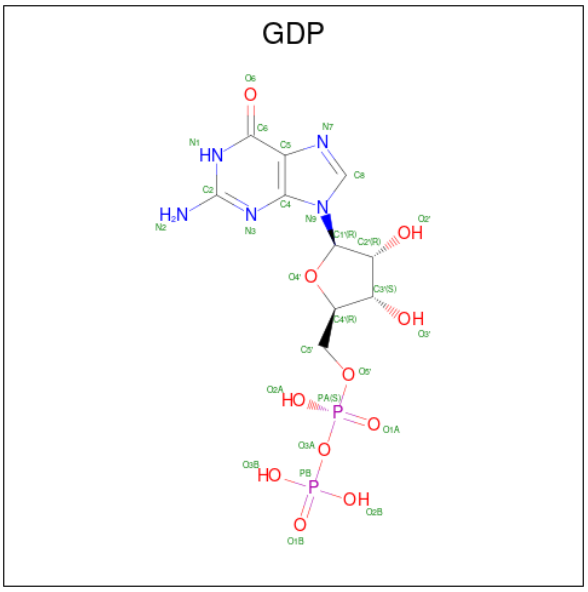
- Molecule 161 is a protein called Cilia- and flagella-associated protein 58 central coiled coil domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
161	9Y	539	Total	C	N	O	S	0	0
			4412	2692	835	860	25		

- Molecule 162 is a protein called Cilia- and flagella-associated protein 58 central coiled coil domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
162	9Z	534	Total	C	N	O	S	0	0
			4339	2668	838	820	13		

- Molecule 163 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
163	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BN	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
163	CA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CI	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CM	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DI	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DM	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	E	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ED	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EL	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
163	F	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	G	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	H	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HL	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
163	I	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JI	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JM	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KI	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KM	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
163	LA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LI	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LM	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	M	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ML	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	N	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ND	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NH	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
163	NJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	O	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	P	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QI	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
163	QK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RI	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	S	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	T	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	U	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
163	UB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	V	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	W	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AP	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
163	AR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CW	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CY	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DW	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
163	DY	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ER	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ET	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HP	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
163	HR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JW	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JY	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KW	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
163	KY	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LW	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	LY	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	MZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QM	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QQ	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
163	QS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QW	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RM	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RW	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ST	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TX	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
163	UN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NR	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
163	NT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ON	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OX	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 164 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
164	A	1	Total	Mg	0
			1	1	
164	AC	1	Total	Mg	0
			1	1	
164	AE	1	Total	Mg	0
			1	1	
164	AG	1	Total	Mg	0
			1	1	
164	AI	1	Total	Mg	0
			1	1	
164	AK	1	Total	Mg	0
			1	1	
164	AM	1	Total	Mg	0
			1	1	
164	BA	1	Total	Mg	0
			1	1	
164	BE	1	Total	Mg	0
			1	1	
164	BG	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	BI	1	Total Mg 1 1	0
164	BK	1	Total Mg 1 1	0
164	BM	1	Total Mg 1 1	0
164	C	1	Total Mg 1 1	0
164	CB	1	Total Mg 1 1	0
164	CD	1	Total Mg 1 1	0
164	CF	1	Total Mg 1 1	0
164	CH	1	Total Mg 1 1	0
164	CJ	1	Total Mg 1 1	0
164	CK	1	Total Mg 1 1	0
164	D	1	Total Mg 1 1	0
164	DB	1	Total Mg 1 1	0
164	DD	1	Total Mg 1 1	0
164	DF	1	Total Mg 1 1	0
164	DH	1	Total Mg 1 1	0
164	DJ	1	Total Mg 1 1	0
164	DK	1	Total Mg 1 1	0
164	EA	1	Total Mg 1 1	0
164	EC	1	Total Mg 1 1	0
164	EE	1	Total Mg 1 1	0
164	EG	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	EI	1	Total Mg 1 1	0
164	EK	1	Total Mg 1 1	0
164	FA	1	Total Mg 1 1	0
164	FC	1	Total Mg 1 1	0
164	FE	1	Total Mg 1 1	0
164	FG	1	Total Mg 1 1	0
164	FI	1	Total Mg 1 1	0
164	FJ	1	Total Mg 1 1	0
164	GA	1	Total Mg 1 1	0
164	GC	1	Total Mg 1 1	0
164	GE	1	Total Mg 1 1	0
164	GG	1	Total Mg 1 1	0
164	GI	1	Total Mg 1 1	0
164	GK	1	Total Mg 1 1	0
164	HA	1	Total Mg 1 1	0
164	HB	1	Total Mg 1 1	0
164	HD	1	Total Mg 1 1	0
164	HG	1	Total Mg 1 1	0
164	HH	1	Total Mg 1 1	0
164	HK	1	Total Mg 1 1	0
164	HL	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	I	1	Total Mg 1 1	0
164	IC	1	Total Mg 1 1	0
164	IE	1	Total Mg 1 1	0
164	IG	1	Total Mg 1 1	0
164	II	1	Total Mg 1 1	0
164	IK	1	Total Mg 1 1	0
164	IL	1	Total Mg 1 1	0
164	J	1	Total Mg 1 1	0
164	JB	1	Total Mg 1 1	0
164	JD	1	Total Mg 1 1	0
164	JF	1	Total Mg 1 1	0
164	JH	1	Total Mg 1 1	0
164	JJ	1	Total Mg 1 1	0
164	JL	1	Total Mg 1 1	0
164	JM	1	Total Mg 1 1	0
164	K	1	Total Mg 1 1	0
164	KB	1	Total Mg 1 1	0
164	KD	1	Total Mg 1 1	0
164	KF	1	Total Mg 1 1	0
164	KH	1	Total Mg 1 1	0
164	KJ	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	KL	1	Total Mg 1 1	0
164	KN	1	Total Mg 1 1	0
164	L	1	Total Mg 1 1	0
164	LB	1	Total Mg 1 1	0
164	LD	1	Total Mg 1 1	0
164	LF	1	Total Mg 1 1	0
164	LG	1	Total Mg 1 1	0
164	LJ	1	Total Mg 1 1	0
164	LL	1	Total Mg 1 1	0
164	LN	1	Total Mg 1 1	0
164	MA	1	Total Mg 1 1	0
164	MC	1	Total Mg 1 1	0
164	ME	1	Total Mg 1 1	0
164	MG	1	Total Mg 1 1	0
164	MI	1	Total Mg 1 1	0
164	MK	1	Total Mg 1 1	0
164	MM	1	Total Mg 1 1	0
164	NA	1	Total Mg 1 1	0
164	NC	1	Total Mg 1 1	0
164	NE	1	Total Mg 1 1	0
164	NG	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	NI	1	Total Mg 1 1	0
164	NJ	1	Total Mg 1 1	0
164	NM	1	Total Mg 1 1	0
164	OA	1	Total Mg 1 1	0
164	OC	1	Total Mg 1 1	0
164	OD	1	Total Mg 1 1	0
164	OG	1	Total Mg 1 1	0
164	OI	1	Total Mg 1 1	0
164	OK	1	Total Mg 1 1	0
164	OM	1	Total Mg 1 1	0
164	PA	1	Total Mg 1 1	0
164	PC	1	Total Mg 1 1	0
164	PE	1	Total Mg 1 1	0
164	PF	1	Total Mg 1 1	0
164	PI	1	Total Mg 1 1	0
164	PK	1	Total Mg 1 1	0
164	PL	1	Total Mg 1 1	0
164	Q	1	Total Mg 1 1	0
164	QB	1	Total Mg 1 1	0
164	QD	1	Total Mg 1 1	0
164	QF	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	QH	1	Total Mg 1 1	0
164	QJ	1	Total Mg 1 1	0
164	QL	1	Total Mg 1 1	0
164	R	1	Total Mg 1 1	0
164	RB	1	Total Mg 1 1	0
164	RD	1	Total Mg 1 1	0
164	RF	1	Total Mg 1 1	0
164	RH	1	Total Mg 1 1	0
164	RJ	1	Total Mg 1 1	0
164	RL	1	Total Mg 1 1	0
164	SA	1	Total Mg 1 1	0
164	SB	1	Total Mg 1 1	0
164	SE	1	Total Mg 1 1	0
164	SG	1	Total Mg 1 1	0
164	SI	1	Total Mg 1 1	0
164	SJ	1	Total Mg 1 1	0
164	T	1	Total Mg 1 1	0
164	TC	1	Total Mg 1 1	0
164	TE	1	Total Mg 1 1	0
164	TG	1	Total Mg 1 1	0
164	TI	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	TK	1	Total Mg 1 1	0
164	TL	1	Total Mg 1 1	0
164	UA	1	Total Mg 1 1	0
164	UC	1	Total Mg 1 1	0
164	UE	1	Total Mg 1 1	0
164	UG	1	Total Mg 1 1	0
164	UI	1	Total Mg 1 1	0
164	UK	1	Total Mg 1 1	0
164	VA	1	Total Mg 1 1	0
164	VC	1	Total Mg 1 1	0
164	VE	1	Total Mg 1 1	0
164	VG	1	Total Mg 1 1	0
164	VI	1	Total Mg 1 1	0
164	VK	1	Total Mg 1 1	0
164	VM	1	Total Mg 1 1	0
164	WA	1	Total Mg 1 1	0
164	WC	1	Total Mg 1 1	0
164	WE	1	Total Mg 1 1	0
164	WF	1	Total Mg 1 1	0
164	WI	1	Total Mg 1 1	0
164	WK	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	WM	1	Total Mg 1 1	0
164	AO	1	Total Mg 1 1	0
164	AQ	1	Total Mg 1 1	0
164	AS	1	Total Mg 1 1	0
164	AU	1	Total Mg 1 1	0
164	AW	1	Total Mg 1 1	0
164	AY	1	Total Mg 1 1	0
164	BO	1	Total Mg 1 1	0
164	BQ	1	Total Mg 1 1	0
164	BS	1	Total Mg 1 1	0
164	BU	1	Total Mg 1 1	0
164	BW	1	Total Mg 1 1	0
164	BY	1	Total Mg 1 1	0
164	CN	1	Total Mg 1 1	0
164	CP	1	Total Mg 1 1	0
164	CR	1	Total Mg 1 1	0
164	CT	1	Total Mg 1 1	0
164	CV	1	Total Mg 1 1	0
164	CX	1	Total Mg 1 1	0
164	DN	1	Total Mg 1 1	0
164	DP	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	DR	1	Total Mg 1 1	0
164	DT	1	Total Mg 1 1	0
164	DV	1	Total Mg 1 1	0
164	DW	1	Total Mg 1 1	0
164	EM	1	Total Mg 1 1	0
164	EO	1	Total Mg 1 1	0
164	EQ	1	Total Mg 1 1	0
164	ES	1	Total Mg 1 1	0
164	EU	1	Total Mg 1 1	0
164	EW	1	Total Mg 1 1	0
164	FM	1	Total Mg 1 1	0
164	FO	1	Total Mg 1 1	0
164	FQ	1	Total Mg 1 1	0
164	FR	1	Total Mg 1 1	0
164	FT	1	Total Mg 1 1	0
164	FV	1	Total Mg 1 1	0
164	GM	1	Total Mg 1 1	0
164	GO	1	Total Mg 1 1	0
164	GQ	1	Total Mg 1 1	0
164	GS	1	Total Mg 1 1	0
164	GT	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	GV	1	Total Mg 1 1	0
164	HN	1	Total Mg 1 1	0
164	HP	1	Total Mg 1 1	0
164	HS	1	Total Mg 1 1	0
164	HT	1	Total Mg 1 1	0
164	HW	1	Total Mg 1 1	0
164	HX	1	Total Mg 1 1	0
164	IO	1	Total Mg 1 1	0
164	IQ	1	Total Mg 1 1	0
164	IS	1	Total Mg 1 1	0
164	IT	1	Total Mg 1 1	0
164	IW	1	Total Mg 1 1	0
164	IX	1	Total Mg 1 1	0
164	JP	1	Total Mg 1 1	0
164	JR	1	Total Mg 1 1	0
164	JT	1	Total Mg 1 1	0
164	JV	1	Total Mg 1 1	0
164	JX	1	Total Mg 1 1	0
164	JY	1	Total Mg 1 1	0
164	KP	1	Total Mg 1 1	0
164	KR	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	KT	1	Total Mg 1 1	0
164	KV	1	Total Mg 1 1	0
164	KX	1	Total Mg 1 1	0
164	KZ	1	Total Mg 1 1	0
164	LP	1	Total Mg 1 1	0
164	LR	1	Total Mg 1 1	0
164	LT	1	Total Mg 1 1	0
164	LV	1	Total Mg 1 1	0
164	LX	1	Total Mg 1 1	0
164	LZ	1	Total Mg 1 1	0
164	MO	1	Total Mg 1 1	0
164	MQ	1	Total Mg 1 1	0
164	MS	1	Total Mg 1 1	0
164	MU	1	Total Mg 1 1	0
164	MW	1	Total Mg 1 1	0
164	MY	1	Total Mg 1 1	0
164	PO	1	Total Mg 1 1	0
164	PQ	1	Total Mg 1 1	0
164	PR	1	Total Mg 1 1	0
164	PU	1	Total Mg 1 1	0
164	PW	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	PX	1	Total Mg 1 1	0
164	QN	1	Total Mg 1 1	0
164	QP	1	Total Mg 1 1	0
164	QR	1	Total Mg 1 1	0
164	QT	1	Total Mg 1 1	0
164	QV	1	Total Mg 1 1	0
164	QX	1	Total Mg 1 1	0
164	RN	1	Total Mg 1 1	0
164	RP	1	Total Mg 1 1	0
164	RR	1	Total Mg 1 1	0
164	RT	1	Total Mg 1 1	0
164	RV	1	Total Mg 1 1	0
164	RX	1	Total Mg 1 1	0
164	SM	1	Total Mg 1 1	0
164	SN	1	Total Mg 1 1	0
164	SQ	1	Total Mg 1 1	0
164	SS	1	Total Mg 1 1	0
164	SU	1	Total Mg 1 1	0
164	SV	1	Total Mg 1 1	0
164	TO	1	Total Mg 1 1	0
164	TQ	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

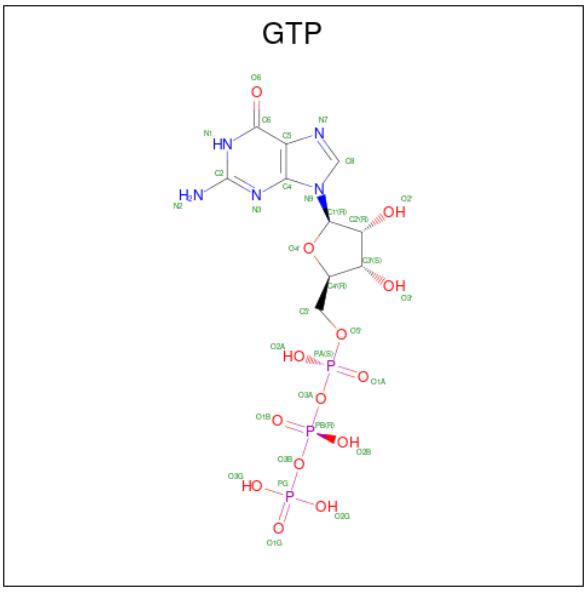
Mol	Chain	Residues	Atoms	AltConf
164	TS	1	Total Mg 1 1	0
164	TU	1	Total Mg 1 1	0
164	TW	1	Total Mg 1 1	0
164	UM	1	Total Mg 1 1	0
164	UO	1	Total Mg 1 1	0
164	UQ	1	Total Mg 1 1	0
164	US	1	Total Mg 1 1	0
164	UU	1	Total Mg 1 1	0
164	UW	1	Total Mg 1 1	0
164	VO	1	Total Mg 1 1	0
164	VQ	1	Total Mg 1 1	0
164	VS	1	Total Mg 1 1	0
164	VU	1	Total Mg 1 1	0
164	VW	1	Total Mg 1 1	0
164	VY	1	Total Mg 1 1	0
164	WO	1	Total Mg 1 1	0
164	WQ	1	Total Mg 1 1	0
164	WR	1	Total Mg 1 1	0
164	WU	1	Total Mg 1 1	0
164	WW	1	Total Mg 1 1	0
164	WY	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
164	NO	1	Total Mg 1 1	0
164	NQ	1	Total Mg 1 1	0
164	NS	1	Total Mg 1 1	0
164	NU	1	Total Mg 1 1	0
164	NV	1	Total Mg 1 1	0
164	NY	1	Total Mg 1 1	0
164	OO	1	Total Mg 1 1	0
164	OP	1	Total Mg 1 1	0
164	OS	1	Total Mg 1 1	0
164	OU	1	Total Mg 1 1	0
164	OW	1	Total Mg 1 1	0
164	OY	1	Total Mg 1 1	0
164	6l	1	Total Mg 1 1	0
164	6p	1	Total Mg 1 1	0
164	9R	1	Total Mg 1 1	0
164	7A	1	Total Mg 1 1	0
164	7D	1	Total Mg 1 1	0

- Molecule 165 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
165	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AD	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	C	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
165	CB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DD	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DH	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DL	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	ED	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FC	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
165	FE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GL	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IE	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
165	IG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	II	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JD	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JF	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JH	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JN	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KD	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KF	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KH	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KL	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KN	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	L	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
165	LB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LD	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LF	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LH	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LL	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LN	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	ME	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NF	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NM	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
165	OA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OD	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	Q	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QF	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QH	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QL	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
165	R	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RB	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RF	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RH	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RL	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	T	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UC	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
165	UE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VH	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WA	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WC	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WE	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WG	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WI	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WK	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AP	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AS	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
165	AU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	AY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	BY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CN	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CT	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	CW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DN	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DP	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DT	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	DX	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
165	EM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EP	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	ES	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	EV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FT	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	FV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	GW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HN	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HU	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
165	HW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	HY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	IY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JP	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JR	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JT	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	JZ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KP	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KR	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KT	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KX	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	KZ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LP	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
165	LR	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LT	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LX	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	LZ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	MY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	PY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QN	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QR	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QT	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
165	QU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	QX	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RN	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RR	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RT	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RV	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	RX	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	SW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TM	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	TW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UM	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
165	UO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	US	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	UW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VT	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	VY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	WY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NR	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NU	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
165	NW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OP	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OY	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 166 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
166	KB	1	Total	Zn	0
			1	1	
166	KD	1	Total	Zn	0
			1	1	
166	KN	1	Total	Zn	0
			1	1	
166	LD	1	Total	Zn	0
			1	1	
166	LF	1	Total	Zn	0
			1	1	
166	LN	1	Total	Zn	0
			1	1	
166	KP	1	Total	Zn	0
			1	1	
166	LP	1	Total	Zn	0
			1	1	
166	LR	1	Total	Zn	0
			1	1	
166	LZ	1	Total	Zn	0
			1	1	
166	0A	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
166	0	1	Total Zn 1 1	0
166	0z	1	Total Zn 1 1	0
166	1V	2	Total Zn 2 2	0
166	1b	2	Total Zn 2 2	0
166	1e	2	Total Zn 2 2	0
166	1q	1	Total Zn 1 1	0
166	1s	1	Total Zn 1 1	0
166	1w	1	Total Zn 1 1	0
166	1x	1	Total Zn 1 1	0
166	3S	1	Total Zn 1 1	0
166	0B	1	Total Zn 1 1	0
166	2A	1	Total Zn 1 1	0
166	1W	2	Total Zn 2 2	0
166	1Z	1	Total Zn 1 1	0
166	1c	2	Total Zn 2 2	0
166	9F	2	Total Zn 2 2	0
166	1f	2	Total Zn 2 2	0
166	1i	2	Total Zn 2 2	0
166	1t	1	Total Zn 1 1	0
166	1v	1	Total Zn 1 1	0
166	1z	1	Total Zn 1 1	0

Continued on next page...

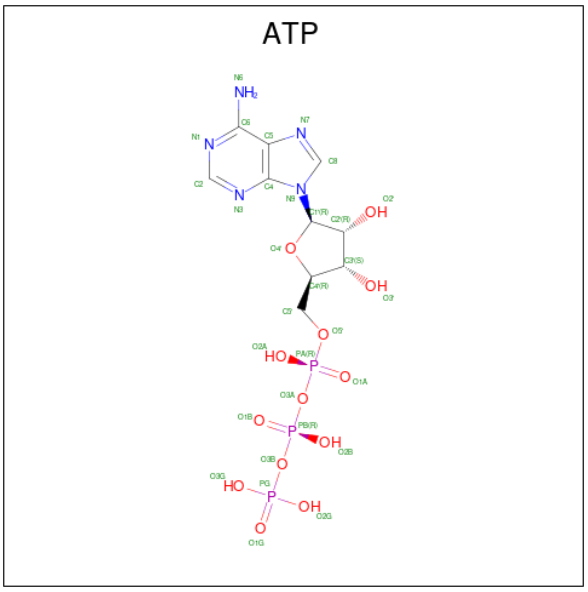
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
166	3T	1	Total Zn 1 1	0
166	4X	2	Total Zn 2 2	0
166	1Y	1	Total Zn 1 1	0
166	5S	1	Total Zn 1 1	0
166	5T	1	Total Zn 1 1	0
166	5U	1	Total Zn 1 1	0
166	5V	1	Total Zn 1 1	0
166	4L	2	Total Zn 2 2	0

- Molecule 167 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
167	1S	1	Total Ca 1 1	0
167	2v	1	Total Ca 1 1	0
167	2w	1	Total Ca 1 1	0
167	1T	1	Total Ca 1 1	0
167	2x	1	Total Ca 1 1	0

- Molecule 168 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
168	2v	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	2w	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	2x	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	6l	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	6p	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	9R	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	6u	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	7A	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	7D	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	8a	1	Total	C	N	O	P	0
			31	10	5	13	3	

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, Not provided	
Number of particles used	281984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	62.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 956 ligands modelled in this entry, 355 are monoatomic - leaving 601 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	$\#\|Z\| > 2$
165	GTP	VK	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	AF	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
165	GTP	FG	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
165	GTP	SW	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	MJ	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	VR	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	TF	500	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	6 (13%)
163	GDP	DS	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	CB	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)
163	GDP	GB	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
163	GDP	HB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	QI	501	164	33,34,34	0.95	2 (6%)	50,54,54	1.58	10 (20%)
165	GTP	SC	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	IW	501	164	33,34,34	1.23	5 (15%)	50,54,54	1.63	10 (20%)
163	GDP	JE	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	MZ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	DQ	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	AU	501	164	33,34,34	0.85	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	VP	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	IB	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	GI	501	164	33,34,34	0.93	2 (6%)	50,54,54	1.60	10 (20%)
163	GDP	AX	500	-	29,30,30	1.15	4 (13%)	45,47,47	1.71	7 (15%)
163	GDP	ON	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	MU	501	164	33,34,34	0.97	2 (6%)	50,54,54	1.54	8 (16%)
165	GTP	AB	501	164	33,34,34	0.93	0	50,54,54	1.51	8 (16%)
163	GDP	NV	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	HE	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.55	9 (18%)
165	GTP	TI	501	164	33,34,34	0.98	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	CO	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	MQ	501	164	33,34,34	0.99	2 (6%)	50,54,54	1.58	9 (18%)
168	ATP	2w	501	-	32,33,33	0.33	0	48,52,52	0.29	0
163	GDP	NX	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	TE	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	LY	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	LT	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
163	GDP	UB	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
168	ATP	7D	601	164	32,33,33	0.42	0	48,52,52	0.30	0
163	GDP	JW	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	FA	501	164	33,34,34	0.91	0	50,54,54	1.54	8 (16%)
165	GTP	QB	501	164	33,34,34	0.96	2 (6%)	50,54,54	1.59	8 (16%)
165	GTP	CC	501	164	33,34,34	0.97	0	50,54,54	1.58	9 (18%)
163	GDP	DA	500	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	6 (13%)
165	GTP	DB	501	164	33,34,34	0.91	0	50,54,54	1.62	10 (20%)
165	GTP	GC	501	164	33,34,34	0.89	0	50,54,54	1.60	10 (20%)
168	ATP	8a	801	-	32,33,33	0.49	1 (3%)	48,52,52	0.30	0
163	GDP	OD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	VV	500	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	8 (17%)
165	GTP	R	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	WY	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	TG	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	MD	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	VH	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	BL	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	BN	500	-	29,30,30	1.16	4 (13%)	45,47,47	1.73	7 (15%)
165	GTP	D	501	-	33,34,34	1.02	2 (6%)	50,54,54	1.62	10 (20%)
165	GTP	NI	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
163	GDP	GJ	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
163	GDP	PX	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	DP	501	164	33,34,34	0.91	0	50,54,54	1.63	12 (24%)
165	GTP	VG	501	164	33,34,34	1.00	2 (6%)	50,54,54	1.58	9 (18%)
163	GDP	GR	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
165	GTP	MJ	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
165	GTP	C	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.58	8 (16%)
163	GDP	RC	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	GE	501	164	33,34,34	0.91	0	50,54,54	1.61	9 (18%)
163	GDP	HR	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	AM	501	164	33,34,34	0.90	0	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	G	501	164	33,34,34	0.89	0	50,54,54	1.54	9 (18%)
165	GTP	LZ	502	164	33,34,34	0.97	1 (3%)	50,54,54	1.55	9 (18%)
165	GTP	OM	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	O	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	QX	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
163	GDP	VX	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
165	GTP	II	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
163	GDP	OJ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	LB	501	164	33,34,34	0.97	2 (6%)	50,54,54	1.56	9 (18%)
163	GDP	PT	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
163	GDP	CI	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
165	GTP	UO	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	PA	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
163	GDP	IH	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	SS	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.59	10 (20%)
163	GDP	QW	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
163	GDP	NH	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	DX	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.62	10 (20%)
163	GDP	AD	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	8 (17%)
163	GDP	NP	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	8 (17%)
165	GTP	EG	501	164	33,34,34	0.92	0	50,54,54	1.63	10 (20%)
165	GTP	HK	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
165	GTP	CO	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.58	8 (16%)
165	GTP	AS	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.54	8 (16%)
163	GDP	SN	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	BV	500	-	29,30,30	1.16	4 (13%)	45,47,47	1.70	5 (11%)
165	GTP	SQ	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.59	10 (20%)
165	GTP	OY	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.55	8 (16%)
163	GDP	WR	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	LC	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
165	GTP	HA	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.54	9 (18%)
165	GTP	FM	501	164	33,34,34	0.89	0	50,54,54	1.53	8 (16%)
163	GDP	SJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	EV	501	164	33,34,34	0.94	0	50,54,54	1.55	9 (18%)
163	GDP	IV	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
163	GDP	TX	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
163	GDP	CG	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	AY	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.52	8 (16%)
163	GDP	NB	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	IX	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
163	GDP	TN	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	HT	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	WJ	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	FP	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	LI	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	BT	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
163	GDP	GD	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)
165	GTP	HU	501	164	33,34,34	0.88	1 (3%)	50,54,54	1.56	9 (18%)
165	GTP	HY	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.55	9 (18%)
165	GTP	BW	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.54	8 (16%)
163	GDP	ET	500	-	29,30,30	1.15	4 (13%)	45,47,47	1.68	5 (11%)
163	GDP	BJ	500	-	29,30,30	1.16	4 (13%)	45,47,47	1.75	7 (15%)
163	GDP	KO	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	HV	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	OC	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	LE	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	RA	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
165	GTP	NK	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
163	GDP	TP	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
165	GTP	NW	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
163	GDP	EJ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	PS	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
163	GDP	PN	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	WI	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.56	8 (16%)
165	GTP	WE	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.59	10 (20%)
165	GTP	BO	501	164	33,34,34	0.95	0	50,54,54	1.56	9 (18%)
163	GDP	HL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	MR	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	CJ	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
163	GDP	FN	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
163	GDP	GH	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
163	GDP	MX	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	FE	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.54	9 (18%)
163	GDP	I	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	QN	501	164	33,34,34	0.98	2 (6%)	50,54,54	1.59	8 (16%)
163	GDP	KY	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
165	GTP	FT	503	164	33,34,34	0.87	2 (6%)	50,54,54	1.65	11 (22%)
165	GTP	EU	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.61	9 (18%)
165	GTP	HI	501	164	33,34,34	0.88	1 (3%)	50,54,54	1.55	9 (18%)
165	GTP	OO	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	DJ	501	164	33,34,34	0.93	0	50,54,54	1.52	8 (16%)
165	GTP	HS	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
165	GTP	NC	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	SO	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	IK	501	164	33,34,34	1.23	5 (15%)	50,54,54	1.62	10 (20%)
165	GTP	JV	501	164	33,34,34	0.98	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	VN	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
163	GDP	HF	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	RS	500	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	JK	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
163	GDP	FD	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
165	GTP	K	501	164	33,34,34	0.97	2 (6%)	50,54,54	1.58	9 (18%)
163	GDP	H	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	MY	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	JJ	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	AJ	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	CE	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	SH	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	BH	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	FX	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	AP	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	LO	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
165	GTP	CH	501	164	33,34,34	0.91	2 (6%)	50,54,54	1.65	9 (18%)
165	GTP	WA	501	164	33,34,34	0.98	1 (3%)	50,54,54	1.56	9 (18%)
165	GTP	DV	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	QF	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	VM	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
165	GTP	UW	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.55	8 (16%)
163	GDP	JM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	AO	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.54	9 (18%)
163	GDP	QK	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)
163	GDP	E	500	-	29,30,30	1.24	4 (13%)	45,47,47	1.80	7 (15%)
163	GDP	ST	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	CE	501	164	33,34,34	0.98	2 (6%)	50,54,54	1.56	9 (18%)
163	GDP	PD	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	OR	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	SA	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
165	GTP	AG	501	164	33,34,34	0.89	0	50,54,54	1.53	8 (16%)
163	GDP	OF	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	BQ	501	164	33,34,34	0.86	1 (3%)	50,54,54	1.56	8 (16%)
168	ATP	7A	402	-	32,33,33	0.45	0	48,52,52	0.29	0
163	GDP	RQ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	8 (17%)
163	GDP	T	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	RN	501	164	33,34,34	0.98	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	EL	500	-	29,30,30	1.20	3 (10%)	45,47,47	1.74	5 (11%)
163	GDP	LM	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	VC	501	164	33,34,34	1.00	2 (6%)	50,54,54	1.56	9 (18%)
163	GDP	MB	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
163	GDP	S	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	CV	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.61	9 (18%)
163	GDP	SP	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
165	GTP	BA	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.55	8 (16%)
163	GDP	QS	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	RL	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
165	GTP	UI	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	PI	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	UJ	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	GL	501	164	33,34,34	0.95	0	50,54,54	1.58	9 (18%)
165	GTP	OG	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
165	GTP	SG	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.59	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	PO	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	TW	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.54	9 (18%)
163	GDP	IN	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	WF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	KS	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	M	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	VT	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	L	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.55	8 (16%)
165	GTP	MV	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
163	GDP	LW	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	DK	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	ID	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	WW	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	AT	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	LX	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.54	8 (16%)
163	GDP	ER	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	VL	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
165	GTP	QL	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)
165	GTP	NQ	501	164	33,34,34	1.00	2 (6%)	50,54,54	1.57	9 (18%)
163	GDP	WL	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	CN	501	164	33,34,34	0.97	0	50,54,54	1.55	8 (16%)
165	GTP	DQ	501	164	33,34,34	0.95	2 (6%)	50,54,54	1.60	9 (18%)
163	GDP	PL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	OK	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.61	9 (18%)
163	GDP	LK	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	OW	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
165	GTP	IO	501	164	33,34,34	0.98	2 (6%)	50,54,54	1.61	9 (18%)
165	GTP	TM	501	164	33,34,34	0.98	2 (6%)	50,54,54	1.58	10 (20%)
165	GTP	IE	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.62	9 (18%)
163	GDP	DU	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	GG	501	164	33,34,34	0.86	1 (3%)	50,54,54	1.62	10 (20%)
163	GDP	CS	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	5 (11%)
165	GTP	TS	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
165	GTP	US	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	SL	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	LL	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.54	8 (16%)
163	GDP	MV	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	HN	503	164	33,34,34	0.97	2 (6%)	50,54,54	1.59	9 (18%)
168	ATP	6l	400	164	32,33,33	0.36	0	48,52,52	0.38	0
165	GTP	LV	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
163	GDP	DM	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	JC	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	KA	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	HP	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	PE	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.59	8 (16%)
163	GDP	LS	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
163	GDP	JQ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	KH	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
163	GDP	FF	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	UK	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.55	8 (16%)
163	GDP	QA	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	GW	501	164	33,34,34	0.93	0	50,54,54	1.59	9 (18%)
165	GTP	HW	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
163	GDP	CC	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
165	GTP	RO	501	164	33,34,34	0.97	2 (6%)	50,54,54	1.55	8 (16%)
165	GTP	JW	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
163	GDP	CY	500	-	29,30,30	1.20	3 (10%)	45,47,47	1.81	7 (15%)
163	GDP	JK	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	HM	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.55	9 (18%)
163	GDP	N	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	CW	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.86	7 (15%)
165	GTP	UA	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.55	9 (18%)
165	GTP	VH	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
163	GDP	A	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.80	7 (15%)
163	GDP	EX	500	-	29,30,30	1.24	4 (13%)	45,47,47	1.71	6 (13%)
165	GTP	OP	503	164	33,34,34	0.95	2 (6%)	50,54,54	1.58	10 (20%)
163	GDP	FL	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	JY	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	IS	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	RV	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.58	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	DH	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.56	9 (18%)
165	GTP	RX	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
163	GDP	EV	500	-	29,30,30	1.14	4 (13%)	45,47,47	1.75	7 (15%)
168	ATP	6p	500	164	32,33,33	0.48	0	48,52,52	0.30	0
163	GDP	KK	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	QH	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.63	10 (20%)
163	GDP	TD	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
163	GDP	SR	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	KZ	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
165	GTP	PG	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	LA	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	RO	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	JZ	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	DE	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	5 (11%)
165	GTP	UQ	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.55	9 (18%)
163	GDP	RG	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	OB	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	JO	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	NJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	GT	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	HQ	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.55	9 (18%)
163	GDP	UF	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	DI	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	PM	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.56	8 (16%)
165	GTP	MG	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	RC	501	164	33,34,34	0.97	2 (6%)	50,54,54	1.55	8 (16%)
163	GDP	QM	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	IF	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	IU	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
165	GTP	LJ	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
163	GDP	CU	500	-	29,30,30	1.15	4 (13%)	45,47,47	1.72	7 (15%)
163	GDP	WN	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	KC	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	BF	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
163	GDP	TV	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	RF	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
163	GDP	ED	500	-	29,30,30	1.17	4 (13%)	45,47,47	1.76	6 (13%)
163	GDP	WD	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	UN	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	FC	501	164	33,34,34	0.89	0	50,54,54	1.55	8 (16%)
163	GDP	GN	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	WX	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	HH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
163	GDP	QC	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	QU	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
165	GTP	T	503	164	33,34,34	0.97	2 (6%)	50,54,54	1.58	10 (20%)
163	GDP	GP	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	PB	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	ES	501	164	33,34,34	0.93	0	50,54,54	1.63	10 (20%)
165	GTP	EJ	501	164	33,34,34	0.99	2 (6%)	50,54,54	1.61	10 (20%)
165	GTP	BK	501	164	33,34,34	0.93	0	50,54,54	1.55	8 (16%)
165	GTP	MA	501	164	33,34,34	0.98	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	DC	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
163	GDP	RI	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	MI	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.54	8 (16%)
165	GTP	DN	501	164	33,34,34	0.92	0	50,54,54	1.60	8 (16%)
163	GDP	U	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	NO	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	HB	503	164	33,34,34	0.97	2 (6%)	50,54,54	1.59	10 (20%)
165	GTP	NA	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
165	GTP	QO	501	164	33,34,34	0.96	2 (6%)	50,54,54	1.59	9 (18%)
165	GTP	PK	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
165	GTP	SE	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.59	10 (20%)
163	GDP	KQ	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	FV	503	-	33,34,34	0.90	1 (3%)	50,54,54	1.62	8 (16%)
165	GTP	LF	502	164	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
163	GDP	TJ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
163	GDP	BR	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	MC	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	WC	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.55	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	MS	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	IR	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	DD	501	164	33,34,34	0.92	0	50,54,54	1.63	10 (20%)
165	GTP	IG	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	FR	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	SU	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	NM	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	CT	501	164	33,34,34	0.93	2 (6%)	50,54,54	1.64	10 (20%)
163	GDP	BP	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	EO	501	164	33,34,34	0.92	0	50,54,54	1.55	9 (18%)
163	GDP	KI	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	JG	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	LH	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
165	GTP	VA	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	HD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	BM	501	164	33,34,34	0.95	0	50,54,54	1.55	8 (16%)
165	GTP	HG	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
165	GTP	AK	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.58	8 (16%)
165	GTP	VS	501	164	33,34,34	1.00	3 (9%)	50,54,54	1.57	9 (18%)
165	GTP	OD	503	164	33,34,34	0.96	2 (6%)	50,54,54	1.59	10 (20%)
163	GDP	SD	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
165	GTP	TU	501	164	33,34,34	0.98	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	TB	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	TT	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	NU	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
163	GDP	EH	500	-	29,30,30	1.17	4 (13%)	45,47,47	1.75	8 (17%)
163	GDP	VF	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	QO	500	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	LP	502	164	33,34,34	0.95	1 (3%)	50,54,54	1.54	8 (16%)
163	GDP	FB	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	SB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	OL	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	IT	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	ED	501	164	33,34,34	0.94	0	50,54,54	1.58	9 (18%)
163	GDP	AH	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
163	GDP	UX	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
165	GTP	WK	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
165	GTP	SM	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
165	GTP	TQ	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	NT	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	WU	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	PJ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	OH	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	SK	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	J	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.55	8 (16%)
165	GTP	QU	501	164	33,34,34	0.95	2 (6%)	50,54,54	1.59	10 (20%)
165	GTP	DL	501	-	33,34,34	0.90	0	50,54,54	1.59	9 (18%)
165	GTP	RR	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
163	GDP	AZ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	QI	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	VY	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	HJ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	OV	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	MO	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	KP	502	164	33,34,34	0.97	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	WM	501	164	33,34,34	0.98	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	KL	501	164	33,34,34	0.96	2 (6%)	50,54,54	1.58	9 (18%)
165	GTP	ME	501	164	33,34,34	0.99	2 (6%)	50,54,54	1.58	9 (18%)
168	ATP	2x	501	-	32,33,33	0.33	0	48,52,52	0.28	0
165	GTP	IM	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	RB	501	164	33,34,34	0.98	2 (6%)	50,54,54	1.56	8 (16%)
163	GDP	EN	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	FI	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.59	10 (20%)
165	GTP	UG	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
163	GDP	F	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
168	ATP	2v	501	-	32,33,33	0.30	0	48,52,52	0.31	0
165	GTP	OS	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	LD	502	164	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
165	GTP	QT	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.63	11 (22%)
165	GTP	TO	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.58	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	TC	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
163	GDP	HN	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
165	GTP	NR	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.60	9 (18%)
165	GTP	KF	501	164	33,34,34	0.98	2 (6%)	50,54,54	1.56	9 (18%)
165	GTP	VE	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
163	GDP	NF	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	VT	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
163	GDP	UR	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	MF	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	KU	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	MP	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	TK	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.53	8 (16%)
163	GDP	QQ	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	FQ	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	NL	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	WT	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	RH	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
163	GDP	RM	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
165	GTP	KB	502	164	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
165	GTP	BS	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.55	8 (16%)
163	GDP	IJ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	IC	501	164	33,34,34	0.98	2 (6%)	50,54,54	1.61	9 (18%)
165	GTP	WO	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.55	9 (18%)
163	GDP	EP	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	BD	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	8 (17%)
165	GTP	KX	501	164	33,34,34	0.96	2 (6%)	50,54,54	1.59	9 (18%)
165	GTP	GO	501	164	33,34,34	0.89	0	50,54,54	1.59	9 (18%)
163	GDP	VB	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
163	GDP	V	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	WP	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
163	GDP	FJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	AP	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	LN	502	164	33,34,34	0.96	1 (3%)	50,54,54	1.55	9 (18%)
165	GTP	WS	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	GK	501	164	33,34,34	0.95	0	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
163	GDP	NR	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	ML	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	LG	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
163	GDP	MH	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	DW	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	EM	501	164	33,34,34	0.94	0	50,54,54	1.56	8 (16%)
165	GTP	GS	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.61	8 (16%)
165	GTP	KT	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
163	GDP	OP	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	UE	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	JI	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	ND	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	8 (17%)
163	GDP	RU	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	HX	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	DT	501	164	33,34,34	0.87	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	NE	501	164	33,34,34	1.00	2 (6%)	50,54,54	1.56	9 (18%)
165	GTP	UC	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
163	GDP	MT	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	PP	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	TL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	UD	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	VQ	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	KN	502	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
163	GDP	PH	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
163	GDP	AR	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
163	GDP	FV	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	WQ	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
163	GDP	CM	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	9 (20%)
163	GDP	W	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	WG	501	164	33,34,34	0.88	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	NF	501	-	33,34,34	1.02	3 (9%)	50,54,54	1.60	9 (18%)
165	GTP	KJ	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
165	GTP	VO	501	164	33,34,34	0.99	2 (6%)	50,54,54	1.55	8 (16%)
165	GTP	BY	501	164	33,34,34	0.94	0	50,54,54	1.53	8 (16%)
165	GTP	KR	501	164	33,34,34	0.99	2 (6%)	50,54,54	1.56	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	PU	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	CK	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)
163	GDP	DY	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
163	GDP	EB	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	6 (13%)
163	GDP	WB	500	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	AL	500	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	8 (17%)
163	GDP	FH	500	-	29,30,30	1.15	4 (13%)	45,47,47	1.72	7 (15%)
163	GDP	NN	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	SI	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	G	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	KD	502	164	33,34,34	0.97	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	RJ	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.57	8 (16%)
163	GDP	CA	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	EP	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
165	GTP	PC	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.56	8 (16%)
163	GDP	UT	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	IQ	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.62	9 (18%)
165	GTP	UU	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.60	9 (18%)
163	GDP	UL	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	LU	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	AI	501	164	33,34,34	0.87	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	PR	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
163	GDP	MN	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	BX	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
165	GTP	JF	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
163	GDP	DG	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
165	GTP	KV	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.58	8 (16%)
163	GDP	GL	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	CQ	501	164	33,34,34	0.96	2 (6%)	50,54,54	1.57	9 (18%)
165	GTP	PQ	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.59	8 (16%)
165	GTP	JR	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
165	GTP	JD	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.55	8 (16%)
163	GDP	EF	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	P	500	-	29,30,30	1.18	3 (10%)	45,47,47	1.82	7 (15%)
165	GTP	AA	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.55	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	EA	501	164	33,34,34	0.96	1 (3%)	50,54,54	1.62	8 (16%)
163	GDP	LQ	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	EC	501	164	33,34,34	0.92	0	50,54,54	1.55	9 (18%)
163	GDP	OT	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
163	GDP	OX	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	RE	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	8 (17%)
163	GDP	QE	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	IL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
165	GTP	PY	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.57	8 (16%)
163	GDP	GX	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	GU	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
163	GDP	KM	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	JA	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	OA	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
165	GTP	JB	501	164	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
163	GDP	JU	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	GV	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	6 (13%)
165	GTP	VW	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
165	GTP	GQ	501	164	33,34,34	0.88	2 (6%)	50,54,54	1.70	10 (20%)
163	GDP	SF	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	UM	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.55	9 (18%)
163	GDP	PV	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
165	GTP	CW	501	164	33,34,34	0.95	0	50,54,54	1.53	8 (16%)
165	GTP	IA	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
163	GDP	WH	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	QG	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	IP	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
163	GDP	UV	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	BU	501	164	33,34,34	0.97	2 (6%)	50,54,54	1.61	10 (20%)
165	GTP	CK	503	164	33,34,34	0.92	1 (3%)	50,54,54	1.57	8 (16%)
165	GTP	IY	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.57	8 (16%)
168	ATP	6u	700	-	32,33,33	0.36	0	48,52,52	0.28	0
163	GDP	VD	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	VJ	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	8 (17%)
163	GDP	WV	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
163	GDP	CQ	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	LR	502	164	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
163	GDP	UP	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)
165	GTP	JN	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	Q	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
165	GTP	JH	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
165	GTP	OU	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
163	GDP	AN	500	-	29,30,30	1.14	4 (13%)	45,47,47	1.71	7 (15%)
165	GTP	EI	501	164	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	FO	501	164	33,34,34	0.90	0	50,54,54	1.55	9 (18%)
165	GTP	PW	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	RT	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
165	GTP	AW	501	164	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
165	GTP	NY	501	164	33,34,34	0.97	2 (6%)	50,54,54	1.56	9 (18%)
165	GTP	BE	501	164	33,34,34	0.91	0	50,54,54	1.58	10 (20%)
163	GDP	KW	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
165	GTP	AD	501	164	33,34,34	0.88	1 (3%)	50,54,54	1.60	10 (20%)
163	GDP	UH	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	BI	501	164	33,34,34	0.97	3 (9%)	50,54,54	1.62	9 (18%)
163	GDP	JS	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	SV	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	AB	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
165	GTP	DE	501	164	33,34,34	0.92	2 (6%)	50,54,54	1.62	9 (18%)
165	GTP	JP	501	164	33,34,34	0.94	1 (3%)	50,54,54	1.55	8 (16%)
163	GDP	TH	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	KE	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
163	GDP	KG	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
163	GDP	DO	500	-	29,30,30	1.16	4 (13%)	45,47,47	1.74	5 (11%)
168	ATP	9R	500	164	32,33,33	0.36	0	48,52,52	0.30	0
165	GTP	JT	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
163	GDP	AV	500	-	29,30,30	1.15	4 (13%)	45,47,47	1.73	7 (15%)
163	GDP	TR	500	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	6 (13%)
163	GDP	RW	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
163	GDP	PF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
163	GDP	GF	500	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
165	GTP	FS	501	164	33,34,34	0.88	0	50,54,54	1.62	8 (16%)
165	GTP	QR	501	164	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
165	GTP	QC	501	164	33,34,34	0.97	2 (6%)	50,54,54	1.58	9 (18%)
165	GTP	BG	501	164	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
165	GTP	FJ	503	164	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
163	GDP	RK	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
165	GTP	OI	501	164	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
163	GDP	FT	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.68	7 (15%)
165	GTP	MM	501	164	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)

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
165	GTP	VK	501	164	-	5/22/38/38	0/3/3/3
163	GDP	AF	500	-	-	1/16/32/32	0/3/3/3
165	GTP	FG	501	164	-	8/22/38/38	0/3/3/3
165	GTP	SW	501	164	-	0/22/38/38	0/3/3/3
163	GDP	MJ	500	-	-	3/16/32/32	0/3/3/3
163	GDP	VR	500	-	-	1/16/32/32	0/3/3/3
163	GDP	TF	500	-	-	1/16/32/32	0/3/3/3
163	GDP	DS	500	-	-	2/16/32/32	0/3/3/3
165	GTP	CB	501	164	-	3/22/38/38	0/3/3/3
163	GDP	GB	500	-	-	2/16/32/32	0/3/3/3
163	GDP	HB	501	-	-	3/16/32/32	0/3/3/3
165	GTP	QI	501	164	-	4/22/38/38	0/3/3/3
165	GTP	SC	501	164	-	6/22/38/38	0/3/3/3
165	GTP	IW	501	164	-	3/22/38/38	0/3/3/3
163	GDP	JE	500	-	-	1/16/32/32	0/3/3/3
163	GDP	MZ	500	-	-	2/16/32/32	0/3/3/3
163	GDP	DQ	500	-	-	3/16/32/32	0/3/3/3
165	GTP	AU	501	164	-	3/22/38/38	0/3/3/3
163	GDP	VP	500	-	-	1/16/32/32	0/3/3/3
163	GDP	IB	500	-	-	3/16/32/32	0/3/3/3
165	GTP	GI	501	164	-	1/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	AX	500	-	-	2/16/32/32	0/3/3/3
163	GDP	ON	500	-	-	5/16/32/32	0/3/3/3
165	GTP	MU	501	164	-	5/22/38/38	0/3/3/3
165	GTP	AB	501	164	-	5/22/38/38	0/3/3/3
163	GDP	NV	501	-	-	1/16/32/32	0/3/3/3
165	GTP	HE	501	164	-	4/22/38/38	0/3/3/3
165	GTP	TI	501	164	-	4/22/38/38	0/3/3/3
163	GDP	CO	500	-	-	0/16/32/32	0/3/3/3
165	GTP	MQ	501	164	-	5/22/38/38	0/3/3/3
168	ATP	2w	501	-	-	7/22/38/38	0/3/3/3
163	GDP	NX	500	-	-	1/16/32/32	0/3/3/3
165	GTP	TE	501	164	-	6/22/38/38	0/3/3/3
163	GDP	LY	500	-	-	1/16/32/32	0/3/3/3
165	GTP	LT	501	164	-	3/22/38/38	0/3/3/3
163	GDP	UB	500	-	-	3/16/32/32	0/3/3/3
168	ATP	7D	601	164	-	10/22/38/38	0/3/3/3
163	GDP	JW	500	-	-	3/16/32/32	0/3/3/3
165	GTP	FA	501	164	-	4/22/38/38	0/3/3/3
165	GTP	QB	501	164	-	2/22/38/38	0/3/3/3
165	GTP	CC	501	164	-	4/22/38/38	0/3/3/3
163	GDP	DA	500	-	-	4/16/32/32	0/3/3/3
165	GTP	DB	501	164	-	3/22/38/38	0/3/3/3
165	GTP	GC	501	164	-	5/22/38/38	0/3/3/3
168	ATP	8a	801	-	-	1/22/38/38	0/3/3/3
163	GDP	OD	501	-	-	2/16/32/32	0/3/3/3
163	GDP	VV	500	-	-	2/16/32/32	0/3/3/3
165	GTP	R	501	164	-	6/22/38/38	0/3/3/3
165	GTP	WY	501	164	-	3/22/38/38	0/3/3/3
165	GTP	TG	501	164	-	1/22/38/38	0/3/3/3
163	GDP	MD	500	-	-	1/16/32/32	0/3/3/3
163	GDP	VH	500	-	-	1/16/32/32	0/3/3/3
163	GDP	BL	500	-	-	4/16/32/32	0/3/3/3
163	GDP	BN	500	-	-	3/16/32/32	0/3/3/3
165	GTP	D	501	-	-	9/22/38/38	0/3/3/3
165	GTP	NI	501	164	-	1/22/38/38	0/3/3/3
163	GDP	GJ	500	-	-	2/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	PX	501	-	-	1/16/32/32	0/3/3/3
165	GTP	DP	501	164	-	3/22/38/38	0/3/3/3
165	GTP	VG	501	164	-	4/22/38/38	0/3/3/3
163	GDP	GR	500	-	-	0/16/32/32	0/3/3/3
165	GTP	MJ	501	164	-	5/22/38/38	0/3/3/3
165	GTP	C	501	164	-	6/22/38/38	0/3/3/3
163	GDP	RC	500	-	-	1/16/32/32	0/3/3/3
165	GTP	GE	501	164	-	5/22/38/38	0/3/3/3
163	GDP	HR	500	-	-	2/16/32/32	0/3/3/3
165	GTP	AM	501	164	-	5/22/38/38	0/3/3/3
165	GTP	G	501	164	-	7/22/38/38	0/3/3/3
165	GTP	LZ	502	164	-	3/22/38/38	0/3/3/3
165	GTP	OM	501	164	-	5/22/38/38	0/3/3/3
163	GDP	O	500	-	-	2/16/32/32	0/3/3/3
165	GTP	QX	501	-	-	3/22/38/38	0/3/3/3
163	GDP	VX	500	-	-	1/16/32/32	0/3/3/3
165	GTP	II	501	164	-	3/22/38/38	0/3/3/3
163	GDP	OJ	500	-	-	3/16/32/32	0/3/3/3
165	GTP	LB	501	164	-	3/22/38/38	0/3/3/3
163	GDP	PT	500	-	-	1/16/32/32	0/3/3/3
163	GDP	CI	500	-	-	4/16/32/32	0/3/3/3
165	GTP	UO	501	164	-	3/22/38/38	0/3/3/3
165	GTP	PA	501	164	-	0/22/38/38	0/3/3/3
163	GDP	IH	500	-	-	2/16/32/32	0/3/3/3
165	GTP	SS	501	164	-	8/22/38/38	0/3/3/3
163	GDP	QW	500	-	-	5/16/32/32	0/3/3/3
163	GDP	NH	500	-	-	2/16/32/32	0/3/3/3
165	GTP	DX	501	-	-	9/22/38/38	0/3/3/3
163	GDP	AD	500	-	-	3/16/32/32	0/3/3/3
163	GDP	NP	500	-	-	0/16/32/32	0/3/3/3
165	GTP	EG	501	164	-	7/22/38/38	0/3/3/3
165	GTP	HK	501	164	-	4/22/38/38	0/3/3/3
165	GTP	CO	501	164	-	4/22/38/38	0/3/3/3
165	GTP	AS	501	164	-	8/22/38/38	0/3/3/3
163	GDP	SN	501	-	-	3/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	BV	500	-	-	2/16/32/32	0/3/3/3
165	GTP	SQ	501	164	-	5/22/38/38	0/3/3/3
165	GTP	OY	501	164	-	5/22/38/38	0/3/3/3
163	GDP	WR	501	-	-	1/16/32/32	0/3/3/3
163	GDP	LC	500	-	-	2/16/32/32	0/3/3/3
165	GTP	HA	501	164	-	3/22/38/38	0/3/3/3
165	GTP	FM	501	164	-	2/22/38/38	0/3/3/3
163	GDP	SJ	501	-	-	2/16/32/32	0/3/3/3
165	GTP	EV	501	164	-	4/22/38/38	0/3/3/3
163	GDP	IV	500	-	-	2/16/32/32	0/3/3/3
163	GDP	TX	500	-	-	0/16/32/32	0/3/3/3
163	GDP	CG	500	-	-	1/16/32/32	0/3/3/3
165	GTP	AY	501	164	-	5/22/38/38	0/3/3/3
163	GDP	NB	500	-	-	3/16/32/32	0/3/3/3
163	GDP	IX	501	-	-	0/16/32/32	0/3/3/3
163	GDP	TN	500	-	-	3/16/32/32	0/3/3/3
163	GDP	HT	501	-	-	1/16/32/32	0/3/3/3
163	GDP	WJ	500	-	-	1/16/32/32	0/3/3/3
163	GDP	FP	500	-	-	1/16/32/32	0/3/3/3
163	GDP	LI	500	-	-	3/16/32/32	0/3/3/3
163	GDP	BT	500	-	-	3/16/32/32	0/3/3/3
163	GDP	GD	500	-	-	4/16/32/32	0/3/3/3
165	GTP	HU	501	164	-	2/22/38/38	0/3/3/3
165	GTP	HY	501	164	-	3/22/38/38	0/3/3/3
165	GTP	BW	501	164	-	3/22/38/38	0/3/3/3
163	GDP	ET	500	-	-	1/16/32/32	0/3/3/3
163	GDP	BJ	500	-	-	3/16/32/32	0/3/3/3
163	GDP	KO	500	-	-	1/16/32/32	0/3/3/3
163	GDP	HV	500	-	-	2/16/32/32	0/3/3/3
165	GTP	OC	501	164	-	1/22/38/38	0/3/3/3
163	GDP	LE	500	-	-	2/16/32/32	0/3/3/3
163	GDP	RA	500	-	-	1/16/32/32	0/3/3/3
165	GTP	NK	501	-	-	3/22/38/38	0/3/3/3
163	GDP	TP	500	-	-	1/16/32/32	0/3/3/3
165	GTP	NW	501	-	-	3/22/38/38	0/3/3/3
163	GDP	EJ	500	-	-	1/16/32/32	0/3/3/3
165	GTP	PS	501	-	-	5/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	PN	500	-	-	1/16/32/32	0/3/3/3
165	GTP	WI	501	164	-	3/22/38/38	0/3/3/3
165	GTP	WE	501	164	-	8/22/38/38	0/3/3/3
165	GTP	BO	501	164	-	4/22/38/38	0/3/3/3
163	GDP	HL	501	-	-	1/16/32/32	0/3/3/3
163	GDP	MR	500	-	-	3/16/32/32	0/3/3/3
165	GTP	CJ	501	164	-	3/22/38/38	0/3/3/3
163	GDP	FN	500	-	-	0/16/32/32	0/3/3/3
163	GDP	GH	500	-	-	3/16/32/32	0/3/3/3
163	GDP	MX	500	-	-	1/16/32/32	0/3/3/3
165	GTP	FE	501	164	-	6/22/38/38	0/3/3/3
163	GDP	I	501	-	-	0/16/32/32	0/3/3/3
165	GTP	QN	501	164	-	2/22/38/38	0/3/3/3
163	GDP	KY	500	-	-	2/16/32/32	0/3/3/3
165	GTP	FT	503	164	-	5/22/38/38	0/3/3/3
165	GTP	EU	501	164	-	4/22/38/38	0/3/3/3
165	GTP	HI	501	164	-	2/22/38/38	0/3/3/3
165	GTP	OO	501	164	-	1/22/38/38	0/3/3/3
165	GTP	DJ	501	164	-	4/22/38/38	0/3/3/3
165	GTP	HS	501	164	-	3/22/38/38	0/3/3/3
165	GTP	NC	501	164	-	3/22/38/38	0/3/3/3
165	GTP	SO	501	164	-	6/22/38/38	0/3/3/3
165	GTP	IK	501	164	-	3/22/38/38	0/3/3/3
165	GTP	JV	501	164	-	3/22/38/38	0/3/3/3
163	GDP	VN	500	-	-	1/16/32/32	0/3/3/3
163	GDP	HF	500	-	-	2/16/32/32	0/3/3/3
163	GDP	RS	500	-	-	1/16/32/32	0/3/3/3
165	GTP	JK	501	164	-	3/22/38/38	0/3/3/3
163	GDP	FD	500	-	-	3/16/32/32	0/3/3/3
165	GTP	K	501	164	-	2/22/38/38	0/3/3/3
163	GDP	H	500	-	-	1/16/32/32	0/3/3/3
165	GTP	MY	501	164	-	2/22/38/38	0/3/3/3
165	GTP	JJ	501	164	-	3/22/38/38	0/3/3/3
163	GDP	AJ	500	-	-	2/16/32/32	0/3/3/3
163	GDP	CE	500	-	-	3/16/32/32	0/3/3/3
163	GDP	SH	500	-	-	2/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	BH	500	-	-	3/16/32/32	0/3/3/3
163	GDP	FX	500	-	-	4/16/32/32	0/3/3/3
163	GDP	AP	500	-	-	1/16/32/32	0/3/3/3
163	GDP	LO	500	-	-	3/16/32/32	0/3/3/3
165	GTP	CH	501	164	-	5/22/38/38	0/3/3/3
165	GTP	WA	501	164	-	2/22/38/38	0/3/3/3
165	GTP	DV	501	164	-	3/22/38/38	0/3/3/3
165	GTP	QF	501	164	-	2/22/38/38	0/3/3/3
165	GTP	VM	501	164	-	5/22/38/38	0/3/3/3
165	GTP	UW	501	164	-	5/22/38/38	0/3/3/3
163	GDP	JM	501	-	-	0/16/32/32	0/3/3/3
165	GTP	AO	501	164	-	4/22/38/38	0/3/3/3
163	GDP	QK	500	-	-	5/16/32/32	0/3/3/3
163	GDP	E	500	-	-	3/16/32/32	0/3/3/3
163	GDP	ST	500	-	-	2/16/32/32	0/3/3/3
165	GTP	CE	501	164	-	6/22/38/38	0/3/3/3
163	GDP	PD	500	-	-	4/16/32/32	0/3/3/3
163	GDP	OR	500	-	-	1/16/32/32	0/3/3/3
165	GTP	SA	501	164	-	3/22/38/38	0/3/3/3
165	GTP	AG	501	164	-	6/22/38/38	0/3/3/3
163	GDP	OF	500	-	-	1/16/32/32	0/3/3/3
165	GTP	BQ	501	164	-	8/22/38/38	0/3/3/3
168	ATP	7A	402	-	-	6/22/38/38	0/3/3/3
163	GDP	RQ	500	-	-	0/16/32/32	0/3/3/3
163	GDP	T	501	-	-	1/16/32/32	0/3/3/3
165	GTP	RN	501	164	-	3/22/38/38	0/3/3/3
163	GDP	EL	500	-	-	3/16/32/32	0/3/3/3
163	GDP	LM	500	-	-	1/16/32/32	0/3/3/3
165	GTP	VC	501	164	-	6/22/38/38	0/3/3/3
163	GDP	MB	500	-	-	2/16/32/32	0/3/3/3
163	GDP	S	500	-	-	2/16/32/32	0/3/3/3
165	GTP	CV	501	164	-	3/22/38/38	0/3/3/3
163	GDP	SP	500	-	-	3/16/32/32	0/3/3/3
165	GTP	BA	501	164	-	3/22/38/38	0/3/3/3
163	GDP	QS	500	-	-	1/16/32/32	0/3/3/3
165	GTP	RL	501	164	-	9/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	UI	501	164	-	3/22/38/38	0/3/3/3
165	GTP	PI	501	164	-	4/22/38/38	0/3/3/3
163	GDP	UJ	500	-	-	1/16/32/32	0/3/3/3
165	GTP	GL	501	164	-	9/22/38/38	0/3/3/3
165	GTP	OG	501	164	-	3/22/38/38	0/3/3/3
165	GTP	SG	501	164	-	8/22/38/38	0/3/3/3
165	GTP	PO	501	164	-	3/22/38/38	0/3/3/3
165	GTP	TW	501	164	-	5/22/38/38	0/3/3/3
163	GDP	IN	500	-	-	3/16/32/32	0/3/3/3
163	GDP	WF	501	-	-	1/16/32/32	0/3/3/3
163	GDP	KS	500	-	-	2/16/32/32	0/3/3/3
163	GDP	M	500	-	-	3/16/32/32	0/3/3/3
163	GDP	VT	500	-	-	1/16/32/32	0/3/3/3
165	GTP	L	501	164	-	4/22/38/38	0/3/3/3
165	GTP	MV	501	164	-	5/22/38/38	0/3/3/3
163	GDP	LW	500	-	-	1/16/32/32	0/3/3/3
163	GDP	DK	501	-	-	2/16/32/32	0/3/3/3
163	GDP	ID	500	-	-	1/16/32/32	0/3/3/3
165	GTP	WW	501	164	-	5/22/38/38	0/3/3/3
163	GDP	AT	500	-	-	4/16/32/32	0/3/3/3
165	GTP	LX	501	164	-	4/22/38/38	0/3/3/3
163	GDP	ER	500	-	-	2/16/32/32	0/3/3/3
163	GDP	VL	500	-	-	1/16/32/32	0/3/3/3
165	GTP	QL	501	-	-	3/22/38/38	0/3/3/3
165	GTP	NQ	501	164	-	4/22/38/38	0/3/3/3
163	GDP	WL	500	-	-	1/16/32/32	0/3/3/3
165	GTP	CN	501	164	-	3/22/38/38	0/3/3/3
165	GTP	DQ	501	164	-	6/22/38/38	0/3/3/3
163	GDP	PL	501	-	-	1/16/32/32	0/3/3/3
165	GTP	OK	501	-	-	6/22/38/38	0/3/3/3
163	GDP	LK	500	-	-	1/16/32/32	0/3/3/3
165	GTP	OW	501	-	-	6/22/38/38	0/3/3/3
165	GTP	IO	501	164	-	4/22/38/38	0/3/3/3
165	GTP	TM	501	164	-	7/22/38/38	0/3/3/3
165	GTP	IE	501	164	-	2/22/38/38	0/3/3/3
163	GDP	DU	500	-	-	2/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	GG	501	164	-	4/22/38/38	0/3/3/3
163	GDP	CS	500	-	-	2/16/32/32	0/3/3/3
165	GTP	TS	501	164	-	1/22/38/38	0/3/3/3
165	GTP	US	501	164	-	5/22/38/38	0/3/3/3
163	GDP	SL	500	-	-	2/16/32/32	0/3/3/3
165	GTP	LL	501	164	-	4/22/38/38	0/3/3/3
163	GDP	MV	500	-	-	3/16/32/32	0/3/3/3
165	GTP	HN	503	164	-	7/22/38/38	0/3/3/3
168	ATP	6l	400	164	-	7/22/38/38	0/3/3/3
165	GTP	LV	501	164	-	5/22/38/38	0/3/3/3
163	GDP	DM	500	-	-	2/16/32/32	0/3/3/3
163	GDP	JC	500	-	-	2/16/32/32	0/3/3/3
163	GDP	KA	500	-	-	3/16/32/32	0/3/3/3
163	GDP	HP	501	-	-	3/16/32/32	0/3/3/3
165	GTP	PE	501	164	-	0/22/38/38	0/3/3/3
163	GDP	LS	500	-	-	2/16/32/32	0/3/3/3
163	GDP	JQ	500	-	-	1/16/32/32	0/3/3/3
165	GTP	KH	501	164	-	5/22/38/38	0/3/3/3
163	GDP	FF	500	-	-	4/16/32/32	0/3/3/3
165	GTP	UK	501	164	-	5/22/38/38	0/3/3/3
163	GDP	QA	500	-	-	1/16/32/32	0/3/3/3
165	GTP	GW	501	164	-	3/22/38/38	0/3/3/3
165	GTP	HW	501	164	-	4/22/38/38	0/3/3/3
163	GDP	CC	500	-	-	3/16/32/32	0/3/3/3
165	GTP	RO	501	164	-	7/22/38/38	0/3/3/3
165	GTP	JW	501	164	-	3/22/38/38	0/3/3/3
163	GDP	CY	500	-	-	5/16/32/32	0/3/3/3
163	GDP	JK	500	-	-	3/16/32/32	0/3/3/3
165	GTP	HM	501	164	-	3/22/38/38	0/3/3/3
163	GDP	N	500	-	-	1/16/32/32	0/3/3/3
163	GDP	CW	500	-	-	5/16/32/32	0/3/3/3
165	GTP	UA	501	164	-	5/22/38/38	0/3/3/3
165	GTP	VH	501	164	-	4/22/38/38	0/3/3/3
163	GDP	A	501	-	-	2/16/32/32	0/3/3/3
163	GDP	EX	500	-	-	2/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	OP	503	164	-	4/22/38/38	0/3/3/3
163	GDP	FL	500	-	-	4/16/32/32	0/3/3/3
163	GDP	JY	501	-	-	0/16/32/32	0/3/3/3
165	GTP	IS	501	164	-	7/22/38/38	0/3/3/3
165	GTP	RV	501	-	-	1/22/38/38	0/3/3/3
165	GTP	DH	501	164	-	1/22/38/38	0/3/3/3
165	GTP	RX	501	164	-	9/22/38/38	0/3/3/3
163	GDP	EV	500	-	-	4/16/32/32	0/3/3/3
168	ATP	6p	500	164	-	9/22/38/38	0/3/3/3
163	GDP	KK	500	-	-	1/16/32/32	0/3/3/3
165	GTP	QH	501	164	-	10/22/38/38	0/3/3/3
163	GDP	TD	500	-	-	1/16/32/32	0/3/3/3
163	GDP	SR	500	-	-	1/16/32/32	0/3/3/3
165	GTP	KZ	501	164	-	3/22/38/38	0/3/3/3
165	GTP	PG	501	-	-	5/22/38/38	0/3/3/3
163	GDP	LA	500	-	-	2/16/32/32	0/3/3/3
163	GDP	RO	500	-	-	1/16/32/32	0/3/3/3
165	GTP	JZ	501	164	-	3/22/38/38	0/3/3/3
163	GDP	DE	500	-	-	4/16/32/32	0/3/3/3
165	GTP	UQ	501	164	-	9/22/38/38	0/3/3/3
163	GDP	RG	500	-	-	1/16/32/32	0/3/3/3
163	GDP	OB	500	-	-	5/16/32/32	0/3/3/3
163	GDP	JO	500	-	-	2/16/32/32	0/3/3/3
163	GDP	NJ	501	-	-	1/16/32/32	0/3/3/3
163	GDP	GT	501	-	-	2/16/32/32	0/3/3/3
165	GTP	HQ	501	164	-	4/22/38/38	0/3/3/3
163	GDP	UF	500	-	-	1/16/32/32	0/3/3/3
163	GDP	DI	500	-	-	2/16/32/32	0/3/3/3
165	GTP	PM	501	164	-	3/22/38/38	0/3/3/3
165	GTP	MG	501	164	-	5/22/38/38	0/3/3/3
165	GTP	RC	501	164	-	7/22/38/38	0/3/3/3
163	GDP	QM	500	-	-	2/16/32/32	0/3/3/3
163	GDP	IF	500	-	-	3/16/32/32	0/3/3/3
165	GTP	IU	501	164	-	3/22/38/38	0/3/3/3
165	GTP	LJ	501	164	-	4/22/38/38	0/3/3/3
163	GDP	CU	500	-	-	0/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	WN	500	-	-	1/16/32/32	0/3/3/3
163	GDP	KC	500	-	-	1/16/32/32	0/3/3/3
163	GDP	BF	500	-	-	1/16/32/32	0/3/3/3
163	GDP	TV	500	-	-	2/16/32/32	0/3/3/3
165	GTP	RF	501	164	-	1/22/38/38	0/3/3/3
163	GDP	ED	500	-	-	4/16/32/32	0/3/3/3
163	GDP	WD	500	-	-	2/16/32/32	0/3/3/3
163	GDP	UN	500	-	-	3/16/32/32	0/3/3/3
165	GTP	FC	501	164	-	4/22/38/38	0/3/3/3
163	GDP	GN	500	-	-	1/16/32/32	0/3/3/3
163	GDP	WX	500	-	-	1/16/32/32	0/3/3/3
163	GDP	HH	501	-	-	1/16/32/32	0/3/3/3
163	GDP	QC	500	-	-	2/16/32/32	0/3/3/3
163	GDP	QU	500	-	-	2/16/32/32	0/3/3/3
165	GTP	T	503	164	-	7/22/38/38	0/3/3/3
163	GDP	GP	500	-	-	4/16/32/32	0/3/3/3
163	GDP	PB	500	-	-	1/16/32/32	0/3/3/3
165	GTP	ES	501	164	-	7/22/38/38	0/3/3/3
165	GTP	EJ	501	164	-	5/22/38/38	0/3/3/3
165	GTP	BK	501	164	-	3/22/38/38	0/3/3/3
165	GTP	MA	501	164	-	0/22/38/38	0/3/3/3
163	GDP	DC	500	-	-	4/16/32/32	0/3/3/3
163	GDP	RI	500	-	-	0/16/32/32	0/3/3/3
165	GTP	MI	501	164	-	5/22/38/38	0/3/3/3
165	GTP	DN	501	164	-	3/22/38/38	0/3/3/3
163	GDP	U	500	-	-	2/16/32/32	0/3/3/3
165	GTP	NO	501	164	-	3/22/38/38	0/3/3/3
165	GTP	HB	503	164	-	7/22/38/38	0/3/3/3
165	GTP	NA	501	-	-	7/22/38/38	0/3/3/3
165	GTP	QO	501	164	-	5/22/38/38	0/3/3/3
165	GTP	PK	501	164	-	3/22/38/38	0/3/3/3
165	GTP	SE	501	164	-	5/22/38/38	0/3/3/3
163	GDP	KQ	500	-	-	1/16/32/32	0/3/3/3
165	GTP	FV	503	-	-	3/22/38/38	0/3/3/3
165	GTP	LF	502	164	-	2/22/38/38	0/3/3/3
163	GDP	TJ	500	-	-	2/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	BR	500	-	-	3/16/32/32	0/3/3/3
165	GTP	MC	501	164	-	4/22/38/38	0/3/3/3
165	GTP	WC	501	164	-	2/22/38/38	0/3/3/3
165	GTP	MS	501	164	-	5/22/38/38	0/3/3/3
163	GDP	IR	500	-	-	3/16/32/32	0/3/3/3
165	GTP	DD	501	164	-	3/22/38/38	0/3/3/3
165	GTP	IG	501	164	-	7/22/38/38	0/3/3/3
163	GDP	FR	501	-	-	3/16/32/32	0/3/3/3
165	GTP	SU	501	164	-	3/22/38/38	0/3/3/3
165	GTP	NM	501	164	-	4/22/38/38	0/3/3/3
165	GTP	CT	501	164	-	6/22/38/38	0/3/3/3
163	GDP	BP	500	-	-	2/16/32/32	0/3/3/3
165	GTP	EO	501	164	-	4/22/38/38	0/3/3/3
163	GDP	KI	500	-	-	3/16/32/32	0/3/3/3
163	GDP	JG	500	-	-	2/16/32/32	0/3/3/3
165	GTP	LH	501	164	-	3/22/38/38	0/3/3/3
165	GTP	VA	501	164	-	4/22/38/38	0/3/3/3
163	GDP	HD	501	-	-	3/16/32/32	0/3/3/3
165	GTP	BM	501	164	-	3/22/38/38	0/3/3/3
165	GTP	HG	501	164	-	3/22/38/38	0/3/3/3
165	GTP	AK	501	164	-	3/22/38/38	0/3/3/3
165	GTP	VS	501	164	-	4/22/38/38	0/3/3/3
165	GTP	OD	503	164	-	4/22/38/38	0/3/3/3
163	GDP	SD	500	-	-	3/16/32/32	0/3/3/3
165	GTP	TU	501	164	-	4/22/38/38	0/3/3/3
163	GDP	TB	500	-	-	3/16/32/32	0/3/3/3
163	GDP	TT	500	-	-	1/16/32/32	0/3/3/3
165	GTP	NU	501	164	-	1/22/38/38	0/3/3/3
163	GDP	EH	500	-	-	1/16/32/32	0/3/3/3
163	GDP	VF	500	-	-	1/16/32/32	0/3/3/3
163	GDP	QO	500	-	-	2/16/32/32	0/3/3/3
165	GTP	LP	502	164	-	6/22/38/38	0/3/3/3
163	GDP	FB	500	-	-	0/16/32/32	0/3/3/3
163	GDP	SB	501	-	-	3/16/32/32	0/3/3/3
163	GDP	OL	500	-	-	2/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	IT	501	-	-	2/16/32/32	0/3/3/3
165	GTP	ED	501	164	-	4/22/38/38	0/3/3/3
163	GDP	AH	500	-	-	3/16/32/32	0/3/3/3
163	GDP	UX	500	-	-	1/16/32/32	0/3/3/3
165	GTP	WK	501	164	-	5/22/38/38	0/3/3/3
165	GTP	SM	501	164	-	3/22/38/38	0/3/3/3
165	GTP	TQ	501	164	-	6/22/38/38	0/3/3/3
163	GDP	NT	500	-	-	2/16/32/32	0/3/3/3
165	GTP	WU	501	164	-	3/22/38/38	0/3/3/3
163	GDP	PJ	500	-	-	3/16/32/32	0/3/3/3
163	GDP	OH	500	-	-	3/16/32/32	0/3/3/3
165	GTP	SK	501	164	-	0/22/38/38	0/3/3/3
165	GTP	J	501	164	-	8/22/38/38	0/3/3/3
165	GTP	QU	501	164	-	4/22/38/38	0/3/3/3
165	GTP	DL	501	-	-	10/22/38/38	0/3/3/3
165	GTP	RR	501	164	-	1/22/38/38	0/3/3/3
163	GDP	AZ	500	-	-	2/16/32/32	0/3/3/3
163	GDP	QI	500	-	-	2/16/32/32	0/3/3/3
165	GTP	VY	501	164	-	5/22/38/38	0/3/3/3
163	GDP	HJ	500	-	-	2/16/32/32	0/3/3/3
163	GDP	OV	500	-	-	3/16/32/32	0/3/3/3
165	GTP	MO	501	164	-	4/22/38/38	0/3/3/3
165	GTP	KP	502	164	-	3/22/38/38	0/3/3/3
165	GTP	WM	501	164	-	3/22/38/38	0/3/3/3
165	GTP	KL	501	164	-	2/22/38/38	0/3/3/3
165	GTP	ME	501	164	-	5/22/38/38	0/3/3/3
168	ATP	2x	501	-	-	7/22/38/38	0/3/3/3
165	GTP	IM	501	164	-	4/22/38/38	0/3/3/3
165	GTP	RB	501	164	-	3/22/38/38	0/3/3/3
163	GDP	EN	500	-	-	3/16/32/32	0/3/3/3
165	GTP	FI	501	164	-	5/22/38/38	0/3/3/3
165	GTP	UG	501	164	-	5/22/38/38	0/3/3/3
163	GDP	F	500	-	-	3/16/32/32	0/3/3/3
168	ATP	2v	501	-	-	5/22/38/38	0/3/3/3
165	GTP	OS	501	164	-	3/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	LD	502	164	-	6/22/38/38	0/3/3/3
165	GTP	QT	501	164	-	10/22/38/38	0/3/3/3
165	GTP	TO	501	164	-	5/22/38/38	0/3/3/3
165	GTP	TC	501	164	-	5/22/38/38	0/3/3/3
163	GDP	HN	501	-	-	3/16/32/32	0/3/3/3
165	GTP	NR	501	-	-	6/22/38/38	0/3/3/3
165	GTP	KF	501	164	-	6/22/38/38	0/3/3/3
165	GTP	VE	501	164	-	1/22/38/38	0/3/3/3
163	GDP	NF	500	-	-	3/16/32/32	0/3/3/3
165	GTP	VT	501	164	-	4/22/38/38	0/3/3/3
163	GDP	UR	500	-	-	1/16/32/32	0/3/3/3
163	GDP	MF	500	-	-	3/16/32/32	0/3/3/3
163	GDP	KU	500	-	-	3/16/32/32	0/3/3/3
163	GDP	MP	500	-	-	1/16/32/32	0/3/3/3
165	GTP	TK	501	164	-	5/22/38/38	0/3/3/3
163	GDP	QQ	500	-	-	2/16/32/32	0/3/3/3
165	GTP	FQ	501	164	-	6/22/38/38	0/3/3/3
163	GDP	NL	500	-	-	1/16/32/32	0/3/3/3
163	GDP	WT	500	-	-	2/16/32/32	0/3/3/3
165	GTP	RH	501	164	-	2/22/38/38	0/3/3/3
163	GDP	RM	500	-	-	1/16/32/32	0/3/3/3
165	GTP	KB	502	164	-	4/22/38/38	0/3/3/3
165	GTP	BS	501	164	-	1/22/38/38	0/3/3/3
163	GDP	IJ	500	-	-	2/16/32/32	0/3/3/3
165	GTP	IC	501	164	-	4/22/38/38	0/3/3/3
165	GTP	WO	501	164	-	2/22/38/38	0/3/3/3
163	GDP	EP	500	-	-	1/16/32/32	0/3/3/3
163	GDP	BD	500	-	-	2/16/32/32	0/3/3/3
165	GTP	KX	501	164	-	2/22/38/38	0/3/3/3
165	GTP	GO	501	164	-	4/22/38/38	0/3/3/3
163	GDP	VB	500	-	-	1/16/32/32	0/3/3/3
163	GDP	V	500	-	-	1/16/32/32	0/3/3/3
163	GDP	WP	500	-	-	2/16/32/32	0/3/3/3
163	GDP	FJ	501	-	-	2/16/32/32	0/3/3/3
165	GTP	AP	501	164	-	4/22/38/38	0/3/3/3
165	GTP	LN	502	164	-	3/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	WS	501	164	-	1/22/38/38	0/3/3/3
165	GTP	GK	501	164	-	3/22/38/38	0/3/3/3
163	GDP	NR	500	-	-	3/16/32/32	0/3/3/3
163	GDP	ML	500	-	-	1/16/32/32	0/3/3/3
163	GDP	LG	501	-	-	2/16/32/32	0/3/3/3
163	GDP	MH	500	-	-	1/16/32/32	0/3/3/3
163	GDP	DW	501	-	-	1/16/32/32	0/3/3/3
165	GTP	EM	501	164	-	4/22/38/38	0/3/3/3
165	GTP	GS	501	164	-	4/22/38/38	0/3/3/3
165	GTP	KT	501	164	-	5/22/38/38	0/3/3/3
163	GDP	OP	501	-	-	2/16/32/32	0/3/3/3
165	GTP	UE	501	164	-	9/22/38/38	0/3/3/3
163	GDP	JI	500	-	-	1/16/32/32	0/3/3/3
163	GDP	ND	500	-	-	0/16/32/32	0/3/3/3
163	GDP	RU	500	-	-	0/16/32/32	0/3/3/3
163	GDP	HX	501	-	-	1/16/32/32	0/3/3/3
165	GTP	DT	501	164	-	3/22/38/38	0/3/3/3
165	GTP	NE	501	164	-	4/22/38/38	0/3/3/3
165	GTP	UC	501	164	-	3/22/38/38	0/3/3/3
163	GDP	MT	500	-	-	1/16/32/32	0/3/3/3
163	GDP	PP	500	-	-	4/16/32/32	0/3/3/3
163	GDP	TL	501	-	-	0/16/32/32	0/3/3/3
163	GDP	UD	500	-	-	3/16/32/32	0/3/3/3
165	GTP	VQ	501	164	-	1/22/38/38	0/3/3/3
165	GTP	KN	502	164	-	3/22/38/38	0/3/3/3
163	GDP	PH	500	-	-	1/16/32/32	0/3/3/3
163	GDP	AR	500	-	-	1/16/32/32	0/3/3/3
163	GDP	FV	501	-	-	1/16/32/32	0/3/3/3
165	GTP	WQ	501	164	-	8/22/38/38	0/3/3/3
163	GDP	CM	500	-	-	3/16/32/32	0/3/3/3
163	GDP	W	500	-	-	1/16/32/32	0/3/3/3
165	GTP	WG	501	164	-	1/22/38/38	0/3/3/3
165	GTP	NF	501	-	-	6/22/38/38	0/3/3/3
165	GTP	KJ	501	164	-	3/22/38/38	0/3/3/3
165	GTP	VO	501	164	-	6/22/38/38	0/3/3/3
165	GTP	BY	501	164	-	4/22/38/38	0/3/3/3
165	GTP	KR	501	164	-	6/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	PU	501	164	-	4/22/38/38	0/3/3/3
163	GDP	CK	501	-	-	6/16/32/32	0/3/3/3
163	GDP	DY	500	-	-	1/16/32/32	0/3/3/3
163	GDP	EB	500	-	-	4/16/32/32	0/3/3/3
163	GDP	WB	500	-	-	1/16/32/32	0/3/3/3
163	GDP	AL	500	-	-	3/16/32/32	0/3/3/3
163	GDP	FH	500	-	-	0/16/32/32	0/3/3/3
163	GDP	NN	500	-	-	3/16/32/32	0/3/3/3
165	GTP	SI	501	164	-	3/22/38/38	0/3/3/3
163	GDP	G	500	-	-	2/16/32/32	0/3/3/3
165	GTP	KD	502	164	-	3/22/38/38	0/3/3/3
165	GTP	RJ	501	-	-	1/22/38/38	0/3/3/3
163	GDP	CA	500	-	-	3/16/32/32	0/3/3/3
165	GTP	EP	501	164	-	5/22/38/38	0/3/3/3
165	GTP	PC	501	164	-	3/22/38/38	0/3/3/3
163	GDP	UT	500	-	-	1/16/32/32	0/3/3/3
165	GTP	IQ	501	164	-	2/22/38/38	0/3/3/3
165	GTP	UU	501	164	-	3/22/38/38	0/3/3/3
163	GDP	UL	500	-	-	1/16/32/32	0/3/3/3
163	GDP	LU	500	-	-	3/16/32/32	0/3/3/3
165	GTP	AI	501	164	-	3/22/38/38	0/3/3/3
163	GDP	PR	501	-	-	3/16/32/32	0/3/3/3
163	GDP	MN	500	-	-	2/16/32/32	0/3/3/3
163	GDP	BX	500	-	-	3/16/32/32	0/3/3/3
165	GTP	JF	501	164	-	3/22/38/38	0/3/3/3
163	GDP	DG	500	-	-	2/16/32/32	0/3/3/3
165	GTP	KV	501	164	-	3/22/38/38	0/3/3/3
163	GDP	GL	500	-	-	3/16/32/32	0/3/3/3
165	GTP	CQ	501	164	-	6/22/38/38	0/3/3/3
165	GTP	PQ	501	164	-	0/22/38/38	0/3/3/3
165	GTP	JR	501	164	-	3/22/38/38	0/3/3/3
165	GTP	JD	501	164	-	5/22/38/38	0/3/3/3
163	GDP	EF	500	-	-	3/16/32/32	0/3/3/3
163	GDP	P	500	-	-	2/16/32/32	0/3/3/3
165	GTP	AA	501	164	-	6/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	EA	501	164	-	2/22/38/38	0/3/3/3
163	GDP	LQ	500	-	-	2/16/32/32	0/3/3/3
165	GTP	EC	501	164	-	3/22/38/38	0/3/3/3
163	GDP	OT	500	-	-	3/16/32/32	0/3/3/3
163	GDP	OX	500	-	-	2/16/32/32	0/3/3/3
163	GDP	RE	500	-	-	0/16/32/32	0/3/3/3
163	GDP	QE	500	-	-	2/16/32/32	0/3/3/3
163	GDP	IL	501	-	-	0/16/32/32	0/3/3/3
165	GTP	PY	501	164	-	3/22/38/38	0/3/3/3
163	GDP	GX	500	-	-	4/16/32/32	0/3/3/3
165	GTP	GU	501	164	-	4/22/38/38	0/3/3/3
163	GDP	KM	500	-	-	2/16/32/32	0/3/3/3
163	GDP	JA	500	-	-	1/16/32/32	0/3/3/3
165	GTP	OA	501	164	-	4/22/38/38	0/3/3/3
165	GTP	JB	501	164	-	2/22/38/38	0/3/3/3
163	GDP	JU	500	-	-	1/16/32/32	0/3/3/3
163	GDP	GV	501	-	-	4/16/32/32	0/3/3/3
165	GTP	VW	501	164	-	5/22/38/38	0/3/3/3
165	GTP	GQ	501	164	-	4/22/38/38	0/3/3/3
163	GDP	SF	500	-	-	1/16/32/32	0/3/3/3
165	GTP	UM	501	164	-	5/22/38/38	0/3/3/3
163	GDP	PV	500	-	-	3/16/32/32	0/3/3/3
165	GTP	CW	501	164	-	4/22/38/38	0/3/3/3
165	GTP	IA	501	164	-	6/22/38/38	0/3/3/3
163	GDP	WH	500	-	-	2/16/32/32	0/3/3/3
163	GDP	QG	500	-	-	1/16/32/32	0/3/3/3
163	GDP	IP	500	-	-	1/16/32/32	0/3/3/3
163	GDP	UV	500	-	-	1/16/32/32	0/3/3/3
165	GTP	BU	501	164	-	4/22/38/38	0/3/3/3
165	GTP	CK	503	164	-	3/22/38/38	0/3/3/3
165	GTP	IY	501	164	-	4/22/38/38	0/3/3/3
168	ATP	6u	700	-	-	7/22/38/38	0/3/3/3
163	GDP	VD	500	-	-	1/16/32/32	0/3/3/3
163	GDP	VJ	500	-	-	2/16/32/32	0/3/3/3
163	GDP	WV	500	-	-	1/16/32/32	0/3/3/3
163	GDP	CQ	500	-	-	3/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	LR	502	164	-	2/22/38/38	0/3/3/3
163	GDP	UP	500	-	-	3/16/32/32	0/3/3/3
165	GTP	JN	501	164	-	3/22/38/38	0/3/3/3
165	GTP	Q	501	164	-	3/22/38/38	0/3/3/3
165	GTP	JH	501	164	-	5/22/38/38	0/3/3/3
165	GTP	OU	501	164	-	6/22/38/38	0/3/3/3
163	GDP	AN	500	-	-	2/16/32/32	0/3/3/3
165	GTP	EI	501	164	-	5/22/38/38	0/3/3/3
165	GTP	FO	501	164	-	3/22/38/38	0/3/3/3
165	GTP	PW	501	164	-	3/22/38/38	0/3/3/3
165	GTP	RT	501	164	-	2/22/38/38	0/3/3/3
165	GTP	AW	501	164	-	3/22/38/38	0/3/3/3
165	GTP	NY	501	164	-	4/22/38/38	0/3/3/3
165	GTP	BE	501	164	-	7/22/38/38	0/3/3/3
163	GDP	KW	500	-	-	1/16/32/32	0/3/3/3
165	GTP	AD	501	164	-	4/22/38/38	0/3/3/3
163	GDP	UH	500	-	-	1/16/32/32	0/3/3/3
165	GTP	BI	501	164	-	5/22/38/38	0/3/3/3
163	GDP	JS	500	-	-	2/16/32/32	0/3/3/3
163	GDP	SV	501	-	-	2/16/32/32	0/3/3/3
163	GDP	AB	500	-	-	3/16/32/32	0/3/3/3
165	GTP	DE	501	164	-	6/22/38/38	0/3/3/3
165	GTP	JP	501	164	-	5/22/38/38	0/3/3/3
163	GDP	TH	500	-	-	1/16/32/32	0/3/3/3
163	GDP	KE	500	-	-	1/16/32/32	0/3/3/3
163	GDP	KG	500	-	-	2/16/32/32	0/3/3/3
163	GDP	DO	500	-	-	1/16/32/32	0/3/3/3
168	ATP	9R	500	164	-	6/22/38/38	0/3/3/3
165	GTP	JT	501	164	-	5/22/38/38	0/3/3/3
163	GDP	AV	500	-	-	3/16/32/32	0/3/3/3
163	GDP	TR	500	-	-	1/16/32/32	0/3/3/3
163	GDP	RW	500	-	-	2/16/32/32	0/3/3/3
163	GDP	PF	501	-	-	3/16/32/32	0/3/3/3
163	GDP	GF	500	-	-	4/16/32/32	0/3/3/3
165	GTP	FS	501	164	-	3/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	QR	501	164	-	2/22/38/38	0/3/3/3
165	GTP	QC	501	164	-	5/22/38/38	0/3/3/3
165	GTP	BG	501	164	-	1/22/38/38	0/3/3/3
165	GTP	FJ	503	164	-	5/22/38/38	0/3/3/3
163	GDP	RK	500	-	-	2/16/32/32	0/3/3/3
165	GTP	OI	501	164	-	6/22/38/38	0/3/3/3
163	GDP	FT	501	-	-	1/16/32/32	0/3/3/3
165	GTP	MM	501	164	-	2/22/38/38	0/3/3/3

All (1224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
165	IK	501	GTP	PB-O3A	3.47	1.63	1.59
165	IW	501	GTP	PB-O3A	3.41	1.63	1.59
163	CK	501	GDP	C5-C4	3.21	1.47	1.38
163	KY	500	GDP	C5-C4	3.13	1.47	1.38
163	O	500	GDP	C5-C4	3.12	1.47	1.38
163	LW	500	GDP	C5-C4	3.12	1.47	1.38
163	QW	500	GDP	C5-C4	3.12	1.47	1.38
163	QK	500	GDP	C5-C4	3.12	1.47	1.38
163	JA	500	GDP	C5-C4	3.11	1.47	1.38
163	M	500	GDP	C5-C4	3.11	1.47	1.38
163	QA	500	GDP	C5-C4	3.11	1.47	1.38
163	WP	500	GDP	C5-C4	3.11	1.47	1.38
163	OB	500	GDP	C5-C4	3.11	1.47	1.38
163	JE	500	GDP	C5-C4	3.10	1.47	1.38
163	JC	500	GDP	C5-C4	3.10	1.47	1.38
163	TX	500	GDP	C5-C4	3.10	1.47	1.38
163	ON	500	GDP	C5-C4	3.10	1.47	1.38
163	NB	500	GDP	C5-C4	3.10	1.47	1.38
163	LM	500	GDP	C5-C4	3.10	1.47	1.38
163	UN	500	GDP	C5-C4	3.10	1.47	1.38
163	OP	501	GDP	C5-C4	3.09	1.47	1.38
163	LY	500	GDP	C5-C4	3.09	1.47	1.38
163	NJ	501	GDP	C5-C4	3.09	1.47	1.38
163	CW	500	GDP	C5-C4	3.09	1.47	1.38
163	NT	500	GDP	C5-C4	3.09	1.47	1.38
163	JO	500	GDP	C5-C4	3.09	1.47	1.38
163	WL	500	GDP	C5-C4	3.09	1.47	1.38
163	KQ	500	GDP	C5-C4	3.09	1.47	1.38
163	EX	500	GDP	C5-C4	3.09	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	UB	500	GDP	C5-C4	3.08	1.47	1.38
163	MR	500	GDP	C5-C4	3.08	1.47	1.38
163	WX	500	GDP	C5-C4	3.08	1.47	1.38
163	NN	500	GDP	C5-C4	3.08	1.47	1.38
163	KE	500	GDP	C5-C4	3.08	1.47	1.38
163	TJ	500	GDP	C5-C4	3.08	1.47	1.38
163	KO	500	GDP	C5-C4	3.08	1.47	1.38
163	IX	501	GDP	C5-C4	3.08	1.47	1.38
163	SL	500	GDP	C5-C4	3.08	1.47	1.38
163	TL	501	GDP	C5-C4	3.08	1.47	1.38
163	SR	500	GDP	C5-C4	3.08	1.47	1.38
163	W	500	GDP	C5-C4	3.08	1.47	1.38
163	WD	500	GDP	C5-C4	3.08	1.47	1.38
163	KU	500	GDP	C5-C4	3.08	1.47	1.38
163	KA	500	GDP	C5-C4	3.08	1.47	1.38
163	JW	500	GDP	C5-C4	3.08	1.47	1.38
163	KM	500	GDP	C5-C4	3.08	1.47	1.38
163	ML	500	GDP	C5-C4	3.08	1.47	1.38
163	HH	501	GDP	C5-C4	3.07	1.47	1.38
163	LE	500	GDP	C5-C4	3.07	1.47	1.38
163	RW	500	GDP	C5-C4	3.07	1.47	1.38
163	TP	500	GDP	C5-C4	3.07	1.47	1.38
163	MH	500	GDP	C5-C4	3.07	1.47	1.38
163	LK	500	GDP	C5-C4	3.07	1.47	1.38
163	MT	500	GDP	C5-C4	3.07	1.47	1.38
163	NP	500	GDP	C5-C4	3.07	1.47	1.38
163	PB	500	GDP	C5-C4	3.07	1.47	1.38
163	NR	500	GDP	C5-C4	3.07	1.47	1.38
163	QM	500	GDP	C5-C4	3.07	1.47	1.38
163	VF	500	GDP	C5-C4	3.07	1.47	1.38
163	WH	500	GDP	C5-C4	3.07	1.47	1.38
163	UH	500	GDP	C5-C4	3.07	1.47	1.38
163	MX	500	GDP	C5-C4	3.07	1.47	1.38
163	KC	500	GDP	C5-C4	3.07	1.47	1.38
163	PJ	500	GDP	C5-C4	3.07	1.47	1.38
163	N	500	GDP	C5-C4	3.07	1.47	1.38
163	UT	500	GDP	C5-C4	3.06	1.47	1.38
163	MB	500	GDP	C5-C4	3.06	1.47	1.38
163	OH	500	GDP	C5-C4	3.06	1.47	1.38
163	VH	500	GDP	C5-C4	3.06	1.47	1.38
163	WF	501	GDP	C5-C4	3.06	1.47	1.38
163	VV	500	GDP	C5-C4	3.06	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	NF	500	GDP	C5-C4	3.06	1.47	1.38
163	IR	500	GDP	C5-C4	3.06	1.47	1.38
163	JQ	500	GDP	C5-C4	3.06	1.47	1.38
163	KI	500	GDP	C5-C4	3.06	1.47	1.38
163	S	500	GDP	C5-C4	3.06	1.47	1.38
163	NH	500	GDP	C5-C4	3.06	1.47	1.38
163	WJ	500	GDP	C5-C4	3.06	1.47	1.38
163	IP	500	GDP	C5-C4	3.06	1.47	1.38
163	TN	500	GDP	C5-C4	3.06	1.47	1.38
163	TR	500	GDP	C5-C4	3.06	1.47	1.38
163	HR	500	GDP	C5-C4	3.06	1.47	1.38
163	IL	501	GDP	C5-C4	3.06	1.47	1.38
163	LC	500	GDP	C5-C4	3.06	1.47	1.38
163	KS	500	GDP	C5-C4	3.06	1.47	1.38
163	OF	500	GDP	C5-C4	3.06	1.47	1.38
163	SF	500	GDP	C5-C4	3.06	1.47	1.38
163	IN	500	GDP	C5-C4	3.06	1.47	1.38
163	PN	500	GDP	C5-C4	3.06	1.47	1.38
163	QU	500	GDP	C5-C4	3.06	1.47	1.38
163	JK	500	GDP	C5-C4	3.06	1.47	1.38
163	VD	500	GDP	C5-C4	3.06	1.47	1.38
163	I	501	GDP	C5-C4	3.06	1.47	1.38
163	HD	501	GDP	C5-C4	3.06	1.47	1.38
163	VN	500	GDP	C5-C4	3.06	1.47	1.38
163	MD	500	GDP	C5-C4	3.06	1.47	1.38
163	VR	500	GDP	C5-C4	3.06	1.47	1.38
163	H	500	GDP	C5-C4	3.05	1.47	1.38
163	LU	500	GDP	C5-C4	3.05	1.47	1.38
163	KG	500	GDP	C5-C4	3.05	1.47	1.38
163	HP	501	GDP	C5-C4	3.05	1.47	1.38
163	IT	501	GDP	C5-C4	3.05	1.47	1.38
163	PR	501	GDP	C5-C4	3.05	1.47	1.38
163	OR	500	GDP	C5-C4	3.05	1.47	1.38
163	IH	500	GDP	C5-C4	3.05	1.47	1.38
163	LG	501	GDP	C5-C4	3.05	1.47	1.38
163	JI	500	GDP	C5-C4	3.05	1.47	1.38
163	OT	500	GDP	C5-C4	3.05	1.47	1.38
163	OV	500	GDP	C5-C4	3.05	1.47	1.38
163	PX	501	GDP	C5-C4	3.05	1.47	1.38
163	TD	500	GDP	C5-C4	3.05	1.47	1.38
163	VT	500	GDP	C5-C4	3.05	1.47	1.38
163	ID	500	GDP	C5-C4	3.05	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	LA	500	GDP	C5-C4	3.05	1.47	1.38
163	HV	500	GDP	C5-C4	3.05	1.47	1.38
163	RU	500	GDP	C5-C4	3.05	1.47	1.38
163	WT	500	GDP	C5-C4	3.05	1.47	1.38
163	OD	501	GDP	C5-C4	3.05	1.47	1.38
163	ND	500	GDP	C5-C4	3.05	1.47	1.38
163	HN	501	GDP	C5-C4	3.05	1.47	1.38
163	PP	500	GDP	C5-C4	3.05	1.47	1.38
163	UF	500	GDP	C5-C4	3.05	1.47	1.38
163	MF	500	GDP	C5-C4	3.05	1.47	1.38
163	T	501	GDP	C5-C4	3.04	1.47	1.38
163	PV	500	GDP	C5-C4	3.04	1.47	1.38
163	SH	500	GDP	C5-C4	3.04	1.47	1.38
163	RE	500	GDP	C5-C4	3.04	1.47	1.38
163	WV	500	GDP	C5-C4	3.04	1.47	1.38
163	RK	500	GDP	C5-C4	3.04	1.47	1.38
163	VJ	500	GDP	C5-C4	3.04	1.47	1.38
163	WR	501	GDP	C5-C4	3.04	1.47	1.38
163	RA	500	GDP	C5-C4	3.04	1.47	1.38
163	RQ	500	GDP	C5-C4	3.04	1.47	1.38
163	RM	500	GDP	C5-C4	3.04	1.47	1.38
163	HF	500	GDP	C5-C4	3.04	1.47	1.38
163	MP	500	GDP	C5-C4	3.04	1.47	1.38
163	SV	501	GDP	C5-C4	3.04	1.47	1.38
163	JM	501	GDP	C5-C4	3.04	1.47	1.38
163	SD	500	GDP	C5-C4	3.04	1.47	1.38
163	G	500	GDP	C5-C4	3.04	1.47	1.38
163	TH	500	GDP	C5-C4	3.04	1.47	1.38
163	JU	500	GDP	C5-C4	3.04	1.47	1.38
163	OJ	500	GDP	C5-C4	3.04	1.47	1.38
163	LI	500	GDP	C5-C4	3.04	1.47	1.38
163	JS	500	GDP	C5-C4	3.04	1.47	1.38
163	HT	501	GDP	C5-C4	3.04	1.47	1.38
163	SN	501	GDP	C5-C4	3.04	1.47	1.38
163	IB	500	GDP	C5-C4	3.04	1.47	1.38
163	QC	500	GDP	C5-C4	3.04	1.47	1.38
163	UL	500	GDP	C5-C4	3.04	1.47	1.38
163	IF	500	GDP	C5-C4	3.04	1.47	1.38
163	SP	500	GDP	C5-C4	3.04	1.47	1.38
163	KK	500	GDP	C5-C4	3.04	1.47	1.38
163	JG	500	GDP	C5-C4	3.03	1.47	1.38
163	HB	501	GDP	C5-C4	3.03	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	RG	500	GDP	C5-C4	3.03	1.47	1.38
163	LS	500	GDP	C5-C4	3.03	1.47	1.38
163	PD	500	GDP	C5-C4	3.03	1.47	1.38
163	SB	501	GDP	C5-C4	3.03	1.47	1.38
163	LO	500	GDP	C5-C4	3.03	1.47	1.38
163	HL	501	GDP	C5-C4	3.03	1.47	1.38
163	LQ	500	GDP	C5-C4	3.03	1.47	1.38
163	OL	500	GDP	C5-C4	3.03	1.47	1.38
163	HX	501	GDP	C5-C4	3.03	1.47	1.38
163	UD	500	GDP	C5-C4	3.03	1.47	1.38
163	QS	500	GDP	C5-C4	3.03	1.47	1.38
163	PF	501	GDP	C5-C4	3.03	1.47	1.38
163	RC	500	GDP	C5-C4	3.03	1.47	1.38
163	FV	501	GDP	C5-C4	3.03	1.47	1.38
163	IJ	500	GDP	C5-C4	3.03	1.47	1.38
163	RS	500	GDP	C5-C4	3.03	1.47	1.38
163	PL	501	GDP	C5-C4	3.03	1.47	1.38
163	HJ	500	GDP	C5-C4	3.03	1.47	1.38
163	UX	500	GDP	C5-C4	3.03	1.47	1.38
163	TF	500	GDP	C5-C4	3.03	1.47	1.38
163	V	500	GDP	C5-C4	3.03	1.47	1.38
163	JY	501	GDP	C5-C4	3.03	1.47	1.38
163	KW	500	GDP	C5-C4	3.03	1.47	1.38
163	QI	500	GDP	C5-C4	3.02	1.47	1.38
163	OX	500	GDP	C5-C4	3.02	1.47	1.38
163	GJ	500	GDP	C5-C4	3.02	1.47	1.38
163	UV	500	GDP	C5-C4	3.02	1.47	1.38
163	VL	500	GDP	C5-C4	3.02	1.47	1.38
163	VB	500	GDP	C5-C4	3.02	1.47	1.38
163	RI	500	GDP	C5-C4	3.02	1.47	1.38
163	IV	500	GDP	C5-C4	3.02	1.47	1.38
163	WB	500	GDP	C5-C4	3.02	1.47	1.38
163	QE	500	GDP	C5-C4	3.02	1.47	1.38
163	SJ	501	GDP	C5-C4	3.02	1.47	1.38
163	CA	500	GDP	C5-C4	3.02	1.47	1.38
163	TT	500	GDP	C5-C4	3.02	1.47	1.38
163	MV	500	GDP	C5-C4	3.02	1.47	1.38
163	QO	500	GDP	C5-C4	3.02	1.47	1.38
163	ST	500	GDP	C5-C4	3.02	1.47	1.38
163	TV	500	GDP	C5-C4	3.01	1.47	1.38
163	MN	500	GDP	C5-C4	3.01	1.47	1.38
163	F	500	GDP	C5-C4	3.01	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	P	500	GDP	C5-C4	3.01	1.47	1.38
163	MZ	500	GDP	C5-C4	3.01	1.47	1.38
163	NL	500	GDP	C5-C4	3.01	1.47	1.38
163	RO	500	GDP	C5-C4	3.01	1.47	1.38
163	QG	500	GDP	C5-C4	3.01	1.47	1.38
163	FF	500	GDP	C5-C4	3.01	1.47	1.38
163	CE	500	GDP	C5-C4	3.01	1.47	1.38
163	UR	500	GDP	C5-C4	3.01	1.47	1.38
163	NV	501	GDP	C5-C4	3.01	1.47	1.38
163	VX	500	GDP	C5-C4	3.01	1.47	1.38
163	U	500	GDP	C5-C4	3.00	1.47	1.38
163	WN	500	GDP	C5-C4	3.00	1.47	1.38
163	TB	500	GDP	C5-C4	3.00	1.47	1.38
163	CQ	500	GDP	C5-C4	3.00	1.47	1.38
163	VP	500	GDP	C5-C4	3.00	1.47	1.38
163	QQ	500	GDP	C5-C4	3.00	1.47	1.38
163	FR	501	GDP	C5-C4	3.00	1.47	1.38
163	EJ	500	GDP	C5-C4	3.00	1.47	1.38
163	PH	500	GDP	C5-C4	3.00	1.47	1.38
163	UJ	500	GDP	C5-C4	2.99	1.47	1.38
163	MJ	500	GDP	C5-C4	2.99	1.47	1.38
163	NX	500	GDP	C5-C4	2.99	1.46	1.38
163	EB	500	GDP	C5-C4	2.99	1.46	1.38
163	UP	500	GDP	C5-C4	2.99	1.46	1.38
163	FB	500	GDP	C5-C4	2.98	1.46	1.38
165	IK	501	GTP	PA-O3A	2.98	1.62	1.59
163	FJ	501	GDP	C5-C4	2.98	1.46	1.38
163	CM	500	GDP	C5-C4	2.98	1.46	1.38
163	GB	500	GDP	C5-C4	2.98	1.46	1.38
163	BL	500	GDP	C5-C4	2.98	1.46	1.38
163	AB	500	GDP	C5-C4	2.98	1.46	1.38
165	IW	501	GTP	PA-O3A	2.98	1.62	1.59
163	CI	500	GDP	C5-C4	2.97	1.46	1.38
163	EN	500	GDP	C5-C4	2.97	1.46	1.38
163	EL	500	GDP	C5-C4	2.97	1.46	1.38
163	GH	500	GDP	C5-C4	2.97	1.46	1.38
163	GT	501	GDP	C5-C4	2.97	1.46	1.38
163	FP	500	GDP	C5-C4	2.97	1.46	1.38
163	E	500	GDP	C5-C4	2.97	1.46	1.38
163	GP	500	GDP	C5-C4	2.96	1.46	1.38
163	DQ	500	GDP	C5-C4	2.96	1.46	1.38
163	AH	500	GDP	C5-C4	2.96	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	CG	500	GDP	C5-C4	2.96	1.46	1.38
163	FL	500	GDP	C5-C4	2.96	1.46	1.38
163	BX	500	GDP	C5-C4	2.95	1.46	1.38
163	BR	500	GDP	C5-C4	2.95	1.46	1.38
163	PT	500	GDP	C5-C4	2.95	1.46	1.38
163	A	501	GDP	C5-C4	2.95	1.46	1.38
163	EP	500	GDP	C5-C4	2.95	1.46	1.38
163	CO	500	GDP	C5-C4	2.95	1.46	1.38
163	DW	501	GDP	C5-C4	2.94	1.46	1.38
163	FX	500	GDP	C5-C4	2.94	1.46	1.38
163	DU	500	GDP	C5-C4	2.94	1.46	1.38
163	AF	500	GDP	C5-C4	2.94	1.46	1.38
163	AT	500	GDP	C5-C4	2.94	1.46	1.38
163	ER	500	GDP	C5-C4	2.94	1.46	1.38
163	GD	500	GDP	C5-C4	2.94	1.46	1.38
163	GN	500	GDP	C5-C4	2.94	1.46	1.38
163	EF	500	GDP	C5-C4	2.94	1.46	1.38
163	DC	500	GDP	C5-C4	2.93	1.46	1.38
163	GX	500	GDP	C5-C4	2.93	1.46	1.38
163	AJ	500	GDP	C5-C4	2.93	1.46	1.38
163	BF	500	GDP	C5-C4	2.93	1.46	1.38
163	BN	500	GDP	C5-C4	2.93	1.46	1.38
163	DY	500	GDP	C5-C4	2.93	1.46	1.38
163	GL	500	GDP	C5-C4	2.92	1.46	1.38
163	AX	500	GDP	C5-C4	2.92	1.46	1.38
163	DK	501	GDP	C5-C4	2.92	1.46	1.38
163	DI	500	GDP	C5-C4	2.92	1.46	1.38
163	AP	500	GDP	C5-C4	2.92	1.46	1.38
163	DE	500	GDP	C5-C4	2.91	1.46	1.38
163	ET	500	GDP	C5-C4	2.91	1.46	1.38
163	BH	500	GDP	C5-C4	2.91	1.46	1.38
163	DO	500	GDP	C5-C4	2.91	1.46	1.38
163	BP	500	GDP	C5-C4	2.91	1.46	1.38
163	AZ	500	GDP	C5-C4	2.91	1.46	1.38
163	DM	500	GDP	C5-C4	2.91	1.46	1.38
163	BD	500	GDP	C5-C4	2.91	1.46	1.38
163	AR	500	GDP	C5-C4	2.91	1.46	1.38
163	FN	500	GDP	C5-C4	2.91	1.46	1.38
163	GV	501	GDP	C5-C4	2.90	1.46	1.38
163	AL	500	GDP	C5-C4	2.90	1.46	1.38
163	BV	500	GDP	C5-C4	2.90	1.46	1.38
163	GF	500	GDP	C5-C4	2.90	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	EH	500	GDP	C5-C4	2.90	1.46	1.38
163	CS	500	GDP	C5-C4	2.89	1.46	1.38
163	DS	500	GDP	C5-C4	2.89	1.46	1.38
163	BT	500	GDP	C5-C4	2.89	1.46	1.38
163	AD	500	GDP	C5-C4	2.89	1.46	1.38
163	AN	500	GDP	C5-C4	2.89	1.46	1.38
163	DA	500	GDP	C5-C4	2.88	1.46	1.38
163	CU	500	GDP	C5-C4	2.88	1.46	1.38
163	ED	500	GDP	C5-C4	2.87	1.46	1.38
163	BJ	500	GDP	C5-C4	2.86	1.46	1.38
163	DG	500	GDP	C5-C4	2.86	1.46	1.38
163	CC	500	GDP	C5-C4	2.86	1.46	1.38
163	FH	500	GDP	C5-C4	2.86	1.46	1.38
163	EV	500	GDP	C5-C4	2.85	1.46	1.38
163	CY	500	GDP	C5-C4	2.84	1.46	1.38
163	AV	500	GDP	C5-C4	2.84	1.46	1.38
163	FD	500	GDP	C5-C4	2.83	1.46	1.38
163	GR	500	GDP	C5-C4	2.82	1.46	1.38
163	FT	501	GDP	C5-C4	2.80	1.46	1.38
163	EL	500	GDP	C6-N1	-2.79	1.33	1.38
163	CY	500	GDP	C6-N1	-2.73	1.33	1.38
163	FL	500	GDP	C6-N1	-2.73	1.33	1.38
163	DO	500	GDP	C6-N1	-2.71	1.33	1.38
163	BP	500	GDP	C6-N1	-2.71	1.33	1.38
163	DE	500	GDP	C6-N1	-2.71	1.33	1.38
163	ED	500	GDP	C6-N1	-2.69	1.33	1.38
163	AL	500	GDP	C6-N1	-2.67	1.33	1.38
163	DI	500	GDP	C6-N1	-2.67	1.33	1.38
163	DW	501	GDP	C6-N1	-2.67	1.33	1.38
163	BD	500	GDP	C6-N1	-2.67	1.33	1.38
163	BT	500	GDP	C6-N1	-2.67	1.33	1.38
163	BJ	500	GDP	C6-N1	-2.66	1.33	1.38
163	A	501	GDP	C6-N1	-2.66	1.33	1.38
163	EP	500	GDP	C6-N1	-2.66	1.33	1.38
163	CM	500	GDP	C6-N1	-2.66	1.33	1.38
163	DC	500	GDP	C6-N1	-2.66	1.33	1.38
163	E	500	GDP	C6-N1	-2.65	1.33	1.38
163	AZ	500	GDP	C6-N1	-2.65	1.33	1.38
163	BX	500	GDP	C6-N1	-2.65	1.33	1.38
163	AV	500	GDP	C6-N1	-2.64	1.33	1.38
163	ET	500	GDP	C6-N1	-2.64	1.33	1.38
163	BF	500	GDP	C6-N1	-2.64	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	FD	500	GDP	C6-N1	-2.64	1.33	1.38
163	DQ	500	GDP	C6-N1	-2.64	1.33	1.38
163	DY	500	GDP	C6-N1	-2.62	1.33	1.38
163	FH	500	GDP	C6-N1	-2.61	1.34	1.38
163	FX	500	GDP	C6-N1	-2.61	1.34	1.38
163	GX	500	GDP	C6-N1	-2.61	1.34	1.38
163	CS	500	GDP	C6-N1	-2.61	1.34	1.38
163	DS	500	GDP	C6-N1	-2.61	1.34	1.38
163	CQ	500	GDP	C6-N1	-2.61	1.34	1.38
163	PX	501	GDP	C6-N1	-2.60	1.34	1.38
163	BV	500	GDP	C6-N1	-2.60	1.34	1.38
163	QU	500	GDP	C6-N1	-2.60	1.34	1.38
163	DU	500	GDP	C6-N1	-2.60	1.34	1.38
163	FP	500	GDP	C6-N1	-2.60	1.34	1.38
163	EN	500	GDP	C6-N1	-2.60	1.34	1.38
163	JU	500	GDP	C6-N1	-2.59	1.34	1.38
163	PL	501	GDP	C6-N1	-2.59	1.34	1.38
163	EH	500	GDP	C6-N1	-2.59	1.34	1.38
163	GN	500	GDP	C6-N1	-2.59	1.34	1.38
163	AF	500	GDP	C6-N1	-2.59	1.34	1.38
163	DM	500	GDP	C6-N1	-2.58	1.34	1.38
163	DA	500	GDP	C6-N1	-2.58	1.34	1.38
163	GF	500	GDP	C6-N1	-2.58	1.34	1.38
163	BN	500	GDP	C6-N1	-2.58	1.34	1.38
163	DG	500	GDP	C6-N1	-2.58	1.34	1.38
163	CA	500	GDP	C6-N1	-2.58	1.34	1.38
163	F	500	GDP	C6-N1	-2.58	1.34	1.38
163	UP	500	GDP	C6-N1	-2.58	1.34	1.38
163	ER	500	GDP	C6-N1	-2.58	1.34	1.38
163	EB	500	GDP	C6-N1	-2.57	1.34	1.38
163	AJ	500	GDP	C6-N1	-2.57	1.34	1.38
163	EF	500	GDP	C6-N1	-2.57	1.34	1.38
163	AP	500	GDP	C6-N1	-2.57	1.34	1.38
163	VX	500	GDP	C6-N1	-2.57	1.34	1.38
163	CC	500	GDP	C6-N1	-2.56	1.34	1.38
163	TH	500	GDP	C6-N1	-2.56	1.34	1.38
163	AB	500	GDP	C6-N1	-2.56	1.34	1.38
163	CO	500	GDP	C6-N1	-2.56	1.34	1.38
163	QG	500	GDP	C6-N1	-2.56	1.34	1.38
163	QS	500	GDP	C6-N1	-2.56	1.34	1.38
163	TT	500	GDP	C6-N1	-2.56	1.34	1.38
163	KG	500	GDP	C6-N1	-2.55	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	UX	500	GDP	C6-N1	-2.55	1.34	1.38
163	WT	500	GDP	C6-N1	-2.55	1.34	1.38
163	N	500	GDP	C6-N1	-2.55	1.34	1.38
163	JI	500	GDP	C6-N1	-2.55	1.34	1.38
163	DK	501	GDP	C6-N1	-2.55	1.34	1.38
163	NN	500	GDP	C6-N1	-2.55	1.34	1.38
163	RE	500	GDP	C6-N1	-2.55	1.34	1.38
163	BR	500	GDP	C6-N1	-2.55	1.34	1.38
163	UN	500	GDP	C6-N1	-2.55	1.34	1.38
163	FT	501	GDP	C6-N1	-2.55	1.34	1.38
163	JS	500	GDP	C6-N1	-2.55	1.34	1.38
163	QI	500	GDP	C6-N1	-2.55	1.34	1.38
163	AT	500	GDP	C6-N1	-2.55	1.34	1.38
163	GH	500	GDP	C6-N1	-2.55	1.34	1.38
163	O	500	GDP	C6-N1	-2.55	1.34	1.38
163	GV	501	GDP	C6-N1	-2.55	1.34	1.38
163	U	500	GDP	C6-N1	-2.54	1.34	1.38
163	FN	500	GDP	C6-N1	-2.54	1.34	1.38
163	UD	500	GDP	C6-N1	-2.54	1.34	1.38
163	GD	500	GDP	C6-N1	-2.54	1.34	1.38
163	NB	500	GDP	C6-N1	-2.54	1.34	1.38
163	TD	500	GDP	C6-N1	-2.54	1.34	1.38
163	GJ	500	GDP	C6-N1	-2.54	1.34	1.38
163	AR	500	GDP	C6-N1	-2.54	1.34	1.38
163	GT	501	GDP	C6-N1	-2.54	1.34	1.38
163	HX	501	GDP	C6-N1	-2.54	1.34	1.38
163	JY	501	GDP	C6-N1	-2.54	1.34	1.38
163	FR	501	GDP	C6-N1	-2.53	1.34	1.38
163	TP	500	GDP	C6-N1	-2.53	1.34	1.38
163	AD	500	GDP	C6-N1	-2.53	1.34	1.38
163	HR	500	GDP	C6-N1	-2.53	1.34	1.38
163	VB	500	GDP	C6-N1	-2.53	1.34	1.38
163	KW	500	GDP	C6-N1	-2.53	1.34	1.38
163	EJ	500	GDP	C6-N1	-2.53	1.34	1.38
163	VL	500	GDP	C6-N1	-2.53	1.34	1.38
163	GB	500	GDP	C6-N1	-2.53	1.34	1.38
163	GR	500	GDP	C6-N1	-2.53	1.34	1.38
163	LK	500	GDP	C6-N1	-2.53	1.34	1.38
163	RO	500	GDP	C6-N1	-2.53	1.34	1.38
163	RK	500	GDP	C6-N1	-2.53	1.34	1.38
163	HT	501	GDP	C6-N1	-2.53	1.34	1.38
163	IT	501	GDP	C6-N1	-2.53	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	BL	500	GDP	C6-N1	-2.53	1.34	1.38
163	AN	500	GDP	C6-N1	-2.53	1.34	1.38
163	MX	500	GDP	C6-N1	-2.53	1.34	1.38
163	MH	500	GDP	C6-N1	-2.52	1.34	1.38
163	RC	500	GDP	C6-N1	-2.52	1.34	1.38
163	AX	500	GDP	C6-N1	-2.52	1.34	1.38
163	JW	500	GDP	C6-N1	-2.52	1.34	1.38
163	P	500	GDP	C6-N1	-2.52	1.34	1.38
163	GP	500	GDP	C6-N1	-2.52	1.34	1.38
163	VF	500	GDP	C6-N1	-2.52	1.34	1.38
163	JC	500	GDP	C6-N1	-2.52	1.34	1.38
163	PH	500	GDP	C6-N1	-2.52	1.34	1.38
163	UB	500	GDP	C6-N1	-2.52	1.34	1.38
163	UL	500	GDP	C6-N1	-2.52	1.34	1.38
163	ON	500	GDP	C6-N1	-2.52	1.34	1.38
163	FB	500	GDP	C6-N1	-2.52	1.34	1.38
163	EV	500	GDP	C6-N1	-2.52	1.34	1.38
163	CE	500	GDP	C6-N1	-2.52	1.34	1.38
163	SD	500	GDP	C6-N1	-2.52	1.34	1.38
163	SR	500	GDP	C6-N1	-2.52	1.34	1.38
163	LS	500	GDP	C6-N1	-2.51	1.34	1.38
163	BH	500	GDP	C6-N1	-2.51	1.34	1.38
163	KY	500	GDP	C6-N1	-2.51	1.34	1.38
163	WD	500	GDP	C6-N1	-2.51	1.34	1.38
163	RG	500	GDP	C6-N1	-2.51	1.34	1.38
163	RW	500	GDP	C6-N1	-2.51	1.34	1.38
163	CG	500	GDP	C6-N1	-2.51	1.34	1.38
163	IJ	500	GDP	C6-N1	-2.51	1.34	1.38
163	CI	500	GDP	C6-N1	-2.51	1.34	1.38
163	TL	501	GDP	C6-N1	-2.51	1.34	1.38
163	CU	500	GDP	C6-N1	-2.51	1.34	1.38
163	PR	501	GDP	C6-N1	-2.51	1.34	1.38
163	GL	500	GDP	C6-N1	-2.51	1.34	1.38
163	SH	500	GDP	C6-N1	-2.51	1.34	1.38
163	HL	501	GDP	C6-N1	-2.51	1.34	1.38
163	EX	500	GDP	C6-N1	-2.51	1.34	1.38
163	RQ	500	GDP	C6-N1	-2.51	1.34	1.38
163	WN	500	GDP	C6-N1	-2.51	1.34	1.38
163	PF	501	GDP	C6-N1	-2.51	1.34	1.38
163	HD	501	GDP	C6-N1	-2.50	1.34	1.38
163	JG	500	GDP	C6-N1	-2.50	1.34	1.38
163	JK	500	GDP	C6-N1	-2.50	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	JM	501	GDP	C6-N1	-2.50	1.34	1.38
163	QC	500	GDP	C6-N1	-2.50	1.34	1.38
163	RU	500	GDP	C6-N1	-2.50	1.34	1.38
163	SV	501	GDP	C6-N1	-2.50	1.34	1.38
163	IV	500	GDP	C6-N1	-2.50	1.34	1.38
163	HH	501	GDP	C6-N1	-2.50	1.34	1.38
163	PN	500	GDP	C6-N1	-2.50	1.34	1.38
163	OL	500	GDP	C6-N1	-2.50	1.34	1.38
163	WP	500	GDP	C6-N1	-2.50	1.34	1.38
163	IL	501	GDP	C6-N1	-2.50	1.34	1.38
163	FF	500	GDP	C6-N1	-2.50	1.34	1.38
163	WV	500	GDP	C6-N1	-2.50	1.34	1.38
163	IH	500	GDP	C6-N1	-2.50	1.34	1.38
163	IP	500	GDP	C6-N1	-2.50	1.34	1.38
163	LW	500	GDP	C6-N1	-2.50	1.34	1.38
163	VR	500	GDP	C6-N1	-2.50	1.34	1.38
163	H	500	GDP	C6-N1	-2.50	1.34	1.38
163	LM	500	GDP	C6-N1	-2.50	1.34	1.38
163	PT	500	GDP	C6-N1	-2.50	1.34	1.38
163	VN	500	GDP	C6-N1	-2.50	1.34	1.38
163	OJ	500	GDP	C6-N1	-2.50	1.34	1.38
163	LU	500	GDP	C6-N1	-2.49	1.34	1.38
163	KI	500	GDP	C6-N1	-2.49	1.34	1.38
163	VJ	500	GDP	C6-N1	-2.49	1.34	1.38
163	NJ	501	GDP	C6-N1	-2.49	1.34	1.38
163	PJ	500	GDP	C6-N1	-2.49	1.34	1.38
163	AH	500	GDP	C6-N1	-2.49	1.34	1.38
163	WX	500	GDP	C6-N1	-2.49	1.34	1.38
163	PD	500	GDP	C6-N1	-2.49	1.34	1.38
163	UJ	500	GDP	C6-N1	-2.49	1.34	1.38
163	WH	500	GDP	C6-N1	-2.49	1.34	1.38
163	TN	500	GDP	C6-N1	-2.49	1.34	1.38
163	QW	500	GDP	C6-N1	-2.49	1.34	1.38
163	TB	500	GDP	C6-N1	-2.49	1.34	1.38
163	UH	500	GDP	C6-N1	-2.49	1.34	1.38
163	MT	500	GDP	C6-N1	-2.49	1.34	1.38
163	JO	500	GDP	C6-N1	-2.49	1.34	1.38
163	JA	500	GDP	C6-N1	-2.49	1.34	1.38
163	KK	500	GDP	C6-N1	-2.49	1.34	1.38
163	HV	500	GDP	C6-N1	-2.49	1.34	1.38
163	KQ	500	GDP	C6-N1	-2.49	1.34	1.38
163	IN	500	GDP	C6-N1	-2.49	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	LI	500	GDP	C6-N1	-2.48	1.34	1.38
163	CW	500	GDP	C6-N1	-2.48	1.34	1.38
163	I	501	GDP	C6-N1	-2.48	1.34	1.38
163	PP	500	GDP	C6-N1	-2.48	1.34	1.38
163	MP	500	GDP	C6-N1	-2.48	1.34	1.38
163	IB	500	GDP	C6-N1	-2.48	1.34	1.38
163	LG	501	GDP	C6-N1	-2.48	1.34	1.38
163	S	500	GDP	C6-N1	-2.48	1.34	1.38
163	NT	500	GDP	C6-N1	-2.48	1.34	1.38
163	LA	500	GDP	C6-N1	-2.48	1.34	1.38
163	NF	500	GDP	C6-N1	-2.48	1.34	1.38
163	SP	500	GDP	C6-N1	-2.48	1.34	1.38
163	FV	501	GDP	C6-N1	-2.48	1.34	1.38
163	OV	500	GDP	C6-N1	-2.48	1.34	1.38
165	IW	501	GTP	PB-O3B	2.48	1.62	1.59
163	LQ	500	GDP	C6-N1	-2.48	1.34	1.38
163	SF	500	GDP	C6-N1	-2.48	1.34	1.38
163	KM	500	GDP	C6-N1	-2.48	1.34	1.38
163	HJ	500	GDP	C6-N1	-2.48	1.34	1.38
163	NX	500	GDP	C6-N1	-2.48	1.34	1.38
163	HF	500	GDP	C6-N1	-2.47	1.34	1.38
163	SN	501	GDP	C6-N1	-2.47	1.34	1.38
163	HP	501	GDP	C6-N1	-2.47	1.34	1.38
163	ID	500	GDP	C6-N1	-2.47	1.34	1.38
163	V	500	GDP	C6-N1	-2.47	1.34	1.38
163	OD	501	GDP	C6-N1	-2.47	1.34	1.38
163	KU	500	GDP	C6-N1	-2.47	1.34	1.38
163	SJ	501	GDP	C6-N1	-2.47	1.34	1.38
163	WJ	500	GDP	C6-N1	-2.47	1.34	1.38
163	TX	500	GDP	C6-N1	-2.47	1.34	1.38
163	KE	500	GDP	C6-N1	-2.47	1.34	1.38
163	NV	501	GDP	C6-N1	-2.47	1.34	1.38
163	ML	500	GDP	C6-N1	-2.47	1.34	1.38
163	QA	500	GDP	C6-N1	-2.47	1.34	1.38
163	KS	500	GDP	C6-N1	-2.47	1.34	1.38
163	WF	501	GDP	C6-N1	-2.47	1.34	1.38
163	MB	500	GDP	C6-N1	-2.46	1.34	1.38
163	OB	500	GDP	C6-N1	-2.46	1.34	1.38
163	VP	500	GDP	C6-N1	-2.46	1.34	1.38
163	IF	500	GDP	C6-N1	-2.46	1.34	1.38
163	JQ	500	GDP	C6-N1	-2.46	1.34	1.38
163	NL	500	GDP	C6-N1	-2.46	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	NH	500	GDP	C6-N1	-2.46	1.34	1.38
163	RI	500	GDP	C6-N1	-2.46	1.34	1.38
163	UV	500	GDP	C6-N1	-2.46	1.34	1.38
163	HN	501	GDP	C6-N1	-2.46	1.34	1.38
163	QQ	500	GDP	C6-N1	-2.46	1.34	1.38
163	LC	500	GDP	C6-N1	-2.46	1.34	1.38
163	PB	500	GDP	C6-N1	-2.46	1.34	1.38
163	OH	500	GDP	C6-N1	-2.46	1.34	1.38
163	TF	500	GDP	C6-N1	-2.46	1.34	1.38
163	MR	500	GDP	C6-N1	-2.46	1.34	1.38
163	VV	500	GDP	C6-N1	-2.46	1.34	1.38
163	JE	500	GDP	C6-N1	-2.46	1.34	1.38
163	LY	500	GDP	C6-N1	-2.46	1.34	1.38
163	ST	500	GDP	C6-N1	-2.45	1.34	1.38
163	UF	500	GDP	C6-N1	-2.45	1.34	1.38
163	MN	500	GDP	C6-N1	-2.45	1.34	1.38
163	VD	500	GDP	C6-N1	-2.45	1.34	1.38
163	SL	500	GDP	C6-N1	-2.45	1.34	1.38
163	G	500	GDP	C6-N1	-2.45	1.34	1.38
163	SB	501	GDP	C6-N1	-2.45	1.34	1.38
163	OX	500	GDP	C6-N1	-2.45	1.34	1.38
163	IX	501	GDP	C6-N1	-2.45	1.34	1.38
163	QM	500	GDP	C6-N1	-2.45	1.34	1.38
163	VT	500	GDP	C6-N1	-2.45	1.34	1.38
163	FJ	501	GDP	C6-N1	-2.45	1.34	1.38
163	OP	501	GDP	C6-N1	-2.45	1.34	1.38
163	MF	500	GDP	C6-N1	-2.45	1.34	1.38
163	P	500	GDP	C5-N7	-2.44	1.34	1.39
163	WB	500	GDP	C6-N1	-2.44	1.34	1.38
163	OT	500	GDP	C6-N1	-2.44	1.34	1.38
163	IR	500	GDP	C6-N1	-2.44	1.34	1.38
163	QO	500	GDP	C6-N1	-2.44	1.34	1.38
163	RM	500	GDP	C6-N1	-2.44	1.34	1.38
163	RA	500	GDP	C6-N1	-2.44	1.34	1.38
163	TJ	500	GDP	C6-N1	-2.44	1.34	1.38
163	MD	500	GDP	C6-N1	-2.43	1.34	1.38
163	UT	500	GDP	C6-N1	-2.43	1.34	1.38
163	WL	500	GDP	C6-N1	-2.43	1.34	1.38
163	HB	501	GDP	C6-N1	-2.43	1.34	1.38
163	NR	500	GDP	C6-N1	-2.43	1.34	1.38
163	LO	500	GDP	C6-N1	-2.43	1.34	1.38
163	PV	500	GDP	C6-N1	-2.43	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	KO	500	GDP	C6-N1	-2.43	1.34	1.38
163	CK	501	GDP	C6-N1	-2.43	1.34	1.38
163	ND	500	GDP	C6-N1	-2.42	1.34	1.38
163	VH	500	GDP	C6-N1	-2.42	1.34	1.38
163	W	500	GDP	C6-N1	-2.42	1.34	1.38
163	MZ	500	GDP	C6-N1	-2.42	1.34	1.38
163	QE	500	GDP	C6-N1	-2.41	1.34	1.38
163	OF	500	GDP	C6-N1	-2.41	1.34	1.38
163	LE	500	GDP	C6-N1	-2.41	1.34	1.38
163	KC	500	GDP	C6-N1	-2.41	1.34	1.38
163	OR	500	GDP	C6-N1	-2.41	1.34	1.38
163	M	500	GDP	C6-N1	-2.41	1.34	1.38
163	QK	500	GDP	C6-N1	-2.41	1.34	1.38
163	UR	500	GDP	C6-N1	-2.41	1.34	1.38
163	T	501	GDP	C6-N1	-2.41	1.34	1.38
163	RS	500	GDP	C6-N1	-2.41	1.34	1.38
163	TV	500	GDP	C6-N1	-2.41	1.34	1.38
163	WR	501	GDP	C6-N1	-2.40	1.34	1.38
163	KA	500	GDP	C6-N1	-2.40	1.34	1.38
163	TR	500	GDP	C6-N1	-2.39	1.34	1.38
163	MV	500	GDP	C6-N1	-2.39	1.34	1.38
163	E	500	GDP	PA-O3A	2.38	1.62	1.59
163	MJ	500	GDP	C6-N1	-2.38	1.34	1.38
165	CE	501	GTP	PB-O3B	2.38	1.62	1.59
165	IK	501	GTP	PB-O3B	2.38	1.62	1.59
163	NP	500	GDP	C6-N1	-2.37	1.34	1.38
165	NF	501	GTP	PA-O3A	2.37	1.62	1.59
163	A	501	GDP	C5-N7	-2.36	1.34	1.39
163	ED	500	GDP	C5-N7	-2.30	1.34	1.39
163	CY	500	GDP	C5-N7	-2.30	1.34	1.39
165	TM	501	GTP	PB-O3B	2.29	1.62	1.59
163	BX	500	GDP	C5-N7	-2.29	1.34	1.39
163	DK	501	GDP	C5-N7	-2.29	1.34	1.39
165	T	503	GTP	PB-O3B	2.29	1.62	1.59
165	VC	501	GTP	PB-O3B	2.28	1.62	1.59
165	QC	501	GTP	PB-O3B	2.28	1.62	1.59
165	VG	501	GTP	PB-O3B	2.27	1.61	1.59
165	HK	501	GTP	C2-N3	2.27	1.38	1.33
163	EX	500	GDP	PA-O3A	2.27	1.61	1.59
163	PL	501	GDP	C5-N7	-2.26	1.34	1.39
165	NR	501	GTP	PA-O3A	2.26	1.61	1.59
165	VQ	501	GTP	C2-N3	2.25	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
165	KT	501	GTP	C2-N3	2.25	1.38	1.33
163	BJ	500	GDP	C5-N7	-2.25	1.34	1.39
165	IC	501	GTP	C2-N3	2.24	1.38	1.33
163	FD	500	GDP	C5-N7	-2.24	1.34	1.39
165	HW	501	GTP	C2-N3	2.24	1.38	1.33
163	WT	500	GDP	C5-N7	-2.23	1.34	1.39
165	HB	503	GTP	C2-N3	2.23	1.38	1.33
165	D	501	GTP	PB-O3B	2.23	1.61	1.59
163	BT	500	GDP	C5-N7	-2.23	1.34	1.39
163	WH	500	GDP	C5-N7	-2.23	1.34	1.39
163	PX	501	GDP	C5-N7	-2.23	1.34	1.39
165	KH	501	GTP	C2-N3	2.23	1.38	1.33
163	CM	500	GDP	C5-N7	-2.22	1.34	1.39
163	CI	500	GDP	C5-N7	-2.22	1.34	1.39
165	KX	501	GTP	PB-O3A	2.22	1.61	1.59
163	FT	501	GDP	C4-N9	-2.22	1.32	1.38
163	BF	500	GDP	C5-N7	-2.22	1.34	1.39
165	VE	501	GTP	C2-N3	2.22	1.38	1.33
165	VO	501	GTP	PB-O3B	2.22	1.61	1.59
163	DG	500	GDP	C5-N7	-2.22	1.34	1.39
163	GD	500	GDP	C5-N7	-2.22	1.34	1.39
165	IK	501	GTP	C2-N3	2.22	1.38	1.33
163	GF	500	GDP	C5-N7	-2.22	1.34	1.39
165	IO	501	GTP	C2-N3	2.22	1.38	1.33
163	OB	500	GDP	C5-N7	-2.22	1.34	1.39
163	GB	500	GDP	C5-N7	-2.21	1.34	1.39
163	DS	500	GDP	C5-N7	-2.21	1.34	1.39
165	LH	501	GTP	C2-N3	2.21	1.38	1.33
165	HN	503	GTP	C2-N3	2.21	1.38	1.33
165	RO	501	GTP	C2-N3	2.21	1.38	1.33
165	OK	501	GTP	C2-N3	2.21	1.38	1.33
165	QF	501	GTP	C2-N3	2.20	1.38	1.33
165	OD	503	GTP	PB-O3B	2.20	1.61	1.59
165	HY	501	GTP	C2-N3	2.20	1.38	1.33
165	NF	501	GTP	C2-N3	2.20	1.38	1.33
165	OW	501	GTP	C2-N3	2.20	1.38	1.33
165	KL	501	GTP	C2-N3	2.20	1.38	1.33
163	DC	500	GDP	C5-N7	-2.20	1.34	1.39
163	GN	500	GDP	C5-N7	-2.20	1.34	1.39
165	SS	501	GTP	C2-N3	2.20	1.38	1.33
165	NR	501	GTP	PB-O3A	2.20	1.61	1.59
163	BP	500	GDP	C5-N7	-2.20	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
165	QR	501	GTP	C2-N3	2.20	1.38	1.33
163	EB	500	GDP	C5-N7	-2.20	1.34	1.39
163	GL	500	GDP	C5-N7	-2.20	1.34	1.39
165	RC	501	GTP	PB-O3B	2.19	1.61	1.59
165	CQ	501	GTP	PB-O3B	2.19	1.61	1.59
163	ON	500	GDP	C5-N7	-2.19	1.34	1.39
165	VO	501	GTP	C2-N3	2.19	1.38	1.33
165	D	501	GTP	PA-O3A	2.19	1.61	1.59
165	IY	501	GTP	C2-N3	2.19	1.38	1.33
163	FL	500	GDP	C5-N7	-2.19	1.34	1.39
165	RO	501	GTP	PB-O3B	2.19	1.61	1.59
165	IK	501	GTP	O4'-C4'	-2.19	1.40	1.45
163	GX	500	GDP	C5-N7	-2.19	1.34	1.39
165	LV	501	GTP	C2-N3	2.19	1.38	1.33
165	JT	501	GTP	C2-N3	2.19	1.38	1.33
165	KX	501	GTP	C2-N3	2.19	1.38	1.33
163	U	500	GDP	C5-N7	-2.19	1.34	1.39
165	IU	501	GTP	C2-N3	2.19	1.38	1.33
163	LU	500	GDP	C5-N7	-2.18	1.34	1.39
163	FN	500	GDP	C5-N7	-2.18	1.34	1.39
165	WE	501	GTP	C2-N3	2.18	1.38	1.33
163	AZ	500	GDP	C5-N7	-2.18	1.34	1.39
163	EP	500	GDP	C5-N7	-2.18	1.34	1.39
165	LT	501	GTP	C2-N3	2.18	1.38	1.33
165	NY	501	GTP	C2-N3	2.18	1.38	1.33
165	RC	501	GTP	C2-N3	2.18	1.38	1.33
165	WQ	501	GTP	C2-N3	2.18	1.38	1.33
165	NQ	501	GTP	C2-N3	2.18	1.38	1.33
165	TU	501	GTP	C2-N3	2.18	1.38	1.33
165	NE	501	GTP	C2-N3	2.18	1.38	1.33
163	GP	500	GDP	C5-N7	-2.18	1.34	1.39
165	IQ	501	GTP	C2-N3	2.18	1.38	1.33
163	AP	500	GDP	C5-N7	-2.18	1.34	1.39
165	QT	501	GTP	C2-N3	2.18	1.38	1.33
163	EL	500	GDP	C5-N7	-2.18	1.34	1.39
165	NM	501	GTP	C2-N3	2.18	1.38	1.33
163	SH	500	GDP	C5-N7	-2.18	1.34	1.39
163	AV	500	GDP	C5-N7	-2.18	1.34	1.39
165	JV	501	GTP	C2-N3	2.17	1.38	1.33
165	IM	501	GTP	C2-N3	2.17	1.38	1.33
165	MV	501	GTP	C2-N3	2.17	1.38	1.33
163	AF	500	GDP	C5-N7	-2.17	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	HL	501	GDP	C5-N7	-2.17	1.34	1.39
163	NP	500	GDP	C5-N7	-2.17	1.34	1.39
165	UI	501	GTP	C2-N3	2.17	1.38	1.33
165	VY	501	GTP	C2-N3	2.17	1.38	1.33
165	HE	501	GTP	C2-N3	2.17	1.38	1.33
165	IG	501	GTP	C2-N3	2.17	1.38	1.33
165	Q	501	GTP	C2-N3	2.17	1.38	1.33
163	QG	500	GDP	C5-N7	-2.17	1.34	1.39
165	WG	501	GTP	C2-N3	2.17	1.38	1.33
163	GR	500	GDP	C5-N7	-2.17	1.34	1.39
163	VL	500	GDP	C5-N7	-2.17	1.34	1.39
165	IA	501	GTP	C2-N3	2.17	1.38	1.33
165	KB	502	GTP	C2-N3	2.17	1.38	1.33
163	BL	500	GDP	C5-N7	-2.17	1.34	1.39
163	KU	500	GDP	C5-N7	-2.17	1.34	1.39
165	SG	501	GTP	C2-N3	2.17	1.38	1.33
165	NC	501	GTP	C2-N3	2.17	1.38	1.33
165	HQ	501	GTP	C2-N3	2.17	1.38	1.33
165	VS	501	GTP	C2-N3	2.17	1.38	1.33
165	OP	503	GTP	PB-O3B	2.17	1.61	1.59
165	VS	501	GTP	PB-O3B	2.17	1.61	1.59
163	FH	500	GDP	C5-N7	-2.17	1.34	1.39
163	DO	500	GDP	C5-N7	-2.16	1.34	1.39
163	DU	500	GDP	C5-N7	-2.16	1.34	1.39
165	IS	501	GTP	C2-N3	2.16	1.38	1.33
163	BN	500	GDP	C5-N7	-2.16	1.34	1.39
163	DW	501	GDP	C5-N7	-2.16	1.34	1.39
163	EN	500	GDP	C5-N7	-2.16	1.34	1.39
163	UT	500	GDP	C5-N7	-2.16	1.34	1.39
165	NO	501	GTP	C2-N3	2.16	1.38	1.33
163	F	500	GDP	C5-N7	-2.16	1.34	1.39
163	WP	500	GDP	C5-N7	-2.16	1.34	1.39
165	IW	501	GTP	C2-N3	2.16	1.38	1.33
163	FT	501	GDP	C5-N7	-2.16	1.34	1.39
165	WS	501	GTP	C2-N3	2.16	1.38	1.33
165	QO	501	GTP	PB-O3B	2.16	1.61	1.59
163	QS	500	GDP	C5-N7	-2.16	1.34	1.39
165	II	501	GTP	C2-N3	2.16	1.38	1.33
165	QH	501	GTP	C2-N3	2.16	1.38	1.33
163	ST	500	GDP	C5-N7	-2.16	1.34	1.39
165	VG	501	GTP	C2-N3	2.16	1.38	1.33
165	LJ	501	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)
165	WC	501	GTP	C2-N3	2.16	1.38	1.33
163	LI	500	GDP	C5-N7	-2.16	1.34	1.39
163	PV	500	GDP	C5-N7	-2.16	1.34	1.39
165	JF	501	GTP	C2-N3	2.16	1.38	1.33
165	KD	502	GTP	C2-N3	2.16	1.38	1.33
165	SO	501	GTP	C2-N3	2.16	1.38	1.33
163	QU	500	GDP	C5-N7	-2.15	1.34	1.39
165	IW	501	GTP	O4'-C4'	-2.15	1.40	1.45
165	VM	501	GTP	C2-N3	2.15	1.38	1.33
163	AL	500	GDP	C5-N7	-2.15	1.34	1.39
163	DA	500	GDP	C5-N7	-2.15	1.34	1.39
163	ER	500	GDP	C5-N7	-2.15	1.34	1.39
163	NT	500	GDP	C5-N7	-2.15	1.34	1.39
165	VH	501	GTP	C2-N3	2.15	1.38	1.33
163	EH	500	GDP	C5-N7	-2.15	1.34	1.39
165	CH	501	GTP	C2-N3	2.15	1.38	1.33
165	KZ	501	GTP	C2-N3	2.15	1.38	1.33
163	ND	500	GDP	C5-N7	-2.15	1.34	1.39
163	PP	500	GDP	C5-N7	-2.15	1.34	1.39
163	GJ	500	GDP	C5-N7	-2.15	1.34	1.39
163	WD	500	GDP	C5-N7	-2.15	1.34	1.39
163	RW	500	GDP	C5-N7	-2.15	1.34	1.39
165	WA	501	GTP	C2-N3	2.15	1.38	1.33
165	UO	501	GTP	C2-N3	2.15	1.38	1.33
163	EV	500	GDP	C5-N7	-2.15	1.34	1.39
163	UH	500	GDP	C5-N7	-2.15	1.34	1.39
163	AB	500	GDP	C5-N7	-2.15	1.34	1.39
163	AJ	500	GDP	C5-N7	-2.15	1.34	1.39
163	BH	500	GDP	C5-N7	-2.15	1.34	1.39
163	CQ	500	GDP	C5-N7	-2.15	1.34	1.39
163	VX	500	GDP	C5-N7	-2.15	1.34	1.39
165	JZ	501	GTP	C2-N3	2.15	1.38	1.33
165	UQ	501	GTP	C2-N3	2.14	1.38	1.33
165	SC	501	GTP	C2-N3	2.14	1.38	1.33
163	KI	500	GDP	C5-N7	-2.14	1.34	1.39
163	UD	500	GDP	C5-N7	-2.14	1.34	1.39
163	O	500	GDP	C5-N7	-2.14	1.34	1.39
165	R	501	GTP	C2-N3	2.14	1.38	1.33
163	AH	500	GDP	C5-N7	-2.14	1.34	1.39
163	HX	501	GDP	C5-N7	-2.14	1.34	1.39
165	JB	501	GTP	C2-N3	2.14	1.38	1.33
163	QI	500	GDP	C5-N7	-2.14	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	S	500	GDP	C5-N7	-2.14	1.34	1.39
163	KS	500	GDP	C5-N7	-2.14	1.34	1.39
165	JW	501	GTP	C2-N3	2.14	1.38	1.33
165	OD	503	GTP	C2-N3	2.14	1.38	1.33
165	MJ	501	GTP	C2-N3	2.14	1.38	1.33
165	KR	501	GTP	C2-N3	2.14	1.38	1.33
165	QX	501	GTP	C2-N3	2.14	1.38	1.33
165	UU	501	GTP	C2-N3	2.14	1.38	1.33
163	GH	500	GDP	C5-N7	-2.14	1.34	1.39
165	CH	501	GTP	C5-N7	-2.14	1.34	1.39
163	FB	500	GDP	C5-N7	-2.14	1.34	1.39
163	DQ	500	GDP	C5-N7	-2.14	1.34	1.39
163	KG	500	GDP	C5-N7	-2.14	1.34	1.39
163	RK	500	GDP	C5-N7	-2.14	1.34	1.39
165	TI	501	GTP	C2-N3	2.14	1.38	1.33
165	NU	501	GTP	C2-N3	2.14	1.38	1.33
165	KF	501	GTP	C2-N3	2.14	1.38	1.33
165	HI	501	GTP	C2-N3	2.14	1.38	1.33
165	JR	501	GTP	C2-N3	2.14	1.38	1.33
165	VA	501	GTP	C2-N3	2.14	1.38	1.33
165	VC	501	GTP	C2-N3	2.14	1.38	1.33
163	M	500	GDP	C5-N7	-2.14	1.34	1.39
163	BR	500	GDP	C5-N7	-2.14	1.34	1.39
165	L	501	GTP	C2-N3	2.14	1.38	1.33
163	QA	500	GDP	C5-N7	-2.14	1.34	1.39
163	AR	500	GDP	C5-N7	-2.14	1.34	1.39
163	JU	500	GDP	C5-N7	-2.14	1.34	1.39
163	OP	501	GDP	C5-N7	-2.14	1.34	1.39
165	US	501	GTP	C2-N3	2.14	1.38	1.33
165	WO	501	GTP	C2-N3	2.14	1.38	1.33
165	NR	501	GTP	C2-N3	2.14	1.38	1.33
163	V	500	GDP	C5-N7	-2.14	1.34	1.39
165	IO	501	GTP	PB-O3B	2.14	1.61	1.59
165	J	501	GTP	C2-N3	2.13	1.38	1.33
163	DM	500	GDP	C5-N7	-2.13	1.34	1.39
163	QO	500	GDP	C5-N7	-2.13	1.34	1.39
163	FP	500	GDP	C5-N7	-2.13	1.34	1.39
163	IV	500	GDP	C5-N7	-2.13	1.34	1.39
165	SK	501	GTP	C2-N3	2.13	1.38	1.33
165	HM	501	GTP	C2-N3	2.13	1.38	1.33
163	TT	500	GDP	C5-N7	-2.13	1.34	1.39
165	JN	501	GTP	C2-N3	2.13	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	EF	500	GDP	C5-N7	-2.13	1.34	1.39
163	UF	500	GDP	C5-N7	-2.13	1.34	1.39
163	RM	500	GDP	C5-N7	-2.13	1.34	1.39
165	JH	501	GTP	C2-N3	2.13	1.38	1.33
165	NI	501	GTP	C2-N3	2.13	1.38	1.33
165	OA	501	GTP	C2-N3	2.13	1.38	1.33
163	OL	500	GDP	C5-N7	-2.13	1.34	1.39
163	GT	501	GDP	C5-N7	-2.13	1.34	1.39
163	UN	500	GDP	C5-N7	-2.13	1.34	1.39
165	IE	501	GTP	C2-N3	2.13	1.38	1.33
165	GI	501	GTP	C2-N3	2.13	1.38	1.33
163	LQ	500	GDP	C5-N7	-2.13	1.34	1.39
165	BU	501	GTP	C5-N7	-2.13	1.34	1.39
163	EH	500	GDP	C4-N9	-2.13	1.32	1.38
165	PA	501	GTP	C2-N3	2.13	1.38	1.33
165	TE	501	GTP	C2-N3	2.13	1.38	1.33
163	CA	500	GDP	C5-N7	-2.13	1.34	1.39
163	IH	500	GDP	C5-N7	-2.13	1.34	1.39
165	KN	502	GTP	C2-N3	2.13	1.38	1.33
165	NE	501	GTP	PB-O3B	2.13	1.61	1.59
163	IJ	500	GDP	C5-N7	-2.13	1.34	1.39
163	JI	500	GDP	C5-N7	-2.13	1.34	1.39
163	VH	500	GDP	C5-N7	-2.13	1.34	1.39
165	HA	501	GTP	C2-N3	2.13	1.38	1.33
163	TH	500	GDP	C5-N7	-2.13	1.34	1.39
163	RG	500	GDP	C5-N7	-2.13	1.34	1.39
163	FX	500	GDP	C5-N7	-2.13	1.34	1.39
165	OP	503	GTP	C2-N3	2.13	1.38	1.33
163	UP	500	GDP	C5-N7	-2.13	1.34	1.39
165	RR	501	GTP	C2-N3	2.13	1.38	1.33
165	OM	501	GTP	C2-N3	2.12	1.38	1.33
165	UG	501	GTP	C2-N3	2.12	1.38	1.33
163	SV	501	GDP	C5-N7	-2.12	1.34	1.39
165	JJ	501	GTP	C2-N3	2.12	1.38	1.33
165	C	501	GTP	C2-N3	2.12	1.38	1.33
163	AN	500	GDP	C5-N7	-2.12	1.34	1.39
163	IT	501	GDP	C5-N7	-2.12	1.34	1.39
165	K	501	GTP	C2-N3	2.12	1.38	1.33
163	FJ	501	GDP	C5-N7	-2.12	1.34	1.39
165	OI	501	GTP	C2-N3	2.12	1.38	1.33
165	RX	501	GTP	C2-N3	2.12	1.38	1.33
165	MG	501	GTP	C2-N3	2.12	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
165	OS	501	GTP	C2-N3	2.12	1.38	1.33
163	AD	500	GDP	C5-N7	-2.12	1.34	1.39
163	FR	501	GDP	C5-N7	-2.12	1.34	1.39
165	MA	501	GTP	C2-N3	2.12	1.38	1.33
165	UC	501	GTP	C2-N3	2.12	1.38	1.33
163	PJ	500	GDP	C5-N7	-2.12	1.34	1.39
165	KL	501	GTP	PB-O3A	2.12	1.61	1.59
165	QI	501	GTP	PB-O3B	2.12	1.61	1.59
165	UE	501	GTP	C2-N3	2.12	1.38	1.33
163	DE	500	GDP	C5-N7	-2.12	1.34	1.39
163	UX	500	GDP	C5-N7	-2.12	1.34	1.39
163	MT	500	GDP	C5-N7	-2.12	1.34	1.39
163	OX	500	GDP	C5-N7	-2.12	1.34	1.39
165	HG	501	GTP	C2-N3	2.12	1.38	1.33
165	OY	501	GTP	C2-N3	2.12	1.38	1.33
165	WM	501	GTP	C2-N3	2.11	1.38	1.33
163	RA	500	GDP	C5-N7	-2.11	1.34	1.39
163	TL	501	GDP	C5-N7	-2.11	1.34	1.39
165	TG	501	GTP	C2-N3	2.11	1.38	1.33
165	SW	501	GTP	C2-N3	2.11	1.38	1.33
163	NN	500	GDP	C5-N7	-2.11	1.34	1.39
165	CB	501	GTP	C2-N3	2.11	1.38	1.33
163	DY	500	GDP	C5-N7	-2.11	1.34	1.39
163	MR	500	GDP	C5-N7	-2.11	1.34	1.39
165	QI	501	GTP	C2-N3	2.11	1.38	1.33
163	NJ	501	GDP	C5-N7	-2.11	1.34	1.39
165	AI	501	GTP	C2-N3	2.11	1.38	1.33
165	KJ	501	GTP	C2-N3	2.11	1.38	1.33
163	DI	500	GDP	C5-N7	-2.11	1.34	1.39
165	VT	501	GTP	C2-N3	2.11	1.38	1.33
163	UB	500	GDP	C5-N7	-2.11	1.34	1.39
163	VF	500	GDP	C5-N7	-2.11	1.34	1.39
163	LW	500	GDP	C5-N7	-2.11	1.34	1.39
165	JK	501	GTP	C2-N3	2.11	1.38	1.33
165	KP	502	GTP	C2-N3	2.11	1.38	1.33
163	UR	500	GDP	C5-N7	-2.11	1.34	1.39
163	ET	500	GDP	C4-N9	-2.11	1.32	1.38
165	RF	501	GTP	C2-N3	2.11	1.38	1.33
165	QL	501	GTP	C2-N3	2.11	1.38	1.33
163	NR	500	GDP	C5-N7	-2.11	1.34	1.39
165	MY	501	GTP	C2-N3	2.11	1.38	1.33
163	WX	500	GDP	C5-N7	-2.11	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
165	UK	501	GTP	C2-N3	2.11	1.38	1.33
165	PC	501	GTP	C2-N3	2.11	1.38	1.33
163	UV	500	GDP	C5-N7	-2.11	1.34	1.39
163	UL	500	GDP	C5-N7	-2.10	1.34	1.39
165	EJ	501	GTP	C2-N3	2.10	1.38	1.33
165	TM	501	GTP	C2-N3	2.10	1.38	1.33
165	MC	501	GTP	C2-N3	2.10	1.38	1.33
163	EJ	500	GDP	C5-N7	-2.10	1.34	1.39
163	GV	501	GDP	C5-N7	-2.10	1.34	1.39
163	PN	500	GDP	C5-N7	-2.10	1.34	1.39
163	PR	501	GDP	C5-N7	-2.10	1.34	1.39
163	I	501	GDP	C5-N7	-2.10	1.34	1.39
163	CO	500	GDP	C5-N7	-2.10	1.34	1.39
165	RH	501	GTP	C2-N3	2.10	1.38	1.33
165	MS	501	GTP	C2-N3	2.10	1.38	1.33
165	HS	501	GTP	C2-N3	2.10	1.38	1.33
163	BD	500	GDP	C5-N7	-2.10	1.34	1.39
163	NH	500	GDP	C5-N7	-2.10	1.34	1.39
163	EX	500	GDP	C5-N7	-2.10	1.34	1.39
163	SL	500	GDP	C5-N7	-2.10	1.34	1.39
165	KF	501	GTP	PB-O3B	2.10	1.61	1.59
163	E	500	GDP	C5-N7	-2.10	1.34	1.39
163	QE	500	GDP	C5-N7	-2.10	1.34	1.39
165	TQ	501	GTP	C2-N3	2.10	1.38	1.33
163	G	500	GDP	C5-N7	-2.10	1.34	1.39
163	NB	500	GDP	C5-N7	-2.10	1.34	1.39
163	NF	500	GDP	C5-N7	-2.10	1.34	1.39
165	IC	501	GTP	PB-O3B	2.10	1.61	1.59
163	KY	500	GDP	C5-N7	-2.10	1.34	1.39
165	T	503	GTP	C2-N3	2.10	1.38	1.33
165	WY	501	GTP	C2-N3	2.10	1.38	1.33
165	LD	502	GTP	C2-N3	2.10	1.38	1.33
163	IF	500	GDP	C5-N7	-2.10	1.34	1.39
163	BV	500	GDP	C5-N7	-2.10	1.34	1.39
163	HR	500	GDP	C5-N7	-2.10	1.34	1.39
163	JS	500	GDP	C5-N7	-2.10	1.34	1.39
163	JQ	500	GDP	C5-N7	-2.10	1.34	1.39
163	TN	500	GDP	C5-N7	-2.10	1.34	1.39
165	UA	501	GTP	C2-N3	2.10	1.38	1.33
163	MD	500	GDP	C5-N7	-2.09	1.34	1.39
163	MZ	500	GDP	C5-N7	-2.09	1.34	1.39
165	LL	501	GTP	C2-N3	2.09	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	JY	501	GDP	C5-N7	-2.09	1.34	1.39
163	AN	500	GDP	C4-N9	-2.09	1.32	1.38
163	HF	500	GDP	C5-N7	-2.09	1.34	1.39
163	AX	500	GDP	C5-N7	-2.09	1.34	1.39
165	DQ	501	GTP	C2-N3	2.09	1.38	1.33
165	DT	501	GTP	C2-N3	2.09	1.38	1.33
165	TW	501	GTP	C2-N3	2.09	1.38	1.33
165	LB	501	GTP	PA-O3A	2.09	1.61	1.59
165	MM	501	GTP	C2-N3	2.09	1.38	1.33
163	QC	500	GDP	C5-N7	-2.09	1.34	1.39
163	WL	500	GDP	C5-N7	-2.09	1.34	1.39
163	OT	500	GDP	C5-N7	-2.09	1.34	1.39
165	LB	501	GTP	C2-N3	2.09	1.38	1.33
165	BI	501	GTP	C2-N3	2.09	1.38	1.33
165	MO	501	GTP	C2-N3	2.09	1.38	1.33
163	IR	500	GDP	C5-N7	-2.09	1.34	1.39
163	IB	500	GDP	C5-N7	-2.09	1.34	1.39
163	CG	500	GDP	C5-N7	-2.09	1.34	1.39
163	LO	500	GDP	C5-N7	-2.09	1.34	1.39
163	OH	500	GDP	C5-N7	-2.09	1.34	1.39
163	TD	500	GDP	C5-N7	-2.09	1.34	1.39
163	SR	500	GDP	C5-N7	-2.09	1.34	1.39
163	OF	500	GDP	C5-N7	-2.09	1.34	1.39
163	PD	500	GDP	C5-N7	-2.09	1.34	1.39
165	SA	501	GTP	C2-N3	2.09	1.38	1.33
163	W	500	GDP	C5-N7	-2.09	1.34	1.39
163	AT	500	GDP	C5-N7	-2.09	1.34	1.39
163	KW	500	GDP	C5-N7	-2.09	1.34	1.39
165	NK	501	GTP	C2-N3	2.09	1.38	1.33
165	CT	501	GTP	C2-N3	2.09	1.38	1.33
163	VN	500	GDP	C5-N7	-2.09	1.34	1.39
163	VJ	500	GDP	C5-N7	-2.09	1.34	1.39
165	EA	501	GTP	C2-N3	2.09	1.38	1.33
163	MP	500	GDP	C5-N7	-2.09	1.34	1.39
163	WV	500	GDP	C5-N7	-2.09	1.34	1.39
163	RE	500	GDP	C5-N7	-2.08	1.34	1.39
165	VK	501	GTP	C2-N3	2.08	1.38	1.33
165	WI	501	GTP	C2-N3	2.08	1.38	1.33
163	CC	500	GDP	C5-N7	-2.08	1.34	1.39
163	N	500	GDP	C5-N7	-2.08	1.34	1.39
165	KR	501	GTP	PB-O3B	2.08	1.61	1.59
168	8a	801	ATP	PA-O3A	-2.08	1.57	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	FV	501	GDP	C5-N7	-2.08	1.34	1.39
165	PI	501	GTP	C2-N3	2.08	1.38	1.33
165	AS	501	GTP	C2-N3	2.08	1.38	1.33
163	JE	500	GDP	C5-N7	-2.08	1.34	1.39
163	LM	500	GDP	C5-N7	-2.08	1.34	1.39
165	PQ	501	GTP	C2-N3	2.08	1.38	1.33
163	JA	500	GDP	C5-N7	-2.08	1.34	1.39
163	RU	500	GDP	C5-N7	-2.08	1.34	1.39
165	OU	501	GTP	C2-N3	2.08	1.38	1.33
165	K	501	GTP	PB-O3A	2.08	1.61	1.59
165	RL	501	GTP	C2-N3	2.08	1.38	1.33
165	VW	501	GTP	C2-N3	2.08	1.38	1.33
163	IX	501	GDP	C5-N7	-2.08	1.34	1.39
165	AK	501	GTP	C2-N3	2.08	1.38	1.33
165	FE	501	GTP	C2-N3	2.08	1.38	1.33
165	LX	501	GTP	C2-N3	2.08	1.38	1.33
163	CE	500	GDP	C5-N7	-2.08	1.34	1.39
163	PF	501	GDP	C5-N7	-2.08	1.34	1.39
163	RC	500	GDP	C5-N7	-2.08	1.34	1.39
163	LS	500	GDP	C5-N7	-2.08	1.34	1.39
163	CK	501	GDP	C5-N7	-2.08	1.34	1.39
163	FF	500	GDP	C5-N7	-2.08	1.34	1.39
163	VV	500	GDP	C5-N7	-2.08	1.34	1.39
165	BQ	501	GTP	C2-N3	2.08	1.38	1.33
163	VD	500	GDP	C5-N7	-2.08	1.34	1.39
163	TX	500	GDP	C5-N7	-2.08	1.34	1.39
165	EI	501	GTP	C2-N3	2.08	1.38	1.33
163	H	500	GDP	C5-N7	-2.08	1.34	1.39
163	JW	500	GDP	C5-N7	-2.08	1.34	1.39
165	RJ	501	GTP	C2-N3	2.08	1.38	1.33
163	LA	500	GDP	C5-N7	-2.08	1.34	1.39
163	MX	500	GDP	C5-N7	-2.08	1.34	1.39
163	NV	501	GDP	C5-N7	-2.08	1.34	1.39
165	UW	501	GTP	C2-N3	2.08	1.38	1.33
163	QQ	500	GDP	C5-N7	-2.08	1.34	1.39
163	JG	500	GDP	C5-N7	-2.08	1.34	1.39
165	EJ	501	GTP	PA-O3A	2.08	1.61	1.59
163	VR	500	GDP	C5-N7	-2.08	1.34	1.39
163	MH	500	GDP	C5-N7	-2.08	1.34	1.39
163	VB	500	GDP	C5-N7	-2.08	1.34	1.39
163	ET	500	GDP	C5-N7	-2.08	1.34	1.39
165	PY	501	GTP	C2-N3	2.08	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	WJ	500	GDP	C5-N7	-2.08	1.34	1.39
163	KQ	500	GDP	C5-N7	-2.08	1.34	1.39
163	PT	500	GDP	C5-N7	-2.07	1.34	1.39
163	QM	500	GDP	C5-N7	-2.07	1.34	1.39
163	RS	500	GDP	C5-N7	-2.07	1.34	1.39
163	CU	500	GDP	C5-N7	-2.07	1.34	1.39
165	GI	501	GTP	C5-N7	-2.07	1.34	1.39
165	HU	501	GTP	C2-N3	2.07	1.38	1.33
165	LZ	502	GTP	C2-N3	2.07	1.38	1.33
163	MN	500	GDP	C5-N7	-2.07	1.34	1.39
163	PB	500	GDP	C5-N7	-2.07	1.34	1.39
163	HP	501	GDP	C5-N7	-2.07	1.34	1.39
163	VT	500	GDP	C5-N7	-2.07	1.34	1.39
165	BG	501	GTP	C2-N3	2.07	1.38	1.33
165	KV	501	GTP	C2-N3	2.07	1.38	1.33
163	WF	501	GDP	C5-N7	-2.07	1.34	1.39
163	VP	500	GDP	C5-N7	-2.07	1.34	1.39
165	PM	501	GTP	C2-N3	2.07	1.38	1.33
165	FQ	501	GTP	C2-N3	2.07	1.38	1.33
163	KK	500	GDP	C5-N7	-2.07	1.34	1.39
165	OG	501	GTP	C2-N3	2.07	1.38	1.33
165	UM	501	GTP	C2-N3	2.07	1.38	1.33
163	ML	500	GDP	C5-N7	-2.07	1.34	1.39
165	ME	501	GTP	PA-O3A	2.07	1.61	1.59
165	PE	501	GTP	C2-N3	2.07	1.38	1.33
163	AX	500	GDP	C4-N9	-2.07	1.32	1.38
163	LE	500	GDP	C5-N7	-2.07	1.34	1.39
165	DE	501	GTP	C5-N7	-2.07	1.34	1.39
163	SB	501	GDP	C5-N7	-2.07	1.34	1.39
165	LN	502	GTP	C2-N3	2.07	1.38	1.33
165	RN	501	GTP	C2-N3	2.07	1.38	1.33
163	TP	500	GDP	C5-N7	-2.07	1.34	1.39
165	RB	501	GTP	C2-N3	2.07	1.38	1.33
165	TO	501	GTP	C2-N3	2.07	1.38	1.33
163	JK	500	GDP	C5-N7	-2.07	1.34	1.39
163	LG	501	GDP	C5-N7	-2.06	1.34	1.39
163	SD	500	GDP	C5-N7	-2.06	1.34	1.39
165	OO	501	GTP	C2-N3	2.06	1.38	1.33
163	AV	500	GDP	C4-N9	-2.06	1.32	1.38
165	WW	501	GTP	C2-N3	2.06	1.38	1.33
165	EP	501	GTP	PB-O3B	2.06	1.61	1.59
163	KE	500	GDP	C5-N7	-2.06	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
165	CE	501	GTP	C2-N3	2.06	1.38	1.33
163	SP	500	GDP	C5-N7	-2.06	1.34	1.39
165	CK	503	GTP	C2-N3	2.06	1.38	1.33
165	WK	501	GTP	C2-N3	2.06	1.38	1.33
163	WR	501	GDP	C5-N7	-2.06	1.34	1.39
165	FT	503	GTP	C5-N7	-2.06	1.34	1.39
163	SF	500	GDP	C5-N7	-2.06	1.34	1.39
163	IN	500	GDP	C5-N7	-2.06	1.34	1.39
165	FT	503	GTP	C2-N3	2.06	1.38	1.33
165	NQ	501	GTP	PB-O3B	2.06	1.61	1.59
165	TC	501	GTP	C2-N3	2.06	1.38	1.33
165	PO	501	GTP	C2-N3	2.06	1.38	1.33
165	PW	501	GTP	C2-N3	2.06	1.38	1.33
163	OD	501	GDP	C5-N7	-2.06	1.34	1.39
165	NA	501	GTP	C2-N3	2.06	1.38	1.33
163	HT	501	GDP	C5-N7	-2.06	1.34	1.39
165	CJ	501	GTP	C2-N3	2.06	1.38	1.33
163	OJ	500	GDP	C5-N7	-2.06	1.34	1.39
163	PH	500	GDP	C5-N7	-2.06	1.34	1.39
163	MV	500	GDP	C5-N7	-2.06	1.34	1.39
165	RT	501	GTP	C2-N3	2.06	1.38	1.33
165	LF	502	GTP	C2-N3	2.06	1.38	1.33
165	TS	501	GTP	C2-N3	2.06	1.38	1.33
163	QW	500	GDP	C5-N7	-2.06	1.34	1.39
165	VS	501	GTP	PB-O3A	2.06	1.61	1.59
165	AW	501	GTP	C2-N3	2.06	1.38	1.33
165	PU	501	GTP	C2-N3	2.06	1.38	1.33
165	RV	501	GTP	C2-N3	2.06	1.38	1.33
163	UJ	500	GDP	C5-N7	-2.06	1.35	1.39
165	FJ	503	GTP	C2-N3	2.05	1.38	1.33
165	LR	502	GTP	C2-N3	2.05	1.38	1.33
165	JP	501	GTP	C2-N3	2.05	1.38	1.33
165	PK	501	GTP	C2-N3	2.05	1.38	1.33
165	BU	501	GTP	C2-N3	2.05	1.38	1.33
163	NL	500	GDP	C5-N7	-2.05	1.35	1.39
163	CS	500	GDP	C5-N7	-2.05	1.35	1.39
165	NF	501	GTP	PB-O3A	2.05	1.61	1.59
165	RB	501	GTP	PA-O3A	2.05	1.61	1.59
165	BA	501	GTP	C2-N3	2.05	1.38	1.33
165	CQ	501	GTP	C2-N3	2.05	1.38	1.33
163	HH	501	GDP	C5-N7	-2.05	1.35	1.39
163	KA	500	GDP	C5-N7	-2.05	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	TJ	500	GDP	C5-N7	-2.05	1.35	1.39
163	RQ	500	GDP	C5-N7	-2.05	1.35	1.39
163	FH	500	GDP	C4-N9	-2.05	1.32	1.38
163	IP	500	GDP	C5-N7	-2.05	1.35	1.39
163	MF	500	GDP	C5-N7	-2.05	1.35	1.39
165	BW	501	GTP	C2-N3	2.05	1.38	1.33
163	TB	500	GDP	C5-N7	-2.05	1.35	1.39
165	DH	501	GTP	C2-N3	2.05	1.38	1.33
165	GU	501	GTP	C2-N3	2.05	1.38	1.33
165	LP	502	GTP	C2-N3	2.05	1.38	1.33
165	HB	503	GTP	PB-O3B	2.05	1.61	1.59
163	BV	500	GDP	C4-N9	-2.05	1.32	1.38
163	KM	500	GDP	C5-N7	-2.05	1.35	1.39
163	WN	500	GDP	C5-N7	-2.05	1.35	1.39
163	SJ	501	GDP	C5-N7	-2.05	1.35	1.39
165	SU	501	GTP	C2-N3	2.05	1.38	1.33
163	LY	500	GDP	C5-N7	-2.05	1.35	1.39
165	BI	501	GTP	PB-O3B	2.05	1.61	1.59
165	FG	501	GTP	C2-N3	2.05	1.38	1.33
165	PG	501	GTP	C2-N3	2.05	1.38	1.33
165	NW	501	GTP	C2-N3	2.05	1.38	1.33
163	MJ	500	GDP	C5-N7	-2.05	1.35	1.39
165	SQ	501	GTP	C2-N3	2.05	1.38	1.33
163	OV	500	GDP	C5-N7	-2.05	1.35	1.39
165	WU	501	GTP	C2-N3	2.04	1.38	1.33
165	TK	501	GTP	C2-N3	2.04	1.38	1.33
163	HJ	500	GDP	C5-N7	-2.04	1.35	1.39
165	MQ	501	GTP	PB-O3A	2.04	1.61	1.59
165	MI	501	GTP	C2-N3	2.04	1.38	1.33
163	T	501	GDP	C5-N7	-2.04	1.35	1.39
163	TV	500	GDP	C5-N7	-2.04	1.35	1.39
165	JD	501	GTP	C2-N3	2.04	1.38	1.33
165	ME	501	GTP	C2-N3	2.04	1.38	1.33
165	QO	501	GTP	C2-N3	2.04	1.38	1.33
165	CT	501	GTP	C5-N7	-2.04	1.35	1.39
165	AD	501	GTP	C2-N3	2.04	1.38	1.33
165	GS	501	GTP	C2-N3	2.04	1.38	1.33
165	CV	501	GTP	C2-N3	2.04	1.38	1.33
163	ID	500	GDP	C5-N7	-2.04	1.35	1.39
163	AL	500	GDP	C4-N9	-2.03	1.32	1.38
163	LC	500	GDP	C5-N7	-2.03	1.35	1.39
165	FV	503	GTP	C2-N3	2.03	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
163	QK	500	GDP	C5-N7	-2.03	1.35	1.39
165	QU	501	GTP	C2-N3	2.03	1.38	1.33
163	TR	500	GDP	C5-N7	-2.03	1.35	1.39
165	QU	501	GTP	PB-O3B	2.03	1.61	1.59
163	IL	501	GDP	C5-N7	-2.03	1.35	1.39
163	RI	500	GDP	C5-N7	-2.03	1.35	1.39
165	AU	501	GTP	C2-N3	2.03	1.38	1.33
165	BS	501	GTP	C2-N3	2.03	1.38	1.33
165	BI	501	GTP	C5-N7	-2.03	1.35	1.39
163	HV	500	GDP	C5-N7	-2.03	1.35	1.39
163	NX	500	GDP	C5-N7	-2.03	1.35	1.39
165	NY	501	GTP	PA-O3A	2.03	1.61	1.59
163	LK	500	GDP	C5-N7	-2.03	1.35	1.39
163	JO	500	GDP	C5-N7	-2.03	1.35	1.39
165	QN	501	GTP	PA-O3A	2.03	1.61	1.59
165	MU	501	GTP	PB-O3B	2.03	1.61	1.59
163	CW	500	GDP	C5-N7	-2.03	1.35	1.39
163	RO	500	GDP	C5-N7	-2.03	1.35	1.39
165	PS	501	GTP	C2-N3	2.03	1.38	1.33
165	QN	501	GTP	C2-N3	2.03	1.38	1.33
163	CU	500	GDP	C4-N9	-2.02	1.32	1.38
165	OC	501	GTP	C2-N3	2.02	1.38	1.33
163	HD	501	GDP	C5-N7	-2.02	1.35	1.39
165	DX	501	GTP	C2-N3	2.02	1.38	1.33
165	SM	501	GTP	C2-N3	2.02	1.38	1.33
165	HN	503	GTP	PB-O3B	2.02	1.61	1.59
165	DE	501	GTP	C2-N3	2.02	1.38	1.33
165	SI	501	GTP	C2-N3	2.02	1.38	1.33
163	BJ	500	GDP	C4-N9	-2.02	1.32	1.38
163	DO	500	GDP	C4-N9	-2.02	1.32	1.38
165	GQ	501	GTP	C2-N3	2.02	1.38	1.33
163	OR	500	GDP	C5-N7	-2.02	1.35	1.39
163	WB	500	GDP	C5-N7	-2.02	1.35	1.39
165	EU	501	GTP	C5-N7	-2.02	1.35	1.39
165	SE	501	GTP	C2-N3	2.02	1.38	1.33
165	MQ	501	GTP	C2-N3	2.02	1.38	1.33
163	JM	501	GDP	C5-N7	-2.02	1.35	1.39
165	MU	501	GTP	C2-N3	2.02	1.38	1.33
163	KC	500	GDP	C5-N7	-2.02	1.35	1.39
163	SN	501	GDP	C5-N7	-2.02	1.35	1.39
165	AO	501	GTP	C2-N3	2.01	1.38	1.33
163	JC	500	GDP	C5-N7	-2.01	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
165	AY	501	GTP	C2-N3	2.01	1.38	1.33
165	CO	501	GTP	C2-N3	2.01	1.38	1.33
163	MB	500	GDP	C5-N7	-2.01	1.35	1.39
163	TF	500	GDP	C5-N7	-2.01	1.35	1.39
163	KO	500	GDP	C5-N7	-2.01	1.35	1.39
165	DV	501	GTP	C2-N3	2.01	1.38	1.33
165	GG	501	GTP	C2-N3	2.01	1.38	1.33
165	QB	501	GTP	PA-O3A	2.01	1.61	1.59
165	AA	501	GTP	C2-N3	2.01	1.38	1.33
163	BN	500	GDP	C4-N9	-2.01	1.32	1.38
163	ED	500	GDP	C4-N9	-2.01	1.33	1.38
165	FI	501	GTP	C2-N3	2.01	1.38	1.33
163	EV	500	GDP	C4-N9	-2.01	1.33	1.38
165	GQ	501	GTP	C5-N7	-2.01	1.35	1.39
163	HB	501	GDP	C5-N7	-2.01	1.35	1.39
165	DQ	501	GTP	PB-O3B	2.01	1.61	1.59
165	QC	501	GTP	C2-N3	2.01	1.38	1.33
165	AP	501	GTP	C5-N7	-2.00	1.35	1.39
165	QB	501	GTP	C2-N3	2.00	1.38	1.33

All (4620) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	CW	500	GDP	C5-C4-N3	-6.47	118.10	128.39
163	P	500	GDP	C5-C4-N3	-6.38	118.23	128.39
163	CK	501	GDP	C5-C4-N3	-6.27	118.41	128.39
163	QK	500	GDP	C5-C4-N3	-6.25	118.45	128.39
163	QW	500	GDP	C5-C4-N3	-6.25	118.45	128.39
163	TX	500	GDP	C5-C4-N3	-6.23	118.48	128.39
163	RQ	500	GDP	C5-C4-N3	-6.23	118.48	128.39
163	TL	501	GDP	C5-C4-N3	-6.22	118.49	128.39
163	A	501	GDP	C5-C4-N3	-6.21	118.50	128.39
163	WT	500	GDP	C5-C4-N3	-6.20	118.52	128.39
163	RE	500	GDP	C5-C4-N3	-6.20	118.52	128.39
163	OL	500	GDP	C5-C4-N3	-6.20	118.53	128.39
163	WH	500	GDP	C5-C4-N3	-6.18	118.55	128.39
163	WL	500	GDP	C5-C4-N3	-6.17	118.57	128.39
163	QI	500	GDP	C5-C4-N3	-6.16	118.58	128.39
163	OX	500	GDP	C5-C4-N3	-6.15	118.59	128.39
163	CY	500	GDP	C5-C4-N3	-6.15	118.60	128.39
163	QU	500	GDP	C5-C4-N3	-6.15	118.60	128.39
163	TD	500	GDP	C5-C4-N3	-6.15	118.61	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	RK	500	GDP	C5-C4-N3	-6.15	118.61	128.39
163	PX	501	GDP	C5-C4-N3	-6.15	118.61	128.39
163	NH	500	GDP	C5-C4-N3	-6.14	118.62	128.39
163	TP	500	GDP	C5-C4-N3	-6.14	118.62	128.39
163	CM	500	GDP	C5-C4-N3	-6.14	118.62	128.39
163	PL	501	GDP	C5-C4-N3	-6.14	118.62	128.39
163	VF	500	GDP	C5-C4-N3	-6.13	118.63	128.39
163	ML	500	GDP	C5-C4-N3	-6.13	118.64	128.39
163	SH	500	GDP	C5-C4-N3	-6.13	118.64	128.39
163	WP	500	GDP	C5-C4-N3	-6.13	118.64	128.39
163	WX	500	GDP	C5-C4-N3	-6.13	118.64	128.39
163	HV	500	GDP	C5-C4-N3	-6.12	118.64	128.39
163	BT	500	GDP	C5-C4-N3	-6.12	118.64	128.39
163	OV	500	GDP	C5-C4-N3	-6.12	118.64	128.39
163	E	500	GDP	C5-C4-N3	-6.12	118.65	128.39
163	JA	500	GDP	C5-C4-N3	-6.12	118.65	128.39
163	KY	500	GDP	C5-C4-N3	-6.12	118.65	128.39
163	RW	500	GDP	C5-C4-N3	-6.11	118.66	128.39
163	KA	500	GDP	C5-C4-N3	-6.11	118.66	128.39
163	KI	500	GDP	C5-C4-N3	-6.11	118.66	128.39
163	WD	500	GDP	C5-C4-N3	-6.11	118.67	128.39
163	KU	500	GDP	C5-C4-N3	-6.11	118.67	128.39
163	U	500	GDP	C5-C4-N3	-6.11	118.67	128.39
163	M	500	GDP	C5-C4-N3	-6.11	118.67	128.39
163	LS	500	GDP	C5-C4-N3	-6.11	118.67	128.39
163	LG	501	GDP	C5-C4-N3	-6.11	118.67	128.39
163	VR	500	GDP	C5-C4-N3	-6.10	118.67	128.39
163	NT	500	GDP	C5-C4-N3	-6.10	118.67	128.39
163	QC	500	GDP	C5-C4-N3	-6.10	118.68	128.39
163	KM	500	GDP	C5-C4-N3	-6.10	118.68	128.39
163	OJ	500	GDP	C5-C4-N3	-6.10	118.68	128.39
163	UH	500	GDP	C5-C4-N3	-6.10	118.68	128.39
163	UL	500	GDP	C5-C4-N3	-6.10	118.68	128.39
163	HJ	500	GDP	C5-C4-N3	-6.10	118.69	128.39
163	JK	500	GDP	C5-C4-N3	-6.10	118.69	128.39
163	JQ	500	GDP	C5-C4-N3	-6.10	118.69	128.39
163	ST	500	GDP	C5-C4-N3	-6.10	118.69	128.39
163	JE	500	GDP	C5-C4-N3	-6.09	118.69	128.39
163	OR	500	GDP	C5-C4-N3	-6.09	118.69	128.39
163	KE	500	GDP	C5-C4-N3	-6.09	118.69	128.39
163	CI	500	GDP	C5-C4-N3	-6.09	118.70	128.39
163	UR	500	GDP	C5-C4-N3	-6.09	118.70	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	O	500	GDP	C5-C4-N3	-6.09	118.70	128.39
163	RG	500	GDP	C5-C4-N3	-6.09	118.70	128.39
163	GB	500	GDP	C5-C4-N3	-6.09	118.70	128.39
163	MX	500	GDP	C5-C4-N3	-6.09	118.70	128.39
163	NP	500	GDP	C5-C4-N3	-6.09	118.70	128.39
163	JM	501	GDP	C5-C4-N3	-6.08	118.71	128.39
163	RS	500	GDP	C5-C4-N3	-6.08	118.72	128.39
163	UX	500	GDP	C5-C4-N3	-6.08	118.72	128.39
163	KS	500	GDP	C5-C4-N3	-6.08	118.72	128.39
163	QA	500	GDP	C5-C4-N3	-6.08	118.72	128.39
163	JY	501	GDP	C5-C4-N3	-6.08	118.72	128.39
163	IL	501	GDP	C5-C4-N3	-6.08	118.72	128.39
163	UN	500	GDP	C5-C4-N3	-6.08	118.72	128.39
163	OP	501	GDP	C5-C4-N3	-6.07	118.72	128.39
163	WF	501	GDP	C5-C4-N3	-6.07	118.72	128.39
163	HP	501	GDP	C5-C4-N3	-6.07	118.72	128.39
163	CQ	500	GDP	C5-C4-N3	-6.07	118.73	128.39
163	MH	500	GDP	C5-C4-N3	-6.07	118.73	128.39
163	JW	500	GDP	C5-C4-N3	-6.07	118.73	128.39
163	BD	500	GDP	C5-C4-N3	-6.07	118.73	128.39
163	UB	500	GDP	C5-C4-N3	-6.07	118.73	128.39
163	QM	500	GDP	C5-C4-N3	-6.07	118.73	128.39
163	S	500	GDP	C5-C4-N3	-6.07	118.73	128.39
163	HH	501	GDP	C5-C4-N3	-6.07	118.73	128.39
163	UF	500	GDP	C5-C4-N3	-6.07	118.74	128.39
163	WN	500	GDP	C5-C4-N3	-6.06	118.74	128.39
163	HD	501	GDP	C5-C4-N3	-6.06	118.74	128.39
163	VN	500	GDP	C5-C4-N3	-6.06	118.74	128.39
163	VB	500	GDP	C5-C4-N3	-6.06	118.74	128.39
163	GN	500	GDP	C5-C4-N3	-6.06	118.74	128.39
163	MT	500	GDP	C5-C4-N3	-6.06	118.74	128.39
163	ND	500	GDP	C5-C4-N3	-6.06	118.74	128.39
163	F	500	GDP	C5-C4-N3	-6.06	118.75	128.39
163	GX	500	GDP	C5-C4-N3	-6.06	118.75	128.39
163	HT	501	GDP	C5-C4-N3	-6.06	118.75	128.39
163	KQ	500	GDP	C5-C4-N3	-6.06	118.75	128.39
163	ON	500	GDP	C5-C4-N3	-6.06	118.75	128.39
163	UT	500	GDP	C5-C4-N3	-6.05	118.75	128.39
163	SN	501	GDP	C5-C4-N3	-6.05	118.75	128.39
163	MB	500	GDP	C5-C4-N3	-6.05	118.76	128.39
163	SL	500	GDP	C5-C4-N3	-6.05	118.76	128.39
163	OB	500	GDP	C5-C4-N3	-6.05	118.76	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	SB	501	GDP	C5-C4-N3	-6.05	118.76	128.39
163	SD	500	GDP	C5-C4-N3	-6.05	118.76	128.39
163	LK	500	GDP	C5-C4-N3	-6.05	118.76	128.39
163	IX	501	GDP	C5-C4-N3	-6.05	118.76	128.39
163	MD	500	GDP	C5-C4-N3	-6.05	118.76	128.39
163	WB	500	GDP	C5-C4-N3	-6.05	118.76	128.39
163	IR	500	GDP	C5-C4-N3	-6.05	118.76	128.39
163	LA	500	GDP	C5-C4-N3	-6.05	118.77	128.39
163	H	500	GDP	C5-C4-N3	-6.05	118.77	128.39
163	T	501	GDP	C5-C4-N3	-6.05	118.77	128.39
163	OD	501	GDP	C5-C4-N3	-6.05	118.77	128.39
163	LY	500	GDP	C5-C4-N3	-6.04	118.77	128.39
163	QO	500	GDP	C5-C4-N3	-6.04	118.77	128.39
163	KG	500	GDP	C5-C4-N3	-6.04	118.77	128.39
163	IF	500	GDP	C5-C4-N3	-6.04	118.77	128.39
163	QQ	500	GDP	C5-C4-N3	-6.04	118.77	128.39
163	QS	500	GDP	C5-C4-N3	-6.04	118.77	128.39
163	VT	500	GDP	C5-C4-N3	-6.04	118.78	128.39
163	N	500	GDP	C5-C4-N3	-6.04	118.78	128.39
163	FV	501	GDP	C5-C4-N3	-6.04	118.78	128.39
163	LW	500	GDP	C5-C4-N3	-6.04	118.78	128.39
163	SP	500	GDP	C5-C4-N3	-6.04	118.78	128.39
163	G	500	GDP	C5-C4-N3	-6.04	118.78	128.39
163	WR	501	GDP	C5-C4-N3	-6.04	118.78	128.39
163	W	500	GDP	C5-C4-N3	-6.03	118.79	128.39
163	GJ	500	GDP	C5-C4-N3	-6.03	118.79	128.39
163	V	500	GDP	C5-C4-N3	-6.03	118.79	128.39
163	PJ	500	GDP	C5-C4-N3	-6.03	118.79	128.39
163	JO	500	GDP	C5-C4-N3	-6.03	118.80	128.39
163	QE	500	GDP	C5-C4-N3	-6.03	118.80	128.39
163	VH	500	GDP	C5-C4-N3	-6.03	118.80	128.39
163	DW	501	GDP	C5-C4-N3	-6.03	118.80	128.39
163	TN	500	GDP	C5-C4-N3	-6.03	118.80	128.39
163	RI	500	GDP	C5-C4-N3	-6.03	118.80	128.39
163	JC	500	GDP	C5-C4-N3	-6.02	118.80	128.39
163	IT	501	GDP	C5-C4-N3	-6.02	118.81	128.39
163	RC	500	GDP	C5-C4-N3	-6.02	118.81	128.39
163	BP	500	GDP	C5-C4-N3	-6.02	118.81	128.39
163	LU	500	GDP	C5-C4-N3	-6.02	118.81	128.39
163	EL	500	GDP	C5-C4-N3	-6.02	118.82	128.39
163	VV	500	GDP	C5-C4-N3	-6.01	118.82	128.39
163	TT	500	GDP	C5-C4-N3	-6.01	118.82	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	TB	500	GDP	C5-C4-N3	-6.01	118.82	128.39
163	MP	500	GDP	C5-C4-N3	-6.01	118.82	128.39
163	LI	500	GDP	C5-C4-N3	-6.01	118.82	128.39
163	LC	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	PV	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	OF	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	TJ	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	CO	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	JG	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	NR	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	EF	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	JU	500	GDP	C5-C4-N3	-6.01	118.83	128.39
163	JI	500	GDP	C5-C4-N3	-6.00	118.83	128.39
163	VJ	500	GDP	C5-C4-N3	-6.00	118.83	128.39
163	TH	500	GDP	C5-C4-N3	-6.00	118.83	128.39
163	LQ	500	GDP	C5-C4-N3	-6.00	118.83	128.39
163	NJ	501	GDP	C5-C4-N3	-6.00	118.84	128.39
163	DA	500	GDP	C5-C4-N3	-6.00	118.84	128.39
163	KK	500	GDP	C5-C4-N3	-6.00	118.84	128.39
163	JS	500	GDP	C5-C4-N3	-6.00	118.84	128.39
163	AP	500	GDP	C5-C4-N3	-6.00	118.84	128.39
163	IV	500	GDP	C5-C4-N3	-5.99	118.85	128.39
163	KO	500	GDP	C5-C4-N3	-5.99	118.85	128.39
163	KW	500	GDP	C5-C4-N3	-5.99	118.85	128.39
163	TR	500	GDP	C5-C4-N3	-5.99	118.85	128.39
163	NN	500	GDP	C5-C4-N3	-5.99	118.85	128.39
163	NF	500	GDP	C5-C4-N3	-5.99	118.86	128.39
163	GH	500	GDP	C5-C4-N3	-5.99	118.86	128.39
163	LM	500	GDP	C5-C4-N3	-5.99	118.86	128.39
163	HN	501	GDP	C5-C4-N3	-5.99	118.86	128.39
163	IH	500	GDP	C5-C4-N3	-5.99	118.86	128.39
163	RO	500	GDP	C5-C4-N3	-5.99	118.86	128.39
163	TV	500	GDP	C5-C4-N3	-5.99	118.86	128.39
163	TF	500	GDP	C5-C4-N3	-5.98	118.86	128.39
163	DI	500	GDP	C5-C4-N3	-5.98	118.87	128.39
163	QG	500	GDP	C5-C4-N3	-5.98	118.87	128.39
163	OH	500	GDP	C5-C4-N3	-5.98	118.87	128.39
163	UV	500	GDP	C5-C4-N3	-5.98	118.87	128.39
163	EJ	500	GDP	C5-C4-N3	-5.98	118.87	128.39
163	LE	500	GDP	C5-C4-N3	-5.98	118.87	128.39
163	NV	501	GDP	C5-C4-N3	-5.98	118.87	128.39
163	RU	500	GDP	C5-C4-N3	-5.98	118.88	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	VX	500	GDP	C5-C4-N3	-5.98	118.88	128.39
163	FF	500	GDP	C5-C4-N3	-5.98	118.88	128.39
163	IJ	500	GDP	C5-C4-N3	-5.98	118.88	128.39
163	UJ	500	GDP	C5-C4-N3	-5.97	118.88	128.39
163	VL	500	GDP	C5-C4-N3	-5.97	118.88	128.39
163	DM	500	GDP	C5-C4-N3	-5.97	118.88	128.39
163	DE	500	GDP	C5-C4-N3	-5.97	118.89	128.39
163	BH	500	GDP	C5-C4-N3	-5.97	118.89	128.39
163	DC	500	GDP	C5-C4-N3	-5.97	118.90	128.39
163	DK	501	GDP	C5-C4-N3	-5.97	118.90	128.39
163	NB	500	GDP	C5-C4-N3	-5.97	118.90	128.39
163	CG	500	GDP	C5-C4-N3	-5.96	118.90	128.39
163	BX	500	GDP	C5-C4-N3	-5.96	118.90	128.39
163	DQ	500	GDP	C5-C4-N3	-5.96	118.90	128.39
163	KC	500	GDP	C5-C4-N3	-5.96	118.90	128.39
163	OT	500	GDP	C5-C4-N3	-5.96	118.91	128.39
163	VD	500	GDP	C5-C4-N3	-5.96	118.91	128.39
163	HR	500	GDP	C5-C4-N3	-5.96	118.91	128.39
163	FL	500	GDP	C5-C4-N3	-5.96	118.91	128.39
163	EP	500	GDP	C5-C4-N3	-5.95	118.92	128.39
163	RA	500	GDP	C5-C4-N3	-5.95	118.92	128.39
163	VP	500	GDP	C5-C4-N3	-5.95	118.92	128.39
163	HX	501	GDP	C5-C4-N3	-5.95	118.92	128.39
163	RM	500	GDP	C5-C4-N3	-5.95	118.92	128.39
163	SJ	501	GDP	C5-C4-N3	-5.94	118.93	128.39
163	ED	500	GDP	C5-C4-N3	-5.94	118.93	128.39
163	MF	500	GDP	C5-C4-N3	-5.94	118.93	128.39
163	SV	501	GDP	C5-C4-N3	-5.94	118.93	128.39
163	MR	500	GDP	C5-C4-N3	-5.94	118.94	128.39
163	HL	501	GDP	C5-C4-N3	-5.94	118.94	128.39
163	DU	500	GDP	C5-C4-N3	-5.94	118.94	128.39
163	PB	500	GDP	C5-C4-N3	-5.94	118.94	128.39
163	I	501	GDP	C5-C4-N3	-5.94	118.94	128.39
163	HB	501	GDP	C5-C4-N3	-5.93	118.95	128.39
163	UD	500	GDP	C5-C4-N3	-5.93	118.95	128.39
163	HF	500	GDP	C5-C4-N3	-5.93	118.95	128.39
163	AB	500	GDP	C5-C4-N3	-5.93	118.95	128.39
163	AF	500	GDP	C5-C4-N3	-5.93	118.96	128.39
163	GT	501	GDP	C5-C4-N3	-5.92	118.97	128.39
163	DS	500	GDP	C5-C4-N3	-5.92	118.97	128.39
163	AT	500	GDP	C5-C4-N3	-5.92	118.97	128.39
163	ER	500	GDP	C5-C4-N3	-5.92	118.97	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	EN	500	GDP	C5-C4-N3	-5.92	118.97	128.39
163	IN	500	GDP	C5-C4-N3	-5.92	118.97	128.39
163	IP	500	GDP	C5-C4-N3	-5.92	118.97	128.39
163	CE	500	GDP	C5-C4-N3	-5.91	118.99	128.39
163	GP	500	GDP	C5-C4-N3	-5.91	118.99	128.39
163	AZ	500	GDP	C5-C4-N3	-5.91	118.99	128.39
163	MZ	500	GDP	C5-C4-N3	-5.91	118.99	128.39
163	FX	500	GDP	C5-C4-N3	-5.91	118.99	128.39
163	FB	500	GDP	C5-C4-N3	-5.91	118.99	128.39
163	AL	500	GDP	C5-C4-N3	-5.90	118.99	128.39
163	IB	500	GDP	C5-C4-N3	-5.90	118.99	128.39
163	SF	500	GDP	C5-C4-N3	-5.90	119.00	128.39
163	SR	500	GDP	C5-C4-N3	-5.90	119.00	128.39
163	LO	500	GDP	C5-C4-N3	-5.90	119.00	128.39
163	PN	500	GDP	C5-C4-N3	-5.90	119.00	128.39
163	UP	500	GDP	C5-C4-N3	-5.90	119.00	128.39
163	BL	500	GDP	C5-C4-N3	-5.89	119.01	128.39
163	FN	500	GDP	C5-C4-N3	-5.89	119.01	128.39
163	ID	500	GDP	C5-C4-N3	-5.89	119.01	128.39
163	FR	501	GDP	C5-C4-N3	-5.88	119.03	128.39
163	PR	501	GDP	C5-C4-N3	-5.88	119.03	128.39
163	PF	501	GDP	C5-C4-N3	-5.87	119.04	128.39
163	MN	500	GDP	C5-C4-N3	-5.87	119.04	128.39
163	WV	500	GDP	C5-C4-N3	-5.87	119.04	128.39
163	NX	500	GDP	C5-C4-N3	-5.87	119.05	128.39
163	WJ	500	GDP	C5-C4-N3	-5.87	119.05	128.39
163	FJ	501	GDP	C5-C4-N3	-5.86	119.06	128.39
163	DO	500	GDP	C5-C4-N3	-5.86	119.06	128.39
163	PT	500	GDP	C5-C4-N3	-5.86	119.06	128.39
163	AJ	500	GDP	C5-C4-N3	-5.86	119.06	128.39
163	FP	500	GDP	C5-C4-N3	-5.86	119.07	128.39
163	PH	500	GDP	C5-C4-N3	-5.86	119.07	128.39
163	GF	500	GDP	C5-C4-N3	-5.85	119.08	128.39
163	PD	500	GDP	C5-C4-N3	-5.85	119.08	128.39
163	PP	500	GDP	C5-C4-N3	-5.85	119.08	128.39
163	NL	500	GDP	C5-C4-N3	-5.85	119.09	128.39
163	BR	500	GDP	C5-C4-N3	-5.85	119.09	128.39
163	DY	500	GDP	C5-C4-N3	-5.84	119.10	128.39
163	GL	500	GDP	C5-C4-N3	-5.83	119.11	128.39
163	BN	500	GDP	C5-C4-N3	-5.82	119.12	128.39
163	CA	500	GDP	C5-C4-N3	-5.82	119.13	128.39
163	GD	500	GDP	C5-C4-N3	-5.82	119.13	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	AD	500	GDP	C5-C4-N3	-5.81	119.14	128.39
163	AH	500	GDP	C5-C4-N3	-5.81	119.15	128.39
163	CS	500	GDP	C5-C4-N3	-5.80	119.16	128.39
163	EX	500	GDP	C5-C4-N3	-5.80	119.16	128.39
163	MV	500	GDP	C5-C4-N3	-5.80	119.17	128.39
163	BJ	500	GDP	C5-C4-N3	-5.79	119.17	128.39
163	AR	500	GDP	C5-C4-N3	-5.79	119.18	128.39
163	GV	501	GDP	C5-C4-N3	-5.78	119.19	128.39
163	DG	500	GDP	C5-C4-N3	-5.77	119.20	128.39
163	MJ	500	GDP	C5-C4-N3	-5.77	119.21	128.39
163	EB	500	GDP	C5-C4-N3	-5.76	119.22	128.39
163	CC	500	GDP	C5-C4-N3	-5.75	119.23	128.39
163	BF	500	GDP	C5-C4-N3	-5.74	119.26	128.39
163	FD	500	GDP	C5-C4-N3	-5.74	119.26	128.39
163	EV	500	GDP	C5-C4-N3	-5.72	119.29	128.39
163	FH	500	GDP	C5-C4-N3	-5.68	119.35	128.39
163	GR	500	GDP	C5-C4-N3	-5.65	119.39	128.39
163	BV	500	GDP	C5-C4-N3	-5.65	119.40	128.39
163	AX	500	GDP	C5-C4-N3	-5.64	119.41	128.39
163	EH	500	GDP	C5-C4-N3	-5.63	119.44	128.39
163	AV	500	GDP	C5-C4-N3	-5.62	119.45	128.39
163	CU	500	GDP	C5-C4-N3	-5.62	119.45	128.39
163	AN	500	GDP	C5-C4-N3	-5.54	119.57	128.39
165	CH	501	GTP	C5-C4-N3	-5.45	119.72	128.39
163	ET	500	GDP	C5-C4-N3	-5.43	119.74	128.39
163	CW	500	GDP	C2-N3-C4	5.39	121.59	112.30
165	GI	501	GTP	C5-C4-N3	-5.35	119.87	128.39
165	EA	501	GTP	C5-C4-N3	-5.31	119.94	128.39
165	GQ	501	GTP	C5-C4-N3	-5.27	120.01	128.39
165	EJ	501	GTP	C5-C4-N3	-5.25	120.03	128.39
165	HW	501	GTP	C5-C4-N3	-5.25	120.03	128.39
165	HK	501	GTP	C5-C4-N3	-5.23	120.07	128.39
165	IO	501	GTP	C5-C4-N3	-5.22	120.08	128.39
165	IC	501	GTP	C5-C4-N3	-5.22	120.08	128.39
163	FT	501	GDP	C5-C4-N3	-5.21	120.09	128.39
165	IU	501	GTP	C5-C4-N3	-5.19	120.12	128.39
165	DE	501	GTP	C5-C4-N3	-5.17	120.17	128.39
165	II	501	GTP	C5-C4-N3	-5.16	120.17	128.39
165	IS	501	GTP	C5-C4-N3	-5.16	120.18	128.39
165	LT	501	GTP	C5-C4-N3	-5.16	120.18	128.39
165	TQ	501	GTP	C5-C4-N3	-5.16	120.18	128.39
165	QT	501	GTP	C5-C4-N3	-5.15	120.19	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	IA	501	GTP	C5-C4-N3	-5.15	120.19	128.39
165	KT	501	GTP	C5-C4-N3	-5.14	120.20	128.39
165	TE	501	GTP	C5-C4-N3	-5.14	120.21	128.39
165	KH	501	GTP	C5-C4-N3	-5.14	120.22	128.39
165	QH	501	GTP	C5-C4-N3	-5.14	120.22	128.39
165	NR	501	GTP	C5-C4-N3	-5.13	120.23	128.39
165	EI	501	GTP	C5-C4-N3	-5.12	120.23	128.39
165	BI	501	GTP	C5-C4-N3	-5.12	120.24	128.39
165	DT	501	GTP	C5-C4-N3	-5.12	120.24	128.39
165	J	501	GTP	C5-C4-N3	-5.12	120.24	128.39
165	CT	501	GTP	C5-C4-N3	-5.12	120.25	128.39
165	KX	501	GTP	C5-C4-N3	-5.12	120.25	128.39
165	QR	501	GTP	C5-C4-N3	-5.12	120.25	128.39
165	NF	501	GTP	C5-C4-N3	-5.12	120.25	128.39
165	IG	501	GTP	C5-C4-N3	-5.11	120.25	128.39
165	FT	503	GTP	C5-C4-N3	-5.11	120.25	128.39
165	LH	501	GTP	C5-C4-N3	-5.11	120.26	128.39
165	JH	501	GTP	C5-C4-N3	-5.11	120.26	128.39
165	OK	501	GTP	C5-C4-N3	-5.11	120.26	128.39
165	NM	501	GTP	C5-C4-N3	-5.10	120.27	128.39
163	E	500	GDP	C2-N3-C4	5.10	121.09	112.30
165	R	501	GTP	C5-C4-N3	-5.10	120.27	128.39
165	JR	501	GTP	C5-C4-N3	-5.10	120.27	128.39
165	KB	502	GTP	C5-C4-N3	-5.10	120.27	128.39
165	QF	501	GTP	C5-C4-N3	-5.10	120.28	128.39
165	HN	503	GTP	C5-C4-N3	-5.10	120.28	128.39
165	IY	501	GTP	C5-C4-N3	-5.10	120.28	128.39
165	QB	501	GTP	C5-C4-N3	-5.10	120.28	128.39
165	UU	501	GTP	C5-C4-N3	-5.10	120.28	128.39
163	QI	500	GDP	C2-N3-C4	5.10	121.08	112.30
165	VG	501	GTP	C5-C4-N3	-5.10	120.28	128.39
165	NQ	501	GTP	C5-C4-N3	-5.10	120.28	128.39
165	BU	501	GTP	C5-C4-N3	-5.09	120.28	128.39
165	CK	503	GTP	C5-C4-N3	-5.09	120.28	128.39
165	KN	502	GTP	C5-C4-N3	-5.09	120.28	128.39
165	IM	501	GTP	C5-C4-N3	-5.09	120.29	128.39
163	CK	501	GDP	C2-N3-C4	5.09	121.07	112.30
165	OU	501	GTP	C5-C4-N3	-5.09	120.29	128.39
165	KL	501	GTP	C5-C4-N3	-5.09	120.29	128.39
165	NO	501	GTP	C5-C4-N3	-5.09	120.29	128.39
165	VS	501	GTP	C5-C4-N3	-5.09	120.30	128.39
163	RQ	500	GDP	C2-N3-C4	5.09	121.06	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	CB	501	GTP	C5-C4-N3	-5.08	120.30	128.39
165	SK	501	GTP	C5-C4-N3	-5.08	120.30	128.39
165	SW	501	GTP	C5-C4-N3	-5.08	120.30	128.39
163	VB	500	GDP	C2-N3-C4	5.08	121.06	112.30
165	VA	501	GTP	C5-C4-N3	-5.08	120.30	128.39
165	JT	501	GTP	C5-C4-N3	-5.08	120.30	128.39
165	QL	501	GTP	C5-C4-N3	-5.08	120.30	128.39
165	K	501	GTP	C5-C4-N3	-5.08	120.30	128.39
165	VH	501	GTP	C5-C4-N3	-5.08	120.30	128.39
163	RE	500	GDP	C2-N3-C4	5.08	121.05	112.30
165	UM	501	GTP	C5-C4-N3	-5.08	120.31	128.39
165	SG	501	GTP	C5-C4-N3	-5.08	120.31	128.39
165	HB	503	GTP	C5-C4-N3	-5.08	120.31	128.39
163	UX	500	GDP	C2-N3-C4	5.08	121.04	112.30
165	QN	501	GTP	C5-C4-N3	-5.08	120.31	128.39
165	SS	501	GTP	C5-C4-N3	-5.08	120.31	128.39
163	LS	500	GDP	C2-N3-C4	5.07	121.04	112.30
165	JJ	501	GTP	C5-C4-N3	-5.07	120.32	128.39
165	GU	501	GTP	C5-C4-N3	-5.07	120.32	128.39
165	UE	501	GTP	C5-C4-N3	-5.07	120.32	128.39
165	WM	501	GTP	C5-C4-N3	-5.07	120.32	128.39
163	QK	500	GDP	C2-N3-C4	5.07	121.03	112.30
165	SC	501	GTP	C5-C4-N3	-5.07	120.32	128.39
165	NI	501	GTP	C5-C4-N3	-5.07	120.33	128.39
163	QW	500	GDP	C2-N3-C4	5.07	121.03	112.30
165	JF	501	GTP	C5-C4-N3	-5.07	120.33	128.39
165	NE	501	GTP	C5-C4-N3	-5.06	120.33	128.39
165	PQ	501	GTP	C5-C4-N3	-5.06	120.33	128.39
163	HV	500	GDP	C2-N3-C4	5.06	121.02	112.30
163	QU	500	GDP	C2-N3-C4	5.06	121.02	112.30
165	UI	501	GTP	C5-C4-N3	-5.06	120.33	128.39
163	WF	501	GDP	C2-N3-C4	5.06	121.02	112.30
163	WD	500	GDP	C2-N3-C4	5.06	121.02	112.30
163	TR	500	GDP	C2-N3-C4	5.06	121.02	112.30
165	WY	501	GTP	C5-C4-N3	-5.06	120.33	128.39
163	QS	500	GDP	C2-N3-C4	5.06	121.02	112.30
165	QX	501	GTP	C5-C4-N3	-5.06	120.34	128.39
163	G	500	GDP	C2-N3-C4	5.06	121.02	112.30
165	VC	501	GTP	C5-C4-N3	-5.06	120.34	128.39
165	EU	501	GTP	C5-C4-N3	-5.06	120.34	128.39
165	PE	501	GTP	C5-C4-N3	-5.06	120.34	128.39
163	BT	500	GDP	C2-N3-C4	5.05	121.00	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	OR	500	GDP	C2-N3-C4	5.05	121.00	112.30
163	LG	501	GDP	C2-N3-C4	5.05	121.00	112.30
165	AD	501	GTP	C5-C4-N3	-5.05	120.35	128.39
165	DD	501	GTP	C5-C4-N3	-5.05	120.35	128.39
165	RV	501	GTP	C5-C4-N3	-5.05	120.35	128.39
163	TX	500	GDP	C2-N3-C4	5.05	121.00	112.30
163	HD	501	GDP	C2-N3-C4	5.05	121.00	112.30
163	PJ	500	GDP	C2-N3-C4	5.05	121.00	112.30
165	NU	501	GTP	C5-C4-N3	-5.05	120.35	128.39
165	VT	501	GTP	C5-C4-N3	-5.05	120.35	128.39
163	TL	501	GDP	C2-N3-C4	5.05	121.00	112.30
165	TI	501	GTP	C5-C4-N3	-5.05	120.35	128.39
165	OW	501	GTP	C5-C4-N3	-5.05	120.35	128.39
165	PW	501	GTP	C5-C4-N3	-5.05	120.35	128.39
163	WP	500	GDP	C2-N3-C4	5.05	121.00	112.30
165	KZ	501	GTP	C5-C4-N3	-5.05	120.36	128.39
163	HJ	500	GDP	C2-N3-C4	5.05	120.99	112.30
165	UQ	501	GTP	C5-C4-N3	-5.05	120.36	128.39
165	IE	501	GTP	C5-C4-N3	-5.05	120.36	128.39
165	UA	501	GTP	C5-C4-N3	-5.05	120.36	128.39
163	QQ	500	GDP	C2-N3-C4	5.05	120.99	112.30
163	MB	500	GDP	C2-N3-C4	5.04	120.99	112.30
163	QE	500	GDP	C2-N3-C4	5.04	120.99	112.30
163	LA	500	GDP	C2-N3-C4	5.04	120.99	112.30
165	Q	501	GTP	C5-C4-N3	-5.04	120.36	128.39
165	FQ	501	GTP	C5-C4-N3	-5.04	120.36	128.39
165	PY	501	GTP	C5-C4-N3	-5.04	120.36	128.39
163	LW	500	GDP	C2-N3-C4	5.04	120.98	112.30
165	PK	501	GTP	C5-C4-N3	-5.04	120.36	128.39
163	VN	500	GDP	C2-N3-C4	5.04	120.98	112.30
165	QU	501	GTP	C5-C4-N3	-5.04	120.37	128.39
163	UR	500	GDP	C2-N3-C4	5.04	120.98	112.30
165	IQ	501	GTP	C5-C4-N3	-5.04	120.37	128.39
165	NY	501	GTP	C5-C4-N3	-5.04	120.37	128.39
163	JE	500	GDP	C2-N3-C4	5.04	120.98	112.30
163	OL	500	GDP	C2-N3-C4	5.04	120.98	112.30
163	HT	501	GDP	C2-N3-C4	5.04	120.98	112.30
163	JO	500	GDP	C2-N3-C4	5.04	120.98	112.30
165	TU	501	GTP	C5-C4-N3	-5.04	120.37	128.39
165	SO	501	GTP	C5-C4-N3	-5.04	120.37	128.39
165	TS	501	GTP	C5-C4-N3	-5.04	120.37	128.39
165	VQ	501	GTP	C5-C4-N3	-5.04	120.37	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	JN	501	GTP	C5-C4-N3	-5.04	120.38	128.39
163	VF	500	GDP	C2-N3-C4	5.04	120.97	112.30
163	NT	500	GDP	C2-N3-C4	5.04	120.97	112.30
165	NC	501	GTP	C5-C4-N3	-5.04	120.38	128.39
163	CO	500	GDP	C2-N3-C4	5.03	120.97	112.30
163	WX	500	GDP	C2-N3-C4	5.03	120.97	112.30
163	WT	500	GDP	C2-N3-C4	5.03	120.97	112.30
165	TG	501	GTP	C5-C4-N3	-5.03	120.38	128.39
163	RK	500	GDP	C2-N3-C4	5.03	120.97	112.30
163	PV	500	GDP	C2-N3-C4	5.03	120.97	112.30
163	KI	500	GDP	C2-N3-C4	5.03	120.97	112.30
163	UB	500	GDP	C2-N3-C4	5.03	120.97	112.30
163	ST	500	GDP	C2-N3-C4	5.03	120.97	112.30
163	U	500	GDP	C2-N3-C4	5.03	120.97	112.30
165	DL	501	GTP	C5-C4-N3	-5.03	120.38	128.39
165	KF	501	GTP	C5-C4-N3	-5.03	120.38	128.39
163	S	500	GDP	C2-N3-C4	5.03	120.96	112.30
165	HQ	501	GTP	C5-C4-N3	-5.03	120.38	128.39
165	IW	501	GTP	C5-C4-N3	-5.03	120.39	128.39
163	RW	500	GDP	C2-N3-C4	5.03	120.96	112.30
165	JZ	501	GTP	C5-C4-N3	-5.03	120.39	128.39
163	MD	500	GDP	C2-N3-C4	5.03	120.96	112.30
163	PL	501	GDP	C2-N3-C4	5.03	120.96	112.30
163	HN	501	GDP	C2-N3-C4	5.03	120.96	112.30
165	KV	501	GTP	C5-C4-N3	-5.03	120.39	128.39
163	UL	500	GDP	C2-N3-C4	5.03	120.96	112.30
163	IR	500	GDP	C2-N3-C4	5.03	120.96	112.30
165	KR	501	GTP	C5-C4-N3	-5.03	120.39	128.39
163	T	501	GDP	C2-N3-C4	5.03	120.96	112.30
165	HM	501	GTP	C5-C4-N3	-5.03	120.39	128.39
163	JC	500	GDP	C2-N3-C4	5.03	120.96	112.30
163	UF	500	GDP	C2-N3-C4	5.03	120.96	112.30
163	OF	500	GDP	C2-N3-C4	5.03	120.96	112.30
163	KU	500	GDP	C2-N3-C4	5.03	120.95	112.30
165	VY	501	GTP	C5-C4-N3	-5.02	120.39	128.39
163	SH	500	GDP	C2-N3-C4	5.02	120.95	112.30
163	DE	500	GDP	C2-N3-C4	5.02	120.95	112.30
163	JA	500	GDP	C2-N3-C4	5.02	120.95	112.30
163	LK	500	GDP	C2-N3-C4	5.02	120.95	112.30
163	ML	500	GDP	C2-N3-C4	5.02	120.95	112.30
163	TT	500	GDP	C2-N3-C4	5.02	120.95	112.30
165	VO	501	GTP	C5-C4-N3	-5.02	120.40	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	AP	500	GDP	C2-N3-C4	5.02	120.95	112.30
165	NA	501	GTP	C5-C4-N3	-5.02	120.40	128.39
165	HY	501	GTP	C5-C4-N3	-5.02	120.40	128.39
165	UC	501	GTP	C5-C4-N3	-5.02	120.40	128.39
163	BH	500	GDP	C2-N3-C4	5.02	120.95	112.30
163	HH	501	GDP	C2-N3-C4	5.02	120.95	112.30
163	UN	500	GDP	C2-N3-C4	5.02	120.95	112.30
163	SD	500	GDP	C2-N3-C4	5.02	120.95	112.30
165	BG	501	GTP	C5-C4-N3	-5.02	120.40	128.39
165	QI	501	GTP	C5-C4-N3	-5.02	120.40	128.39
163	OX	500	GDP	C2-N3-C4	5.02	120.94	112.30
165	PM	501	GTP	C5-C4-N3	-5.02	120.40	128.39
163	O	500	GDP	C2-N3-C4	5.02	120.94	112.30
163	KY	500	GDP	C2-N3-C4	5.02	120.94	112.30
163	TD	500	GDP	C2-N3-C4	5.02	120.94	112.30
163	SB	501	GDP	C2-N3-C4	5.02	120.94	112.30
163	OV	500	GDP	C2-N3-C4	5.02	120.94	112.30
165	BQ	501	GTP	C5-C4-N3	-5.02	120.41	128.39
163	WH	500	GDP	C2-N3-C4	5.02	120.94	112.30
163	BP	500	GDP	C2-N3-C4	5.02	120.94	112.30
165	DV	501	GTP	C5-C4-N3	-5.02	120.41	128.39
163	CY	500	GDP	C2-N3-C4	5.02	120.94	112.30
163	HP	501	GDP	C2-N3-C4	5.02	120.94	112.30
165	WQ	501	GTP	C5-C4-N3	-5.02	120.41	128.39
163	PX	501	GDP	C2-N3-C4	5.01	120.94	112.30
165	HU	501	GTP	C5-C4-N3	-5.01	120.41	128.39
165	RR	501	GTP	C5-C4-N3	-5.01	120.41	128.39
163	KA	500	GDP	C2-N3-C4	5.01	120.94	112.30
163	IL	501	GDP	C2-N3-C4	5.01	120.94	112.30
165	HE	501	GTP	C5-C4-N3	-5.01	120.41	128.39
163	JQ	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	IF	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	TF	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	KS	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	VV	500	GDP	C2-N3-C4	5.01	120.93	112.30
165	KD	502	GTP	C5-C4-N3	-5.01	120.41	128.39
165	OI	501	GTP	C5-C4-N3	-5.01	120.41	128.39
163	NH	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	IX	501	GDP	C2-N3-C4	5.01	120.93	112.30
163	VX	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	WL	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	JS	500	GDP	C2-N3-C4	5.01	120.93	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	UJ	500	GDP	C2-N3-C4	5.01	120.93	112.30
165	RJ	501	GTP	C5-C4-N3	-5.01	120.42	128.39
163	V	500	GDP	C2-N3-C4	5.01	120.93	112.30
165	CV	501	GTP	C5-C4-N3	-5.01	120.42	128.39
163	JK	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	M	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	QO	500	GDP	C2-N3-C4	5.01	120.93	112.30
163	QC	500	GDP	C2-N3-C4	5.01	120.92	112.30
163	JY	501	GDP	C2-N3-C4	5.01	120.92	112.30
165	C	501	GTP	C5-C4-N3	-5.01	120.42	128.39
165	OD	503	GTP	C5-C4-N3	-5.01	120.42	128.39
165	VM	501	GTP	C5-C4-N3	-5.01	120.42	128.39
163	RS	500	GDP	C2-N3-C4	5.01	120.92	112.30
163	NP	500	GDP	C2-N3-C4	5.01	120.92	112.30
165	KJ	501	GTP	C5-C4-N3	-5.01	120.42	128.39
163	EV	500	GDP	C2-N3-C4	5.01	120.92	112.30
163	A	501	GDP	C2-N3-C4	5.00	120.92	112.30
163	CG	500	GDP	C2-N3-C4	5.00	120.92	112.30
163	TH	500	GDP	C2-N3-C4	5.00	120.92	112.30
163	VH	500	GDP	C2-N3-C4	5.00	120.92	112.30
163	SL	500	GDP	C2-N3-C4	5.00	120.92	112.30
165	UG	501	GTP	C5-C4-N3	-5.00	120.43	128.39
165	VE	501	GTP	C5-C4-N3	-5.00	120.43	128.39
165	RT	501	GTP	C5-C4-N3	-5.00	120.43	128.39
163	SN	501	GDP	C2-N3-C4	5.00	120.92	112.30
165	WS	501	GTP	C5-C4-N3	-5.00	120.43	128.39
163	VJ	500	GDP	C2-N3-C4	5.00	120.92	112.30
163	OP	501	GDP	C2-N3-C4	5.00	120.92	112.30
165	JB	501	GTP	C5-C4-N3	-5.00	120.43	128.39
165	IK	501	GTP	C5-C4-N3	-5.00	120.43	128.39
163	UV	500	GDP	C2-N3-C4	5.00	120.92	112.30
163	UH	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	CI	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	H	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	SV	501	GDP	C2-N3-C4	5.00	120.91	112.30
163	KO	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	VL	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	MX	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	SP	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	W	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	VT	500	GDP	C2-N3-C4	5.00	120.91	112.30
163	JG	500	GDP	C2-N3-C4	5.00	120.91	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	KP	502	GTP	C5-C4-N3	-5.00	120.44	128.39
163	WR	501	GDP	C2-N3-C4	5.00	120.91	112.30
165	CO	501	GTP	C5-C4-N3	-5.00	120.44	128.39
163	JW	500	GDP	C2-N3-C4	5.00	120.90	112.30
163	WN	500	GDP	C2-N3-C4	5.00	120.90	112.30
163	MT	500	GDP	C2-N3-C4	4.99	120.90	112.30
163	LQ	500	GDP	C2-N3-C4	4.99	120.90	112.30
165	UO	501	GTP	C5-C4-N3	-4.99	120.44	128.39
163	RG	500	GDP	C2-N3-C4	4.99	120.90	112.30
165	JV	501	GTP	C5-C4-N3	-4.99	120.44	128.39
163	FV	501	GDP	C2-N3-C4	4.99	120.90	112.30
163	BD	500	GDP	C2-N3-C4	4.99	120.90	112.30
163	KW	500	GDP	C2-N3-C4	4.99	120.90	112.30
165	AI	501	GTP	C5-C4-N3	-4.99	120.44	128.39
163	MH	500	GDP	C2-N3-C4	4.99	120.90	112.30
163	ND	500	GDP	C2-N3-C4	4.99	120.90	112.30
163	KE	500	GDP	C2-N3-C4	4.99	120.90	112.30
165	T	503	GTP	C5-C4-N3	-4.99	120.45	128.39
163	TB	500	GDP	C2-N3-C4	4.99	120.89	112.30
165	OP	503	GTP	C5-C4-N3	-4.99	120.45	128.39
163	DW	501	GDP	C2-N3-C4	4.99	120.89	112.30
163	LY	500	GDP	C2-N3-C4	4.99	120.89	112.30
163	RC	500	GDP	C2-N3-C4	4.99	120.89	112.30
163	TJ	500	GDP	C2-N3-C4	4.99	120.89	112.30
163	LC	500	GDP	C2-N3-C4	4.99	120.89	112.30
163	WB	500	GDP	C2-N3-C4	4.99	120.89	112.30
163	JM	501	GDP	C2-N3-C4	4.99	120.89	112.30
163	SF	500	GDP	C2-N3-C4	4.99	120.89	112.30
165	DQ	501	GTP	C5-C4-N3	-4.98	120.46	128.39
163	DI	500	GDP	C2-N3-C4	4.98	120.89	112.30
163	OJ	500	GDP	C2-N3-C4	4.98	120.89	112.30
163	P	500	GDP	C2-N3-C4	4.98	120.89	112.30
165	WE	501	GTP	C5-C4-N3	-4.98	120.46	128.39
163	AD	500	GDP	C2-N3-C4	4.98	120.88	112.30
163	GB	500	GDP	C2-N3-C4	4.98	120.88	112.30
163	KK	500	GDP	C2-N3-C4	4.98	120.88	112.30
163	OD	501	GDP	C2-N3-C4	4.98	120.88	112.30
163	GT	501	GDP	C2-N3-C4	4.98	120.88	112.30
163	QG	500	GDP	C2-N3-C4	4.98	120.88	112.30
163	IP	500	GDP	C2-N3-C4	4.98	120.88	112.30
163	RO	500	GDP	C2-N3-C4	4.98	120.88	112.30
165	CE	501	GTP	C5-C4-N3	-4.98	120.46	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	ES	501	GTP	C5-C4-N3	-4.98	120.46	128.39
163	N	500	GDP	C2-N3-C4	4.98	120.88	112.30
163	GJ	500	GDP	C2-N3-C4	4.98	120.88	112.30
163	VR	500	GDP	C2-N3-C4	4.98	120.88	112.30
165	LB	501	GTP	C5-C4-N3	-4.98	120.46	128.39
163	TP	500	GDP	C2-N3-C4	4.98	120.88	112.30
165	RX	501	GTP	C5-C4-N3	-4.98	120.47	128.39
163	PR	501	GDP	C2-N3-C4	4.98	120.88	112.30
165	OG	501	GTP	C5-C4-N3	-4.98	120.47	128.39
163	SR	500	GDP	C2-N3-C4	4.98	120.87	112.30
163	ON	500	GDP	C2-N3-C4	4.98	120.87	112.30
165	WK	501	GTP	C5-C4-N3	-4.98	120.47	128.39
163	TN	500	GDP	C2-N3-C4	4.98	120.87	112.30
163	MR	500	GDP	C2-N3-C4	4.98	120.87	112.30
165	RF	501	GTP	C5-C4-N3	-4.97	120.47	128.39
163	GH	500	GDP	C2-N3-C4	4.97	120.87	112.30
163	VD	500	GDP	C2-N3-C4	4.97	120.87	112.30
163	NJ	501	GDP	C2-N3-C4	4.97	120.87	112.30
165	WA	501	GTP	C5-C4-N3	-4.97	120.47	128.39
165	WO	501	GTP	C5-C4-N3	-4.97	120.47	128.39
163	KG	500	GDP	C2-N3-C4	4.97	120.86	112.30
163	EJ	500	GDP	C2-N3-C4	4.97	120.86	112.30
163	DQ	500	GDP	C2-N3-C4	4.97	120.86	112.30
165	MM	501	GTP	C5-C4-N3	-4.97	120.48	128.39
165	WG	501	GTP	C5-C4-N3	-4.97	120.48	128.39
163	AT	500	GDP	C2-N3-C4	4.97	120.86	112.30
163	AF	500	GDP	C2-N3-C4	4.97	120.86	112.30
165	LF	502	GTP	C5-C4-N3	-4.97	120.48	128.39
165	SQ	501	GTP	C5-C4-N3	-4.97	120.48	128.39
165	UW	501	GTP	C5-C4-N3	-4.97	120.48	128.39
163	CC	500	GDP	C2-N3-C4	4.97	120.86	112.30
163	LE	500	GDP	C2-N3-C4	4.97	120.86	112.30
163	PH	500	GDP	C2-N3-C4	4.97	120.86	112.30
163	HX	501	GDP	C2-N3-C4	4.97	120.86	112.30
163	KC	500	GDP	C2-N3-C4	4.97	120.86	112.30
163	MZ	500	GDP	C2-N3-C4	4.97	120.86	112.30
165	US	501	GTP	C5-C4-N3	-4.97	120.48	128.39
163	UT	500	GDP	C2-N3-C4	4.97	120.86	112.30
165	RC	501	GTP	C5-C4-N3	-4.97	120.48	128.39
165	RL	501	GTP	C5-C4-N3	-4.97	120.48	128.39
163	KM	500	GDP	C2-N3-C4	4.97	120.85	112.30
163	OB	500	GDP	C2-N3-C4	4.97	120.85	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	PT	500	GDP	C2-N3-C4	4.97	120.85	112.30
165	HI	501	GTP	C5-C4-N3	-4.97	120.49	128.39
163	MF	500	GDP	C2-N3-C4	4.97	120.85	112.30
165	JW	501	GTP	C5-C4-N3	-4.97	120.49	128.39
163	EF	500	GDP	C2-N3-C4	4.97	120.85	112.30
163	NR	500	GDP	C2-N3-C4	4.97	120.85	112.30
165	MS	501	GTP	C5-C4-N3	-4.96	120.49	128.39
163	DA	500	GDP	C2-N3-C4	4.96	120.85	112.30
163	ED	500	GDP	C2-N3-C4	4.96	120.85	112.30
163	HB	501	GDP	C2-N3-C4	4.96	120.85	112.30
163	LI	500	GDP	C2-N3-C4	4.96	120.85	112.30
163	MP	500	GDP	C2-N3-C4	4.96	120.85	112.30
165	MO	501	GTP	C5-C4-N3	-4.96	120.49	128.39
165	WW	501	GTP	C5-C4-N3	-4.96	120.49	128.39
165	RO	501	GTP	C5-C4-N3	-4.96	120.49	128.39
163	LM	500	GDP	C2-N3-C4	4.96	120.85	112.30
165	FA	501	GTP	C5-C4-N3	-4.96	120.49	128.39
165	QO	501	GTP	C5-C4-N3	-4.96	120.49	128.39
163	VP	500	GDP	C2-N3-C4	4.96	120.84	112.30
163	LO	500	GDP	C2-N3-C4	4.96	120.84	112.30
165	WC	501	GTP	C5-C4-N3	-4.96	120.50	128.39
165	CJ	501	GTP	C5-C4-N3	-4.96	120.50	128.39
165	AP	501	GTP	C5-C4-N3	-4.96	120.50	128.39
165	MY	501	GTP	C5-C4-N3	-4.96	120.50	128.39
163	I	501	GDP	C2-N3-C4	4.96	120.84	112.30
165	UK	501	GTP	C5-C4-N3	-4.96	120.50	128.39
165	MC	501	GTP	C5-C4-N3	-4.96	120.50	128.39
163	ER	500	GDP	C2-N3-C4	4.96	120.84	112.30
163	SJ	501	GDP	C2-N3-C4	4.96	120.84	112.30
163	KQ	500	GDP	C2-N3-C4	4.96	120.84	112.30
165	FI	501	GTP	C5-C4-N3	-4.96	120.50	128.39
163	F	500	GDP	C2-N3-C4	4.96	120.84	112.30
163	PF	501	GDP	C2-N3-C4	4.96	120.84	112.30
163	CQ	500	GDP	C2-N3-C4	4.96	120.84	112.30
163	CS	500	GDP	C2-N3-C4	4.96	120.84	112.30
163	HR	500	GDP	C2-N3-C4	4.96	120.84	112.30
165	L	501	GTP	C5-C4-N3	-4.96	120.50	128.39
163	GN	500	GDP	C2-N3-C4	4.96	120.83	112.30
163	IT	501	GDP	C2-N3-C4	4.96	120.83	112.30
165	EC	501	GTP	C5-C4-N3	-4.95	120.50	128.39
163	ID	500	GDP	C2-N3-C4	4.95	120.83	112.30
165	RH	501	GTP	C5-C4-N3	-4.95	120.50	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	HS	501	GTP	C5-C4-N3	-4.95	120.50	128.39
165	QC	501	GTP	C5-C4-N3	-4.95	120.51	128.39
163	JU	500	GDP	C2-N3-C4	4.95	120.83	112.30
165	HG	501	GTP	C5-C4-N3	-4.95	120.51	128.39
163	IH	500	GDP	C2-N3-C4	4.95	120.83	112.30
163	DU	500	GDP	C2-N3-C4	4.95	120.83	112.30
163	LU	500	GDP	C2-N3-C4	4.95	120.83	112.30
163	WV	500	GDP	C2-N3-C4	4.95	120.83	112.30
163	HL	501	GDP	C2-N3-C4	4.95	120.83	112.30
165	OM	501	GTP	C5-C4-N3	-4.95	120.51	128.39
163	RM	500	GDP	C2-N3-C4	4.95	120.82	112.30
165	SM	501	GTP	C5-C4-N3	-4.95	120.51	128.39
163	OH	500	GDP	C2-N3-C4	4.95	120.82	112.30
163	UD	500	GDP	C2-N3-C4	4.95	120.82	112.30
165	JK	501	GTP	C5-C4-N3	-4.95	120.52	128.39
165	LR	502	GTP	C5-C4-N3	-4.95	120.52	128.39
163	EP	500	GDP	C2-N3-C4	4.95	120.82	112.30
165	AK	501	GTP	C5-C4-N3	-4.95	120.52	128.39
165	TM	501	GTP	C5-C4-N3	-4.95	120.52	128.39
163	QA	500	GDP	C2-N3-C4	4.95	120.82	112.30
163	IV	500	GDP	C2-N3-C4	4.95	120.82	112.30
165	SA	501	GTP	C5-C4-N3	-4.95	120.52	128.39
165	SE	501	GTP	C5-C4-N3	-4.95	120.52	128.39
165	FG	501	GTP	C5-C4-N3	-4.94	120.52	128.39
163	FF	500	GDP	C2-N3-C4	4.94	120.82	112.30
165	PO	501	GTP	C5-C4-N3	-4.94	120.52	128.39
163	FX	500	GDP	C2-N3-C4	4.94	120.81	112.30
165	MA	501	GTP	C5-C4-N3	-4.94	120.52	128.39
163	AL	500	GDP	C2-N3-C4	4.94	120.81	112.30
165	TW	501	GTP	C5-C4-N3	-4.94	120.52	128.39
163	NF	500	GDP	C2-N3-C4	4.94	120.81	112.30
163	GV	501	GDP	C2-N3-C4	4.94	120.81	112.30
163	MV	500	GDP	C2-N3-C4	4.94	120.81	112.30
165	EG	501	GTP	C5-C4-N3	-4.94	120.53	128.39
163	AB	500	GDP	C2-N3-C4	4.94	120.81	112.30
163	PP	500	GDP	C2-N3-C4	4.94	120.81	112.30
165	WU	501	GTP	C5-C4-N3	-4.94	120.53	128.39
165	AU	501	GTP	C5-C4-N3	-4.94	120.53	128.39
163	NV	501	GDP	C2-N3-C4	4.94	120.80	112.30
163	WJ	500	GDP	C2-N3-C4	4.94	120.80	112.30
163	GX	500	GDP	C2-N3-C4	4.94	120.80	112.30
163	IN	500	GDP	C2-N3-C4	4.94	120.80	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	DO	500	GDP	C2-N3-C4	4.94	120.80	112.30
163	RA	500	GDP	C2-N3-C4	4.93	120.80	112.30
165	MJ	501	GTP	C5-C4-N3	-4.93	120.54	128.39
165	PC	501	GTP	C5-C4-N3	-4.93	120.54	128.39
163	TV	500	GDP	C2-N3-C4	4.93	120.80	112.30
163	NX	500	GDP	C2-N3-C4	4.93	120.80	112.30
163	P	500	GDP	N9-C4-N3	4.93	135.81	125.95
163	DS	500	GDP	C2-N3-C4	4.93	120.79	112.30
163	BL	500	GDP	C2-N3-C4	4.93	120.79	112.30
163	IB	500	GDP	C2-N3-C4	4.93	120.79	112.30
163	GP	500	GDP	C2-N3-C4	4.93	120.79	112.30
165	AS	501	GTP	C5-C4-N3	-4.93	120.54	128.39
163	DM	500	GDP	C2-N3-C4	4.93	120.79	112.30
163	HF	500	GDP	C2-N3-C4	4.93	120.79	112.30
163	PB	500	GDP	C2-N3-C4	4.93	120.79	112.30
163	OT	500	GDP	C2-N3-C4	4.93	120.79	112.30
163	JI	500	GDP	C2-N3-C4	4.93	120.79	112.30
163	NL	500	GDP	C2-N3-C4	4.93	120.78	112.30
163	FJ	501	GDP	C2-N3-C4	4.93	120.78	112.30
163	AR	500	GDP	C2-N3-C4	4.93	120.78	112.30
165	BA	501	GTP	C5-C4-N3	-4.92	120.55	128.39
165	MG	501	GTP	C5-C4-N3	-4.92	120.55	128.39
165	LN	502	GTP	C5-C4-N3	-4.92	120.55	128.39
163	EL	500	GDP	C2-N3-C4	4.92	120.78	112.30
163	UP	500	GDP	C2-N3-C4	4.92	120.78	112.30
165	EP	501	GTP	C5-C4-N3	-4.92	120.56	128.39
163	NN	500	GDP	C2-N3-C4	4.92	120.78	112.30
163	MN	500	GDP	C2-N3-C4	4.92	120.78	112.30
165	FE	501	GTP	C5-C4-N3	-4.92	120.56	128.39
163	IJ	500	GDP	C2-N3-C4	4.92	120.77	112.30
163	RU	500	GDP	C2-N3-C4	4.92	120.77	112.30
165	VW	501	GTP	C5-C4-N3	-4.92	120.56	128.39
163	NB	500	GDP	C2-N3-C4	4.92	120.77	112.30
163	AJ	500	GDP	C2-N3-C4	4.91	120.77	112.30
165	LL	501	GTP	C5-C4-N3	-4.91	120.57	128.39
165	LX	501	GTP	C5-C4-N3	-4.91	120.57	128.39
165	NK	501	GTP	C5-C4-N3	-4.91	120.57	128.39
165	WI	501	GTP	C5-C4-N3	-4.91	120.57	128.39
165	LJ	501	GTP	C5-C4-N3	-4.91	120.57	128.39
165	NW	501	GTP	C5-C4-N3	-4.91	120.57	128.39
163	CE	500	GDP	C2-N3-C4	4.91	120.76	112.30
163	QM	500	GDP	C2-N3-C4	4.91	120.76	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	TK	501	GTP	C5-C4-N3	-4.91	120.57	128.39
165	BE	501	GTP	C5-C4-N3	-4.91	120.57	128.39
163	BJ	500	GDP	C2-N3-C4	4.91	120.76	112.30
165	OS	501	GTP	C5-C4-N3	-4.91	120.58	128.39
163	DC	500	GDP	C2-N3-C4	4.91	120.76	112.30
163	DG	500	GDP	C2-N3-C4	4.91	120.76	112.30
163	RI	500	GDP	C2-N3-C4	4.91	120.76	112.30
163	FP	500	GDP	C2-N3-C4	4.91	120.76	112.30
165	TO	501	GTP	C5-C4-N3	-4.91	120.58	128.39
165	VK	501	GTP	C5-C4-N3	-4.91	120.58	128.39
165	EM	501	GTP	C5-C4-N3	-4.91	120.58	128.39
165	LV	501	GTP	C5-C4-N3	-4.91	120.58	128.39
165	OO	501	GTP	C5-C4-N3	-4.91	120.58	128.39
163	MJ	500	GDP	C2-N3-C4	4.91	120.75	112.30
165	LZ	502	GTP	C5-C4-N3	-4.90	120.59	128.39
163	PN	500	GDP	C2-N3-C4	4.90	120.74	112.30
165	FV	503	GTP	C5-C4-N3	-4.90	120.59	128.39
163	FN	500	GDP	C2-N3-C4	4.90	120.74	112.30
163	EN	500	GDP	C2-N3-C4	4.90	120.74	112.30
165	FS	501	GTP	C5-C4-N3	-4.90	120.59	128.39
163	GD	500	GDP	C2-N3-C4	4.90	120.74	112.30
163	BN	500	GDP	C2-N3-C4	4.90	120.73	112.30
163	CM	500	GDP	C2-N3-C4	4.90	120.73	112.30
163	AH	500	GDP	C2-N3-C4	4.90	120.73	112.30
163	FB	500	GDP	C2-N3-C4	4.90	120.73	112.30
165	GW	501	GTP	C5-C4-N3	-4.90	120.60	128.39
165	TC	501	GTP	C5-C4-N3	-4.89	120.60	128.39
165	OY	501	GTP	C5-C4-N3	-4.89	120.60	128.39
163	BR	500	GDP	C2-N3-C4	4.89	120.73	112.30
163	AZ	500	GDP	C2-N3-C4	4.89	120.73	112.30
165	OC	501	GTP	C5-C4-N3	-4.89	120.60	128.39
165	AW	501	GTP	C5-C4-N3	-4.89	120.61	128.39
165	AY	501	GTP	C5-C4-N3	-4.89	120.61	128.39
165	MU	501	GTP	C5-C4-N3	-4.89	120.61	128.39
165	PI	501	GTP	C5-C4-N3	-4.89	120.61	128.39
165	JD	501	GTP	C5-C4-N3	-4.89	120.61	128.39
165	PS	501	GTP	C5-C4-N3	-4.89	120.61	128.39
163	GF	500	GDP	C2-N3-C4	4.88	120.71	112.30
163	CU	500	GDP	C2-N3-C4	4.88	120.71	112.30
165	JP	501	GTP	C5-C4-N3	-4.88	120.62	128.39
165	GG	501	GTP	C5-C4-N3	-4.88	120.62	128.39
165	CW	501	GTP	C5-C4-N3	-4.88	120.62	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	MI	501	GTP	C5-C4-N3	-4.88	120.62	128.39
165	PA	501	GTP	C5-C4-N3	-4.88	120.62	128.39
163	PD	500	GDP	C2-N3-C4	4.88	120.70	112.30
165	RN	501	GTP	C5-C4-N3	-4.88	120.63	128.39
165	FC	501	GTP	C5-C4-N3	-4.87	120.63	128.39
165	PU	501	GTP	C5-C4-N3	-4.87	120.63	128.39
163	GR	500	GDP	C2-N3-C4	4.87	120.69	112.30
165	OA	501	GTP	C5-C4-N3	-4.87	120.63	128.39
165	MV	501	GTP	C5-C4-N3	-4.87	120.63	128.39
165	CC	501	GTP	C5-C4-N3	-4.87	120.64	128.39
163	FD	500	GDP	C2-N3-C4	4.87	120.69	112.30
163	EX	500	GDP	C2-N3-C4	4.87	120.69	112.30
165	RB	501	GTP	C5-C4-N3	-4.87	120.64	128.39
165	CQ	501	GTP	C5-C4-N3	-4.87	120.64	128.39
163	FR	501	GDP	C2-N3-C4	4.87	120.69	112.30
163	FL	500	GDP	C2-N3-C4	4.87	120.68	112.30
163	CA	500	GDP	C2-N3-C4	4.86	120.68	112.30
165	EO	501	GTP	C5-C4-N3	-4.86	120.65	128.39
163	FH	500	GDP	C2-N3-C4	4.86	120.68	112.30
163	GL	500	GDP	C2-N3-C4	4.86	120.68	112.30
163	BF	500	GDP	C2-N3-C4	4.86	120.67	112.30
163	DK	501	GDP	C2-N3-C4	4.86	120.67	112.30
163	DY	500	GDP	C2-N3-C4	4.86	120.67	112.30
165	DX	501	GTP	C5-C4-N3	-4.86	120.66	128.39
165	FO	501	GTP	C5-C4-N3	-4.86	120.66	128.39
165	SU	501	GTP	C5-C4-N3	-4.86	120.66	128.39
165	BW	501	GTP	C5-C4-N3	-4.86	120.66	128.39
165	FJ	503	GTP	C5-C4-N3	-4.85	120.67	128.39
165	LD	502	GTP	C5-C4-N3	-4.85	120.67	128.39
165	SI	501	GTP	C5-C4-N3	-4.85	120.68	128.39
165	AO	501	GTP	C5-C4-N3	-4.85	120.68	128.39
165	AM	501	GTP	C5-C4-N3	-4.84	120.68	128.39
165	LP	502	GTP	C5-C4-N3	-4.84	120.68	128.39
163	EH	500	GDP	C2-N3-C4	4.84	120.63	112.30
163	BX	500	GDP	C2-N3-C4	4.84	120.63	112.30
165	AG	501	GTP	C5-C4-N3	-4.83	120.70	128.39
163	CW	500	GDP	N9-C4-N3	4.83	135.61	125.95
165	DH	501	GTP	C5-C4-N3	-4.83	120.71	128.39
163	AV	500	GDP	C2-N3-C4	4.82	120.60	112.30
165	PG	501	GTP	C5-C4-N3	-4.82	120.72	128.39
163	AX	500	GDP	C2-N3-C4	4.81	120.59	112.30
165	HA	501	GTP	C5-C4-N3	-4.81	120.73	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	GE	501	GTP	C5-C4-N3	-4.81	120.74	128.39
165	DN	501	GTP	C5-C4-N3	-4.81	120.74	128.39
165	BK	501	GTP	C5-C4-N3	-4.81	120.74	128.39
163	EB	500	GDP	C2-N3-C4	4.81	120.58	112.30
165	BS	501	GTP	C5-C4-N3	-4.81	120.74	128.39
163	BV	500	GDP	C2-N3-C4	4.80	120.57	112.30
165	CN	501	GTP	C5-C4-N3	-4.80	120.75	128.39
165	AA	501	GTP	C5-C4-N3	-4.79	120.76	128.39
165	DD	501	GTP	C2-N3-C4	4.79	120.55	112.30
165	GS	501	GTP	C5-C4-N3	-4.79	120.77	128.39
165	D	501	GTP	C5-C4-N3	-4.78	120.78	128.39
165	MQ	501	GTP	C5-C4-N3	-4.78	120.78	128.39
165	ME	501	GTP	C5-C4-N3	-4.78	120.78	128.39
165	EA	501	GTP	C2-N3-C4	4.78	120.53	112.30
165	ED	501	GTP	C5-C4-N3	-4.78	120.79	128.39
165	DP	501	GTP	C5-C4-N3	-4.78	120.79	128.39
165	QB	501	GTP	C2-N3-C4	4.77	120.52	112.30
165	GO	501	GTP	C5-C4-N3	-4.77	120.80	128.39
165	BY	501	GTP	C5-C4-N3	-4.76	120.81	128.39
165	CH	501	GTP	C2-N3-C4	4.76	120.49	112.30
163	AN	500	GDP	C2-N3-C4	4.75	120.48	112.30
163	A	501	GDP	N9-C4-N3	4.74	135.44	125.95
165	BO	501	GTP	C5-C4-N3	-4.74	120.85	128.39
165	DB	501	GTP	C5-C4-N3	-4.74	120.85	128.39
165	DJ	501	GTP	C5-C4-N3	-4.73	120.86	128.39
165	AB	501	GTP	C5-C4-N3	-4.73	120.87	128.39
165	GK	501	GTP	C5-C4-N3	-4.73	120.87	128.39
165	QN	501	GTP	C2-N3-C4	4.72	120.42	112.30
165	QL	501	GTP	C2-N3-C4	4.71	120.41	112.30
165	RV	501	GTP	C2-N3-C4	4.71	120.41	112.30
165	UE	501	GTP	C2-N3-C4	4.70	120.40	112.30
163	FT	501	GDP	C2-N3-C4	4.70	120.40	112.30
165	IU	501	GTP	C2-N3-C4	4.70	120.40	112.30
165	UI	501	GTP	C2-N3-C4	4.70	120.39	112.30
165	EI	501	GTP	C2-N3-C4	4.70	120.39	112.30
165	HW	501	GTP	C2-N3-C4	4.70	120.39	112.30
165	KN	502	GTP	C2-N3-C4	4.70	120.39	112.30
165	IO	501	GTP	C2-N3-C4	4.69	120.38	112.30
165	CC	501	GTP	C2-N3-C4	4.69	120.38	112.30
165	SK	501	GTP	C2-N3-C4	4.69	120.37	112.30
165	HN	503	GTP	C2-N3-C4	4.69	120.37	112.30
165	KZ	501	GTP	C2-N3-C4	4.69	120.37	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	GL	501	GTP	C5-C4-N3	-4.68	120.93	128.39
165	IA	501	GTP	C2-N3-C4	4.68	120.37	112.30
165	II	501	GTP	C2-N3-C4	4.68	120.37	112.30
165	JJ	501	GTP	C2-N3-C4	4.68	120.37	112.30
165	UC	501	GTP	C2-N3-C4	4.68	120.37	112.30
165	IY	501	GTP	C2-N3-C4	4.68	120.36	112.30
165	UU	501	GTP	C2-N3-C4	4.68	120.36	112.30
163	CK	501	GDP	N9-C4-N3	4.68	135.30	125.95
165	FM	501	GTP	C5-C4-N3	-4.68	120.95	128.39
165	HK	501	GTP	C2-N3-C4	4.68	120.35	112.30
165	CE	501	GTP	C2-N3-C4	4.67	120.35	112.30
165	GQ	501	GTP	C2-N3-C4	4.67	120.35	112.30
165	CB	501	GTP	C2-N3-C4	4.67	120.35	112.30
165	WK	501	GTP	C2-N3-C4	4.67	120.35	112.30
165	KP	502	GTP	C2-N3-C4	4.67	120.35	112.30
165	PE	501	GTP	C2-N3-C4	4.67	120.34	112.30
165	IC	501	GTP	C2-N3-C4	4.67	120.34	112.30
165	IE	501	GTP	C2-N3-C4	4.67	120.34	112.30
165	EJ	501	GTP	C2-N3-C4	4.67	120.34	112.30
165	WW	501	GTP	C2-N3-C4	4.67	120.34	112.30
165	NA	501	GTP	C2-N3-C4	4.67	120.34	112.30
165	IM	501	GTP	C2-N3-C4	4.67	120.33	112.30
165	NQ	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	IW	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	PW	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	DP	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	KV	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	PQ	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	OW	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	OM	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	RJ	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	SW	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	JB	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	VA	501	GTP	C2-N3-C4	4.66	120.33	112.30
165	KD	502	GTP	C2-N3-C4	4.66	120.32	112.30
165	PO	501	GTP	C2-N3-C4	4.66	120.32	112.30
165	QX	501	GTP	C2-N3-C4	4.65	120.32	112.30
165	VH	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	IS	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	VS	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	LH	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	KR	501	GTP	C2-N3-C4	4.65	120.31	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	VY	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	VT	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	WS	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	JV	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	UQ	501	GTP	C2-N3-C4	4.65	120.31	112.30
165	Q	501	GTP	C2-N3-C4	4.65	120.30	112.30
165	UO	501	GTP	C2-N3-C4	4.65	120.30	112.30
165	TE	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	KX	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	SC	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	AD	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	VG	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	SM	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	OK	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	CO	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	R	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	RF	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	PY	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	WU	501	GTP	C2-N3-C4	4.64	120.30	112.30
165	GI	501	GTP	C2-N3-C4	4.64	120.29	112.30
165	WG	501	GTP	C2-N3-C4	4.64	120.29	112.30
165	KF	501	GTP	C2-N3-C4	4.64	120.29	112.30
165	TQ	501	GTP	C2-N3-C4	4.64	120.29	112.30
165	KL	501	GTP	C2-N3-C4	4.64	120.29	112.30
165	VM	501	GTP	C2-N3-C4	4.64	120.29	112.30
165	SQ	501	GTP	C2-N3-C4	4.64	120.29	112.30
165	JH	501	GTP	C2-N3-C4	4.64	120.29	112.30
165	LT	501	GTP	C2-N3-C4	4.64	120.28	112.30
165	LJ	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	NR	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	US	501	GTP	C2-N3-C4	4.63	120.28	112.30
163	CY	500	GDP	N9-C4-N3	4.63	135.22	125.95
165	OU	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	VC	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	DN	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	KT	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	PC	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	CQ	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	NM	501	GTP	C2-N3-C4	4.63	120.28	112.30
165	IG	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	WQ	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	SA	501	GTP	C2-N3-C4	4.63	120.27	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	KH	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	IQ	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	PK	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	JW	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	QH	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	DE	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	UG	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	DV	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	QU	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	VK	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	HM	501	GTP	C2-N3-C4	4.63	120.27	112.30
165	GG	501	GTP	C2-N3-C4	4.62	120.27	112.30
165	TI	501	GTP	C2-N3-C4	4.62	120.27	112.30
165	WO	501	GTP	C2-N3-C4	4.62	120.27	112.30
163	ET	500	GDP	C2-N3-C4	4.62	120.26	112.30
165	LF	502	GTP	C2-N3-C4	4.62	120.26	112.30
165	SG	501	GTP	C2-N3-C4	4.62	120.26	112.30
165	PM	501	GTP	C2-N3-C4	4.62	120.26	112.30
165	WC	501	GTP	C2-N3-C4	4.62	120.26	112.30
165	CT	501	GTP	C2-N3-C4	4.62	120.26	112.30
165	JR	501	GTP	C2-N3-C4	4.62	120.26	112.30
165	BM	501	GTP	C5-C4-N3	-4.62	121.04	128.39
165	KJ	501	GTP	C2-N3-C4	4.62	120.25	112.30
165	MS	501	GTP	C2-N3-C4	4.62	120.25	112.30
165	QI	501	GTP	C2-N3-C4	4.62	120.25	112.30
165	HB	503	GTP	C2-N3-C4	4.62	120.25	112.30
165	JK	501	GTP	C2-N3-C4	4.62	120.25	112.30
165	GU	501	GTP	C2-N3-C4	4.62	120.25	112.30
165	NI	501	GTP	C2-N3-C4	4.61	120.25	112.30
165	VQ	501	GTP	C2-N3-C4	4.61	120.25	112.30
165	IK	501	GTP	C2-N3-C4	4.61	120.25	112.30
165	RL	501	GTP	C2-N3-C4	4.61	120.25	112.30
165	WE	501	GTP	C2-N3-C4	4.61	120.25	112.30
165	JF	501	GTP	C2-N3-C4	4.61	120.25	112.30
165	J	501	GTP	C2-N3-C4	4.61	120.25	112.30
165	WM	501	GTP	C2-N3-C4	4.61	120.25	112.30
165	CV	501	GTP	C2-N3-C4	4.61	120.24	112.30
165	NF	501	GTP	C2-N3-C4	4.61	120.24	112.30
165	SO	501	GTP	C2-N3-C4	4.61	120.24	112.30
163	QW	500	GDP	N9-C4-N3	4.61	135.17	125.95
165	VW	501	GTP	C2-N3-C4	4.61	120.24	112.30
165	DT	501	GTP	C2-N3-C4	4.61	120.24	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	OI	501	GTP	C2-N3-C4	4.61	120.24	112.30
165	QF	501	GTP	C2-N3-C4	4.61	120.24	112.30
165	KB	502	GTP	C2-N3-C4	4.61	120.24	112.30
165	PS	501	GTP	C2-N3-C4	4.61	120.24	112.30
163	QU	500	GDP	N9-C4-N3	4.61	135.17	125.95
163	WT	500	GDP	N9-C4-N3	4.61	135.17	125.95
165	AP	501	GTP	C2-N3-C4	4.61	120.23	112.30
165	LZ	502	GTP	C2-N3-C4	4.61	120.23	112.30
165	MO	501	GTP	C2-N3-C4	4.61	120.23	112.30
165	QT	501	GTP	C2-N3-C4	4.61	120.23	112.30
165	UM	501	GTP	C2-N3-C4	4.61	120.23	112.30
163	NP	500	GDP	N9-C4-N3	4.61	135.16	125.95
165	JT	501	GTP	C2-N3-C4	4.61	120.23	112.30
165	RR	501	GTP	C2-N3-C4	4.61	120.23	112.30
165	WA	501	GTP	C2-N3-C4	4.61	120.23	112.30
165	LV	501	GTP	C2-N3-C4	4.61	120.23	112.30
165	OG	501	GTP	C2-N3-C4	4.60	120.23	112.30
165	UA	501	GTP	C2-N3-C4	4.60	120.23	112.30
165	NU	501	GTP	C2-N3-C4	4.60	120.23	112.30
165	TO	501	GTP	C2-N3-C4	4.60	120.23	112.30
165	QR	501	GTP	C2-N3-C4	4.60	120.23	112.30
165	WY	501	GTP	C2-N3-C4	4.60	120.23	112.30
163	QK	500	GDP	N9-C4-N3	4.60	135.16	125.95
165	NE	501	GTP	C2-N3-C4	4.60	120.23	112.30
163	WH	500	GDP	N9-C4-N3	4.60	135.15	125.95
165	OD	503	GTP	C2-N3-C4	4.60	120.22	112.30
163	F	500	GDP	N9-C4-N3	4.60	135.15	125.95
165	CJ	501	GTP	C2-N3-C4	4.60	120.22	112.30
165	VO	501	GTP	C2-N3-C4	4.60	120.22	112.30
165	TU	501	GTP	C2-N3-C4	4.60	120.22	112.30
165	LR	502	GTP	C2-N3-C4	4.60	120.22	112.30
165	MG	501	GTP	C2-N3-C4	4.60	120.22	112.30
165	TC	501	GTP	C2-N3-C4	4.60	120.22	112.30
165	OO	501	GTP	C2-N3-C4	4.60	120.22	112.30
165	LN	502	GTP	C2-N3-C4	4.59	120.21	112.30
165	HY	501	GTP	C2-N3-C4	4.59	120.21	112.30
163	TX	500	GDP	N9-C4-N3	4.59	135.14	125.95
165	LP	502	GTP	C2-N3-C4	4.59	120.21	112.30
165	JN	501	GTP	C2-N3-C4	4.59	120.21	112.30
163	GX	500	GDP	N9-C4-N3	4.59	135.14	125.95
165	C	501	GTP	C2-N3-C4	4.59	120.21	112.30
165	DQ	501	GTP	C2-N3-C4	4.59	120.21	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	NW	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	SS	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	AS	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	EV	501	GTP	C5-C4-N3	-4.59	121.09	128.39
165	FI	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	RT	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	OC	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	WI	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	AW	501	GTP	C2-N3-C4	4.59	120.20	112.30
163	RW	500	GDP	N9-C4-N3	4.59	135.12	125.95
165	MC	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	AM	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	LD	502	GTP	C2-N3-C4	4.59	120.20	112.30
165	MA	501	GTP	C2-N3-C4	4.59	120.20	112.30
165	TM	501	GTP	C2-N3-C4	4.59	120.20	112.30
163	QI	500	GDP	N9-C4-N3	4.58	135.12	125.95
165	K	501	GTP	C2-N3-C4	4.58	120.20	112.30
165	VE	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	AK	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	NK	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	SE	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	MI	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	MJ	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	FV	503	GTP	C2-N3-C4	4.58	120.19	112.30
165	RX	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	MU	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	TS	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	EP	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	EG	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	FT	503	GTP	C2-N3-C4	4.58	120.19	112.30
165	UW	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	EU	501	GTP	C2-N3-C4	4.58	120.19	112.30
165	OA	501	GTP	C2-N3-C4	4.58	120.18	112.30
163	NH	500	GDP	N9-C4-N3	4.58	135.10	125.95
165	FQ	501	GTP	C2-N3-C4	4.58	120.18	112.30
165	JP	501	GTP	C2-N3-C4	4.58	120.18	112.30
165	JD	501	GTP	C2-N3-C4	4.58	120.18	112.30
163	RK	500	GDP	N9-C4-N3	4.58	135.10	125.95
165	FC	501	GTP	C2-N3-C4	4.57	120.18	112.30
165	T	503	GTP	C2-N3-C4	4.57	120.18	112.30
165	HE	501	GTP	C2-N3-C4	4.57	120.18	112.30
163	BT	500	GDP	N9-C4-N3	4.57	135.10	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	MM	501	GTP	C2-N3-C4	4.57	120.18	112.30
165	TG	501	GTP	C2-N3-C4	4.57	120.18	112.30
165	QC	501	GTP	C2-N3-C4	4.57	120.18	112.30
163	QA	500	GDP	N9-C4-N3	4.57	135.10	125.95
163	TL	501	GDP	N9-C4-N3	4.57	135.10	125.95
165	RB	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	MY	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	HU	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	NY	501	GTP	C2-N3-C4	4.57	120.17	112.30
163	ON	500	GDP	N9-C4-N3	4.57	135.09	125.95
165	NC	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	BW	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	QO	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	HQ	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	JZ	501	GTP	C2-N3-C4	4.57	120.17	112.30
163	OL	500	GDP	N9-C4-N3	4.57	135.09	125.95
165	LB	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	UK	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	BG	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	SI	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	BQ	501	GTP	C2-N3-C4	4.57	120.17	112.30
165	GC	501	GTP	C5-C4-N3	-4.57	121.12	128.39
165	BU	501	GTP	C2-N3-C4	4.57	120.16	112.30
165	MQ	501	GTP	C2-N3-C4	4.57	120.16	112.30
165	OY	501	GTP	C2-N3-C4	4.57	120.16	112.30
165	D	501	GTP	C2-N3-C4	4.56	120.16	112.30
165	BE	501	GTP	C2-N3-C4	4.56	120.16	112.30
163	WP	500	GDP	N9-C4-N3	4.56	135.07	125.95
165	BK	501	GTP	C2-N3-C4	4.56	120.15	112.30
165	BI	501	GTP	C2-N3-C4	4.56	120.15	112.30
163	ND	500	GDP	N9-C4-N3	4.56	135.07	125.95
165	FG	501	GTP	C2-N3-C4	4.56	120.15	112.30
165	SU	501	GTP	C2-N3-C4	4.56	120.15	112.30
163	QS	500	GDP	N9-C4-N3	4.56	135.06	125.95
165	PG	501	GTP	C2-N3-C4	4.55	120.14	112.30
165	GW	501	GTP	C2-N3-C4	4.55	120.14	112.30
163	VF	500	GDP	N9-C4-N3	4.55	135.06	125.95
165	PU	501	GTP	C2-N3-C4	4.55	120.14	112.30
165	NO	501	GTP	C2-N3-C4	4.55	120.14	112.30
163	JE	500	GDP	N9-C4-N3	4.55	135.05	125.95
165	FO	501	GTP	C2-N3-C4	4.55	120.14	112.30
165	FS	501	GTP	C2-N3-C4	4.55	120.14	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	HH	501	GDP	N9-C4-N3	4.55	135.05	125.95
165	AU	501	GTP	C2-N3-C4	4.55	120.13	112.30
163	O	500	GDP	N9-C4-N3	4.55	135.05	125.95
165	CK	503	GTP	C2-N3-C4	4.55	120.13	112.30
165	ME	501	GTP	C2-N3-C4	4.55	120.13	112.30
165	RO	501	GTP	C2-N3-C4	4.55	120.13	112.30
163	NT	500	GDP	N9-C4-N3	4.55	135.04	125.95
165	DH	501	GTP	C2-N3-C4	4.55	120.13	112.30
165	ED	501	GTP	C2-N3-C4	4.55	120.13	112.30
163	OB	500	GDP	N9-C4-N3	4.55	135.04	125.95
163	ML	500	GDP	N9-C4-N3	4.55	135.04	125.95
165	RC	501	GTP	C2-N3-C4	4.54	120.13	112.30
163	HT	501	GDP	N9-C4-N3	4.54	135.04	125.95
163	JQ	500	GDP	N9-C4-N3	4.54	135.04	125.95
165	OP	503	GTP	C2-N3-C4	4.54	120.12	112.30
165	HG	501	GTP	C2-N3-C4	4.54	120.12	112.30
165	BA	501	GTP	C2-N3-C4	4.54	120.12	112.30
165	OS	501	GTP	C2-N3-C4	4.54	120.12	112.30
165	RH	501	GTP	C2-N3-C4	4.54	120.12	112.30
163	PX	501	GDP	N9-C4-N3	4.54	135.03	125.95
165	LX	501	GTP	C2-N3-C4	4.54	120.12	112.30
165	MV	501	GTP	C2-N3-C4	4.54	120.12	112.30
165	FJ	503	GTP	C2-N3-C4	4.54	120.12	112.30
163	KU	500	GDP	N9-C4-N3	4.54	135.03	125.95
165	EC	501	GTP	C2-N3-C4	4.54	120.11	112.30
165	L	501	GTP	C2-N3-C4	4.54	120.11	112.30
165	LL	501	GTP	C2-N3-C4	4.54	120.11	112.30
165	HS	501	GTP	C2-N3-C4	4.53	120.11	112.30
163	FL	500	GDP	N9-C4-N3	4.53	135.02	125.95
163	OX	500	GDP	N9-C4-N3	4.53	135.02	125.95
163	KI	500	GDP	N9-C4-N3	4.53	135.02	125.95
165	DB	501	GTP	C2-N3-C4	4.53	120.11	112.30
165	DX	501	GTP	C2-N3-C4	4.53	120.11	112.30
163	KY	500	GDP	N9-C4-N3	4.53	135.02	125.95
165	PA	501	GTP	C2-N3-C4	4.53	120.11	112.30
163	SH	500	GDP	N9-C4-N3	4.53	135.01	125.95
165	PI	501	GTP	C2-N3-C4	4.53	120.10	112.30
163	CQ	500	GDP	N9-C4-N3	4.53	135.01	125.95
163	QM	500	GDP	N9-C4-N3	4.53	135.01	125.95
163	RE	500	GDP	N9-C4-N3	4.53	135.01	125.95
165	GK	501	GTP	C2-N3-C4	4.53	120.10	112.30
163	UH	500	GDP	N9-C4-N3	4.53	135.01	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	EM	501	GTP	C2-N3-C4	4.53	120.10	112.30
163	WL	500	GDP	N9-C4-N3	4.53	135.01	125.95
165	HI	501	GTP	C2-N3-C4	4.53	120.10	112.30
163	JA	500	GDP	N9-C4-N3	4.53	135.00	125.95
163	ST	500	GDP	N9-C4-N3	4.53	135.00	125.95
165	TW	501	GTP	C2-N3-C4	4.53	120.10	112.30
163	M	500	GDP	N9-C4-N3	4.53	135.00	125.95
165	AI	501	GTP	C2-N3-C4	4.52	120.09	112.30
165	BM	501	GTP	C2-N3-C4	4.52	120.09	112.30
165	CW	501	GTP	C2-N3-C4	4.52	120.09	112.30
163	PL	501	GDP	N9-C4-N3	4.52	134.99	125.95
163	WD	500	GDP	N9-C4-N3	4.52	134.99	125.95
163	VR	500	GDP	N9-C4-N3	4.52	134.99	125.95
165	AY	501	GTP	C2-N3-C4	4.52	120.09	112.30
165	RN	501	GTP	C2-N3-C4	4.52	120.09	112.30
163	WX	500	GDP	N9-C4-N3	4.52	134.99	125.95
163	RQ	500	GDP	N9-C4-N3	4.52	134.99	125.95
163	KA	500	GDP	N9-C4-N3	4.52	134.99	125.95
163	MH	500	GDP	N9-C4-N3	4.52	134.99	125.95
165	HA	501	GTP	C2-N3-C4	4.52	120.08	112.30
165	FE	501	GTP	C2-N3-C4	4.52	120.08	112.30
163	DM	500	GDP	N9-C4-N3	4.52	134.99	125.95
165	BO	501	GTP	C2-N3-C4	4.52	120.08	112.30
163	QC	500	GDP	N9-C4-N3	4.52	134.98	125.95
165	G	501	GTP	C5-C4-N3	-4.51	121.20	128.39
165	AG	501	GTP	C2-N3-C4	4.51	120.08	112.30
163	UT	500	GDP	N9-C4-N3	4.51	134.98	125.95
165	AO	501	GTP	C2-N3-C4	4.51	120.07	112.30
165	GS	501	GTP	C2-N3-C4	4.51	120.07	112.30
163	LI	500	GDP	N9-C4-N3	4.51	134.97	125.95
163	KE	500	GDP	N9-C4-N3	4.51	134.97	125.95
163	MX	500	GDP	N9-C4-N3	4.51	134.97	125.95
165	ES	501	GTP	C2-N3-C4	4.51	120.06	112.30
165	AA	501	GTP	C2-N3-C4	4.51	120.06	112.30
165	DL	501	GTP	C2-N3-C4	4.50	120.06	112.30
163	QO	500	GDP	N9-C4-N3	4.50	134.95	125.95
163	OP	501	GDP	N9-C4-N3	4.50	134.95	125.95
163	CI	500	GDP	N9-C4-N3	4.50	134.95	125.95
163	MT	500	GDP	N9-C4-N3	4.50	134.95	125.95
163	LU	500	GDP	N9-C4-N3	4.50	134.95	125.95
163	LA	500	GDP	N9-C4-N3	4.50	134.94	125.95
163	LW	500	GDP	N9-C4-N3	4.50	134.94	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	AB	501	GTP	C2-N3-C4	4.50	120.04	112.30
163	QG	500	GDP	N9-C4-N3	4.50	134.94	125.95
163	OV	500	GDP	N9-C4-N3	4.50	134.94	125.95
163	U	500	GDP	N9-C4-N3	4.50	134.94	125.95
163	LS	500	GDP	N9-C4-N3	4.50	134.94	125.95
165	EO	501	GTP	C2-N3-C4	4.50	120.04	112.30
165	TK	501	GTP	C2-N3-C4	4.49	120.04	112.30
163	GB	500	GDP	N9-C4-N3	4.49	134.94	125.95
165	CN	501	GTP	C2-N3-C4	4.49	120.04	112.30
163	IX	501	GDP	N9-C4-N3	4.49	134.93	125.95
163	JW	500	GDP	N9-C4-N3	4.49	134.93	125.95
163	JK	500	GDP	N9-C4-N3	4.49	134.93	125.95
163	DK	501	GDP	N9-C4-N3	4.49	134.93	125.95
163	LG	501	GDP	N9-C4-N3	4.49	134.93	125.95
163	FV	501	GDP	N9-C4-N3	4.49	134.93	125.95
163	AP	500	GDP	N9-C4-N3	4.49	134.93	125.95
165	DJ	501	GTP	C2-N3-C4	4.49	120.03	112.30
163	OD	501	GDP	N9-C4-N3	4.49	134.93	125.95
165	FA	501	GTP	C2-N3-C4	4.49	120.03	112.30
163	WF	501	GDP	N9-C4-N3	4.49	134.92	125.95
163	LY	500	GDP	N9-C4-N3	4.49	134.92	125.95
163	KQ	500	GDP	N9-C4-N3	4.48	134.92	125.95
163	VB	500	GDP	N9-C4-N3	4.48	134.92	125.95
163	TD	500	GDP	N9-C4-N3	4.48	134.91	125.95
163	VN	500	GDP	N9-C4-N3	4.48	134.91	125.95
163	N	500	GDP	N9-C4-N3	4.48	134.91	125.95
163	IR	500	GDP	N9-C4-N3	4.48	134.91	125.95
163	MD	500	GDP	N9-C4-N3	4.48	134.91	125.95
163	HV	500	GDP	N9-C4-N3	4.48	134.90	125.95
163	KG	500	GDP	N9-C4-N3	4.47	134.90	125.95
163	LK	500	GDP	N9-C4-N3	4.47	134.90	125.95
163	RU	500	GDP	N9-C4-N3	4.47	134.90	125.95
163	GN	500	GDP	N9-C4-N3	4.47	134.89	125.95
165	GE	501	GTP	C2-N3-C4	4.47	120.00	112.30
163	EF	500	GDP	N9-C4-N3	4.47	134.89	125.95
163	GP	500	GDP	N9-C4-N3	4.47	134.88	125.95
163	KS	500	GDP	N9-C4-N3	4.47	134.88	125.95
163	LM	500	GDP	N9-C4-N3	4.47	134.88	125.95
163	OJ	500	GDP	N9-C4-N3	4.47	134.88	125.95
163	IL	501	GDP	N9-C4-N3	4.46	134.88	125.95
163	MB	500	GDP	N9-C4-N3	4.46	134.88	125.95
163	SN	501	GDP	N9-C4-N3	4.46	134.87	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	RI	500	GDP	N9-C4-N3	4.46	134.87	125.95
163	OT	500	GDP	N9-C4-N3	4.46	134.87	125.95
165	BS	501	GTP	C2-N3-C4	4.46	119.98	112.30
163	JM	501	GDP	N9-C4-N3	4.46	134.87	125.95
163	NR	500	GDP	N9-C4-N3	4.46	134.87	125.95
163	KM	500	GDP	N9-C4-N3	4.46	134.87	125.95
163	QE	500	GDP	N9-C4-N3	4.46	134.87	125.95
165	GO	501	GTP	C2-N3-C4	4.46	119.97	112.30
163	EL	500	GDP	N9-C4-N3	4.45	134.86	125.95
163	H	500	GDP	N9-C4-N3	4.45	134.86	125.95
163	IT	501	GDP	N9-C4-N3	4.45	134.86	125.95
163	HJ	500	GDP	N9-C4-N3	4.45	134.86	125.95
163	I	501	GDP	N9-C4-N3	4.45	134.86	125.95
163	HD	501	GDP	N9-C4-N3	4.45	134.85	125.95
163	IF	500	GDP	N9-C4-N3	4.45	134.85	125.95
163	NF	500	GDP	N9-C4-N3	4.45	134.85	125.95
163	BD	500	GDP	N9-C4-N3	4.45	134.85	125.95
163	JY	501	GDP	N9-C4-N3	4.45	134.85	125.95
163	LE	500	GDP	N9-C4-N3	4.45	134.85	125.95
163	W	500	GDP	N9-C4-N3	4.45	134.85	125.95
163	RO	500	GDP	N9-C4-N3	4.45	134.85	125.95
165	BY	501	GTP	C2-N3-C4	4.45	119.96	112.30
163	RG	500	GDP	N9-C4-N3	4.45	134.84	125.95
163	RS	500	GDP	N9-C4-N3	4.45	134.84	125.95
163	UD	500	GDP	N9-C4-N3	4.45	134.84	125.95
163	HP	501	GDP	N9-C4-N3	4.44	134.84	125.95
163	LQ	500	GDP	N9-C4-N3	4.44	134.84	125.95
163	OH	500	GDP	N9-C4-N3	4.44	134.84	125.95
163	GH	500	GDP	N9-C4-N3	4.44	134.83	125.95
163	MP	500	GDP	N9-C4-N3	4.44	134.83	125.95
163	GJ	500	GDP	N9-C4-N3	4.44	134.83	125.95
163	RC	500	GDP	N9-C4-N3	4.44	134.83	125.95
163	SV	501	GDP	N9-C4-N3	4.43	134.82	125.95
163	SB	501	GDP	N9-C4-N3	4.43	134.82	125.95
163	IH	500	GDP	N9-C4-N3	4.43	134.82	125.95
163	TP	500	GDP	N9-C4-N3	4.43	134.82	125.95
163	DS	500	GDP	N9-C4-N3	4.43	134.81	125.95
163	OR	500	GDP	N9-C4-N3	4.43	134.81	125.95
163	KO	500	GDP	N9-C4-N3	4.43	134.81	125.95
163	UR	500	GDP	N9-C4-N3	4.43	134.80	125.95
163	WN	500	GDP	N9-C4-N3	4.43	134.80	125.95
163	DA	500	GDP	N9-C4-N3	4.42	134.80	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	UB	500	GDP	N9-C4-N3	4.42	134.80	125.95
163	VV	500	GDP	N9-C4-N3	4.42	134.80	125.95
163	T	501	GDP	N9-C4-N3	4.42	134.80	125.95
163	UF	500	GDP	N9-C4-N3	4.42	134.80	125.95
163	AZ	500	GDP	N9-C4-N3	4.42	134.80	125.95
163	NN	500	GDP	N9-C4-N3	4.42	134.80	125.95
163	V	500	GDP	N9-C4-N3	4.42	134.80	125.95
163	QQ	500	GDP	N9-C4-N3	4.42	134.80	125.95
163	WR	501	GDP	N9-C4-N3	4.42	134.80	125.95
163	VJ	500	GDP	N9-C4-N3	4.42	134.79	125.95
163	TT	500	GDP	N9-C4-N3	4.42	134.79	125.95
163	CM	500	GDP	N9-C4-N3	4.42	134.79	125.95
163	UN	500	GDP	N9-C4-N3	4.42	134.79	125.95
163	HX	501	GDP	N9-C4-N3	4.42	134.79	125.95
163	OF	500	GDP	N9-C4-N3	4.42	134.79	125.95
163	JS	500	GDP	N9-C4-N3	4.42	134.79	125.95
163	SD	500	GDP	N9-C4-N3	4.42	134.79	125.95
163	NJ	501	GDP	N9-C4-N3	4.42	134.79	125.95
163	TB	500	GDP	N9-C4-N3	4.42	134.78	125.95
163	TR	500	GDP	N9-C4-N3	4.42	134.78	125.95
163	S	500	GDP	N9-C4-N3	4.41	134.78	125.95
163	AF	500	GDP	N9-C4-N3	4.41	134.78	125.95
163	TH	500	GDP	N9-C4-N3	4.41	134.78	125.95
163	AT	500	GDP	N9-C4-N3	4.41	134.78	125.95
163	TN	500	GDP	N9-C4-N3	4.41	134.78	125.95
163	JG	500	GDP	N9-C4-N3	4.41	134.78	125.95
163	AL	500	GDP	N9-C4-N3	4.41	134.78	125.95
163	GL	500	GDP	N9-C4-N3	4.41	134.78	125.95
163	HL	501	GDP	N9-C4-N3	4.41	134.78	125.95
163	LC	500	GDP	N9-C4-N3	4.41	134.77	125.95
163	WB	500	GDP	N9-C4-N3	4.41	134.77	125.95
163	IN	500	GDP	N9-C4-N3	4.41	134.77	125.95
163	IB	500	GDP	N9-C4-N3	4.41	134.77	125.95
165	FM	501	GTP	C2-N3-C4	4.41	119.89	112.30
163	KC	500	GDP	N9-C4-N3	4.41	134.77	125.95
163	G	500	GDP	N9-C4-N3	4.41	134.76	125.95
163	EP	500	GDP	N9-C4-N3	4.41	134.76	125.95
163	UL	500	GDP	N9-C4-N3	4.41	134.76	125.95
163	FF	500	GDP	N9-C4-N3	4.40	134.76	125.95
163	BL	500	GDP	N9-C4-N3	4.40	134.76	125.95
163	GF	500	GDP	N9-C4-N3	4.40	134.76	125.95
163	HN	501	GDP	N9-C4-N3	4.40	134.76	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	TF	500	GDP	N9-C4-N3	4.40	134.75	125.95
163	FP	500	GDP	N9-C4-N3	4.40	134.75	125.95
163	MR	500	GDP	N9-C4-N3	4.40	134.75	125.95
163	UP	500	GDP	N9-C4-N3	4.40	134.75	125.95
163	TJ	500	GDP	N9-C4-N3	4.40	134.75	125.95
163	VX	500	GDP	N9-C4-N3	4.40	134.75	125.95
163	JC	500	GDP	N9-C4-N3	4.40	134.75	125.95
163	NB	500	GDP	N9-C4-N3	4.40	134.75	125.95
165	GC	501	GTP	C2-N3-C4	4.40	119.88	112.30
163	PV	500	GDP	N9-C4-N3	4.40	134.75	125.95
163	PJ	500	GDP	N9-C4-N3	4.39	134.74	125.95
163	VD	500	GDP	N9-C4-N3	4.39	134.74	125.95
163	HR	500	GDP	N9-C4-N3	4.39	134.74	125.95
163	MN	500	GDP	N9-C4-N3	4.39	134.74	125.95
163	IJ	500	GDP	N9-C4-N3	4.39	134.74	125.95
163	SL	500	GDP	N9-C4-N3	4.39	134.73	125.95
163	TV	500	GDP	N9-C4-N3	4.39	134.73	125.95
163	DW	501	GDP	N9-C4-N3	4.39	134.73	125.95
163	IV	500	GDP	N9-C4-N3	4.39	134.73	125.95
163	HF	500	GDP	N9-C4-N3	4.39	134.73	125.95
163	SJ	501	GDP	N9-C4-N3	4.39	134.73	125.95
163	JO	500	GDP	N9-C4-N3	4.39	134.73	125.95
163	VT	500	GDP	N9-C4-N3	4.39	134.73	125.95
163	CG	500	GDP	N9-C4-N3	4.39	134.73	125.95
163	BX	500	GDP	N9-C4-N3	4.39	134.73	125.95
163	EJ	500	GDP	N9-C4-N3	4.39	134.72	125.95
163	FB	500	GDP	N9-C4-N3	4.39	134.72	125.95
163	MZ	500	GDP	N9-C4-N3	4.39	134.72	125.95
163	SP	500	GDP	N9-C4-N3	4.39	134.72	125.95
163	UX	500	GDP	N9-C4-N3	4.39	134.72	125.95
163	LO	500	GDP	N9-C4-N3	4.39	134.72	125.95
163	MV	500	GDP	N9-C4-N3	4.38	134.72	125.95
163	BH	500	GDP	N9-C4-N3	4.38	134.72	125.95
163	KW	500	GDP	N9-C4-N3	4.38	134.72	125.95
163	DQ	500	GDP	N9-C4-N3	4.38	134.72	125.95
165	EV	501	GTP	C2-N3-C4	4.38	119.85	112.30
163	MF	500	GDP	N9-C4-N3	4.38	134.71	125.95
163	VH	500	GDP	N9-C4-N3	4.38	134.71	125.95
165	GL	501	GTP	C2-N3-C4	4.38	119.84	112.30
163	VL	500	GDP	N9-C4-N3	4.38	134.71	125.95
163	MJ	500	GDP	N9-C4-N3	4.38	134.71	125.95
163	KK	500	GDP	N9-C4-N3	4.38	134.71	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	G	501	GTP	C2-N3-C4	4.38	119.84	112.30
163	FR	501	GDP	N9-C4-N3	4.38	134.70	125.95
163	IP	500	GDP	N9-C4-N3	4.38	134.70	125.95
163	EN	500	GDP	N9-C4-N3	4.37	134.70	125.95
163	NV	501	GDP	N9-C4-N3	4.37	134.69	125.95
163	SF	500	GDP	N9-C4-N3	4.37	134.69	125.95
163	ID	500	GDP	N9-C4-N3	4.37	134.69	125.95
163	SR	500	GDP	N9-C4-N3	4.37	134.69	125.95
163	RA	500	GDP	N9-C4-N3	4.37	134.69	125.95
163	RM	500	GDP	N9-C4-N3	4.37	134.69	125.95
163	UV	500	GDP	N9-C4-N3	4.36	134.68	125.95
163	JI	500	GDP	N9-C4-N3	4.36	134.68	125.95
163	JU	500	GDP	N9-C4-N3	4.36	134.68	125.95
163	FX	500	GDP	N9-C4-N3	4.36	134.67	125.95
163	GD	500	GDP	N9-C4-N3	4.35	134.65	125.95
163	CO	500	GDP	N9-C4-N3	4.35	134.65	125.95
163	ED	500	GDP	N9-C4-N3	4.35	134.65	125.95
163	WV	500	GDP	N9-C4-N3	4.35	134.65	125.95
163	DI	500	GDP	N9-C4-N3	4.34	134.64	125.95
163	DG	500	GDP	N9-C4-N3	4.34	134.64	125.95
163	CA	500	GDP	N9-C4-N3	4.34	134.63	125.95
163	AB	500	GDP	N9-C4-N3	4.34	134.63	125.95
163	UJ	500	GDP	N9-C4-N3	4.34	134.62	125.95
163	VP	500	GDP	N9-C4-N3	4.34	134.62	125.95
163	PB	500	GDP	N9-C4-N3	4.33	134.61	125.95
163	WJ	500	GDP	N9-C4-N3	4.33	134.61	125.95
163	DC	500	GDP	N9-C4-N3	4.32	134.60	125.95
163	HB	501	GDP	N9-C4-N3	4.32	134.60	125.95
163	PP	500	GDP	N9-C4-N3	4.32	134.59	125.95
163	CE	500	GDP	N9-C4-N3	4.32	134.59	125.95
163	FJ	501	GDP	N9-C4-N3	4.32	134.58	125.95
163	AJ	500	GDP	N9-C4-N3	4.31	134.57	125.95
163	PH	500	GDP	N9-C4-N3	4.30	134.55	125.95
163	BR	500	GDP	N9-C4-N3	4.30	134.55	125.95
163	GT	501	GDP	N9-C4-N3	4.29	134.54	125.95
163	BP	500	GDP	N9-C4-N3	4.29	134.54	125.95
163	PN	500	GDP	N9-C4-N3	4.29	134.54	125.95
163	FN	500	GDP	N9-C4-N3	4.29	134.53	125.95
163	PR	501	GDP	N9-C4-N3	4.28	134.51	125.95
163	DY	500	GDP	N9-C4-N3	4.28	134.50	125.95
163	PT	500	GDP	N9-C4-N3	4.28	134.50	125.95
163	PF	501	GDP	N9-C4-N3	4.27	134.50	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	GV	501	GDP	N9-C4-N3	4.27	134.50	125.95
163	DU	500	GDP	N9-C4-N3	4.26	134.48	125.95
163	AD	500	GDP	N9-C4-N3	4.26	134.47	125.95
163	AH	500	GDP	N9-C4-N3	4.25	134.45	125.95
163	BJ	500	GDP	N9-C4-N3	4.25	134.45	125.95
163	FD	500	GDP	N9-C4-N3	4.25	134.44	125.95
163	PD	500	GDP	N9-C4-N3	4.24	134.44	125.95
163	NL	500	GDP	N9-C4-N3	4.23	134.42	125.95
163	ER	500	GDP	N9-C4-N3	4.23	134.42	125.95
163	BN	500	GDP	N9-C4-N3	4.23	134.41	125.95
163	AR	500	GDP	N9-C4-N3	4.22	134.40	125.95
163	DE	500	GDP	N9-C4-N3	4.22	134.39	125.95
163	NX	500	GDP	N9-C4-N3	4.21	134.37	125.95
163	EB	500	GDP	N9-C4-N3	4.20	134.34	125.95
163	BF	500	GDP	N9-C4-N3	4.19	134.33	125.95
163	CS	500	GDP	N9-C4-N3	4.17	134.30	125.95
163	CC	500	GDP	N9-C4-N3	4.16	134.27	125.95
163	FH	500	GDP	N9-C4-N3	4.15	134.26	125.95
163	AV	500	GDP	N9-C4-N3	4.15	134.26	125.95
163	EV	500	GDP	N9-C4-N3	4.15	134.25	125.95
163	GR	500	GDP	N9-C4-N3	4.15	134.25	125.95
163	DO	500	GDP	N9-C4-N3	4.14	134.23	125.95
163	EH	500	GDP	N9-C4-N3	4.13	134.21	125.95
163	AN	500	GDP	N9-C4-N3	4.11	134.16	125.95
163	AX	500	GDP	N9-C4-N3	4.09	134.13	125.95
163	ET	500	GDP	N9-C4-N3	4.08	134.11	125.95
163	BV	500	GDP	N9-C4-N3	4.07	134.09	125.95
163	CU	500	GDP	N9-C4-N3	4.06	134.08	125.95
163	E	500	GDP	N9-C4-N3	4.05	134.05	125.95
163	EX	500	GDP	N9-C4-N3	3.87	133.69	125.95
163	FT	501	GDP	N9-C4-N3	3.85	133.66	125.95
163	EX	500	GDP	C6-C5-N7	3.73	137.08	130.29
163	E	500	GDP	C6-C5-N7	3.72	137.05	130.29
165	EJ	501	GTP	N9-C4-N3	3.70	133.36	125.95
163	FT	501	GDP	C6-C5-N7	3.63	136.90	130.29
163	DE	500	GDP	C6-C5-N7	3.62	136.88	130.29
163	EV	500	GDP	C6-C5-N7	3.60	136.84	130.29
165	CH	501	GTP	N9-C4-N3	3.60	133.15	125.95
163	CS	500	GDP	C6-C5-N7	3.59	136.83	130.29
163	CU	500	GDP	C6-C5-N7	3.58	136.81	130.29
163	CC	500	GDP	C6-C5-N7	3.57	136.79	130.29
163	DO	500	GDP	C6-C5-N7	3.54	136.73	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	BP	500	GDP	C6-C5-N7	3.53	136.72	130.29
163	EH	500	GDP	C6-C5-N7	3.53	136.71	130.29
163	AX	500	GDP	C6-C5-N7	3.52	136.70	130.29
163	DI	500	GDP	C6-C5-N7	3.52	136.70	130.29
163	BV	500	GDP	C6-C5-N7	3.51	136.68	130.29
163	AR	500	GDP	C6-C5-N7	3.50	136.66	130.29
163	GR	500	GDP	C6-C5-N7	3.50	136.66	130.29
163	PR	501	GDP	C6-C5-N7	3.48	136.63	130.29
163	DY	500	GDP	C6-C5-N7	3.48	136.62	130.29
163	GT	501	GDP	C6-C5-N7	3.47	136.60	130.29
165	GQ	501	GTP	N9-C4-N3	3.46	132.88	125.95
163	BF	500	GDP	C6-C5-N7	3.46	136.59	130.29
163	GV	501	GDP	C6-C5-N7	3.45	136.58	130.29
163	AV	500	GDP	C6-C5-N7	3.45	136.57	130.29
163	EL	500	GDP	C6-C5-N7	3.45	136.56	130.29
163	ET	500	GDP	C6-C5-N7	3.44	136.56	130.29
163	AN	500	GDP	C6-C5-N7	3.44	136.56	130.29
163	PF	501	GDP	C6-C5-N7	3.44	136.56	130.29
163	ER	500	GDP	C6-C5-N7	3.44	136.55	130.29
163	AD	500	GDP	C6-C5-N7	3.44	136.54	130.29
163	PH	500	GDP	C6-C5-N7	3.43	136.53	130.29
165	GI	501	GTP	N9-C4-N3	3.43	132.80	125.95
163	DQ	500	GDP	C6-C5-N7	3.43	136.52	130.29
163	DU	500	GDP	C6-C5-N7	3.42	136.52	130.29
163	NL	500	GDP	C6-C5-N7	3.42	136.52	130.29
163	NX	500	GDP	C6-C5-N7	3.42	136.51	130.29
163	PD	500	GDP	C6-C5-N7	3.42	136.51	130.29
165	QH	501	GTP	N9-C4-N3	3.42	132.78	125.95
163	UJ	500	GDP	C6-C5-N7	3.42	136.50	130.29
165	HW	501	GTP	N9-C4-N3	3.42	132.78	125.95
163	FH	500	GDP	C6-C5-N7	3.41	136.50	130.29
165	DE	501	GTP	N9-C4-N3	3.41	132.77	125.95
163	BJ	500	GDP	C6-C5-N7	3.41	136.50	130.29
163	UV	500	GDP	C6-C5-N7	3.41	136.49	130.29
165	EA	501	GTP	N9-C4-N3	3.41	132.76	125.95
165	IE	501	GTP	N9-C4-N3	3.40	132.76	125.95
163	CG	500	GDP	C6-C5-N7	3.40	136.48	130.29
165	HK	501	GTP	N9-C4-N3	3.40	132.75	125.95
163	PT	500	GDP	C6-C5-N7	3.39	136.47	130.29
163	BN	500	GDP	C6-C5-N7	3.39	136.46	130.29
163	KK	500	GDP	C6-C5-N7	3.39	136.46	130.29
163	PJ	500	GDP	C6-C5-N7	3.39	136.46	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	AH	500	GDP	C6-C5-N7	3.39	136.46	130.29
165	IQ	501	GTP	N9-C4-N3	3.39	132.72	125.95
165	QT	501	GTP	N9-C4-N3	3.38	132.72	125.95
165	NR	501	GTP	N9-C4-N3	3.38	132.72	125.95
165	IO	501	GTP	N9-C4-N3	3.38	132.72	125.95
163	PP	500	GDP	C6-C5-N7	3.38	136.44	130.29
163	SL	500	GDP	C6-C5-N7	3.38	136.44	130.29
163	WJ	500	GDP	C6-C5-N7	3.38	136.44	130.29
163	BR	500	GDP	C6-C5-N7	3.38	136.43	130.29
163	PN	500	GDP	C6-C5-N7	3.37	136.43	130.29
163	SR	500	GDP	C6-C5-N7	3.37	136.43	130.29
163	AF	500	GDP	C6-C5-N7	3.37	136.43	130.29
163	UX	500	GDP	C6-C5-N7	3.37	136.43	130.29
163	DW	501	GDP	C6-C5-N7	3.37	136.43	130.29
163	CO	500	GDP	C6-C5-N7	3.37	136.43	130.29
165	IC	501	GTP	N9-C4-N3	3.37	132.69	125.95
163	DC	500	GDP	C6-C5-N7	3.37	136.42	130.29
163	PB	500	GDP	C6-C5-N7	3.37	136.42	130.29
163	FD	500	GDP	C6-C5-N7	3.37	136.42	130.29
163	FX	500	GDP	C6-C5-N7	3.37	136.41	130.29
163	WV	500	GDP	C6-C5-N7	3.36	136.41	130.29
163	KW	500	GDP	C6-C5-N7	3.36	136.41	130.29
163	TF	500	GDP	C6-C5-N7	3.36	136.41	130.29
163	EJ	500	GDP	C6-C5-N7	3.36	136.41	130.29
165	KH	501	GTP	N9-C4-N3	3.36	132.67	125.95
163	VL	500	GDP	C6-C5-N7	3.36	136.40	130.29
163	JO	500	GDP	C6-C5-N7	3.36	136.40	130.29
163	VV	500	GDP	C6-C5-N7	3.36	136.40	130.29
163	CE	500	GDP	C6-C5-N7	3.35	136.40	130.29
163	TR	500	GDP	C6-C5-N7	3.35	136.40	130.29
163	SF	500	GDP	C6-C5-N7	3.35	136.39	130.29
163	S	500	GDP	C6-C5-N7	3.35	136.39	130.29
163	IP	500	GDP	C6-C5-N7	3.35	136.39	130.29
163	NJ	501	GDP	C6-C5-N7	3.35	136.39	130.29
163	EB	500	GDP	C6-C5-N7	3.35	136.39	130.29
163	HB	501	GDP	C6-C5-N7	3.35	136.39	130.29
163	ID	500	GDP	C6-C5-N7	3.35	136.38	130.29
163	JC	500	GDP	C6-C5-N7	3.34	136.37	130.29
163	UL	500	GDP	C6-C5-N7	3.34	136.37	130.29
165	IS	501	GTP	N9-C4-N3	3.34	132.64	125.95
163	SJ	501	GDP	C6-C5-N7	3.34	136.37	130.29
163	EP	500	GDP	C6-C5-N7	3.34	136.37	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	AT	500	GDP	C6-C5-N7	3.34	136.37	130.29
163	ED	500	GDP	C6-C5-N7	3.34	136.37	130.29
163	PV	500	GDP	C6-C5-N7	3.34	136.37	130.29
165	CT	501	GTP	N9-C4-N3	3.34	132.63	125.95
163	UF	500	GDP	C6-C5-N7	3.34	136.36	130.29
163	VX	500	GDP	C6-C5-N7	3.34	136.36	130.29
163	G	500	GDP	C6-C5-N7	3.34	136.36	130.29
163	VJ	500	GDP	C6-C5-N7	3.34	136.36	130.29
163	SV	501	GDP	C6-C5-N7	3.34	136.36	130.29
163	TH	500	GDP	C6-C5-N7	3.33	136.36	130.29
163	MZ	500	GDP	C6-C5-N7	3.33	136.35	130.29
165	R	501	GTP	N9-C4-N3	3.33	132.62	125.95
163	AL	500	GDP	C6-C5-N7	3.33	136.35	130.29
163	TJ	500	GDP	C6-C5-N7	3.33	136.35	130.29
163	JG	500	GDP	C6-C5-N7	3.33	136.35	130.29
165	IU	501	GTP	N9-C4-N3	3.33	132.61	125.95
165	BI	501	GTP	N9-C4-N3	3.33	132.61	125.95
163	VP	500	GDP	C6-C5-N7	3.33	136.35	130.29
165	KT	501	GTP	N9-C4-N3	3.33	132.61	125.95
163	VH	500	GDP	C6-C5-N7	3.33	136.35	130.29
163	CA	500	GDP	C6-C5-N7	3.33	136.35	130.29
163	JS	500	GDP	C6-C5-N7	3.33	136.35	130.29
163	MV	500	GDP	C6-C5-N7	3.33	136.35	130.29
163	TP	500	GDP	C6-C5-N7	3.33	136.34	130.29
163	UN	500	GDP	C6-C5-N7	3.33	136.34	130.29
165	SG	501	GTP	N9-C4-N3	3.33	132.60	125.95
165	JH	501	GTP	N9-C4-N3	3.32	132.60	125.95
163	AJ	500	GDP	C6-C5-N7	3.32	136.34	130.29
165	QF	501	GTP	N9-C4-N3	3.32	132.60	125.95
163	BH	500	GDP	C6-C5-N7	3.32	136.34	130.29
163	OF	500	GDP	C6-C5-N7	3.32	136.34	130.29
163	SP	500	GDP	C6-C5-N7	3.32	136.34	130.29
165	CK	503	GTP	N9-C4-N3	3.32	132.60	125.95
163	OR	500	GDP	C6-C5-N7	3.32	136.34	130.29
165	NF	501	GTP	N9-C4-N3	3.32	132.59	125.95
165	SS	501	GTP	N9-C4-N3	3.32	132.59	125.95
165	IG	501	GTP	N9-C4-N3	3.32	132.59	125.95
163	VN	500	GDP	C6-C5-N7	3.32	136.33	130.29
163	VT	500	GDP	C6-C5-N7	3.32	136.33	130.29
163	BD	500	GDP	C6-C5-N7	3.32	136.32	130.29
163	KY	500	GDP	C6-C5-N7	3.32	136.32	130.29
165	LH	501	GTP	N9-C4-N3	3.31	132.58	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	MN	500	GDP	C6-C5-N7	3.31	136.32	130.29
163	LW	500	GDP	C6-C5-N7	3.31	136.32	130.29
163	AB	500	GDP	C6-C5-N7	3.31	136.32	130.29
163	HN	501	GDP	C6-C5-N7	3.31	136.32	130.29
165	IA	501	GTP	N9-C4-N3	3.31	132.57	125.95
163	FJ	501	GDP	C6-C5-N7	3.31	136.31	130.29
165	FT	503	GTP	N9-C4-N3	3.31	132.57	125.95
163	HP	501	GDP	C6-C5-N7	3.31	136.31	130.29
163	MR	500	GDP	C6-C5-N7	3.31	136.31	130.29
163	LO	500	GDP	C6-C5-N7	3.31	136.31	130.29
163	T	501	GDP	C6-C5-N7	3.30	136.30	130.29
163	IT	501	GDP	C6-C5-N7	3.30	136.30	130.29
165	II	501	GTP	N9-C4-N3	3.30	132.56	125.95
165	LT	501	GTP	N9-C4-N3	3.30	132.56	125.95
163	VD	500	GDP	C6-C5-N7	3.30	136.30	130.29
163	NV	501	GDP	C6-C5-N7	3.30	136.30	130.29
163	MJ	500	GDP	C6-C5-N7	3.30	136.30	130.29
163	V	500	GDP	C6-C5-N7	3.30	136.30	130.29
163	VB	500	GDP	C6-C5-N7	3.30	136.30	130.29
163	BL	500	GDP	C6-C5-N7	3.30	136.30	130.29
165	SW	501	GTP	N9-C4-N3	3.30	132.55	125.95
163	JY	501	GDP	C6-C5-N7	3.30	136.30	130.29
165	DT	501	GTP	N9-C4-N3	3.30	132.55	125.95
163	DA	500	GDP	C6-C5-N7	3.30	136.29	130.29
163	LS	500	GDP	C6-C5-N7	3.30	136.29	130.29
163	UR	500	GDP	C6-C5-N7	3.30	136.29	130.29
165	FQ	501	GTP	N9-C4-N3	3.30	132.55	125.95
163	HD	501	GDP	C6-C5-N7	3.30	136.29	130.29
163	EN	500	GDP	C6-C5-N7	3.30	136.29	130.29
165	NQ	501	GTP	N9-C4-N3	3.30	132.55	125.95
163	SD	500	GDP	C6-C5-N7	3.30	136.29	130.29
165	BU	501	GTP	N9-C4-N3	3.30	132.55	125.95
163	DG	500	GDP	C6-C5-N7	3.30	136.29	130.29
163	MB	500	GDP	C6-C5-N7	3.30	136.29	130.29
163	GD	500	GDP	C6-C5-N7	3.30	136.29	130.29
165	QR	501	GTP	N9-C4-N3	3.29	132.54	125.95
163	TT	500	GDP	C6-C5-N7	3.29	136.29	130.29
163	HJ	500	GDP	C6-C5-N7	3.29	136.28	130.29
165	JT	501	GTP	N9-C4-N3	3.29	132.54	125.95
163	TV	500	GDP	C6-C5-N7	3.29	136.28	130.29
163	LG	501	GDP	C6-C5-N7	3.29	136.28	130.29
163	UB	500	GDP	C6-C5-N7	3.29	136.28	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	IW	501	GTP	N9-C4-N3	3.29	132.53	125.95
163	HV	500	GDP	C6-C5-N7	3.29	136.28	130.29
163	HR	500	GDP	C6-C5-N7	3.29	136.28	130.29
163	KM	500	GDP	C6-C5-N7	3.29	136.28	130.29
163	LC	500	GDP	C6-C5-N7	3.29	136.28	130.29
165	K	501	GTP	N9-C4-N3	3.29	132.53	125.95
163	LM	500	GDP	C6-C5-N7	3.29	136.27	130.29
163	WB	500	GDP	C6-C5-N7	3.29	136.27	130.29
163	AZ	500	GDP	C6-C5-N7	3.29	136.27	130.29
163	I	501	GDP	C6-C5-N7	3.28	136.27	130.29
163	KC	500	GDP	C6-C5-N7	3.28	136.27	130.29
163	SB	501	GDP	C6-C5-N7	3.28	136.27	130.29
165	NM	501	GTP	N9-C4-N3	3.28	132.52	125.95
163	IR	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	IF	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	N	500	GDP	C6-C5-N7	3.28	136.26	130.29
165	VG	501	GTP	N9-C4-N3	3.28	132.52	125.95
165	KX	501	GTP	N9-C4-N3	3.28	132.51	125.95
163	CI	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	GH	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	GJ	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	TN	500	GDP	C6-C5-N7	3.28	136.26	130.29
165	KL	501	GTP	N9-C4-N3	3.28	132.51	125.95
165	VC	501	GTP	N9-C4-N3	3.28	132.51	125.95
165	HN	503	GTP	N9-C4-N3	3.28	132.51	125.95
163	JI	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	NB	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	FP	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	LY	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	MP	500	GDP	C6-C5-N7	3.28	136.26	130.29
163	LA	500	GDP	C6-C5-N7	3.28	136.26	130.29
165	WY	501	GTP	N9-C4-N3	3.28	132.51	125.95
163	JU	500	GDP	C6-C5-N7	3.28	136.25	130.29
165	NY	501	GTP	N9-C4-N3	3.28	132.50	125.95
165	JR	501	GTP	N9-C4-N3	3.28	132.50	125.95
163	FF	500	GDP	C6-C5-N7	3.28	136.25	130.29
163	IL	501	GDP	C6-C5-N7	3.28	136.25	130.29
163	TD	500	GDP	C6-C5-N7	3.28	136.25	130.29
163	IV	500	GDP	C6-C5-N7	3.28	136.25	130.29
165	OK	501	GTP	N9-C4-N3	3.27	132.50	125.95
163	W	500	GDP	C6-C5-N7	3.27	136.25	130.29
163	IH	500	GDP	C6-C5-N7	3.27	136.25	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	HF	500	GDP	C6-C5-N7	3.27	136.25	130.29
163	LK	500	GDP	C6-C5-N7	3.27	136.25	130.29
163	RM	500	GDP	C6-C5-N7	3.27	136.25	130.29
165	VA	501	GTP	N9-C4-N3	3.27	132.49	125.95
163	WN	500	GDP	C6-C5-N7	3.27	136.24	130.29
163	JA	500	GDP	C6-C5-N7	3.27	136.24	130.29
165	J	501	GTP	N9-C4-N3	3.27	132.49	125.95
163	MD	500	GDP	C6-C5-N7	3.27	136.24	130.29
165	OW	501	GTP	N9-C4-N3	3.27	132.49	125.95
163	WF	501	GDP	C6-C5-N7	3.27	136.24	130.29
165	AD	501	GTP	N9-C4-N3	3.27	132.49	125.95
163	MF	500	GDP	C6-C5-N7	3.27	136.23	130.29
163	H	500	GDP	C6-C5-N7	3.27	136.23	130.29
163	JM	501	GDP	C6-C5-N7	3.27	136.23	130.29
165	SK	501	GTP	N9-C4-N3	3.26	132.48	125.95
165	TE	501	GTP	N9-C4-N3	3.26	132.48	125.95
163	IJ	500	GDP	C6-C5-N7	3.26	136.23	130.29
163	DS	500	GDP	C6-C5-N7	3.26	136.23	130.29
165	NE	501	GTP	N9-C4-N3	3.26	132.48	125.95
163	RC	500	GDP	C6-C5-N7	3.26	136.23	130.29
163	MH	500	GDP	C6-C5-N7	3.26	136.22	130.29
163	JW	500	GDP	C6-C5-N7	3.26	136.22	130.29
163	FR	501	GDP	C6-C5-N7	3.26	136.22	130.29
165	WM	501	GTP	N9-C4-N3	3.26	132.47	125.95
165	TQ	501	GTP	N9-C4-N3	3.26	132.47	125.95
163	GF	500	GDP	C6-C5-N7	3.26	136.22	130.29
163	HH	501	GDP	C6-C5-N7	3.26	136.22	130.29
163	OP	501	GDP	C6-C5-N7	3.26	136.22	130.29
165	DQ	501	GTP	N9-C4-N3	3.26	132.47	125.95
165	IY	501	GTP	N9-C4-N3	3.26	132.47	125.95
165	VS	501	GTP	N9-C4-N3	3.26	132.47	125.95
163	HX	501	GDP	C6-C5-N7	3.26	136.22	130.29
163	GP	500	GDP	C6-C5-N7	3.25	136.21	130.29
163	KO	500	GDP	C6-C5-N7	3.25	136.21	130.29
165	JF	501	GTP	N9-C4-N3	3.25	132.46	125.95
165	SC	501	GTP	N9-C4-N3	3.25	132.46	125.95
165	HM	501	GTP	N9-C4-N3	3.25	132.46	125.95
165	GU	501	GTP	N9-C4-N3	3.25	132.46	125.95
163	RA	500	GDP	C6-C5-N7	3.25	136.21	130.29
163	SN	501	GDP	C6-C5-N7	3.25	136.21	130.29
163	QE	500	GDP	C6-C5-N7	3.25	136.21	130.29
163	IX	501	GDP	C6-C5-N7	3.25	136.21	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	FN	500	GDP	C6-C5-N7	3.25	136.21	130.29
163	QS	500	GDP	C6-C5-N7	3.25	136.21	130.29
165	TI	501	GTP	N9-C4-N3	3.25	132.45	125.95
165	EI	501	GTP	N9-C4-N3	3.25	132.45	125.95
163	AP	500	GDP	C6-C5-N7	3.25	136.20	130.29
163	WR	501	GDP	C6-C5-N7	3.25	136.20	130.29
163	NN	500	GDP	C6-C5-N7	3.25	136.20	130.29
165	IM	501	GTP	N9-C4-N3	3.25	132.45	125.95
163	TB	500	GDP	C6-C5-N7	3.25	136.20	130.29
163	MT	500	GDP	C6-C5-N7	3.25	136.20	130.29
163	QQ	500	GDP	C6-C5-N7	3.25	136.20	130.29
163	GL	500	GDP	C6-C5-N7	3.25	136.20	130.29
165	IK	501	GTP	N9-C4-N3	3.25	132.45	125.95
165	VO	501	GTP	N9-C4-N3	3.25	132.44	125.95
163	U	500	GDP	C6-C5-N7	3.25	136.20	130.29
163	KQ	500	GDP	C6-C5-N7	3.25	136.20	130.29
165	AI	501	GTP	N9-C4-N3	3.24	132.44	125.95
163	DM	500	GDP	C6-C5-N7	3.24	136.19	130.29
165	VQ	501	GTP	N9-C4-N3	3.24	132.44	125.95
163	QG	500	GDP	C6-C5-N7	3.24	136.19	130.29
163	VR	500	GDP	C6-C5-N7	3.24	136.19	130.29
163	HL	501	GDP	C6-C5-N7	3.24	136.19	130.29
165	KB	502	GTP	N9-C4-N3	3.24	132.43	125.95
163	LU	500	GDP	C6-C5-N7	3.24	136.19	130.29
163	FB	500	GDP	C6-C5-N7	3.24	136.18	130.29
163	JK	500	GDP	C6-C5-N7	3.24	136.18	130.29
165	DL	501	GTP	C2-N1-C6	-3.24	119.24	125.11
163	WX	500	GDP	C6-C5-N7	3.24	136.18	130.29
165	NU	501	GTP	N9-C4-N3	3.24	132.42	125.95
163	WL	500	GDP	C6-C5-N7	3.24	136.18	130.29
165	HB	503	GTP	N9-C4-N3	3.24	132.42	125.95
165	VT	501	GTP	N9-C4-N3	3.24	132.42	125.95
165	VH	501	GTP	N9-C4-N3	3.23	132.42	125.95
163	O	500	GDP	C6-C5-N7	3.23	136.17	130.29
163	QU	500	GDP	C6-C5-N7	3.23	136.17	130.29
165	QU	501	GTP	N9-C4-N3	3.23	132.42	125.95
163	NT	500	GDP	C6-C5-N7	3.23	136.17	130.29
165	HE	501	GTP	N9-C4-N3	3.23	132.41	125.95
165	Q	501	GTP	N9-C4-N3	3.23	132.41	125.95
165	TU	501	GTP	N9-C4-N3	3.23	132.41	125.95
163	IB	500	GDP	C6-C5-N7	3.23	136.17	130.29
163	OH	500	GDP	C6-C5-N7	3.23	136.17	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	HQ	501	GTP	N9-C4-N3	3.23	132.41	125.95
163	UD	500	GDP	C6-C5-N7	3.23	136.17	130.29
165	AP	501	GTP	N9-C4-N3	3.23	132.41	125.95
165	HY	501	GTP	N9-C4-N3	3.23	132.41	125.95
163	WD	500	GDP	C6-C5-N7	3.23	136.16	130.29
163	HT	501	GDP	C6-C5-N7	3.23	136.16	130.29
165	SO	501	GTP	N9-C4-N3	3.23	132.41	125.95
163	IN	500	GDP	C6-C5-N7	3.23	136.16	130.29
165	PY	501	GTP	N9-C4-N3	3.23	132.41	125.95
163	M	500	GDP	C6-C5-N7	3.23	136.16	130.29
165	UA	501	GTP	N9-C4-N3	3.23	132.40	125.95
163	OJ	500	GDP	C6-C5-N7	3.23	136.16	130.29
163	RG	500	GDP	C6-C5-N7	3.23	136.16	130.29
163	VF	500	GDP	C6-C5-N7	3.22	136.16	130.29
165	NO	501	GTP	N9-C4-N3	3.22	132.40	125.95
163	FV	501	GDP	C6-C5-N7	3.22	136.16	130.29
163	OD	501	GDP	C6-C5-N7	3.22	136.16	130.29
163	SH	500	GDP	C6-C5-N7	3.22	136.16	130.29
163	JQ	500	GDP	C6-C5-N7	3.22	136.16	130.29
165	UM	501	GTP	N9-C4-N3	3.22	132.40	125.95
165	NC	501	GTP	N9-C4-N3	3.22	132.39	125.95
163	KA	500	GDP	C6-C5-N7	3.22	136.15	130.29
163	TL	501	GDP	C6-C5-N7	3.22	136.15	130.29
163	KS	500	GDP	C6-C5-N7	3.22	136.15	130.29
163	EF	500	GDP	C6-C5-N7	3.22	136.15	130.29
165	T	503	GTP	N9-C4-N3	3.22	132.38	125.95
163	UH	500	GDP	C6-C5-N7	3.22	136.14	130.29
163	TX	500	GDP	C6-C5-N7	3.22	136.14	130.29
165	VE	501	GTP	N9-C4-N3	3.22	132.38	125.95
163	UP	500	GDP	C6-C5-N7	3.22	136.14	130.29
163	OV	500	GDP	C6-C5-N7	3.22	136.14	130.29
165	KN	502	GTP	N9-C4-N3	3.22	132.38	125.95
165	JN	501	GTP	N9-C4-N3	3.21	132.38	125.95
163	JE	500	GDP	C6-C5-N7	3.21	136.14	130.29
165	TM	501	GTP	N9-C4-N3	3.21	132.38	125.95
163	NF	500	GDP	C6-C5-N7	3.21	136.14	130.29
163	KE	500	GDP	C6-C5-N7	3.21	136.14	130.29
163	PX	501	GDP	C6-C5-N7	3.21	136.14	130.29
165	CB	501	GTP	N9-C4-N3	3.21	132.38	125.95
163	OT	500	GDP	C6-C5-N7	3.21	136.14	130.29
165	JZ	501	GTP	N9-C4-N3	3.21	132.38	125.95
163	KG	500	GDP	C6-C5-N7	3.21	136.13	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	DL	501	GTP	N9-C4-N3	3.21	132.37	125.95
165	QL	501	GTP	N9-C4-N3	3.21	132.37	125.95
165	KF	501	GTP	N9-C4-N3	3.21	132.37	125.95
163	RS	500	GDP	C6-C5-N7	3.21	136.13	130.29
163	WP	500	GDP	C6-C5-N7	3.21	136.13	130.29
165	HU	501	GTP	N9-C4-N3	3.21	132.37	125.95
163	NR	500	GDP	C6-C5-N7	3.21	136.13	130.29
165	QI	501	GTP	N9-C4-N3	3.21	132.37	125.95
165	KD	502	GTP	N9-C4-N3	3.21	132.37	125.95
165	KP	502	GTP	N9-C4-N3	3.21	132.37	125.95
163	BT	500	GDP	C6-C5-N7	3.21	136.12	130.29
163	RE	500	GDP	C6-C5-N7	3.21	136.12	130.29
163	RO	500	GDP	C6-C5-N7	3.21	136.12	130.29
165	JJ	501	GTP	N9-C4-N3	3.20	132.36	125.95
163	MX	500	GDP	C6-C5-N7	3.20	136.12	130.29
165	QX	501	GTP	N9-C4-N3	3.20	132.36	125.95
165	C	501	GTP	N9-C4-N3	3.20	132.36	125.95
163	CQ	500	GDP	C6-C5-N7	3.20	136.12	130.29
165	RC	501	GTP	N9-C4-N3	3.20	132.36	125.95
163	PL	501	GDP	C6-C5-N7	3.20	136.12	130.29
165	BG	501	GTP	N9-C4-N3	3.20	132.36	125.95
165	TG	501	GTP	N9-C4-N3	3.20	132.36	125.95
165	EA	501	GTP	C2-N1-C6	-3.20	119.30	125.11
165	NI	501	GTP	N9-C4-N3	3.20	132.35	125.95
163	KI	500	GDP	C6-C5-N7	3.20	136.12	130.29
165	AK	501	GTP	N9-C4-N3	3.20	132.35	125.95
165	KZ	501	GTP	N9-C4-N3	3.20	132.35	125.95
163	UT	500	GDP	C6-C5-N7	3.20	136.11	130.29
163	LI	500	GDP	C6-C5-N7	3.20	136.11	130.29
163	QI	500	GDP	C6-C5-N7	3.20	136.11	130.29
163	QO	500	GDP	C6-C5-N7	3.20	136.11	130.29
165	OD	503	GTP	N9-C4-N3	3.20	132.34	125.95
163	LE	500	GDP	C6-C5-N7	3.19	136.10	130.29
165	UC	501	GTP	N9-C4-N3	3.19	132.34	125.95
165	EU	501	GTP	N9-C4-N3	3.19	132.34	125.95
163	CM	500	GDP	C6-C5-N7	3.19	136.10	130.29
163	ST	500	GDP	C6-C5-N7	3.19	136.10	130.29
165	EM	501	GTP	N9-C4-N3	3.19	132.34	125.95
163	QC	500	GDP	C6-C5-N7	3.19	136.10	130.29
165	AW	501	GTP	N9-C4-N3	3.19	132.34	125.95
163	LQ	500	GDP	C6-C5-N7	3.19	136.10	130.29
165	PM	501	GTP	N9-C4-N3	3.19	132.34	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	UU	501	GTP	N9-C4-N3	3.19	132.34	125.95
163	CW	500	GDP	C6-C5-N7	3.19	136.10	130.29
165	KR	501	GTP	N9-C4-N3	3.19	132.33	125.95
165	PW	501	GTP	N9-C4-N3	3.19	132.33	125.95
165	HI	501	GTP	N9-C4-N3	3.19	132.33	125.95
165	UI	501	GTP	N9-C4-N3	3.19	132.33	125.95
163	KU	500	GDP	C6-C5-N7	3.19	136.09	130.29
163	ML	500	GDP	C6-C5-N7	3.19	136.09	130.29
165	BA	501	GTP	N9-C4-N3	3.19	132.32	125.95
165	TS	501	GTP	N9-C4-N3	3.19	132.32	125.95
165	HS	501	GTP	N9-C4-N3	3.18	132.32	125.95
165	MM	501	GTP	N9-C4-N3	3.18	132.32	125.95
165	BQ	501	GTP	N9-C4-N3	3.18	132.32	125.95
165	WQ	501	GTP	N9-C4-N3	3.18	132.32	125.95
165	FJ	503	GTP	N9-C4-N3	3.18	132.32	125.95
165	L	501	GTP	N9-C4-N3	3.18	132.32	125.95
165	WE	501	GTP	N9-C4-N3	3.18	132.31	125.95
165	CV	501	GTP	C2-N1-C6	-3.18	119.34	125.11
165	VY	501	GTP	N9-C4-N3	3.18	132.31	125.95
163	GN	500	GDP	C6-C5-N7	3.18	136.08	130.29
165	UO	501	GTP	N9-C4-N3	3.18	132.31	125.95
165	DD	501	GTP	C2-N1-C6	-3.18	119.35	125.11
165	HG	501	GTP	N9-C4-N3	3.18	132.31	125.95
165	WS	501	GTP	N9-C4-N3	3.18	132.30	125.95
165	US	501	GTP	N9-C4-N3	3.18	132.30	125.95
165	MA	501	GTP	N9-C4-N3	3.17	132.30	125.95
163	RQ	500	GDP	C6-C5-N7	3.17	136.06	130.29
165	JV	501	GTP	N9-C4-N3	3.17	132.30	125.95
165	GQ	501	GTP	C2-N1-C6	-3.17	119.36	125.11
163	RW	500	GDP	C6-C5-N7	3.17	136.06	130.29
163	OL	500	GDP	C6-C5-N7	3.17	136.06	130.29
163	QW	500	GDP	C6-C5-N7	3.17	136.06	130.29
163	RU	500	GDP	C6-C5-N7	3.17	136.06	130.29
165	OU	501	GTP	N9-C4-N3	3.17	132.29	125.95
163	RI	500	GDP	C6-C5-N7	3.17	136.06	130.29
165	FE	501	GTP	N9-C4-N3	3.17	132.29	125.95
165	QB	501	GTP	N9-C4-N3	3.17	132.29	125.95
163	FL	500	GDP	C6-C5-N7	3.17	136.05	130.29
165	UE	501	GTP	N9-C4-N3	3.17	132.28	125.95
165	PK	501	GTP	N9-C4-N3	3.16	132.28	125.95
165	KV	501	GTP	N9-C4-N3	3.16	132.28	125.95
165	WA	501	GTP	N9-C4-N3	3.16	132.28	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	MY	501	GTP	N9-C4-N3	3.16	132.28	125.95
163	OX	500	GDP	C6-C5-N7	3.16	136.04	130.29
165	FV	503	GTP	N9-C4-N3	3.16	132.28	125.95
163	NH	500	GDP	C6-C5-N7	3.16	136.04	130.29
165	NA	501	GTP	N9-C4-N3	3.16	132.27	125.95
165	FG	501	GTP	N9-C4-N3	3.16	132.27	125.95
165	ES	501	GTP	N9-C4-N3	3.16	132.27	125.95
163	WH	500	GDP	C6-C5-N7	3.16	136.04	130.29
165	OG	501	GTP	N9-C4-N3	3.16	132.27	125.95
165	RT	501	GTP	N9-C4-N3	3.16	132.27	125.95
165	WO	501	GTP	N9-C4-N3	3.16	132.26	125.95
163	QM	500	GDP	C6-C5-N7	3.16	136.03	130.29
165	DP	501	GTP	C2-N1-C6	-3.16	119.39	125.11
163	QA	500	GDP	C6-C5-N7	3.16	136.03	130.29
165	OI	501	GTP	N9-C4-N3	3.16	132.26	125.95
163	DK	501	GDP	C6-C5-N7	3.16	136.03	130.29
165	FC	501	GTP	N9-C4-N3	3.15	132.26	125.95
163	RK	500	GDP	C6-C5-N7	3.15	136.03	130.29
165	PA	501	GTP	N9-C4-N3	3.15	132.26	125.95
165	RO	501	GTP	N9-C4-N3	3.15	132.26	125.95
163	GB	500	GDP	C6-C5-N7	3.15	136.03	130.29
165	RV	501	GTP	N9-C4-N3	3.15	132.26	125.95
165	WG	501	GTP	N9-C4-N3	3.15	132.25	125.95
165	MS	501	GTP	N9-C4-N3	3.15	132.25	125.95
165	OA	501	GTP	N9-C4-N3	3.15	132.25	125.95
165	RF	501	GTP	N9-C4-N3	3.15	132.25	125.95
165	UG	501	GTP	N9-C4-N3	3.15	132.25	125.95
165	EG	501	GTP	N9-C4-N3	3.15	132.25	125.95
165	QN	501	GTP	N9-C4-N3	3.15	132.25	125.95
165	LF	502	GTP	N9-C4-N3	3.15	132.25	125.95
165	OP	503	GTP	N9-C4-N3	3.15	132.25	125.95
165	VM	501	GTP	N9-C4-N3	3.14	132.24	125.95
165	FA	501	GTP	N9-C4-N3	3.14	132.24	125.95
165	RR	501	GTP	N9-C4-N3	3.14	132.24	125.95
165	MG	501	GTP	N9-C4-N3	3.14	132.24	125.95
165	WC	501	GTP	N9-C4-N3	3.14	132.24	125.95
165	FI	501	GTP	N9-C4-N3	3.14	132.23	125.95
165	LJ	501	GTP	N9-C4-N3	3.14	132.23	125.95
163	QK	500	GDP	C6-C5-N7	3.14	136.00	130.29
165	LX	501	GTP	N9-C4-N3	3.14	132.23	125.95
163	F	500	GDP	C6-C5-N7	3.14	136.00	130.29
163	ND	500	GDP	C6-C5-N7	3.14	136.00	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	AS	501	GTP	N9-C4-N3	3.14	132.22	125.95
163	BX	500	GDP	C6-C5-N7	3.14	136.00	130.29
165	OM	501	GTP	N9-C4-N3	3.14	132.22	125.95
165	RH	501	GTP	N9-C4-N3	3.13	132.22	125.95
165	RL	501	GTP	N9-C4-N3	3.13	132.22	125.95
165	PE	501	GTP	N9-C4-N3	3.13	132.22	125.95
165	LL	501	GTP	N9-C4-N3	3.13	132.22	125.95
165	EP	501	GTP	N9-C4-N3	3.13	132.22	125.95
165	UQ	501	GTP	N9-C4-N3	3.13	132.21	125.95
165	GS	501	GTP	N9-C4-N3	3.13	132.21	125.95
165	FT	503	GTP	C2-N1-C6	-3.13	119.44	125.11
165	PQ	501	GTP	N9-C4-N3	3.13	132.21	125.95
163	NP	500	GDP	C6-C5-N7	3.13	135.98	130.29
165	EC	501	GTP	N9-C4-N3	3.13	132.21	125.95
165	JB	501	GTP	N9-C4-N3	3.13	132.21	125.95
165	GG	501	GTP	N9-C4-N3	3.13	132.20	125.95
163	GX	500	GDP	C6-C5-N7	3.13	135.98	130.29
165	NW	501	GTP	N9-C4-N3	3.13	132.20	125.95
165	LR	502	GTP	N9-C4-N3	3.12	132.20	125.95
165	KJ	501	GTP	N9-C4-N3	3.12	132.20	125.95
165	BE	501	GTP	N9-C4-N3	3.12	132.20	125.95
163	CK	501	GDP	C6-C5-N7	3.12	135.97	130.29
163	CY	500	GDP	C6-C5-N7	3.12	135.97	130.29
163	WT	500	GDP	C6-C5-N7	3.12	135.97	130.29
165	PC	501	GTP	N9-C4-N3	3.12	132.19	125.95
165	SM	501	GTP	N9-C4-N3	3.12	132.19	125.95
165	CB	501	GTP	C2-N1-C6	-3.12	119.46	125.11
165	GE	501	GTP	N9-C4-N3	3.11	132.18	125.95
165	TO	501	GTP	N9-C4-N3	3.11	132.17	125.95
165	EM	501	GTP	C2-N1-C6	-3.11	119.47	125.11
165	FS	501	GTP	N9-C4-N3	3.11	132.17	125.95
165	RX	501	GTP	N9-C4-N3	3.11	132.17	125.95
165	FO	501	GTP	N9-C4-N3	3.11	132.17	125.95
165	QO	501	GTP	N9-C4-N3	3.11	132.17	125.95
165	CH	501	GTP	C2-N1-C6	-3.11	119.47	125.11
165	NK	501	GTP	N9-C4-N3	3.11	132.16	125.95
165	LB	501	GTP	N9-C4-N3	3.11	132.16	125.95
163	OB	500	GDP	C6-C5-N7	3.11	135.94	130.29
165	LV	501	GTP	N9-C4-N3	3.10	132.16	125.95
165	EU	501	GTP	C2-N1-C6	-3.10	119.48	125.11
165	QC	501	GTP	N9-C4-N3	3.10	132.16	125.95
165	UK	501	GTP	N9-C4-N3	3.10	132.16	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	DV	501	GTP	N9-C4-N3	3.10	132.16	125.95
165	RB	501	GTP	N9-C4-N3	3.10	132.15	125.95
165	CJ	501	GTP	N9-C4-N3	3.10	132.15	125.95
165	MJ	501	GTP	N9-C4-N3	3.10	132.15	125.95
165	AU	501	GTP	N9-C4-N3	3.10	132.15	125.95
165	GI	501	GTP	C2-N1-C6	-3.10	119.49	125.11
165	PO	501	GTP	N9-C4-N3	3.10	132.15	125.95
165	DH	501	GTP	N9-C4-N3	3.10	132.15	125.95
165	OS	501	GTP	N9-C4-N3	3.10	132.15	125.95
165	DE	501	GTP	C2-N1-C6	-3.10	119.49	125.11
165	UW	501	GTP	N9-C4-N3	3.10	132.15	125.95
165	OY	501	GTP	N9-C4-N3	3.09	132.14	125.95
165	ES	501	GTP	C2-N1-C6	-3.09	119.50	125.11
165	RJ	501	GTP	N9-C4-N3	3.09	132.14	125.95
165	SA	501	GTP	N9-C4-N3	3.09	132.14	125.95
163	ON	500	GDP	C6-C5-N7	3.09	135.92	130.29
165	DB	501	GTP	C2-N1-C6	-3.09	119.51	125.11
165	DX	501	GTP	C2-N1-C6	-3.09	119.51	125.11
165	MO	501	GTP	N9-C4-N3	3.09	132.13	125.95
165	IA	501	GTP	C2-N1-C6	-3.09	119.51	125.11
165	SQ	501	GTP	N9-C4-N3	3.09	132.12	125.95
165	BS	501	GTP	N9-C4-N3	3.09	132.12	125.95
165	TC	501	GTP	N9-C4-N3	3.08	132.12	125.95
165	WW	501	GTP	N9-C4-N3	3.08	132.12	125.95
165	GW	501	GTP	N9-C4-N3	3.08	132.11	125.95
165	WK	501	GTP	N9-C4-N3	3.08	132.11	125.95
165	RN	501	GTP	N9-C4-N3	3.08	132.11	125.95
165	VW	501	GTP	N9-C4-N3	3.08	132.11	125.95
165	AY	501	GTP	N9-C4-N3	3.08	132.11	125.95
165	MV	501	GTP	N9-C4-N3	3.08	132.10	125.95
165	HA	501	GTP	N9-C4-N3	3.08	132.10	125.95
165	DT	501	GTP	C2-N1-C6	-3.08	119.53	125.11
165	EC	501	GTP	C2-N1-C6	-3.07	119.54	125.11
165	TW	501	GTP	N9-C4-N3	3.07	132.10	125.95
165	VK	501	GTP	N9-C4-N3	3.07	132.09	125.95
165	DN	501	GTP	C2-N1-C6	-3.07	119.54	125.11
165	MC	501	GTP	N9-C4-N3	3.06	132.08	125.95
165	EI	501	GTP	C2-N1-C6	-3.06	119.55	125.11
165	BI	501	GTP	C2-N1-C6	-3.06	119.56	125.11
165	WU	501	GTP	N9-C4-N3	3.06	132.07	125.95
165	TK	501	GTP	N9-C4-N3	3.06	132.07	125.95
165	MU	501	GTP	N9-C4-N3	3.06	132.07	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	LN	502	GTP	N9-C4-N3	3.06	132.07	125.95
165	SE	501	GTP	N9-C4-N3	3.06	132.07	125.95
165	CK	503	GTP	C2-N1-C6	-3.06	119.56	125.11
165	GL	501	GTP	N9-C4-N3	3.06	132.07	125.95
165	MI	501	GTP	N9-C4-N3	3.06	132.07	125.95
165	CV	501	GTP	N9-C4-N3	3.06	132.07	125.95
165	HW	501	GTP	C2-N1-C6	-3.06	119.57	125.11
165	WI	501	GTP	N9-C4-N3	3.06	132.06	125.95
165	LZ	502	GTP	N9-C4-N3	3.06	132.06	125.95
163	E	500	GDP	C4-C5-N7	-3.06	105.83	110.67
165	CE	501	GTP	N9-C4-N3	3.05	132.06	125.95
165	IC	501	GTP	C2-N1-C6	-3.05	119.57	125.11
165	PU	501	GTP	N9-C4-N3	3.05	132.06	125.95
165	BU	501	GTP	C2-N1-C6	-3.05	119.58	125.11
165	EO	501	GTP	C2-N1-C6	-3.05	119.58	125.11
165	CW	501	GTP	C2-N1-C6	-3.05	119.58	125.11
165	CO	501	GTP	N9-C4-N3	3.05	132.04	125.95
165	D	501	GTP	C2-N1-C6	-3.04	119.59	125.11
165	FS	501	GTP	C2-N1-C6	-3.04	119.60	125.11
165	LF	502	GTP	C2-N1-C6	-3.04	119.60	125.11
165	PI	501	GTP	N9-C4-N3	3.04	132.03	125.95
165	AK	501	GTP	C2-N1-C6	-3.04	119.60	125.11
165	PS	501	GTP	N9-C4-N3	3.03	132.02	125.95
165	IO	501	GTP	C2-N1-C6	-3.03	119.61	125.11
165	FA	501	GTP	C2-N1-C6	-3.03	119.61	125.11
165	AP	501	GTP	C2-N1-C6	-3.03	119.61	125.11
165	QN	501	GTP	C2-N1-C6	-3.03	119.61	125.11
165	C	501	GTP	C2-N1-C6	-3.03	119.61	125.11
165	HK	501	GTP	C2-N1-C6	-3.03	119.62	125.11
165	AO	501	GTP	N9-C4-N3	3.03	132.01	125.95
163	EX	500	GDP	C4-C5-N7	-3.03	105.87	110.67
165	AA	501	GTP	N9-C4-N3	3.03	132.01	125.95
165	AY	501	GTP	C2-N1-C6	-3.02	119.62	125.11
165	WM	501	GTP	C2-N1-C6	-3.02	119.63	125.11
165	CO	501	GTP	C2-N1-C6	-3.02	119.63	125.11
165	ED	501	GTP	N9-C4-N3	3.02	132.00	125.95
165	PA	501	GTP	C2-N1-C6	-3.02	119.63	125.11
165	DQ	501	GTP	C2-N1-C6	-3.02	119.63	125.11
165	QB	501	GTP	C2-N1-C6	-3.02	119.63	125.11
165	LH	501	GTP	C2-N1-C6	-3.02	119.63	125.11
165	BK	501	GTP	N9-C4-N3	3.02	131.99	125.95
165	WY	501	GTP	C2-N1-C6	-3.02	119.64	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	FQ	501	GTP	C2-N1-C6	-3.02	119.64	125.11
165	EG	501	GTP	C2-N1-C6	-3.02	119.64	125.11
165	FV	503	GTP	C2-N1-C6	-3.01	119.64	125.11
165	PW	501	GTP	C2-N1-C6	-3.01	119.65	125.11
165	PK	501	GTP	C2-N1-C6	-3.01	119.65	125.11
165	DV	501	GTP	C2-N1-C6	-3.01	119.65	125.11
165	AS	501	GTP	C2-N1-C6	-3.01	119.66	125.11
165	TQ	501	GTP	C2-N1-C6	-3.01	119.66	125.11
165	GU	501	GTP	C2-N1-C6	-3.01	119.66	125.11
165	LR	502	GTP	C2-N1-C6	-3.01	119.66	125.11
165	AG	501	GTP	C2-N1-C6	-3.01	119.66	125.11
165	CT	501	GTP	C2-N1-C6	-3.01	119.66	125.11
165	LP	502	GTP	N9-C4-N3	3.01	131.96	125.95
165	BQ	501	GTP	C2-N1-C6	-3.01	119.66	125.11
165	EO	501	GTP	N9-C4-N3	3.01	131.96	125.95
165	BO	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	JH	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	NU	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	FM	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	AM	501	GTP	N9-C4-N3	3.00	131.95	125.95
165	GE	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	LT	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	BA	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	NR	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	TE	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	LD	502	GTP	N9-C4-N3	3.00	131.95	125.95
165	OO	501	GTP	N9-C4-N3	3.00	131.95	125.95
165	CJ	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	SQ	501	GTP	C2-N1-C6	-3.00	119.67	125.11
165	GK	501	GTP	C2-N1-C6	-3.00	119.68	125.11
165	FC	501	GTP	C2-N1-C6	-3.00	119.68	125.11
165	PG	501	GTP	N9-C4-N3	2.99	131.94	125.95
165	BE	501	GTP	C2-N1-C6	-2.99	119.68	125.11
165	QO	501	GTP	C2-N1-C6	-2.99	119.68	125.11
165	JW	501	GTP	N9-C4-N3	2.99	131.94	125.95
165	QU	501	GTP	C2-N1-C6	-2.99	119.69	125.11
165	SU	501	GTP	C2-N1-C6	-2.99	119.69	125.11
165	KB	502	GTP	C2-N1-C6	-2.99	119.69	125.11
165	RJ	501	GTP	C2-N1-C6	-2.99	119.69	125.11
165	LB	501	GTP	C2-N1-C6	-2.99	119.69	125.11
165	OW	501	GTP	C2-N1-C6	-2.99	119.69	125.11
165	NQ	501	GTP	C2-N1-C6	-2.99	119.69	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	JK	501	GTP	N9-C4-N3	2.99	131.93	125.95
165	GO	501	GTP	C2-N1-C6	-2.99	119.69	125.11
165	KT	501	GTP	C2-N1-C6	-2.99	119.69	125.11
165	LZ	502	GTP	C2-N1-C6	-2.99	119.69	125.11
165	VO	501	GTP	C2-N1-C6	-2.99	119.70	125.11
165	GO	501	GTP	N9-C4-N3	2.98	131.92	125.95
165	BG	501	GTP	C2-N1-C6	-2.98	119.70	125.11
165	EJ	501	GTP	C2-N1-C6	-2.98	119.70	125.11
165	OC	501	GTP	N9-C4-N3	2.98	131.92	125.95
165	JD	501	GTP	C2-N1-C6	-2.98	119.70	125.11
165	RV	501	GTP	C2-N1-C6	-2.98	119.70	125.11
165	SE	501	GTP	C2-N1-C6	-2.98	119.70	125.11
165	PI	501	GTP	C2-N1-C6	-2.98	119.70	125.11
165	RN	501	GTP	C2-N1-C6	-2.98	119.70	125.11
165	AI	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	AO	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	FO	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	OU	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	OY	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	VT	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	SI	501	GTP	N9-C4-N3	2.98	131.91	125.95
165	NA	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	EP	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	NM	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	QC	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	QH	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	UA	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	IY	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	TU	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	BW	501	GTP	N9-C4-N3	2.98	131.91	125.95
165	MQ	501	GTP	N9-C4-N3	2.98	131.91	125.95
165	MA	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	OC	501	GTP	C2-N1-C6	-2.98	119.71	125.11
165	FG	501	GTP	C2-N1-C6	-2.98	119.72	125.11
165	ME	501	GTP	N9-C4-N3	2.97	131.90	125.95
165	II	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	KP	502	GTP	C2-N1-C6	-2.97	119.72	125.11
165	IG	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	NI	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	NY	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	OG	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	DX	501	GTP	N9-C4-N3	2.97	131.90	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	JJ	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	LN	502	GTP	C2-N1-C6	-2.97	119.72	125.11
165	MM	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	TI	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	QT	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	OO	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	KD	502	GTP	C2-N1-C6	-2.97	119.72	125.11
165	VG	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	JV	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	KX	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	QF	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	AD	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	CQ	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	MY	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	VS	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	NF	501	GTP	C2-N1-C6	-2.97	119.72	125.11
165	UU	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	PC	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	NO	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	WU	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	AM	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	CE	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	VM	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	UM	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	KF	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	L	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	SU	501	GTP	N9-C4-N3	2.97	131.88	125.95
165	FI	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	KL	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	LX	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	AG	501	GTP	N9-C4-N3	2.97	131.88	125.95
165	J	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	KH	501	GTP	C2-N1-C6	-2.97	119.73	125.11
165	TG	501	GTP	C2-N1-C6	-2.96	119.73	125.11
165	HB	503	GTP	C2-N1-C6	-2.96	119.73	125.11
165	IQ	501	GTP	C2-N1-C6	-2.96	119.73	125.11
163	A	501	GDP	C6-C5-N7	2.96	135.68	130.29
165	R	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	QL	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	VW	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	QX	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	UC	501	GTP	C2-N1-C6	-2.96	119.74	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	CN	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	JP	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	PQ	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	OK	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	JR	501	GTP	C2-N1-C6	-2.96	119.74	125.11
165	RB	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	KZ	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	QR	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	SS	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	AA	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	AU	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	AW	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	IS	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	RR	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	IE	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	SG	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	VC	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	RT	501	GTP	C2-N1-C6	-2.96	119.75	125.11
165	Q	501	GTP	C2-N1-C6	-2.95	119.75	125.11
165	BY	501	GTP	C2-N1-C6	-2.95	119.75	125.11
165	OP	503	GTP	C2-N1-C6	-2.95	119.75	125.11
165	CN	501	GTP	N9-C4-N3	2.95	131.86	125.95
165	OI	501	GTP	C2-N1-C6	-2.95	119.75	125.11
165	WI	501	GTP	C2-N1-C6	-2.95	119.75	125.11
165	OD	503	GTP	C2-N1-C6	-2.95	119.75	125.11
165	UI	501	GTP	C2-N1-C6	-2.95	119.75	125.11
165	PU	501	GTP	C2-N1-C6	-2.95	119.75	125.11
165	QI	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	SI	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	NC	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	TK	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	UG	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	VH	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	PO	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	JZ	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	KR	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	TW	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	IM	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	K	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	MJ	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	JT	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	BY	501	GTP	N9-C4-N3	2.95	131.85	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	VA	501	GTP	C2-N1-C6	-2.95	119.76	125.11
165	NE	501	GTP	C2-N1-C6	-2.95	119.77	125.11
165	JN	501	GTP	C2-N1-C6	-2.95	119.77	125.11
165	IU	501	GTP	C2-N1-C6	-2.95	119.77	125.11
165	TS	501	GTP	C2-N1-C6	-2.95	119.77	125.11
165	OA	501	GTP	C2-N1-C6	-2.95	119.77	125.11
165	VY	501	GTP	C2-N1-C6	-2.95	119.77	125.11
165	CQ	501	GTP	N9-C4-N3	2.94	131.84	125.95
165	JF	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	HG	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	WA	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	WG	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	AB	501	GTP	N9-C4-N3	2.94	131.83	125.95
165	WE	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	PG	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	OM	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	HS	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	RH	501	GTP	C2-N1-C6	-2.94	119.78	125.11
165	GG	501	GTP	C2-N1-C6	-2.94	119.79	125.11
165	SO	501	GTP	C2-N1-C6	-2.94	119.79	125.11
165	CC	501	GTP	N9-C4-N3	2.94	131.82	125.95
165	MI	501	GTP	C2-N1-C6	-2.94	119.79	125.11
165	GW	501	GTP	C2-N1-C6	-2.94	119.79	125.11
165	OS	501	GTP	C2-N1-C6	-2.93	119.79	125.11
165	MV	501	GTP	C2-N1-C6	-2.93	119.79	125.11
165	WW	501	GTP	C2-N1-C6	-2.93	119.79	125.11
165	JD	501	GTP	N9-C4-N3	2.93	131.82	125.95
165	CW	501	GTP	N9-C4-N3	2.93	131.82	125.95
165	ED	501	GTP	C2-N1-C6	-2.93	119.79	125.11
165	RF	501	GTP	C2-N1-C6	-2.93	119.79	125.11
165	PE	501	GTP	C2-N1-C6	-2.93	119.79	125.11
165	DD	501	GTP	N9-C4-N3	2.93	131.82	125.95
165	BK	501	GTP	C2-N1-C6	-2.93	119.79	125.11
165	JK	501	GTP	C2-N1-C6	-2.93	119.80	125.11
165	WS	501	GTP	C2-N1-C6	-2.93	119.80	125.11
165	WO	501	GTP	C2-N1-C6	-2.93	119.80	125.11
165	VK	501	GTP	C2-N1-C6	-2.93	119.80	125.11
165	JP	501	GTP	N9-C4-N3	2.93	131.81	125.95
165	LD	502	GTP	C2-N1-C6	-2.93	119.80	125.11
165	LP	502	GTP	C2-N1-C6	-2.93	119.80	125.11
165	KN	502	GTP	C2-N1-C6	-2.93	119.80	125.11
165	NK	501	GTP	C2-N1-C6	-2.93	119.80	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	BM	501	GTP	N9-C8-N7	-2.92	107.98	113.40
165	UQ	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	BW	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	HE	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	SK	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	BM	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	VE	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	WC	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	UW	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	PY	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	MC	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	ME	501	GTP	C2-N1-C6	-2.92	119.81	125.11
165	PS	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	LL	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	MG	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	SM	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	SC	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	UO	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	GC	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	UK	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	SW	501	GTP	C2-N1-C6	-2.92	119.82	125.11
165	MO	501	GTP	C2-N1-C6	-2.91	119.83	125.11
165	PM	501	GTP	C2-N1-C6	-2.91	119.83	125.11
165	CC	501	GTP	C2-N1-C6	-2.91	119.83	125.11
165	MQ	501	GTP	C2-N1-C6	-2.91	119.83	125.11
165	MU	501	GTP	C2-N1-C6	-2.91	119.83	125.11
165	RC	501	GTP	C2-N1-C6	-2.91	119.84	125.11
165	HN	503	GTP	C2-N1-C6	-2.91	119.84	125.11
165	UE	501	GTP	C2-N1-C6	-2.91	119.84	125.11
165	RO	501	GTP	C2-N1-C6	-2.91	119.84	125.11
165	JB	501	GTP	C2-N1-C6	-2.91	119.84	125.11
165	WK	501	GTP	C2-N1-C6	-2.90	119.84	125.11
165	JW	501	GTP	C2-N1-C6	-2.90	119.84	125.11
165	EV	501	GTP	C2-N1-C6	-2.90	119.85	125.11
165	WQ	501	GTP	C2-N1-C6	-2.90	119.85	125.11
165	NW	501	GTP	C2-N1-C6	-2.90	119.85	125.11
165	KV	501	GTP	C2-N1-C6	-2.90	119.86	125.11
165	SA	501	GTP	C2-N1-C6	-2.89	119.86	125.11
165	GL	501	GTP	C2-N1-C6	-2.89	119.86	125.11
165	VQ	501	GTP	C2-N1-C6	-2.89	119.87	125.11
165	GS	501	GTP	C2-N1-C6	-2.89	119.88	125.11
165	US	501	GTP	C2-N1-C6	-2.89	119.88	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	FJ	503	GTP	C2-N1-C6	-2.88	119.88	125.11
165	HQ	501	GTP	C2-N1-C6	-2.88	119.88	125.11
165	TC	501	GTP	C2-N1-C6	-2.88	119.89	125.11
165	ED	501	GTP	N9-C8-N7	-2.88	108.06	113.40
165	AK	501	GTP	N9-C8-N7	-2.88	108.06	113.40
165	KJ	501	GTP	C2-N1-C6	-2.88	119.89	125.11
165	BO	501	GTP	N9-C4-N3	2.88	131.71	125.95
165	DH	501	GTP	C2-N1-C6	-2.87	119.90	125.11
165	MS	501	GTP	C2-N1-C6	-2.87	119.90	125.11
165	BS	501	GTP	C2-N1-C6	-2.87	119.90	125.11
165	D	501	GTP	N9-C8-N7	-2.87	108.08	113.40
165	T	503	GTP	C2-N1-C6	-2.87	119.91	125.11
165	AP	501	GTP	N9-C8-N7	-2.87	108.08	113.40
165	TO	501	GTP	C2-N1-C6	-2.87	119.92	125.11
165	LV	501	GTP	C2-N1-C6	-2.86	119.92	125.11
165	RL	501	GTP	C2-N1-C6	-2.86	119.92	125.11
165	DX	501	GTP	N9-C8-N7	-2.86	108.09	113.40
165	HI	501	GTP	C2-N1-C6	-2.86	119.92	125.11
165	LJ	501	GTP	C2-N1-C6	-2.86	119.92	125.11
165	GK	501	GTP	N9-C8-N7	-2.86	108.10	113.40
165	RX	501	GTP	C2-N1-C6	-2.85	119.94	125.11
165	HM	501	GTP	C2-N1-C6	-2.85	119.94	125.11
165	HU	501	GTP	C2-N1-C6	-2.85	119.94	125.11
165	FM	501	GTP	N9-C4-N3	2.85	131.66	125.95
165	TM	501	GTP	C2-N1-C6	-2.85	119.94	125.11
165	DB	501	GTP	N9-C8-N7	-2.84	108.13	113.40
165	DJ	501	GTP	N9-C8-N7	-2.84	108.13	113.40
165	D	501	GTP	N9-C4-N3	2.84	131.63	125.95
165	DJ	501	GTP	N9-C4-N3	2.84	131.63	125.95
165	HY	501	GTP	C2-N1-C6	-2.83	119.97	125.11
165	ED	501	GTP	O3G-PG-O3B	2.83	114.13	104.64
165	EV	501	GTP	N9-C8-N7	-2.83	108.15	113.40
165	EV	501	GTP	N9-C4-N3	2.83	131.61	125.95
165	BY	501	GTP	N9-C8-N7	-2.83	108.16	113.40
165	GK	501	GTP	N9-C4-N3	2.83	131.60	125.95
165	BK	501	GTP	N9-C8-N7	-2.82	108.17	113.40
165	DL	501	GTP	N9-C8-N7	-2.82	108.17	113.40
165	BM	501	GTP	N9-C4-N3	2.81	131.58	125.95
165	CC	501	GTP	N9-C8-N7	-2.81	108.19	113.40
165	AW	501	GTP	N9-C8-N7	-2.81	108.19	113.40
165	DH	501	GTP	N9-C8-N7	-2.80	108.20	113.40
165	AA	501	GTP	N9-C8-N7	-2.80	108.20	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	DN	501	GTP	N9-C8-N7	-2.80	108.20	113.40
165	CN	501	GTP	N9-C8-N7	-2.80	108.21	113.40
165	BW	501	GTP	N9-C8-N7	-2.80	108.21	113.40
165	GS	501	GTP	N9-C8-N7	-2.80	108.21	113.40
165	DN	501	GTP	N9-C4-N3	2.79	131.54	125.95
165	G	501	GTP	N9-C4-N3	2.79	131.53	125.95
165	EU	501	GTP	N9-C8-N7	-2.79	108.23	113.40
163	DE	500	GDP	C4-C5-N7	-2.78	106.27	110.67
165	FE	501	GTP	C2-N1-C6	-2.78	120.07	125.11
165	FV	503	GTP	N9-C8-N7	-2.78	108.25	113.40
165	DP	501	GTP	N9-C8-N7	-2.77	108.25	113.40
165	AM	501	GTP	N9-C8-N7	-2.77	108.26	113.40
165	AB	501	GTP	C2-N1-C6	-2.77	120.08	125.11
165	DD	501	GTP	N9-C8-N7	-2.77	108.26	113.40
165	MQ	501	GTP	N9-C8-N7	-2.77	108.26	113.40
165	CV	501	GTP	N9-C8-N7	-2.77	108.26	113.40
165	GC	501	GTP	N9-C4-N3	2.77	131.49	125.95
165	FO	501	GTP	N9-C8-N7	-2.77	108.27	113.40
165	CQ	501	GTP	N9-C8-N7	-2.77	108.27	113.40
165	HA	501	GTP	C2-N1-C6	-2.76	120.10	125.11
165	SI	501	GTP	N9-C8-N7	-2.76	108.28	113.40
165	DE	501	GTP	N9-C8-N7	-2.76	108.28	113.40
165	BO	501	GTP	N9-C8-N7	-2.76	108.28	113.40
165	GC	501	GTP	N9-C8-N7	-2.76	108.28	113.40
165	ME	501	GTP	N9-C8-N7	-2.76	108.28	113.40
165	JP	501	GTP	N9-C8-N7	-2.76	108.29	113.40
165	LP	502	GTP	N9-C8-N7	-2.76	108.29	113.40
165	UO	501	GTP	N9-C8-N7	-2.76	108.29	113.40
165	FC	501	GTP	N9-C8-N7	-2.76	108.29	113.40
165	OA	501	GTP	N9-C8-N7	-2.76	108.29	113.40
165	BE	501	GTP	N9-C8-N7	-2.76	108.29	113.40
165	LD	502	GTP	N9-C8-N7	-2.75	108.29	113.40
165	MI	501	GTP	N9-C8-N7	-2.75	108.30	113.40
165	GW	501	GTP	N9-C8-N7	-2.75	108.30	113.40
165	KP	502	GTP	N9-C8-N7	-2.75	108.30	113.40
165	GG	501	GTP	N9-C8-N7	-2.75	108.31	113.40
165	EM	501	GTP	N9-C8-N7	-2.75	108.31	113.40
165	JD	501	GTP	N9-C8-N7	-2.74	108.31	113.40
165	LX	501	GTP	N9-C8-N7	-2.74	108.31	113.40
165	KD	502	GTP	N9-C8-N7	-2.74	108.32	113.40
165	FT	503	GTP	O3G-PG-O3B	2.74	113.82	104.64
165	UC	501	GTP	N9-C8-N7	-2.74	108.32	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	SU	501	GTP	N9-C8-N7	-2.74	108.32	113.40
165	EO	501	GTP	N9-C8-N7	-2.74	108.32	113.40
165	GO	501	GTP	N9-C8-N7	-2.74	108.33	113.40
165	UU	501	GTP	N9-C8-N7	-2.73	108.33	113.40
165	OO	501	GTP	N9-C8-N7	-2.73	108.33	113.40
165	FJ	503	GTP	N9-C8-N7	-2.73	108.33	113.40
165	FM	501	GTP	N9-C8-N7	-2.73	108.33	113.40
165	CJ	501	GTP	N9-C8-N7	-2.73	108.34	113.40
165	G	501	GTP	N9-C8-N7	-2.73	108.34	113.40
165	RN	501	GTP	N9-C8-N7	-2.73	108.34	113.40
165	GQ	501	GTP	O2A-PA-O3A	2.73	114.65	107.27
165	AO	501	GTP	N9-C8-N7	-2.73	108.34	113.40
165	PY	501	GTP	N9-C8-N7	-2.73	108.35	113.40
165	OC	501	GTP	N9-C8-N7	-2.73	108.35	113.40
163	BP	500	GDP	C4-C5-N7	-2.72	106.36	110.67
165	GE	501	GTP	N9-C8-N7	-2.72	108.36	113.40
165	PM	501	GTP	N9-C8-N7	-2.72	108.36	113.40
165	BA	501	GTP	N9-C8-N7	-2.72	108.36	113.40
165	MU	501	GTP	N9-C8-N7	-2.72	108.36	113.40
165	WI	501	GTP	N9-C8-N7	-2.72	108.36	113.40
165	AD	501	GTP	N9-C8-N7	-2.72	108.36	113.40
165	LL	501	GTP	N9-C8-N7	-2.72	108.36	113.40
165	FQ	501	GTP	N9-C8-N7	-2.72	108.36	113.40
165	UI	501	GTP	N9-C8-N7	-2.71	108.37	113.40
165	DV	501	GTP	N9-C8-N7	-2.71	108.37	113.40
165	IY	501	GTP	N9-C8-N7	-2.71	108.37	113.40
163	DO	500	GDP	C4-C5-N7	-2.71	106.38	110.67
165	PI	501	GTP	N9-C8-N7	-2.71	108.38	113.40
165	FI	501	GTP	N9-C8-N7	-2.71	108.38	113.40
163	DI	500	GDP	C4-C5-N7	-2.71	106.38	110.67
165	IA	501	GTP	N9-C8-N7	-2.71	108.38	113.40
165	LZ	502	GTP	N9-C8-N7	-2.71	108.38	113.40
165	BG	501	GTP	N9-C8-N7	-2.71	108.38	113.40
165	WG	501	GTP	N9-C8-N7	-2.71	108.38	113.40
165	EV	501	GTP	O3G-PG-O3B	2.70	113.70	104.64
165	FA	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	TU	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	PO	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	SQ	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	SA	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	PS	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	AG	501	GTP	N9-C8-N7	-2.70	108.39	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	TC	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	VY	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	WU	501	GTP	N9-C8-N7	-2.70	108.39	113.40
163	DY	500	GDP	C4-C5-N7	-2.70	106.39	110.67
165	BS	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	PQ	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	RR	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	OM	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	PA	501	GTP	N9-C8-N7	-2.70	108.39	113.40
165	L	501	GTP	N9-C8-N7	-2.70	108.40	113.40
165	MG	501	GTP	N9-C8-N7	-2.70	108.40	113.40
165	IW	501	GTP	N9-C8-N7	-2.70	108.40	113.40
165	QU	501	GTP	N9-C8-N7	-2.70	108.40	113.40
165	HM	501	GTP	N9-C8-N7	-2.70	108.40	113.40
163	P	500	GDP	C6-C5-N7	2.70	135.20	130.29
165	SC	501	GTP	N9-C8-N7	-2.70	108.40	113.40
165	NW	501	GTP	N9-C8-N7	-2.70	108.40	113.40
165	MA	501	GTP	N9-C8-N7	-2.69	108.40	113.40
165	EP	501	GTP	N9-C8-N7	-2.69	108.40	113.40
165	OY	501	GTP	N9-C8-N7	-2.69	108.40	113.40
165	EA	501	GTP	C5-C6-N1	2.69	120.11	113.25
165	IK	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	RB	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	CE	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	CO	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	GL	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	DT	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	LV	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	EI	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	KF	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	HA	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	VC	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	RF	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	RJ	501	GTP	N9-C8-N7	-2.69	108.41	113.40
165	PU	501	GTP	N9-C8-N7	-2.69	108.41	113.40
163	TP	500	GDP	C4-C5-N7	-2.69	106.41	110.67
165	OK	501	GTP	N9-C8-N7	-2.69	108.42	113.40
165	QX	501	GTP	N9-C8-N7	-2.69	108.42	113.40
165	LN	502	GTP	N9-C8-N7	-2.69	108.42	113.40
165	PE	501	GTP	N9-C8-N7	-2.69	108.42	113.40
165	SE	501	GTP	N9-C8-N7	-2.69	108.42	113.40
165	DQ	501	GTP	N9-C8-N7	-2.69	108.42	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	GU	501	GTP	N9-C8-N7	-2.69	108.42	113.40
165	AY	501	GTP	N9-C8-N7	-2.69	108.42	113.40
165	BQ	501	GTP	N9-C8-N7	-2.69	108.42	113.40
165	IM	501	GTP	N9-C8-N7	-2.68	108.42	113.40
165	NC	501	GTP	N9-C8-N7	-2.68	108.42	113.40
165	IK	501	GTP	C8-N7-C5	2.68	109.04	104.26
165	PC	501	GTP	N9-C8-N7	-2.68	108.42	113.40
165	LR	502	GTP	N9-C8-N7	-2.68	108.42	113.40
165	AS	501	GTP	N9-C8-N7	-2.68	108.42	113.40
165	QL	501	GTP	N9-C8-N7	-2.68	108.43	113.40
165	QN	501	GTP	N9-C8-N7	-2.68	108.43	113.40
165	RL	501	GTP	N9-C8-N7	-2.68	108.43	113.40
165	NY	501	GTP	N9-C8-N7	-2.68	108.43	113.40
165	JJ	501	GTP	N9-C8-N7	-2.68	108.43	113.40
163	UL	500	GDP	C4-C5-N7	-2.68	106.42	110.67
165	FT	503	GTP	N9-C8-N7	-2.68	108.43	113.40
165	WS	501	GTP	N9-C8-N7	-2.68	108.43	113.40
165	HY	501	GTP	N9-C8-N7	-2.68	108.43	113.40
165	EP	501	GTP	O3G-PG-O3B	2.68	113.62	104.64
165	DB	501	GTP	N9-C4-N3	2.68	131.31	125.95
165	NK	501	GTP	N9-C8-N7	-2.68	108.43	113.40
165	TI	501	GTP	N9-C8-N7	-2.68	108.43	113.40
165	US	501	GTP	N9-C8-N7	-2.68	108.44	113.40
163	CS	500	GDP	C4-C5-N7	-2.68	106.43	110.67
165	LF	502	GTP	N9-C8-N7	-2.68	108.44	113.40
165	T	503	GTP	N9-C8-N7	-2.68	108.44	113.40
165	NM	501	GTP	N9-C8-N7	-2.68	108.44	113.40
165	PG	501	GTP	N9-C8-N7	-2.68	108.44	113.40
165	KZ	501	GTP	N9-C8-N7	-2.68	108.44	113.40
163	CM	500	GDP	C2'-C1'-N9	-2.68	105.80	113.25
163	SL	500	GDP	C4-C5-N7	-2.67	106.43	110.67
165	VM	501	GTP	N9-C8-N7	-2.67	108.44	113.40
165	IW	501	GTP	C8-N7-C5	2.67	109.02	104.26
165	VK	501	GTP	N9-C8-N7	-2.67	108.44	113.40
165	UM	501	GTP	N9-C8-N7	-2.67	108.44	113.40
165	VW	501	GTP	N9-C8-N7	-2.67	108.44	113.40
165	OS	501	GTP	N9-C8-N7	-2.67	108.44	113.40
165	IE	501	GTP	N9-C8-N7	-2.67	108.44	113.40
165	KN	502	GTP	N9-C8-N7	-2.67	108.44	113.40
165	UA	501	GTP	N9-C8-N7	-2.67	108.44	113.40
165	JB	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	MM	501	GTP	N9-C8-N7	-2.67	108.45	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	UG	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	MS	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	QT	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	SM	501	GTP	N9-C8-N7	-2.67	108.45	113.40
163	UX	500	GDP	C4-C5-N7	-2.67	106.44	110.67
165	OG	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	JV	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	QC	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	JN	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	KR	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	EA	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	JH	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	QO	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	EC	501	GTP	N9-C8-N7	-2.67	108.45	113.40
165	EG	501	GTP	N9-C8-N7	-2.67	108.45	113.40
163	IX	501	GDP	C3'-C2'-C1'	2.67	106.51	101.46
165	RT	501	GTP	N9-C8-N7	-2.67	108.46	113.40
165	DJ	501	GTP	C2-N1-C6	-2.66	120.28	125.11
165	QI	501	GTP	N9-C8-N7	-2.66	108.46	113.40
165	WW	501	GTP	N9-C8-N7	-2.66	108.46	113.40
165	OU	501	GTP	N9-C8-N7	-2.66	108.46	113.40
165	TO	501	GTP	N9-C8-N7	-2.66	108.46	113.40
163	KM	500	GDP	C4-C5-N7	-2.66	106.45	110.67
165	EJ	501	GTP	N9-C8-N7	-2.66	108.46	113.40
165	NA	501	GTP	N9-C8-N7	-2.66	108.46	113.40
163	DU	500	GDP	C4-C5-N7	-2.66	106.45	110.67
165	LJ	501	GTP	N9-C8-N7	-2.66	108.47	113.40
165	AI	501	GTP	N9-C8-N7	-2.66	108.47	113.40
165	NO	501	GTP	N9-C8-N7	-2.66	108.47	113.40
165	RX	501	GTP	N9-C8-N7	-2.66	108.47	113.40
165	CV	501	GTP	C5-C6-N1	2.66	120.02	113.25
165	JT	501	GTP	N9-C8-N7	-2.66	108.47	113.40
165	FG	501	GTP	N9-C8-N7	-2.66	108.47	113.40
165	QB	501	GTP	N9-C8-N7	-2.66	108.47	113.40
163	DC	500	GDP	C4-C5-N7	-2.66	106.46	110.67
165	SS	501	GTP	N9-C8-N7	-2.66	108.47	113.40
165	DB	501	GTP	C8-N7-C5	2.66	108.99	104.26
165	SG	501	GTP	N9-C8-N7	-2.66	108.47	113.40
163	DW	501	GDP	C4-C5-N7	-2.66	106.46	110.67
165	OI	501	GTP	N9-C8-N7	-2.66	108.48	113.40
165	FC	501	GTP	O6-C6-C5	-2.66	119.52	126.53
165	QH	501	GTP	N9-C8-N7	-2.66	108.48	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	FS	501	GTP	N9-C8-N7	-2.66	108.48	113.40
165	TM	501	GTP	N9-C8-N7	-2.66	108.48	113.40
165	SW	501	GTP	N9-C8-N7	-2.65	108.48	113.40
165	WC	501	GTP	N9-C8-N7	-2.65	108.48	113.40
165	JZ	501	GTP	N9-C8-N7	-2.65	108.48	113.40
165	AK	501	GTP	C5-C6-N1	2.65	120.00	113.25
165	RV	501	GTP	N9-C8-N7	-2.65	108.48	113.40
165	AB	501	GTP	N9-C8-N7	-2.65	108.48	113.40
165	RH	501	GTP	N9-C8-N7	-2.65	108.48	113.40
163	UF	500	GDP	C4-C5-N7	-2.65	106.47	110.67
165	CB	501	GTP	C5-C6-N1	2.65	120.00	113.25
165	MY	501	GTP	N9-C8-N7	-2.65	108.49	113.40
163	IL	501	GDP	C3'-C2'-C1'	2.65	106.47	101.46
163	NL	500	GDP	C4-C5-N7	-2.65	106.47	110.67
163	S	500	GDP	C4-C5-N7	-2.65	106.48	110.67
163	UR	500	GDP	C4-C5-N7	-2.65	106.48	110.67
165	WY	501	GTP	N9-C8-N7	-2.65	108.50	113.40
165	GQ	501	GTP	C5-C6-N1	2.65	119.99	113.25
165	VO	501	GTP	N9-C8-N7	-2.64	108.50	113.40
163	ER	500	GDP	C4-C5-N7	-2.64	106.48	110.67
165	VA	501	GTP	N9-C8-N7	-2.64	108.50	113.40
165	WO	501	GTP	N9-C8-N7	-2.64	108.50	113.40
165	DL	501	GTP	C5-C6-N1	2.64	119.98	113.25
163	KY	500	GDP	C4-C5-N7	-2.64	106.48	110.67
165	ES	501	GTP	N9-C8-N7	-2.64	108.50	113.40
163	TX	500	GDP	C4-C5-N7	-2.64	106.48	110.67
163	CC	500	GDP	C4-C5-N7	-2.64	106.48	110.67
165	JR	501	GTP	N9-C8-N7	-2.64	108.50	113.40
165	SO	501	GTP	N9-C8-N7	-2.64	108.50	113.40
165	CW	501	GTP	N9-C8-N7	-2.64	108.50	113.40
163	PR	501	GDP	C4-C5-N7	-2.64	106.49	110.67
163	NX	500	GDP	C4-C5-N7	-2.64	106.49	110.67
165	MJ	501	GTP	N9-C8-N7	-2.64	108.51	113.40
165	WE	501	GTP	N9-C8-N7	-2.64	108.51	113.40
163	EL	500	GDP	C4-C5-N7	-2.64	106.49	110.67
163	TD	500	GDP	C4-C5-N7	-2.64	106.49	110.67
165	K	501	GTP	N9-C8-N7	-2.64	108.51	113.40
165	VS	501	GTP	N9-C8-N7	-2.64	108.51	113.40
165	FE	501	GTP	N9-C8-N7	-2.64	108.51	113.40
165	WA	501	GTP	N9-C8-N7	-2.64	108.51	113.40
163	TL	501	GDP	C4-C5-N7	-2.63	106.50	110.67
165	DX	501	GTP	C8-N7-C5	2.63	108.95	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	MO	501	GTP	N9-C8-N7	-2.63	108.52	113.40
165	IW	501	GTP	O2A-PA-O5'	2.63	119.50	107.57
163	VH	500	GDP	C4-C5-N7	-2.63	106.50	110.67
165	DE	501	GTP	C8-N7-C5	2.63	108.95	104.26
165	NF	501	GTP	N9-C8-N7	-2.63	108.52	113.40
165	OW	501	GTP	N9-C8-N7	-2.63	108.52	113.40
163	WL	500	GDP	C4-C5-N7	-2.63	106.50	110.67
165	WM	501	GTP	N9-C8-N7	-2.63	108.52	113.40
165	MV	501	GTP	N9-C8-N7	-2.63	108.52	113.40
165	CB	501	GTP	N9-C8-N7	-2.63	108.52	113.40
165	DD	501	GTP	C5-C6-N1	2.63	119.95	113.25
165	WK	501	GTP	N9-C8-N7	-2.63	108.52	113.40
165	BM	501	GTP	C5-C6-N1	2.63	119.95	113.25
163	HV	500	GDP	C4-C5-N7	-2.63	106.50	110.67
165	OD	503	GTP	N9-C8-N7	-2.63	108.53	113.40
163	PF	501	GDP	C4-C5-N7	-2.63	106.51	110.67
163	GT	501	GDP	C4-C5-N7	-2.63	106.51	110.67
163	JM	501	GDP	C4-C5-N7	-2.63	106.51	110.67
163	PB	500	GDP	C4-C5-N7	-2.63	106.51	110.67
163	UN	500	GDP	C4-C5-N7	-2.63	106.51	110.67
163	OR	500	GDP	C4-C5-N7	-2.63	106.51	110.67
165	IU	501	GTP	N9-C8-N7	-2.63	108.53	113.40
165	JF	501	GTP	N9-C8-N7	-2.63	108.53	113.40
165	IK	501	GTP	O2A-PA-O5'	2.63	119.47	107.57
163	KK	500	GDP	C4-C5-N7	-2.63	106.51	110.67
163	CO	500	GDP	C4-C5-N7	-2.63	106.51	110.67
163	SP	500	GDP	C4-C5-N7	-2.63	106.51	110.67
165	PA	501	GTP	O6-C6-C5	-2.63	119.60	126.53
165	NE	501	GTP	N9-C8-N7	-2.63	108.53	113.40
165	QF	501	GTP	N9-C8-N7	-2.63	108.53	113.40
163	PJ	500	GDP	C4-C5-N7	-2.63	106.51	110.67
163	KA	500	GDP	C4-C5-N7	-2.62	106.51	110.67
163	T	501	GDP	C4-C5-N7	-2.62	106.51	110.67
165	KL	501	GTP	N9-C8-N7	-2.62	108.53	113.40
165	OP	503	GTP	N9-C8-N7	-2.62	108.53	113.40
163	VT	500	GDP	C4-C5-N7	-2.62	106.51	110.67
165	HG	501	GTP	N9-C8-N7	-2.62	108.54	113.40
165	II	501	GTP	N9-C8-N7	-2.62	108.54	113.40
163	WB	500	GDP	C4-C5-N7	-2.62	106.51	110.67
165	KJ	501	GTP	N9-C8-N7	-2.62	108.54	113.40
165	KX	501	GTP	N9-C8-N7	-2.62	108.54	113.40
165	VG	501	GTP	N9-C8-N7	-2.62	108.54	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	JY	501	GDP	C4-C5-N7	-2.62	106.52	110.67
165	EJ	501	GTP	C5-C6-N1	2.62	119.92	113.25
163	QK	500	GDP	C4-C5-N7	-2.62	106.52	110.67
163	UJ	500	GDP	C4-C5-N7	-2.62	106.52	110.67
165	HB	503	GTP	N9-C8-N7	-2.62	108.54	113.40
165	NU	501	GTP	N9-C8-N7	-2.62	108.54	113.40
165	QR	501	GTP	N9-C8-N7	-2.62	108.55	113.40
165	DP	501	GTP	C5-C6-N1	2.62	119.92	113.25
163	CU	500	GDP	C4-C5-N7	-2.62	106.52	110.67
165	AM	501	GTP	C5-C6-N1	2.62	119.91	113.25
165	D	501	GTP	C5-C6-N1	2.62	119.91	113.25
165	G	501	GTP	C2-N1-C6	-2.62	120.37	125.11
165	R	501	GTP	N9-C8-N7	-2.62	108.55	113.40
165	LH	501	GTP	N9-C8-N7	-2.61	108.55	113.40
165	IQ	501	GTP	N9-C8-N7	-2.61	108.55	113.40
165	FT	503	GTP	C5-C6-N1	2.61	119.91	113.25
163	PD	500	GDP	C4-C5-N7	-2.61	106.53	110.67
163	JO	500	GDP	C4-C5-N7	-2.61	106.53	110.67
165	DB	501	GTP	C5-C6-N1	2.61	119.90	113.25
163	QW	500	GDP	C4-C5-N7	-2.61	106.53	110.67
165	SK	501	GTP	N9-C8-N7	-2.61	108.56	113.40
165	PE	501	GTP	C8-N7-C5	2.61	108.91	104.26
165	CC	501	GTP	C5-C6-N1	2.61	119.90	113.25
165	MC	501	GTP	N9-C8-N7	-2.61	108.56	113.40
165	LB	501	GTP	N9-C8-N7	-2.61	108.56	113.40
165	KB	502	GTP	N9-C8-N7	-2.61	108.56	113.40
163	PN	500	GDP	C4-C5-N7	-2.61	106.53	110.67
165	IK	501	GTP	C2-N1-C6	-2.61	120.38	125.11
163	NJ	501	GDP	C4-C5-N7	-2.61	106.54	110.67
163	BV	500	GDP	C4-C5-N7	-2.61	106.54	110.67
165	AU	501	GTP	N9-C8-N7	-2.61	108.56	113.40
165	CQ	501	GTP	C5-C6-N1	2.61	119.89	113.25
163	SB	501	GDP	C4-C5-N7	-2.61	106.54	110.67
163	AX	500	GDP	C4-C5-N7	-2.61	106.54	110.67
165	HS	501	GTP	N9-C8-N7	-2.61	108.56	113.40
165	NR	501	GTP	N9-C8-N7	-2.61	108.57	113.40
163	CM	500	GDP	C4-C5-N7	-2.61	106.54	110.67
165	LH	501	GTP	C5-C6-N1	2.61	119.89	113.25
163	HB	501	GDP	C4-C5-N7	-2.60	106.54	110.67
163	HJ	500	GDP	C4-C5-N7	-2.60	106.54	110.67
163	PX	501	GDP	C4-C5-N7	-2.60	106.54	110.67
165	VT	501	GTP	N9-C8-N7	-2.60	108.57	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	C	501	GTP	O6-C6-C5	-2.60	119.66	126.53
163	WN	500	GDP	C4-C5-N7	-2.60	106.55	110.67
165	DX	501	GTP	C5-C6-N1	2.60	119.88	113.25
165	C	501	GTP	N9-C8-N7	-2.60	108.58	113.40
163	CG	500	GDP	C4-C5-N7	-2.60	106.55	110.67
165	PK	501	GTP	N9-C8-N7	-2.60	108.58	113.40
163	UV	500	GDP	C4-C5-N7	-2.60	106.55	110.67
163	VN	500	GDP	C4-C5-N7	-2.60	106.55	110.67
165	VY	501	GTP	C5-C6-N1	2.60	119.87	113.25
165	DD	501	GTP	C8-N7-C5	2.60	108.89	104.26
165	C	501	GTP	C5-C6-N1	2.60	119.87	113.25
165	VM	501	GTP	C5-C6-N1	2.60	119.87	113.25
165	NQ	501	GTP	N9-C8-N7	-2.60	108.58	113.40
165	IA	501	GTP	C5-C6-N1	2.60	119.86	113.25
163	JC	500	GDP	C4-C5-N7	-2.60	106.55	110.67
163	V	500	GDP	C4-C5-N7	-2.60	106.55	110.67
165	VH	501	GTP	N9-C8-N7	-2.60	108.58	113.40
165	PQ	501	GTP	C8-N7-C5	2.60	108.89	104.26
165	JV	501	GTP	C5-C6-N1	2.60	119.86	113.25
163	TJ	500	GDP	C4-C5-N7	-2.60	106.56	110.67
165	AS	501	GTP	C5-C6-N1	2.60	119.86	113.25
165	VE	501	GTP	N9-C8-N7	-2.59	108.59	113.40
165	PA	501	GTP	C5-C6-N1	2.59	119.86	113.25
163	H	500	GDP	C4-C5-N7	-2.59	106.56	110.67
163	SD	500	GDP	C4-C5-N7	-2.59	106.56	110.67
165	GQ	501	GTP	O6-C6-C5	-2.59	119.69	126.53
165	HQ	501	GTP	N9-C8-N7	-2.59	108.59	113.40
163	EJ	500	GDP	C4-C5-N7	-2.59	106.56	110.67
165	KN	502	GTP	C8-N7-C5	2.59	108.88	104.26
165	OO	501	GTP	C8-N7-C5	2.59	108.88	104.26
165	KV	501	GTP	N9-C8-N7	-2.59	108.59	113.40
165	EI	501	GTP	C5-C6-N1	2.59	119.85	113.25
165	GG	501	GTP	C5-C6-N1	2.59	119.85	113.25
163	PL	501	GDP	C4-C5-N7	-2.59	106.56	110.67
165	DE	501	GTP	C5-C6-N1	2.59	119.85	113.25
165	HW	501	GTP	C5-C6-N1	2.59	119.85	113.25
165	IQ	501	GTP	C5-C6-N1	2.59	119.85	113.25
165	JJ	501	GTP	C5-C6-N1	2.59	119.85	113.25
165	DP	501	GTP	N9-C4-N3	2.59	131.13	125.95
165	VQ	501	GTP	N9-C8-N7	-2.59	108.60	113.40
165	CK	503	GTP	N9-C8-N7	-2.59	108.60	113.40
163	BF	500	GDP	C4-C5-N7	-2.59	106.57	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	UQ	501	GTP	N9-C8-N7	-2.59	108.60	113.40
163	LS	500	GDP	C4-C5-N7	-2.59	106.57	110.67
165	CV	501	GTP	C8-N7-C5	2.59	108.87	104.26
165	NI	501	GTP	N9-C8-N7	-2.59	108.60	113.40
165	EM	501	GTP	C5-C6-N1	2.59	119.84	113.25
163	LG	501	GDP	C4-C5-N7	-2.59	106.57	110.67
165	CT	501	GTP	N9-C8-N7	-2.59	108.60	113.40
165	OW	501	GTP	C5-C6-N1	2.59	119.84	113.25
163	UB	500	GDP	C4-C5-N7	-2.59	106.57	110.67
163	HN	501	GDP	C4-C5-N7	-2.59	106.57	110.67
163	IR	500	GDP	C4-C5-N7	-2.59	106.57	110.67
163	WX	500	GDP	C4-C5-N7	-2.59	106.57	110.67
165	FV	503	GTP	C5-C6-N1	2.59	119.84	113.25
165	FI	501	GTP	C5-C6-N1	2.59	119.84	113.25
165	LT	501	GTP	C5-C6-N1	2.59	119.84	113.25
163	OB	500	GDP	C3'-C2'-C1'	2.59	106.36	101.46
163	VV	500	GDP	C4-C5-N7	-2.59	106.57	110.67
165	IE	501	GTP	C5-C6-N1	2.59	119.83	113.25
163	CE	500	GDP	C4-C5-N7	-2.59	106.57	110.67
163	MB	500	GDP	C4-C5-N7	-2.59	106.57	110.67
163	CW	500	GDP	C4-C5-N7	-2.59	106.57	110.67
163	RQ	500	GDP	C4-C5-N7	-2.59	106.57	110.67
165	PW	501	GTP	N9-C8-N7	-2.58	108.61	113.40
165	D	501	GTP	C8-N7-C5	2.58	108.86	104.26
163	IF	500	GDP	C4-C5-N7	-2.58	106.57	110.67
163	VP	500	GDP	C4-C5-N7	-2.58	106.57	110.67
165	KL	501	GTP	C5-C6-N1	2.58	119.83	113.25
165	EU	501	GTP	C8-N7-C5	2.58	108.86	104.26
163	JA	500	GDP	C4-C5-N7	-2.58	106.58	110.67
165	IC	501	GTP	O6-C6-C5	-2.58	119.71	126.53
165	DN	501	GTP	C8-N7-C5	2.58	108.86	104.26
165	JB	501	GTP	C5-C6-N1	2.58	119.83	113.25
163	CI	500	GDP	C4-C5-N7	-2.58	106.58	110.67
163	G	500	GDP	C4-C5-N7	-2.58	106.58	110.67
163	HP	501	GDP	C4-C5-N7	-2.58	106.58	110.67
165	KZ	501	GTP	C8-N7-C5	2.58	108.86	104.26
165	DN	501	GTP	C5-C6-N1	2.58	119.83	113.25
165	DP	501	GTP	C8-N7-C5	2.58	108.86	104.26
165	ED	501	GTP	C5-C6-N1	2.58	119.82	113.25
163	SN	501	GDP	C4-C5-N7	-2.58	106.58	110.67
165	LT	501	GTP	N9-C8-N7	-2.58	108.61	113.40
165	RO	501	GTP	N9-C8-N7	-2.58	108.61	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	RG	500	GDP	C4-C5-N7	-2.58	106.58	110.67
163	RS	500	GDP	C4-C5-N7	-2.58	106.58	110.67
165	CQ	501	GTP	C8-N7-C5	2.58	108.86	104.26
163	IL	501	GDP	C4-C5-N7	-2.58	106.58	110.67
163	JI	500	GDP	C4-C5-N7	-2.58	106.58	110.67
165	IG	501	GTP	N9-C8-N7	-2.58	108.62	113.40
165	TK	501	GTP	N9-C8-N7	-2.58	108.62	113.40
165	JW	501	GTP	N9-C8-N7	-2.58	108.62	113.40
163	RE	500	GDP	C4-C5-N7	-2.58	106.58	110.67
165	AW	501	GTP	C5-C6-N1	2.58	119.82	113.25
165	EG	501	GTP	O2A-PA-O3A	2.58	114.24	107.27
165	TS	501	GTP	N9-C8-N7	-2.58	108.62	113.40
163	DQ	500	GDP	C4-C5-N7	-2.58	106.58	110.67
165	SU	501	GTP	C5-C6-N1	2.58	119.81	113.25
163	BN	500	GDP	C4-C5-N7	-2.58	106.59	110.67
163	RM	500	GDP	C4-C5-N7	-2.58	106.59	110.67
163	TR	500	GDP	C4-C5-N7	-2.58	106.59	110.67
165	KX	501	GTP	C5-C6-N1	2.58	119.81	113.25
165	OC	501	GTP	C8-N7-C5	2.58	108.85	104.26
165	JK	501	GTP	N9-C8-N7	-2.58	108.62	113.40
165	CO	501	GTP	C5-C6-N1	2.58	119.81	113.25
165	DQ	501	GTP	C5-C6-N1	2.58	119.81	113.25
163	JK	500	GDP	C4-C5-N7	-2.58	106.59	110.67
163	LC	500	GDP	C4-C5-N7	-2.58	106.59	110.67
163	OF	500	GDP	C4-C5-N7	-2.58	106.59	110.67
163	TF	500	GDP	C4-C5-N7	-2.58	106.59	110.67
163	AR	500	GDP	C4-C5-N7	-2.58	106.59	110.67
165	CE	501	GTP	C5-C6-N1	2.58	119.81	113.25
165	GU	501	GTP	C5-C6-N1	2.58	119.81	113.25
163	DA	500	GDP	C4-C5-N7	-2.58	106.59	110.67
165	TW	501	GTP	N9-C8-N7	-2.58	108.62	113.40
165	WG	501	GTP	C5-C6-N1	2.57	119.81	113.25
163	OV	500	GDP	C4-C5-N7	-2.57	106.59	110.67
165	IO	501	GTP	O6-C6-C5	-2.57	119.74	126.53
165	HE	501	GTP	N9-C8-N7	-2.57	108.63	113.40
163	EH	500	GDP	C4-C5-N7	-2.57	106.59	110.67
163	OL	500	GDP	C4-C5-N7	-2.57	106.59	110.67
165	IW	501	GTP	C2-N1-C6	-2.57	120.44	125.11
163	JW	500	GDP	C4-C5-N7	-2.57	106.59	110.67
163	NN	500	GDP	C4-C5-N7	-2.57	106.59	110.67
165	UU	501	GTP	C8-N7-C5	2.57	108.84	104.26
165	HN	503	GTP	N9-C8-N7	-2.57	108.63	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	WS	501	GTP	C5-C6-N1	2.57	119.80	113.25
163	KE	500	GDP	C4-C5-N7	-2.57	106.59	110.67
163	VJ	500	GDP	C4-C5-N7	-2.57	106.59	110.67
163	KS	500	GDP	C4-C5-N7	-2.57	106.59	110.67
163	KW	500	GDP	C4-C5-N7	-2.57	106.59	110.67
165	HK	501	GTP	C5-C6-N1	2.57	119.80	113.25
165	AP	501	GTP	C5-C6-N1	2.57	119.80	113.25
165	IO	501	GTP	C5-C6-N1	2.57	119.80	113.25
165	BW	501	GTP	C8-N7-C5	2.57	108.84	104.26
165	WQ	501	GTP	N9-C8-N7	-2.57	108.63	113.40
163	OJ	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	IV	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	KQ	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	NV	501	GDP	C4-C5-N7	-2.57	106.60	110.67
165	SA	501	GTP	C8-N7-C5	2.57	108.84	104.26
165	CH	501	GTP	C5-C6-N1	2.57	119.80	113.25
165	UW	501	GTP	N9-C8-N7	-2.57	108.63	113.40
163	N	500	GDP	C4-C5-N7	-2.57	106.60	110.67
165	OA	501	GTP	C5-C6-N1	2.57	119.80	113.25
165	SM	501	GTP	C8-N7-C5	2.57	108.84	104.26
165	AY	501	GTP	C5-C6-N1	2.57	119.79	113.25
163	GJ	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	VR	500	GDP	C4-C5-N7	-2.57	106.60	110.67
165	KZ	501	GTP	C5-C6-N1	2.57	119.79	113.25
163	PH	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	IT	501	GDP	C4-C5-N7	-2.57	106.60	110.67
165	BA	501	GTP	O6-C6-C5	-2.57	119.75	126.53
165	TG	501	GTP	N9-C8-N7	-2.57	108.64	113.40
165	JD	501	GTP	C8-N7-C5	2.57	108.83	104.26
163	TH	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	TN	500	GDP	C4-C5-N7	-2.57	106.60	110.67
165	UC	501	GTP	C8-N7-C5	2.57	108.83	104.26
163	NB	500	GDP	C4-C5-N7	-2.57	106.60	110.67
165	JP	501	GTP	C8-N7-C5	2.57	108.83	104.26
163	EV	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	U	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	HR	500	GDP	C4-C5-N7	-2.57	106.60	110.67
163	SR	500	GDP	C4-C5-N7	-2.57	106.60	110.67
165	CE	501	GTP	C8-N7-C5	2.57	108.83	104.26
165	BE	501	GTP	C5-C6-N1	2.57	119.78	113.25
163	BD	500	GDP	C4-C5-N7	-2.57	106.61	110.67
163	SF	500	GDP	C4-C5-N7	-2.57	106.61	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	JU	500	GDP	C4-C5-N7	-2.57	106.61	110.67
163	PV	500	GDP	C4-C5-N7	-2.57	106.61	110.67
163	TV	500	GDP	C4-C5-N7	-2.57	106.61	110.67
163	VX	500	GDP	C4-C5-N7	-2.57	106.61	110.67
163	OP	501	GDP	C4-C5-N7	-2.57	106.61	110.67
165	CK	503	GTP	O6-C6-C5	-2.57	119.76	126.53
165	FJ	503	GTP	C5-C6-N1	2.56	119.78	113.25
165	OK	501	GTP	C5-C6-N1	2.56	119.78	113.25
165	NO	501	GTP	C8-N7-C5	2.56	108.83	104.26
165	WE	501	GTP	C5-C6-N1	2.56	119.78	113.25
165	BW	501	GTP	C5-C6-N1	2.56	119.78	113.25
165	DT	501	GTP	C5-C6-N1	2.56	119.78	113.25
163	ON	500	GDP	C3'-C2'-C1'	2.56	106.31	101.46
165	AU	501	GTP	C5-C6-N1	2.56	119.78	113.25
163	BR	500	GDP	C4-C5-N7	-2.56	106.61	110.67
165	JT	501	GTP	C5-C6-N1	2.56	119.78	113.25
163	W	500	GDP	C4-C5-N7	-2.56	106.61	110.67
163	AH	500	GDP	C4-C5-N7	-2.56	106.61	110.67
163	VB	500	GDP	C4-C5-N7	-2.56	106.61	110.67
163	GV	501	GDP	C4-C5-N7	-2.56	106.61	110.67
163	LU	500	GDP	C4-C5-N7	-2.56	106.61	110.67
165	AD	501	GTP	C5-C6-N1	2.56	119.77	113.25
165	UK	501	GTP	N9-C8-N7	-2.56	108.65	113.40
165	KD	502	GTP	C5-C6-N1	2.56	119.77	113.25
165	CT	501	GTP	C5-C6-N1	2.56	119.77	113.25
163	FF	500	GDP	C4-C5-N7	-2.56	106.61	110.67
165	RJ	501	GTP	C8-N7-C5	2.56	108.82	104.26
165	GE	501	GTP	O6-C6-C5	-2.56	119.77	126.53
165	WI	501	GTP	C8-N7-C5	2.56	108.82	104.26
165	QN	501	GTP	C8-N7-C5	2.56	108.82	104.26
165	OY	501	GTP	C8-N7-C5	2.56	108.82	104.26
163	GR	500	GDP	C4-C5-N7	-2.56	106.61	110.67
163	QU	500	GDP	C4-C5-N7	-2.56	106.61	110.67
165	FC	501	GTP	C5-C6-N1	2.56	119.77	113.25
165	NY	501	GTP	C8-N7-C5	2.56	108.82	104.26
165	KT	501	GTP	N9-C8-N7	-2.56	108.65	113.40
163	KC	500	GDP	C4-C5-N7	-2.56	106.61	110.67
165	RJ	501	GTP	C5-C6-N1	2.56	119.77	113.25
165	BA	501	GTP	C5-C6-N1	2.56	119.77	113.25
165	PQ	501	GTP	C5-C6-N1	2.56	119.77	113.25
163	M	500	GDP	C4-C5-N7	-2.56	106.61	110.67
165	UI	501	GTP	C8-N7-C5	2.56	108.82	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	PO	501	GTP	C8-N7-C5	2.56	108.82	104.26
165	VE	501	GTP	C5-C6-N1	2.56	119.77	113.25
165	VW	501	GTP	C5-C6-N1	2.56	119.77	113.25
163	RA	500	GDP	C4-C5-N7	-2.56	106.62	110.67
163	WF	501	GDP	C4-C5-N7	-2.56	106.62	110.67
165	EM	501	GTP	O6-C6-C5	-2.56	119.78	126.53
165	QU	501	GTP	C5-C6-N1	2.56	119.76	113.25
165	OY	501	GTP	C5-C6-N1	2.56	119.76	113.25
163	HD	501	GDP	C4-C5-N7	-2.56	106.62	110.67
163	VD	500	GDP	C4-C5-N7	-2.56	106.62	110.67
165	RC	501	GTP	N9-C8-N7	-2.56	108.66	113.40
165	UO	501	GTP	C8-N7-C5	2.56	108.81	104.26
165	GI	501	GTP	C5-C6-N1	2.56	119.76	113.25
165	JH	501	GTP	C5-C6-N1	2.56	119.76	113.25
165	QT	501	GTP	C5-C6-N1	2.56	119.76	113.25
163	UH	500	GDP	C4-C5-N7	-2.56	106.62	110.67
163	WR	501	GDP	C4-C5-N7	-2.56	106.62	110.67
165	QH	501	GTP	C5-C6-N1	2.56	119.76	113.25
165	KF	501	GTP	C5-C6-N1	2.56	119.76	113.25
163	BJ	500	GDP	C4-C5-N7	-2.56	106.62	110.67
163	EB	500	GDP	C4-C5-N7	-2.56	106.62	110.67
163	MX	500	GDP	C4-C5-N7	-2.56	106.62	110.67
165	NF	501	GTP	C8-N7-C5	2.56	108.81	104.26
165	CO	501	GTP	C8-N7-C5	2.56	108.81	104.26
165	DV	501	GTP	C5-C6-N1	2.56	119.76	113.25
165	GK	501	GTP	C8-N7-C5	2.55	108.81	104.26
163	MH	500	GDP	C4-C5-N7	-2.55	106.62	110.67
165	AP	501	GTP	C8-N7-C5	2.55	108.81	104.26
165	WU	501	GTP	C5-C6-N1	2.55	119.75	113.25
163	CK	501	GDP	C4-C5-N7	-2.55	106.62	110.67
163	VL	500	GDP	C4-C5-N7	-2.55	106.62	110.67
165	KP	502	GTP	C5-C6-N1	2.55	119.75	113.25
165	CK	503	GTP	C5-C6-N1	2.55	119.75	113.25
165	WQ	501	GTP	C5-C6-N1	2.55	119.75	113.25
165	UE	501	GTP	N9-C8-N7	-2.55	108.67	113.40
165	GQ	501	GTP	N9-C8-N7	-2.55	108.67	113.40
165	KH	501	GTP	N9-C8-N7	-2.55	108.67	113.40
165	UI	501	GTP	C5-C6-N1	2.55	119.75	113.25
165	SU	501	GTP	C8-N7-C5	2.55	108.81	104.26
163	LW	500	GDP	C4-C5-N7	-2.55	106.63	110.67
165	CC	501	GTP	C8-N7-C5	2.55	108.81	104.26
165	EC	501	GTP	C5-C6-N1	2.55	119.75	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	QF	501	GTP	C5-C6-N1	2.55	119.75	113.25
163	AB	500	GDP	C4-C5-N7	-2.55	106.63	110.67
163	ML	500	GDP	C4-C5-N7	-2.55	106.63	110.67
163	NT	500	GDP	C4-C5-N7	-2.55	106.63	110.67
165	TE	501	GTP	C5-C6-N1	2.55	119.74	113.25
165	IO	501	GTP	N9-C8-N7	-2.55	108.67	113.40
165	CJ	501	GTP	C5-C6-N1	2.55	119.74	113.25
165	IC	501	GTP	C5-C6-N1	2.55	119.74	113.25
165	PC	501	GTP	C5-C6-N1	2.55	119.74	113.25
163	JG	500	GDP	C4-C5-N7	-2.55	106.63	110.67
163	PT	500	GDP	C4-C5-N7	-2.55	106.63	110.67
163	OX	500	GDP	C4-C5-N7	-2.55	106.63	110.67
165	BQ	501	GTP	C5-C6-N1	2.55	119.74	113.25
165	EU	501	GTP	C5-C6-N1	2.55	119.74	113.25
163	HF	500	GDP	C4-C5-N7	-2.55	106.63	110.67
165	KD	502	GTP	C8-N7-C5	2.55	108.80	104.26
165	LP	502	GTP	C8-N7-C5	2.55	108.80	104.26
165	HI	501	GTP	N9-C8-N7	-2.55	108.67	113.40
163	ID	500	GDP	C4-C5-N7	-2.55	106.63	110.67
163	QQ	500	GDP	C4-C5-N7	-2.55	106.63	110.67
165	AK	501	GTP	C8-N7-C5	2.55	108.80	104.26
165	LJ	501	GTP	C5-C6-N1	2.55	119.74	113.25
163	MP	500	GDP	C4-C5-N7	-2.55	106.63	110.67
165	OM	501	GTP	C8-N7-C5	2.55	108.80	104.26
163	RC	500	GDP	C4-C5-N7	-2.55	106.63	110.67
163	SJ	501	GDP	C4-C5-N7	-2.55	106.63	110.67
163	MR	500	GDP	C4-C5-N7	-2.55	106.63	110.67
165	RB	501	GTP	C5-C6-N1	2.55	119.74	113.25
165	UC	501	GTP	C5-C6-N1	2.55	119.74	113.25
165	MJ	501	GTP	C5-C6-N1	2.55	119.73	113.25
163	IJ	500	GDP	C4-C5-N7	-2.55	106.64	110.67
165	IS	501	GTP	N9-C8-N7	-2.55	108.68	113.40
165	UU	501	GTP	C5-C6-N1	2.55	119.73	113.25
165	II	501	GTP	C5-C6-N1	2.55	119.73	113.25
165	VK	501	GTP	C5-C6-N1	2.55	119.73	113.25
165	FO	501	GTP	C5-C6-N1	2.55	119.73	113.25
165	IY	501	GTP	C5-C6-N1	2.55	119.73	113.25
163	AD	500	GDP	C4-C5-N7	-2.55	106.64	110.67
165	MI	501	GTP	C8-N7-C5	2.55	108.80	104.26
165	PM	501	GTP	C8-N7-C5	2.55	108.80	104.26
165	SI	501	GTP	C8-N7-C5	2.55	108.80	104.26
165	VS	501	GTP	C5-C6-N1	2.55	119.73	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	NQ	501	GTP	C5-C6-N1	2.55	119.73	113.25
165	EI	501	GTP	C8-N7-C5	2.55	108.79	104.26
165	NM	501	GTP	C8-N7-C5	2.55	108.79	104.26
163	KI	500	GDP	C4-C5-N7	-2.54	106.64	110.67
165	FS	501	GTP	C5-C6-N1	2.54	119.73	113.25
165	LF	502	GTP	C5-C6-N1	2.54	119.73	113.25
165	WM	501	GTP	C5-C6-N1	2.54	119.73	113.25
165	JJ	501	GTP	C8-N7-C5	2.54	108.79	104.26
165	SI	501	GTP	C5-C6-N1	2.54	119.73	113.25
165	KH	501	GTP	O6-C6-C5	-2.54	119.82	126.53
165	TE	501	GTP	N9-C8-N7	-2.54	108.68	113.40
165	JV	501	GTP	C8-N7-C5	2.54	108.79	104.26
165	DL	501	GTP	C8-N7-C5	2.54	108.79	104.26
165	QU	501	GTP	C8-N7-C5	2.54	108.79	104.26
163	LK	500	GDP	C4-C5-N7	-2.54	106.64	110.67
163	WH	500	GDP	C4-C5-N7	-2.54	106.64	110.67
165	BO	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	UQ	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	IM	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	LR	502	GTP	C5-C6-N1	2.54	119.72	113.25
165	MV	501	GTP	C5-C6-N1	2.54	119.72	113.25
163	ED	500	GDP	C4-C5-N7	-2.54	106.64	110.67
163	OD	501	GDP	C4-C5-N7	-2.54	106.64	110.67
163	QE	500	GDP	C4-C5-N7	-2.54	106.64	110.67
163	LY	500	GDP	C4-C5-N7	-2.54	106.64	110.67
165	WI	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	LV	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	CB	501	GTP	C8-N7-C5	2.54	108.79	104.26
165	JB	501	GTP	C8-N7-C5	2.54	108.79	104.26
165	BI	501	GTP	O6-C6-C5	-2.54	119.82	126.53
163	O	500	GDP	C4-C5-N7	-2.54	106.64	110.67
163	FN	500	GDP	C4-C5-N7	-2.54	106.64	110.67
163	MT	500	GDP	C4-C5-N7	-2.54	106.64	110.67
165	QI	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	WW	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	KH	501	GTP	C5-C6-N1	2.54	119.72	113.25
163	JE	500	GDP	C4-C5-N7	-2.54	106.64	110.67
163	VF	500	GDP	C4-C5-N7	-2.54	106.64	110.67
165	HB	503	GTP	C8-N7-C5	2.54	108.78	104.26
163	RK	500	GDP	C4-C5-N7	-2.54	106.64	110.67
165	BU	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	TQ	501	GTP	N9-C8-N7	-2.54	108.69	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	BI	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	KB	502	GTP	C5-C6-N1	2.54	119.72	113.25
165	OO	501	GTP	C5-C6-N1	2.54	119.72	113.25
163	JQ	500	GDP	C4-C5-N7	-2.54	106.65	110.67
163	KO	500	GDP	C4-C5-N7	-2.54	106.65	110.67
165	PE	501	GTP	C5-C6-N1	2.54	119.72	113.25
165	KX	501	GTP	C8-N7-C5	2.54	108.78	104.26
163	SH	500	GDP	C4-C5-N7	-2.54	106.65	110.67
165	CJ	501	GTP	C8-N7-C5	2.54	108.78	104.26
165	MA	501	GTP	C5-C6-N1	2.54	119.71	113.25
163	WJ	500	GDP	C4-C5-N7	-2.54	106.65	110.67
163	FX	500	GDP	C4-C5-N7	-2.54	106.65	110.67
163	IP	500	GDP	C4-C5-N7	-2.54	106.65	110.67
165	UA	501	GTP	C8-N7-C5	2.54	108.78	104.26
165	WU	501	GTP	C8-N7-C5	2.54	108.78	104.26
165	NW	501	GTP	C8-N7-C5	2.54	108.78	104.26
165	HB	503	GTP	C5-C6-N1	2.54	119.71	113.25
165	KT	501	GTP	C5-C6-N1	2.54	119.71	113.25
163	QC	500	GDP	C4-C5-N7	-2.54	106.65	110.67
165	UG	501	GTP	C5-C6-N1	2.54	119.71	113.25
163	GH	500	GDP	C4-C5-N7	-2.54	106.65	110.67
163	WD	500	GDP	C4-C5-N7	-2.54	106.65	110.67
165	RV	501	GTP	C5-C6-N1	2.54	119.71	113.25
165	VQ	501	GTP	C5-C6-N1	2.54	119.71	113.25
165	IM	501	GTP	C8-N7-C5	2.54	108.78	104.26
165	WG	501	GTP	C8-N7-C5	2.54	108.78	104.26
165	VG	501	GTP	C5-C6-N1	2.54	119.71	113.25
165	DJ	501	GTP	C8-N7-C5	2.54	108.78	104.26
165	FS	501	GTP	O6-C6-C5	-2.54	119.84	126.53
165	KN	502	GTP	C5-C6-N1	2.54	119.71	113.25
163	QI	500	GDP	C4-C5-N7	-2.54	106.65	110.67
165	OM	501	GTP	C5-C6-N1	2.54	119.71	113.25
165	RR	501	GTP	C8-N7-C5	2.53	108.78	104.26
163	KG	500	GDP	C4-C5-N7	-2.53	106.65	110.67
163	OH	500	GDP	C4-C5-N7	-2.53	106.65	110.67
165	GI	501	GTP	O6-C6-C5	-2.53	119.84	126.53
165	QO	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	WY	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	LD	502	GTP	C8-N7-C5	2.53	108.78	104.26
165	EG	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	QN	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	TQ	501	GTP	C5-C6-N1	2.53	119.70	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	FV	501	GDP	C4-C5-N7	-2.53	106.65	110.67
165	GK	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	R	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	NC	501	GTP	C8-N7-C5	2.53	108.77	104.26
165	RB	501	GTP	O6-C6-C5	-2.53	119.84	126.53
165	NA	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	SW	501	GTP	C8-N7-C5	2.53	108.77	104.26
165	J	501	GTP	N9-C8-N7	-2.53	108.70	113.40
165	NU	501	GTP	C5-C6-N1	2.53	119.70	113.25
163	AF	500	GDP	C4-C5-N7	-2.53	106.66	110.67
165	UE	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	QR	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	TO	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	VO	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	KJ	501	GTP	C8-N7-C5	2.53	108.77	104.26
165	KP	502	GTP	C8-N7-C5	2.53	108.77	104.26
165	LZ	502	GTP	C8-N7-C5	2.53	108.77	104.26
165	Q	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	FG	501	GTP	C5-C6-N1	2.53	119.70	113.25
165	QX	501	GTP	C5-C6-N1	2.53	119.70	113.25
163	JS	500	GDP	C4-C5-N7	-2.53	106.66	110.67
163	TT	500	GDP	C4-C5-N7	-2.53	106.66	110.67
165	BK	501	GTP	C8-N7-C5	2.53	108.77	104.26
165	SE	501	GTP	C8-N7-C5	2.53	108.77	104.26
165	Q	501	GTP	N9-C8-N7	-2.53	108.71	113.40
165	QL	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	EP	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	RN	501	GTP	C5-C6-N1	2.53	119.69	113.25
163	MF	500	GDP	C4-C5-N7	-2.53	106.66	110.67
165	RC	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	KR	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	PC	501	GTP	C8-N7-C5	2.53	108.77	104.26
163	WV	500	GDP	C4-C5-N7	-2.53	106.66	110.67
165	IE	501	GTP	O6-C6-C5	-2.53	119.86	126.53
165	EA	501	GTP	C8-N7-C5	2.53	108.77	104.26
165	ED	501	GTP	C8-N7-C5	2.53	108.77	104.26
163	MD	500	GDP	C4-C5-N7	-2.53	106.66	110.67
163	QM	500	GDP	C4-C5-N7	-2.53	106.66	110.67
165	RF	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	PO	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	RR	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	QT	501	GTP	C8-N7-C5	2.53	108.77	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	RV	501	GTP	C8-N7-C5	2.53	108.77	104.26
163	EP	500	GDP	C4-C5-N7	-2.53	106.66	110.67
165	JD	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	IC	501	GTP	N9-C8-N7	-2.53	108.71	113.40
165	SK	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	ES	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	GS	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	SO	501	GTP	C5-C6-N1	2.53	119.69	113.25
163	IX	501	GDP	C4-C5-N7	-2.53	106.66	110.67
165	OI	501	GTP	C8-N7-C5	2.53	108.76	104.26
165	PY	501	GTP	C8-N7-C5	2.53	108.76	104.26
163	MZ	500	GDP	C4-C5-N7	-2.53	106.67	110.67
165	NM	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	WA	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	EO	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	LX	501	GTP	C8-N7-C5	2.53	108.76	104.26
165	PS	501	GTP	C8-N7-C5	2.53	108.76	104.26
165	OC	501	GTP	C5-C6-N1	2.53	119.69	113.25
165	KL	501	GTP	C8-N7-C5	2.53	108.76	104.26
165	QX	501	GTP	C8-N7-C5	2.53	108.76	104.26
165	BK	501	GTP	C5-C6-N1	2.53	119.68	113.25
165	IU	501	GTP	C5-C6-N1	2.53	119.68	113.25
165	PW	501	GTP	C5-C6-N1	2.53	119.68	113.25
165	HU	501	GTP	N9-C8-N7	-2.53	108.72	113.40
163	GB	500	GDP	C4-C5-N7	-2.53	106.67	110.67
163	TB	500	GDP	C4-C5-N7	-2.53	106.67	110.67
163	WP	500	GDP	C4-C5-N7	-2.53	106.67	110.67
165	TI	501	GTP	C5-C6-N1	2.53	119.68	113.25
165	MQ	501	GTP	C8-N7-C5	2.53	108.76	104.26
165	AG	501	GTP	C5-C6-N1	2.53	119.68	113.25
165	PY	501	GTP	C5-C6-N1	2.53	119.68	113.25
165	HK	501	GTP	N9-C8-N7	-2.53	108.72	113.40
165	KT	501	GTP	O6-C6-C5	-2.53	119.87	126.53
165	NC	501	GTP	C5-C6-N1	2.53	119.68	113.25
165	FQ	501	GTP	C5-C6-N1	2.52	119.68	113.25
165	IY	501	GTP	C8-N7-C5	2.52	108.76	104.26
165	PG	501	GTP	C5-C6-N1	2.52	119.68	113.25
165	SE	501	GTP	C5-C6-N1	2.52	119.68	113.25
165	SW	501	GTP	C5-C6-N1	2.52	119.68	113.25
165	PU	501	GTP	C8-N7-C5	2.52	108.76	104.26
165	WS	501	GTP	C8-N7-C5	2.52	108.76	104.26
163	NH	500	GDP	C4-C5-N7	-2.52	106.67	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	RI	500	GDP	C4-C5-N7	-2.52	106.67	110.67
163	KU	500	GDP	C4-C5-N7	-2.52	106.67	110.67
165	LL	501	GTP	C8-N7-C5	2.52	108.76	104.26
165	DH	501	GTP	C5-C6-N1	2.52	119.68	113.25
165	VH	501	GTP	C5-C6-N1	2.52	119.68	113.25
163	IH	500	GDP	C4-C5-N7	-2.52	106.67	110.67
163	LI	500	GDP	C4-C5-N7	-2.52	106.67	110.67
163	WT	500	GDP	C4-C5-N7	-2.52	106.67	110.67
165	RO	501	GTP	C5-C6-N1	2.52	119.68	113.25
165	VY	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	JP	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	CN	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	TU	501	GTP	C5-C6-N1	2.52	119.67	113.25
163	NF	500	GDP	C4-C5-N7	-2.52	106.67	110.67
163	PP	500	GDP	C4-C5-N7	-2.52	106.67	110.67
163	RW	500	GDP	C4-C5-N7	-2.52	106.67	110.67
165	PI	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	OK	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	GW	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	DP	501	GTP	O4'-C1'-N9	2.52	114.07	108.36
165	BG	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	JK	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	WK	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	AA	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	BM	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	MG	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	DV	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	NI	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	VT	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	QB	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	JR	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	NY	501	GTP	C5-C6-N1	2.52	119.67	113.25
163	FJ	501	GDP	C4-C5-N7	-2.52	106.68	110.67
163	LM	500	GDP	C4-C5-N7	-2.52	106.68	110.67
163	EN	500	GDP	C4-C5-N7	-2.52	106.68	110.67
165	UO	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	JN	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	OU	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	TC	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	WO	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	BG	501	GTP	C8-N7-C5	2.52	108.75	104.26
163	AN	500	GDP	C4-C5-N7	-2.52	106.68	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	DM	500	GDP	C4-C5-N7	-2.52	106.68	110.67
163	FR	501	GDP	C4-C5-N7	-2.52	106.68	110.67
163	NR	500	GDP	C4-C5-N7	-2.52	106.68	110.67
165	AA	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	RT	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	SQ	501	GTP	C5-C6-N1	2.52	119.67	113.25
165	DX	501	GTP	O3G-PG-O3B	2.52	113.08	104.64
165	ME	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	JR	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	UM	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	OG	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	RH	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	BY	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	FV	503	GTP	O6-C6-C5	-2.52	119.89	126.53
163	BT	500	GDP	C4-C5-N7	-2.52	106.68	110.67
163	HX	501	GDP	C4-C5-N7	-2.52	106.68	110.67
165	BQ	501	GTP	C8-N7-C5	2.52	108.75	104.26
165	MM	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	OD	503	GTP	C5-C6-N1	2.52	119.66	113.25
163	ST	500	GDP	C4-C5-N7	-2.52	106.68	110.67
165	MJ	501	GTP	O6-C6-C5	-2.52	119.89	126.53
165	IG	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	NF	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	QC	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	SC	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	US	501	GTP	C8-N7-C5	2.52	108.74	104.26
165	SM	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	HM	501	GTP	C8-N7-C5	2.52	108.74	104.26
165	TC	501	GTP	C8-N7-C5	2.52	108.74	104.26
165	VQ	501	GTP	C8-N7-C5	2.52	108.74	104.26
165	GE	501	GTP	C5-C6-N1	2.52	119.66	113.25
163	AZ	500	GDP	C4-C5-N7	-2.52	106.68	110.67
163	OT	500	GDP	C4-C5-N7	-2.52	106.68	110.67
165	HK	501	GTP	C8-N7-C5	2.52	108.74	104.26
165	HY	501	GTP	C8-N7-C5	2.52	108.74	104.26
165	PK	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	LX	501	GTP	C5-C6-N1	2.52	119.66	113.25
165	NA	501	GTP	C8-N7-C5	2.52	108.74	104.26
165	NO	501	GTP	C5-C6-N1	2.51	119.65	113.25
165	BU	501	GTP	O6-C6-C5	-2.51	119.89	126.53
165	DQ	501	GTP	O6-C6-C5	-2.51	119.89	126.53
165	KF	501	GTP	C8-N7-C5	2.51	108.74	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	L	501	GTP	C8-N7-C5	2.51	108.74	104.26
165	L	501	GTP	C5-C6-N1	2.51	119.65	113.25
165	NK	501	GTP	C5-C6-N1	2.51	119.65	113.25
163	LA	500	GDP	C4-C5-N7	-2.51	106.69	110.67
165	FO	501	GTP	O6-C6-C5	-2.51	119.90	126.53
165	UA	501	GTP	C5-C6-N1	2.51	119.65	113.25
165	PI	501	GTP	C8-N7-C5	2.51	108.74	104.26
165	VW	501	GTP	C8-N7-C5	2.51	108.74	104.26
163	BH	500	GDP	C4-C5-N7	-2.51	106.69	110.67
165	MV	501	GTP	O6-C6-C5	-2.51	119.90	126.53
165	RT	501	GTP	C8-N7-C5	2.51	108.74	104.26
163	FH	500	GDP	C4-C5-N7	-2.51	106.69	110.67
163	HH	501	GDP	C4-C5-N7	-2.51	106.69	110.67
165	LV	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	NU	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	LD	502	GTP	C5-C6-N1	2.51	119.65	113.25
165	VC	501	GTP	C5-C6-N1	2.51	119.65	113.25
165	HN	503	GTP	C5-C6-N1	2.51	119.65	113.25
165	JW	501	GTP	C5-C6-N1	2.51	119.65	113.25
165	SS	501	GTP	C5-C6-N1	2.51	119.65	113.25
163	MN	500	GDP	C4-C5-N7	-2.51	106.69	110.67
165	AK	501	GTP	O6-C6-C5	-2.51	119.90	126.53
165	ES	501	GTP	O6-C6-C5	-2.51	119.90	126.53
165	GS	501	GTP	O6-C6-C5	-2.51	119.90	126.53
165	LN	502	GTP	C8-N7-C5	2.51	108.73	104.26
165	VC	501	GTP	C8-N7-C5	2.51	108.73	104.26
163	AL	500	GDP	C4-C5-N7	-2.51	106.69	110.67
165	EG	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	SC	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	US	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	TG	501	GTP	C5-C6-N1	2.51	119.64	113.25
163	AJ	500	GDP	C4-C5-N7	-2.51	106.69	110.67
165	MY	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	GW	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	JZ	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	K	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	BO	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	HW	501	GTP	N9-C8-N7	-2.51	108.75	113.40
165	AM	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	IA	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	RH	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	RX	501	GTP	C8-N7-C5	2.51	108.73	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	AI	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	ME	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	OI	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	IQ	501	GTP	O6-C6-C5	-2.51	119.91	126.53
165	JT	501	GTP	O6-C6-C5	-2.51	119.91	126.53
165	MG	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	LL	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	EO	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	FQ	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	SQ	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	SG	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	KV	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	PU	501	GTP	C5-C6-N1	2.51	119.64	113.25
165	KB	502	GTP	C8-N7-C5	2.51	108.73	104.26
165	OD	503	GTP	C8-N7-C5	2.51	108.73	104.26
165	QL	501	GTP	C8-N7-C5	2.51	108.73	104.26
165	WC	501	GTP	C5-C6-N1	2.51	119.63	113.25
165	NR	501	GTP	C5-C6-N1	2.51	119.63	113.25
165	AD	501	GTP	C8-N7-C5	2.51	108.72	104.26
165	MA	501	GTP	C8-N7-C5	2.51	108.72	104.26
165	K	501	GTP	C5-C6-N1	2.51	119.63	113.25
163	UT	500	GDP	C4-C5-N7	-2.51	106.70	110.67
165	VS	501	GTP	C8-N7-C5	2.51	108.72	104.26
165	PM	501	GTP	C5-C6-N1	2.51	119.63	113.25
163	P	500	GDP	C3'-C2'-C1'	2.51	106.20	101.46
165	CW	501	GTP	C5-C6-N1	2.51	119.63	113.25
165	NW	501	GTP	C5-C6-N1	2.51	119.63	113.25
165	HA	501	GTP	C8-N7-C5	2.51	108.72	104.26
165	SK	501	GTP	C8-N7-C5	2.51	108.72	104.26
165	J	501	GTP	C5-C6-N1	2.50	119.63	113.25
165	BY	501	GTP	C5-C6-N1	2.50	119.63	113.25
165	II	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	HN	503	GTP	C8-N7-C5	2.50	108.72	104.26
165	MQ	501	GTP	C5-C6-N1	2.50	119.63	113.25
165	TS	501	GTP	C5-C6-N1	2.50	119.63	113.25
165	LN	502	GTP	C5-C6-N1	2.50	119.63	113.25
165	HE	501	GTP	C5-C6-N1	2.50	119.63	113.25
165	MM	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	IU	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	RN	501	GTP	O6-C6-C5	-2.50	119.92	126.53
165	QB	501	GTP	C8-N7-C5	2.50	108.72	104.26
163	QO	500	GDP	C4-C5-N7	-2.50	106.70	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	JF	501	GTP	C5-C6-N1	2.50	119.62	113.25
165	PS	501	GTP	C5-C6-N1	2.50	119.62	113.25
165	WA	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	IO	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	SA	501	GTP	C5-C6-N1	2.50	119.62	113.25
165	DB	501	GTP	O4'-C1'-N9	2.50	114.03	108.36
165	MS	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	VA	501	GTP	C5-C6-N1	2.50	119.62	113.25
165	CN	501	GTP	C5-C6-N1	2.50	119.62	113.25
165	KV	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	MU	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	TO	501	GTP	C8-N7-C5	2.50	108.72	104.26
165	OW	501	GTP	C8-N7-C5	2.50	108.72	104.26
163	FD	500	GDP	C4-C5-N7	-2.50	106.71	110.67
165	QI	501	GTP	C8-N7-C5	2.50	108.71	104.26
165	RF	501	GTP	C8-N7-C5	2.50	108.71	104.26
165	FT	503	GTP	O6-C6-C5	-2.50	119.93	126.53
165	WW	501	GTP	C8-N7-C5	2.50	108.71	104.26
163	AP	500	GDP	C4-C5-N7	-2.50	106.71	110.67
165	NK	501	GTP	C8-N7-C5	2.50	108.71	104.26
163	GN	500	GDP	C4-C5-N7	-2.50	106.71	110.67
165	MY	501	GTP	C8-N7-C5	2.50	108.71	104.26
163	HL	501	GDP	C4-C5-N7	-2.50	106.71	110.67
165	QR	501	GTP	C8-N7-C5	2.50	108.71	104.26
165	WK	501	GTP	C8-N7-C5	2.50	108.71	104.26
163	LE	500	GDP	C4-C5-N7	-2.50	106.71	110.67
163	LQ	500	GDP	C4-C5-N7	-2.50	106.71	110.67
165	OP	503	GTP	C5-C6-N1	2.50	119.61	113.25
165	EA	501	GTP	O6-C6-C5	-2.50	119.94	126.53
165	FT	503	GTP	C8-N7-C5	2.50	108.71	104.26
165	NE	501	GTP	C5-C6-N1	2.50	119.61	113.25
165	LP	502	GTP	C5-C6-N1	2.50	119.61	113.25
163	QA	500	GDP	C4-C5-N7	-2.50	106.72	110.67
165	NE	501	GTP	C8-N7-C5	2.50	108.71	104.26
165	OG	501	GTP	C8-N7-C5	2.50	108.71	104.26
165	WE	501	GTP	C8-N7-C5	2.50	108.71	104.26
163	CQ	500	GDP	C4-C5-N7	-2.50	106.72	110.67
165	QH	501	GTP	C8-N7-C5	2.50	108.70	104.26
165	TI	501	GTP	C8-N7-C5	2.50	108.70	104.26
165	GO	501	GTP	C8-N7-C5	2.50	108.70	104.26
165	TU	501	GTP	C8-N7-C5	2.50	108.70	104.26
165	KR	501	GTP	C8-N7-C5	2.49	108.70	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	BL	500	GDP	C4-C5-N7	-2.49	106.72	110.67
163	DK	501	GDP	C4-C5-N7	-2.49	106.72	110.67
163	AT	500	GDP	C4-C5-N7	-2.49	106.72	110.67
163	SV	501	GDP	C4-C5-N7	-2.49	106.72	110.67
165	T	503	GTP	C5-C6-N1	2.49	119.60	113.25
165	EJ	501	GTP	O6-C6-C5	-2.49	119.95	126.53
165	VG	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	VK	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	DT	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	ES	501	GTP	C8-N7-C5	2.49	108.70	104.26
163	LO	500	GDP	C4-C5-N7	-2.49	106.72	110.67
163	CK	501	GDP	C3'-C2'-C1'	2.49	106.18	101.46
165	GG	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	DQ	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	HG	501	GTP	C5-C6-N1	2.49	119.60	113.25
165	LZ	502	GTP	C5-C6-N1	2.49	119.60	113.25
165	UM	501	GTP	C5-C6-N1	2.49	119.60	113.25
165	VA	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	BE	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	OS	501	GTP	C5-C6-N1	2.49	119.59	113.25
165	HW	501	GTP	O6-C6-C5	-2.49	119.96	126.53
165	WC	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	CW	501	GTP	C8-N7-C5	2.49	108.70	104.26
165	BI	501	GTP	N9-C8-N7	-2.49	108.78	113.40
165	FJ	503	GTP	O6-C6-C5	-2.49	119.96	126.53
165	T	503	GTP	C8-N7-C5	2.49	108.69	104.26
165	OP	503	GTP	C8-N7-C5	2.49	108.69	104.26
165	TM	501	GTP	C5-C6-N1	2.49	119.59	113.25
165	GO	501	GTP	C5-C6-N1	2.49	119.59	113.25
165	FO	501	GTP	C8-N7-C5	2.49	108.69	104.26
165	GU	501	GTP	C8-N7-C5	2.49	108.69	104.26
165	LB	501	GTP	C5-C6-N1	2.49	119.58	113.25
165	RC	501	GTP	O6-C6-C5	-2.49	119.97	126.53
165	KJ	501	GTP	C5-C6-N1	2.49	119.58	113.25
165	GS	501	GTP	C8-N7-C5	2.49	108.69	104.26
165	WO	501	GTP	C8-N7-C5	2.49	108.69	104.26
165	HK	501	GTP	O6-C6-C5	-2.49	119.97	126.53
165	MI	501	GTP	C5-C6-N1	2.49	119.58	113.25
163	BX	500	GDP	C4-C5-N7	-2.49	106.73	110.67
165	IG	501	GTP	C8-N7-C5	2.49	108.69	104.26
165	AW	501	GTP	C8-N7-C5	2.49	108.69	104.26
165	HQ	501	GTP	C5-C6-N1	2.49	119.58	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	IS	501	GTP	C5-C6-N1	2.49	119.58	113.25
165	JK	501	GTP	C8-N7-C5	2.49	108.69	104.26
165	MV	501	GTP	C8-N7-C5	2.49	108.69	104.26
165	JF	501	GTP	C8-N7-C5	2.48	108.69	104.26
165	PG	501	GTP	C8-N7-C5	2.48	108.69	104.26
165	QF	501	GTP	C8-N7-C5	2.48	108.69	104.26
165	SO	501	GTP	C8-N7-C5	2.48	108.69	104.26
165	OU	501	GTP	C8-N7-C5	2.48	108.69	104.26
165	AG	501	GTP	C8-N7-C5	2.48	108.69	104.26
165	MU	501	GTP	C5-C6-N1	2.48	119.58	113.25
165	TQ	501	GTP	C8-N7-C5	2.48	108.69	104.26
165	BE	501	GTP	O6-C6-C5	-2.48	119.98	126.53
163	EF	500	GDP	C4-C5-N7	-2.48	106.73	110.67
165	UK	501	GTP	C5-C6-N1	2.48	119.58	113.25
165	AO	501	GTP	C5-C6-N1	2.48	119.58	113.25
165	OA	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	R	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	RL	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	VE	501	GTP	C8-N7-C5	2.48	108.68	104.26
163	CA	500	GDP	C4-C5-N7	-2.48	106.73	110.67
163	A	501	GDP	C3'-C2'-C1'	2.48	106.16	101.46
163	HT	501	GDP	C4-C5-N7	-2.48	106.74	110.67
165	EV	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	HS	501	GTP	C5-C6-N1	2.48	119.57	113.25
165	WM	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	JW	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	RL	501	GTP	C5-C6-N1	2.48	119.57	113.25
165	AS	501	GTP	O6-C6-C5	-2.48	119.98	126.53
165	DH	501	GTP	C8-N7-C5	2.48	108.68	104.26
163	I	501	GDP	C4-C5-N7	-2.48	106.74	110.67
163	FT	501	GDP	C4-C5-N7	-2.48	106.74	110.67
163	RO	500	GDP	C4-C5-N7	-2.48	106.74	110.67
165	AO	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	HS	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	QH	501	GTP	O6-C6-C5	-2.48	119.98	126.53
165	FM	501	GTP	C5-C6-N1	2.48	119.57	113.25
165	MS	501	GTP	C5-C6-N1	2.48	119.57	113.25
163	ET	500	GDP	C4-C5-N7	-2.48	106.74	110.67
165	FG	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	UG	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	HM	501	GTP	C5-C6-N1	2.48	119.56	113.25
165	EV	501	GTP	O6-C6-C5	-2.48	119.99	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	AI	501	GTP	C8-N7-C5	2.48	108.68	104.26
165	CT	501	GTP	C8-N7-C5	2.48	108.68	104.26
163	IB	500	GDP	C4-C5-N7	-2.48	106.74	110.67
165	BS	501	GTP	C5-C6-N1	2.48	119.56	113.25
165	MO	501	GTP	C5-C6-N1	2.48	119.56	113.25
165	QC	501	GTP	C8-N7-C5	2.48	108.67	104.26
165	NR	501	GTP	C8-N7-C5	2.48	108.67	104.26
165	MO	501	GTP	C8-N7-C5	2.48	108.67	104.26
163	AV	500	GDP	C4-C5-N7	-2.48	106.74	110.67
165	LB	501	GTP	C8-N7-C5	2.48	108.67	104.26
165	MJ	501	GTP	C8-N7-C5	2.48	108.67	104.26
165	MC	501	GTP	C8-N7-C5	2.48	108.67	104.26
165	SG	501	GTP	C8-N7-C5	2.48	108.67	104.26
165	HY	501	GTP	C5-C6-N1	2.48	119.56	113.25
165	WE	501	GTP	O6-C6-C5	-2.48	120.00	126.53
165	TM	501	GTP	C8-N7-C5	2.48	108.67	104.26
165	WY	501	GTP	C8-N7-C5	2.48	108.67	104.26
165	MC	501	GTP	C5-C6-N1	2.48	119.55	113.25
165	RF	501	GTP	O6-C6-C5	-2.48	120.00	126.53
165	EG	501	GTP	O6-C6-C5	-2.47	120.00	126.53
165	LH	501	GTP	O6-C6-C5	-2.47	120.00	126.53
163	RU	500	GDP	C4-C5-N7	-2.47	106.75	110.67
165	IY	501	GTP	O6-C6-C5	-2.47	120.00	126.53
165	UW	501	GTP	C5-C6-N1	2.47	119.55	113.25
165	PK	501	GTP	C8-N7-C5	2.47	108.67	104.26
165	FG	501	GTP	O6-C6-C5	-2.47	120.00	126.53
165	JN	501	GTP	C8-N7-C5	2.47	108.67	104.26
165	RN	501	GTP	C8-N7-C5	2.47	108.67	104.26
163	CA	500	GDP	C2'-C1'-N9	-2.47	106.37	113.25
165	RO	501	GTP	O6-C6-C5	-2.47	120.01	126.53
165	Q	501	GTP	C8-N7-C5	2.47	108.66	104.26
165	CT	501	GTP	O3G-PG-O3B	2.47	112.92	104.64
163	FB	500	GDP	C4-C5-N7	-2.47	106.75	110.67
165	EV	501	GTP	C5-C6-N1	2.47	119.54	113.25
165	RX	501	GTP	C5-C6-N1	2.47	119.54	113.25
165	AI	501	GTP	O6-C6-C5	-2.47	120.01	126.53
165	GL	501	GTP	O6-C6-C5	-2.47	120.01	126.53
165	GL	501	GTP	C5-C6-N1	2.47	119.54	113.25
165	QT	501	GTP	O6-C6-C5	-2.47	120.01	126.53
165	LT	501	GTP	O6-C6-C5	-2.47	120.02	126.53
165	GC	501	GTP	C8-N7-C5	2.47	108.66	104.26
165	IA	501	GTP	O6-C6-C5	-2.47	120.02	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	RR	501	GTP	O6-C6-C5	-2.47	120.02	126.53
165	FV	503	GTP	C8-N7-C5	2.47	108.66	104.26
163	NP	500	GDP	C4-C5-N7	-2.47	106.76	110.67
165	JH	501	GTP	O6-C6-C5	-2.47	120.02	126.53
165	JH	501	GTP	C8-N7-C5	2.47	108.66	104.26
163	ND	500	GDP	C4-C5-N7	-2.47	106.76	110.67
163	FP	500	GDP	C4-C5-N7	-2.47	106.76	110.67
163	IN	500	GDP	C4-C5-N7	-2.47	106.76	110.67
163	GX	500	GDP	C4-C5-N7	-2.47	106.76	110.67
165	NQ	501	GTP	C8-N7-C5	2.47	108.65	104.26
165	OS	501	GTP	C8-N7-C5	2.47	108.65	104.26
165	AB	501	GTP	C5-C6-N1	2.47	119.53	113.25
165	UK	501	GTP	C8-N7-C5	2.47	108.65	104.26
165	QO	501	GTP	C8-N7-C5	2.47	108.65	104.26
165	EP	501	GTP	C8-N7-C5	2.47	108.65	104.26
165	HW	501	GTP	C8-N7-C5	2.47	108.65	104.26
165	FI	501	GTP	O6-C6-C5	-2.47	120.03	126.53
165	FI	501	GTP	C8-N7-C5	2.46	108.65	104.26
165	NI	501	GTP	C8-N7-C5	2.46	108.65	104.26
163	CM	500	GDP	C3'-C2'-C1'	2.46	106.12	101.46
165	WM	501	GTP	O6-C6-C5	-2.46	120.03	126.53
165	HI	501	GTP	C5-C6-N1	2.46	119.53	113.25
165	TK	501	GTP	C8-N7-C5	2.46	108.65	104.26
165	LR	502	GTP	C8-N7-C5	2.46	108.65	104.26
165	VT	501	GTP	C8-N7-C5	2.46	108.65	104.26
165	TK	501	GTP	C5-C6-N1	2.46	119.52	113.25
165	IM	501	GTP	O6-C6-C5	-2.46	120.03	126.53
165	FM	501	GTP	C8-N7-C5	2.46	108.65	104.26
165	DE	501	GTP	O6-C6-C5	-2.46	120.03	126.53
165	DJ	501	GTP	C5-C6-N1	2.46	119.52	113.25
165	WQ	501	GTP	O6-C6-C5	-2.46	120.04	126.53
165	NW	501	GTP	O6-C6-C5	-2.46	120.04	126.53
165	J	501	GTP	C8-N7-C5	2.46	108.64	104.26
165	SS	501	GTP	C8-N7-C5	2.46	108.64	104.26
165	GC	501	GTP	C5-C6-N1	2.46	119.52	113.25
165	AU	501	GTP	O6-C6-C5	-2.46	120.04	126.53
165	FQ	501	GTP	O6-C6-C5	-2.46	120.04	126.53
163	DS	500	GDP	C4-C5-N7	-2.46	106.77	110.67
165	FA	501	GTP	C8-N7-C5	2.46	108.64	104.26
165	OD	503	GTP	O6-C6-C5	-2.46	120.04	126.53
165	CT	501	GTP	O6-C6-C5	-2.46	120.04	126.53
165	CH	501	GTP	O6-C6-C5	-2.46	120.04	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	TS	501	GTP	C8-N7-C5	2.46	108.64	104.26
165	BU	501	GTP	N9-C8-N7	-2.46	108.84	113.40
165	WA	501	GTP	O6-C6-C5	-2.46	120.04	126.53
165	VM	501	GTP	C8-N7-C5	2.46	108.64	104.26
165	JZ	501	GTP	C8-N7-C5	2.46	108.64	104.26
165	OP	503	GTP	O6-C6-C5	-2.46	120.05	126.53
165	IC	501	GTP	C8-N7-C5	2.46	108.64	104.26
165	AS	501	GTP	C8-N7-C5	2.46	108.64	104.26
163	QS	500	GDP	C4-C5-N7	-2.46	106.78	110.67
165	SS	501	GTP	O6-C6-C5	-2.46	120.05	126.53
165	UU	501	GTP	O6-C6-C5	-2.45	120.05	126.53
163	GP	500	GDP	C4-C5-N7	-2.45	106.78	110.67
165	LB	501	GTP	O6-C6-C5	-2.45	120.05	126.53
165	AM	501	GTP	O6-C6-C5	-2.45	120.06	126.53
165	VE	501	GTP	O6-C6-C5	-2.45	120.06	126.53
165	TE	501	GTP	C8-N7-C5	2.45	108.63	104.26
165	TW	501	GTP	C8-N7-C5	2.45	108.63	104.26
165	EC	501	GTP	C8-N7-C5	2.45	108.63	104.26
163	P	500	GDP	O6-C6-C5	-2.45	120.06	126.53
165	GG	501	GTP	O6-C6-C5	-2.45	120.06	126.53
165	TO	501	GTP	O6-C6-C5	-2.45	120.06	126.53
163	QG	500	GDP	C4-C5-N7	-2.45	106.78	110.67
165	WQ	501	GTP	C8-N7-C5	2.45	108.63	104.26
165	UE	501	GTP	C8-N7-C5	2.45	108.63	104.26
165	SO	501	GTP	O6-C6-C5	-2.45	120.06	126.53
165	LF	502	GTP	C8-N7-C5	2.45	108.63	104.26
165	RB	501	GTP	C8-N7-C5	2.45	108.62	104.26
165	AW	501	GTP	O6-C6-C5	-2.45	120.07	126.53
165	TS	501	GTP	O6-C6-C5	-2.45	120.07	126.53
165	PA	501	GTP	C8-N7-C5	2.45	108.62	104.26
165	EJ	501	GTP	O3G-PG-O3B	2.45	112.85	104.64
165	HA	501	GTP	C5-C6-N1	2.45	119.49	113.25
165	AY	501	GTP	C8-N7-C5	2.45	108.62	104.26
165	DH	501	GTP	O6-C6-C5	-2.45	120.07	126.53
165	FC	501	GTP	C8-N7-C5	2.45	108.62	104.26
165	FE	501	GTP	C8-N7-C5	2.45	108.62	104.26
163	GL	500	GDP	C4-C5-N7	-2.45	106.79	110.67
165	TW	501	GTP	C5-C6-N1	2.45	119.48	113.25
165	UI	501	GTP	O6-C6-C5	-2.45	120.07	126.53
165	VO	501	GTP	C8-N7-C5	2.45	108.62	104.26
165	HS	501	GTP	O6-C6-C5	-2.45	120.07	126.53
165	TG	501	GTP	O6-C6-C5	-2.45	120.07	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	LJ	501	GTP	C8-N7-C5	2.45	108.62	104.26
165	PK	501	GTP	O6-C6-C5	-2.45	120.08	126.53
165	SG	501	GTP	O6-C6-C5	-2.45	120.08	126.53
165	UQ	501	GTP	C8-N7-C5	2.45	108.62	104.26
165	FA	501	GTP	C5-C6-N1	2.45	119.48	113.25
163	UD	500	GDP	C4-C5-N7	-2.45	106.80	110.67
165	WE	501	GTP	O3G-PG-O3B	2.45	112.83	104.64
165	WQ	501	GTP	O3G-PG-O3B	2.45	112.83	104.64
165	HG	501	GTP	C8-N7-C5	2.44	108.61	104.26
165	R	501	GTP	O6-C6-C5	-2.44	120.08	126.53
165	BK	501	GTP	O6-C6-C5	-2.44	120.08	126.53
165	IS	501	GTP	C8-N7-C5	2.44	108.61	104.26
163	GD	500	GDP	C4-C5-N7	-2.44	106.80	110.67
165	VO	501	GTP	O6-C6-C5	-2.44	120.08	126.53
165	VH	501	GTP	C8-N7-C5	2.44	108.61	104.26
165	DT	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	KB	502	GTP	O6-C6-C5	-2.44	120.09	126.53
165	WY	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	KT	501	GTP	C8-N7-C5	2.44	108.61	104.26
165	NU	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	DL	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	AP	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	LH	501	GTP	C8-N7-C5	2.44	108.61	104.26
165	GW	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	II	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	FA	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	JF	501	GTP	O6-C6-C5	-2.44	120.09	126.53
165	NF	501	GTP	O6-C6-C5	-2.44	120.09	126.53
163	EF	500	GDP	C3'-C2'-C1'	2.44	106.08	101.46
165	KH	501	GTP	C8-N7-C5	2.44	108.60	104.26
165	JT	501	GTP	C8-N7-C5	2.44	108.60	104.26
165	HQ	501	GTP	O6-C6-C5	-2.44	120.10	126.53
165	GO	501	GTP	O6-C6-C5	-2.44	120.10	126.53
163	GF	500	GDP	C4-C5-N7	-2.44	106.81	110.67
165	TG	501	GTP	C8-N7-C5	2.44	108.60	104.26
165	EC	501	GTP	O6-C6-C5	-2.44	120.10	126.53
165	EU	501	GTP	O6-C6-C5	-2.44	120.10	126.53
165	HE	501	GTP	O6-C6-C5	-2.44	120.10	126.53
165	IG	501	GTP	O6-C6-C5	-2.44	120.10	126.53
165	K	501	GTP	O6-C6-C5	-2.44	120.10	126.53
165	NK	501	GTP	O6-C6-C5	-2.44	120.10	126.53
165	HU	501	GTP	C5-C6-N1	2.44	119.45	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	HE	501	GTP	C8-N7-C5	2.43	108.60	104.26
163	CW	500	GDP	C3'-C2'-C1'	2.43	106.07	101.46
165	FM	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	HG	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	KV	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	QN	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	AD	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	AY	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	HY	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	GE	501	GTP	C8-N7-C5	2.43	108.59	104.26
165	IE	501	GTP	C8-N7-C5	2.43	108.59	104.26
165	RH	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	TE	501	GTP	O6-C6-C5	-2.43	120.11	126.53
163	CY	500	GDP	C4-C5-N7	-2.43	106.82	110.67
163	OB	500	GDP	C4-C5-N7	-2.43	106.82	110.67
165	EI	501	GTP	O6-C6-C5	-2.43	120.11	126.53
165	UW	501	GTP	C8-N7-C5	2.43	108.59	104.26
165	EP	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	SM	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	MM	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	GC	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	IU	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	US	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	BA	501	GTP	C8-N7-C5	2.43	108.59	104.26
165	AO	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	VQ	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	GI	501	GTP	N9-C8-N7	-2.43	108.90	113.40
165	PW	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	KR	501	GTP	O6-C6-C5	-2.43	120.12	126.53
165	HM	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	QC	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	SC	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	AU	501	GTP	C8-N7-C5	2.43	108.58	104.26
165	SW	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	NI	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	PW	501	GTP	C8-N7-C5	2.43	108.58	104.26
165	LL	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	PU	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	HQ	501	GTP	C8-N7-C5	2.43	108.58	104.26
165	BS	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	TQ	501	GTP	O6-C6-C5	-2.43	120.13	126.53
165	JR	501	GTP	O6-C6-C5	-2.43	120.13	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	GK	501	GTP	O6-C6-C5	-2.42	120.13	126.53
165	MC	501	GTP	O6-C6-C5	-2.42	120.13	126.53
165	Q	501	GTP	O6-C6-C5	-2.42	120.13	126.53
165	AA	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	J	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	AB	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	KF	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	FJ	503	GTP	C8-N7-C5	2.42	108.57	104.26
165	UG	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	PS	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	GQ	501	GTP	C8-N7-C5	2.42	108.57	104.26
165	NQ	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	CK	503	GTP	C8-N7-C5	2.42	108.57	104.26
165	BS	501	GTP	C8-N7-C5	2.42	108.57	104.26
165	OK	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	LX	501	GTP	O6-C6-C5	-2.42	120.14	126.53
165	MG	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	TM	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	GI	501	GTP	C8-N7-C5	2.42	108.57	104.26
165	LT	501	GTP	C8-N7-C5	2.42	108.57	104.26
165	G	501	GTP	C5-C6-N1	2.42	119.41	113.25
165	PG	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	HI	501	GTP	C8-N7-C5	2.42	108.57	104.26
165	FS	501	GTP	C8-N7-C5	2.42	108.57	104.26
165	NA	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	OG	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	PI	501	GTP	O6-C6-C5	-2.42	120.15	126.53
163	UP	500	GDP	C4-C5-N7	-2.42	106.84	110.67
165	QF	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	TC	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	UC	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	MQ	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	QO	501	GTP	O6-C6-C5	-2.42	120.15	126.53
165	KZ	501	GTP	O6-C6-C5	-2.42	120.16	126.53
165	NC	501	GTP	O6-C6-C5	-2.42	120.16	126.53
163	WD	500	GDP	C3'-C2'-C1'	2.42	106.03	101.46
165	QB	501	GTP	O6-C6-C5	-2.42	120.16	126.53
165	OW	501	GTP	O6-C6-C5	-2.42	120.16	126.53
163	DG	500	GDP	C4-C5-N7	-2.41	106.84	110.67
165	LR	502	GTP	O6-C6-C5	-2.41	120.16	126.53
165	OC	501	GTP	O6-C6-C5	-2.41	120.16	126.53
165	BQ	501	GTP	O6-C6-C5	-2.41	120.16	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	TU	501	GTP	O6-C6-C5	-2.41	120.16	126.53
165	RC	501	GTP	C8-N7-C5	2.41	108.56	104.26
165	MA	501	GTP	O6-C6-C5	-2.41	120.16	126.53
165	NR	501	GTP	O6-C6-C5	-2.41	120.17	126.53
165	MU	501	GTP	O6-C6-C5	-2.41	120.17	126.53
165	RT	501	GTP	O6-C6-C5	-2.41	120.17	126.53
165	VC	501	GTP	O6-C6-C5	-2.41	120.17	126.53
165	FE	501	GTP	C5-C6-N1	2.41	119.39	113.25
165	OS	501	GTP	O6-C6-C5	-2.41	120.17	126.53
165	DX	501	GTP	O6-C6-C5	-2.41	120.17	126.53
165	HA	501	GTP	O6-C6-C5	-2.41	120.17	126.53
165	LN	502	GTP	O6-C6-C5	-2.41	120.17	126.53
165	LZ	502	GTP	O6-C6-C5	-2.41	120.17	126.53
165	AG	501	GTP	O6-C6-C5	-2.41	120.17	126.53
165	PC	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	WO	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	NO	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	T	503	GTP	O6-C6-C5	-2.41	120.18	126.53
165	MO	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	ED	501	GTP	O6-C6-C5	-2.41	120.18	126.53
163	FL	500	GDP	C4-C5-N7	-2.41	106.86	110.67
165	SE	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	KJ	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	NE	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	AD	501	GTP	O3G-PG-O3B	2.41	112.70	104.64
165	TI	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	BO	501	GTP	O6-C6-C5	-2.41	120.18	126.53
165	HU	501	GTP	C8-N7-C5	2.41	108.55	104.26
165	CN	501	GTP	O6-C6-C5	-2.40	120.18	126.53
165	EO	501	GTP	O6-C6-C5	-2.40	120.18	126.53
163	ON	500	GDP	C4-C5-N7	-2.40	106.86	110.67
165	CW	501	GTP	O6-C6-C5	-2.40	120.19	126.53
165	PY	501	GTP	O6-C6-C5	-2.40	120.19	126.53
165	BY	501	GTP	O6-C6-C5	-2.40	120.19	126.53
165	HN	503	GTP	O6-C6-C5	-2.40	120.19	126.53
163	F	500	GDP	C4-C5-N7	-2.40	106.86	110.67
165	ME	501	GTP	O6-C6-C5	-2.40	120.19	126.53
163	MV	500	GDP	C4-C5-N7	-2.40	106.86	110.67
165	G	501	GTP	C8-N7-C5	2.40	108.54	104.26
165	LP	502	GTP	O6-C6-C5	-2.40	120.19	126.53
165	EJ	501	GTP	C8-N7-C5	2.40	108.54	104.26
165	SK	501	GTP	O6-C6-C5	-2.40	120.20	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	PO	501	GTP	O6-C6-C5	-2.40	120.20	126.53
165	QL	501	GTP	O6-C6-C5	-2.40	120.20	126.53
165	QX	501	GTP	O6-C6-C5	-2.40	120.20	126.53
165	ES	501	GTP	O2A-PA-O3A	2.40	113.76	107.27
165	MY	501	GTP	O6-C6-C5	-2.40	120.20	126.53
165	BG	501	GTP	O6-C6-C5	-2.40	120.20	126.53
165	HU	501	GTP	O6-C6-C5	-2.40	120.20	126.53
165	IS	501	GTP	O6-C6-C5	-2.40	120.20	126.53
165	HI	501	GTP	O6-C6-C5	-2.40	120.20	126.53
165	VH	501	GTP	O6-C6-C5	-2.40	120.21	126.53
165	WC	501	GTP	O6-C6-C5	-2.40	120.21	126.53
165	MI	501	GTP	O6-C6-C5	-2.40	120.21	126.53
165	UE	501	GTP	O6-C6-C5	-2.40	120.21	126.53
165	OO	501	GTP	O6-C6-C5	-2.40	120.21	126.53
165	RO	501	GTP	C8-N7-C5	2.40	108.53	104.26
165	VA	501	GTP	O6-C6-C5	-2.39	120.21	126.53
165	KX	501	GTP	O6-C6-C5	-2.39	120.21	126.53
165	GU	501	GTP	O6-C6-C5	-2.39	120.21	126.53
163	MJ	500	GDP	C4-C5-N7	-2.39	106.88	110.67
165	L	501	GTP	O6-C6-C5	-2.39	120.22	126.53
165	SA	501	GTP	O6-C6-C5	-2.39	120.22	126.53
165	WS	501	GTP	O6-C6-C5	-2.39	120.22	126.53
165	PM	501	GTP	O6-C6-C5	-2.39	120.22	126.53
165	UQ	501	GTP	O6-C6-C5	-2.39	120.22	126.53
165	WK	501	GTP	O6-C6-C5	-2.39	120.22	126.53
165	CB	501	GTP	O6-C6-C5	-2.39	120.22	126.53
165	KN	502	GTP	O6-C6-C5	-2.39	120.22	126.53
165	MS	501	GTP	O6-C6-C5	-2.39	120.22	126.53
163	RE	500	GDP	C3'-C2'-C1'	2.39	105.98	101.46
165	LF	502	GTP	O6-C6-C5	-2.39	120.22	126.53
165	HB	503	GTP	O6-C6-C5	-2.39	120.22	126.53
165	PE	501	GTP	O6-C6-C5	-2.39	120.23	126.53
165	IQ	501	GTP	C8-N7-C5	2.39	108.52	104.26
165	JN	501	GTP	O6-C6-C5	-2.39	120.23	126.53
165	SI	501	GTP	O6-C6-C5	-2.39	120.23	126.53
165	VG	501	GTP	O6-C6-C5	-2.39	120.23	126.53
165	EM	501	GTP	C8-N7-C5	2.39	108.51	104.26
163	WP	500	GDP	C3'-C2'-C1'	2.39	105.98	101.46
165	SU	501	GTP	O6-C6-C5	-2.39	120.23	126.53
165	OA	501	GTP	O6-C6-C5	-2.39	120.23	126.53
165	PQ	501	GTP	O6-C6-C5	-2.39	120.23	126.53
165	UO	501	GTP	O6-C6-C5	-2.39	120.23	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	GL	501	GTP	C8-N7-C5	2.39	108.51	104.26
165	OY	501	GTP	O6-C6-C5	-2.38	120.24	126.53
165	NM	501	GTP	O6-C6-C5	-2.38	120.24	126.53
165	FT	503	GTP	C3'-C2'-C1'	2.38	105.97	101.46
165	JZ	501	GTP	O6-C6-C5	-2.38	120.24	126.53
165	WW	501	GTP	O6-C6-C5	-2.38	120.24	126.53
165	WU	501	GTP	O6-C6-C5	-2.38	120.24	126.53
165	LD	502	GTP	O6-C6-C5	-2.38	120.24	126.53
165	VT	501	GTP	O6-C6-C5	-2.38	120.25	126.53
165	AB	501	GTP	C8-N7-C5	2.38	108.50	104.26
165	VY	501	GTP	O6-C6-C5	-2.38	120.25	126.53
165	WI	501	GTP	O6-C6-C5	-2.38	120.25	126.53
165	OI	501	GTP	O6-C6-C5	-2.38	120.25	126.53
165	NY	501	GTP	O6-C6-C5	-2.38	120.25	126.53
163	G	500	GDP	C3'-C2'-C1'	2.38	105.96	101.46
165	TK	501	GTP	O6-C6-C5	-2.38	120.25	126.53
165	JB	501	GTP	O6-C6-C5	-2.38	120.26	126.53
165	CJ	501	GTP	O6-C6-C5	-2.38	120.26	126.53
165	CH	501	GTP	C3'-C2'-C1'	2.38	105.96	101.46
165	VS	501	GTP	O6-C6-C5	-2.38	120.26	126.53
165	UA	501	GTP	O6-C6-C5	-2.38	120.26	126.53
165	KL	501	GTP	O6-C6-C5	-2.38	120.26	126.53
165	VM	501	GTP	O6-C6-C5	-2.38	120.26	126.53
165	CV	501	GTP	O6-C6-C5	-2.38	120.26	126.53
165	C	501	GTP	C8-N7-C5	2.37	108.49	104.26
165	OU	501	GTP	O6-C6-C5	-2.37	120.27	126.53
165	BI	501	GTP	C8-N7-C5	2.37	108.49	104.26
165	KP	502	GTP	O6-C6-C5	-2.37	120.27	126.53
165	QR	501	GTP	O6-C6-C5	-2.37	120.27	126.53
165	DJ	501	GTP	O6-C6-C5	-2.37	120.28	126.53
165	OM	501	GTP	O6-C6-C5	-2.37	120.28	126.53
165	QT	501	GTP	O3G-PG-O3B	2.37	112.58	104.64
165	UK	501	GTP	O6-C6-C5	-2.37	120.28	126.53
165	VK	501	GTP	O6-C6-C5	-2.37	120.28	126.53
165	RV	501	GTP	O6-C6-C5	-2.37	120.28	126.53
163	V	500	GDP	C3'-C2'-C1'	2.36	105.94	101.46
165	WG	501	GTP	O6-C6-C5	-2.36	120.29	126.53
165	DD	501	GTP	O6-C6-C5	-2.36	120.30	126.53
165	KD	502	GTP	O6-C6-C5	-2.36	120.30	126.53
165	SQ	501	GTP	O6-C6-C5	-2.36	120.30	126.53
163	P	500	GDP	C4-C5-N7	-2.36	106.93	110.67
163	I	501	GDP	C3'-C2'-C1'	2.36	105.93	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	CQ	500	GDP	C3'-C2'-C1'	2.36	105.93	101.46
163	MV	500	GDP	C2'-C3'-C4'	2.36	107.17	102.61
163	JK	500	GDP	C3'-C2'-C1'	2.36	105.93	101.46
163	A	501	GDP	C4-C5-N7	-2.36	106.93	110.67
163	JW	500	GDP	C3'-C2'-C1'	2.36	105.93	101.46
165	UW	501	GTP	O6-C6-C5	-2.36	120.31	126.53
165	D	501	GTP	O3G-PG-O3B	2.36	112.54	104.64
165	LJ	501	GTP	O6-C6-C5	-2.36	120.31	126.53
165	UM	501	GTP	O6-C6-C5	-2.35	120.32	126.53
165	QH	501	GTP	O3G-PG-O3B	2.35	112.53	104.64
163	RQ	500	GDP	C3'-C2'-C1'	2.35	105.92	101.46
165	JV	501	GTP	O6-C6-C5	-2.35	120.32	126.53
165	CH	501	GTP	C8-N7-C5	2.35	108.45	104.26
165	LV	501	GTP	O6-C6-C5	-2.35	120.33	126.53
165	BM	501	GTP	O6-C6-C5	-2.35	120.33	126.53
165	RJ	501	GTP	O6-C6-C5	-2.35	120.33	126.53
165	JD	501	GTP	O6-C6-C5	-2.35	120.33	126.53
165	JP	501	GTP	O6-C6-C5	-2.35	120.33	126.53
163	KG	500	GDP	C3'-C2'-C1'	2.35	105.91	101.46
165	TW	501	GTP	O6-C6-C5	-2.35	120.33	126.53
165	VW	501	GTP	O6-C6-C5	-2.35	120.34	126.53
165	G	501	GTP	O6-C6-C5	-2.34	120.34	126.53
163	CI	500	GDP	C3'-C2'-C1'	2.34	105.90	101.46
165	CT	501	GTP	C3'-C2'-C1'	2.34	105.89	101.46
163	GJ	500	GDP	C3'-C2'-C1'	2.34	105.89	101.46
163	MH	500	GDP	C3'-C2'-C1'	2.34	105.89	101.46
165	QI	501	GTP	O6-C6-C5	-2.34	120.35	126.53
163	PX	501	GDP	C3'-C2'-C1'	2.34	105.89	101.46
163	LE	500	GDP	C3'-C2'-C1'	2.34	105.89	101.46
165	RL	501	GTP	O6-C6-C5	-2.34	120.36	126.53
165	JJ	501	GTP	O6-C6-C5	-2.34	120.36	126.53
163	U	500	GDP	C3'-C2'-C1'	2.34	105.88	101.46
163	F	500	GDP	C3'-C2'-C1'	2.33	105.88	101.46
165	RX	501	GTP	O6-C6-C5	-2.33	120.37	126.53
165	QU	501	GTP	O6-C6-C5	-2.33	120.37	126.53
163	KS	500	GDP	C3'-C2'-C1'	2.33	105.88	101.46
163	TT	500	GDP	C3'-C2'-C1'	2.33	105.88	101.46
163	W	500	GDP	C3'-C2'-C1'	2.33	105.88	101.46
163	MT	500	GDP	C3'-C2'-C1'	2.33	105.87	101.46
163	MJ	500	GDP	C2'-C3'-C4'	2.33	107.11	102.61
163	O	500	GDP	C3'-C2'-C1'	2.33	105.87	101.46
163	PL	501	GDP	C3'-C2'-C1'	2.33	105.87	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	BN	500	GDP	C2'-C3'-C4'	2.33	107.11	102.61
165	FE	501	GTP	O6-C6-C5	-2.33	120.39	126.53
165	DV	501	GTP	O6-C6-C5	-2.33	120.39	126.53
165	BU	501	GTP	C8-N7-C5	2.32	108.40	104.26
163	OL	500	GDP	C3'-C2'-C1'	2.32	105.85	101.46
163	NH	500	GDP	C3'-C2'-C1'	2.32	105.84	101.46
163	GX	500	GDP	C3'-C2'-C1'	2.32	105.84	101.46
163	M	500	GDP	C3'-C2'-C1'	2.31	105.83	101.46
163	OX	500	GDP	C3'-C2'-C1'	2.31	105.83	101.46
163	LQ	500	GDP	C3'-C2'-C1'	2.31	105.83	101.46
165	DP	501	GTP	O6-C6-C5	-2.31	120.44	126.53
165	CO	501	GTP	O6-C6-C5	-2.31	120.45	126.53
163	NB	500	GDP	C3'-C2'-C1'	2.30	105.82	101.46
165	IW	501	GTP	O2A-PA-O1A	-2.30	101.73	112.44
163	UN	500	GDP	C3'-C2'-C1'	2.30	105.82	101.46
165	CQ	501	GTP	O6-C6-C5	-2.30	120.46	126.53
163	HT	501	GDP	C3'-C2'-C1'	2.30	105.81	101.46
163	MX	500	GDP	C3'-C2'-C1'	2.30	105.81	101.46
163	HJ	500	GDP	C3'-C2'-C1'	2.30	105.81	101.46
163	UB	500	GDP	C3'-C2'-C1'	2.30	105.81	101.46
165	CH	501	GTP	N9-C8-N7	-2.30	109.14	113.40
163	NT	500	GDP	C3'-C2'-C1'	2.30	105.81	101.46
165	IK	501	GTP	O2A-PA-O1A	-2.30	101.76	112.44
163	ML	500	GDP	C3'-C2'-C1'	2.30	105.81	101.46
163	WX	500	GDP	C3'-C2'-C1'	2.30	105.81	101.46
163	VD	500	GDP	C3'-C2'-C1'	2.29	105.80	101.46
165	D	501	GTP	O6-C6-C5	-2.29	120.47	126.53
163	NN	500	GDP	C3'-C2'-C1'	2.29	105.80	101.46
163	LY	500	GDP	C3'-C2'-C1'	2.29	105.80	101.46
163	WL	500	GDP	C3'-C2'-C1'	2.29	105.80	101.46
163	GL	500	GDP	C3'-C2'-C1'	2.29	105.80	101.46
165	CC	501	GTP	O6-C6-C5	-2.29	120.49	126.53
163	JC	500	GDP	C3'-C2'-C1'	2.29	105.79	101.46
165	HK	501	GTP	C3'-C2'-C1'	2.29	105.79	101.46
163	VP	500	GDP	C3'-C2'-C1'	2.29	105.79	101.46
163	TH	500	GDP	C3'-C2'-C1'	2.29	105.79	101.46
163	AP	500	GDP	C3'-C2'-C1'	2.29	105.79	101.46
163	VR	500	GDP	C3'-C2'-C1'	2.29	105.79	101.46
165	DN	501	GTP	O6-C6-C5	-2.29	120.50	126.53
165	QH	501	GTP	O2B-PB-O3A	2.28	113.45	107.27
163	KI	500	GDP	C3'-C2'-C1'	2.28	105.78	101.46
163	CY	500	GDP	C3'-C2'-C1'	2.28	105.78	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	KU	500	GDP	C3'-C2'-C1'	2.28	105.78	101.46
165	QT	501	GTP	O2B-PB-O3A	2.28	113.44	107.27
163	MP	500	GDP	C3'-C2'-C1'	2.28	105.77	101.46
163	HH	501	GDP	C3'-C2'-C1'	2.28	105.77	101.46
163	MD	500	GDP	C3'-C2'-C1'	2.28	105.77	101.46
163	TD	500	GDP	C3'-C2'-C1'	2.28	105.77	101.46
163	GN	500	GDP	O6-C6-C5	-2.28	120.52	126.53
163	BT	500	GDP	C3'-C2'-C1'	2.28	105.77	101.46
165	BW	501	GTP	O6-C6-C5	-2.28	120.53	126.53
163	KY	500	GDP	C3'-C2'-C1'	2.28	105.77	101.46
165	GQ	501	GTP	C3'-C2'-C1'	2.27	105.77	101.46
165	JW	501	GTP	O6-C6-C5	-2.27	120.53	126.53
163	LM	500	GDP	C3'-C2'-C1'	2.27	105.76	101.46
163	HV	500	GDP	C3'-C2'-C1'	2.27	105.76	101.46
163	FL	500	GDP	C3'-C2'-C1'	2.27	105.75	101.46
163	KM	500	GDP	C3'-C2'-C1'	2.27	105.75	101.46
163	TP	500	GDP	C3'-C2'-C1'	2.27	105.75	101.46
163	HR	500	GDP	C3'-C2'-C1'	2.27	105.75	101.46
163	UT	500	GDP	C3'-C2'-C1'	2.27	105.75	101.46
163	FX	500	GDP	C3'-C2'-C1'	2.27	105.75	101.46
163	QQ	500	GDP	C3'-C2'-C1'	2.26	105.75	101.46
165	CE	501	GTP	O6-C6-C5	-2.26	120.56	126.53
165	JK	501	GTP	O6-C6-C5	-2.26	120.57	126.53
163	BD	500	GDP	C3'-C2'-C1'	2.26	105.73	101.46
163	QE	500	GDP	C3'-C2'-C1'	2.26	105.73	101.46
163	ER	500	GDP	C3'-C2'-C1'	2.26	105.73	101.46
163	UH	500	GDP	C3'-C2'-C1'	2.26	105.73	101.46
163	JO	500	GDP	C3'-C2'-C1'	2.26	105.73	101.46
163	FV	501	GDP	C3'-C2'-C1'	2.25	105.73	101.46
165	DT	501	GTP	C3'-C2'-C1'	2.25	105.73	101.46
163	F	500	GDP	O6-C6-C5	-2.25	120.58	126.53
163	AB	500	GDP	C3'-C2'-C1'	2.25	105.72	101.46
163	H	500	GDP	C3'-C2'-C1'	2.25	105.72	101.46
165	HW	501	GTP	C3'-C2'-C1'	2.25	105.72	101.46
163	CY	500	GDP	O6-C6-C5	-2.25	120.59	126.53
165	IK	501	GTP	C5-C6-N1	2.25	118.97	113.25
165	DB	501	GTP	O6-C6-C5	-2.24	120.61	126.53
163	OF	500	GDP	C3'-C2'-C1'	2.24	105.71	101.46
163	UF	500	GDP	C3'-C2'-C1'	2.24	105.70	101.46
163	HF	500	GDP	C3'-C2'-C1'	2.24	105.70	101.46
165	DE	501	GTP	O2B-PB-O3B	2.24	113.33	107.27
163	QI	500	GDP	C3'-C2'-C1'	2.24	105.70	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	QO	500	GDP	C3'-C2'-C1'	2.24	105.70	101.46
163	EV	500	GDP	C2'-C3'-C4'	2.23	106.92	102.61
163	VF	500	GDP	C3'-C2'-C1'	2.23	105.69	101.46
163	TX	500	GDP	C3'-C2'-C1'	2.23	105.69	101.46
163	MV	500	GDP	O6-C6-C5	-2.23	120.64	126.53
163	IB	500	GDP	C3'-C2'-C1'	2.23	105.68	101.46
163	WH	500	GDP	C3'-C2'-C1'	2.23	105.68	101.46
163	JS	500	GDP	C3'-C2'-C1'	2.23	105.68	101.46
165	IW	501	GTP	C5-C6-N1	2.23	118.93	113.25
163	QU	500	GDP	C3'-C2'-C1'	2.23	105.68	101.46
163	IJ	500	GDP	C3'-C2'-C1'	2.23	105.67	101.46
163	QC	500	GDP	C3'-C2'-C1'	2.23	105.67	101.46
163	T	501	GDP	C3'-C2'-C1'	2.23	105.67	101.46
163	WN	500	GDP	C3'-C2'-C1'	2.23	105.67	101.46
163	OR	500	GDP	C3'-C2'-C1'	2.22	105.67	101.46
165	IQ	501	GTP	C3'-C2'-C1'	2.22	105.67	101.46
163	RK	500	GDP	C3'-C2'-C1'	2.22	105.67	101.46
163	IN	500	GDP	C3'-C2'-C1'	2.22	105.67	101.46
163	IR	500	GDP	C3'-C2'-C1'	2.22	105.67	101.46
165	OK	501	GTP	C3'-C2'-C1'	2.22	105.67	101.46
163	MJ	500	GDP	O6-C6-C5	-2.22	120.68	126.53
163	JG	500	GDP	C3'-C2'-C1'	2.21	105.65	101.46
165	RL	501	GTP	O3G-PG-O3B	2.21	112.05	104.64
163	DG	500	GDP	O6-C6-C5	-2.21	120.70	126.53
163	A	501	GDP	O6-C6-C5	-2.21	120.70	126.53
163	TL	501	GDP	C3'-C2'-C1'	2.21	105.64	101.46
163	LK	500	GDP	C3'-C2'-C1'	2.21	105.64	101.46
165	AU	501	GTP	C3'-C2'-C1'	2.21	105.64	101.46
163	AN	500	GDP	C2'-C3'-C4'	2.21	106.87	102.61
163	JA	500	GDP	C3'-C2'-C1'	2.21	105.64	101.46
165	SS	501	GTP	O3G-PG-O3B	2.20	112.03	104.64
165	IE	501	GTP	C3'-C2'-C1'	2.20	105.63	101.46
165	RX	501	GTP	O3G-PG-O3B	2.20	112.02	104.64
163	AN	500	GDP	O6-C6-C5	-2.20	120.72	126.53
163	VN	500	GDP	C3'-C2'-C1'	2.20	105.63	101.46
163	IV	500	GDP	C3'-C2'-C1'	2.20	105.62	101.46
165	IW	501	GTP	O6-C6-C5	-2.20	120.72	126.53
165	QO	501	GTP	O3G-PG-O3B	2.20	112.01	104.64
165	SG	501	GTP	O3G-PG-O3B	2.20	112.01	104.64
165	FI	501	GTP	O2A-PA-O3A	2.20	113.21	107.27
165	QC	501	GTP	O3G-PG-O3B	2.20	112.00	104.64
163	LW	500	GDP	C3'-C2'-C1'	2.19	105.61	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	VE	501	GTP	C3'-C2'-C1'	2.19	105.61	101.46
163	KA	500	GDP	C3'-C2'-C1'	2.19	105.61	101.46
163	WB	500	GDP	C3'-C2'-C1'	2.19	105.61	101.46
163	JY	501	GDP	C3'-C2'-C1'	2.19	105.61	101.46
165	EC	501	GTP	C3'-C2'-C1'	2.19	105.61	101.46
165	GI	501	GTP	C3'-C2'-C1'	2.19	105.61	101.46
165	BU	501	GTP	O2B-PB-O3B	2.19	113.19	107.27
165	IK	501	GTP	O6-C6-C5	-2.19	120.75	126.53
165	VQ	501	GTP	C3'-C2'-C1'	2.19	105.61	101.46
163	FR	501	GDP	C3'-C2'-C1'	2.19	105.61	101.46
165	GC	501	GTP	O2A-PA-O3A	2.19	113.19	107.27
163	WT	500	GDP	C3'-C2'-C1'	2.19	105.60	101.46
163	IF	500	GDP	C3'-C2'-C1'	2.19	105.60	101.46
163	EN	500	GDP	C3'-C2'-C1'	2.19	105.60	101.46
163	DA	500	GDP	O6-C6-C5	-2.18	120.77	126.53
165	CV	501	GTP	C3'-C2'-C1'	2.18	105.59	101.46
163	AZ	500	GDP	C3'-C2'-C1'	2.18	105.59	101.46
163	NV	501	GDP	C3'-C2'-C1'	2.18	105.59	101.46
165	OW	501	GTP	C3'-C2'-C1'	2.18	105.59	101.46
163	FT	501	GDP	C2'-C3'-C4'	2.18	106.82	102.61
165	KH	501	GTP	C3'-C2'-C1'	2.18	105.58	101.46
163	RC	500	GDP	C3'-C2'-C1'	2.18	105.58	101.46
163	BL	500	GDP	O6-C6-C5	-2.18	120.79	126.53
163	BH	500	GDP	O6-C6-C5	-2.17	120.79	126.53
165	FE	501	GTP	C3'-C2'-C1'	2.17	105.58	101.46
163	GP	500	GDP	O6-C6-C5	-2.17	120.80	126.53
165	NC	501	GTP	C3'-C2'-C1'	2.17	105.57	101.46
163	NJ	501	GDP	C3'-C2'-C1'	2.17	105.57	101.46
163	JM	501	GDP	C3'-C2'-C1'	2.17	105.57	101.46
163	FL	500	GDP	O6-C6-C5	-2.17	120.81	126.53
163	EV	500	GDP	O6-C6-C5	-2.17	120.81	126.53
165	VG	501	GTP	C3'-C2'-C1'	2.17	105.56	101.46
163	PP	500	GDP	C3'-C2'-C1'	2.17	105.56	101.46
165	AI	501	GTP	C3'-C2'-C1'	2.17	105.56	101.46
163	VB	500	GDP	C3'-C2'-C1'	2.16	105.56	101.46
163	RU	500	GDP	C3'-C2'-C1'	2.16	105.56	101.46
163	RW	500	GDP	C3'-C2'-C1'	2.16	105.55	101.46
163	NR	500	GDP	C3'-C2'-C1'	2.16	105.55	101.46
165	VS	501	GTP	C3'-C2'-C1'	2.16	105.55	101.46
163	UR	500	GDP	C3'-C2'-C1'	2.16	105.55	101.46
163	DM	500	GDP	O6-C6-C5	-2.16	120.83	126.53
163	BT	500	GDP	O6-C6-C5	-2.16	120.83	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	GL	500	GDP	O6-C6-C5	-2.16	120.83	126.53
163	QG	500	GDP	C3'-C2'-C1'	2.16	105.55	101.46
163	AJ	500	GDP	C3'-C2'-C1'	2.16	105.55	101.46
163	GD	500	GDP	O6-C6-C5	-2.16	120.84	126.53
163	AH	500	GDP	O6-C6-C5	-2.16	120.84	126.53
163	HP	501	GDP	C3'-C2'-C1'	2.16	105.54	101.46
165	WS	501	GTP	C3'-C2'-C1'	2.16	105.54	101.46
163	AD	500	GDP	O6-C6-C5	-2.16	120.84	126.53
163	GX	500	GDP	O6-C6-C5	-2.16	120.84	126.53
163	NF	500	GDP	C3'-C2'-C1'	2.15	105.54	101.46
163	JA	500	GDP	O6-C6-C5	-2.15	120.85	126.53
163	IT	501	GDP	O6-C6-C5	-2.15	120.85	126.53
165	IU	501	GTP	C3'-C2'-C1'	2.15	105.53	101.46
165	II	501	GTP	C3'-C2'-C1'	2.15	105.53	101.46
163	HB	501	GDP	C3'-C2'-C1'	2.15	105.53	101.46
165	K	501	GTP	C3'-C2'-C1'	2.15	105.53	101.46
163	RI	500	GDP	C3'-C2'-C1'	2.15	105.53	101.46
163	AZ	500	GDP	O6-C6-C5	-2.15	120.86	126.53
163	DK	501	GDP	O6-C6-C5	-2.15	120.86	126.53
163	GF	500	GDP	O6-C6-C5	-2.15	120.86	126.53
163	TN	500	GDP	C3'-C2'-C1'	2.15	105.53	101.46
163	RO	500	GDP	C3'-C2'-C1'	2.15	105.53	101.46
163	BX	500	GDP	O6-C6-C5	-2.15	120.86	126.53
163	AP	500	GDP	O6-C6-C5	-2.15	120.86	126.53
165	GC	501	GTP	C2'-C3'-C4'	2.15	106.76	102.61
165	SA	501	GTP	C3'-C2'-C1'	2.15	105.53	101.46
165	NO	501	GTP	C3'-C2'-C1'	2.15	105.52	101.46
163	TB	500	GDP	C3'-C2'-C1'	2.15	105.52	101.46
163	GP	500	GDP	C3'-C2'-C1'	2.15	105.52	101.46
163	WJ	500	GDP	C3'-C2'-C1'	2.14	105.52	101.46
165	KT	501	GTP	C3'-C2'-C1'	2.14	105.52	101.46
165	JR	501	GTP	C3'-C2'-C1'	2.14	105.52	101.46
163	GH	500	GDP	O6-C6-C5	-2.14	120.88	126.53
165	FI	501	GTP	C3'-C2'-C1'	2.14	105.52	101.46
165	GL	501	GTP	O2A-PA-O3A	2.14	113.06	107.27
163	GJ	500	GDP	O6-C6-C5	-2.14	120.88	126.53
163	LU	500	GDP	C3'-C2'-C1'	2.14	105.51	101.46
165	GE	501	GTP	O2A-PA-O3A	2.14	113.06	107.27
165	BI	501	GTP	C3'-C2'-C1'	2.14	105.51	101.46
163	GV	501	GDP	O6-C6-C5	-2.14	120.88	126.53
163	FF	500	GDP	C3'-C2'-C1'	2.14	105.51	101.46
163	LA	500	GDP	C3'-C2'-C1'	2.14	105.51	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	NP	500	GDP	C3'-C2'-C1'	2.14	105.51	101.46
163	QG	500	GDP	O6-C6-C5	-2.14	120.89	126.53
163	JU	500	GDP	O6-C6-C5	-2.14	120.89	126.53
163	KQ	500	GDP	O6-C6-C5	-2.14	120.89	126.53
163	GD	500	GDP	C3'-C2'-C1'	2.14	105.51	101.46
163	SH	500	GDP	O6-C6-C5	-2.14	120.89	126.53
163	LW	500	GDP	O6-C6-C5	-2.14	120.89	126.53
163	JQ	500	GDP	C3'-C2'-C1'	2.14	105.51	101.46
165	WG	501	GTP	C3'-C2'-C1'	2.14	105.51	101.46
163	CW	500	GDP	O6-C6-C5	-2.14	120.89	126.53
163	NT	500	GDP	O6-C6-C5	-2.14	120.89	126.53
163	N	500	GDP	C3'-C2'-C1'	2.14	105.51	101.46
163	AT	500	GDP	O6-C6-C5	-2.14	120.89	126.53
165	AD	501	GTP	C3'-C2'-C1'	2.14	105.50	101.46
163	HD	501	GDP	C3'-C2'-C1'	2.14	105.50	101.46
165	GG	501	GTP	O2A-PA-O3A	2.14	113.05	107.27
163	AB	500	GDP	O6-C6-C5	-2.14	120.89	126.53
163	QS	500	GDP	O6-C6-C5	-2.14	120.89	126.53
165	G	501	GTP	C2'-C3'-C4'	2.13	106.73	102.61
163	JQ	500	GDP	O6-C6-C5	-2.13	120.90	126.53
165	LH	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
163	RG	500	GDP	C3'-C2'-C1'	2.13	105.50	101.46
165	JF	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
163	IH	500	GDP	O6-C6-C5	-2.13	120.90	126.53
165	BU	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
165	TS	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
165	TG	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
165	TM	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
165	T	503	GTP	O3G-PG-O3B	2.13	111.78	104.64
163	ST	500	GDP	O6-C6-C5	-2.13	120.91	126.53
163	RS	500	GDP	C3'-C2'-C1'	2.13	105.49	101.46
163	I	501	GDP	O6-C6-C5	-2.13	120.91	126.53
165	EU	501	GTP	C3'-C2'-C1'	2.13	105.49	101.46
163	LK	500	GDP	O6-C6-C5	-2.13	120.91	126.53
163	BL	500	GDP	C3'-C2'-C1'	2.13	105.49	101.46
163	SV	501	GDP	C3'-C2'-C1'	2.13	105.49	101.46
165	SM	501	GTP	C3'-C2'-C1'	2.13	105.49	101.46
163	TJ	500	GDP	O6-C6-C5	-2.13	120.92	126.53
163	ON	500	GDP	O6-C6-C5	-2.13	120.92	126.53
163	PD	500	GDP	C3'-C2'-C1'	2.13	105.49	101.46
163	JE	500	GDP	O6-C6-C5	-2.13	120.92	126.53
163	LI	500	GDP	C3'-C2'-C1'	2.13	105.48	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	ES	501	GTP	C3'-C2'-C1'	2.13	105.48	101.46
165	LT	501	GTP	C3'-C2'-C1'	2.13	105.48	101.46
165	UM	501	GTP	C3'-C2'-C1'	2.13	105.48	101.46
163	MH	500	GDP	O6-C6-C5	-2.13	120.92	126.53
163	OP	501	GDP	O6-C6-C5	-2.13	120.92	126.53
165	VT	501	GTP	C3'-C2'-C1'	2.13	105.48	101.46
163	JK	500	GDP	O6-C6-C5	-2.12	120.92	126.53
163	QA	500	GDP	C3'-C2'-C1'	2.12	105.48	101.46
163	KY	500	GDP	O6-C6-C5	-2.12	120.92	126.53
163	JE	500	GDP	C3'-C2'-C1'	2.12	105.48	101.46
165	SE	501	GTP	O2A-PA-O3A	2.12	113.01	107.27
163	CQ	500	GDP	O6-C6-C5	-2.12	120.93	126.53
163	SV	501	GDP	O6-C6-C5	-2.12	120.93	126.53
165	KR	501	GTP	C3'-C2'-C1'	2.12	105.48	101.46
165	NW	501	GTP	C3'-C2'-C1'	2.12	105.48	101.46
163	MT	500	GDP	O6-C6-C5	-2.12	120.93	126.53
163	VR	500	GDP	O6-C6-C5	-2.12	120.93	126.53
163	AV	500	GDP	O6-C6-C5	-2.12	120.93	126.53
163	DQ	500	GDP	C3'-C2'-C1'	2.12	105.48	101.46
165	KX	501	GTP	C3'-C2'-C1'	2.12	105.48	101.46
165	DL	501	GTP	O3G-PG-O3B	2.12	111.75	104.64
163	ND	500	GDP	O6-C6-C5	-2.12	120.93	126.53
163	S	500	GDP	C3'-C2'-C1'	2.12	105.47	101.46
163	VF	500	GDP	O6-C6-C5	-2.12	120.94	126.53
163	WV	500	GDP	C3'-C2'-C1'	2.12	105.47	101.46
163	AL	500	GDP	O6-C6-C5	-2.12	120.94	126.53
165	GO	501	GTP	C3'-C2'-C1'	2.12	105.47	101.46
163	SF	500	GDP	C3'-C2'-C1'	2.12	105.47	101.46
163	QS	500	GDP	C3'-C2'-C1'	2.12	105.47	101.46
163	OB	500	GDP	O6-C6-C5	-2.12	120.94	126.53
163	UN	500	GDP	O6-C6-C5	-2.12	120.94	126.53
163	IF	500	GDP	O6-C6-C5	-2.12	120.94	126.53
163	KI	500	GDP	O6-C6-C5	-2.12	120.95	126.53
163	GF	500	GDP	C3'-C2'-C1'	2.12	105.47	101.46
163	OD	501	GDP	O6-C6-C5	-2.12	120.95	126.53
163	AJ	500	GDP	O6-C6-C5	-2.12	120.95	126.53
165	QI	501	GTP	C3'-C2'-C1'	2.12	105.46	101.46
165	TM	501	GTP	O3G-PG-O3B	2.11	111.73	104.64
163	VH	500	GDP	C3'-C2'-C1'	2.11	105.46	101.46
165	GW	501	GTP	O3G-PG-O3B	2.11	111.72	104.64
163	W	500	GDP	O6-C6-C5	-2.11	120.95	126.53
163	WD	500	GDP	O6-C6-C5	-2.11	120.95	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	FV	501	GDP	O6-C6-C5	-2.11	120.95	126.53
163	LA	500	GDP	O6-C6-C5	-2.11	120.96	126.53
163	RE	500	GDP	O6-C6-C5	-2.11	120.96	126.53
163	WX	500	GDP	O6-C6-C5	-2.11	120.96	126.53
165	QU	501	GTP	C3'-C2'-C1'	2.11	105.46	101.46
163	KE	500	GDP	O6-C6-C5	-2.11	120.96	126.53
163	IX	501	GDP	O6-C6-C5	-2.11	120.96	126.53
163	WP	500	GDP	O6-C6-C5	-2.11	120.96	126.53
163	FB	500	GDP	O6-C6-C5	-2.11	120.96	126.53
163	QC	500	GDP	O6-C6-C5	-2.11	120.96	126.53
163	T	501	GDP	O6-C6-C5	-2.11	120.96	126.53
163	IT	501	GDP	C3'-C2'-C1'	2.11	105.45	101.46
163	NH	500	GDP	O6-C6-C5	-2.11	120.97	126.53
163	FR	501	GDP	O6-C6-C5	-2.11	120.97	126.53
163	QO	500	GDP	O6-C6-C5	-2.11	120.97	126.53
163	TF	500	GDP	O6-C6-C5	-2.11	120.97	126.53
165	OI	501	GTP	C3'-C2'-C1'	2.11	105.45	101.46
165	WA	501	GTP	C3'-C2'-C1'	2.11	105.45	101.46
165	SQ	501	GTP	O2A-PA-O3A	2.11	112.97	107.27
163	JI	500	GDP	O6-C6-C5	-2.11	120.97	126.53
163	IR	500	GDP	O6-C6-C5	-2.11	120.97	126.53
165	NI	501	GTP	C3'-C2'-C1'	2.11	105.45	101.46
163	FF	500	GDP	O6-C6-C5	-2.11	120.97	126.53
163	JW	500	GDP	O6-C6-C5	-2.11	120.97	126.53
163	KM	500	GDP	O6-C6-C5	-2.11	120.97	126.53
163	WN	500	GDP	O6-C6-C5	-2.11	120.97	126.53
163	UD	500	GDP	C3'-C2'-C1'	2.11	105.45	101.46
165	HI	501	GTP	C3'-C2'-C1'	2.11	105.45	101.46
165	T	503	GTP	C3'-C2'-C1'	2.11	105.45	101.46
163	UB	500	GDP	O6-C6-C5	-2.11	120.97	126.53
163	SB	501	GDP	O6-C6-C5	-2.11	120.97	126.53
163	HN	501	GDP	C3'-C2'-C1'	2.11	105.44	101.46
165	KB	502	GTP	C3'-C2'-C1'	2.11	105.44	101.46
163	BN	500	GDP	O6-C6-C5	-2.10	120.98	126.53
163	WF	501	GDP	O6-C6-C5	-2.10	120.98	126.53
163	VV	500	GDP	C3'-C2'-C1'	2.10	105.44	101.46
165	OD	503	GTP	C3'-C2'-C1'	2.10	105.44	101.46
163	EJ	500	GDP	O6-C6-C5	-2.10	120.98	126.53
163	IJ	500	GDP	O6-C6-C5	-2.10	120.98	126.53
163	NJ	501	GDP	O6-C6-C5	-2.10	120.98	126.53
163	QU	500	GDP	O6-C6-C5	-2.10	120.98	126.53
163	IH	500	GDP	C3'-C2'-C1'	2.10	105.44	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	NK	501	GTP	C3'-C2'-C1'	2.10	105.44	101.46
163	PP	500	GDP	O6-C6-C5	-2.10	120.98	126.53
163	UP	500	GDP	C3'-C2'-C1'	2.10	105.44	101.46
163	G	500	GDP	O6-C6-C5	-2.10	120.98	126.53
163	QM	500	GDP	C3'-C2'-C1'	2.10	105.44	101.46
163	ST	500	GDP	C3'-C2'-C1'	2.10	105.44	101.46
165	HY	501	GTP	C3'-C2'-C1'	2.10	105.44	101.46
163	TR	500	GDP	O6-C6-C5	-2.10	120.98	126.53
163	ND	500	GDP	C3'-C2'-C1'	2.10	105.44	101.46
163	KQ	500	GDP	C3'-C2'-C1'	2.10	105.44	101.46
163	VP	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	CM	500	GDP	O4'-C1'-N9	2.10	113.12	108.36
163	IL	501	GDP	O6-C6-C5	-2.10	120.99	126.53
165	VM	501	GTP	C3'-C2'-C1'	2.10	105.44	101.46
163	OR	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	U	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	AR	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	SL	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	SP	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	EF	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	WL	500	GDP	O6-C6-C5	-2.10	120.99	126.53
165	DX	501	GTP	O2B-PB-O3B	2.10	112.95	107.27
163	PD	500	GDP	O6-C6-C5	-2.10	120.99	126.53
165	FQ	501	GTP	C3'-C2'-C1'	2.10	105.43	101.46
163	IV	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	WT	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	CI	500	GDP	O6-C6-C5	-2.10	120.99	126.53
163	QW	500	GDP	O6-C6-C5	-2.10	120.99	126.53
165	EG	501	GTP	C3'-C2'-C1'	2.10	105.43	101.46
165	OP	503	GTP	C3'-C2'-C1'	2.10	105.43	101.46
165	DP	501	GTP	C4-C5-N7	-2.10	107.34	110.67
163	UT	500	GDP	O6-C6-C5	-2.10	121.00	126.53
165	KL	501	GTP	C3'-C2'-C1'	2.10	105.43	101.46
163	WH	500	GDP	O6-C6-C5	-2.10	121.00	126.53
163	KU	500	GDP	O6-C6-C5	-2.10	121.00	126.53
163	UR	500	GDP	O6-C6-C5	-2.10	121.00	126.53
163	MN	500	GDP	O6-C6-C5	-2.10	121.00	126.53
163	M	500	GDP	O6-C6-C5	-2.10	121.00	126.53
163	MX	500	GDP	O6-C6-C5	-2.10	121.00	126.53
165	MS	501	GTP	C3'-C2'-C1'	2.10	105.43	101.46
163	TB	500	GDP	O6-C6-C5	-2.10	121.00	126.53
163	BR	500	GDP	O6-C6-C5	-2.10	121.00	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	SJ	501	GDP	C3'-C2'-C1'	2.09	105.43	101.46
165	IC	501	GTP	C3'-C2'-C1'	2.09	105.43	101.46
165	ME	501	GTP	C3'-C2'-C1'	2.09	105.43	101.46
165	UQ	501	GTP	C3'-C2'-C1'	2.09	105.42	101.46
163	SJ	501	GDP	O6-C6-C5	-2.09	121.00	126.53
163	VT	500	GDP	C3'-C2'-C1'	2.09	105.42	101.46
165	IO	501	GTP	C3'-C2'-C1'	2.09	105.42	101.46
163	CA	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	NV	501	GDP	O6-C6-C5	-2.09	121.01	126.53
163	NB	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	MZ	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	UH	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	SR	500	GDP	C3'-C2'-C1'	2.09	105.42	101.46
165	MQ	501	GTP	C3'-C2'-C1'	2.09	105.42	101.46
163	GB	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	SD	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	FX	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	TP	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	KO	500	GDP	C3'-C2'-C1'	2.09	105.42	101.46
163	S	500	GDP	O6-C6-C5	-2.09	121.01	126.53
163	O	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	KE	500	GDP	C3'-C2'-C1'	2.09	105.42	101.46
163	OV	500	GDP	C3'-C2'-C1'	2.09	105.42	101.46
165	CC	501	GTP	O3G-PG-O3B	2.09	111.64	104.64
163	ED	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	OJ	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	UF	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	NN	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	DW	501	GDP	C3'-C2'-C1'	2.09	105.41	101.46
165	GU	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46
163	DS	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	IP	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	VJ	500	GDP	C3'-C2'-C1'	2.09	105.41	101.46
165	JH	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46
163	KG	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	OF	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	JS	500	GDP	O6-C6-C5	-2.09	121.02	126.53
163	SH	500	GDP	C3'-C2'-C1'	2.09	105.41	101.46
165	IS	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46
163	WR	501	GDP	O6-C6-C5	-2.09	121.03	126.53
163	EN	500	GDP	O6-C6-C5	-2.09	121.03	126.53
165	VH	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	BF	500	GDP	O6-C6-C5	-2.09	121.03	126.53
165	VA	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46
165	EO	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46
163	ML	500	GDP	O6-C6-C5	-2.09	121.03	126.53
163	QI	500	GDP	O6-C6-C5	-2.09	121.03	126.53
163	VD	500	GDP	O6-C6-C5	-2.09	121.03	126.53
165	NF	501	GTP	C3'-C2'-C1'	2.08	105.41	101.46
165	VY	501	GTP	C3'-C2'-C1'	2.08	105.41	101.46
163	HD	501	GDP	O6-C6-C5	-2.08	121.03	126.53
163	HJ	500	GDP	O6-C6-C5	-2.08	121.03	126.53
163	OH	500	GDP	O6-C6-C5	-2.08	121.03	126.53
165	HB	503	GTP	C3'-C2'-C1'	2.08	105.41	101.46
165	UA	501	GTP	C3'-C2'-C1'	2.08	105.41	101.46
165	QF	501	GTP	C3'-C2'-C1'	2.08	105.41	101.46
165	HN	503	GTP	C3'-C2'-C1'	2.08	105.41	101.46
163	PN	500	GDP	C3'-C2'-C1'	2.08	105.40	101.46
163	SL	500	GDP	C3'-C2'-C1'	2.08	105.40	101.46
165	KF	501	GTP	C3'-C2'-C1'	2.08	105.40	101.46
163	TV	500	GDP	O6-C6-C5	-2.08	121.03	126.53
163	HL	501	GDP	C3'-C2'-C1'	2.08	105.40	101.46
165	NR	501	GTP	C3'-C2'-C1'	2.08	105.40	101.46
163	FD	500	GDP	O6-C6-C5	-2.08	121.04	126.53
163	PL	501	GDP	O6-C6-C5	-2.08	121.04	126.53
163	RQ	500	GDP	O6-C6-C5	-2.08	121.04	126.53
163	GT	501	GDP	O6-C6-C5	-2.08	121.04	126.53
163	MP	500	GDP	O6-C6-C5	-2.08	121.04	126.53
165	OU	501	GTP	C3'-C2'-C1'	2.08	105.40	101.46
163	TD	500	GDP	O6-C6-C5	-2.08	121.04	126.53
163	WB	500	GDP	O6-C6-C5	-2.08	121.04	126.53
163	FH	500	GDP	O6-C6-C5	-2.08	121.04	126.53
163	OJ	500	GDP	C3'-C2'-C1'	2.08	105.40	101.46
165	GG	501	GTP	C3'-C2'-C1'	2.08	105.40	101.46
163	CE	500	GDP	C3'-C2'-C1'	2.08	105.40	101.46
163	KW	500	GDP	C3'-C2'-C1'	2.08	105.40	101.46
163	HV	500	GDP	O6-C6-C5	-2.08	121.04	126.53
163	UX	500	GDP	O6-C6-C5	-2.08	121.04	126.53
163	OD	501	GDP	C3'-C2'-C1'	2.08	105.40	101.46
163	QE	500	GDP	O6-C6-C5	-2.08	121.04	126.53
163	EH	500	GDP	C2'-C3'-C4'	2.08	106.63	102.61
163	NX	500	GDP	C3'-C2'-C1'	2.08	105.40	101.46
163	H	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	EP	500	GDP	O6-C6-C5	-2.08	121.05	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	SN	501	GDP	O6-C6-C5	-2.08	121.05	126.53
163	JC	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	RG	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	HP	501	GDP	O6-C6-C5	-2.08	121.05	126.53
163	MR	500	GDP	C2'-C3'-C4'	2.08	106.62	102.61
163	CK	501	GDP	O6-C6-C5	-2.08	121.05	126.53
163	LU	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	MD	500	GDP	O6-C6-C5	-2.08	121.05	126.53
165	DP	501	GTP	N2-C2-N1	2.08	121.14	116.76
163	SR	500	GDP	O6-C6-C5	-2.08	121.05	126.53
165	SG	501	GTP	C3'-C2'-C1'	2.08	105.39	101.46
163	TL	501	GDP	O6-C6-C5	-2.08	121.05	126.53
163	FP	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	RW	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	TN	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	NP	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	NR	500	GDP	O6-C6-C5	-2.08	121.05	126.53
165	SS	501	GTP	C3'-C2'-C1'	2.08	105.39	101.46
163	BJ	500	GDP	O6-C6-C5	-2.08	121.05	126.53
163	FJ	501	GDP	O6-C6-C5	-2.08	121.05	126.53
163	UJ	500	GDP	O6-C6-C5	-2.08	121.05	126.53
165	BO	501	GTP	O3G-PG-O3B	2.08	111.59	104.64
163	PJ	500	GDP	O6-C6-C5	-2.08	121.06	126.53
163	HX	501	GDP	C3'-C2'-C1'	2.07	105.39	101.46
165	UG	501	GTP	C3'-C2'-C1'	2.07	105.39	101.46
165	WM	501	GTP	C3'-C2'-C1'	2.07	105.39	101.46
163	IB	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	LI	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	AF	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	CO	500	GDP	O6-C6-C5	-2.07	121.06	126.53
165	WY	501	GTP	C3'-C2'-C1'	2.07	105.39	101.46
163	NF	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	AD	500	GDP	C3'-C2'-C1'	2.07	105.39	101.46
163	KA	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	VH	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	FJ	501	GDP	C3'-C2'-C1'	2.07	105.38	101.46
165	MG	501	GTP	C3'-C2'-C1'	2.07	105.38	101.46
163	UP	500	GDP	O6-C6-C5	-2.07	121.06	126.53
165	IG	501	GTP	C3'-C2'-C1'	2.07	105.38	101.46
163	KS	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	PN	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	PX	501	GDP	O6-C6-C5	-2.07	121.06	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	RK	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	VB	500	GDP	O6-C6-C5	-2.07	121.06	126.53
163	FN	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	UV	500	GDP	O6-C6-C5	-2.07	121.07	126.53
165	BG	501	GTP	C3'-C2'-C1'	2.07	105.38	101.46
163	TH	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	LO	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	UD	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	N	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	RU	500	GDP	O6-C6-C5	-2.07	121.07	126.53
165	UE	501	GTP	C3'-C2'-C1'	2.07	105.38	101.46
165	US	501	GTP	C3'-C2'-C1'	2.07	105.38	101.46
163	SF	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	IN	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	HX	501	GDP	O6-C6-C5	-2.07	121.07	126.53
163	FB	500	GDP	C2'-C3'-C4'	2.07	106.61	102.61
163	QK	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	QQ	500	GDP	O6-C6-C5	-2.07	121.07	126.53
163	DU	500	GDP	O6-C6-C5	-2.07	121.08	126.53
165	HA	501	GTP	C3'-C2'-C1'	2.07	105.37	101.46
163	ID	500	GDP	O6-C6-C5	-2.07	121.08	126.53
163	JG	500	GDP	O6-C6-C5	-2.07	121.08	126.53
165	OP	503	GTP	O3G-PG-O3B	2.07	111.57	104.64
165	OS	501	GTP	C3'-C2'-C1'	2.07	105.37	101.46
163	PV	500	GDP	O6-C6-C5	-2.07	121.08	126.53
163	EH	500	GDP	C3'-C2'-C1'	2.07	105.37	101.46
163	PB	500	GDP	C3'-C2'-C1'	2.07	105.37	101.46
165	OG	501	GTP	C3'-C2'-C1'	2.07	105.37	101.46
163	HF	500	GDP	O6-C6-C5	-2.07	121.08	126.53
163	HT	501	GDP	O6-C6-C5	-2.07	121.08	126.53
165	EI	501	GTP	C3'-C2'-C1'	2.06	105.37	101.46
165	QR	501	GTP	C3'-C2'-C1'	2.06	105.37	101.46
163	HR	500	GDP	O6-C6-C5	-2.06	121.08	126.53
163	JO	500	GDP	O6-C6-C5	-2.06	121.08	126.53
163	KO	500	GDP	O6-C6-C5	-2.06	121.08	126.53
163	MR	500	GDP	O6-C6-C5	-2.06	121.08	126.53
163	CO	500	GDP	C3'-C2'-C1'	2.06	105.37	101.46
163	KC	500	GDP	O6-C6-C5	-2.06	121.08	126.53
163	OT	500	GDP	O6-C6-C5	-2.06	121.08	126.53
163	SB	501	GDP	C3'-C2'-C1'	2.06	105.37	101.46
165	HU	501	GTP	C3'-C2'-C1'	2.06	105.37	101.46
163	PR	501	GDP	O6-C6-C5	-2.06	121.09	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
165	QU	501	GTP	O3G-PG-O3B	2.06	111.55	104.64
163	LS	500	GDP	O6-C6-C5	-2.06	121.09	126.53
163	KC	500	GDP	C3'-C2'-C1'	2.06	105.36	101.46
163	VV	500	GDP	O6-C6-C5	-2.06	121.09	126.53
163	OV	500	GDP	O6-C6-C5	-2.06	121.09	126.53
165	AO	501	GTP	C3'-C2'-C1'	2.06	105.36	101.46
163	DI	500	GDP	C2'-C3'-C4'	2.06	106.59	102.61
163	PV	500	GDP	C3'-C2'-C1'	2.06	105.36	101.46
165	HM	501	GTP	C3'-C2'-C1'	2.06	105.36	101.46
163	KW	500	GDP	O6-C6-C5	-2.06	121.09	126.53
165	DH	501	GTP	C3'-C2'-C1'	2.06	105.36	101.46
163	LQ	500	GDP	O6-C6-C5	-2.06	121.10	126.53
163	VT	500	GDP	O6-C6-C5	-2.06	121.10	126.53
163	MN	500	GDP	C2'-C3'-C4'	2.06	106.59	102.61
163	TX	500	GDP	O6-C6-C5	-2.06	121.10	126.53
165	JT	501	GTP	C3'-C2'-C1'	2.06	105.36	101.46
165	DP	501	GTP	O3G-PG-O3B	2.06	111.54	104.64
163	OP	501	GDP	C3'-C2'-C1'	2.06	105.36	101.46
165	TE	501	GTP	C3'-C2'-C1'	2.06	105.36	101.46
163	BD	500	GDP	O6-C6-C5	-2.06	121.10	126.53
163	HB	501	GDP	O6-C6-C5	-2.06	121.10	126.53
163	HL	501	GDP	O6-C6-C5	-2.06	121.10	126.53
163	LC	500	GDP	O6-C6-C5	-2.06	121.10	126.53
163	VJ	500	GDP	O6-C6-C5	-2.06	121.10	126.53
163	NX	500	GDP	O6-C6-C5	-2.06	121.10	126.53
163	NL	500	GDP	C3'-C2'-C1'	2.06	105.35	101.46
163	BH	500	GDP	C2'-C3'-C4'	2.06	106.58	102.61
163	FN	500	GDP	C2'-C3'-C4'	2.06	106.58	102.61
163	DY	500	GDP	O6-C6-C5	-2.06	121.11	126.53
165	GK	501	GTP	O3G-PG-O3B	2.06	111.53	104.64
165	TU	501	GTP	C3'-C2'-C1'	2.06	105.35	101.46
163	VN	500	GDP	O6-C6-C5	-2.06	121.11	126.53
163	CG	500	GDP	C2'-C3'-C4'	2.06	106.58	102.61
163	HH	501	GDP	O6-C6-C5	-2.06	121.11	126.53
163	AL	500	GDP	C3'-C2'-C1'	2.06	105.35	101.46
165	AP	501	GTP	C3'-C2'-C1'	2.05	105.35	101.46
163	QA	500	GDP	O6-C6-C5	-2.05	121.11	126.53
165	TQ	501	GTP	C3'-C2'-C1'	2.05	105.35	101.46
163	EJ	500	GDP	C3'-C2'-C1'	2.05	105.35	101.46
165	HE	501	GTP	C3'-C2'-C1'	2.05	105.35	101.46
163	DC	500	GDP	O6-C6-C5	-2.05	121.11	126.53
163	RA	500	GDP	O6-C6-C5	-2.05	121.11	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	HN	501	GDP	O6-C6-C5	-2.05	121.11	126.53
163	LG	501	GDP	O6-C6-C5	-2.05	121.11	126.53
165	EJ	501	GTP	C3'-C2'-C1'	2.05	105.34	101.46
163	VJ	500	GDP	C2'-C3'-C4'	2.05	106.57	102.61
163	MF	500	GDP	O6-C6-C5	-2.05	121.12	126.53
165	NQ	501	GTP	C3'-C2'-C1'	2.05	105.34	101.46
165	QI	501	GTP	O3G-PG-O3B	2.05	111.51	104.64
163	PB	500	GDP	O6-C6-C5	-2.05	121.12	126.53
163	JY	501	GDP	O6-C6-C5	-2.05	121.12	126.53
163	EP	500	GDP	C3'-C2'-C1'	2.05	105.34	101.46
163	RM	500	GDP	O6-C6-C5	-2.05	121.12	126.53
163	RI	500	GDP	O6-C6-C5	-2.05	121.12	126.53
165	NU	501	GTP	C3'-C2'-C1'	2.05	105.34	101.46
163	PF	501	GDP	O6-C6-C5	-2.05	121.13	126.53
163	V	500	GDP	O6-C6-C5	-2.05	121.13	126.53
165	OD	503	GTP	O3G-PG-O3B	2.05	111.50	104.64
163	PH	500	GDP	O6-C6-C5	-2.05	121.13	126.53
163	WJ	500	GDP	O6-C6-C5	-2.05	121.13	126.53
163	QM	500	GDP	O6-C6-C5	-2.05	121.13	126.53
163	LY	500	GDP	O6-C6-C5	-2.05	121.13	126.53
163	UL	500	GDP	O6-C6-C5	-2.05	121.13	126.53
165	DD	501	GTP	N2-C2-N1	2.05	121.08	116.76
165	HQ	501	GTP	C3'-C2'-C1'	2.05	105.33	101.46
163	BP	500	GDP	O6-C6-C5	-2.05	121.13	126.53
163	TT	500	GDP	O6-C6-C5	-2.05	121.13	126.53
163	ER	500	GDP	O6-C6-C5	-2.04	121.14	126.53
163	BP	500	GDP	C2'-C3'-C4'	2.04	106.56	102.61
163	OH	500	GDP	C3'-C2'-C1'	2.04	105.33	101.46
163	OL	500	GDP	O6-C6-C5	-2.04	121.14	126.53
165	JN	501	GTP	C3'-C2'-C1'	2.04	105.33	101.46
165	UC	501	GTP	C3'-C2'-C1'	2.04	105.33	101.46
163	CG	500	GDP	O6-C6-C5	-2.04	121.14	126.53
163	UJ	500	GDP	C3'-C2'-C1'	2.04	105.33	101.46
163	UV	500	GDP	C3'-C2'-C1'	2.04	105.33	101.46
165	JV	501	GTP	C3'-C2'-C1'	2.04	105.33	101.46
165	GI	501	GTP	O3G-PG-O3B	2.04	111.48	104.64
163	DS	500	GDP	C3'-C2'-C1'	2.04	105.32	101.46
165	LJ	501	GTP	C3'-C2'-C1'	2.04	105.32	101.46
163	CE	500	GDP	O6-C6-C5	-2.04	121.14	126.53
163	LM	500	GDP	O6-C6-C5	-2.04	121.15	126.53
165	Q	501	GTP	C3'-C2'-C1'	2.04	105.32	101.46
165	UO	501	GTP	C3'-C2'-C1'	2.04	105.32	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	JM	501	GDP	O6-C6-C5	-2.04	121.15	126.53
165	LN	502	GTP	C3'-C2'-C1'	2.04	105.32	101.46
163	LE	500	GDP	O6-C6-C5	-2.04	121.15	126.53
163	AV	500	GDP	C2'-C3'-C4'	2.04	106.55	102.61
163	DK	501	GDP	C3'-C2'-C1'	2.04	105.32	101.46
163	DM	500	GDP	C3'-C2'-C1'	2.04	105.32	101.46
165	UU	501	GTP	C3'-C2'-C1'	2.04	105.32	101.46
163	VL	500	GDP	O6-C6-C5	-2.04	121.15	126.53
163	DQ	500	GDP	O6-C6-C5	-2.04	121.15	126.53
163	AD	500	GDP	C2'-C3'-C4'	2.04	106.55	102.61
163	KK	500	GDP	C3'-C2'-C1'	2.04	105.32	101.46
163	WV	500	GDP	O6-C6-C5	-2.04	121.15	126.53
163	RA	500	GDP	C2'-C3'-C4'	2.04	106.55	102.61
165	JZ	501	GTP	C3'-C2'-C1'	2.04	105.32	101.46
163	AL	500	GDP	C2'-C3'-C4'	2.04	106.55	102.61
163	FN	500	GDP	C3'-C2'-C1'	2.04	105.32	101.46
163	RS	500	GDP	O6-C6-C5	-2.04	121.16	126.53
163	GT	501	GDP	C3'-C2'-C1'	2.04	105.31	101.46
163	OX	500	GDP	O6-C6-C5	-2.03	121.16	126.53
163	RQ	500	GDP	C2'-C3'-C4'	2.03	106.54	102.61
163	AT	500	GDP	C2'-C3'-C4'	2.03	106.54	102.61
163	FP	500	GDP	C3'-C2'-C1'	2.03	105.31	101.46
163	NP	500	GDP	O2A-PA-O3A	2.03	112.77	107.27
163	RM	500	GDP	C2'-C3'-C4'	2.03	106.54	102.61
163	SN	501	GDP	C3'-C2'-C1'	2.03	105.31	101.46
165	JJ	501	GTP	C3'-C2'-C1'	2.03	105.31	101.46
165	LV	501	GTP	C3'-C2'-C1'	2.03	105.31	101.46
163	NL	500	GDP	O6-C6-C5	-2.03	121.17	126.53
165	OO	501	GTP	C3'-C2'-C1'	2.03	105.31	101.46
163	FT	501	GDP	O6-C6-C5	-2.03	121.17	126.53
165	CE	501	GTP	O3G-PG-O3B	2.03	111.45	104.64
165	MY	501	GTP	C3'-C2'-C1'	2.03	105.30	101.46
163	CM	500	GDP	O6-C6-C5	-2.03	121.17	126.53
165	DB	501	GTP	C4-C5-N7	-2.03	107.45	110.67
165	WC	501	GTP	C3'-C2'-C1'	2.03	105.30	101.46
163	KK	500	GDP	O6-C6-C5	-2.03	121.18	126.53
165	OC	501	GTP	C3'-C2'-C1'	2.03	105.30	101.46
165	BE	501	GTP	O3G-PG-O3B	2.03	111.44	104.64
163	GR	500	GDP	O6-C6-C5	-2.03	121.18	126.53
163	PT	500	GDP	O6-C6-C5	-2.03	121.18	126.53
163	UL	500	GDP	C3'-C2'-C1'	2.03	105.30	101.46
163	RE	500	GDP	C2'-C3'-C4'	2.03	106.53	102.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	AX	500	GDP	C2'-C3'-C4'	2.03	106.53	102.61
163	OT	500	GDP	C2'-C3'-C4'	2.03	106.52	102.61
163	PJ	500	GDP	C3'-C2'-C1'	2.03	105.30	101.46
165	NY	501	GTP	C3'-C2'-C1'	2.03	105.30	101.46
163	RC	500	GDP	O6-C6-C5	-2.03	121.19	126.53
163	MF	500	GDP	C2'-C3'-C4'	2.02	106.52	102.61
165	DQ	501	GTP	C3'-C2'-C1'	2.02	105.29	101.46
165	LZ	502	GTP	C3'-C2'-C1'	2.02	105.29	101.46
165	WW	501	GTP	C3'-C2'-C1'	2.02	105.29	101.46
163	AX	500	GDP	O6-C6-C5	-2.02	121.19	126.53
163	ID	500	GDP	C3'-C2'-C1'	2.02	105.29	101.46
163	VX	500	GDP	O6-C6-C5	-2.02	121.20	126.53
163	VV	500	GDP	C2'-C3'-C4'	2.02	106.51	102.61
163	BJ	500	GDP	C3'-C2'-C1'	2.02	105.28	101.46
163	DU	500	GDP	C3'-C2'-C1'	2.02	105.28	101.46
163	DI	500	GDP	O6-C6-C5	-2.02	121.20	126.53
163	WF	501	GDP	C3'-C2'-C1'	2.02	105.28	101.46
165	SE	501	GTP	C3'-C2'-C1'	2.02	105.28	101.46
165	SW	501	GTP	C3'-C2'-C1'	2.02	105.28	101.46
165	DD	501	GTP	C4-C5-N7	-2.02	107.48	110.67
163	CC	500	GDP	C2'-C3'-C4'	2.02	106.50	102.61
163	BR	500	GDP	C2'-C3'-C4'	2.02	106.50	102.61
163	CU	500	GDP	C2'-C3'-C4'	2.02	106.50	102.61
165	NE	501	GTP	C3'-C2'-C1'	2.02	105.28	101.46
163	RO	500	GDP	O6-C6-C5	-2.01	121.21	126.53
163	FH	500	GDP	C2'-C3'-C4'	2.01	106.50	102.61
165	RT	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
163	E	500	GDP	C8-N7-C5	2.01	107.85	104.26
163	EH	500	GDP	O6-C6-C5	-2.01	121.22	126.53
165	TI	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
165	CQ	501	GTP	O3G-PG-O3B	2.01	111.39	104.64
163	ND	500	GDP	O2A-PA-O3A	2.01	112.71	107.27
165	SQ	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
165	FT	503	GTP	O2A-PA-O3A	2.01	112.71	107.27
165	NA	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
165	PW	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
165	R	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
165	WE	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
165	QT	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
165	UI	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
165	D	501	GTP	O2B-PB-O3B	2.01	112.70	107.27
165	MM	501	GTP	C3'-C2'-C1'	2.01	105.26	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
163	MZ	500	GDP	C2'-C3'-C4'	2.01	106.49	102.61
165	LF	502	GTP	C3'-C2'-C1'	2.01	105.26	101.46
163	E	500	GDP	O3B-PB-O3A	2.01	111.37	104.64
165	HB	503	GTP	O3G-PG-O3B	2.01	111.37	104.64
163	EB	500	GDP	O6-C6-C5	-2.01	121.23	126.53
163	JU	500	GDP	C2'-C3'-C4'	2.01	106.49	102.61
163	CU	500	GDP	O6-C6-C5	-2.01	121.23	126.53
165	LB	501	GTP	C3'-C2'-C1'	2.01	105.26	101.46
163	PF	501	GDP	C3'-C2'-C1'	2.01	105.26	101.46
163	MB	500	GDP	C3'-C2'-C1'	2.01	105.26	101.46
163	DW	501	GDP	O6-C6-C5	-2.01	121.24	126.53
163	GN	500	GDP	C2'-C3'-C4'	2.01	106.48	102.61
163	WR	501	GDP	C3'-C2'-C1'	2.01	105.26	101.46
165	TW	501	GTP	C3'-C2'-C1'	2.01	105.26	101.46
165	VC	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46
163	BD	500	GDP	O3B-PB-O3A	2.00	111.36	104.64
165	BE	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46
165	MO	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46
163	JI	500	GDP	C2'-C3'-C4'	2.00	106.48	102.61
165	WO	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46
163	AH	500	GDP	C2'-C3'-C4'	2.00	106.47	102.61
163	EX	500	GDP	C2'-C3'-C4'	2.00	106.47	102.61
165	FO	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (1851) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
163	AB	500	GDP	C5'-O5'-PA-O3A
163	AB	500	GDP	C5'-O5'-PA-O1A
163	AD	500	GDP	C5'-O5'-PA-O3A
163	AD	500	GDP	C5'-O5'-PA-O1A
163	AF	500	GDP	C5'-O5'-PA-O1A
163	AH	500	GDP	C5'-O5'-PA-O1A
163	AJ	500	GDP	C5'-O5'-PA-O3A
163	AL	500	GDP	C5'-O5'-PA-O1A
163	AN	500	GDP	C5'-O5'-PA-O3A
163	BD	500	GDP	C5'-O5'-PA-O3A
163	BD	500	GDP	C5'-O5'-PA-O1A
163	BF	500	GDP	C5'-O5'-PA-O1A
163	BH	500	GDP	C5'-O5'-PA-O3A
163	BH	500	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	BH	500	GDP	C5'-O5'-PA-O2A
163	BJ	500	GDP	C5'-O5'-PA-O3A
163	BL	500	GDP	C5'-O5'-PA-O3A
163	BL	500	GDP	C5'-O5'-PA-O1A
163	BN	500	GDP	C5'-O5'-PA-O3A
163	BN	500	GDP	C5'-O5'-PA-O2A
163	CA	500	GDP	C5'-O5'-PA-O3A
163	CA	500	GDP	C5'-O5'-PA-O1A
163	CA	500	GDP	C5'-O5'-PA-O2A
163	CE	500	GDP	C5'-O5'-PA-O3A
163	CE	500	GDP	C5'-O5'-PA-O1A
163	CG	500	GDP	C5'-O5'-PA-O1A
163	CI	500	GDP	C5'-O5'-PA-O3A
163	CI	500	GDP	C5'-O5'-PA-O1A
163	CK	501	GDP	C5'-O5'-PA-O3A
163	CK	501	GDP	C5'-O5'-PA-O2A
163	CK	501	GDP	O4'-C4'-C5'-O5'
163	CM	500	GDP	C5'-O5'-PA-O3A
163	CM	500	GDP	C5'-O5'-PA-O1A
163	CM	500	GDP	C5'-O5'-PA-O2A
163	DA	500	GDP	C5'-O5'-PA-O3A
163	DA	500	GDP	C5'-O5'-PA-O1A
163	DC	500	GDP	C5'-O5'-PA-O3A
163	DC	500	GDP	C5'-O5'-PA-O1A
163	DE	500	GDP	C5'-O5'-PA-O3A
163	DE	500	GDP	C5'-O5'-PA-O1A
163	DG	500	GDP	C5'-O5'-PA-O3A
163	DI	500	GDP	C5'-O5'-PA-O3A
163	DK	501	GDP	C5'-O5'-PA-O3A
163	DM	500	GDP	C5'-O5'-PA-O3A
163	DM	500	GDP	C5'-O5'-PA-O1A
163	E	500	GDP	PA-O3A-PB-O2B
163	E	500	GDP	C5'-O5'-PA-O3A
163	E	500	GDP	C5'-O5'-PA-O2A
163	EB	500	GDP	C5'-O5'-PA-O3A
163	EB	500	GDP	C5'-O5'-PA-O1A
163	ED	500	GDP	C5'-O5'-PA-O3A
163	ED	500	GDP	C5'-O5'-PA-O1A
163	EF	500	GDP	C5'-O5'-PA-O3A
163	EF	500	GDP	C5'-O5'-PA-O2A
163	EJ	500	GDP	C5'-O5'-PA-O1A
163	EL	500	GDP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	EL	500	GDP	C5'-O5'-PA-O1A
163	EL	500	GDP	C5'-O5'-PA-O2A
163	FD	500	GDP	C5'-O5'-PA-O3A
163	FD	500	GDP	C5'-O5'-PA-O1A
163	FF	500	GDP	C5'-O5'-PA-O3A
163	FF	500	GDP	C5'-O5'-PA-O1A
163	FJ	501	GDP	C5'-O5'-PA-O1A
163	FL	500	GDP	C5'-O5'-PA-O3A
163	GB	500	GDP	C5'-O5'-PA-O1A
163	GD	500	GDP	C5'-O5'-PA-O3A
163	GF	500	GDP	C5'-O5'-PA-O1A
163	GH	500	GDP	C5'-O5'-PA-O3A
163	GJ	500	GDP	C5'-O5'-PA-O3A
163	GJ	500	GDP	C5'-O5'-PA-O1A
163	GL	500	GDP	C5'-O5'-PA-O1A
163	H	500	GDP	C5'-O5'-PA-O1A
163	HD	501	GDP	C5'-O5'-PA-O1A
163	HH	501	GDP	C5'-O5'-PA-O1A
163	HJ	500	GDP	C5'-O5'-PA-O3A
163	HJ	500	GDP	C5'-O5'-PA-O1A
163	IB	500	GDP	C5'-O5'-PA-O1A
163	IF	500	GDP	C5'-O5'-PA-O1A
163	IJ	500	GDP	C5'-O5'-PA-O3A
163	IJ	500	GDP	C5'-O5'-PA-O1A
163	JI	500	GDP	C5'-O5'-PA-O1A
163	JK	500	GDP	C5'-O5'-PA-O3A
163	JK	500	GDP	C5'-O5'-PA-O1A
163	JK	500	GDP	C5'-O5'-PA-O2A
163	KC	500	GDP	C5'-O5'-PA-O1A
163	KG	500	GDP	C5'-O5'-PA-O3A
163	KG	500	GDP	C5'-O5'-PA-O1A
163	LC	500	GDP	C5'-O5'-PA-O3A
163	LC	500	GDP	C5'-O5'-PA-O1A
163	LE	500	GDP	C5'-O5'-PA-O1A
163	LG	501	GDP	C5'-O5'-PA-O1A
163	LO	500	GDP	C5'-O5'-PA-O3A
163	LO	500	GDP	C5'-O5'-PA-O1A
163	M	500	GDP	C5'-O5'-PA-O1A
163	MD	500	GDP	C5'-O5'-PA-O1A
163	MH	500	GDP	C5'-O5'-PA-O1A
163	MJ	500	GDP	O4'-C4'-C5'-O5'
163	N	500	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	NB	500	GDP	C5'-O5'-PA-O1A
163	NF	500	GDP	C5'-O5'-PA-O1A
163	NH	500	GDP	C5'-O5'-PA-O1A
163	OB	500	GDP	C5'-O5'-PA-O3A
163	OB	500	GDP	C5'-O5'-PA-O1A
163	OB	500	GDP	C5'-O5'-PA-O2A
163	OF	500	GDP	C5'-O5'-PA-O1A
163	OH	500	GDP	C5'-O5'-PA-O1A
163	PB	500	GDP	C5'-O5'-PA-O1A
163	PD	500	GDP	C5'-O5'-PA-O1A
163	PH	500	GDP	C5'-O5'-PA-O1A
163	PL	501	GDP	C5'-O5'-PA-O1A
163	QA	500	GDP	C5'-O5'-PA-O1A
163	QC	500	GDP	C5'-O5'-PA-O3A
163	QE	500	GDP	C5'-O5'-PA-O1A
163	QG	500	GDP	C5'-O5'-PA-O1A
163	QI	500	GDP	C5'-O5'-PA-O3A
163	QK	500	GDP	C5'-O5'-PA-O3A
163	QK	500	GDP	C5'-O5'-PA-O2A
163	QK	500	GDP	C3'-C4'-C5'-O5'
163	RA	500	GDP	C5'-O5'-PA-O1A
163	RC	500	GDP	C5'-O5'-PA-O1A
163	RG	500	GDP	C5'-O5'-PA-O1A
163	S	500	GDP	C5'-O5'-PA-O3A
163	S	500	GDP	C5'-O5'-PA-O1A
163	SB	501	GDP	C5'-O5'-PA-O1A
163	SD	500	GDP	C5'-O5'-PA-O1A
163	SF	500	GDP	C5'-O5'-PA-O1A
163	TB	500	GDP	C5'-O5'-PA-O3A
163	TB	500	GDP	C5'-O5'-PA-O1A
163	TB	500	GDP	C5'-O5'-PA-O2A
163	TF	500	GDP	C5'-O5'-PA-O1A
163	TH	500	GDP	C5'-O5'-PA-O1A
163	TJ	500	GDP	C5'-O5'-PA-O3A
163	TJ	500	GDP	C5'-O5'-PA-O1A
163	U	500	GDP	C5'-O5'-PA-O3A
163	U	500	GDP	C5'-O5'-PA-O1A
163	UB	500	GDP	C5'-O5'-PA-O3A
163	UB	500	GDP	C5'-O5'-PA-O2A
163	UD	500	GDP	C5'-O5'-PA-O3A
163	UD	500	GDP	C5'-O5'-PA-O1A
163	UD	500	GDP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	UF	500	GDP	C5'-O5'-PA-O1A
163	UH	500	GDP	C5'-O5'-PA-O1A
163	VB	500	GDP	C5'-O5'-PA-O1A
163	VD	500	GDP	C5'-O5'-PA-O1A
163	VF	500	GDP	C5'-O5'-PA-O1A
163	VJ	500	GDP	C5'-O5'-PA-O3A
163	VJ	500	GDP	C5'-O5'-PA-O1A
163	VL	500	GDP	C5'-O5'-PA-O1A
163	WD	500	GDP	C5'-O5'-PA-O3A
163	WD	500	GDP	C5'-O5'-PA-O1A
163	WH	500	GDP	C5'-O5'-PA-O1A
163	WJ	500	GDP	C5'-O5'-PA-O1A
163	WL	500	GDP	C5'-O5'-PA-O1A
163	AR	500	GDP	C5'-O5'-PA-O1A
163	AT	500	GDP	C5'-O5'-PA-O3A
163	AT	500	GDP	C5'-O5'-PA-O1A
163	AV	500	GDP	C5'-O5'-PA-O3A
163	AX	500	GDP	C5'-O5'-PA-O1A
163	AZ	500	GDP	C5'-O5'-PA-O3A
163	BP	500	GDP	C5'-O5'-PA-O1A
163	BR	500	GDP	C5'-O5'-PA-O3A
163	BT	500	GDP	C5'-O5'-PA-O3A
163	BT	500	GDP	C5'-O5'-PA-O1A
163	BT	500	GDP	C5'-O5'-PA-O2A
163	BV	500	GDP	C5'-O5'-PA-O3A
163	BX	500	GDP	C5'-O5'-PA-O1A
163	CQ	500	GDP	C5'-O5'-PA-O3A
163	CQ	500	GDP	C5'-O5'-PA-O1A
163	CS	500	GDP	C5'-O5'-PA-O3A
163	CS	500	GDP	C5'-O5'-PA-O1A
163	CW	500	GDP	C5'-O5'-PA-O3A
163	CW	500	GDP	C5'-O5'-PA-O2A
163	CW	500	GDP	O4'-C4'-C5'-O5'
163	CY	500	GDP	C5'-O5'-PA-O3A
163	CY	500	GDP	C5'-O5'-PA-O1A
163	CY	500	GDP	C5'-O5'-PA-O2A
163	DO	500	GDP	C5'-O5'-PA-O1A
163	DQ	500	GDP	C5'-O5'-PA-O3A
163	DQ	500	GDP	C5'-O5'-PA-O1A
163	DS	500	GDP	C5'-O5'-PA-O3A
163	DU	500	GDP	C5'-O5'-PA-O3A
163	DU	500	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	DW	501	GDP	C5'-O5'-PA-O1A
163	EN	500	GDP	C5'-O5'-PA-O1A
163	EP	500	GDP	C5'-O5'-PA-O1A
163	ER	500	GDP	C5'-O5'-PA-O3A
163	EV	500	GDP	C5'-O5'-PA-O3A
163	EX	500	GDP	C5'-O5'-PA-O3A
163	EX	500	GDP	C5'-O5'-PA-O2A
163	FP	500	GDP	C5'-O5'-PA-O1A
163	FR	501	GDP	C5'-O5'-PA-O1A
163	FX	500	GDP	C5'-O5'-PA-O3A
163	FX	500	GDP	C5'-O5'-PA-O1A
163	GN	500	GDP	C5'-O5'-PA-O1A
163	GP	500	GDP	C5'-O5'-PA-O3A
163	GT	501	GDP	C5'-O5'-PA-O3A
163	GV	501	GDP	C5'-O5'-PA-O3A
163	GV	501	GDP	C5'-O5'-PA-O1A
163	GX	500	GDP	C5'-O5'-PA-O3A
163	GX	500	GDP	C5'-O5'-PA-O1A
163	HP	501	GDP	C5'-O5'-PA-O1A
163	HT	501	GDP	C5'-O5'-PA-O1A
163	HV	500	GDP	C5'-O5'-PA-O3A
163	HV	500	GDP	C5'-O5'-PA-O1A
163	IN	500	GDP	C5'-O5'-PA-O1A
163	IR	500	GDP	C5'-O5'-PA-O1A
163	IV	500	GDP	C5'-O5'-PA-O3A
163	IV	500	GDP	C5'-O5'-PA-O1A
163	JU	500	GDP	C5'-O5'-PA-O1A
163	JW	500	GDP	C5'-O5'-PA-O3A
163	JW	500	GDP	C5'-O5'-PA-O1A
163	JW	500	GDP	C5'-O5'-PA-O2A
163	KO	500	GDP	C5'-O5'-PA-O1A
163	KS	500	GDP	C5'-O5'-PA-O3A
163	KS	500	GDP	C5'-O5'-PA-O1A
163	LQ	500	GDP	C5'-O5'-PA-O1A
163	LS	500	GDP	C5'-O5'-PA-O1A
163	MP	500	GDP	C5'-O5'-PA-O1A
163	MT	500	GDP	C5'-O5'-PA-O1A
163	MV	500	GDP	O4'-C4'-C5'-O5'
163	PN	500	GDP	C5'-O5'-PA-O1A
163	PP	500	GDP	C5'-O5'-PA-O1A
163	PT	500	GDP	C5'-O5'-PA-O1A
163	PX	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	QM	500	GDP	C5'-O5'-PA-O1A
163	QO	500	GDP	C5'-O5'-PA-O3A
163	QQ	500	GDP	C5'-O5'-PA-O1A
163	QS	500	GDP	C5'-O5'-PA-O1A
163	QU	500	GDP	C5'-O5'-PA-O3A
163	QW	500	GDP	C5'-O5'-PA-O3A
163	QW	500	GDP	C5'-O5'-PA-O2A
163	QW	500	GDP	C3'-C4'-C5'-O5'
163	RM	500	GDP	C5'-O5'-PA-O1A
163	RO	500	GDP	C5'-O5'-PA-O1A
163	RS	500	GDP	C5'-O5'-PA-O1A
163	SL	500	GDP	C5'-O5'-PA-O3A
163	SL	500	GDP	C5'-O5'-PA-O1A
163	SN	501	GDP	C5'-O5'-PA-O1A
163	SP	500	GDP	C5'-O5'-PA-O1A
163	SR	500	GDP	C5'-O5'-PA-O1A
163	TN	500	GDP	C5'-O5'-PA-O3A
163	TN	500	GDP	C5'-O5'-PA-O1A
163	TN	500	GDP	C5'-O5'-PA-O2A
163	TR	500	GDP	C5'-O5'-PA-O1A
163	TT	500	GDP	C5'-O5'-PA-O1A
163	TV	500	GDP	C5'-O5'-PA-O3A
163	TV	500	GDP	C5'-O5'-PA-O1A
163	UN	500	GDP	C5'-O5'-PA-O3A
163	UN	500	GDP	C5'-O5'-PA-O2A
163	UP	500	GDP	C5'-O5'-PA-O3A
163	UP	500	GDP	C5'-O5'-PA-O1A
163	UP	500	GDP	C5'-O5'-PA-O2A
163	UR	500	GDP	C5'-O5'-PA-O1A
163	UT	500	GDP	C5'-O5'-PA-O1A
163	VN	500	GDP	C5'-O5'-PA-O1A
163	VP	500	GDP	C5'-O5'-PA-O1A
163	VR	500	GDP	C5'-O5'-PA-O1A
163	VV	500	GDP	C5'-O5'-PA-O3A
163	VV	500	GDP	C5'-O5'-PA-O1A
163	VX	500	GDP	C5'-O5'-PA-O1A
163	WP	500	GDP	C5'-O5'-PA-O3A
163	WP	500	GDP	C5'-O5'-PA-O1A
163	WT	500	GDP	C5'-O5'-PA-O1A
163	WV	500	GDP	C5'-O5'-PA-O1A
163	WX	500	GDP	C5'-O5'-PA-O1A
163	NN	500	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	NR	500	GDP	C5'-O5'-PA-O1A
163	NT	500	GDP	C5'-O5'-PA-O1A
163	ON	500	GDP	C5'-O5'-PA-O3A
163	ON	500	GDP	C5'-O5'-PA-O1A
163	ON	500	GDP	C5'-O5'-PA-O2A
163	OR	500	GDP	C5'-O5'-PA-O1A
163	OT	500	GDP	C5'-O5'-PA-O1A
165	AB	501	GTP	C5'-O5'-PA-O3A
165	AB	501	GTP	C5'-O5'-PA-O1A
165	AB	501	GTP	C5'-O5'-PA-O2A
165	AD	501	GTP	C5'-O5'-PA-O3A
165	AD	501	GTP	C5'-O5'-PA-O1A
165	AD	501	GTP	C5'-O5'-PA-O2A
165	AG	501	GTP	C5'-O5'-PA-O3A
165	AG	501	GTP	C5'-O5'-PA-O1A
165	AG	501	GTP	C5'-O5'-PA-O2A
165	AI	501	GTP	O4'-C4'-C5'-O5'
165	AK	501	GTP	C5'-O5'-PA-O3A
165	AK	501	GTP	C5'-O5'-PA-O1A
165	AK	501	GTP	C5'-O5'-PA-O2A
165	AM	501	GTP	PB-O3A-PA-O5'
165	BA	501	GTP	C5'-O5'-PA-O3A
165	BA	501	GTP	C5'-O5'-PA-O1A
165	BA	501	GTP	C5'-O5'-PA-O2A
165	BE	501	GTP	C5'-O5'-PA-O3A
165	BE	501	GTP	C5'-O5'-PA-O1A
165	BE	501	GTP	C5'-O5'-PA-O2A
165	BI	501	GTP	C5'-O5'-PA-O3A
165	BI	501	GTP	C5'-O5'-PA-O1A
165	BI	501	GTP	C5'-O5'-PA-O2A
165	BK	501	GTP	C5'-O5'-PA-O3A
165	BK	501	GTP	C5'-O5'-PA-O1A
165	BK	501	GTP	C5'-O5'-PA-O2A
165	BM	501	GTP	C5'-O5'-PA-O3A
165	BM	501	GTP	C5'-O5'-PA-O1A
165	BM	501	GTP	C5'-O5'-PA-O2A
165	C	501	GTP	PB-O3B-PG-O3G
165	C	501	GTP	C5'-O5'-PA-O3A
165	CB	501	GTP	C5'-O5'-PA-O3A
165	CB	501	GTP	C5'-O5'-PA-O1A
165	CB	501	GTP	C5'-O5'-PA-O2A
165	CC	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	CC	501	GTP	C5'-O5'-PA-O1A
165	CE	501	GTP	C5'-O5'-PA-O3A
165	CH	501	GTP	O4'-C4'-C5'-O5'
165	CH	501	GTP	C3'-C4'-C5'-O5'
165	CJ	501	GTP	C5'-O5'-PA-O3A
165	CJ	501	GTP	C5'-O5'-PA-O1A
165	CJ	501	GTP	C5'-O5'-PA-O2A
165	D	501	GTP	PB-O3B-PG-O3G
165	D	501	GTP	C5'-O5'-PA-O3A
165	DB	501	GTP	C5'-O5'-PA-O3A
165	DB	501	GTP	C5'-O5'-PA-O2A
165	DD	501	GTP	C5'-O5'-PA-O3A
165	DD	501	GTP	C5'-O5'-PA-O1A
165	DD	501	GTP	C5'-O5'-PA-O2A
165	DE	501	GTP	C5'-O5'-PA-O1A
165	DJ	501	GTP	C5'-O5'-PA-O3A
165	DJ	501	GTP	C5'-O5'-PA-O1A
165	DL	501	GTP	PB-O3B-PG-O2G
165	DL	501	GTP	PB-O3B-PG-O3G
165	DL	501	GTP	PB-O3A-PA-O5'
165	DL	501	GTP	C5'-O5'-PA-O3A
165	EA	501	GTP	C5'-O5'-PA-O3A
165	EA	501	GTP	C5'-O5'-PA-O1A
165	EC	501	GTP	C5'-O5'-PA-O3A
165	EC	501	GTP	C5'-O5'-PA-O1A
165	EC	501	GTP	C5'-O5'-PA-O2A
165	ED	501	GTP	C5'-O5'-PA-O3A
165	ED	501	GTP	C5'-O5'-PA-O1A
165	EG	501	GTP	C5'-O5'-PA-O3A
165	EG	501	GTP	C5'-O5'-PA-O1A
165	EG	501	GTP	C5'-O5'-PA-O2A
165	EI	501	GTP	C5'-O5'-PA-O3A
165	EI	501	GTP	C5'-O5'-PA-O2A
165	EI	501	GTP	O4'-C4'-C5'-O5'
165	EI	501	GTP	C3'-C4'-C5'-O5'
165	EJ	501	GTP	C5'-O5'-PA-O3A
165	EJ	501	GTP	C5'-O5'-PA-O1A
165	EJ	501	GTP	C5'-O5'-PA-O2A
165	FA	501	GTP	C5'-O5'-PA-O3A
165	FA	501	GTP	C5'-O5'-PA-O1A
165	FA	501	GTP	C5'-O5'-PA-O2A
165	FC	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	FC	501	GTP	C5'-O5'-PA-O1A
165	FC	501	GTP	C5'-O5'-PA-O2A
165	FE	501	GTP	C5'-O5'-PA-O3A
165	FE	501	GTP	C5'-O5'-PA-O1A
165	FE	501	GTP	C5'-O5'-PA-O2A
165	FG	501	GTP	C5'-O5'-PA-O3A
165	FG	501	GTP	C5'-O5'-PA-O1A
165	FG	501	GTP	C5'-O5'-PA-O2A
165	FI	501	GTP	O4'-C4'-C5'-O5'
165	FJ	503	GTP	C5'-O5'-PA-O3A
165	FJ	503	GTP	C5'-O5'-PA-O2A
165	G	501	GTP	C5'-O5'-PA-O3A
165	G	501	GTP	C5'-O5'-PA-O1A
165	G	501	GTP	C5'-O5'-PA-O2A
165	GC	501	GTP	C5'-O5'-PA-O3A
165	GC	501	GTP	C5'-O5'-PA-O1A
165	GC	501	GTP	C5'-O5'-PA-O2A
165	GE	501	GTP	C5'-O5'-PA-O3A
165	GE	501	GTP	C5'-O5'-PA-O2A
165	GG	501	GTP	C5'-O5'-PA-O3A
165	GG	501	GTP	C5'-O5'-PA-O2A
165	GG	501	GTP	C4'-C5'-O5'-PA
165	GK	501	GTP	C5'-O5'-PA-O3A
165	GK	501	GTP	C5'-O5'-PA-O1A
165	GK	501	GTP	C5'-O5'-PA-O2A
165	GL	501	GTP	PB-O3B-PG-O2G
165	GL	501	GTP	PB-O3B-PG-O3G
165	GL	501	GTP	C5'-O5'-PA-O3A
165	GL	501	GTP	C5'-O5'-PA-O1A
165	GL	501	GTP	C5'-O5'-PA-O2A
165	HA	501	GTP	C5'-O5'-PA-O3A
165	HA	501	GTP	C5'-O5'-PA-O2A
165	HB	503	GTP	C5'-O5'-PA-O3A
165	HB	503	GTP	C5'-O5'-PA-O1A
165	HB	503	GTP	C5'-O5'-PA-O2A
165	HE	501	GTP	C5'-O5'-PA-O3A
165	HE	501	GTP	C5'-O5'-PA-O1A
165	HE	501	GTP	C5'-O5'-PA-O2A
165	HG	501	GTP	C5'-O5'-PA-O3A
165	HG	501	GTP	C5'-O5'-PA-O2A
165	HK	501	GTP	C5'-O5'-PA-O3A
165	HK	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	HK	501	GTP	C5'-O5'-PA-O2A
165	HM	501	GTP	C5'-O5'-PA-O3A
165	HM	501	GTP	C5'-O5'-PA-O2A
165	IA	501	GTP	PB-O3A-PA-O5'
165	IA	501	GTP	C5'-O5'-PA-O3A
165	IA	501	GTP	C5'-O5'-PA-O1A
165	IC	501	GTP	C5'-O5'-PA-O3A
165	IC	501	GTP	C5'-O5'-PA-O1A
165	IC	501	GTP	C5'-O5'-PA-O2A
165	IG	501	GTP	C5'-O5'-PA-O3A
165	IG	501	GTP	C5'-O5'-PA-O1A
165	IG	501	GTP	C5'-O5'-PA-O2A
165	IG	501	GTP	O4'-C4'-C5'-O5'
165	IM	501	GTP	PB-O3A-PA-O5'
165	IM	501	GTP	C5'-O5'-PA-O3A
165	J	501	GTP	C5'-O5'-PA-O3A
165	J	501	GTP	C5'-O5'-PA-O1A
165	JB	501	GTP	C5'-O5'-PA-O3A
165	JD	501	GTP	C5'-O5'-PA-O3A
165	JD	501	GTP	C5'-O5'-PA-O2A
165	JF	501	GTP	C5'-O5'-PA-O3A
165	JF	501	GTP	C5'-O5'-PA-O2A
165	JF	501	GTP	C4'-C5'-O5'-PA
165	JH	501	GTP	C5'-O5'-PA-O2A
165	JH	501	GTP	O4'-C4'-C5'-O5'
165	JH	501	GTP	C3'-C4'-C5'-O5'
165	JJ	501	GTP	C5'-O5'-PA-O3A
165	JJ	501	GTP	C5'-O5'-PA-O1A
165	JJ	501	GTP	C5'-O5'-PA-O2A
165	JN	501	GTP	C5'-O5'-PA-O3A
165	JN	501	GTP	C5'-O5'-PA-O2A
165	K	501	GTP	O4'-C4'-C5'-O5'
165	KB	502	GTP	C5'-O5'-PA-O3A
165	KB	502	GTP	C5'-O5'-PA-O2A
165	KD	502	GTP	C5'-O5'-PA-O3A
165	KD	502	GTP	C5'-O5'-PA-O2A
165	KF	501	GTP	C5'-O5'-PA-O3A
165	KF	501	GTP	C5'-O5'-PA-O1A
165	KF	501	GTP	C5'-O5'-PA-O2A
165	KH	501	GTP	PB-O3B-PG-O3G
165	KH	501	GTP	O4'-C4'-C5'-O5'
165	KH	501	GTP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	KJ	501	GTP	C5'-O5'-PA-O3A
165	KJ	501	GTP	C5'-O5'-PA-O1A
165	KL	501	GTP	O4'-C4'-C5'-O5'
165	KN	502	GTP	O4'-C4'-C5'-O5'
165	L	501	GTP	C5'-O5'-PA-O1A
165	LB	501	GTP	C5'-O5'-PA-O3A
165	LB	501	GTP	C5'-O5'-PA-O2A
165	LD	502	GTP	C5'-O5'-PA-O3A
165	LF	502	GTP	C5'-O5'-PA-O3A
165	LJ	501	GTP	C5'-O5'-PA-O3A
165	LJ	501	GTP	C5'-O5'-PA-O1A
165	LJ	501	GTP	C5'-O5'-PA-O2A
165	LN	502	GTP	C5'-O5'-PA-O3A
165	LN	502	GTP	C5'-O5'-PA-O1A
165	LN	502	GTP	C5'-O5'-PA-O2A
165	MC	501	GTP	C5'-O5'-PA-O3A
165	MC	501	GTP	C5'-O5'-PA-O1A
165	ME	501	GTP	C5'-O5'-PA-O3A
165	ME	501	GTP	C5'-O5'-PA-O2A
165	MG	501	GTP	C5'-O5'-PA-O3A
165	MG	501	GTP	O4'-C4'-C5'-O5'
165	MG	501	GTP	C3'-C4'-C5'-O5'
165	MI	501	GTP	PB-O3B-PG-O3G
165	MI	501	GTP	C5'-O5'-PA-O3A
165	MI	501	GTP	C5'-O5'-PA-O1A
165	MI	501	GTP	C5'-O5'-PA-O2A
165	MJ	501	GTP	PB-O3A-PA-O5'
165	MJ	501	GTP	C5'-O5'-PA-O3A
165	NA	501	GTP	PB-O3B-PG-O3G
165	NA	501	GTP	PB-O3A-PA-O5'
165	NA	501	GTP	C5'-O5'-PA-O3A
165	NA	501	GTP	C5'-O5'-PA-O2A
165	NC	501	GTP	C5'-O5'-PA-O3A
165	NC	501	GTP	C5'-O5'-PA-O2A
165	NE	501	GTP	PB-O3B-PG-O2G
165	NE	501	GTP	C5'-O5'-PA-O3A
165	NE	501	GTP	C5'-O5'-PA-O1A
165	NE	501	GTP	C5'-O5'-PA-O2A
165	NF	501	GTP	C5'-O5'-PA-O3A
165	NF	501	GTP	C5'-O5'-PA-O1A
165	NK	501	GTP	C5'-O5'-PA-O3A
165	NK	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	NM	501	GTP	C5'-O5'-PA-O3A
165	OA	501	GTP	PB-O3A-PA-O5'
165	OA	501	GTP	C5'-O5'-PA-O3A
165	OA	501	GTP	C5'-O5'-PA-O1A
165	OD	503	GTP	C5'-O5'-PA-O3A
165	OD	503	GTP	C5'-O5'-PA-O1A
165	OD	503	GTP	C5'-O5'-PA-O2A
165	OG	501	GTP	C5'-O5'-PA-O3A
165	OG	501	GTP	C5'-O5'-PA-O2A
165	OG	501	GTP	C4'-C5'-O5'-PA
165	OI	501	GTP	C5'-O5'-PA-O3A
165	OI	501	GTP	C5'-O5'-PA-O2A
165	OI	501	GTP	O4'-C4'-C5'-O5'
165	OI	501	GTP	C3'-C4'-C5'-O5'
165	OK	501	GTP	C5'-O5'-PA-O3A
165	OK	501	GTP	C5'-O5'-PA-O1A
165	OK	501	GTP	C5'-O5'-PA-O2A
165	OM	501	GTP	PB-O3A-PA-O5'
165	OM	501	GTP	C5'-O5'-PA-O3A
165	OM	501	GTP	C5'-O5'-PA-O1A
165	PC	501	GTP	C5'-O5'-PA-O3A
165	PC	501	GTP	C5'-O5'-PA-O1A
165	PC	501	GTP	C5'-O5'-PA-O2A
165	PG	501	GTP	C5'-O5'-PA-O1A
165	PI	501	GTP	C5'-O5'-PA-O3A
165	PI	501	GTP	C5'-O5'-PA-O2A
165	PI	501	GTP	O4'-C4'-C5'-O5'
165	PK	501	GTP	C5'-O5'-PA-O1A
165	PM	501	GTP	C5'-O5'-PA-O3A
165	PM	501	GTP	C5'-O5'-PA-O1A
165	PM	501	GTP	C5'-O5'-PA-O2A
165	Q	501	GTP	C5'-O5'-PA-O3A
165	Q	501	GTP	C5'-O5'-PA-O2A
165	QC	501	GTP	C5'-O5'-PA-O3A
165	QC	501	GTP	C5'-O5'-PA-O1A
165	QC	501	GTP	C5'-O5'-PA-O2A
165	QH	501	GTP	PB-O3B-PG-O2G
165	QH	501	GTP	PB-O3B-PG-O3G
165	QH	501	GTP	C5'-O5'-PA-O3A
165	QH	501	GTP	C5'-O5'-PA-O1A
165	QH	501	GTP	C5'-O5'-PA-O2A
165	QH	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	QH	501	GTP	O4'-C4'-C5'-O5'
165	QI	501	GTP	C5'-O5'-PA-O3A
165	QI	501	GTP	C5'-O5'-PA-O1A
165	QI	501	GTP	C5'-O5'-PA-O2A
165	QL	501	GTP	C5'-O5'-PA-O3A
165	QL	501	GTP	C5'-O5'-PA-O1A
165	QL	501	GTP	C5'-O5'-PA-O2A
165	R	501	GTP	C5'-O5'-PA-O3A
165	R	501	GTP	C5'-O5'-PA-O1A
165	R	501	GTP	C5'-O5'-PA-O2A
165	RB	501	GTP	C5'-O5'-PA-O3A
165	RB	501	GTP	C5'-O5'-PA-O1A
165	RB	501	GTP	C5'-O5'-PA-O2A
165	RC	501	GTP	PB-O3A-PA-O5'
165	RC	501	GTP	C5'-O5'-PA-O3A
165	RC	501	GTP	C5'-O5'-PA-O1A
165	RH	501	GTP	O4'-C4'-C5'-O5'
165	RL	501	GTP	PB-O3A-PA-O5'
165	RL	501	GTP	C5'-O5'-PA-O3A
165	SA	501	GTP	C5'-O5'-PA-O3A
165	SA	501	GTP	C5'-O5'-PA-O2A
165	SC	501	GTP	C5'-O5'-PA-O3A
165	SC	501	GTP	C5'-O5'-PA-O1A
165	SE	501	GTP	C5'-O5'-PA-O3A
165	SE	501	GTP	C5'-O5'-PA-O1A
165	SE	501	GTP	C5'-O5'-PA-O2A
165	SG	501	GTP	PB-O3B-PG-O3G
165	SG	501	GTP	C5'-O5'-PA-O2A
165	SG	501	GTP	O4'-C4'-C5'-O5'
165	SI	501	GTP	C5'-O5'-PA-O3A
165	SI	501	GTP	C5'-O5'-PA-O2A
165	T	503	GTP	C5'-O5'-PA-O3A
165	T	503	GTP	C5'-O5'-PA-O1A
165	T	503	GTP	C5'-O5'-PA-O2A
165	TC	501	GTP	C5'-O5'-PA-O1A
165	TE	501	GTP	C5'-O5'-PA-O3A
165	TE	501	GTP	C5'-O5'-PA-O1A
165	TE	501	GTP	C5'-O5'-PA-O2A
165	TI	501	GTP	C5'-O5'-PA-O3A
165	TI	501	GTP	C5'-O5'-PA-O1A
165	TI	501	GTP	C5'-O5'-PA-O2A
165	UA	501	GTP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	UA	501	GTP	C5'-O5'-PA-O3A
165	UA	501	GTP	C5'-O5'-PA-O2A
165	UC	501	GTP	C5'-O5'-PA-O3A
165	UC	501	GTP	C5'-O5'-PA-O1A
165	UC	501	GTP	C5'-O5'-PA-O2A
165	UE	501	GTP	C5'-O5'-PA-O3A
165	UE	501	GTP	C5'-O5'-PA-O1A
165	UE	501	GTP	C5'-O5'-PA-O2A
165	UG	501	GTP	C5'-O5'-PA-O3A
165	UG	501	GTP	C5'-O5'-PA-O2A
165	UG	501	GTP	O4'-C4'-C5'-O5'
165	UI	501	GTP	C5'-O5'-PA-O3A
165	UI	501	GTP	C5'-O5'-PA-O1A
165	UI	501	GTP	C5'-O5'-PA-O2A
165	UK	501	GTP	C5'-O5'-PA-O1A
165	VA	501	GTP	C5'-O5'-PA-O3A
165	VA	501	GTP	C5'-O5'-PA-O1A
165	VC	501	GTP	C5'-O5'-PA-O3A
165	VC	501	GTP	C5'-O5'-PA-O1A
165	VC	501	GTP	C5'-O5'-PA-O2A
165	VG	501	GTP	O4'-C4'-C5'-O5'
165	VH	501	GTP	C5'-O5'-PA-O3A
165	VH	501	GTP	C5'-O5'-PA-O1A
165	VH	501	GTP	C5'-O5'-PA-O2A
165	VM	501	GTP	C5'-O5'-PA-O3A
165	VM	501	GTP	C5'-O5'-PA-O2A
165	WE	501	GTP	PB-O3B-PG-O3G
165	WI	501	GTP	C5'-O5'-PA-O3A
165	WI	501	GTP	C5'-O5'-PA-O1A
165	WI	501	GTP	C5'-O5'-PA-O2A
165	WK	501	GTP	C5'-O5'-PA-O3A
165	WK	501	GTP	C5'-O5'-PA-O1A
165	WM	501	GTP	C5'-O5'-PA-O3A
165	WM	501	GTP	C5'-O5'-PA-O2A
165	AO	501	GTP	C5'-O5'-PA-O3A
165	AO	501	GTP	C5'-O5'-PA-O1A
165	AO	501	GTP	C5'-O5'-PA-O2A
165	AP	501	GTP	C5'-O5'-PA-O3A
165	AP	501	GTP	C5'-O5'-PA-O1A
165	AP	501	GTP	C5'-O5'-PA-O2A
165	AS	501	GTP	C5'-O5'-PA-O3A
165	AS	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	AS	501	GTP	C5'-O5'-PA-O2A
165	AS	501	GTP	O4'-C4'-C5'-O5'
165	AW	501	GTP	C5'-O5'-PA-O3A
165	AW	501	GTP	C5'-O5'-PA-O2A
165	AY	501	GTP	PB-O3A-PA-O5'
165	BO	501	GTP	C5'-O5'-PA-O3A
165	BO	501	GTP	C5'-O5'-PA-O1A
165	BO	501	GTP	C5'-O5'-PA-O2A
165	BQ	501	GTP	PB-O3B-PG-O2G
165	BQ	501	GTP	C5'-O5'-PA-O3A
165	BQ	501	GTP	C5'-O5'-PA-O1A
165	BQ	501	GTP	C5'-O5'-PA-O2A
165	BQ	501	GTP	O4'-C4'-C5'-O5'
165	BU	501	GTP	C5'-O5'-PA-O3A
165	BU	501	GTP	C5'-O5'-PA-O1A
165	BU	501	GTP	C5'-O5'-PA-O2A
165	BW	501	GTP	C5'-O5'-PA-O3A
165	BW	501	GTP	C5'-O5'-PA-O1A
165	BW	501	GTP	C5'-O5'-PA-O2A
165	BY	501	GTP	C5'-O5'-PA-O3A
165	BY	501	GTP	C5'-O5'-PA-O2A
165	CN	501	GTP	C5'-O5'-PA-O3A
165	CN	501	GTP	C5'-O5'-PA-O1A
165	CN	501	GTP	C5'-O5'-PA-O2A
165	CO	501	GTP	C5'-O5'-PA-O1A
165	CQ	501	GTP	PB-O3B-PG-O2G
165	CQ	501	GTP	C5'-O5'-PA-O3A
165	CQ	501	GTP	C5'-O5'-PA-O1A
165	CT	501	GTP	PB-O3B-PG-O3G
165	CT	501	GTP	O4'-C4'-C5'-O5'
165	CV	501	GTP	C5'-O5'-PA-O3A
165	CV	501	GTP	C5'-O5'-PA-O1A
165	CV	501	GTP	C5'-O5'-PA-O2A
165	DN	501	GTP	C5'-O5'-PA-O3A
165	DN	501	GTP	C5'-O5'-PA-O1A
165	DN	501	GTP	C5'-O5'-PA-O2A
165	DP	501	GTP	C5'-O5'-PA-O3A
165	DP	501	GTP	C5'-O5'-PA-O1A
165	DP	501	GTP	C5'-O5'-PA-O2A
165	DQ	501	GTP	C5'-O5'-PA-O3A
165	DQ	501	GTP	C5'-O5'-PA-O1A
165	DV	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	DV	501	GTP	C5'-O5'-PA-O1A
165	DV	501	GTP	C5'-O5'-PA-O2A
165	DX	501	GTP	PB-O3B-PG-O3G
165	DX	501	GTP	C5'-O5'-PA-O3A
165	DX	501	GTP	C5'-O5'-PA-O2A
165	EM	501	GTP	C5'-O5'-PA-O3A
165	EO	501	GTP	C5'-O5'-PA-O3A
165	EO	501	GTP	C5'-O5'-PA-O1A
165	EO	501	GTP	C5'-O5'-PA-O2A
165	EP	501	GTP	C5'-O5'-PA-O3A
165	EP	501	GTP	C5'-O5'-PA-O1A
165	ES	501	GTP	C5'-O5'-PA-O3A
165	ES	501	GTP	C5'-O5'-PA-O2A
165	EU	501	GTP	C5'-O5'-PA-O3A
165	EU	501	GTP	C5'-O5'-PA-O2A
165	EU	501	GTP	O4'-C4'-C5'-O5'
165	EV	501	GTP	C5'-O5'-PA-O3A
165	EV	501	GTP	C5'-O5'-PA-O1A
165	FO	501	GTP	C5'-O5'-PA-O3A
165	FO	501	GTP	C5'-O5'-PA-O1A
165	FO	501	GTP	C5'-O5'-PA-O2A
165	FQ	501	GTP	C5'-O5'-PA-O3A
165	FQ	501	GTP	C5'-O5'-PA-O1A
165	FQ	501	GTP	C5'-O5'-PA-O2A
165	FS	501	GTP	C5'-O5'-PA-O3A
165	FS	501	GTP	C4'-C5'-O5'-PA
165	FT	503	GTP	O4'-C4'-C5'-O5'
165	FV	503	GTP	C5'-O5'-PA-O3A
165	GO	501	GTP	C5'-O5'-PA-O3A
165	GO	501	GTP	C5'-O5'-PA-O1A
165	GO	501	GTP	C5'-O5'-PA-O2A
165	GQ	501	GTP	C5'-O5'-PA-O3A
165	GQ	501	GTP	C5'-O5'-PA-O2A
165	GS	501	GTP	C5'-O5'-PA-O3A
165	GS	501	GTP	C5'-O5'-PA-O2A
165	GU	501	GTP	C5'-O5'-PA-O3A
165	GU	501	GTP	O4'-C4'-C5'-O5'
165	GW	501	GTP	C5'-O5'-PA-O3A
165	GW	501	GTP	C5'-O5'-PA-O1A
165	GW	501	GTP	C5'-O5'-PA-O2A
165	HN	503	GTP	C5'-O5'-PA-O3A
165	HN	503	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	HN	503	GTP	C5'-O5'-PA-O2A
165	HQ	501	GTP	C5'-O5'-PA-O3A
165	HQ	501	GTP	C5'-O5'-PA-O1A
165	HQ	501	GTP	C5'-O5'-PA-O2A
165	HS	501	GTP	C5'-O5'-PA-O3A
165	HS	501	GTP	C5'-O5'-PA-O2A
165	HW	501	GTP	C5'-O5'-PA-O3A
165	HW	501	GTP	C5'-O5'-PA-O1A
165	HW	501	GTP	C5'-O5'-PA-O2A
165	HY	501	GTP	C5'-O5'-PA-O3A
165	HY	501	GTP	C5'-O5'-PA-O2A
165	IO	501	GTP	C5'-O5'-PA-O3A
165	IO	501	GTP	C5'-O5'-PA-O1A
165	IO	501	GTP	C5'-O5'-PA-O2A
165	IS	501	GTP	C5'-O5'-PA-O3A
165	IS	501	GTP	C5'-O5'-PA-O1A
165	IS	501	GTP	C5'-O5'-PA-O2A
165	IS	501	GTP	O4'-C4'-C5'-O5'
165	IY	501	GTP	PB-O3A-PA-O5'
165	IY	501	GTP	C5'-O5'-PA-O3A
165	JP	501	GTP	C5'-O5'-PA-O3A
165	JP	501	GTP	C5'-O5'-PA-O2A
165	JR	501	GTP	C5'-O5'-PA-O3A
165	JR	501	GTP	C5'-O5'-PA-O2A
165	JR	501	GTP	C4'-C5'-O5'-PA
165	JT	501	GTP	C5'-O5'-PA-O2A
165	JT	501	GTP	O4'-C4'-C5'-O5'
165	JT	501	GTP	C3'-C4'-C5'-O5'
165	JV	501	GTP	C5'-O5'-PA-O3A
165	JV	501	GTP	C5'-O5'-PA-O1A
165	JV	501	GTP	C5'-O5'-PA-O2A
165	JZ	501	GTP	C5'-O5'-PA-O3A
165	JZ	501	GTP	C5'-O5'-PA-O2A
165	KP	502	GTP	C5'-O5'-PA-O3A
165	KP	502	GTP	C5'-O5'-PA-O2A
165	KR	501	GTP	C5'-O5'-PA-O3A
165	KR	501	GTP	C5'-O5'-PA-O1A
165	KR	501	GTP	C5'-O5'-PA-O2A
165	KT	501	GTP	PB-O3B-PG-O3G
165	KT	501	GTP	O4'-C4'-C5'-O5'
165	KT	501	GTP	C3'-C4'-C5'-O5'
165	KV	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	KV	501	GTP	C5'-O5'-PA-O1A
165	KX	501	GTP	O4'-C4'-C5'-O5'
165	KZ	501	GTP	O4'-C4'-C5'-O5'
165	LP	502	GTP	C5'-O5'-PA-O3A
165	LR	502	GTP	C5'-O5'-PA-O3A
165	LV	501	GTP	C5'-O5'-PA-O3A
165	LV	501	GTP	C5'-O5'-PA-O1A
165	LV	501	GTP	C5'-O5'-PA-O2A
165	LZ	502	GTP	C5'-O5'-PA-O3A
165	LZ	502	GTP	C5'-O5'-PA-O1A
165	LZ	502	GTP	C5'-O5'-PA-O2A
165	MO	501	GTP	C5'-O5'-PA-O3A
165	MO	501	GTP	C5'-O5'-PA-O1A
165	MQ	501	GTP	C5'-O5'-PA-O3A
165	MQ	501	GTP	C5'-O5'-PA-O2A
165	MS	501	GTP	C5'-O5'-PA-O3A
165	MS	501	GTP	O4'-C4'-C5'-O5'
165	MS	501	GTP	C3'-C4'-C5'-O5'
165	MU	501	GTP	PB-O3B-PG-O3G
165	MU	501	GTP	C5'-O5'-PA-O3A
165	MU	501	GTP	C5'-O5'-PA-O1A
165	MU	501	GTP	C5'-O5'-PA-O2A
165	MV	501	GTP	PB-O3A-PA-O5'
165	MV	501	GTP	C5'-O5'-PA-O3A
165	PO	501	GTP	C5'-O5'-PA-O3A
165	PO	501	GTP	C5'-O5'-PA-O1A
165	PO	501	GTP	C5'-O5'-PA-O2A
165	PS	501	GTP	C5'-O5'-PA-O1A
165	PU	501	GTP	C5'-O5'-PA-O3A
165	PU	501	GTP	C5'-O5'-PA-O2A
165	PU	501	GTP	O4'-C4'-C5'-O5'
165	PW	501	GTP	C5'-O5'-PA-O1A
165	PY	501	GTP	C5'-O5'-PA-O3A
165	PY	501	GTP	C5'-O5'-PA-O1A
165	PY	501	GTP	C5'-O5'-PA-O2A
165	QO	501	GTP	C5'-O5'-PA-O3A
165	QO	501	GTP	C5'-O5'-PA-O1A
165	QO	501	GTP	C5'-O5'-PA-O2A
165	QT	501	GTP	PB-O3B-PG-O2G
165	QT	501	GTP	PB-O3B-PG-O3G
165	QT	501	GTP	C5'-O5'-PA-O3A
165	QT	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	QT	501	GTP	C5'-O5'-PA-O2A
165	QT	501	GTP	C4'-C5'-O5'-PA
165	QT	501	GTP	O4'-C4'-C5'-O5'
165	QU	501	GTP	C5'-O5'-PA-O3A
165	QU	501	GTP	C5'-O5'-PA-O1A
165	QU	501	GTP	C5'-O5'-PA-O2A
165	QX	501	GTP	C5'-O5'-PA-O3A
165	QX	501	GTP	C5'-O5'-PA-O1A
165	QX	501	GTP	C5'-O5'-PA-O2A
165	RN	501	GTP	C5'-O5'-PA-O3A
165	RN	501	GTP	C5'-O5'-PA-O1A
165	RN	501	GTP	C5'-O5'-PA-O2A
165	RO	501	GTP	PB-O3A-PA-O5'
165	RO	501	GTP	C5'-O5'-PA-O3A
165	RO	501	GTP	C5'-O5'-PA-O1A
165	RT	501	GTP	O4'-C4'-C5'-O5'
165	RX	501	GTP	PB-O3A-PA-O5'
165	RX	501	GTP	C5'-O5'-PA-O3A
165	SM	501	GTP	C5'-O5'-PA-O3A
165	SM	501	GTP	C5'-O5'-PA-O2A
165	SO	501	GTP	C5'-O5'-PA-O3A
165	SO	501	GTP	C5'-O5'-PA-O1A
165	SQ	501	GTP	C5'-O5'-PA-O3A
165	SQ	501	GTP	C5'-O5'-PA-O1A
165	SQ	501	GTP	C5'-O5'-PA-O2A
165	SS	501	GTP	PB-O3B-PG-O3G
165	SS	501	GTP	C5'-O5'-PA-O2A
165	SS	501	GTP	O4'-C4'-C5'-O5'
165	SU	501	GTP	C5'-O5'-PA-O3A
165	SU	501	GTP	C5'-O5'-PA-O2A
165	TM	501	GTP	C5'-O5'-PA-O3A
165	TM	501	GTP	C5'-O5'-PA-O1A
165	TM	501	GTP	C5'-O5'-PA-O2A
165	TO	501	GTP	C5'-O5'-PA-O1A
165	TQ	501	GTP	C5'-O5'-PA-O3A
165	TQ	501	GTP	C5'-O5'-PA-O1A
165	TQ	501	GTP	C5'-O5'-PA-O2A
165	TU	501	GTP	C5'-O5'-PA-O3A
165	TU	501	GTP	C5'-O5'-PA-O1A
165	TU	501	GTP	C5'-O5'-PA-O2A
165	UM	501	GTP	PB-O3B-PG-O3G
165	UM	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	UM	501	GTP	C5'-O5'-PA-O2A
165	UO	501	GTP	C5'-O5'-PA-O3A
165	UO	501	GTP	C5'-O5'-PA-O1A
165	UO	501	GTP	C5'-O5'-PA-O2A
165	UQ	501	GTP	C5'-O5'-PA-O3A
165	UQ	501	GTP	C5'-O5'-PA-O1A
165	UQ	501	GTP	C5'-O5'-PA-O2A
165	US	501	GTP	C5'-O5'-PA-O3A
165	US	501	GTP	C5'-O5'-PA-O2A
165	US	501	GTP	O4'-C4'-C5'-O5'
165	UU	501	GTP	C5'-O5'-PA-O3A
165	UU	501	GTP	C5'-O5'-PA-O1A
165	UU	501	GTP	C5'-O5'-PA-O2A
165	UW	501	GTP	C5'-O5'-PA-O1A
165	VO	501	GTP	C5'-O5'-PA-O3A
165	VO	501	GTP	C5'-O5'-PA-O1A
165	VO	501	GTP	C5'-O5'-PA-O2A
165	VS	501	GTP	O4'-C4'-C5'-O5'
165	VT	501	GTP	C5'-O5'-PA-O3A
165	VT	501	GTP	C5'-O5'-PA-O1A
165	VT	501	GTP	C5'-O5'-PA-O2A
165	VY	501	GTP	C5'-O5'-PA-O3A
165	VY	501	GTP	C5'-O5'-PA-O2A
165	WQ	501	GTP	PB-O3B-PG-O3G
165	WU	501	GTP	C5'-O5'-PA-O3A
165	WU	501	GTP	C5'-O5'-PA-O1A
165	WU	501	GTP	C5'-O5'-PA-O2A
165	WW	501	GTP	C5'-O5'-PA-O3A
165	WW	501	GTP	C5'-O5'-PA-O1A
165	WY	501	GTP	C5'-O5'-PA-O3A
165	WY	501	GTP	C5'-O5'-PA-O2A
165	NO	501	GTP	C5'-O5'-PA-O3A
165	NO	501	GTP	C5'-O5'-PA-O2A
165	NQ	501	GTP	PB-O3B-PG-O2G
165	NQ	501	GTP	C5'-O5'-PA-O3A
165	NQ	501	GTP	C5'-O5'-PA-O1A
165	NQ	501	GTP	C5'-O5'-PA-O2A
165	NR	501	GTP	C5'-O5'-PA-O3A
165	NR	501	GTP	C5'-O5'-PA-O1A
165	NW	501	GTP	C5'-O5'-PA-O3A
165	NW	501	GTP	C4'-C5'-O5'-PA
165	NY	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	OP	503	GTP	C5'-O5'-PA-O3A
165	OP	503	GTP	C5'-O5'-PA-O1A
165	OP	503	GTP	C5'-O5'-PA-O2A
165	OS	501	GTP	C5'-O5'-PA-O3A
165	OS	501	GTP	C5'-O5'-PA-O2A
165	OS	501	GTP	C4'-C5'-O5'-PA
165	OU	501	GTP	C5'-O5'-PA-O3A
165	OU	501	GTP	C5'-O5'-PA-O2A
165	OU	501	GTP	O4'-C4'-C5'-O5'
165	OU	501	GTP	C3'-C4'-C5'-O5'
165	OW	501	GTP	C5'-O5'-PA-O3A
165	OW	501	GTP	C5'-O5'-PA-O1A
165	OW	501	GTP	C5'-O5'-PA-O2A
165	OY	501	GTP	PB-O3A-PA-O5'
165	OY	501	GTP	C5'-O5'-PA-O3A
165	OY	501	GTP	C5'-O5'-PA-O1A
168	2v	501	ATP	O4'-C4'-C5'-O5'
168	2w	501	ATP	C2'-C1'-N9-C8
168	2x	501	ATP	C2'-C1'-N9-C8
168	6l	400	ATP	C5'-O5'-PA-O2A
168	6l	400	ATP	C5'-O5'-PA-O3A
168	6l	400	ATP	O4'-C4'-C5'-O5'
168	6p	500	ATP	PB-O3B-PG-O2G
168	6p	500	ATP	C5'-O5'-PA-O1A
168	6p	500	ATP	C5'-O5'-PA-O2A
168	6p	500	ATP	C5'-O5'-PA-O3A
168	9R	500	ATP	PB-O3B-PG-O2G
168	9R	500	ATP	C5'-O5'-PA-O2A
168	9R	500	ATP	C5'-O5'-PA-O3A
168	6u	700	ATP	C5'-O5'-PA-O2A
168	6u	700	ATP	C5'-O5'-PA-O3A
168	6u	700	ATP	O4'-C4'-C5'-O5'
168	6u	700	ATP	C3'-C4'-C5'-O5'
168	7D	601	ATP	C5'-O5'-PA-O1A
168	7D	601	ATP	C5'-O5'-PA-O3A
168	7D	601	ATP	O4'-C4'-C5'-O5'
163	FL	500	GDP	O4'-C4'-C5'-O5'
163	FL	500	GDP	C3'-C4'-C5'-O5'
163	MJ	500	GDP	C3'-C4'-C5'-O5'
163	O	500	GDP	C3'-C4'-C5'-O5'
163	PF	501	GDP	O4'-C4'-C5'-O5'
163	PF	501	GDP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	FX	500	GDP	O4'-C4'-C5'-O5'
163	FX	500	GDP	C3'-C4'-C5'-O5'
163	MV	500	GDP	C3'-C4'-C5'-O5'
163	PR	501	GDP	O4'-C4'-C5'-O5'
163	PR	501	GDP	C3'-C4'-C5'-O5'
165	AA	501	GTP	O4'-C4'-C5'-O5'
165	AA	501	GTP	C3'-C4'-C5'-O5'
165	AG	501	GTP	O4'-C4'-C5'-O5'
165	AG	501	GTP	C3'-C4'-C5'-O5'
165	AM	501	GTP	O4'-C4'-C5'-O5'
165	AM	501	GTP	C3'-C4'-C5'-O5'
165	CK	503	GTP	O4'-C4'-C5'-O5'
165	CK	503	GTP	C3'-C4'-C5'-O5'
165	DE	501	GTP	O4'-C4'-C5'-O5'
165	DE	501	GTP	C3'-C4'-C5'-O5'
165	DJ	501	GTP	O4'-C4'-C5'-O5'
165	DJ	501	GTP	C3'-C4'-C5'-O5'
165	DL	501	GTP	O4'-C4'-C5'-O5'
165	DL	501	GTP	C3'-C4'-C5'-O5'
165	IG	501	GTP	C3'-C4'-C5'-O5'
165	K	501	GTP	C3'-C4'-C5'-O5'
165	KL	501	GTP	C3'-C4'-C5'-O5'
165	L	501	GTP	O4'-C4'-C5'-O5'
165	L	501	GTP	C3'-C4'-C5'-O5'
165	LL	501	GTP	O4'-C4'-C5'-O5'
165	LL	501	GTP	C3'-C4'-C5'-O5'
165	QH	501	GTP	C3'-C4'-C5'-O5'
165	RH	501	GTP	C3'-C4'-C5'-O5'
165	SC	501	GTP	O4'-C4'-C5'-O5'
165	SC	501	GTP	C3'-C4'-C5'-O5'
165	TE	501	GTP	O4'-C4'-C5'-O5'
165	TE	501	GTP	C3'-C4'-C5'-O5'
165	UE	501	GTP	O4'-C4'-C5'-O5'
165	UE	501	GTP	C3'-C4'-C5'-O5'
165	UG	501	GTP	C3'-C4'-C5'-O5'
165	VA	501	GTP	O4'-C4'-C5'-O5'
165	VA	501	GTP	C3'-C4'-C5'-O5'
165	AS	501	GTP	C3'-C4'-C5'-O5'
165	AU	501	GTP	O4'-C4'-C5'-O5'
165	BQ	501	GTP	C3'-C4'-C5'-O5'
165	CT	501	GTP	C3'-C4'-C5'-O5'
165	CW	501	GTP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	EU	501	GTP	C3'-C4'-C5'-O5'
165	EV	501	GTP	O4'-C4'-C5'-O5'
165	EV	501	GTP	C3'-C4'-C5'-O5'
165	FT	503	GTP	C3'-C4'-C5'-O5'
165	IS	501	GTP	C3'-C4'-C5'-O5'
165	KX	501	GTP	C3'-C4'-C5'-O5'
165	LX	501	GTP	O4'-C4'-C5'-O5'
165	LX	501	GTP	C3'-C4'-C5'-O5'
165	QT	501	GTP	C3'-C4'-C5'-O5'
165	RT	501	GTP	C3'-C4'-C5'-O5'
165	SO	501	GTP	O4'-C4'-C5'-O5'
165	SO	501	GTP	C3'-C4'-C5'-O5'
165	TQ	501	GTP	O4'-C4'-C5'-O5'
165	TQ	501	GTP	C3'-C4'-C5'-O5'
165	UQ	501	GTP	O4'-C4'-C5'-O5'
165	UQ	501	GTP	C3'-C4'-C5'-O5'
165	US	501	GTP	C3'-C4'-C5'-O5'
168	6l	400	ATP	C3'-C4'-C5'-O5'
168	7D	601	ATP	C3'-C4'-C5'-O5'
165	SI	501	GTP	C4'-C5'-O5'-PA
165	GQ	501	GTP	C4'-C5'-O5'-PA
165	GS	501	GTP	C4'-C5'-O5'-PA
165	SU	501	GTP	C4'-C5'-O5'-PA
163	O	500	GDP	O4'-C4'-C5'-O5'
163	PJ	500	GDP	O4'-C4'-C5'-O5'
163	PJ	500	GDP	C3'-C4'-C5'-O5'
163	QK	500	GDP	O4'-C4'-C5'-O5'
163	PV	500	GDP	O4'-C4'-C5'-O5'
163	PV	500	GDP	C3'-C4'-C5'-O5'
163	QW	500	GDP	O4'-C4'-C5'-O5'
165	BE	501	GTP	O4'-C4'-C5'-O5'
165	BE	501	GTP	C3'-C4'-C5'-O5'
165	ED	501	GTP	O4'-C4'-C5'-O5'
165	ED	501	GTP	C3'-C4'-C5'-O5'
165	IE	501	GTP	O4'-C4'-C5'-O5'
165	JK	501	GTP	O4'-C4'-C5'-O5'
165	JK	501	GTP	C3'-C4'-C5'-O5'
165	LH	501	GTP	O4'-C4'-C5'-O5'
165	TK	501	GTP	O4'-C4'-C5'-O5'
165	TK	501	GTP	C3'-C4'-C5'-O5'
165	CO	501	GTP	O4'-C4'-C5'-O5'
165	CO	501	GTP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	CW	501	GTP	C3'-C4'-C5'-O5'
165	EP	501	GTP	C3'-C4'-C5'-O5'
165	IQ	501	GTP	O4'-C4'-C5'-O5'
165	JW	501	GTP	O4'-C4'-C5'-O5'
165	JW	501	GTP	C3'-C4'-C5'-O5'
165	LT	501	GTP	O4'-C4'-C5'-O5'
165	TW	501	GTP	O4'-C4'-C5'-O5'
165	TW	501	GTP	C3'-C4'-C5'-O5'
168	2v	501	ATP	C3'-C4'-C5'-O5'
168	2w	501	ATP	O4'-C4'-C5'-O5'
168	2w	501	ATP	C3'-C4'-C5'-O5'
168	2x	501	ATP	O4'-C4'-C5'-O5'
168	2w	501	ATP	C2'-C1'-N9-C4
168	2x	501	ATP	C2'-C1'-N9-C4
165	GC	501	GTP	C4'-C5'-O5'-PA
165	HG	501	GTP	C4'-C5'-O5'-PA
165	FV	503	GTP	C4'-C5'-O5'-PA
165	HS	501	GTP	C4'-C5'-O5'-PA
168	7A	402	ATP	C4'-C5'-O5'-PA
163	CI	500	GDP	C3'-C4'-C5'-O5'
163	CW	500	GDP	C3'-C4'-C5'-O5'
165	AI	501	GTP	C3'-C4'-C5'-O5'
165	FI	501	GTP	C3'-C4'-C5'-O5'
165	PI	501	GTP	C3'-C4'-C5'-O5'
165	SG	501	GTP	C3'-C4'-C5'-O5'
165	VG	501	GTP	C3'-C4'-C5'-O5'
165	VK	501	GTP	C3'-C4'-C5'-O5'
165	AY	501	GTP	O4'-C4'-C5'-O5'
165	AY	501	GTP	C3'-C4'-C5'-O5'
165	GU	501	GTP	C3'-C4'-C5'-O5'
165	IQ	501	GTP	C3'-C4'-C5'-O5'
165	PU	501	GTP	C3'-C4'-C5'-O5'
165	SS	501	GTP	C3'-C4'-C5'-O5'
165	VS	501	GTP	C3'-C4'-C5'-O5'
165	VW	501	GTP	C3'-C4'-C5'-O5'
168	2x	501	ATP	C3'-C4'-C5'-O5'
165	FJ	503	GTP	C4'-C5'-O5'-PA
165	RF	501	GTP	C4'-C5'-O5'-PA
165	RR	501	GTP	C4'-C5'-O5'-PA
163	A	501	GDP	C3'-C4'-C5'-O5'
163	CK	501	GDP	C3'-C4'-C5'-O5'
163	DC	500	GDP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	DE	500	GDP	C3'-C4'-C5'-O5'
163	FF	500	GDP	C3'-C4'-C5'-O5'
163	GF	500	GDP	C3'-C4'-C5'-O5'
163	LI	500	GDP	C3'-C4'-C5'-O5'
163	M	500	GDP	C3'-C4'-C5'-O5'
163	OB	500	GDP	O4'-C4'-C5'-O5'
163	OH	500	GDP	C3'-C4'-C5'-O5'
163	BX	500	GDP	C3'-C4'-C5'-O5'
163	EV	500	GDP	C3'-C4'-C5'-O5'
163	GP	500	GDP	C3'-C4'-C5'-O5'
163	LU	500	GDP	C3'-C4'-C5'-O5'
163	ON	500	GDP	O4'-C4'-C5'-O5'
163	OT	500	GDP	C3'-C4'-C5'-O5'
165	CC	501	GTP	C3'-C4'-C5'-O5'
165	IE	501	GTP	C3'-C4'-C5'-O5'
165	KN	502	GTP	C3'-C4'-C5'-O5'
165	LH	501	GTP	C3'-C4'-C5'-O5'
165	QB	501	GTP	C3'-C4'-C5'-O5'
165	RC	501	GTP	C3'-C4'-C5'-O5'
165	UK	501	GTP	C3'-C4'-C5'-O5'
165	WE	501	GTP	C3'-C4'-C5'-O5'
165	CQ	501	GTP	C3'-C4'-C5'-O5'
165	DQ	501	GTP	C3'-C4'-C5'-O5'
165	KZ	501	GTP	C3'-C4'-C5'-O5'
165	LT	501	GTP	C3'-C4'-C5'-O5'
165	QN	501	GTP	C3'-C4'-C5'-O5'
165	RO	501	GTP	C3'-C4'-C5'-O5'
165	UW	501	GTP	C3'-C4'-C5'-O5'
165	WQ	501	GTP	C3'-C4'-C5'-O5'
168	6p	500	ATP	C3'-C4'-C5'-O5'
163	A	501	GDP	O4'-C4'-C5'-O5'
163	CI	500	GDP	O4'-C4'-C5'-O5'
163	EB	500	GDP	C3'-C4'-C5'-O5'
163	ED	500	GDP	C3'-C4'-C5'-O5'
163	IB	500	GDP	C3'-C4'-C5'-O5'
163	IF	500	GDP	C3'-C4'-C5'-O5'
163	PD	500	GDP	C3'-C4'-C5'-O5'
163	SD	500	GDP	C3'-C4'-C5'-O5'
163	IN	500	GDP	C3'-C4'-C5'-O5'
163	IR	500	GDP	C3'-C4'-C5'-O5'
163	PP	500	GDP	C3'-C4'-C5'-O5'
163	SP	500	GDP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	D	501	GTP	C3'-C4'-C5'-O5'
165	FG	501	GTP	C3'-C4'-C5'-O5'
165	HI	501	GTP	O4'-C4'-C5'-O5'
165	HI	501	GTP	C3'-C4'-C5'-O5'
165	IA	501	GTP	C3'-C4'-C5'-O5'
165	VK	501	GTP	O4'-C4'-C5'-O5'
165	AU	501	GTP	C3'-C4'-C5'-O5'
165	EP	501	GTP	O4'-C4'-C5'-O5'
165	HU	501	GTP	O4'-C4'-C5'-O5'
165	HU	501	GTP	C3'-C4'-C5'-O5'
165	VW	501	GTP	O4'-C4'-C5'-O5'
168	6p	500	ATP	O4'-C4'-C5'-O5'
163	DC	500	GDP	O4'-C4'-C5'-O5'
163	GF	500	GDP	O4'-C4'-C5'-O5'
163	OJ	500	GDP	C3'-C4'-C5'-O5'
163	OV	500	GDP	C3'-C4'-C5'-O5'
165	WE	501	GTP	O4'-C4'-C5'-O5'
165	CQ	501	GTP	O4'-C4'-C5'-O5'
165	DT	501	GTP	O4'-C4'-C5'-O5'
165	DX	501	GTP	C3'-C4'-C5'-O5'
165	WQ	501	GTP	O4'-C4'-C5'-O5'
165	RL	501	GTP	PB-O3B-PG-O1G
165	RX	501	GTP	PB-O3B-PG-O1G
163	AL	500	GDP	C3'-C4'-C5'-O5'
163	CC	500	GDP	C3'-C4'-C5'-O5'
163	DA	500	GDP	C3'-C4'-C5'-O5'
163	NB	500	GDP	C3'-C4'-C5'-O5'
163	OL	500	GDP	C3'-C4'-C5'-O5'
163	NN	500	GDP	C3'-C4'-C5'-O5'
163	OX	500	GDP	C3'-C4'-C5'-O5'
165	PG	501	GTP	C3'-C4'-C5'-O5'
165	CH	501	GTP	PB-O3A-PA-O1A
165	GL	501	GTP	PB-O3A-PA-O1A
165	ME	501	GTP	PA-O3A-PB-O1B
165	NF	501	GTP	PB-O3A-PA-O1A
165	VG	501	GTP	PB-O3A-PA-O1A
165	CT	501	GTP	PB-O3A-PA-O1A
165	MQ	501	GTP	PA-O3A-PB-O1B
165	VS	501	GTP	PB-O3A-PA-O1A
165	NR	501	GTP	PB-O3A-PA-O1A
165	GL	501	GTP	C4'-C5'-O5'-PA
165	LF	502	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	LJ	501	GTP	C4'-C5'-O5'-PA
165	OI	501	GTP	C4'-C5'-O5'-PA
165	OK	501	GTP	C4'-C5'-O5'-PA
165	BU	501	GTP	C4'-C5'-O5'-PA
165	GO	501	GTP	C4'-C5'-O5'-PA
165	LR	502	GTP	C4'-C5'-O5'-PA
165	LV	501	GTP	C4'-C5'-O5'-PA
165	OU	501	GTP	C4'-C5'-O5'-PA
165	OW	501	GTP	C4'-C5'-O5'-PA
163	FF	500	GDP	O4'-C4'-C5'-O5'
163	M	500	GDP	O4'-C4'-C5'-O5'
163	OH	500	GDP	O4'-C4'-C5'-O5'
163	BX	500	GDP	O4'-C4'-C5'-O5'
163	GP	500	GDP	O4'-C4'-C5'-O5'
165	UK	501	GTP	O4'-C4'-C5'-O5'
165	DQ	501	GTP	O4'-C4'-C5'-O5'
165	UW	501	GTP	O4'-C4'-C5'-O5'
165	BI	501	GTP	C4'-C5'-O5'-PA
165	G	501	GTP	C4'-C5'-O5'-PA
165	GE	501	GTP	C4'-C5'-O5'-PA
165	IC	501	GTP	C4'-C5'-O5'-PA
165	ME	501	GTP	C4'-C5'-O5'-PA
165	QF	501	GTP	C4'-C5'-O5'-PA
165	ES	501	GTP	C4'-C5'-O5'-PA
165	IO	501	GTP	C4'-C5'-O5'-PA
165	MQ	501	GTP	C4'-C5'-O5'-PA
165	QR	501	GTP	C4'-C5'-O5'-PA
168	6l	400	ATP	C4'-C5'-O5'-PA
163	LI	500	GDP	O4'-C4'-C5'-O5'
163	LU	500	GDP	O4'-C4'-C5'-O5'
163	OT	500	GDP	O4'-C4'-C5'-O5'
165	CC	501	GTP	O4'-C4'-C5'-O5'
165	D	501	GTP	O4'-C4'-C5'-O5'
165	IA	501	GTP	O4'-C4'-C5'-O5'
165	RC	501	GTP	O4'-C4'-C5'-O5'
165	DT	501	GTP	C3'-C4'-C5'-O5'
165	PS	501	GTP	C3'-C4'-C5'-O5'
165	RO	501	GTP	O4'-C4'-C5'-O5'
165	AA	501	GTP	PB-O3A-PA-O5'
165	C	501	GTP	PB-O3A-PA-O5'
165	CE	501	GTP	PB-O3A-PA-O5'
165	D	501	GTP	PB-O3A-PA-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	KB	502	GTP	PB-O3A-PA-O5'
165	LD	502	GTP	PB-O3A-PA-O5'
165	NM	501	GTP	PB-O3A-PA-O5'
165	QH	501	GTP	PB-O3A-PA-O5'
165	R	501	GTP	PB-O3A-PA-O5'
165	UA	501	GTP	PB-O3A-PA-O5'
165	UE	501	GTP	PB-O3A-PA-O5'
165	UK	501	GTP	PB-O3A-PA-O5'
165	VK	501	GTP	PB-O3A-PA-O5'
165	WE	501	GTP	PB-O3A-PA-O5'
165	WK	501	GTP	PB-O3A-PA-O5'
165	BO	501	GTP	PB-O3A-PA-O5'
165	CQ	501	GTP	PB-O3A-PA-O5'
165	CW	501	GTP	PB-O3A-PA-O5'
165	DX	501	GTP	PB-O3A-PA-O5'
165	EM	501	GTP	PB-O3A-PA-O5'
165	LP	502	GTP	PB-O3A-PA-O5'
165	QT	501	GTP	PB-O3A-PA-O5'
165	UM	501	GTP	PB-O3A-PA-O5'
165	UQ	501	GTP	PB-O3A-PA-O5'
165	UW	501	GTP	PB-O3A-PA-O5'
165	VW	501	GTP	PB-O3A-PA-O5'
165	WQ	501	GTP	PB-O3A-PA-O5'
165	WW	501	GTP	PB-O3A-PA-O5'
165	NY	501	GTP	PB-O3A-PA-O5'
165	EG	501	GTP	C4'-C5'-O5'-PA
168	6p	500	ATP	C4'-C5'-O5'-PA
163	F	500	GDP	C3'-C4'-C5'-O5'
163	G	500	GDP	C3'-C4'-C5'-O5'
163	GV	501	GDP	C3'-C4'-C5'-O5'
165	FG	501	GTP	O4'-C4'-C5'-O5'
165	FJ	503	GTP	C3'-C4'-C5'-O5'
165	TC	501	GTP	C3'-C4'-C5'-O5'
165	VM	501	GTP	C3'-C4'-C5'-O5'
165	TO	501	GTP	C3'-C4'-C5'-O5'
165	VY	501	GTP	C3'-C4'-C5'-O5'
165	KF	501	GTP	PB-O3B-PG-O1G
165	T	503	GTP	PB-O3B-PG-O1G
165	VC	501	GTP	PB-O3B-PG-O1G
165	WE	501	GTP	PB-O3B-PG-O1G
165	DX	501	GTP	PB-O3B-PG-O1G
165	KR	501	GTP	PB-O3B-PG-O1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	TM	501	GTP	PB-O3B-PG-O1G
165	VO	501	GTP	PB-O3B-PG-O1G
165	WQ	501	GTP	PB-O3B-PG-O1G
163	CY	500	GDP	PA-O3A-PB-O3B
165	C	501	GTP	PB-O3B-PG-O2G
165	CH	501	GTP	PB-O3B-PG-O3G
165	G	501	GTP	PB-O3B-PG-O3G
165	NA	501	GTP	PB-O3B-PG-O2G
165	RC	501	GTP	PB-O3B-PG-O2G
165	RL	501	GTP	PB-O3B-PG-O3G
165	SG	501	GTP	PB-O3B-PG-O2G
165	RO	501	GTP	PB-O3B-PG-O2G
165	RX	501	GTP	PB-O3B-PG-O3G
165	SS	501	GTP	PB-O3B-PG-O2G
163	DE	500	GDP	O4'-C4'-C5'-O5'
163	EB	500	GDP	O4'-C4'-C5'-O5'
163	GD	500	GDP	C3'-C4'-C5'-O5'
163	HD	501	GDP	C3'-C4'-C5'-O5'
163	IB	500	GDP	O4'-C4'-C5'-O5'
163	JG	500	GDP	C3'-C4'-C5'-O5'
163	KI	500	GDP	C3'-C4'-C5'-O5'
163	MF	500	GDP	C3'-C4'-C5'-O5'
163	NF	500	GDP	C3'-C4'-C5'-O5'
163	EV	500	GDP	O4'-C4'-C5'-O5'
163	HP	501	GDP	C3'-C4'-C5'-O5'
163	IN	500	GDP	O4'-C4'-C5'-O5'
163	JS	500	GDP	C3'-C4'-C5'-O5'
163	KU	500	GDP	C3'-C4'-C5'-O5'
163	MR	500	GDP	C3'-C4'-C5'-O5'
163	NR	500	GDP	C3'-C4'-C5'-O5'
165	II	501	GTP	C3'-C4'-C5'-O5'
165	JD	501	GTP	C3'-C4'-C5'-O5'
165	FS	501	GTP	C3'-C4'-C5'-O5'
165	IU	501	GTP	C3'-C4'-C5'-O5'
165	JP	501	GTP	C3'-C4'-C5'-O5'
165	DL	501	GTP	C4'-C5'-O5'-PA
165	NA	501	GTP	C4'-C5'-O5'-PA
165	DX	501	GTP	C4'-C5'-O5'-PA
165	MV	501	GTP	C4'-C5'-O5'-PA
168	2v	501	ATP	C2'-C1'-N9-C8
165	GL	501	GTP	PA-O3A-PB-O1B
165	QH	501	GTP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	UE	501	GTP	PA-O3A-PB-O1B
165	QT	501	GTP	PA-O3A-PB-O2B
165	UQ	501	GTP	PA-O3A-PB-O1B
168	2w	501	ATP	PA-O3A-PB-O1B
168	2x	501	ATP	PA-O3A-PB-O1B
168	6p	500	ATP	PB-O3A-PA-O2A
168	6u	700	ATP	PA-O3A-PB-O1B
168	7D	601	ATP	PG-O3B-PB-O2B
168	7D	601	ATP	PA-O3A-PB-O2B
168	8a	801	ATP	PG-O3B-PB-O2B
163	AH	500	GDP	C3'-C4'-C5'-O5'
163	BL	500	GDP	C3'-C4'-C5'-O5'
163	AT	500	GDP	C3'-C4'-C5'-O5'
163	FR	501	GDP	C3'-C4'-C5'-O5'
165	LD	502	GTP	C3'-C4'-C5'-O5'
165	FV	503	GTP	C3'-C4'-C5'-O5'
165	LP	502	GTP	C3'-C4'-C5'-O5'
165	MJ	501	GTP	C4'-C5'-O5'-PA
163	ED	500	GDP	O4'-C4'-C5'-O5'
163	HB	501	GDP	C3'-C4'-C5'-O5'
163	IF	500	GDP	O4'-C4'-C5'-O5'
163	OJ	500	GDP	O4'-C4'-C5'-O5'
163	PD	500	GDP	O4'-C4'-C5'-O5'
163	SB	501	GDP	C3'-C4'-C5'-O5'
163	SD	500	GDP	O4'-C4'-C5'-O5'
163	GX	500	GDP	C3'-C4'-C5'-O5'
163	HN	501	GDP	C3'-C4'-C5'-O5'
163	IR	500	GDP	O4'-C4'-C5'-O5'
163	PP	500	GDP	O4'-C4'-C5'-O5'
163	SN	501	GDP	C3'-C4'-C5'-O5'
163	SP	500	GDP	O4'-C4'-C5'-O5'
163	OV	500	GDP	O4'-C4'-C5'-O5'
165	II	501	GTP	O4'-C4'-C5'-O5'
165	DX	501	GTP	O4'-C4'-C5'-O5'
165	IU	501	GTP	O4'-C4'-C5'-O5'
165	RX	501	GTP	C3'-C4'-C5'-O5'
163	AJ	500	GDP	C5'-O5'-PA-O1A
163	AN	500	GDP	C5'-O5'-PA-O1A
163	BJ	500	GDP	C5'-O5'-PA-O1A
163	BN	500	GDP	C5'-O5'-PA-O1A
163	CC	500	GDP	C5'-O5'-PA-O1A
163	CK	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	DG	500	GDP	C5'-O5'-PA-O1A
163	DI	500	GDP	C5'-O5'-PA-O1A
163	DK	501	GDP	C5'-O5'-PA-O1A
163	EF	500	GDP	C5'-O5'-PA-O1A
163	EH	500	GDP	C5'-O5'-PA-O1A
163	F	500	GDP	C5'-O5'-PA-O1A
163	FL	500	GDP	C5'-O5'-PA-O1A
163	GD	500	GDP	C5'-O5'-PA-O1A
163	GF	500	GDP	C5'-O5'-PA-O3A
163	GH	500	GDP	C5'-O5'-PA-O1A
163	HB	501	GDP	C5'-O5'-PA-O1A
163	HL	501	GDP	C5'-O5'-PA-O1A
163	ID	500	GDP	C5'-O5'-PA-O1A
163	IH	500	GDP	C5'-O5'-PA-O1A
163	JA	500	GDP	C5'-O5'-PA-O1A
163	JC	500	GDP	C5'-O5'-PA-O1A
163	JE	500	GDP	C5'-O5'-PA-O1A
163	KA	500	GDP	C5'-O5'-PA-O1A
163	KE	500	GDP	C5'-O5'-PA-O1A
163	KI	500	GDP	C5'-O5'-PA-O1A
163	KK	500	GDP	C5'-O5'-PA-O1A
163	KM	500	GDP	C5'-O5'-PA-O1A
163	LA	500	GDP	C5'-O5'-PA-O1A
163	LE	500	GDP	C5'-O5'-PA-O3A
163	LI	500	GDP	C5'-O5'-PA-O1A
163	LK	500	GDP	C5'-O5'-PA-O1A
163	MB	500	GDP	C5'-O5'-PA-O1A
163	MF	500	GDP	C5'-O5'-PA-O1A
163	MJ	500	GDP	C5'-O5'-PA-O1A
163	ML	500	GDP	C5'-O5'-PA-O1A
163	MN	500	GDP	C5'-O5'-PA-O1A
163	NJ	501	GDP	C5'-O5'-PA-O1A
163	NL	500	GDP	C5'-O5'-PA-O1A
163	OD	501	GDP	C5'-O5'-PA-O1A
163	OJ	500	GDP	C5'-O5'-PA-O1A
163	P	500	GDP	C5'-O5'-PA-O1A
163	PD	500	GDP	C5'-O5'-PA-O3A
163	PF	501	GDP	C5'-O5'-PA-O1A
163	PJ	500	GDP	C5'-O5'-PA-O1A
163	QC	500	GDP	C5'-O5'-PA-O1A
163	QI	500	GDP	C5'-O5'-PA-O1A
163	RK	500	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	SH	500	GDP	C5'-O5'-PA-O1A
163	SJ	501	GDP	C5'-O5'-PA-O1A
163	T	501	GDP	C5'-O5'-PA-O1A
163	TD	500	GDP	C5'-O5'-PA-O1A
163	UB	500	GDP	C5'-O5'-PA-O1A
163	UJ	500	GDP	C5'-O5'-PA-O1A
163	UL	500	GDP	C5'-O5'-PA-O1A
163	V	500	GDP	C5'-O5'-PA-O1A
163	VH	500	GDP	C5'-O5'-PA-O1A
163	W	500	GDP	C5'-O5'-PA-O1A
163	WB	500	GDP	C5'-O5'-PA-O1A
163	WF	501	GDP	C5'-O5'-PA-O1A
163	WH	500	GDP	C5'-O5'-PA-O3A
163	AP	500	GDP	C5'-O5'-PA-O1A
163	AV	500	GDP	C5'-O5'-PA-O1A
163	AZ	500	GDP	C5'-O5'-PA-O1A
163	BP	500	GDP	C5'-O5'-PA-O3A
163	BR	500	GDP	C5'-O5'-PA-O1A
163	BV	500	GDP	C5'-O5'-PA-O1A
163	CW	500	GDP	C5'-O5'-PA-O1A
163	DS	500	GDP	C5'-O5'-PA-O1A
163	DY	500	GDP	C5'-O5'-PA-O1A
163	EN	500	GDP	C5'-O5'-PA-O3A
163	ER	500	GDP	C5'-O5'-PA-O1A
163	ET	500	GDP	C5'-O5'-PA-O1A
163	EV	500	GDP	C5'-O5'-PA-O1A
163	FT	501	GDP	C5'-O5'-PA-O1A
163	FV	501	GDP	C5'-O5'-PA-O1A
163	GP	500	GDP	C5'-O5'-PA-O1A
163	GT	501	GDP	C5'-O5'-PA-O1A
163	HN	501	GDP	C5'-O5'-PA-O1A
163	HX	501	GDP	C5'-O5'-PA-O1A
163	IP	500	GDP	C5'-O5'-PA-O1A
163	IT	501	GDP	C5'-O5'-PA-O1A
163	JO	500	GDP	C5'-O5'-PA-O1A
163	JQ	500	GDP	C5'-O5'-PA-O1A
163	KQ	500	GDP	C5'-O5'-PA-O1A
163	KU	500	GDP	C5'-O5'-PA-O1A
163	KW	500	GDP	C5'-O5'-PA-O1A
163	KY	500	GDP	C5'-O5'-PA-O1A
163	LQ	500	GDP	C5'-O5'-PA-O3A
163	LU	500	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	LW	500	GDP	C5'-O5'-PA-O1A
163	MR	500	GDP	C5'-O5'-PA-O1A
163	MV	500	GDP	C5'-O5'-PA-O1A
163	MX	500	GDP	C5'-O5'-PA-O1A
163	MZ	500	GDP	C5'-O5'-PA-O1A
163	PP	500	GDP	C5'-O5'-PA-O3A
163	PR	501	GDP	C5'-O5'-PA-O1A
163	PV	500	GDP	C5'-O5'-PA-O1A
163	QO	500	GDP	C5'-O5'-PA-O1A
163	QU	500	GDP	C5'-O5'-PA-O1A
163	RW	500	GDP	C5'-O5'-PA-O1A
163	ST	500	GDP	C5'-O5'-PA-O1A
163	SV	501	GDP	C5'-O5'-PA-O1A
163	TP	500	GDP	C5'-O5'-PA-O1A
163	UN	500	GDP	C5'-O5'-PA-O1A
163	UV	500	GDP	C5'-O5'-PA-O1A
163	UX	500	GDP	C5'-O5'-PA-O1A
163	VT	500	GDP	C5'-O5'-PA-O1A
163	WN	500	GDP	C5'-O5'-PA-O1A
163	WR	501	GDP	C5'-O5'-PA-O1A
163	WT	500	GDP	C5'-O5'-PA-O3A
163	NV	501	GDP	C5'-O5'-PA-O1A
163	NX	500	GDP	C5'-O5'-PA-O1A
163	OP	501	GDP	C5'-O5'-PA-O1A
163	OV	500	GDP	C5'-O5'-PA-O1A
165	AA	501	GTP	C5'-O5'-PA-O1A
165	AM	501	GTP	C5'-O5'-PA-O1A
165	C	501	GTP	C5'-O5'-PA-O1A
165	CE	501	GTP	C5'-O5'-PA-O1A
165	D	501	GTP	C5'-O5'-PA-O1A
165	DB	501	GTP	C5'-O5'-PA-O1A
165	DE	501	GTP	C5'-O5'-PA-O3A
165	DE	501	GTP	C5'-O5'-PA-O2A
165	DL	501	GTP	C5'-O5'-PA-O1A
165	IM	501	GTP	C5'-O5'-PA-O1A
165	JD	501	GTP	C5'-O5'-PA-O1A
165	JH	501	GTP	C5'-O5'-PA-O3A
165	JH	501	GTP	C5'-O5'-PA-O1A
165	KD	502	GTP	C5'-O5'-PA-O1A
165	LB	501	GTP	C5'-O5'-PA-O1A
165	LD	502	GTP	C5'-O5'-PA-O1A
165	LL	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	ME	501	GTP	C5'-O5'-PA-O1A
165	MG	501	GTP	C5'-O5'-PA-O2A
165	MJ	501	GTP	C5'-O5'-PA-O1A
165	MM	501	GTP	C5'-O5'-PA-O3A
165	MM	501	GTP	C5'-O5'-PA-O1A
165	NA	501	GTP	C5'-O5'-PA-O1A
165	NC	501	GTP	C5'-O5'-PA-O1A
165	NF	501	GTP	C5'-O5'-PA-O2A
165	NM	501	GTP	C5'-O5'-PA-O1A
165	OI	501	GTP	C5'-O5'-PA-O1A
165	PG	501	GTP	C5'-O5'-PA-O3A
165	Q	501	GTP	C5'-O5'-PA-O1A
165	QF	501	GTP	C5'-O5'-PA-O3A
165	RL	501	GTP	C5'-O5'-PA-O1A
165	SC	501	GTP	C5'-O5'-PA-O2A
165	SG	501	GTP	C5'-O5'-PA-O3A
165	SG	501	GTP	C5'-O5'-PA-O1A
165	TC	501	GTP	C5'-O5'-PA-O3A
165	TK	501	GTP	C5'-O5'-PA-O1A
165	UG	501	GTP	C5'-O5'-PA-O1A
165	VK	501	GTP	C5'-O5'-PA-O1A
165	VM	501	GTP	C5'-O5'-PA-O1A
165	WA	501	GTP	C5'-O5'-PA-O3A
165	WA	501	GTP	C5'-O5'-PA-O1A
165	WC	501	GTP	C5'-O5'-PA-O3A
165	WC	501	GTP	C5'-O5'-PA-O1A
165	WE	501	GTP	C5'-O5'-PA-O1A
165	WM	501	GTP	C5'-O5'-PA-O1A
165	AU	501	GTP	C5'-O5'-PA-O3A
165	AW	501	GTP	C5'-O5'-PA-O1A
165	AY	501	GTP	C5'-O5'-PA-O1A
165	BY	501	GTP	C5'-O5'-PA-O1A
165	DQ	501	GTP	C5'-O5'-PA-O2A
165	DX	501	GTP	C5'-O5'-PA-O1A
165	EM	501	GTP	C5'-O5'-PA-O1A
165	FM	501	GTP	C5'-O5'-PA-O3A
165	GU	501	GTP	C5'-O5'-PA-O2A
165	IY	501	GTP	C5'-O5'-PA-O1A
165	JP	501	GTP	C5'-O5'-PA-O1A
165	JT	501	GTP	C5'-O5'-PA-O3A
165	JT	501	GTP	C5'-O5'-PA-O1A
165	KP	502	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	LP	502	GTP	C5'-O5'-PA-O1A
165	LX	501	GTP	C5'-O5'-PA-O1A
165	MQ	501	GTP	C5'-O5'-PA-O1A
165	MS	501	GTP	C5'-O5'-PA-O2A
165	MV	501	GTP	C5'-O5'-PA-O1A
165	MY	501	GTP	C5'-O5'-PA-O3A
165	MY	501	GTP	C5'-O5'-PA-O1A
165	PS	501	GTP	C5'-O5'-PA-O3A
165	QR	501	GTP	C5'-O5'-PA-O3A
165	RX	501	GTP	C5'-O5'-PA-O1A
165	SO	501	GTP	C5'-O5'-PA-O2A
165	SS	501	GTP	C5'-O5'-PA-O3A
165	SS	501	GTP	C5'-O5'-PA-O1A
165	TO	501	GTP	C5'-O5'-PA-O3A
165	TW	501	GTP	C5'-O5'-PA-O1A
165	US	501	GTP	C5'-O5'-PA-O1A
165	VW	501	GTP	C5'-O5'-PA-O1A
165	VY	501	GTP	C5'-O5'-PA-O1A
165	WO	501	GTP	C5'-O5'-PA-O3A
165	WO	501	GTP	C5'-O5'-PA-O1A
165	WQ	501	GTP	C5'-O5'-PA-O1A
165	WY	501	GTP	C5'-O5'-PA-O1A
165	NO	501	GTP	C5'-O5'-PA-O1A
165	NR	501	GTP	C5'-O5'-PA-O2A
165	NY	501	GTP	C5'-O5'-PA-O1A
165	OU	501	GTP	C5'-O5'-PA-O1A
168	2w	501	ATP	C5'-O5'-PA-O1A
168	2x	501	ATP	C5'-O5'-PA-O1A
168	7A	402	ATP	C5'-O5'-PA-O1A
168	7A	402	ATP	C5'-O5'-PA-O2A
168	7A	402	ATP	C5'-O5'-PA-O3A
168	7D	601	ATP	C5'-O5'-PA-O2A
165	AG	501	GTP	C4'-C5'-O5'-PA
165	AM	501	GTP	C4'-C5'-O5'-PA
165	D	501	GTP	C4'-C5'-O5'-PA
165	FG	501	GTP	C4'-C5'-O5'-PA
165	HA	501	GTP	C4'-C5'-O5'-PA
165	HB	503	GTP	C4'-C5'-O5'-PA
165	IG	501	GTP	C4'-C5'-O5'-PA
165	J	501	GTP	C4'-C5'-O5'-PA
165	JK	501	GTP	C4'-C5'-O5'-PA
165	KJ	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	KN	502	GTP	C4'-C5'-O5'-PA
165	NF	501	GTP	C4'-C5'-O5'-PA
165	OA	501	GTP	C4'-C5'-O5'-PA
165	OM	501	GTP	C4'-C5'-O5'-PA
165	RC	501	GTP	C4'-C5'-O5'-PA
165	RL	501	GTP	C4'-C5'-O5'-PA
165	SC	501	GTP	C4'-C5'-O5'-PA
165	SE	501	GTP	C4'-C5'-O5'-PA
165	T	503	GTP	C4'-C5'-O5'-PA
165	TC	501	GTP	C4'-C5'-O5'-PA
165	TE	501	GTP	C4'-C5'-O5'-PA
165	UE	501	GTP	C4'-C5'-O5'-PA
165	VE	501	GTP	C4'-C5'-O5'-PA
165	AS	501	GTP	C4'-C5'-O5'-PA
165	BQ	501	GTP	C4'-C5'-O5'-PA
165	FT	503	GTP	C4'-C5'-O5'-PA
165	HN	503	GTP	C4'-C5'-O5'-PA
165	IS	501	GTP	C4'-C5'-O5'-PA
165	JW	501	GTP	C4'-C5'-O5'-PA
165	KV	501	GTP	C4'-C5'-O5'-PA
165	KZ	501	GTP	C4'-C5'-O5'-PA
165	RO	501	GTP	C4'-C5'-O5'-PA
165	RX	501	GTP	C4'-C5'-O5'-PA
165	SO	501	GTP	C4'-C5'-O5'-PA
165	SQ	501	GTP	C4'-C5'-O5'-PA
165	TM	501	GTP	C4'-C5'-O5'-PA
165	TO	501	GTP	C4'-C5'-O5'-PA
165	TQ	501	GTP	C4'-C5'-O5'-PA
165	UQ	501	GTP	C4'-C5'-O5'-PA
165	VQ	501	GTP	C4'-C5'-O5'-PA
165	NR	501	GTP	C4'-C5'-O5'-PA
165	OY	501	GTP	C4'-C5'-O5'-PA
168	7D	601	ATP	C4'-C5'-O5'-PA
163	G	500	GDP	O4'-C4'-C5'-O5'
163	NB	500	GDP	O4'-C4'-C5'-O5'
163	SH	500	GDP	C3'-C4'-C5'-O5'
163	ST	500	GDP	C3'-C4'-C5'-O5'
163	NN	500	GDP	O4'-C4'-C5'-O5'
165	RJ	501	GTP	C3'-C4'-C5'-O5'
165	RL	501	GTP	C3'-C4'-C5'-O5'
165	RV	501	GTP	C3'-C4'-C5'-O5'
165	BE	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	QK	500	GDP	PB-O3A-PA-O2A
163	QW	500	GDP	PB-O3A-PA-O2A
165	AA	501	GTP	PG-O3B-PB-O1B
165	EG	501	GTP	PB-O3A-PA-O2A
165	FI	501	GTP	PA-O3A-PB-O2B
165	G	501	GTP	PB-O3A-PA-O2A
165	GE	501	GTP	PB-O3A-PA-O2A
165	IK	501	GTP	PG-O3B-PB-O1B
165	J	501	GTP	PG-O3B-PB-O2B
165	RL	501	GTP	PG-O3B-PB-O1B
165	SE	501	GTP	PB-O3A-PA-O2A
165	ES	501	GTP	PB-O3A-PA-O2A
165	FT	503	GTP	PA-O3A-PB-O2B
165	IW	501	GTP	PG-O3B-PB-O1B
165	RX	501	GTP	PG-O3B-PB-O1B
165	SQ	501	GTP	PB-O3A-PA-O2A
168	6u	700	ATP	PA-O3A-PB-O2B
163	FD	500	GDP	C3'-C4'-C5'-O5'
163	HF	500	GDP	C3'-C4'-C5'-O5'
163	KA	500	GDP	C3'-C4'-C5'-O5'
163	SJ	501	GDP	C3'-C4'-C5'-O5'
163	AV	500	GDP	C3'-C4'-C5'-O5'
163	HR	500	GDP	C3'-C4'-C5'-O5'
163	SV	501	GDP	C3'-C4'-C5'-O5'
165	LD	502	GTP	C4'-C5'-O5'-PA
165	PG	501	GTP	C4'-C5'-O5'-PA
165	EM	501	GTP	C4'-C5'-O5'-PA
165	LP	502	GTP	C4'-C5'-O5'-PA
165	PS	501	GTP	C4'-C5'-O5'-PA
165	J	501	GTP	PA-O3A-PB-O3B
163	GL	500	GDP	C3'-C4'-C5'-O5'
165	GG	501	GTP	C3'-C4'-C5'-O5'
165	QB	501	GTP	O4'-C4'-C5'-O5'
165	QN	501	GTP	O4'-C4'-C5'-O5'
165	CK	503	GTP	C4'-C5'-O5'-PA
165	JB	501	GTP	C4'-C5'-O5'-PA
165	JN	501	GTP	C4'-C5'-O5'-PA
165	MC	501	GTP	C4'-C5'-O5'-PA
165	TK	501	GTP	C4'-C5'-O5'-PA
165	UK	501	GTP	C4'-C5'-O5'-PA
165	CW	501	GTP	C4'-C5'-O5'-PA
165	EO	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	FM	501	GTP	C4'-C5'-O5'-PA
165	JZ	501	GTP	C4'-C5'-O5'-PA
165	MO	501	GTP	C4'-C5'-O5'-PA
165	TW	501	GTP	C4'-C5'-O5'-PA
165	UW	501	GTP	C4'-C5'-O5'-PA
165	HB	503	GTP	PB-O3B-PG-O1G
165	HN	503	GTP	PB-O3B-PG-O1G
163	IH	500	GDP	C3'-C4'-C5'-O5'
163	OL	500	GDP	O4'-C4'-C5'-O5'
163	IT	501	GDP	C3'-C4'-C5'-O5'
165	IK	501	GTP	PA-O3A-PB-O3B
165	IW	501	GTP	PA-O3A-PB-O3B
165	FI	501	GTP	C4'-C5'-O5'-PA
165	KB	502	GTP	C4'-C5'-O5'-PA
165	NM	501	GTP	C4'-C5'-O5'-PA
165	QC	501	GTP	C4'-C5'-O5'-PA
165	WK	501	GTP	C4'-C5'-O5'-PA
165	DQ	501	GTP	C4'-C5'-O5'-PA
165	FQ	501	GTP	C4'-C5'-O5'-PA
165	QO	501	GTP	C4'-C5'-O5'-PA
165	WW	501	GTP	C4'-C5'-O5'-PA
165	NY	501	GTP	C4'-C5'-O5'-PA
163	AL	500	GDP	O4'-C4'-C5'-O5'
163	CC	500	GDP	O4'-C4'-C5'-O5'
163	DA	500	GDP	O4'-C4'-C5'-O5'
163	F	500	GDP	O4'-C4'-C5'-O5'
163	JG	500	GDP	O4'-C4'-C5'-O5'
163	KM	500	GDP	C3'-C4'-C5'-O5'
163	AX	500	GDP	C3'-C4'-C5'-O5'
163	CQ	500	GDP	C3'-C4'-C5'-O5'
163	DQ	500	GDP	C3'-C4'-C5'-O5'
163	GV	501	GDP	O4'-C4'-C5'-O5'
163	KY	500	GDP	C3'-C4'-C5'-O5'
163	OX	500	GDP	O4'-C4'-C5'-O5'
165	OK	501	GTP	C3'-C4'-C5'-O5'
165	PG	501	GTP	O4'-C4'-C5'-O5'
165	PK	501	GTP	C3'-C4'-C5'-O5'
165	TC	501	GTP	O4'-C4'-C5'-O5'
165	TI	501	GTP	C3'-C4'-C5'-O5'
165	VM	501	GTP	O4'-C4'-C5'-O5'
165	PS	501	GTP	O4'-C4'-C5'-O5'
165	PW	501	GTP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	TO	501	GTP	O4'-C4'-C5'-O5'
165	VY	501	GTP	O4'-C4'-C5'-O5'
165	OW	501	GTP	C3'-C4'-C5'-O5'
165	AI	501	GTP	PA-O3A-PB-O1B
165	BI	501	GTP	PG-O3B-PB-O1B
165	D	501	GTP	PG-O3B-PB-O1B
165	DL	501	GTP	PG-O3B-PB-O1B
165	EI	501	GTP	PA-O3A-PB-O1B
165	FG	501	GTP	PA-O3A-PB-O1B
165	FI	501	GTP	PA-O3A-PB-O1B
165	IK	501	GTP	PA-O3A-PB-O1B
165	OK	501	GTP	PA-O3A-PB-O1B
165	OM	501	GTP	PG-O3B-PB-O1B
165	R	501	GTP	PG-O3B-PB-O1B
165	WE	501	GTP	PG-O3B-PB-O1B
165	AS	501	GTP	PA-O3A-PB-O1B
165	ES	501	GTP	PB-O3A-PA-O1A
165	IW	501	GTP	PA-O3A-PB-O1B
165	WQ	501	GTP	PG-O3B-PB-O1B
165	OW	501	GTP	PA-O3A-PB-O1B
165	OY	501	GTP	PG-O3B-PB-O1B
168	6l	400	ATP	PB-O3A-PA-O2A
168	9R	500	ATP	PA-O3A-PB-O1B
168	7A	402	ATP	PA-O3A-PB-O1B
165	TK	501	GTP	PB-O3A-PA-O5'
165	TW	501	GTP	PB-O3A-PA-O5'
163	GH	500	GDP	C4'-C5'-O5'-PA
165	AA	501	GTP	C4'-C5'-O5'-PA
165	AD	501	GTP	C4'-C5'-O5'-PA
165	C	501	GTP	C4'-C5'-O5'-PA
165	DE	501	GTP	C4'-C5'-O5'-PA
165	HE	501	GTP	C4'-C5'-O5'-PA
165	HM	501	GTP	C4'-C5'-O5'-PA
165	IA	501	GTP	C4'-C5'-O5'-PA
165	IM	501	GTP	C4'-C5'-O5'-PA
165	L	501	GTP	C4'-C5'-O5'-PA
165	OD	503	GTP	C4'-C5'-O5'-PA
165	R	501	GTP	C4'-C5'-O5'-PA
165	SA	501	GTP	C4'-C5'-O5'-PA
165	VH	501	GTP	C4'-C5'-O5'-PA
165	VK	501	GTP	C4'-C5'-O5'-PA
165	WE	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	AO	501	GTP	C4'-C5'-O5'-PA
165	AY	501	GTP	C4'-C5'-O5'-PA
165	HQ	501	GTP	C4'-C5'-O5'-PA
165	HY	501	GTP	C4'-C5'-O5'-PA
165	IY	501	GTP	C4'-C5'-O5'-PA
165	SM	501	GTP	C4'-C5'-O5'-PA
165	VT	501	GTP	C4'-C5'-O5'-PA
165	VW	501	GTP	C4'-C5'-O5'-PA
165	OP	503	GTP	C4'-C5'-O5'-PA
168	2v	501	ATP	O4'-C1'-N9-C8
163	CE	500	GDP	C3'-C4'-C5'-O5'
163	HD	501	GDP	O4'-C4'-C5'-O5'
163	LA	500	GDP	C3'-C4'-C5'-O5'
163	LO	500	GDP	C3'-C4'-C5'-O5'
163	MF	500	GDP	O4'-C4'-C5'-O5'
163	HP	501	GDP	O4'-C4'-C5'-O5'
163	JS	500	GDP	O4'-C4'-C5'-O5'
163	MR	500	GDP	O4'-C4'-C5'-O5'
165	TU	501	GTP	C3'-C4'-C5'-O5'
165	HK	501	GTP	C4'-C5'-O5'-PA
165	LL	501	GTP	C4'-C5'-O5'-PA
165	PK	501	GTP	C4'-C5'-O5'-PA
165	UA	501	GTP	C4'-C5'-O5'-PA
165	HW	501	GTP	C4'-C5'-O5'-PA
165	LX	501	GTP	C4'-C5'-O5'-PA
165	PW	501	GTP	C4'-C5'-O5'-PA
165	UM	501	GTP	C4'-C5'-O5'-PA
165	WQ	501	GTP	C4'-C5'-O5'-PA
163	KI	500	GDP	O4'-C4'-C5'-O5'
163	MN	500	GDP	C3'-C4'-C5'-O5'
163	NF	500	GDP	O4'-C4'-C5'-O5'
163	KU	500	GDP	O4'-C4'-C5'-O5'
163	MZ	500	GDP	C3'-C4'-C5'-O5'
163	NR	500	GDP	O4'-C4'-C5'-O5'
165	JD	501	GTP	O4'-C4'-C5'-O5'
165	JP	501	GTP	O4'-C4'-C5'-O5'
165	CE	501	GTP	PB-O3B-PG-O1G
165	SG	501	GTP	PB-O3B-PG-O1G
165	FQ	501	GTP	PB-O3B-PG-O1G
165	SS	501	GTP	PB-O3B-PG-O1G
163	CK	501	GDP	PA-O3A-PB-O2B
163	CY	500	GDP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	AB	501	GTP	PB-O3B-PG-O2G
165	BE	501	GTP	PB-O3B-PG-O2G
165	CE	501	GTP	PB-O3B-PG-O2G
165	CE	501	GTP	PB-O3B-PG-O3G
165	CH	501	GTP	PB-O3B-PG-O2G
165	D	501	GTP	PB-O3B-PG-O2G
165	EJ	501	GTP	PB-O3B-PG-O2G
165	EJ	501	GTP	PB-O3B-PG-O3G
165	FE	501	GTP	PB-O3B-PG-O2G
165	G	501	GTP	PB-O3B-PG-O2G
165	HB	503	GTP	PB-O3B-PG-O2G
165	HB	503	GTP	PB-O3B-PG-O3G
165	KF	501	GTP	PB-O3B-PG-O2G
165	KF	501	GTP	PB-O3B-PG-O3G
165	KH	501	GTP	PB-O3B-PG-O2G
165	QC	501	GTP	PB-O3B-PG-O2G
165	T	503	GTP	PB-O3B-PG-O2G
165	T	503	GTP	PB-O3B-PG-O3G
165	VC	501	GTP	PB-O3B-PG-O2G
165	VC	501	GTP	PB-O3B-PG-O3G
165	BQ	501	GTP	PB-O3B-PG-O3G
165	CO	501	GTP	PB-O3B-PG-O2G
165	CT	501	GTP	PB-O3B-PG-O2G
165	EP	501	GTP	PB-O3B-PG-O2G
165	FQ	501	GTP	PB-O3B-PG-O2G
165	HN	503	GTP	PB-O3B-PG-O2G
165	HN	503	GTP	PB-O3B-PG-O3G
165	KR	501	GTP	PB-O3B-PG-O2G
165	KR	501	GTP	PB-O3B-PG-O3G
165	KT	501	GTP	PB-O3B-PG-O2G
165	QO	501	GTP	PB-O3B-PG-O2G
165	TM	501	GTP	PB-O3B-PG-O2G
165	TM	501	GTP	PB-O3B-PG-O3G
165	VO	501	GTP	PB-O3B-PG-O2G
165	VO	501	GTP	PB-O3B-PG-O3G
165	FE	501	GTP	C4'-C5'-O5'-PA
165	KH	501	GTP	C4'-C5'-O5'-PA
165	MI	501	GTP	C4'-C5'-O5'-PA
165	QI	501	GTP	C4'-C5'-O5'-PA
165	KT	501	GTP	C4'-C5'-O5'-PA
165	MU	501	GTP	C4'-C5'-O5'-PA
165	QU	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
163	GD	500	GDP	O4'-C4'-C5'-O5'
163	JC	500	GDP	C3'-C4'-C5'-O5'
163	MB	500	GDP	C3'-C4'-C5'-O5'
163	QE	500	GDP	C3'-C4'-C5'-O5'
163	RK	500	GDP	C3'-C4'-C5'-O5'
163	BR	500	GDP	C3'-C4'-C5'-O5'
163	JO	500	GDP	C3'-C4'-C5'-O5'
163	QQ	500	GDP	C3'-C4'-C5'-O5'
163	RW	500	GDP	C3'-C4'-C5'-O5'
165	LD	502	GTP	O4'-C4'-C5'-O5'
165	GS	501	GTP	C3'-C4'-C5'-O5'
165	LP	502	GTP	O4'-C4'-C5'-O5'
168	9R	500	ATP	O4'-C4'-C5'-O5'
163	BJ	500	GDP	C3'-C4'-C5'-O5'
163	FJ	501	GDP	C3'-C4'-C5'-O5'
163	GB	500	GDP	C3'-C4'-C5'-O5'
163	OD	501	GDP	C3'-C4'-C5'-O5'
163	EN	500	GDP	C3'-C4'-C5'-O5'
163	OP	501	GDP	C3'-C4'-C5'-O5'
165	MJ	501	GTP	C3'-C4'-C5'-O5'
165	NK	501	GTP	C3'-C4'-C5'-O5'
165	OC	501	GTP	C3'-C4'-C5'-O5'
165	WK	501	GTP	C3'-C4'-C5'-O5'
165	BY	501	GTP	C3'-C4'-C5'-O5'
165	MV	501	GTP	C3'-C4'-C5'-O5'
165	WW	501	GTP	C3'-C4'-C5'-O5'
165	NW	501	GTP	C3'-C4'-C5'-O5'
165	OO	501	GTP	C3'-C4'-C5'-O5'
165	FA	501	GTP	C4'-C5'-O5'-PA
165	EG	501	GTP	PA-O3A-PB-O2B
165	GC	501	GTP	PA-O3A-PB-O2B
165	GE	501	GTP	PB-O3A-PA-O1A
165	IG	501	GTP	PA-O3A-PB-O2B
165	II	501	GTP	PB-O3A-PA-O2A
165	J	501	GTP	PA-O3A-PB-O1B
165	NF	501	GTP	PB-O3A-PA-O2A
165	NI	501	GTP	PB-O3A-PA-O2A
165	TG	501	GTP	PB-O3A-PA-O2A
165	VG	501	GTP	PB-O3A-PA-O2A
165	WG	501	GTP	PG-O3B-PB-O2B
165	AS	501	GTP	PA-O3A-PB-O2B
165	BS	501	GTP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	ES	501	GTP	PA-O3A-PB-O1B
165	FT	503	GTP	PA-O3A-PB-O1B
165	GQ	501	GTP	PA-O3A-PB-O2B
165	IS	501	GTP	PA-O3A-PB-O2B
165	IU	501	GTP	PB-O3A-PA-O2A
165	TS	501	GTP	PB-O3A-PA-O2A
165	WS	501	GTP	PG-O3B-PB-O2B
165	NR	501	GTP	PB-O3A-PA-O2A
165	NU	501	GTP	PB-O3A-PA-O2A
168	6l	400	ATP	PB-O3A-PA-O1A
168	9R	500	ATP	PA-O3A-PB-O2B
168	6u	700	ATP	PG-O3B-PB-O2B
168	7D	601	ATP	PG-O3B-PB-O1B
163	AB	500	GDP	C3'-C4'-C5'-O5'
163	AD	500	GDP	C3'-C4'-C5'-O5'
165	J	501	GTP	C3'-C4'-C5'-O5'
165	FC	501	GTP	C4'-C5'-O5'-PA
168	2v	501	ATP	C2'-C1'-N9-C4
165	DL	501	GTP	PB-O3B-PG-O1G
165	FE	501	GTP	PB-O3B-PG-O1G
163	AH	500	GDP	O4'-C4'-C5'-O5'
163	BL	500	GDP	O4'-C4'-C5'-O5'
163	HB	501	GDP	O4'-C4'-C5'-O5'
163	HF	500	GDP	O4'-C4'-C5'-O5'
163	LM	500	GDP	C3'-C4'-C5'-O5'
163	SB	501	GDP	O4'-C4'-C5'-O5'
163	FR	501	GDP	O4'-C4'-C5'-O5'
163	GX	500	GDP	O4'-C4'-C5'-O5'
163	HN	501	GDP	O4'-C4'-C5'-O5'
163	LY	500	GDP	C3'-C4'-C5'-O5'
163	SN	501	GDP	O4'-C4'-C5'-O5'
165	MC	501	GTP	C3'-C4'-C5'-O5'
165	RL	501	GTP	O4'-C4'-C5'-O5'
165	MO	501	GTP	C3'-C4'-C5'-O5'
165	RX	501	GTP	O4'-C4'-C5'-O5'
165	AB	501	GTP	C4'-C5'-O5'-PA
165	AP	501	GTP	C4'-C5'-O5'-PA
163	OB	500	GDP	C3'-C4'-C5'-O5'
163	HR	500	GDP	O4'-C4'-C5'-O5'
165	FJ	503	GTP	O4'-C4'-C5'-O5'
165	DH	501	GTP	C4'-C5'-O5'-PA
165	BG	501	GTP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
165	EG	501	GTP	PB-O3A-PA-O1A
165	FG	501	GTP	PA-O3A-PB-O2B
165	GI	501	GTP	PB-O3A-PA-O2A
165	GL	501	GTP	PA-O3A-PB-O2B
165	J	501	GTP	PG-O3B-PB-O1B
165	LH	501	GTP	PB-O3A-PA-O2A
165	MG	501	GTP	PG-O3B-PB-O2B
165	UE	501	GTP	PA-O3A-PB-O2B
165	CT	501	GTP	PB-O3A-PA-O2A
165	DT	501	GTP	PB-O3A-PA-O2A
165	ES	501	GTP	PA-O3A-PB-O2B
165	LT	501	GTP	PB-O3A-PA-O2A
165	LV	501	GTP	PA-O3A-PB-O2B
165	MS	501	GTP	PG-O3B-PB-O2B
165	UQ	501	GTP	PA-O3A-PB-O2B
165	VS	501	GTP	PB-O3A-PA-O2A
168	2w	501	ATP	PA-O3A-PB-O2B
168	2x	501	ATP	PA-O3A-PB-O2B
168	6p	500	ATP	PG-O3B-PB-O2B
168	7A	402	ATP	PA-O3A-PB-O2B
168	7D	601	ATP	PA-O3A-PB-O1B
163	GL	500	GDP	O4'-C4'-C5'-O5'
163	KA	500	GDP	O4'-C4'-C5'-O5'
163	LG	501	GDP	C3'-C4'-C5'-O5'
163	NH	500	GDP	C3'-C4'-C5'-O5'
163	P	500	GDP	C3'-C4'-C5'-O5'
163	AT	500	GDP	O4'-C4'-C5'-O5'
163	LS	500	GDP	C3'-C4'-C5'-O5'
163	QM	500	GDP	C3'-C4'-C5'-O5'
163	NT	500	GDP	C3'-C4'-C5'-O5'
163	ON	500	GDP	C3'-C4'-C5'-O5'

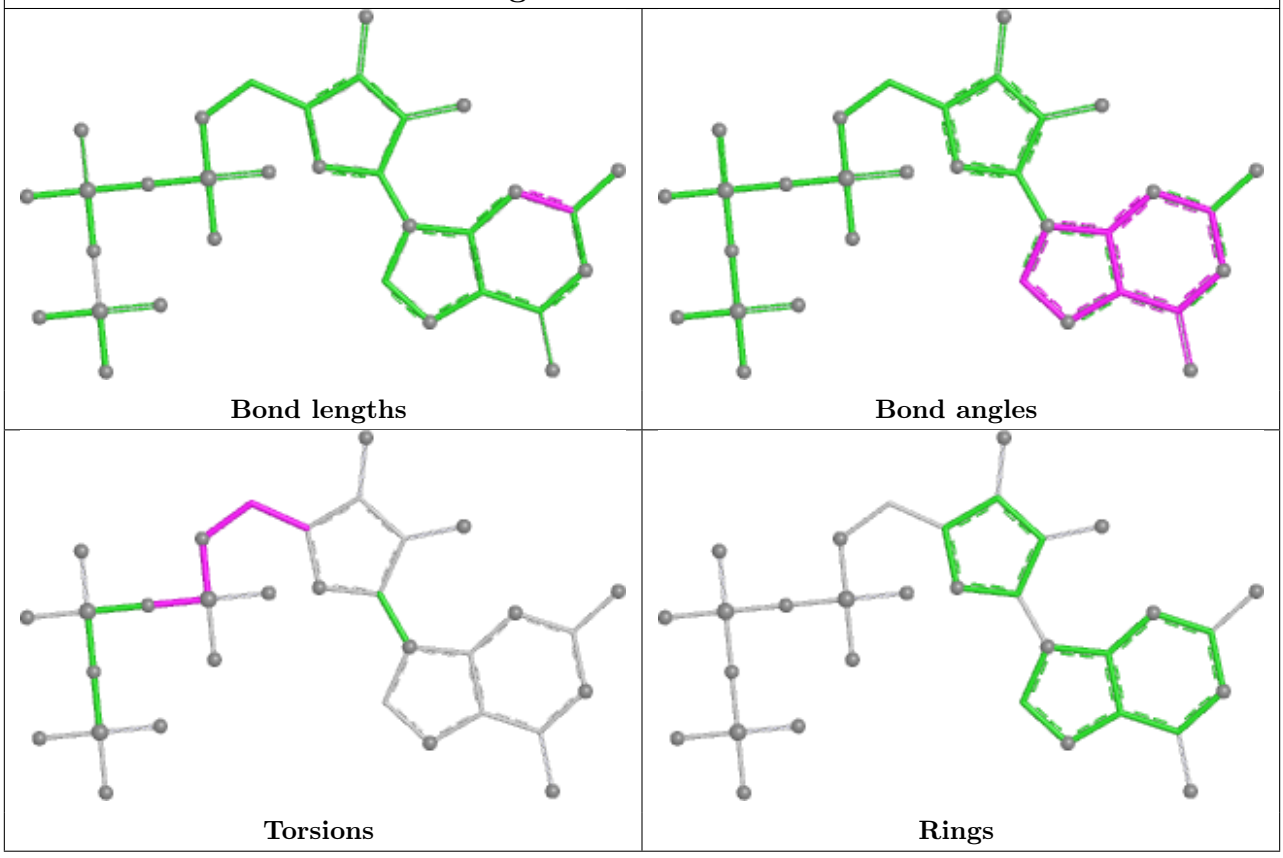
There are no ring outliers.

No monomer is involved in short contacts.

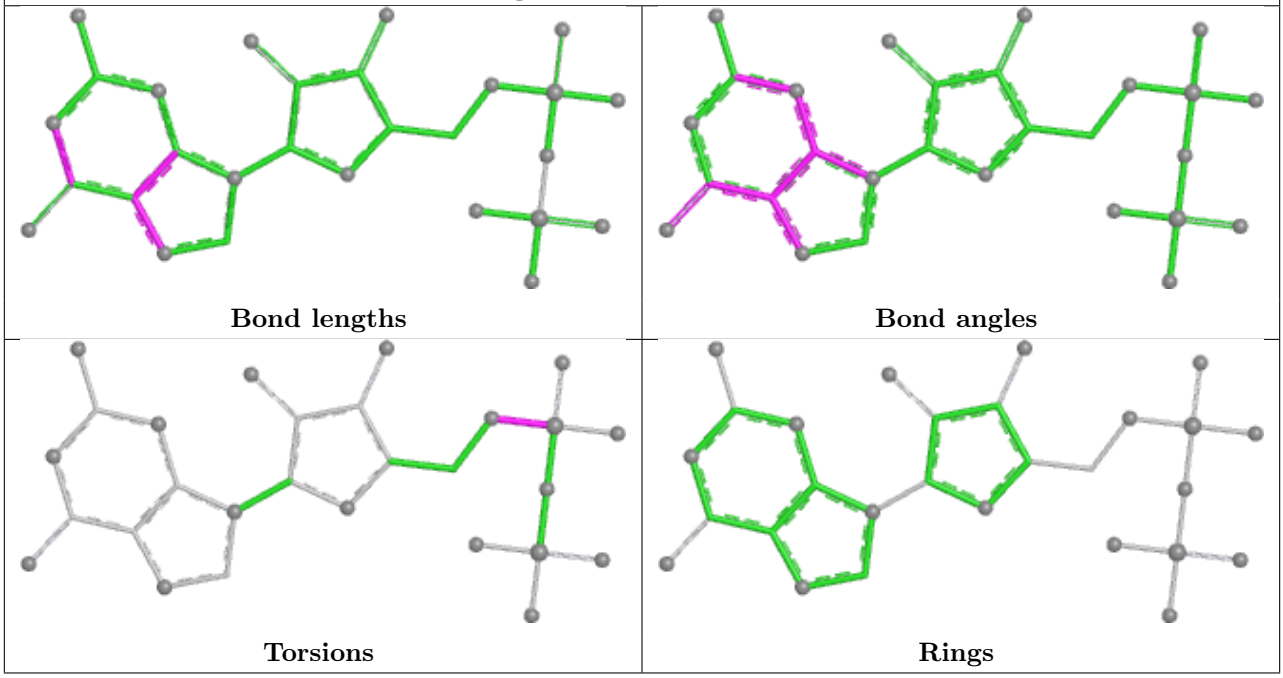
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

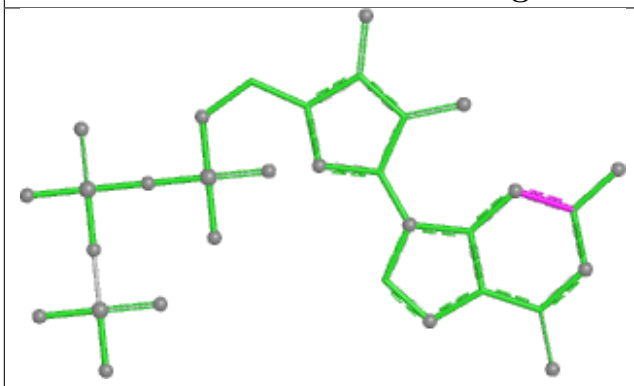
Ligand GTP VK 501



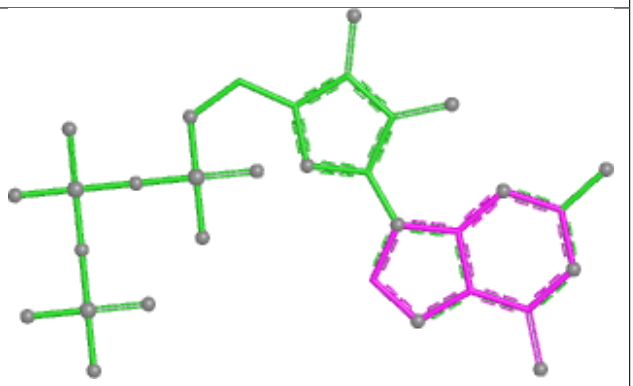
Ligand GDP AF 500



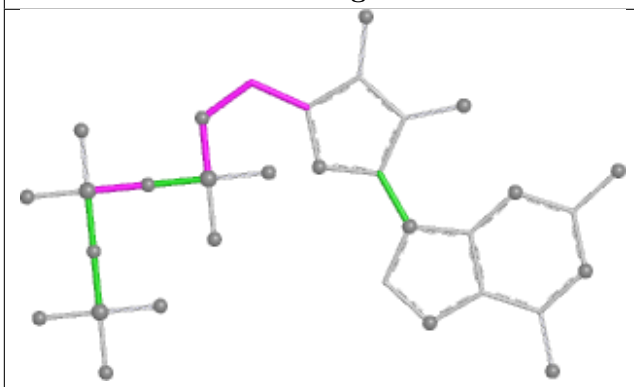
Ligand GTP FG 501



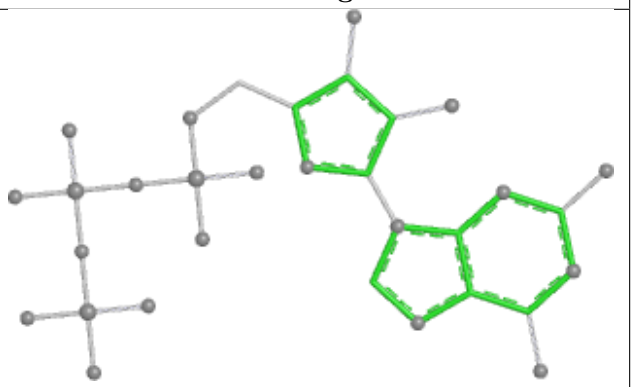
Bond lengths



Bond angles

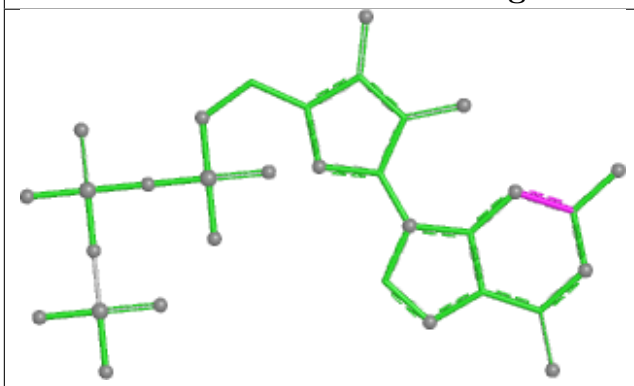


Torsions

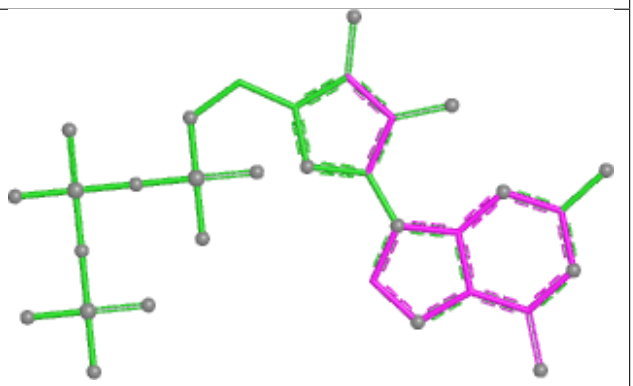


Rings

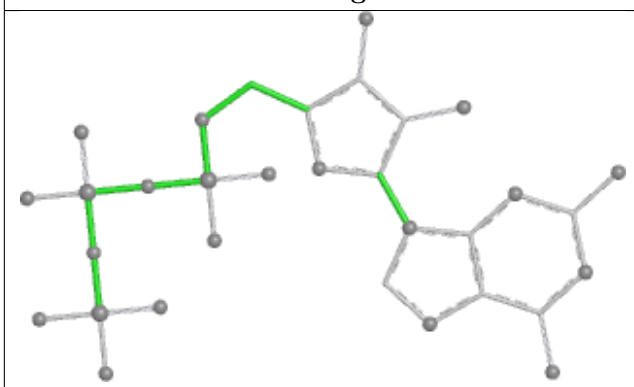
Ligand GTP SW 501



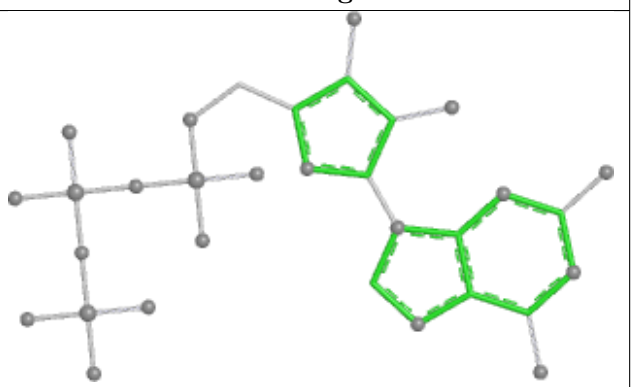
Bond lengths



Bond angles

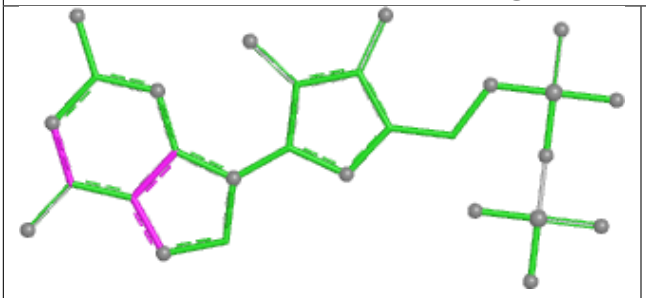


Torsions

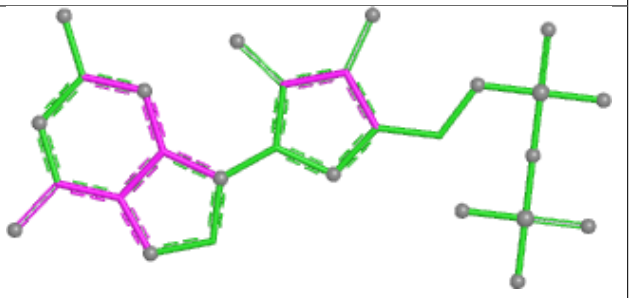


Rings

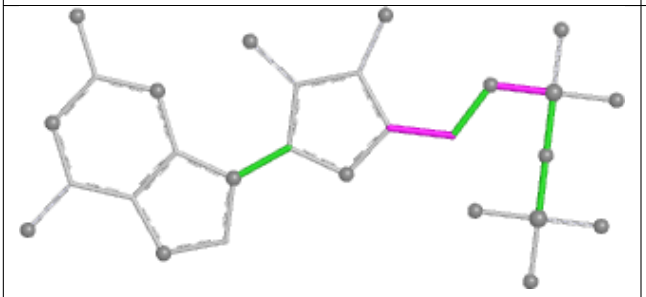
Ligand GDP MJ 500



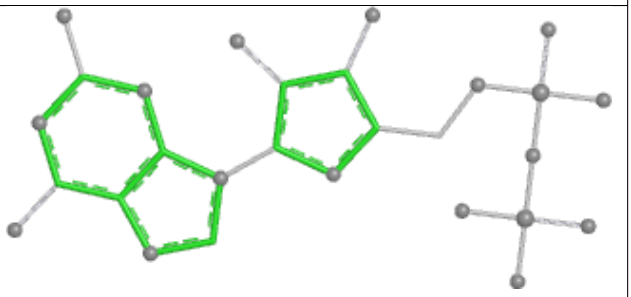
Bond lengths



Bond angles

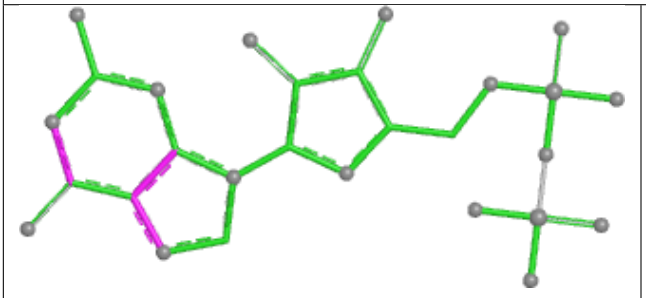


Torsions

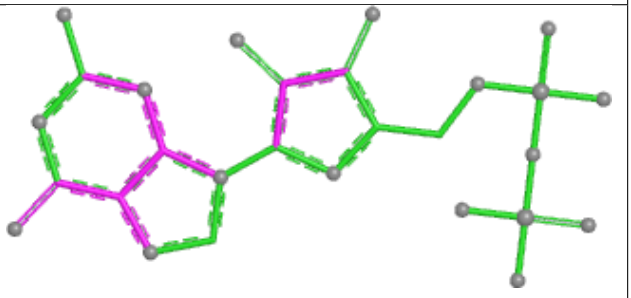


Rings

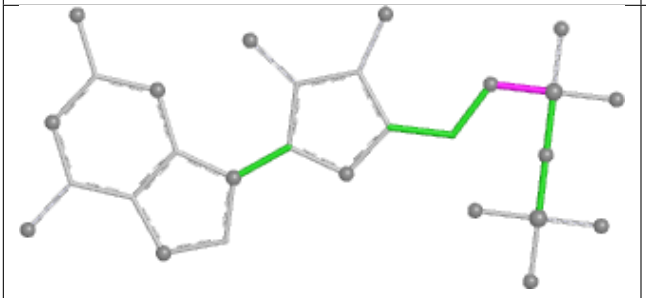
Ligand GDP VR 500



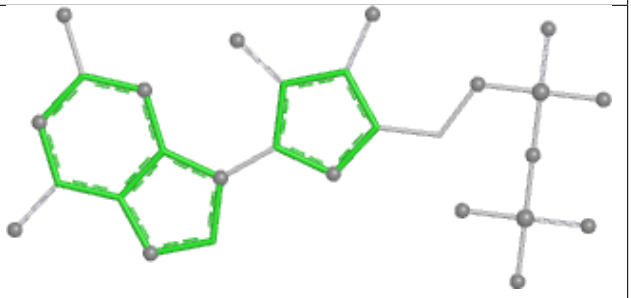
Bond lengths



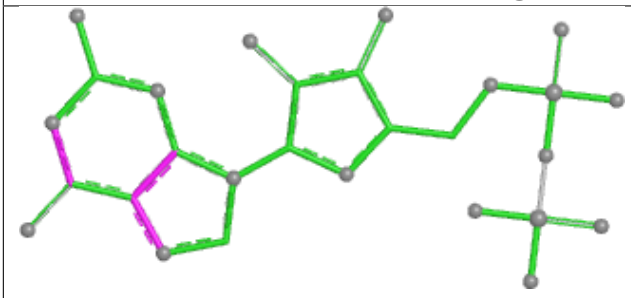
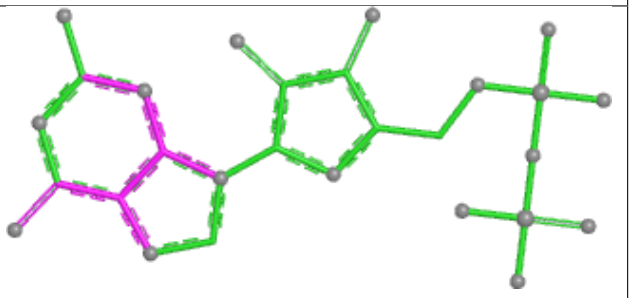
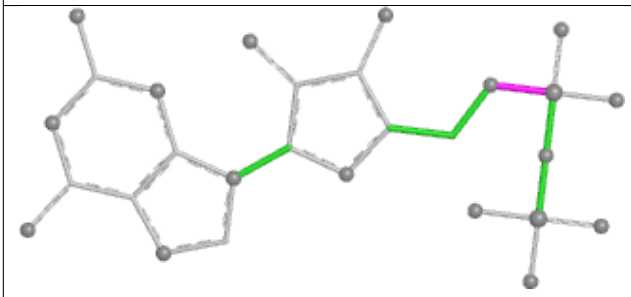
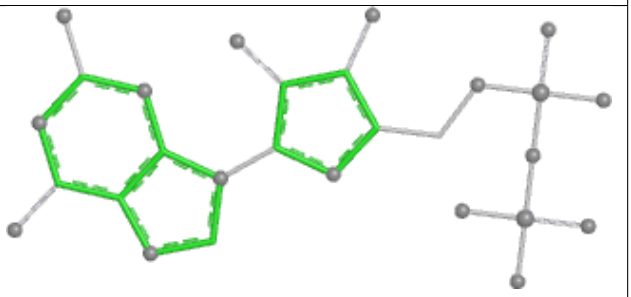
Bond angles

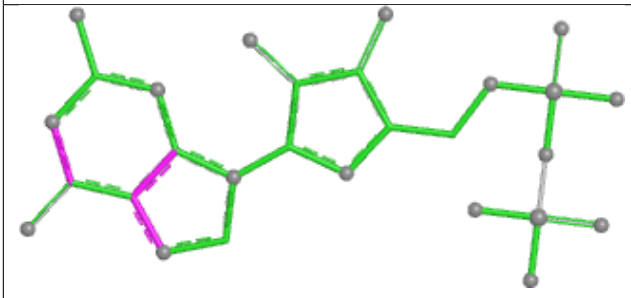
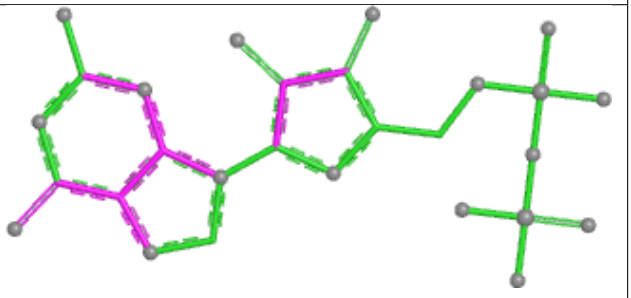
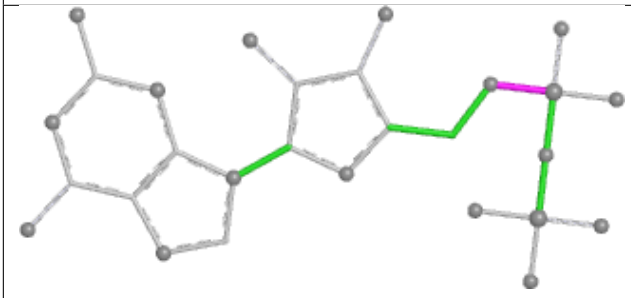
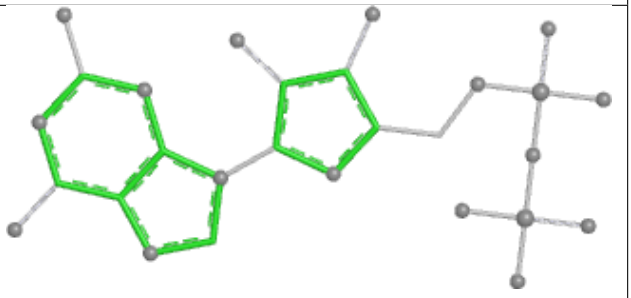


Torsions

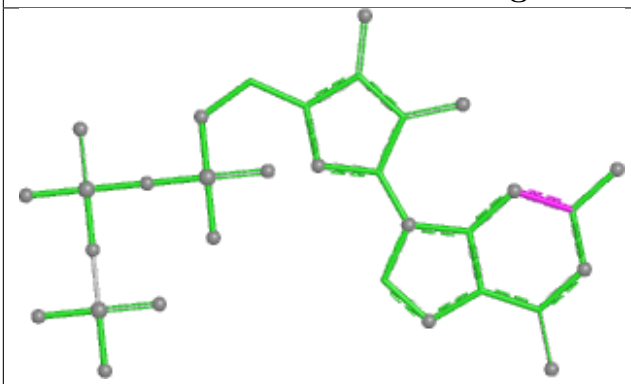


Rings

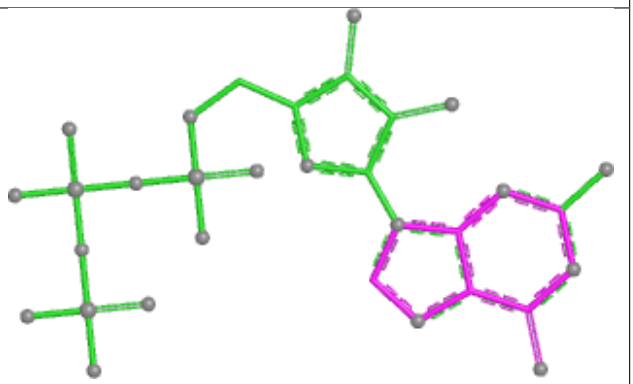
Ligand GDP TF 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP DS 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

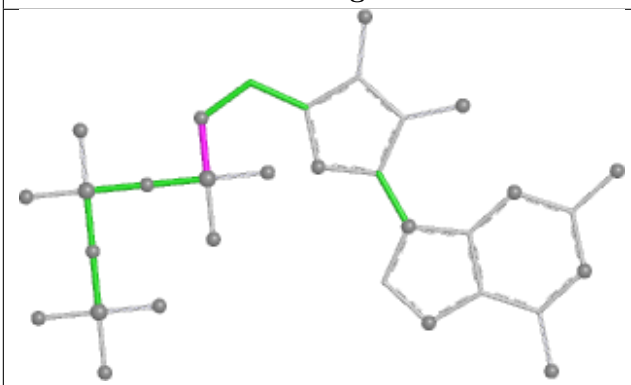
Ligand GTP CB 501



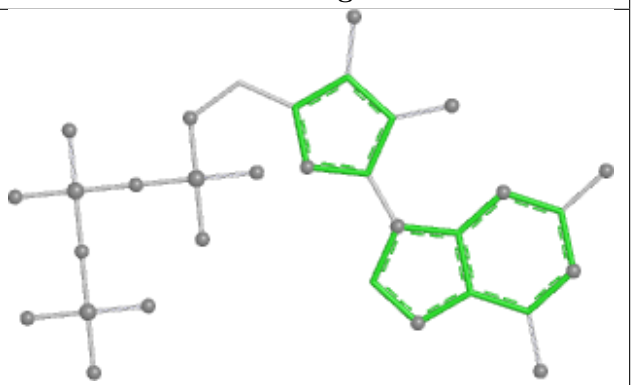
Bond lengths



Bond angles

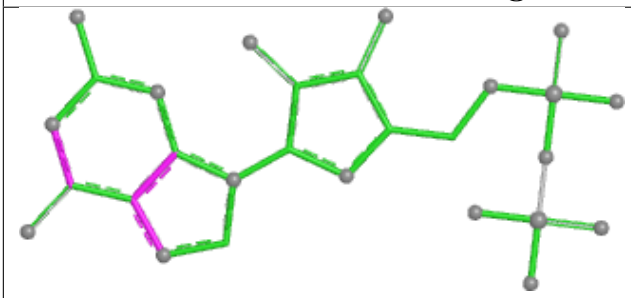


Torsions

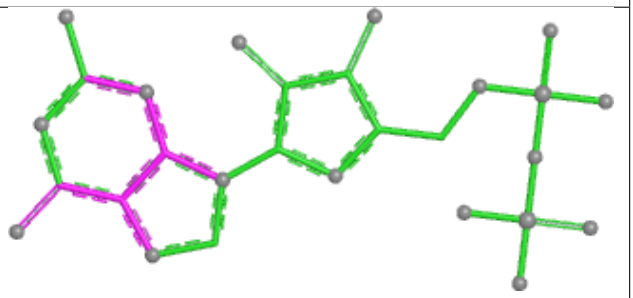


Rings

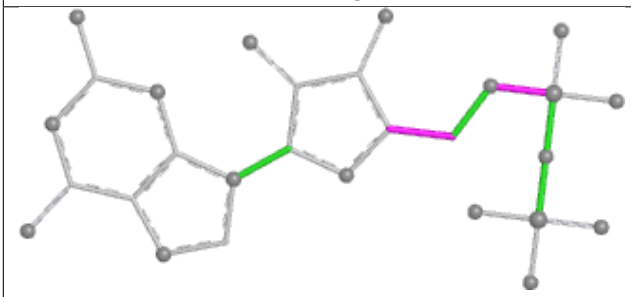
Ligand GDP GB 500



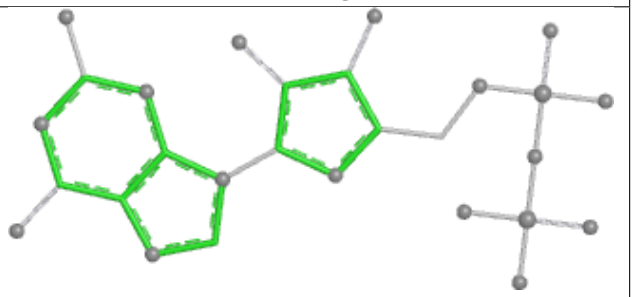
Bond lengths



Bond angles

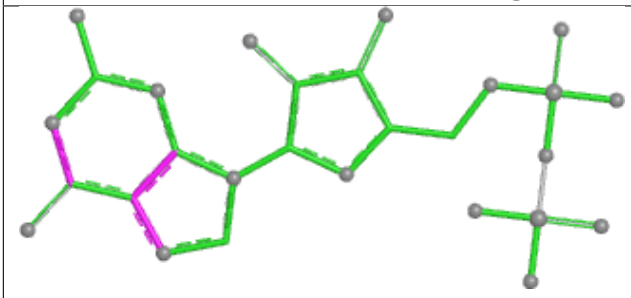


Torsions

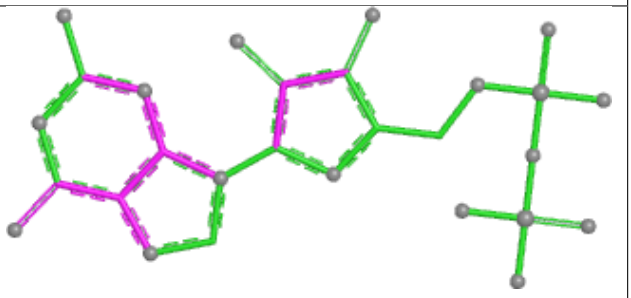


Rings

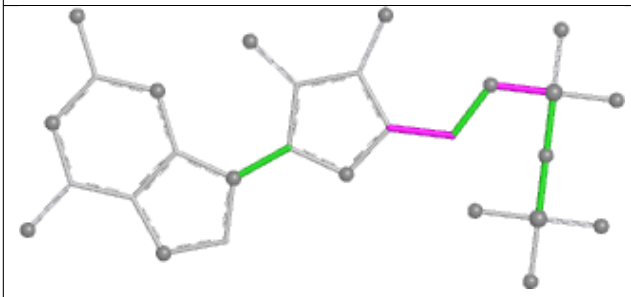
Ligand GDP HB 501



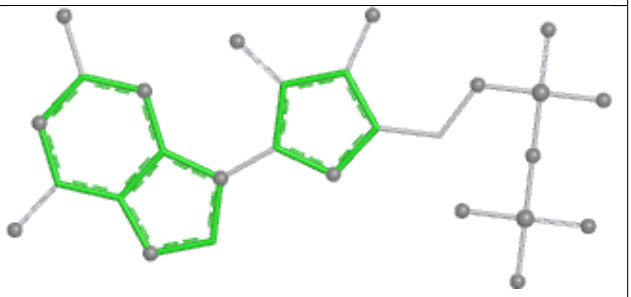
Bond lengths



Bond angles

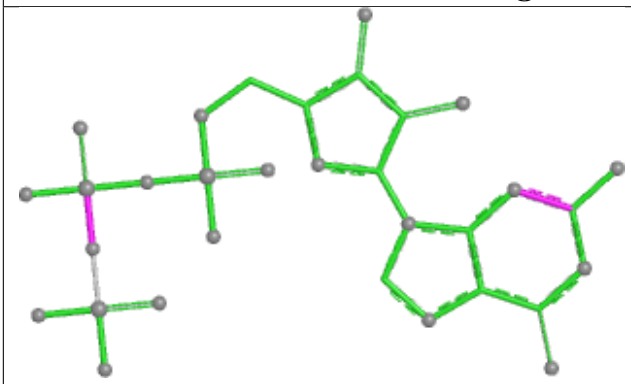


Torsions

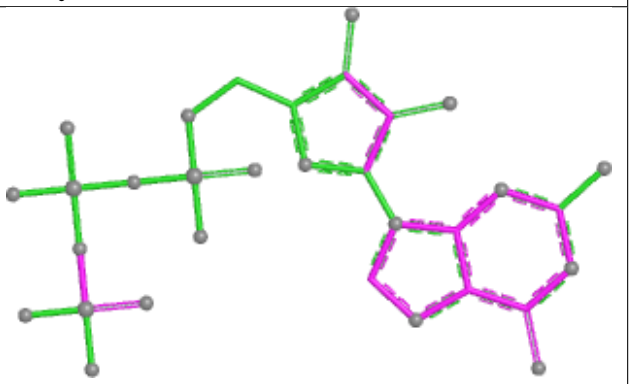


Rings

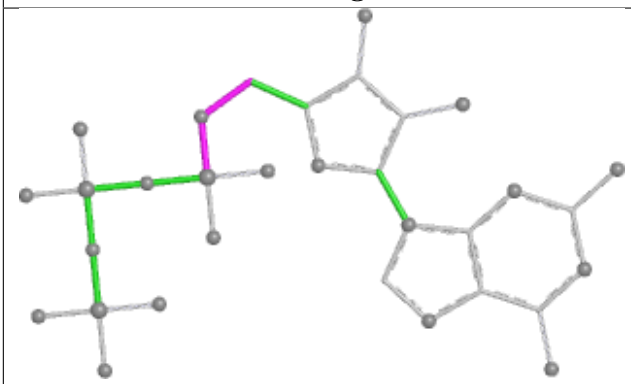
Ligand GTP QI 501



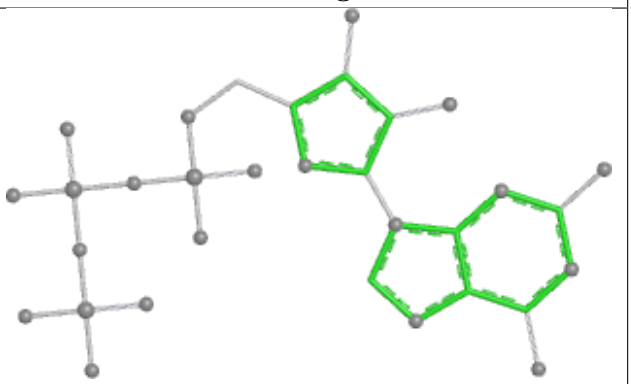
Bond lengths



Bond angles

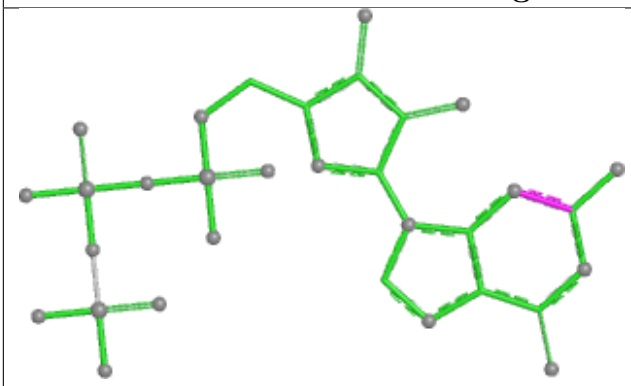


Torsions

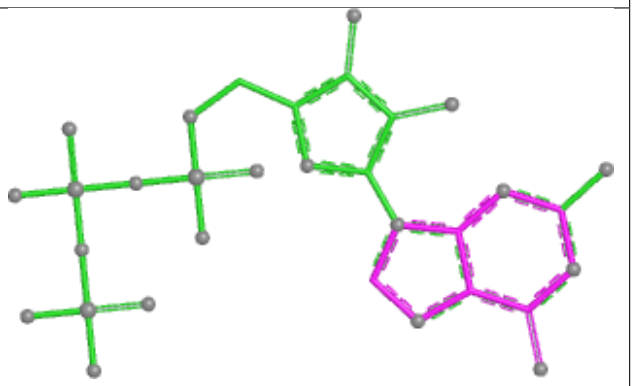


Rings

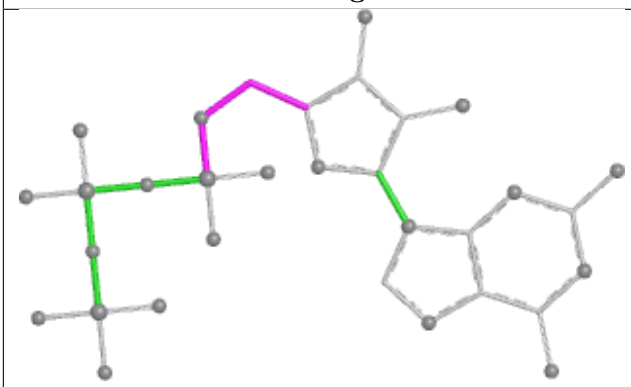
Ligand GTP SC 501



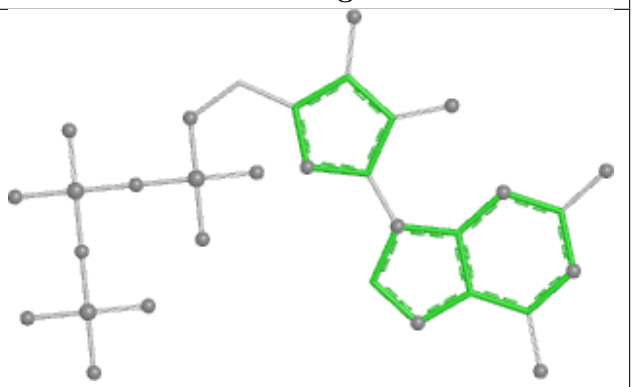
Bond lengths



Bond angles

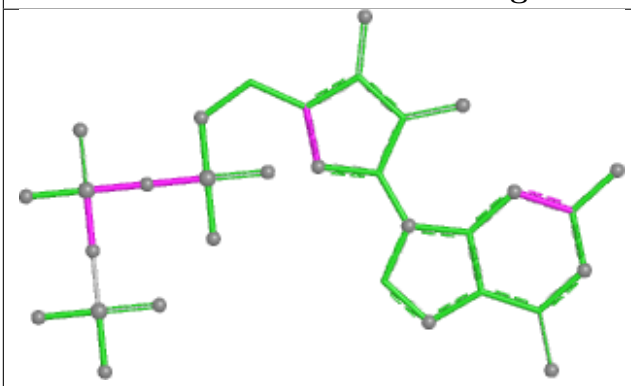


Torsions

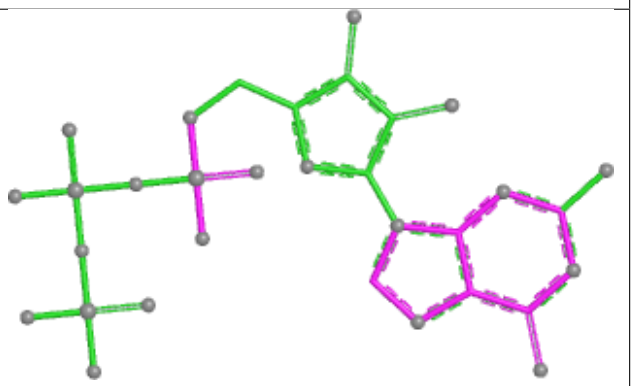


Rings

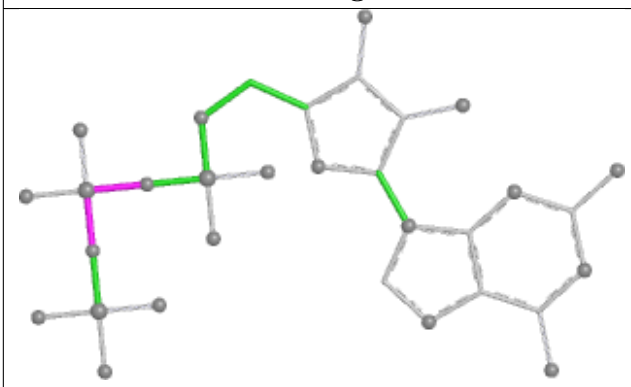
Ligand GTP IW 501



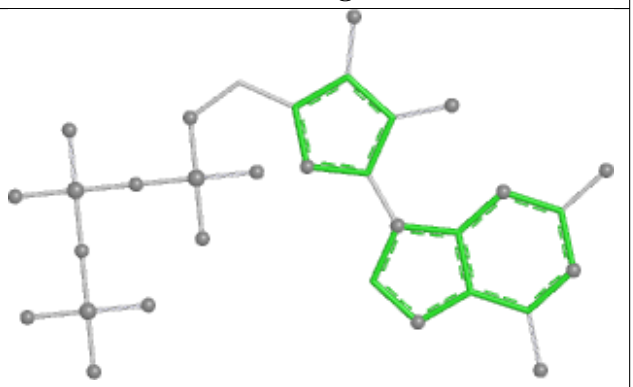
Bond lengths



Bond angles

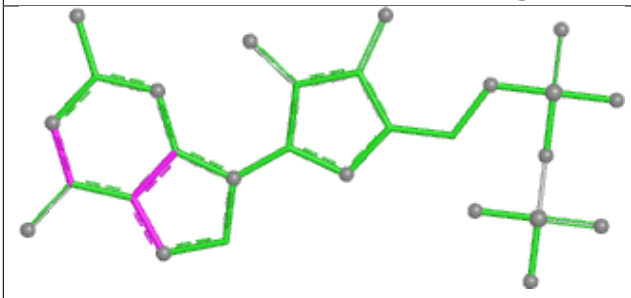


Torsions

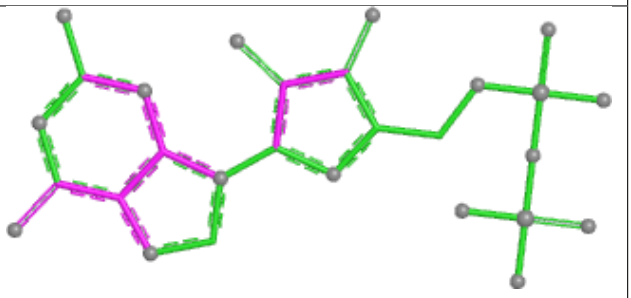


Rings

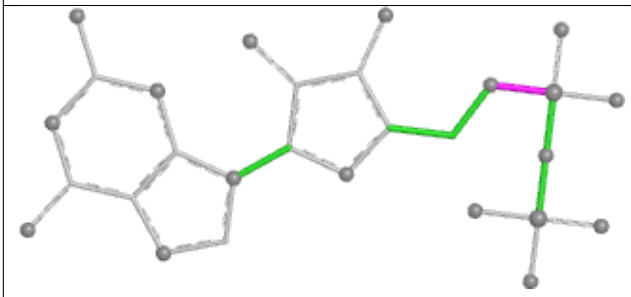
Ligand GDP JE 500



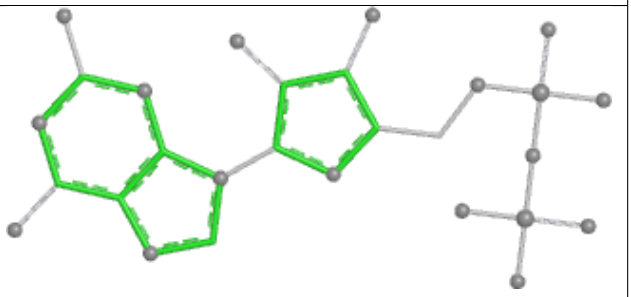
Bond lengths



Bond angles

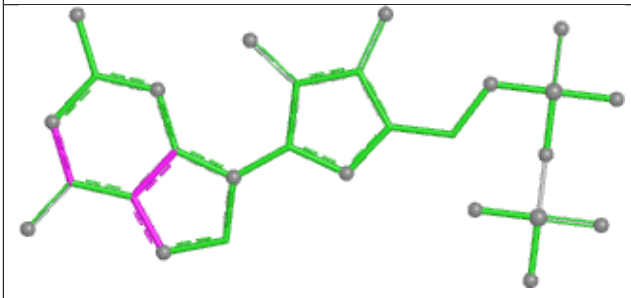


Torsions

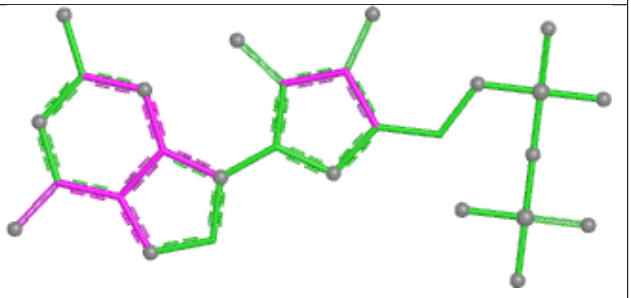


Rings

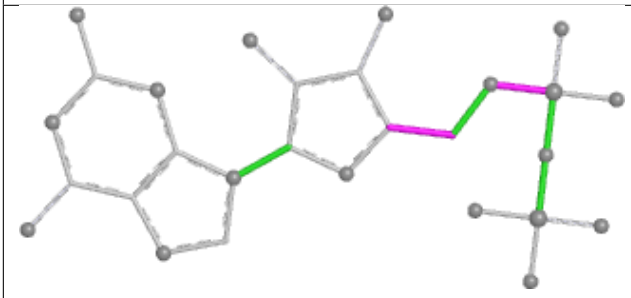
Ligand GDP MZ 500



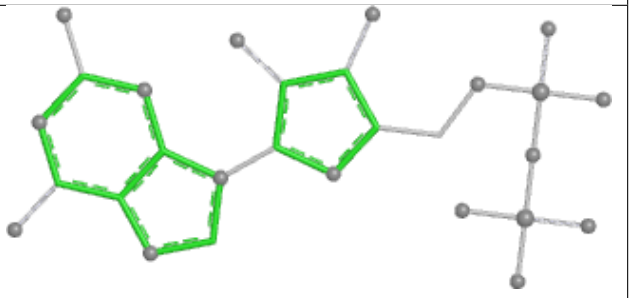
Bond lengths



Bond angles

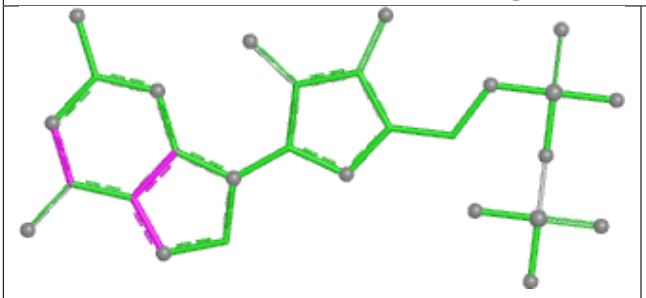


Torsions

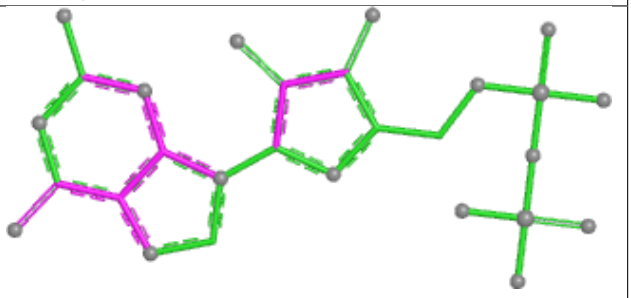


Rings

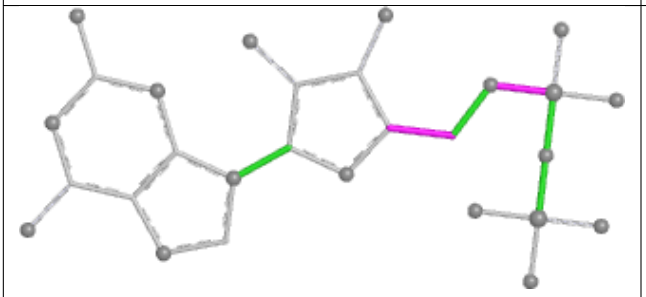
Ligand GDP DQ 500



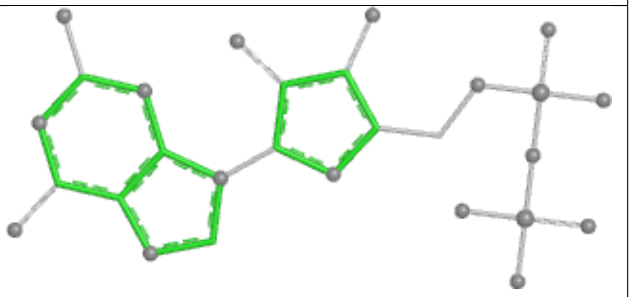
Bond lengths



Bond angles

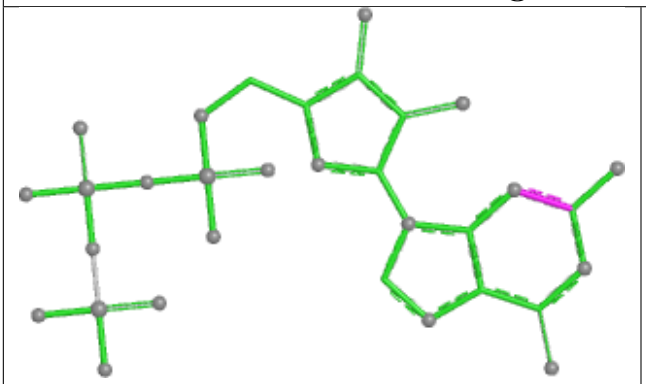


Torsions

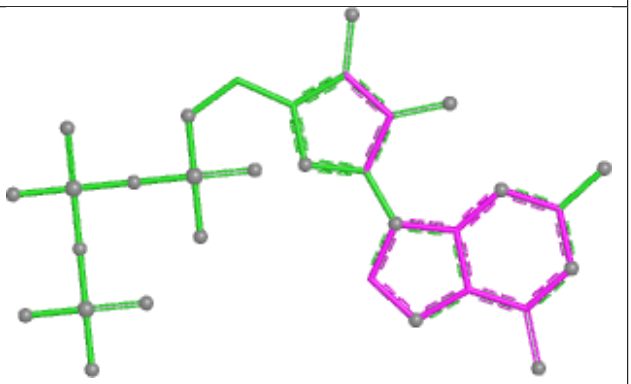


Rings

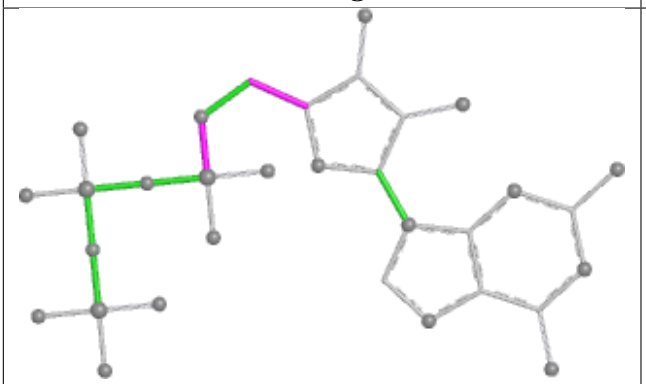
Ligand GTP AU 501



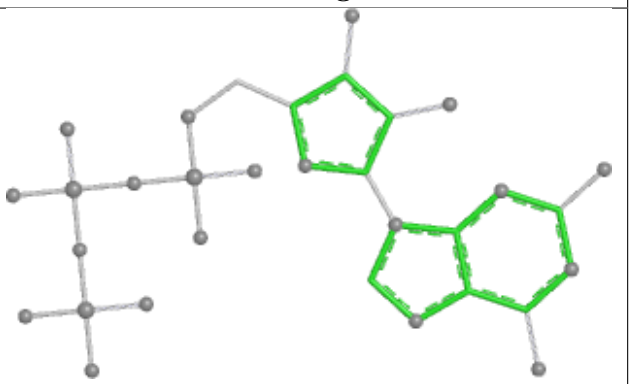
Bond lengths



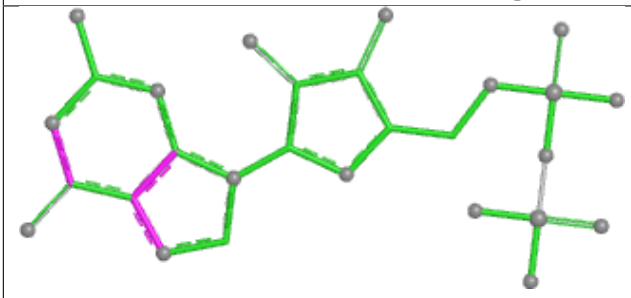
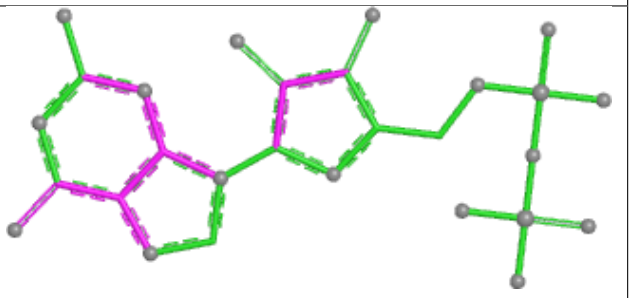
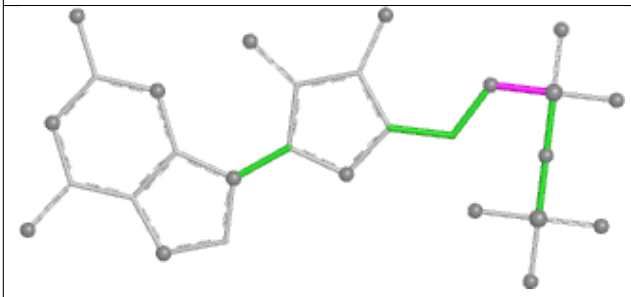
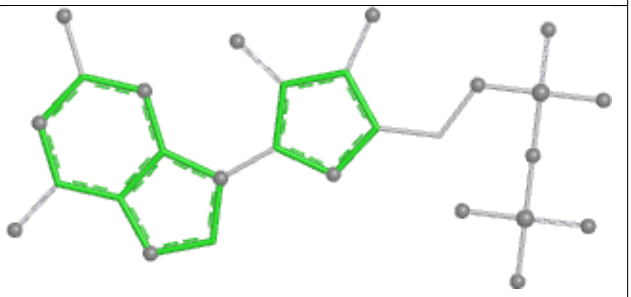
Bond angles

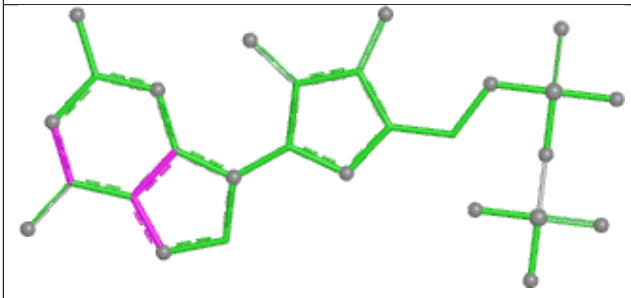
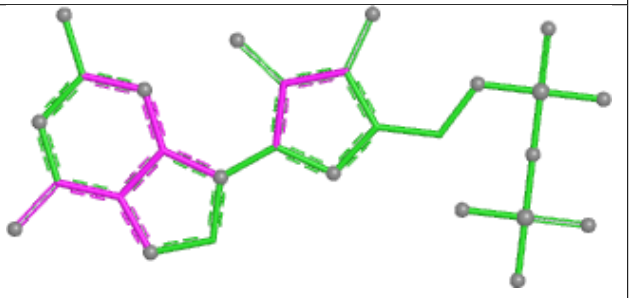
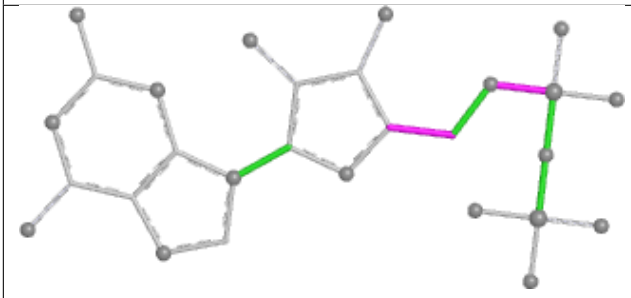
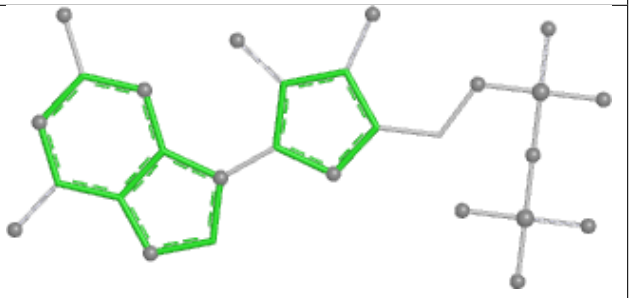


Torsions

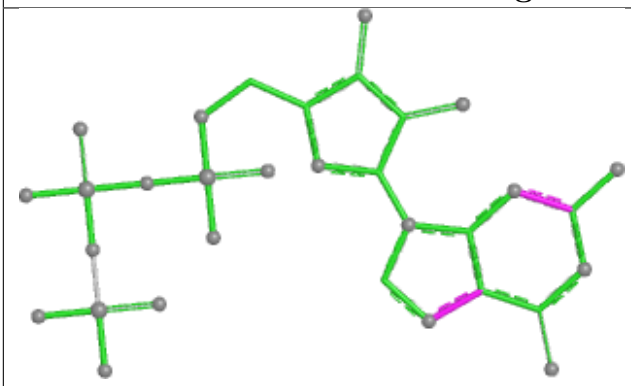


Rings

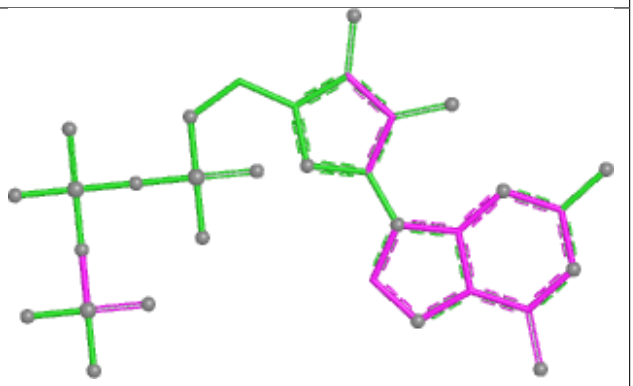
Ligand GDP VP 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP IB 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

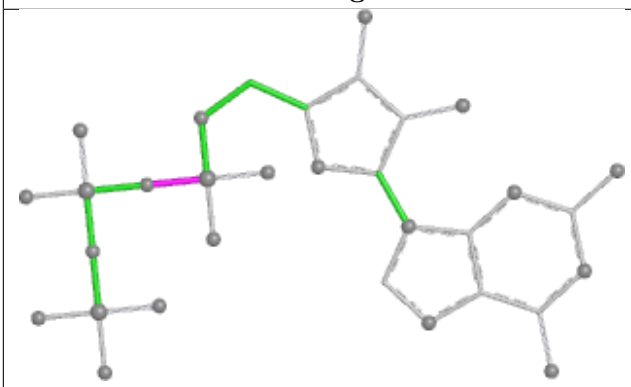
Ligand GTP GI 501



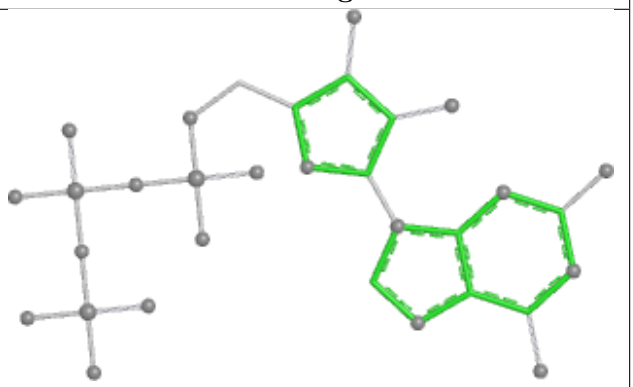
Bond lengths



Bond angles

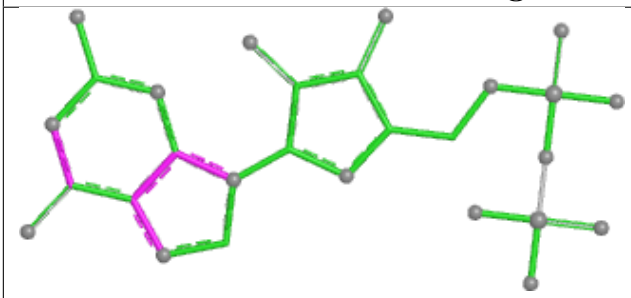


Torsions

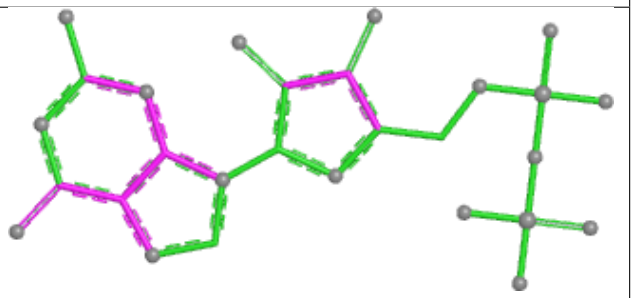


Rings

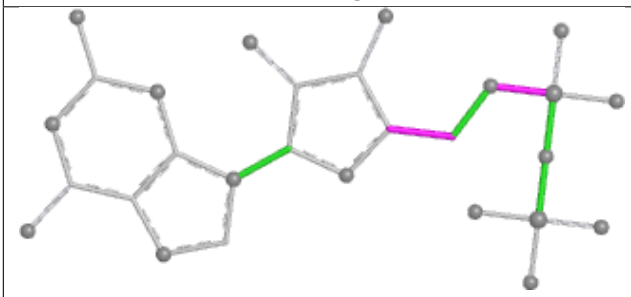
Ligand GDP AX 500



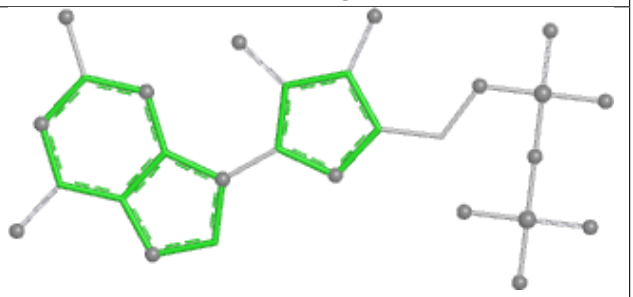
Bond lengths



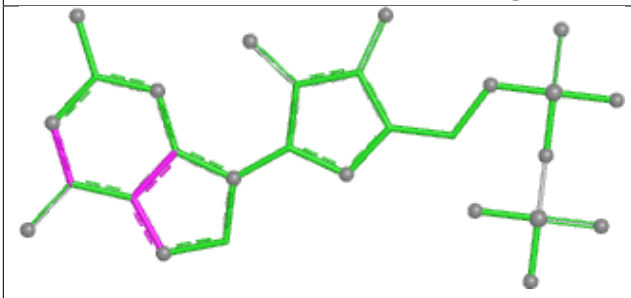
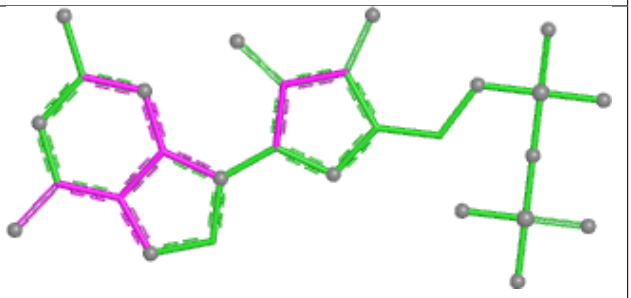
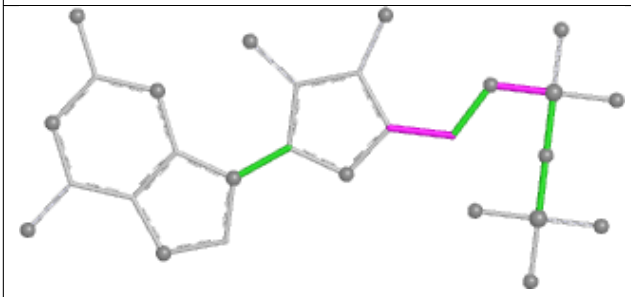
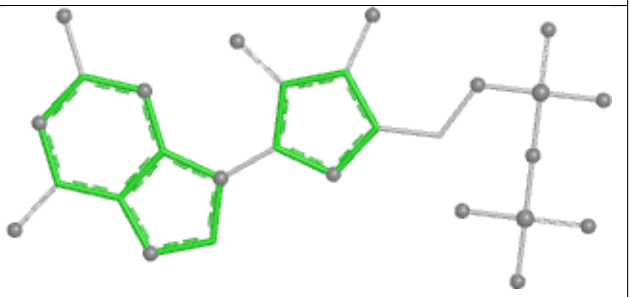
Bond angles

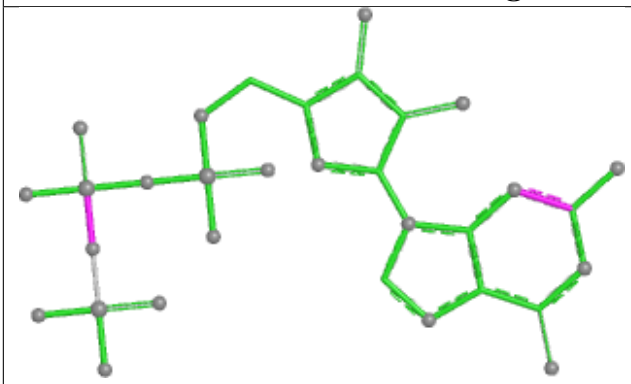
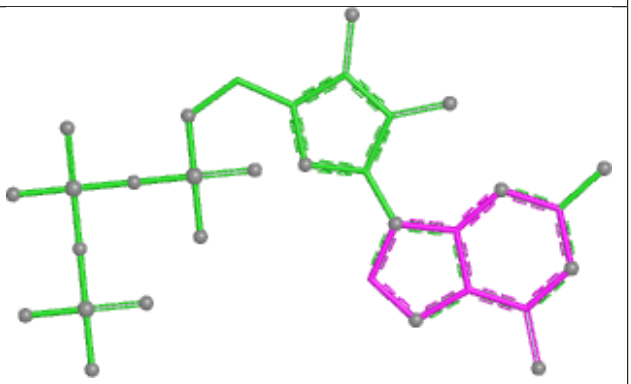
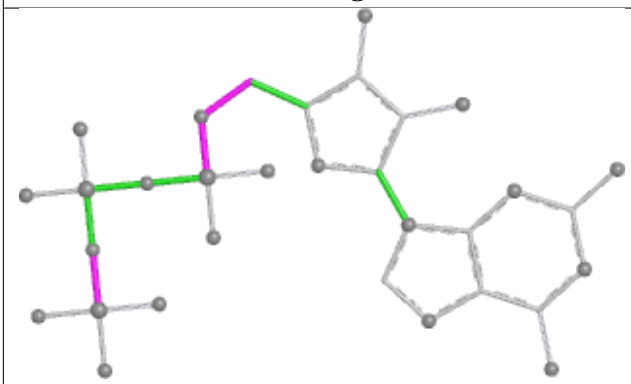
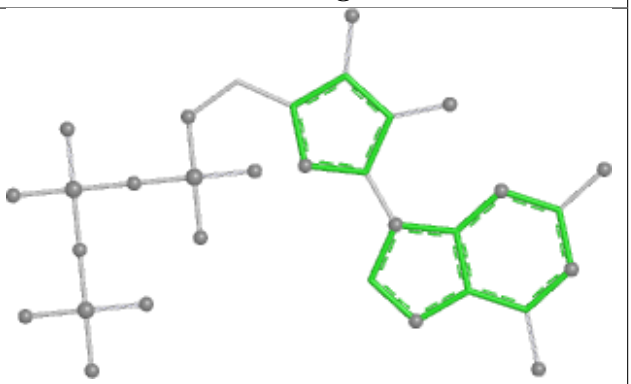


Torsions

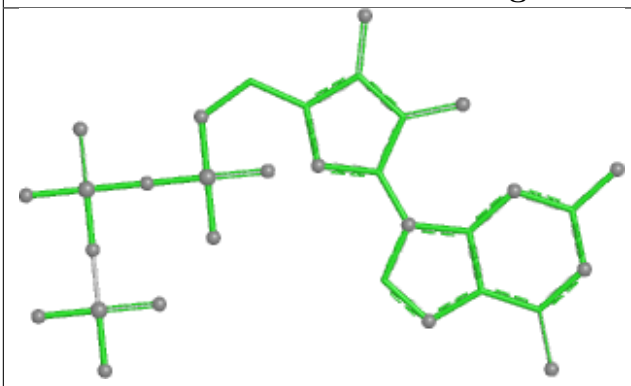


Rings

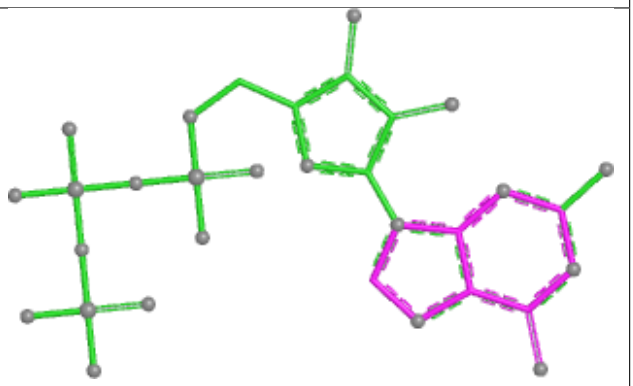
Ligand GDP ON 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP MU 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

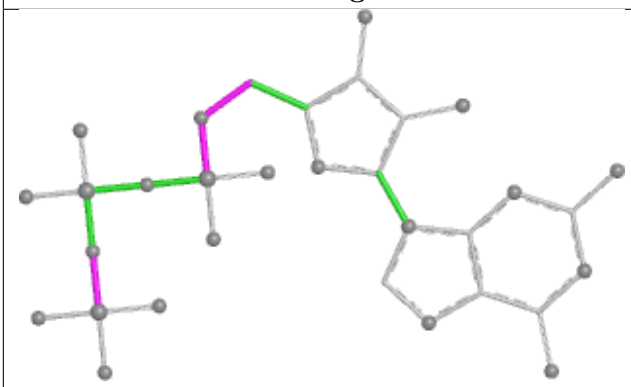
Ligand GTP AB 501



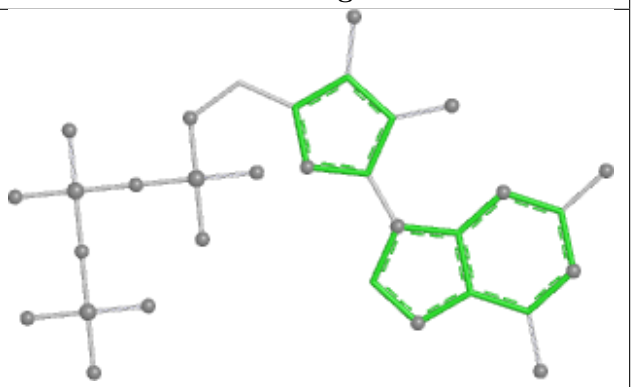
Bond lengths



Bond angles

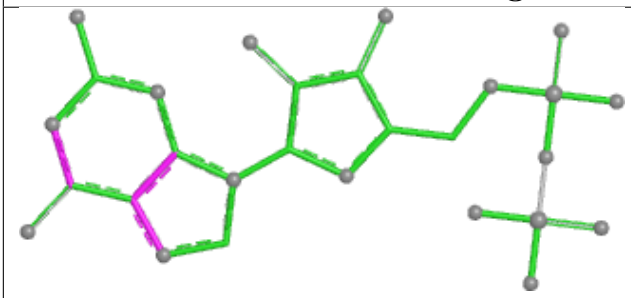


Torsions

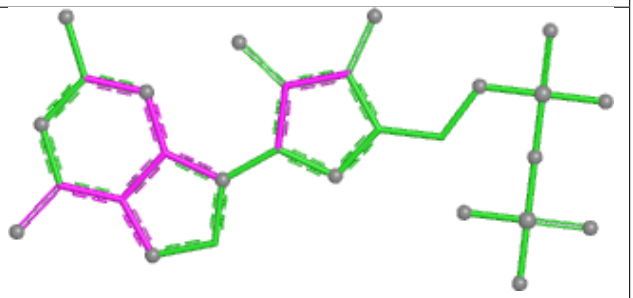


Rings

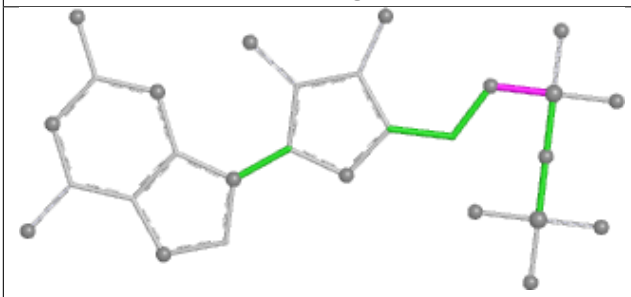
Ligand GDP NV 501



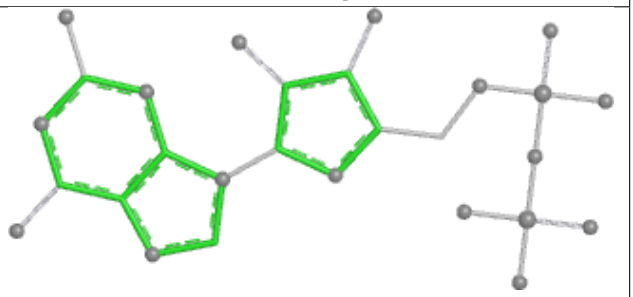
Bond lengths



Bond angles

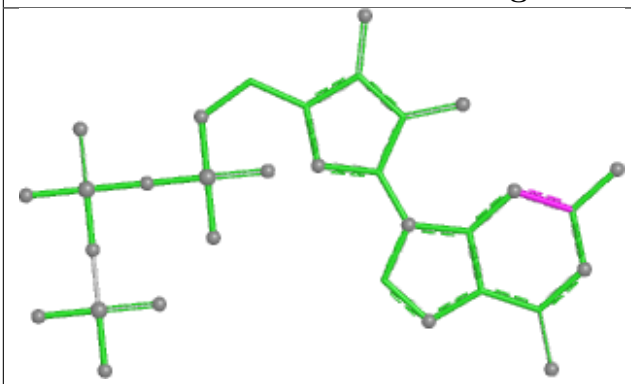


Torsions

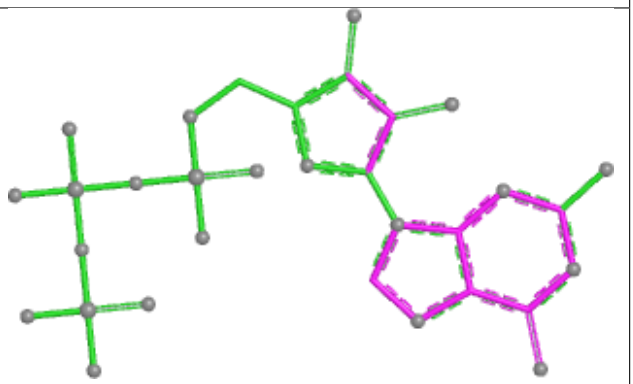


Rings

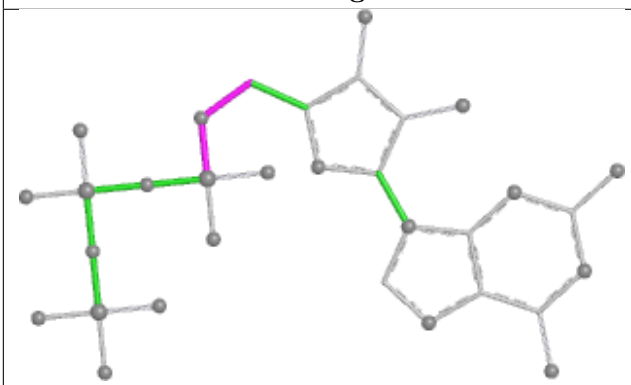
Ligand GTP HE 501



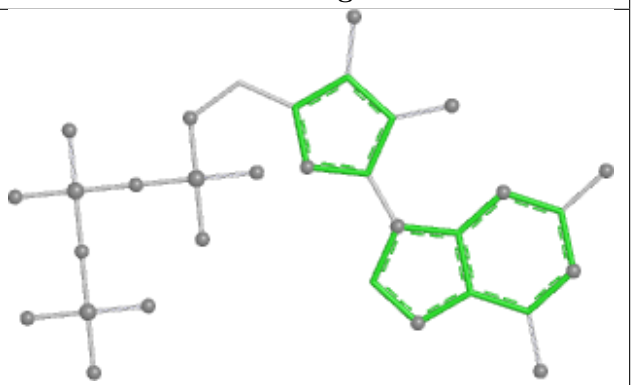
Bond lengths



Bond angles

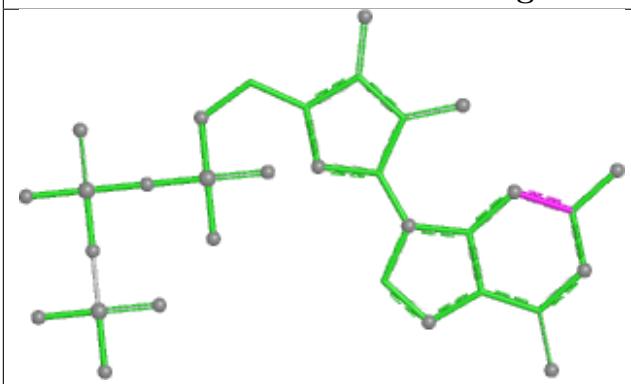


Torsions

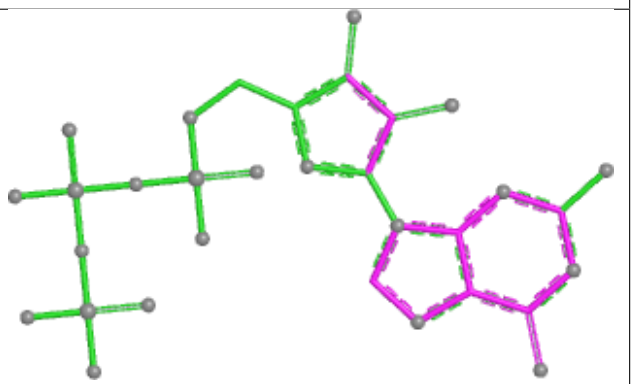


Rings

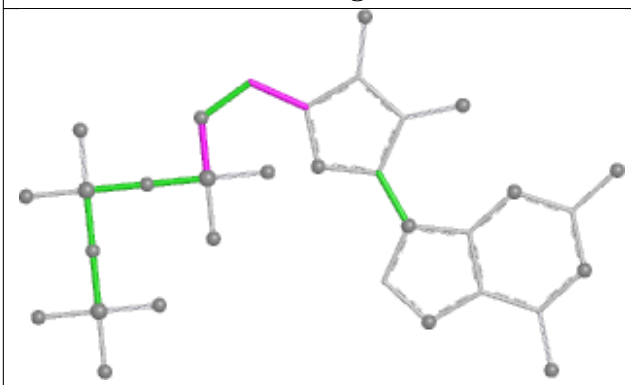
Ligand GTP TI 501



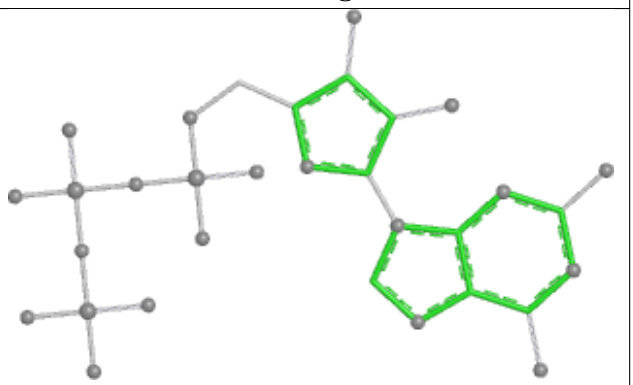
Bond lengths



Bond angles

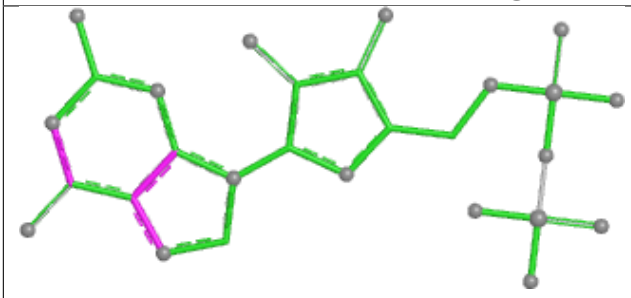


Torsions

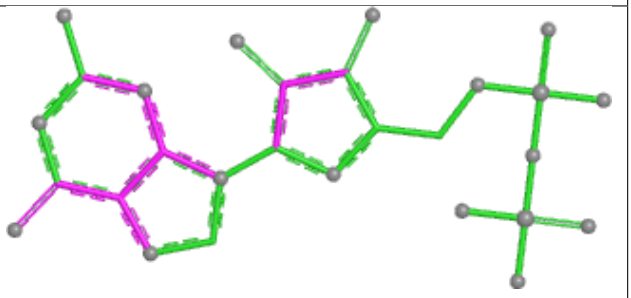


Rings

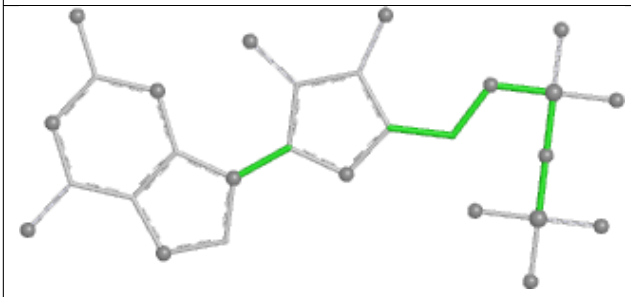
Ligand GDP CO 500



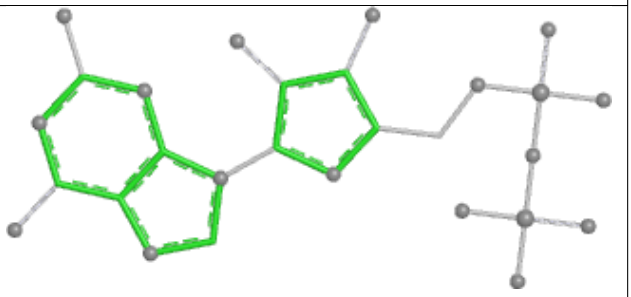
Bond lengths



Bond angles

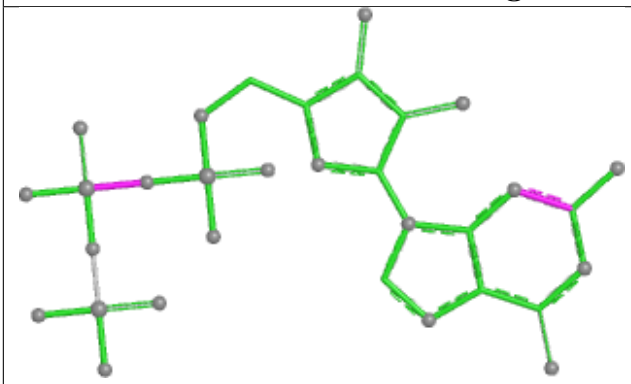


Torsions

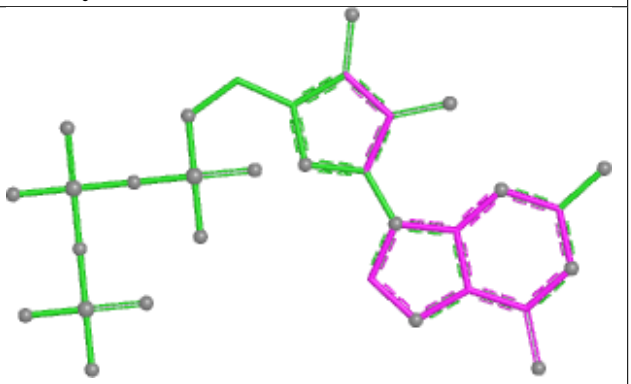


Rings

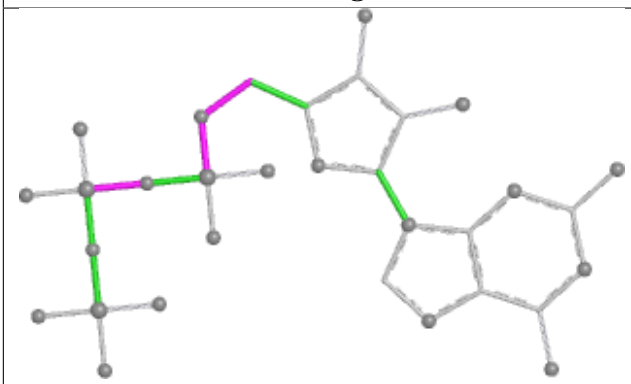
Ligand GTP MQ 501



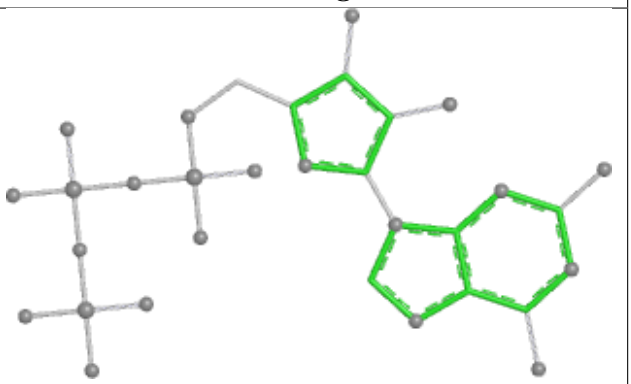
Bond lengths



Bond angles

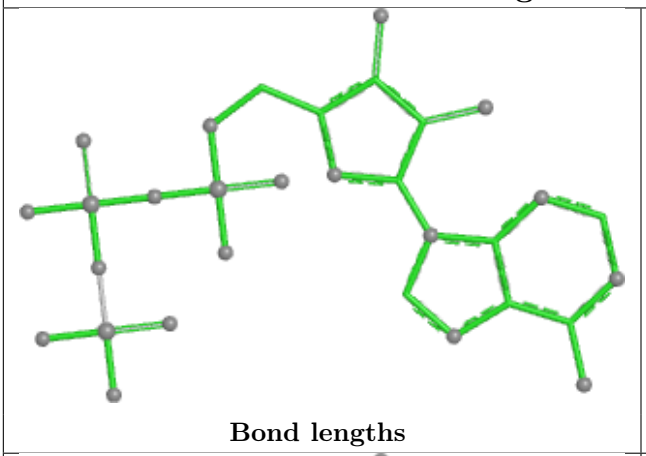


Torsions

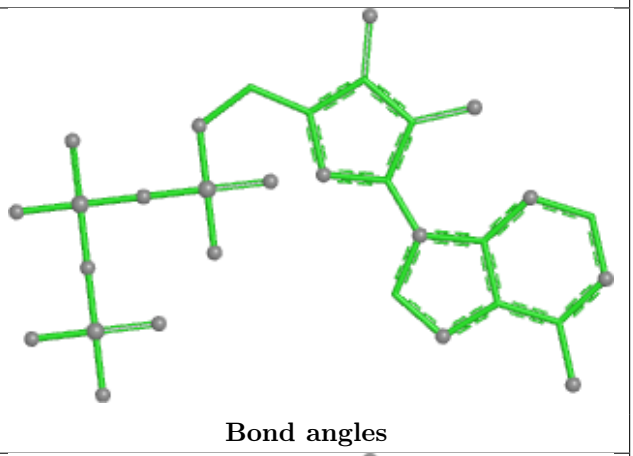


Rings

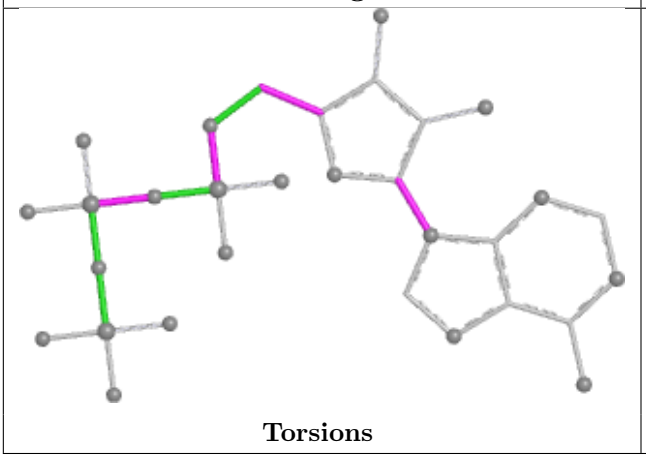
Ligand ATP 2w 501



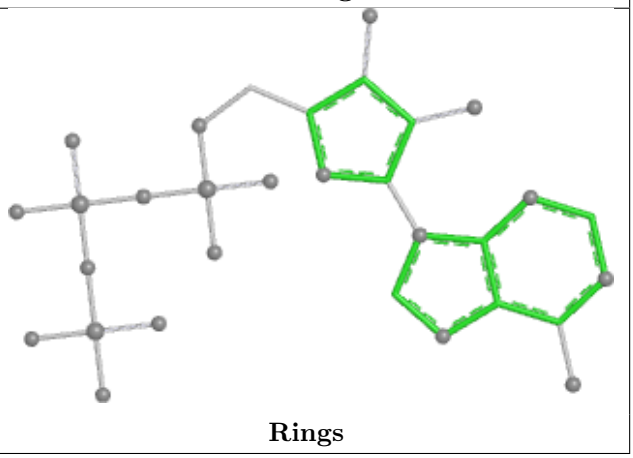
Bond lengths



Bond angles

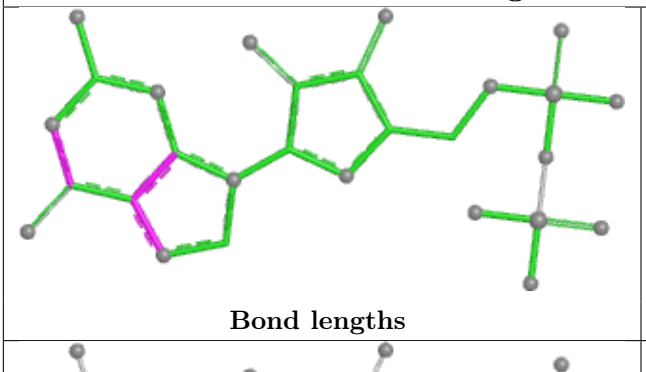


Torsions

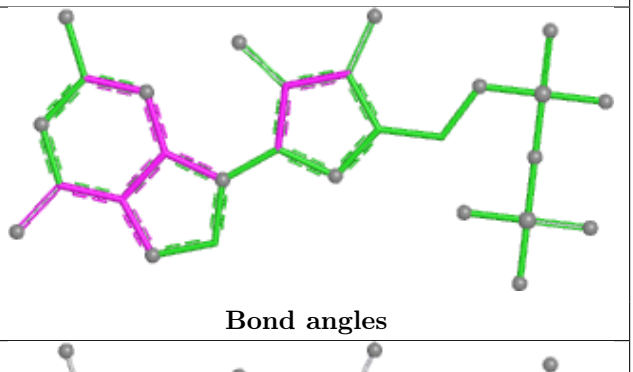


Rings

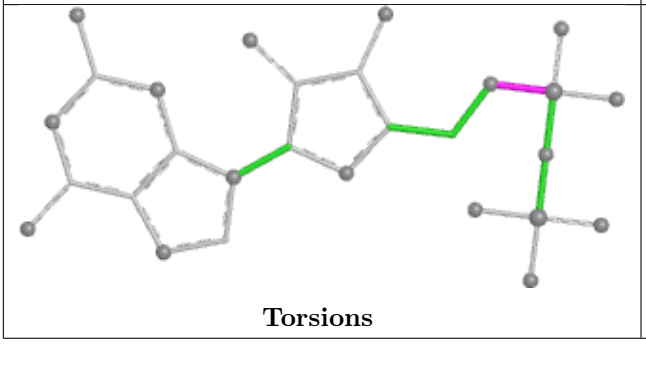
Ligand GDP NX 500



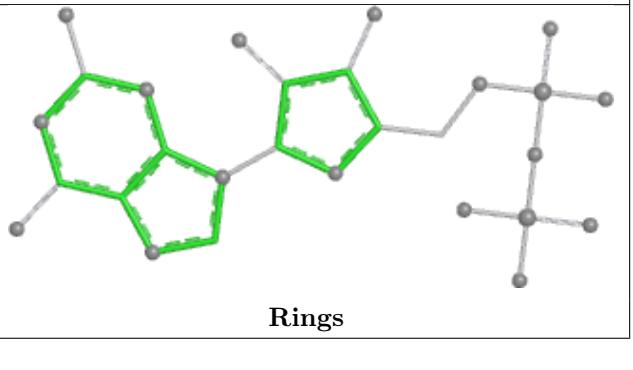
Bond lengths



Bond angles

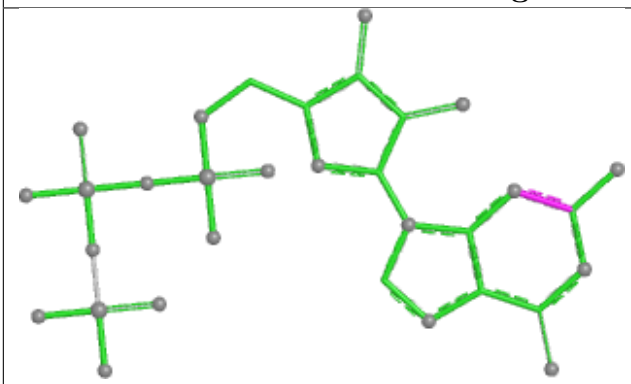


Torsions

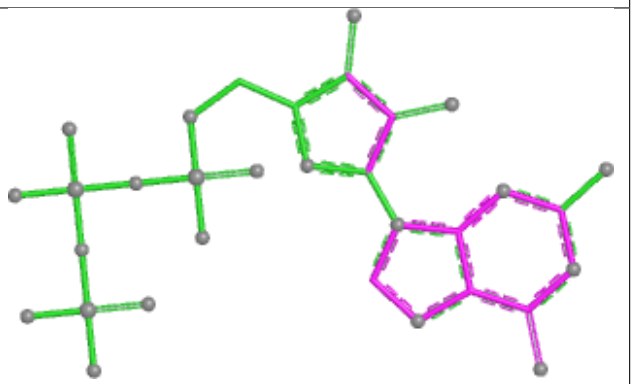


Rings

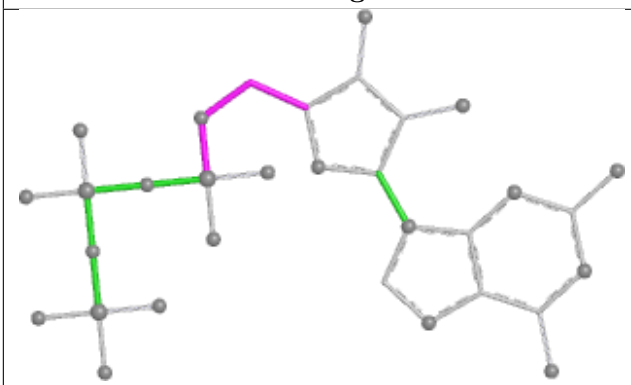
Ligand GTP TE 501



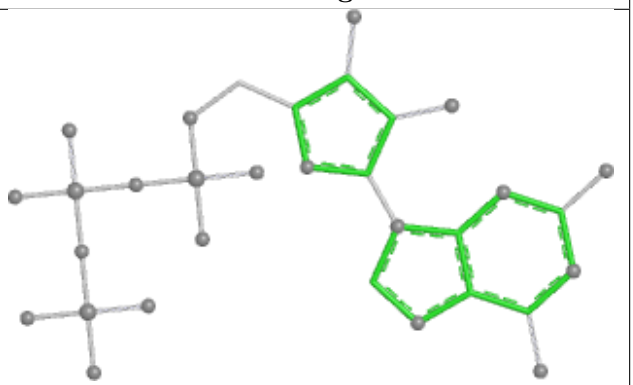
Bond lengths



Bond angles

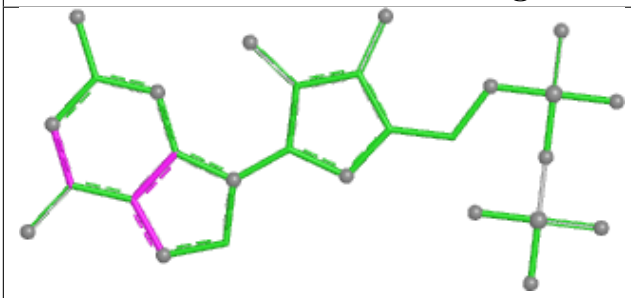


Torsions

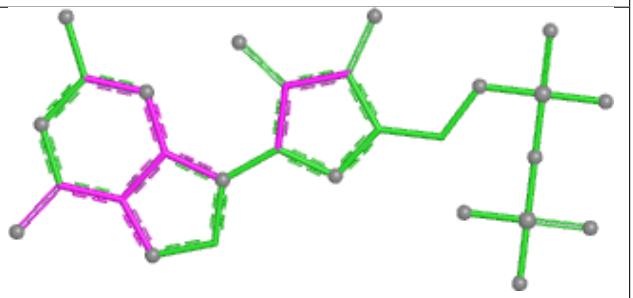


Rings

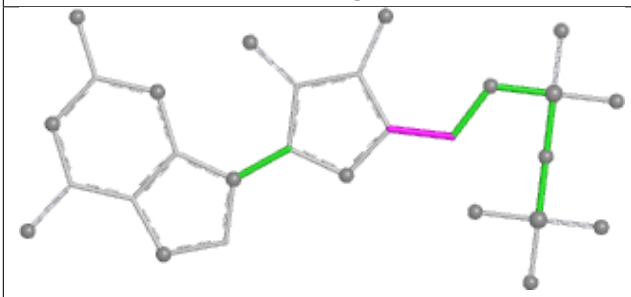
Ligand GDP LY 500



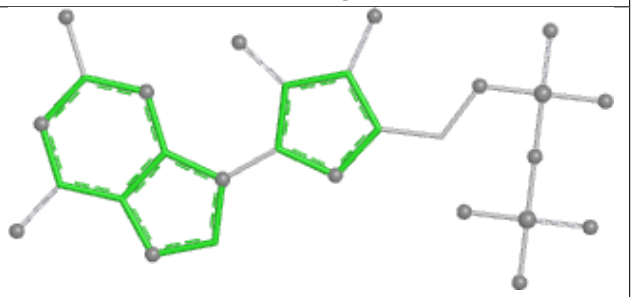
Bond lengths



Bond angles

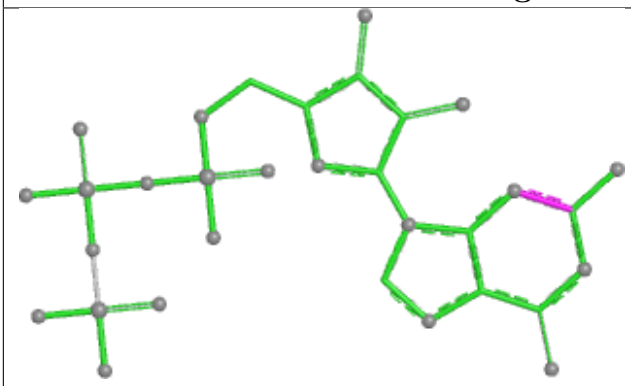


Torsions

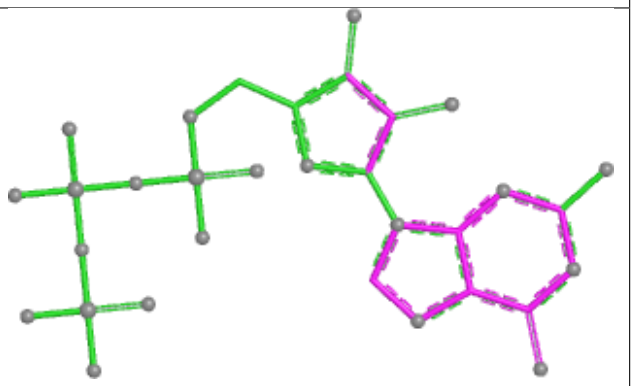


Rings

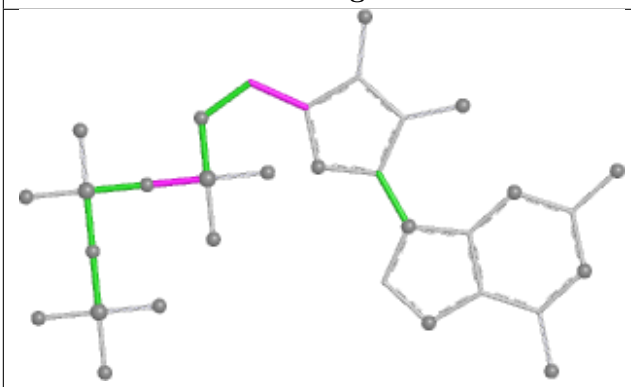
Ligand GTP LT 501



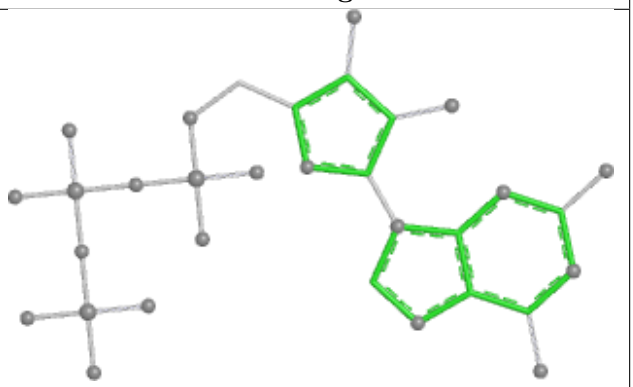
Bond lengths



Bond angles

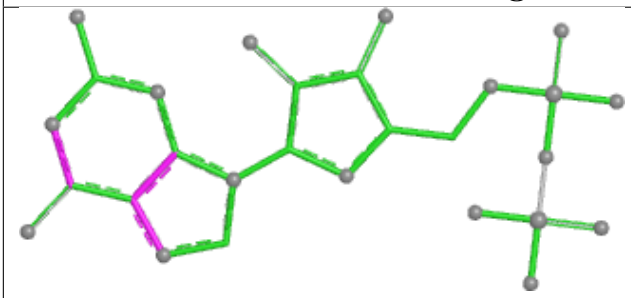


Torsions

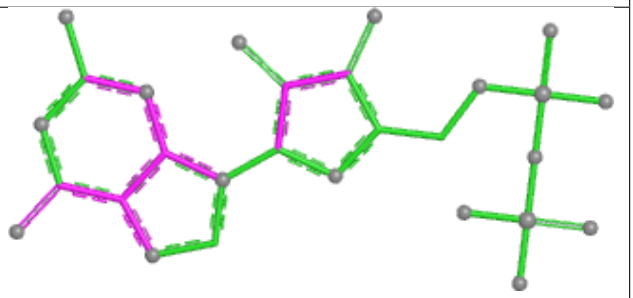


Rings

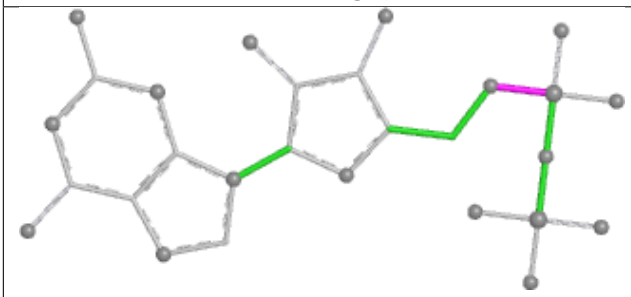
Ligand GDP UB 500



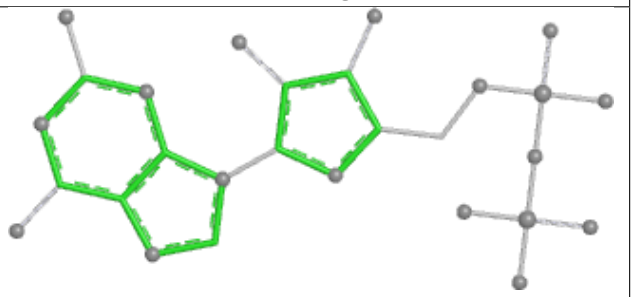
Bond lengths



Bond angles

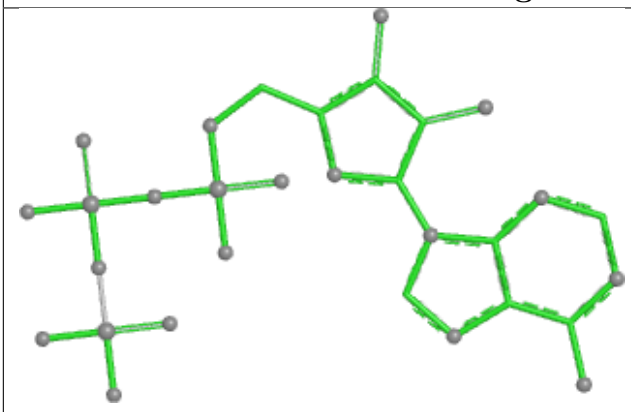


Torsions

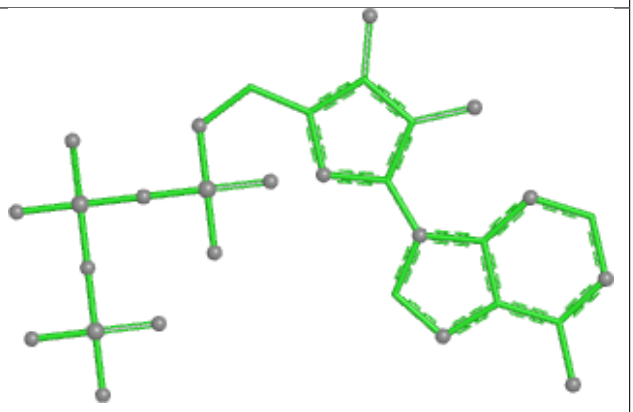


Rings

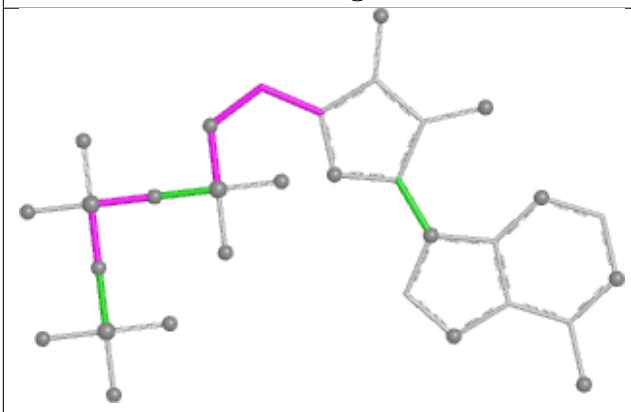
Ligand ATP 7D 601



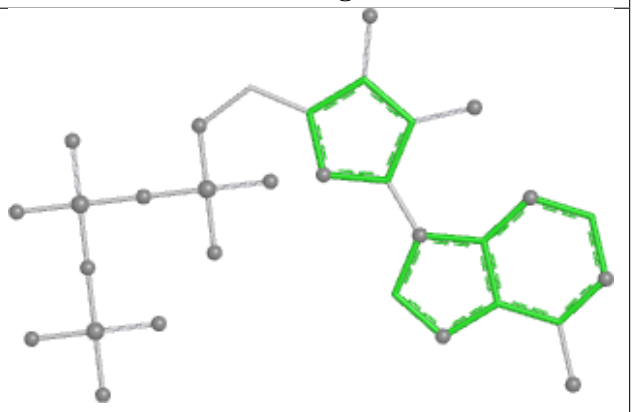
Bond lengths



Bond angles

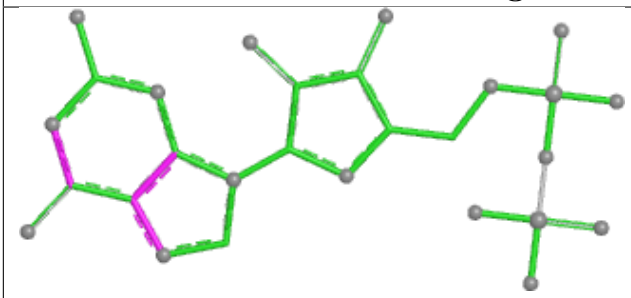


Torsions

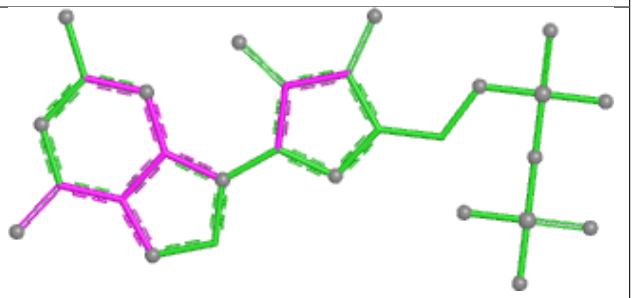


Rings

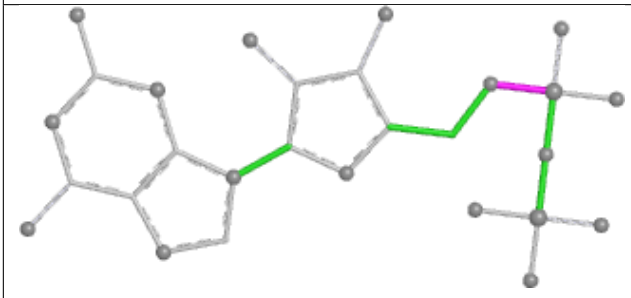
Ligand GDP JW 500



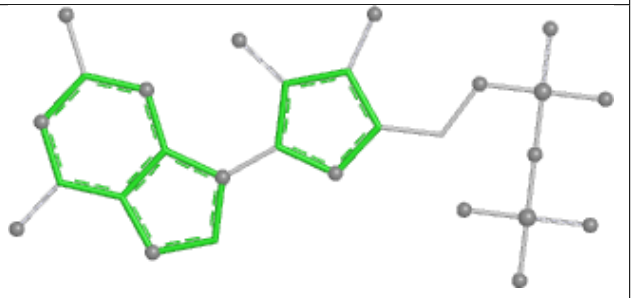
Bond lengths



Bond angles

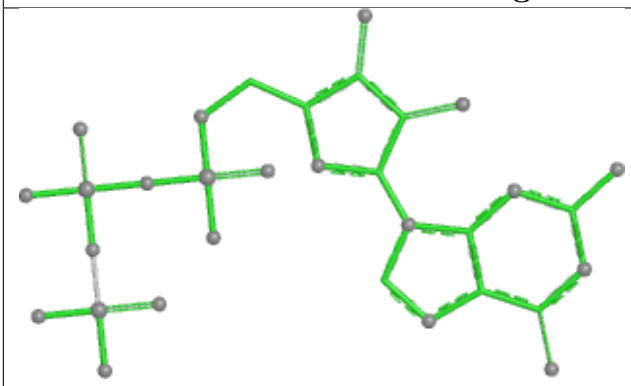


Torsions

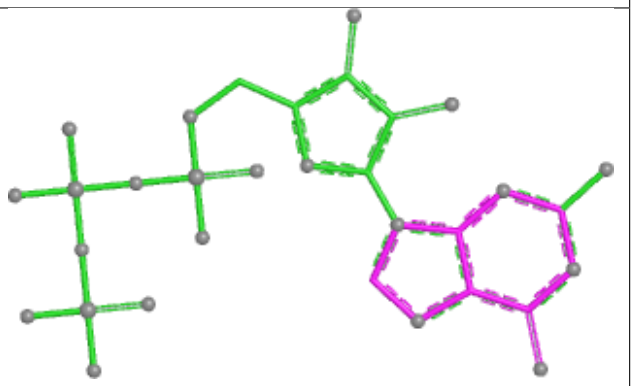


Rings

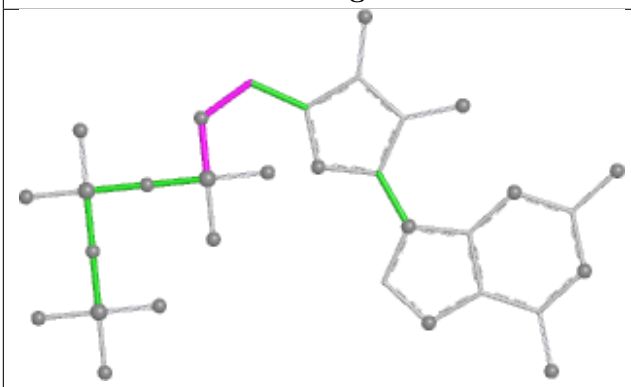
Ligand GTP FA 501



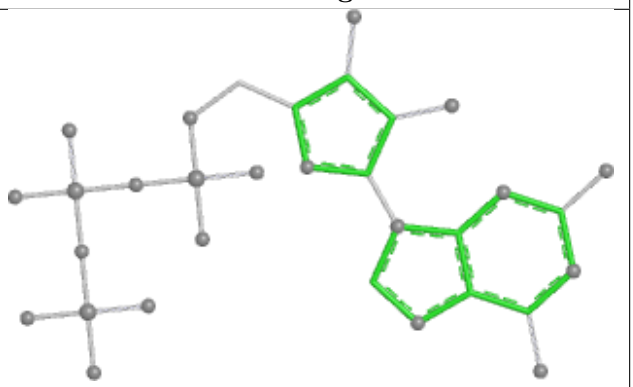
Bond lengths



Bond angles

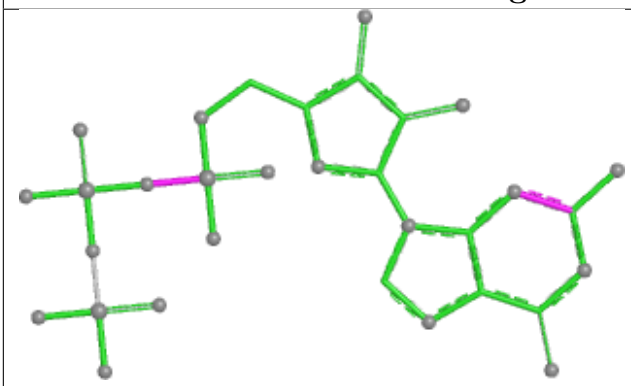


Torsions

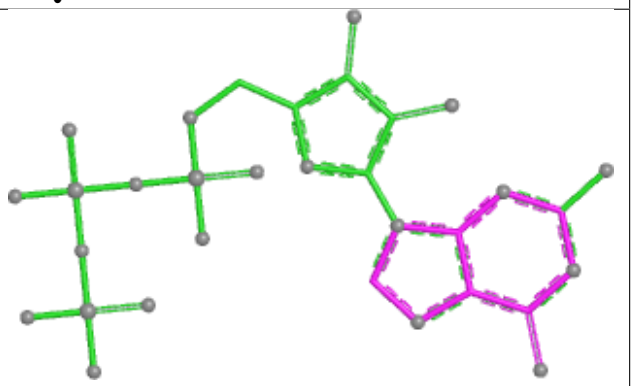


Rings

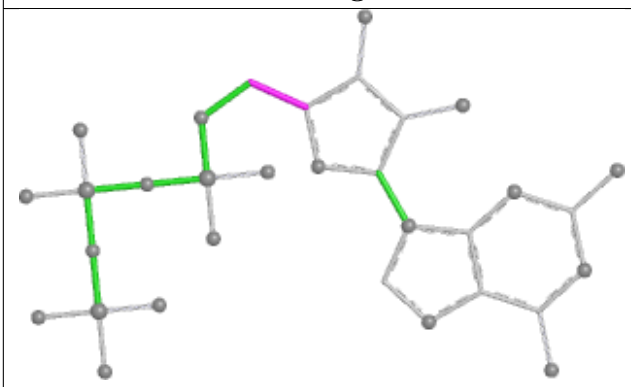
Ligand GTP QB 501



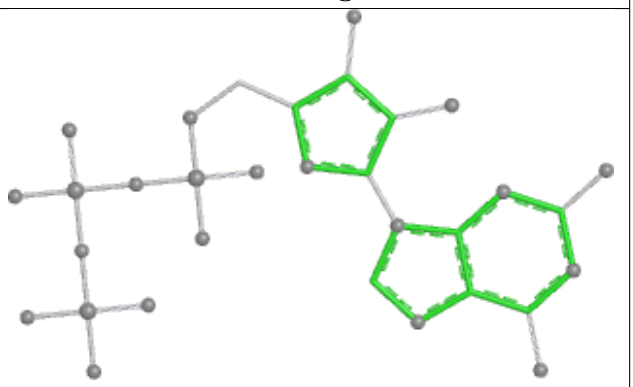
Bond lengths



Bond angles

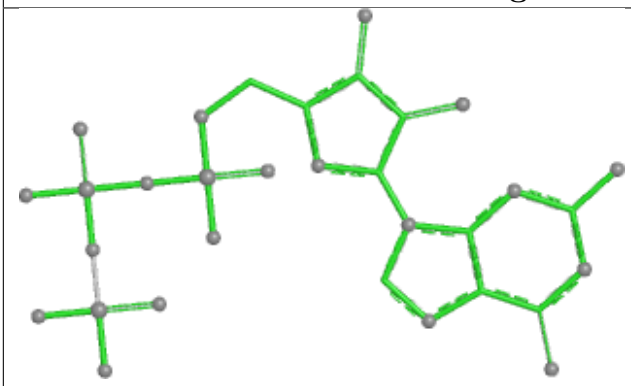


Torsions

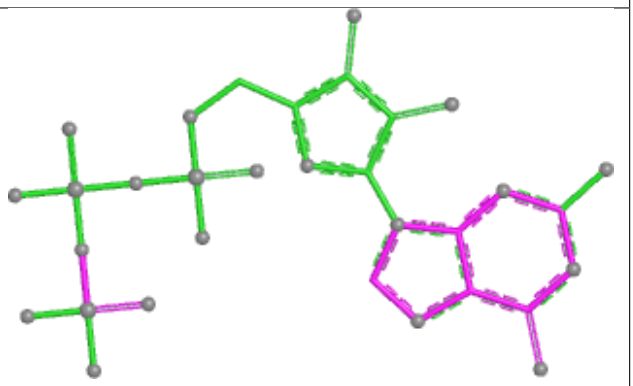


Rings

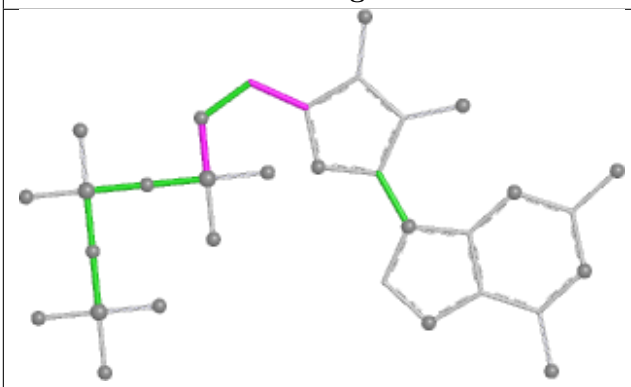
Ligand GTP CC 501



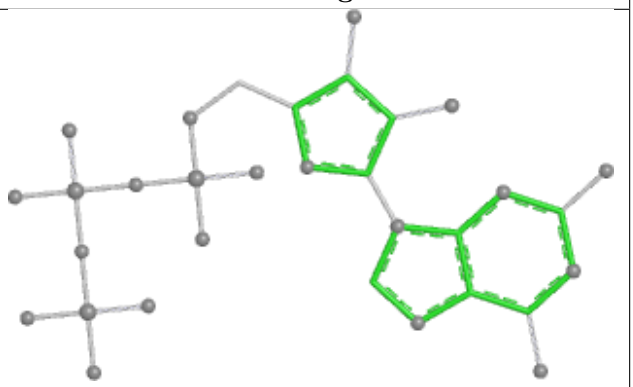
Bond lengths



Bond angles

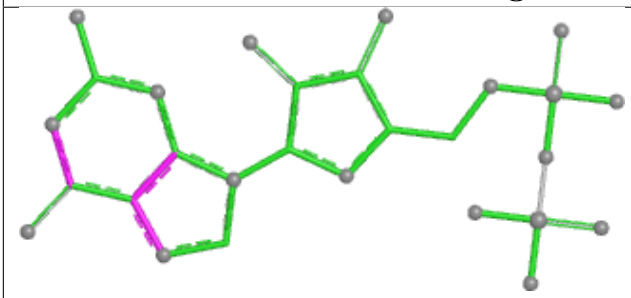


Torsions

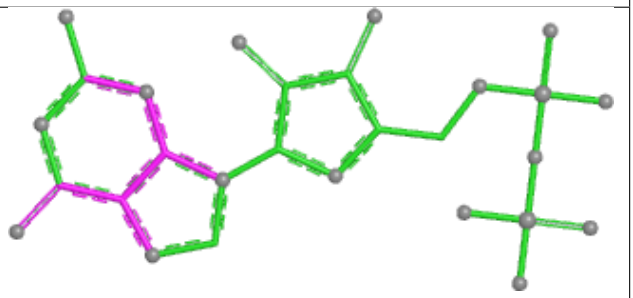


Rings

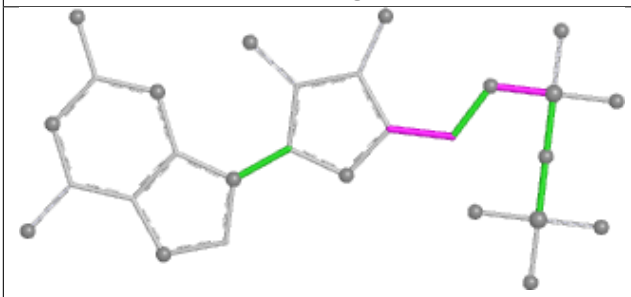
Ligand GDP DA 500



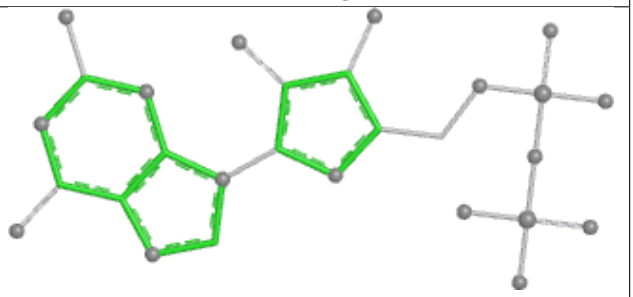
Bond lengths



Bond angles

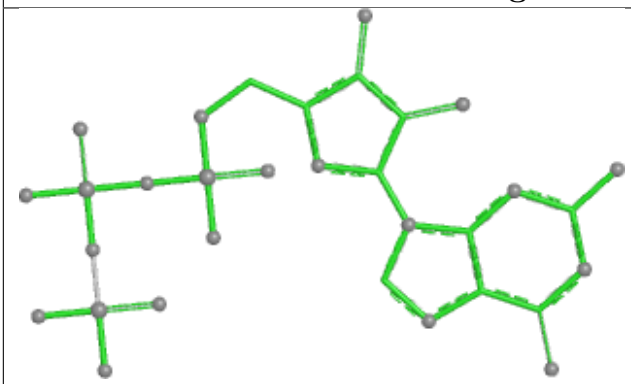


Torsions

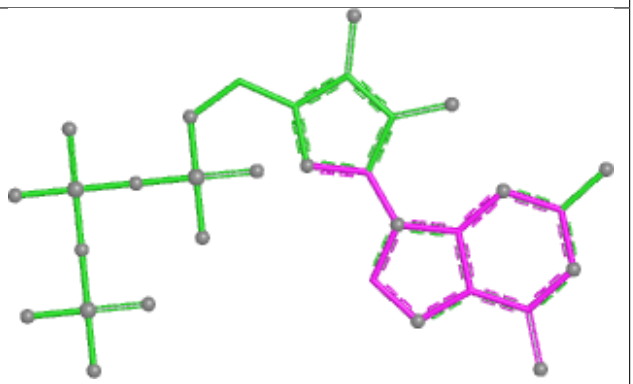


Rings

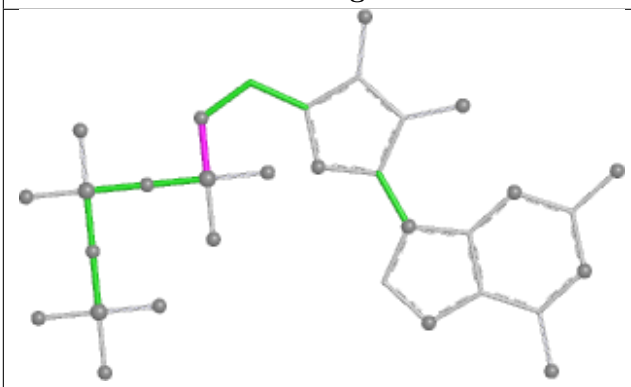
Ligand GTP DB 501



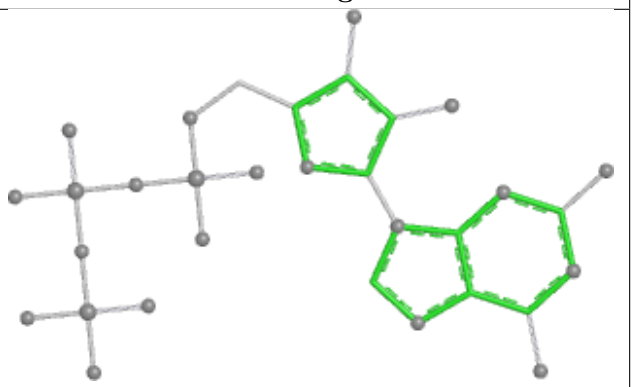
Bond lengths



Bond angles

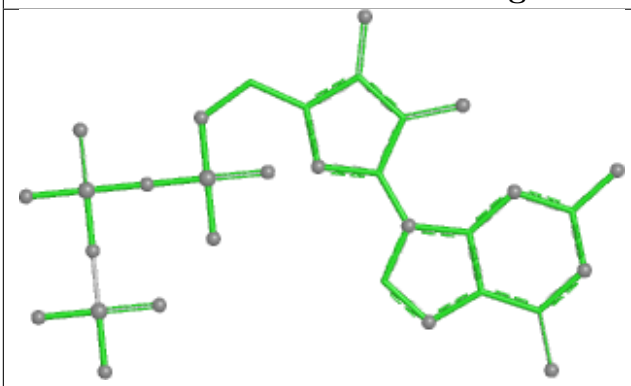


Torsions

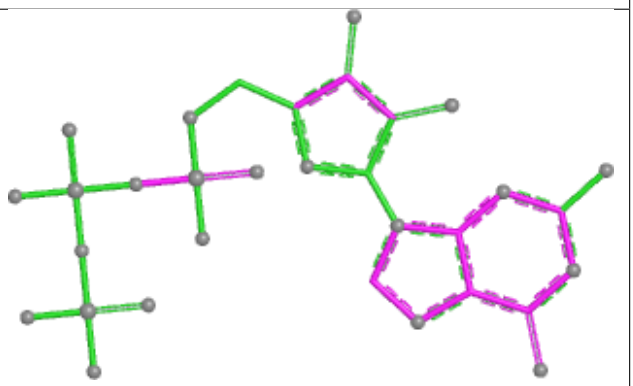


Rings

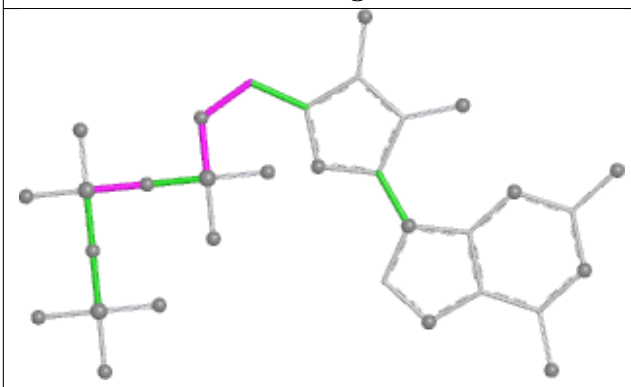
Ligand GTP GC 501



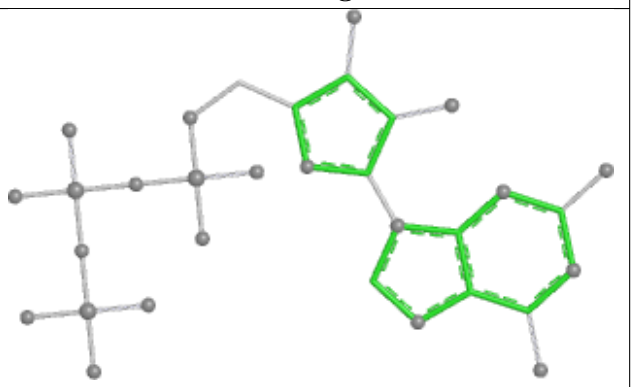
Bond lengths



Bond angles

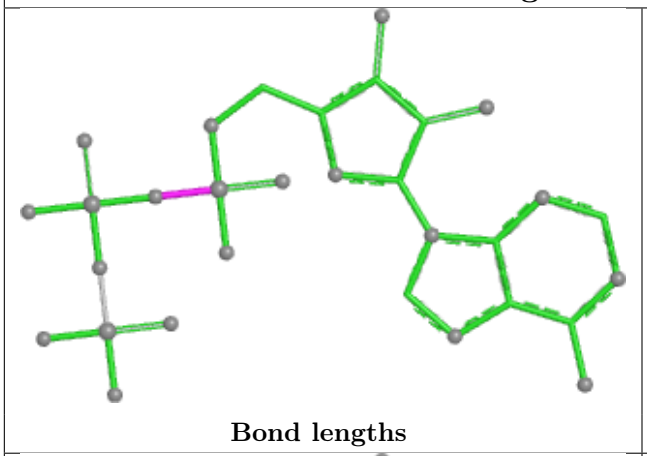


Torsions

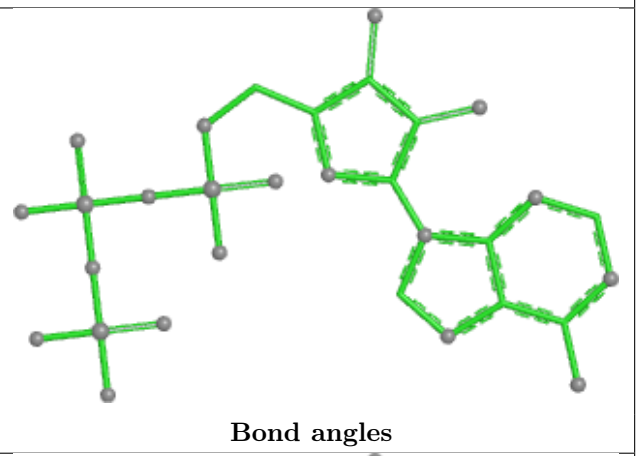


Rings

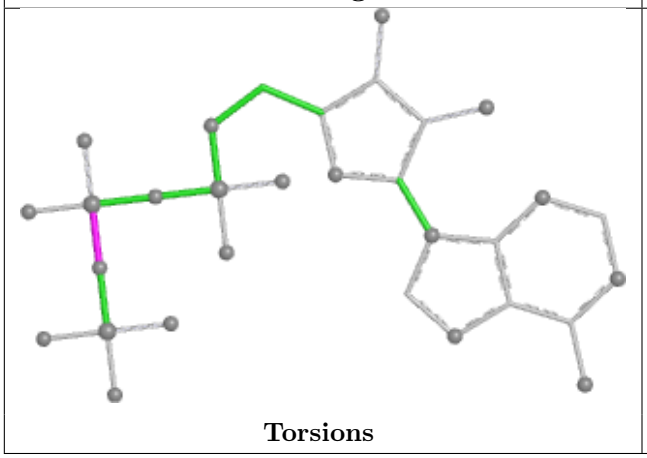
Ligand ATP 8a 801



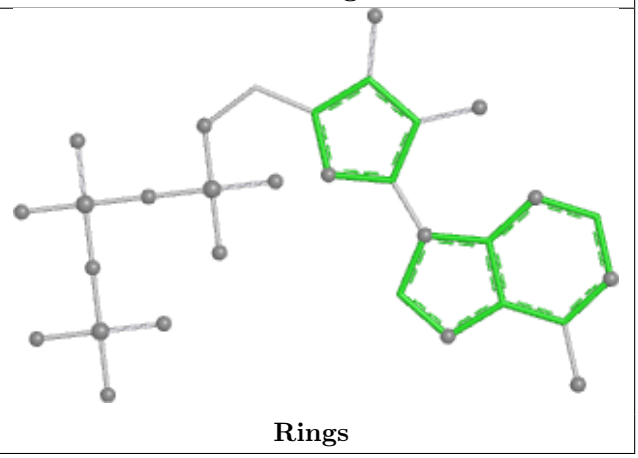
Bond lengths



Bond angles

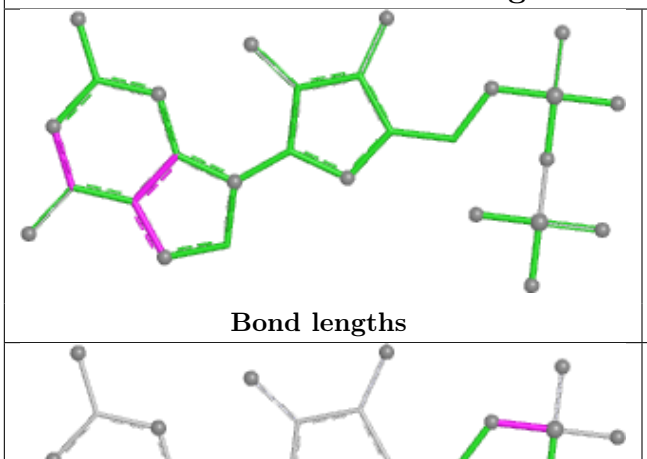


Torsions

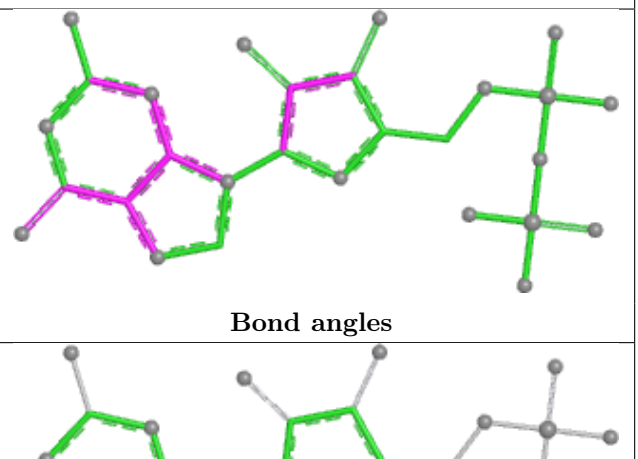


Rings

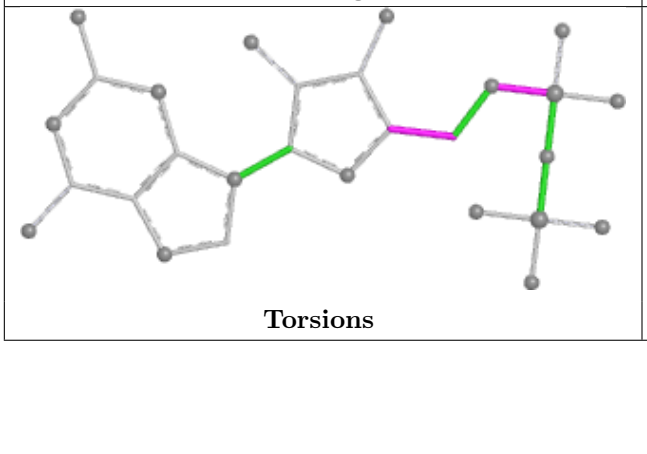
Ligand GDP OD 501



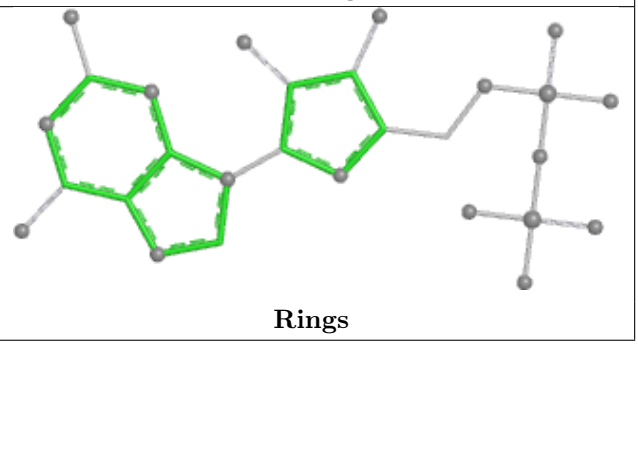
Bond lengths



Bond angles

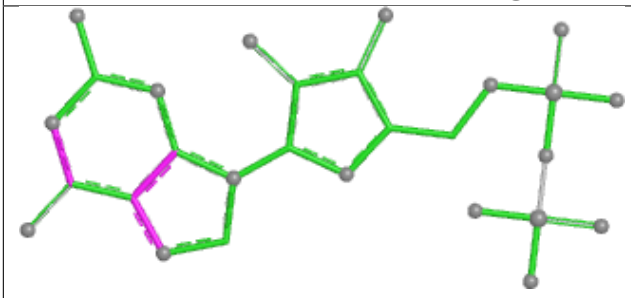


Torsions

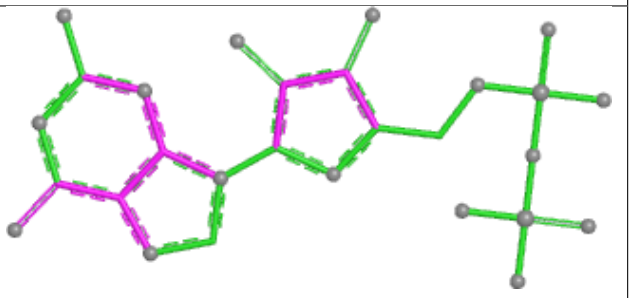


Rings

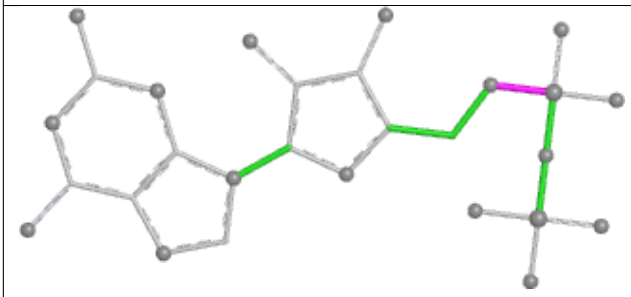
Ligand GDP VV 500



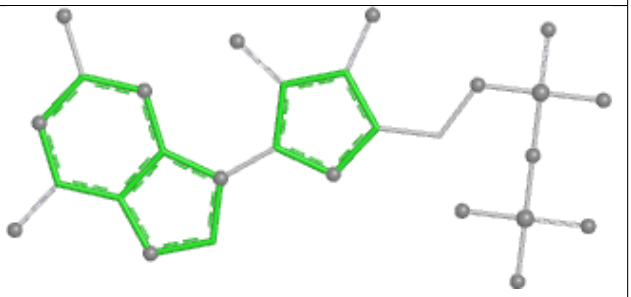
Bond lengths



Bond angles

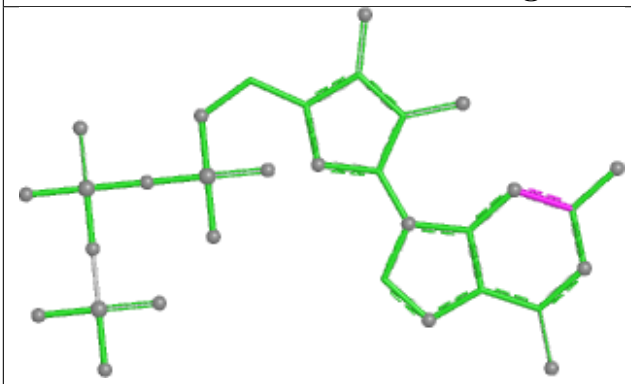


Torsions

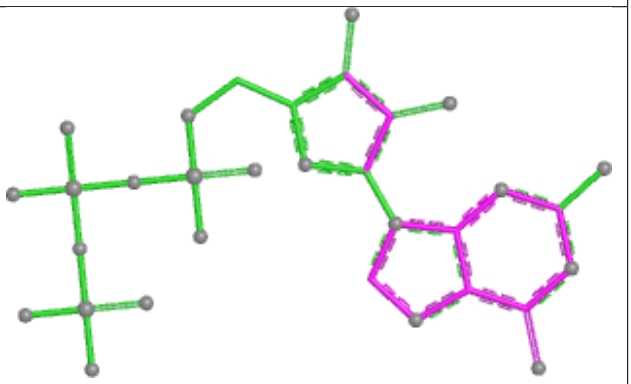


Rings

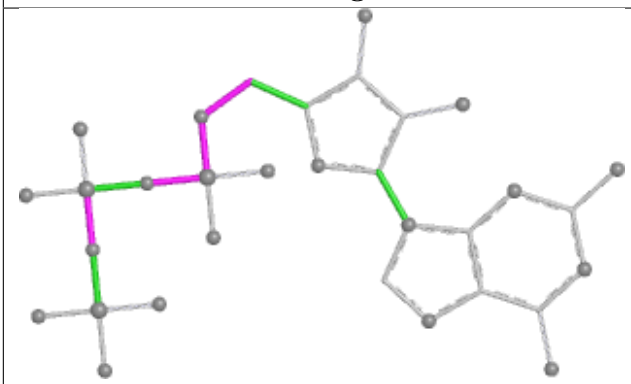
Ligand GTP R 501



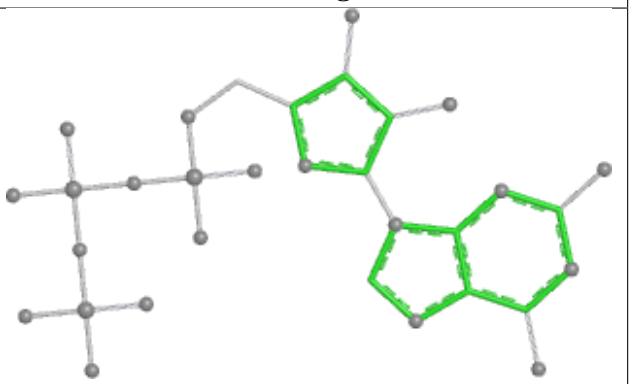
Bond lengths



Bond angles

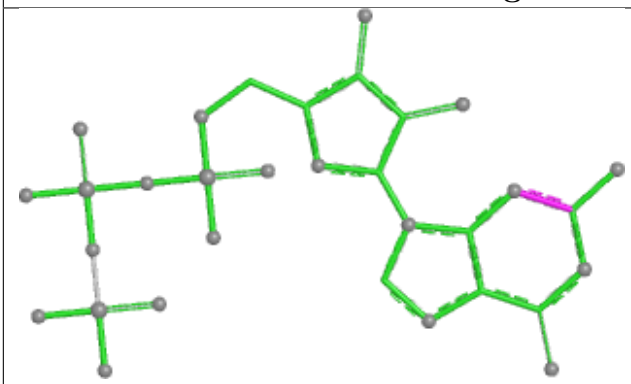


Torsions

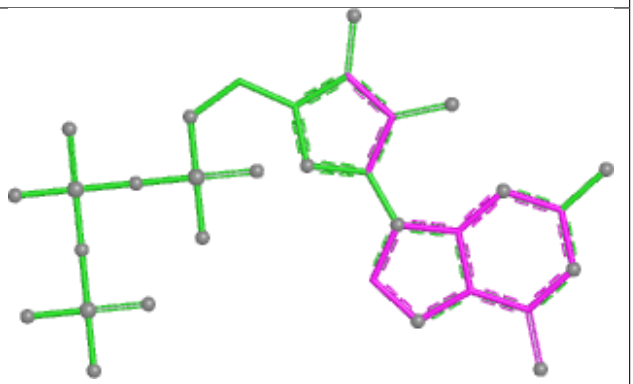


Rings

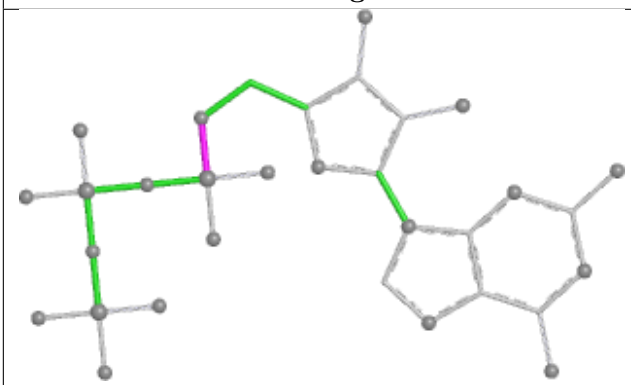
Ligand GTP WY 501



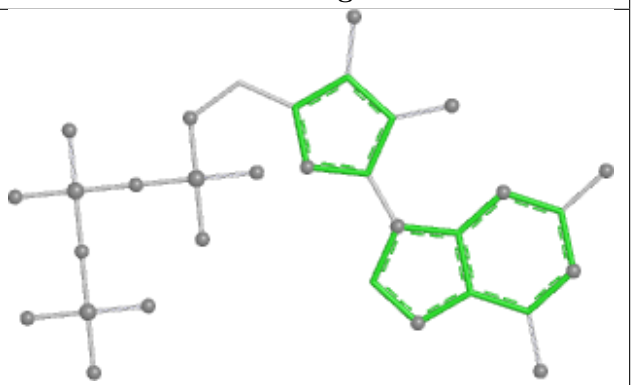
Bond lengths



Bond angles

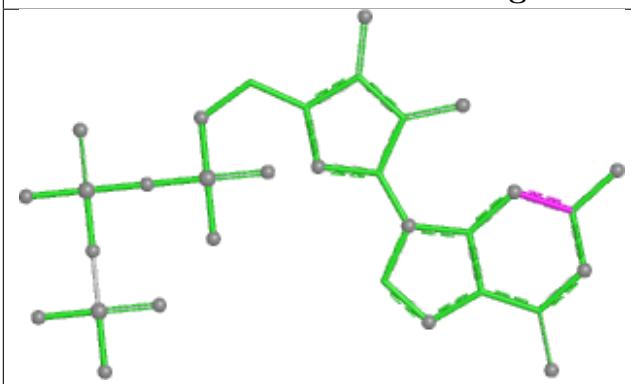


Torsions

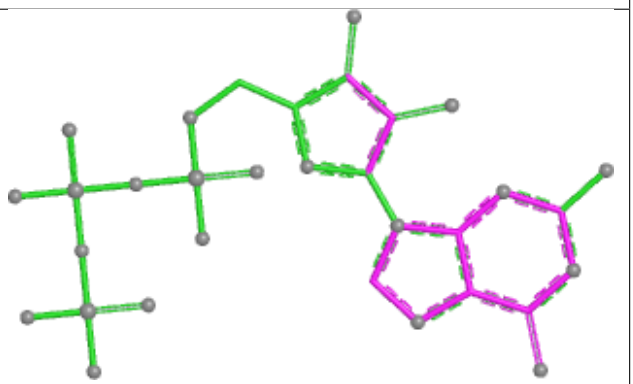


Rings

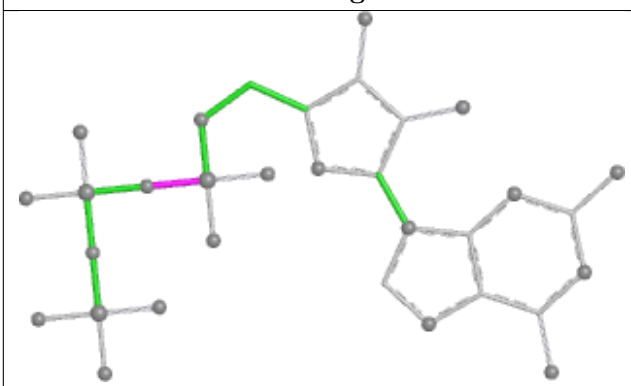
Ligand GTP TG 501



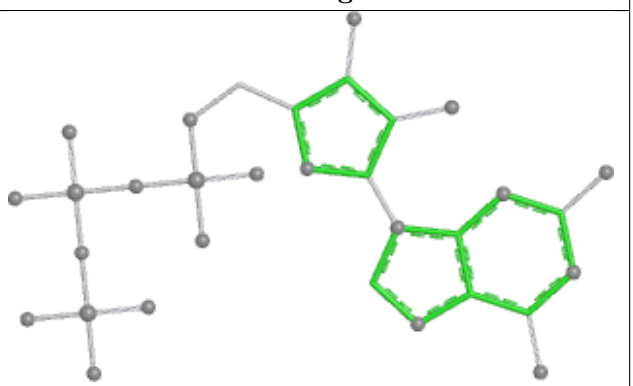
Bond lengths



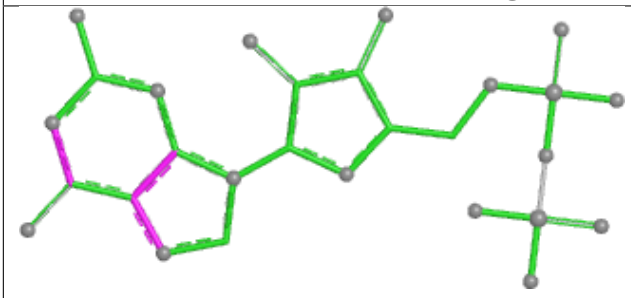
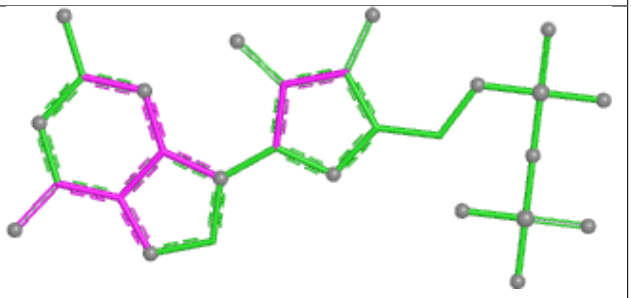
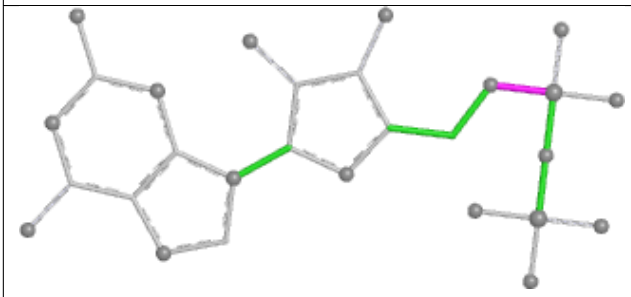
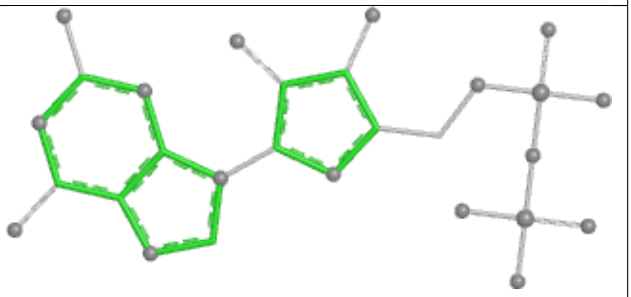
Bond angles

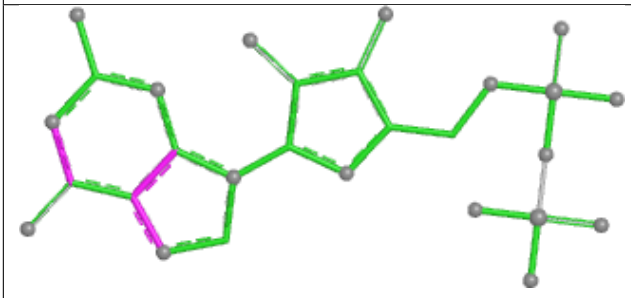
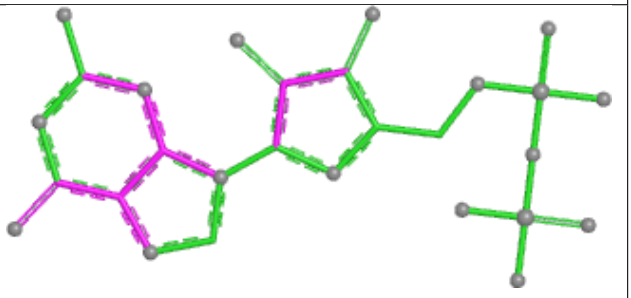
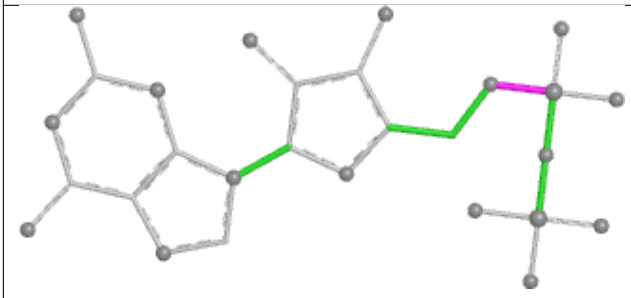
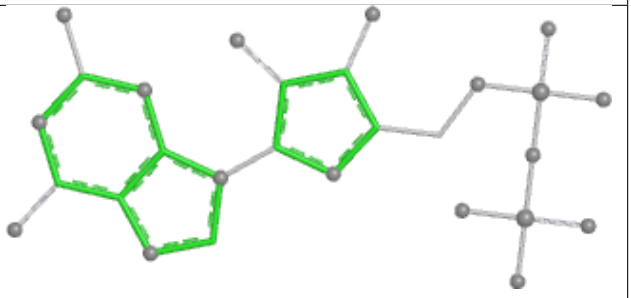


Torsions

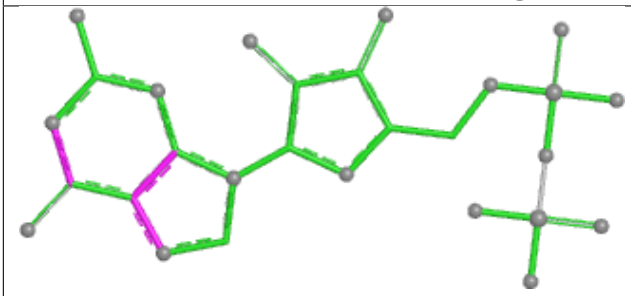


Rings

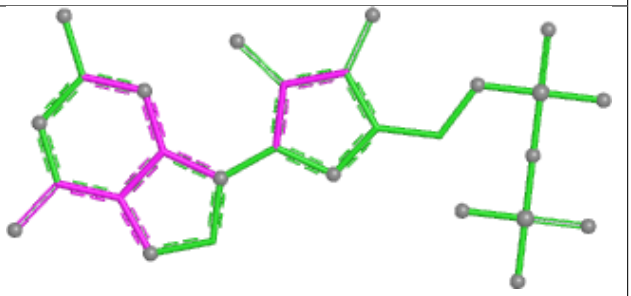
Ligand GDP MD 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP VH 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

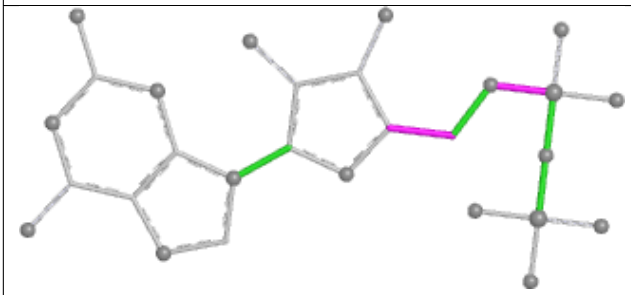
Ligand GDP BL 500



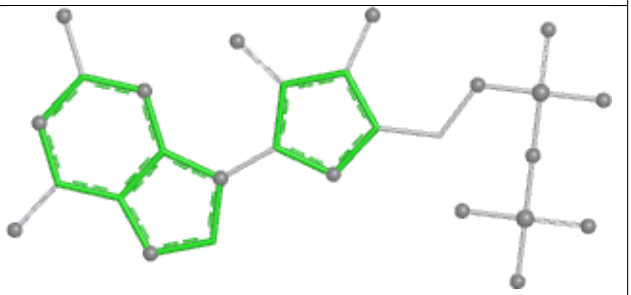
Bond lengths



Bond angles

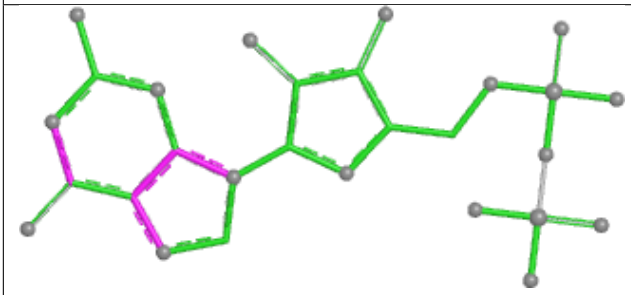


Torsions

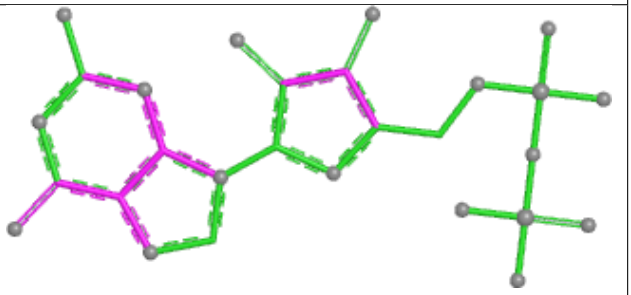


Rings

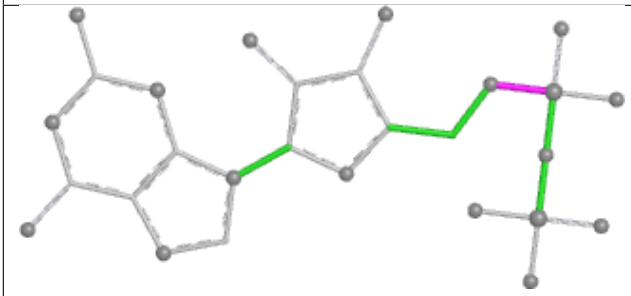
Ligand GDP BN 500



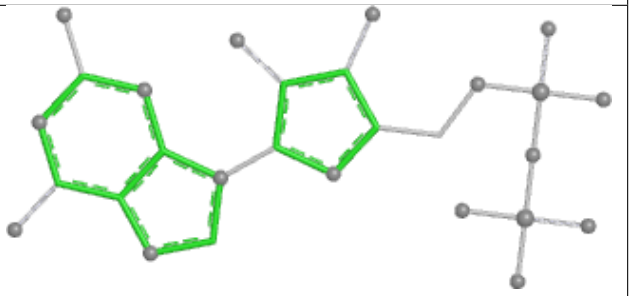
Bond lengths



Bond angles

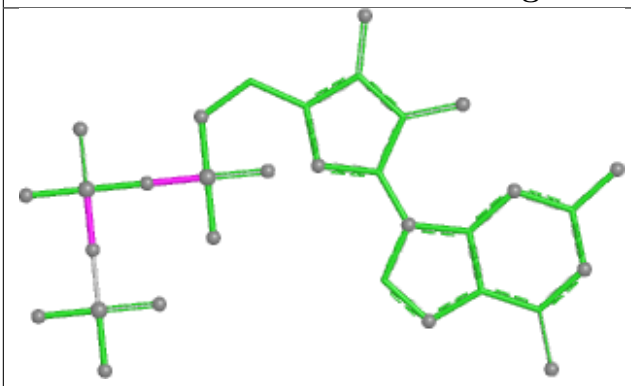


Torsions

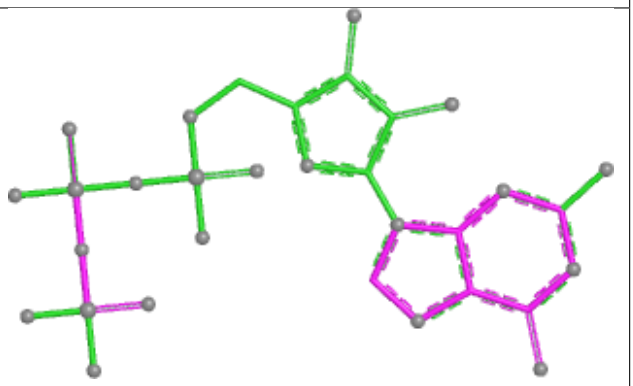


Rings

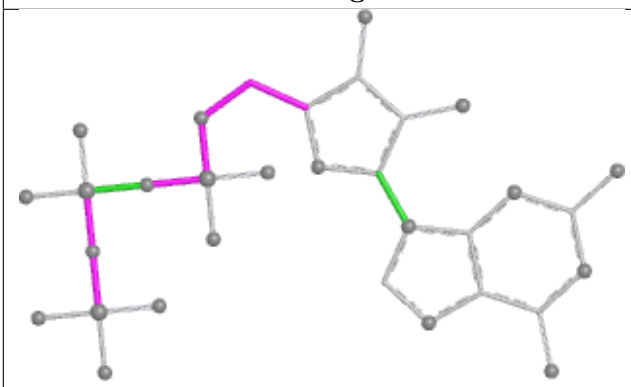
Ligand GTP D 501



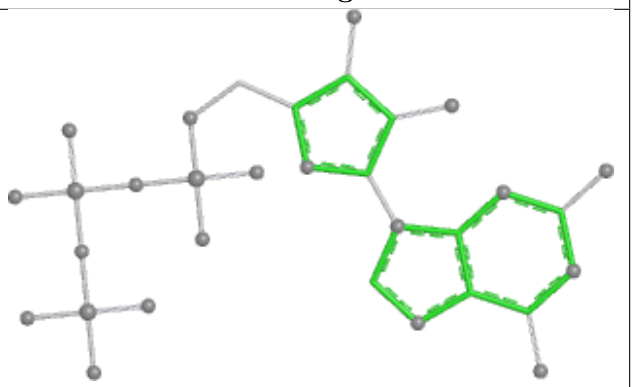
Bond lengths



Bond angles

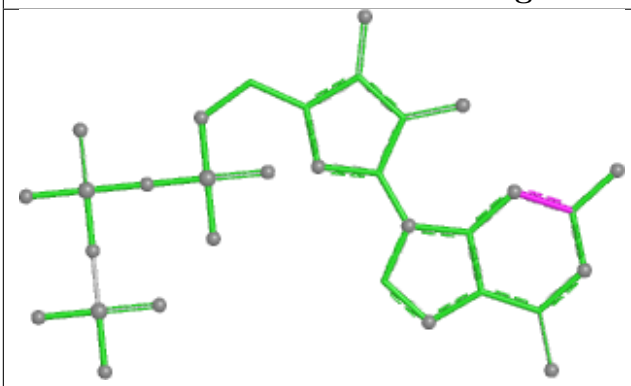


Torsions

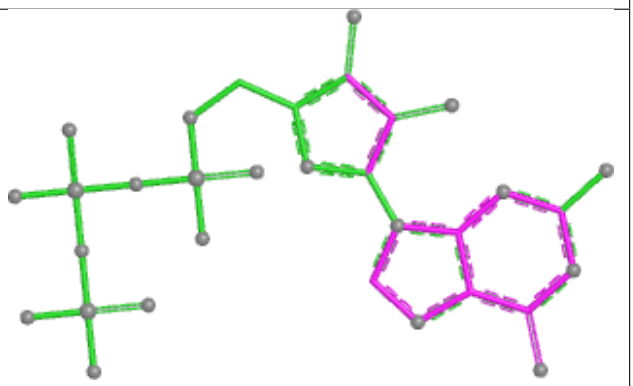


Rings

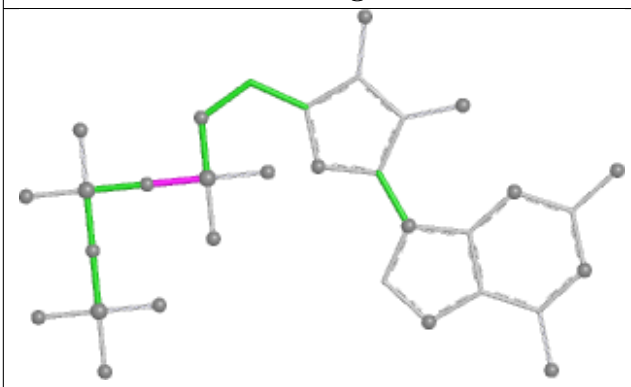
Ligand GTP NI 501



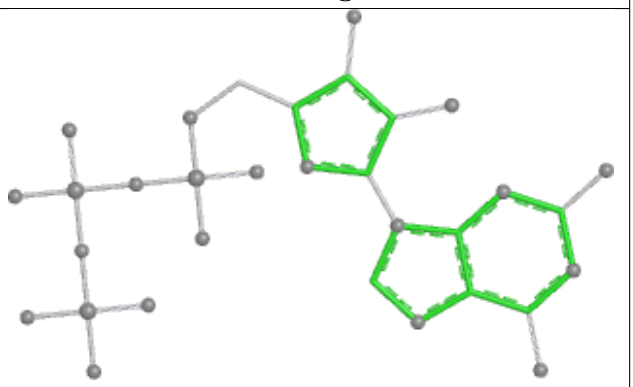
Bond lengths



Bond angles

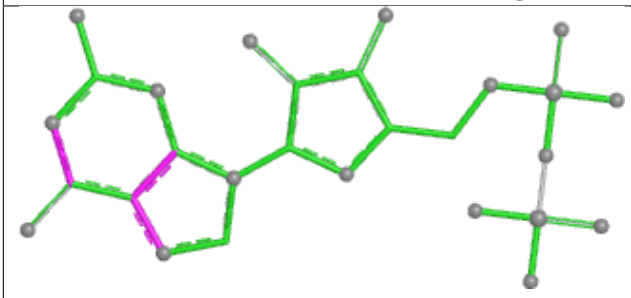


Torsions

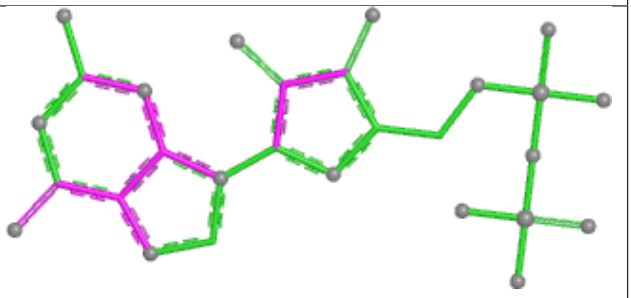


Rings

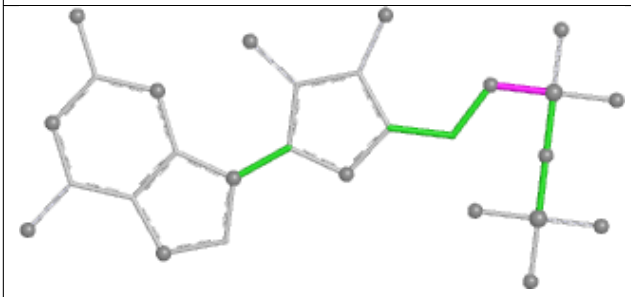
Ligand GDP GJ 500



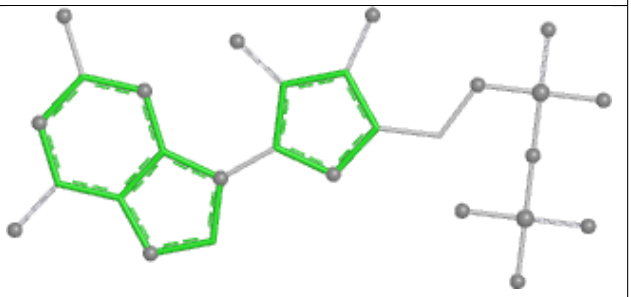
Bond lengths



Bond angles

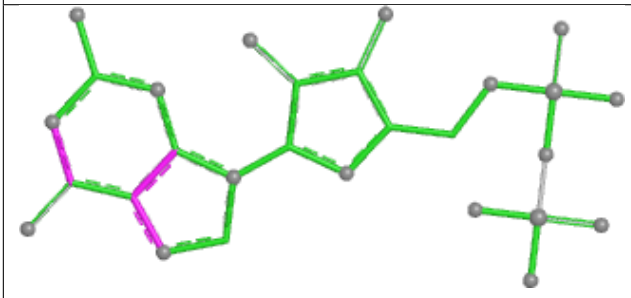


Torsions

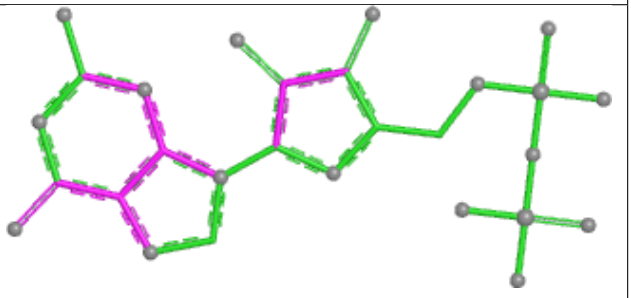


Rings

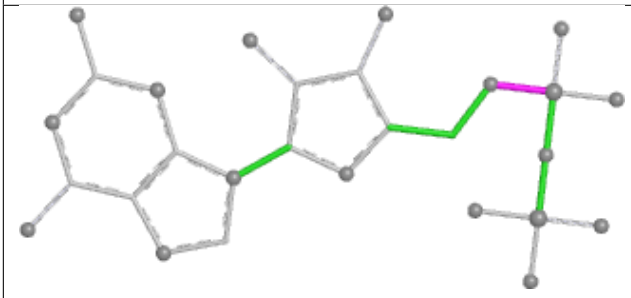
Ligand GDP PX 501



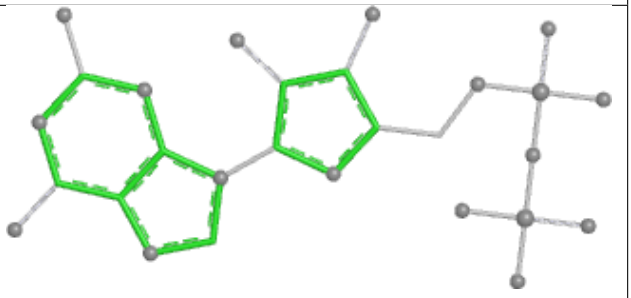
Bond lengths



Bond angles

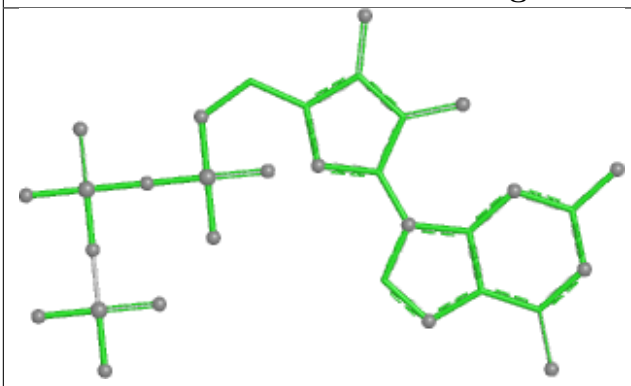


Torsions

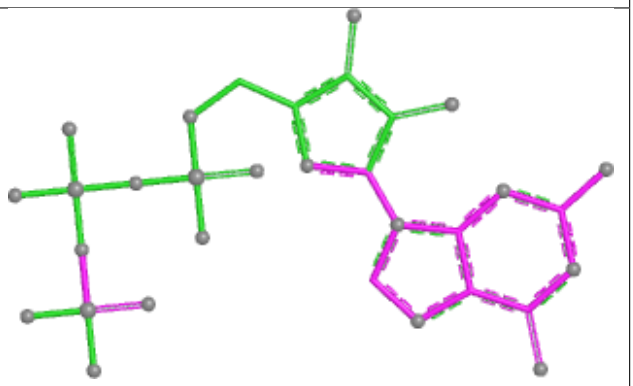


Rings

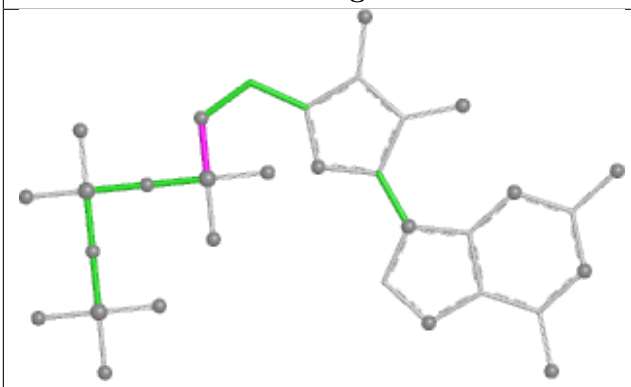
Ligand GTP DP 501



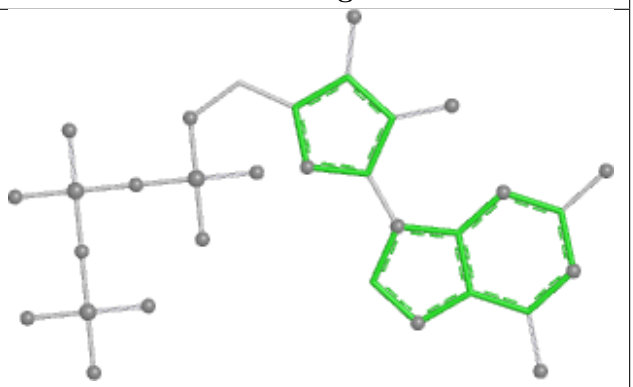
Bond lengths



Bond angles

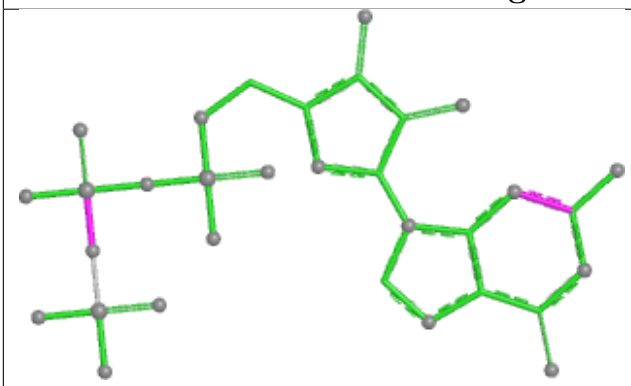


Torsions

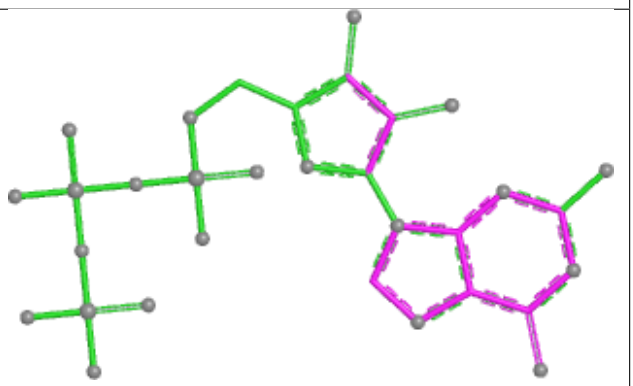


Rings

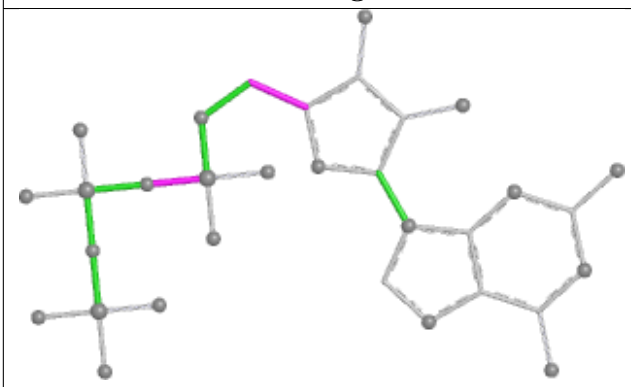
Ligand GTP VG 501



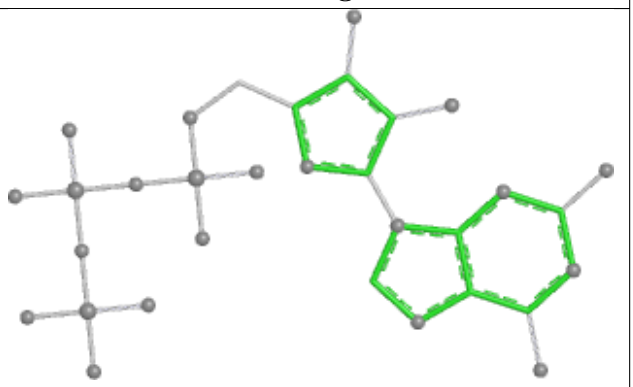
Bond lengths



Bond angles

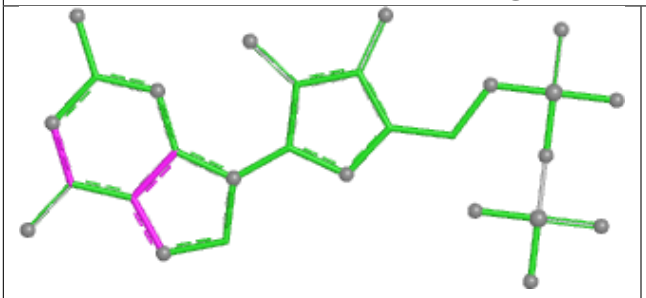


Torsions

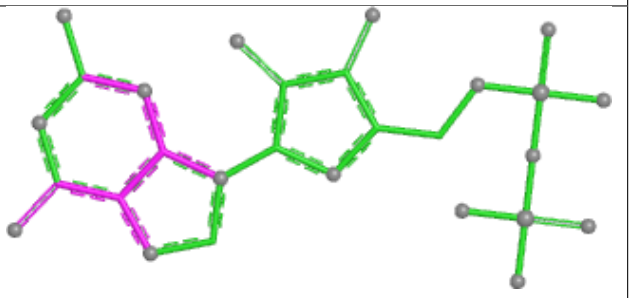


Rings

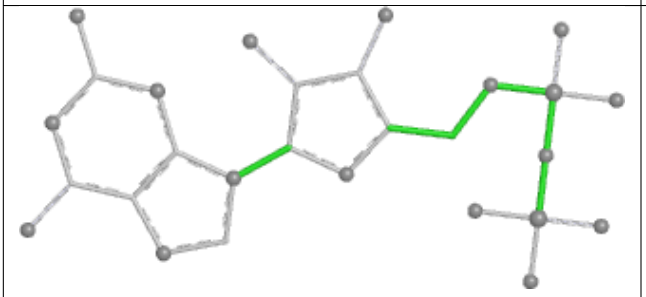
Ligand GDP GR 500



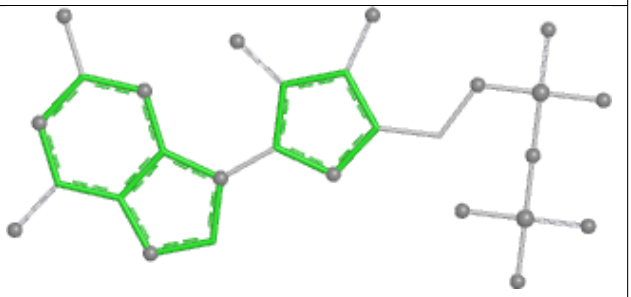
Bond lengths



Bond angles

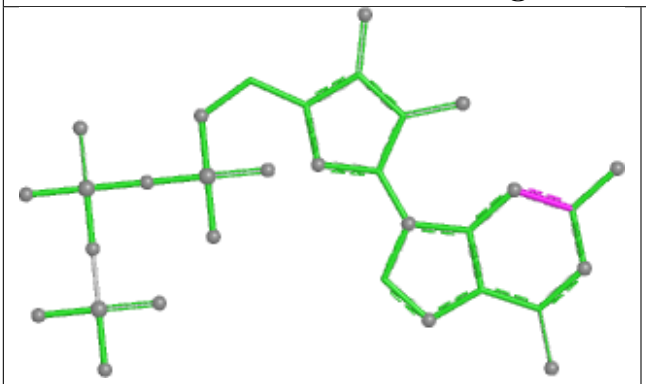


Torsions

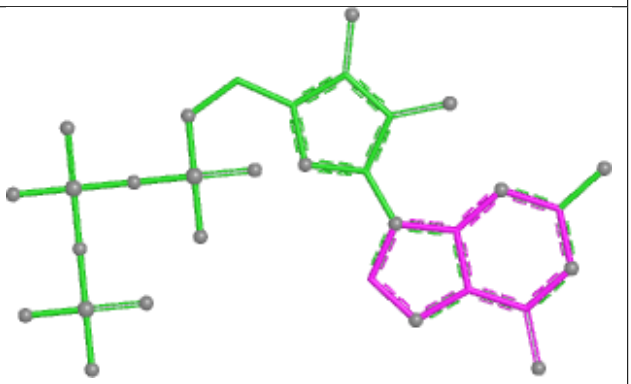


Rings

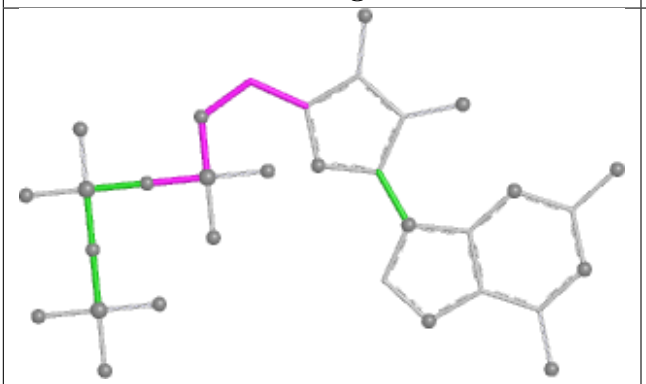
Ligand GTP MJ 501



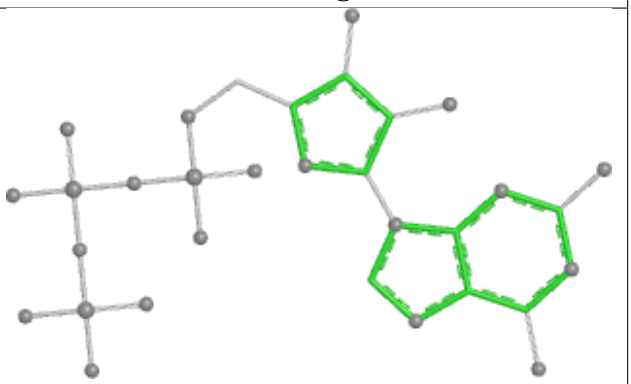
Bond lengths



Bond angles

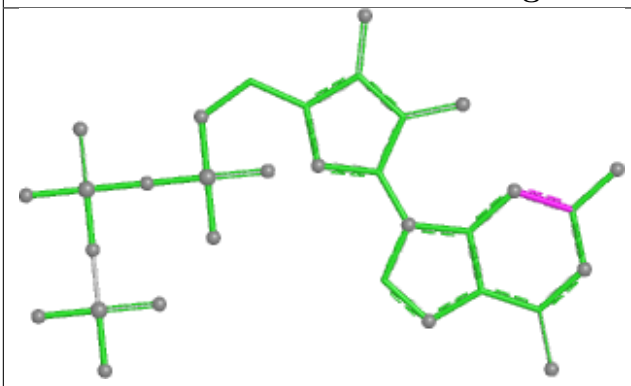


Torsions

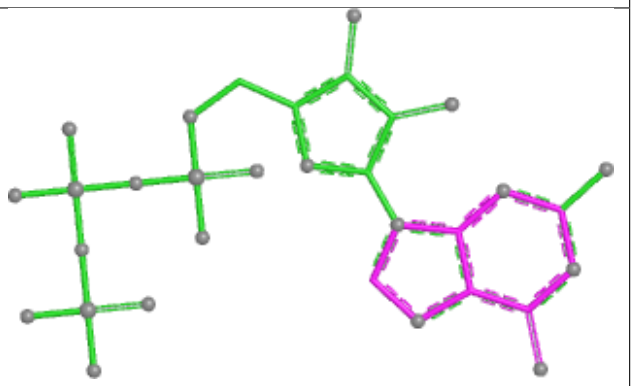


Rings

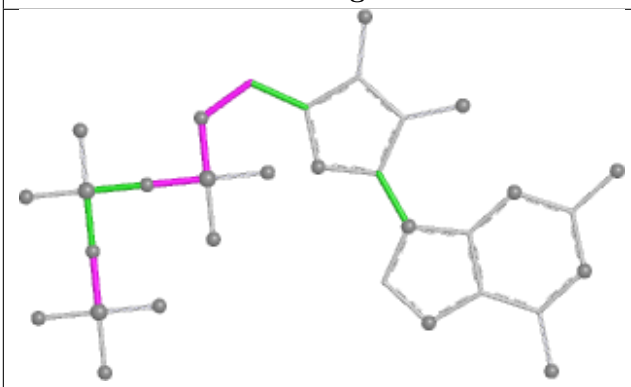
Ligand GTP C 501



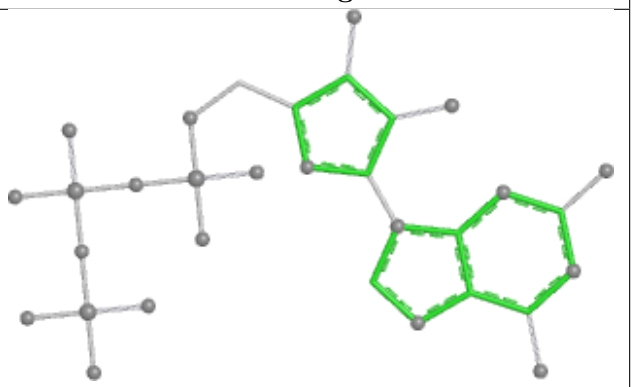
Bond lengths



Bond angles

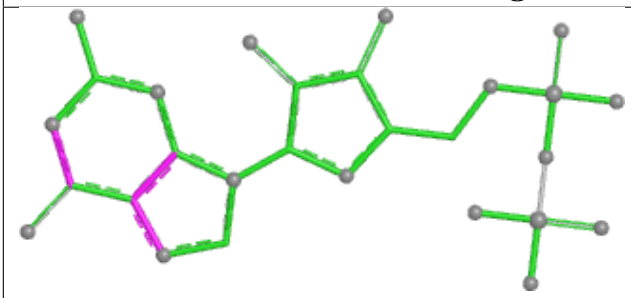


Torsions

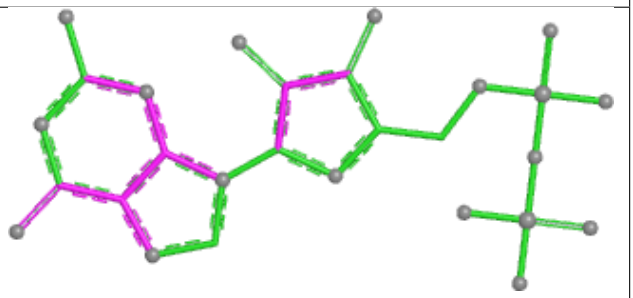


Rings

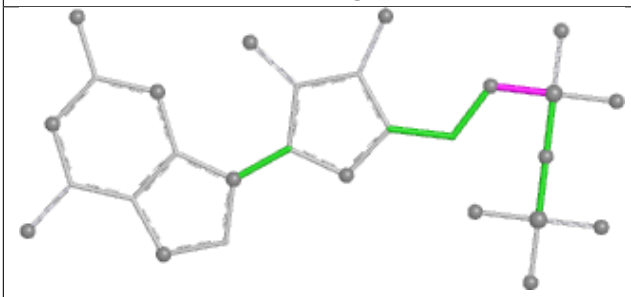
Ligand GDP RC 500



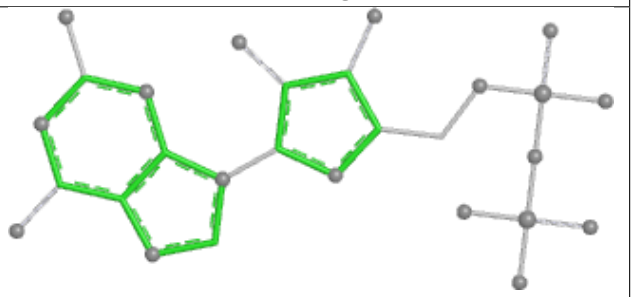
Bond lengths



Bond angles

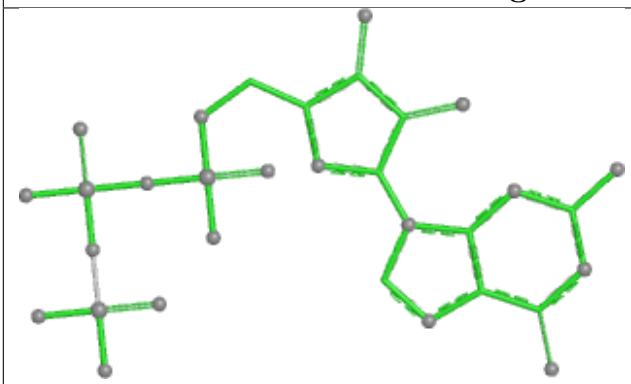


Torsions

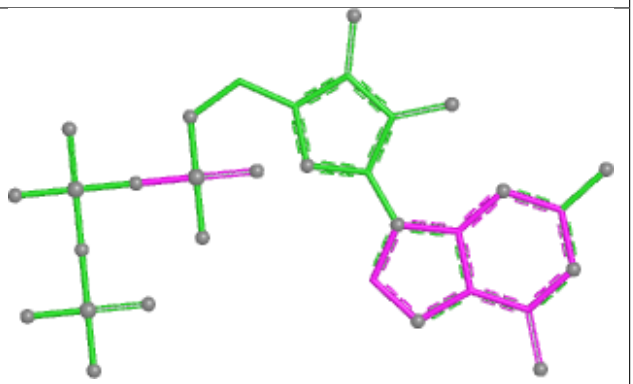


Rings

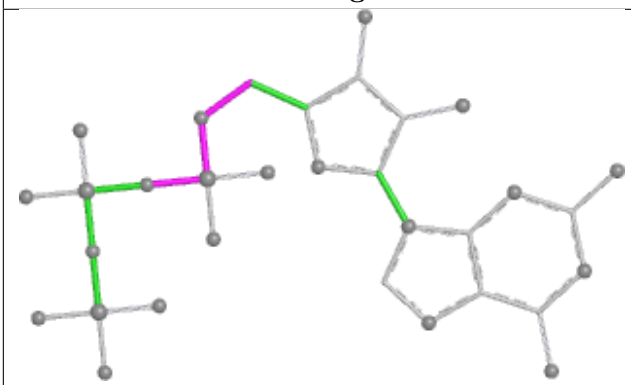
Ligand GTP GE 501



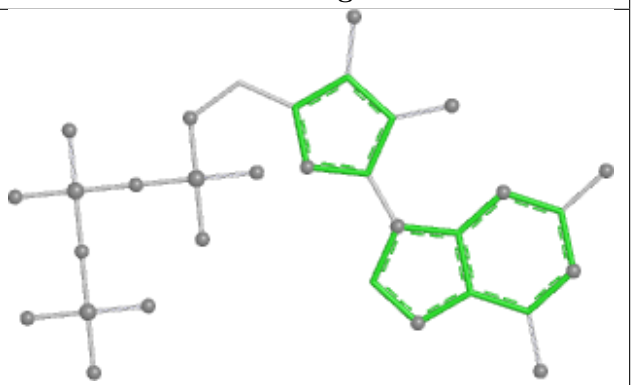
Bond lengths



Bond angles

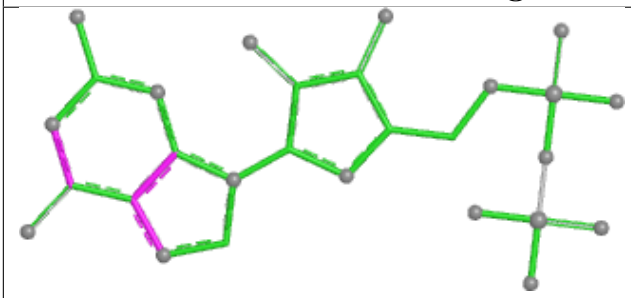


Torsions

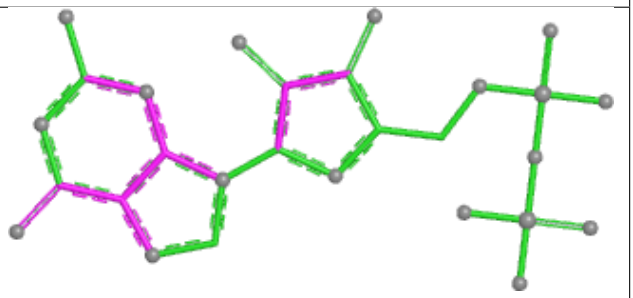


Rings

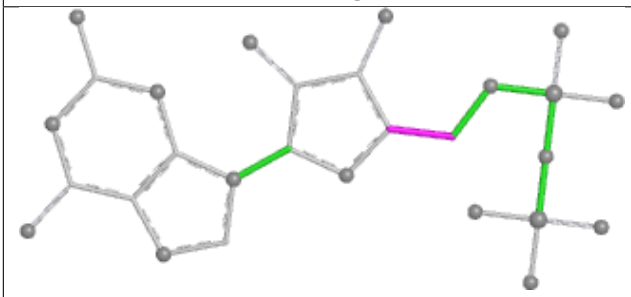
Ligand GDP HR 500



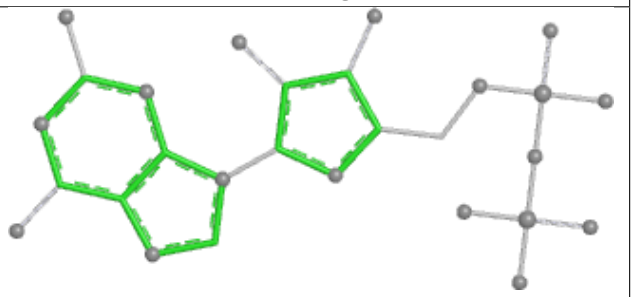
Bond lengths



Bond angles

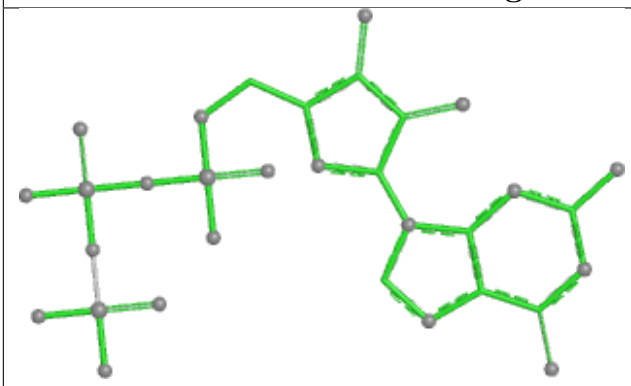


Torsions

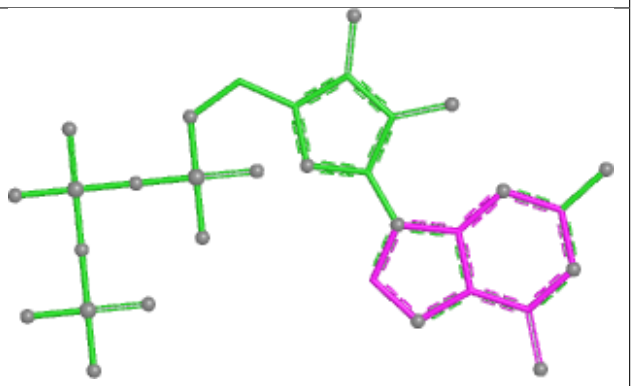


Rings

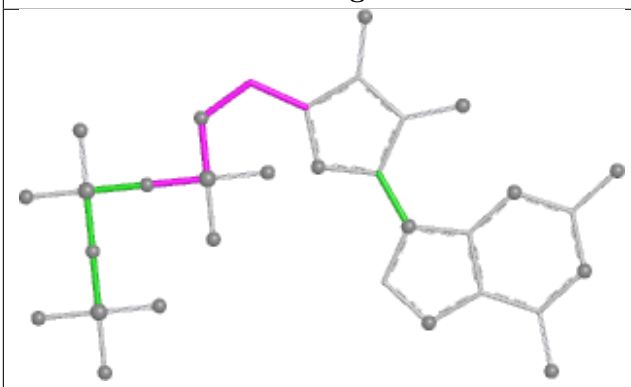
Ligand GTP AM 501



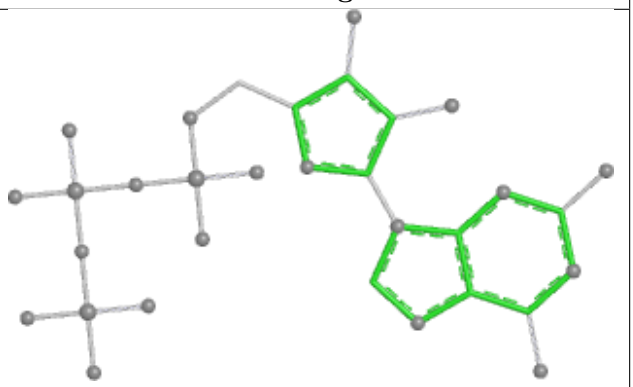
Bond lengths



Bond angles

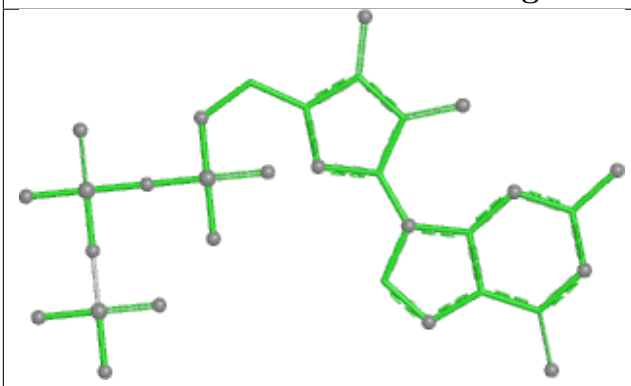


Torsions

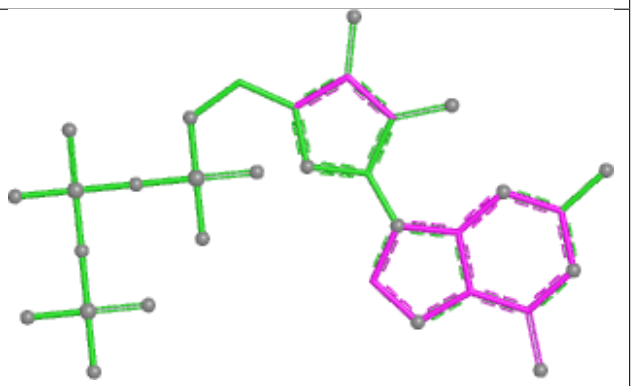


Rings

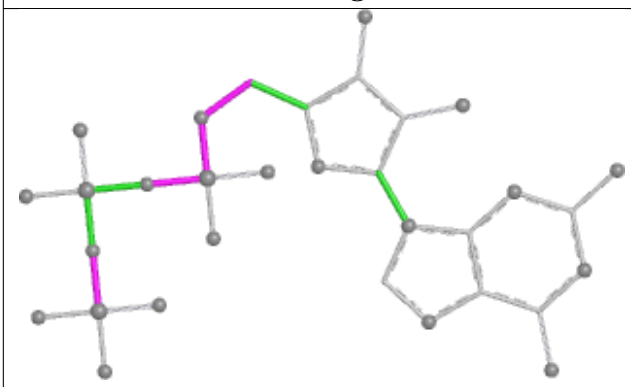
Ligand GTP G 501



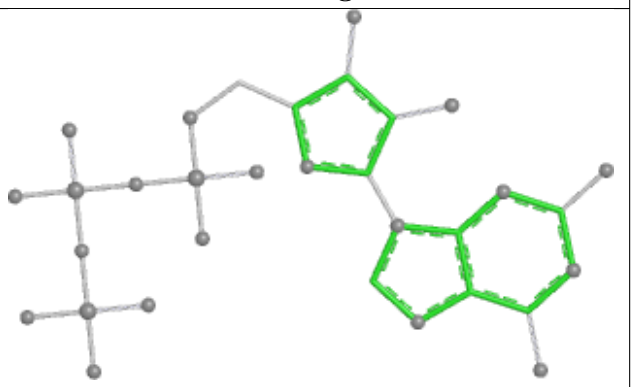
Bond lengths



Bond angles

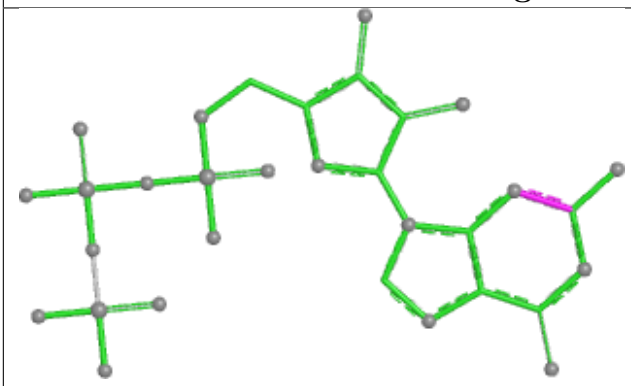


Torsions

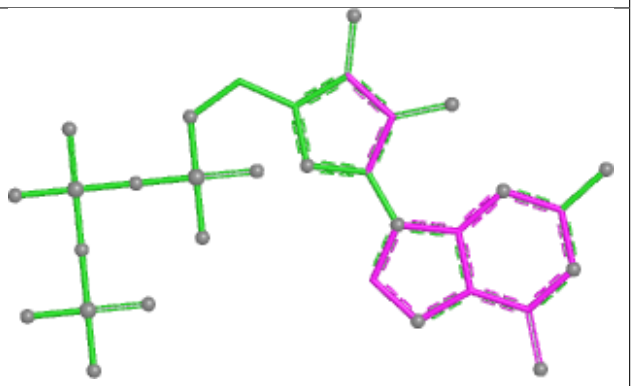


Rings

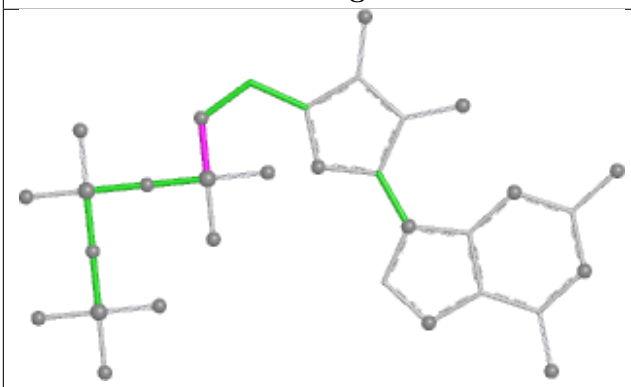
Ligand GTP LZ 502



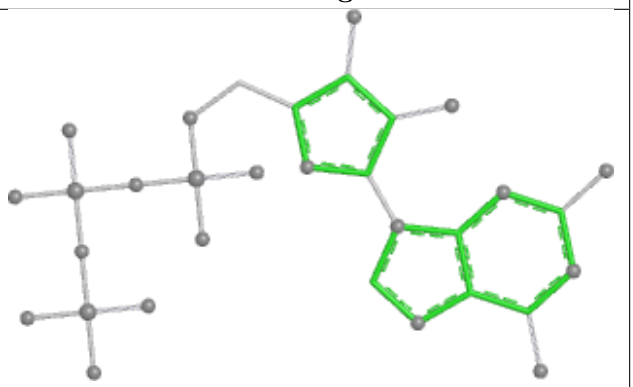
Bond lengths



Bond angles

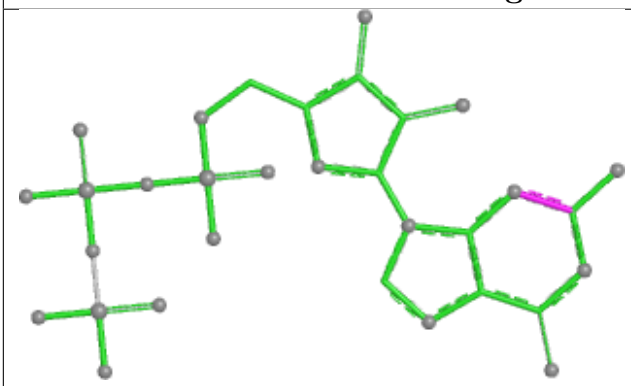


Torsions

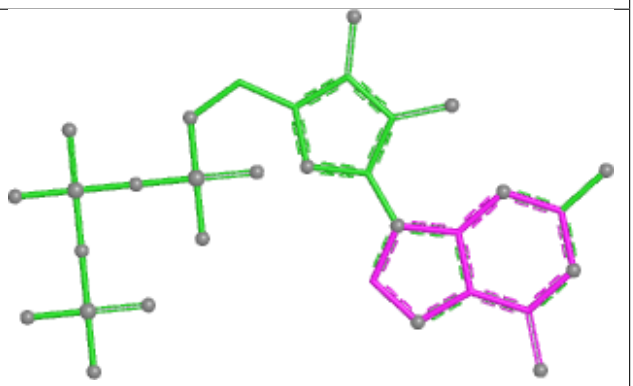


Rings

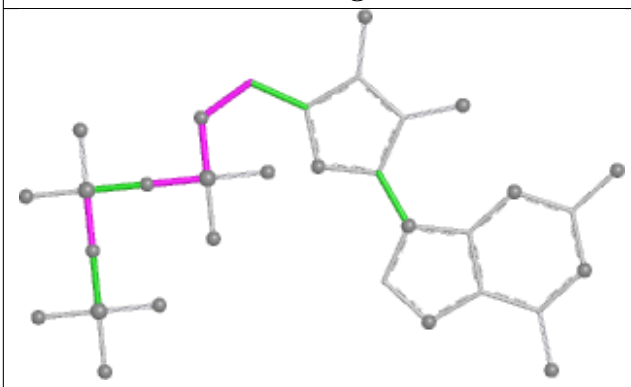
Ligand GTP OM 501



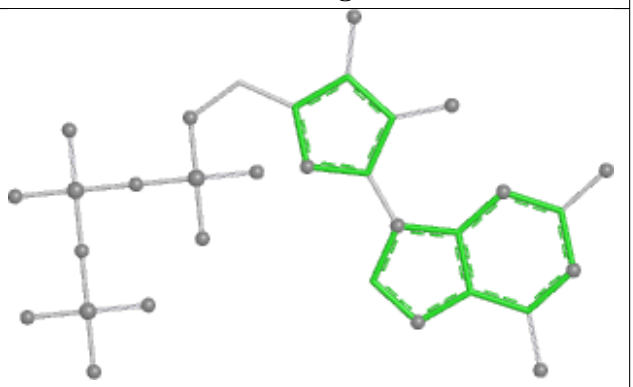
Bond lengths



Bond angles

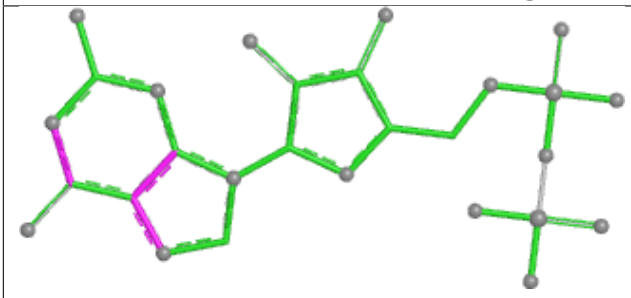


Torsions

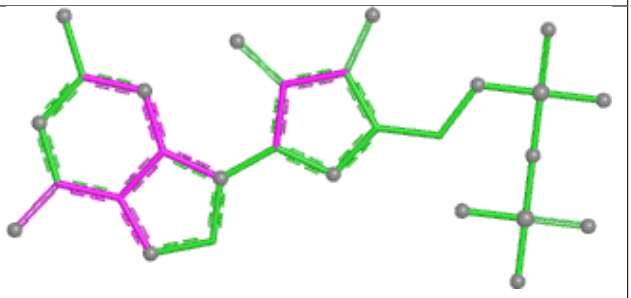


Rings

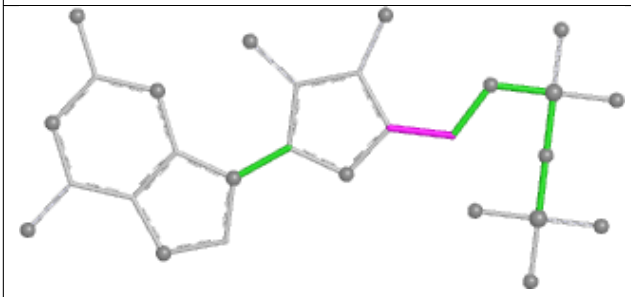
Ligand GDP O 500



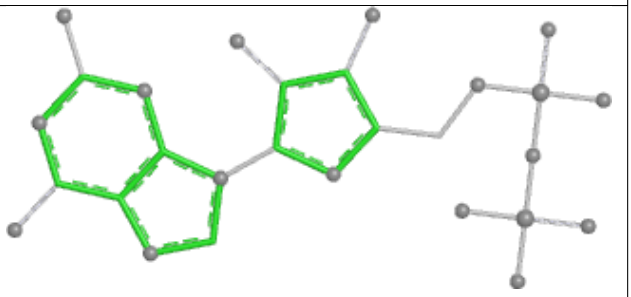
Bond lengths



Bond angles

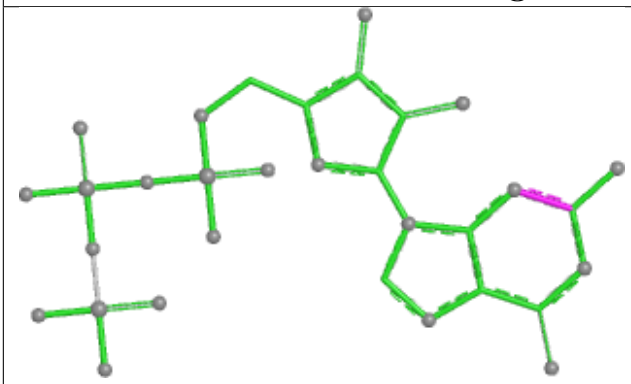


Torsions

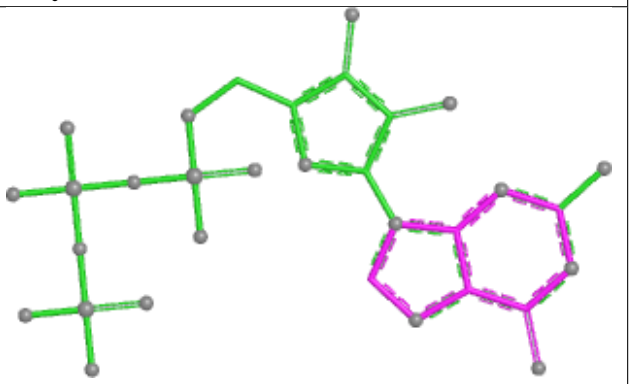


Rings

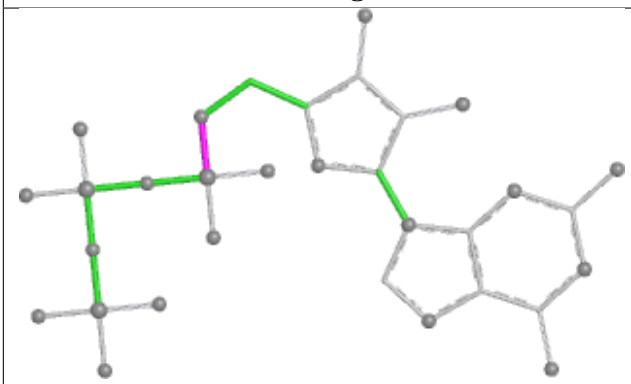
Ligand GTP QX 501



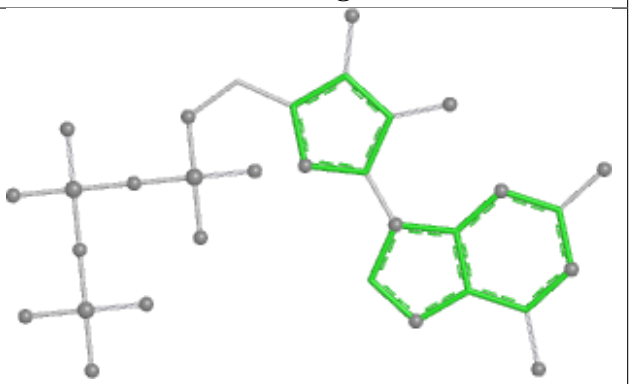
Bond lengths



Bond angles

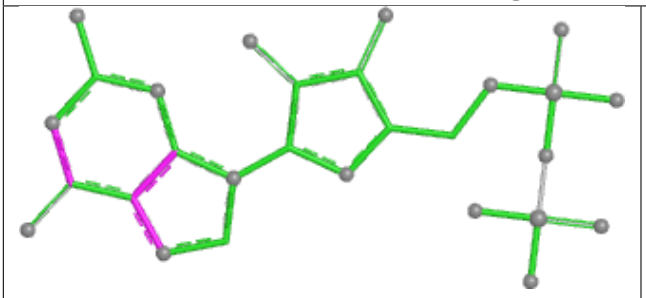


Torsions

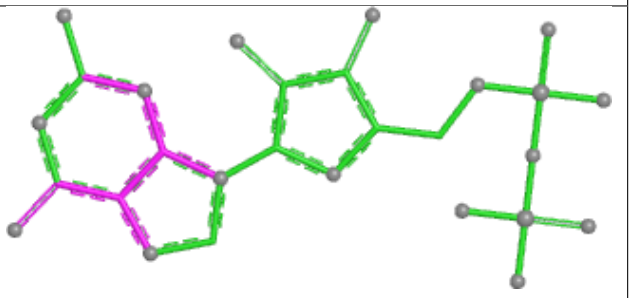


Rings

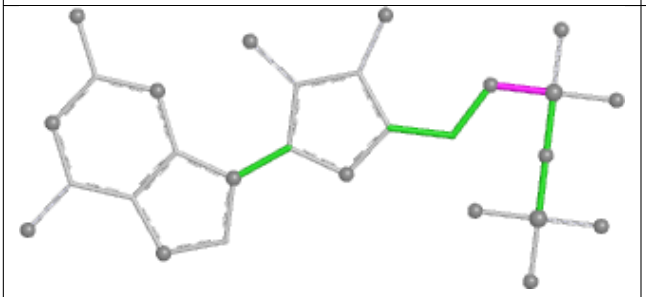
Ligand GDP VX 500



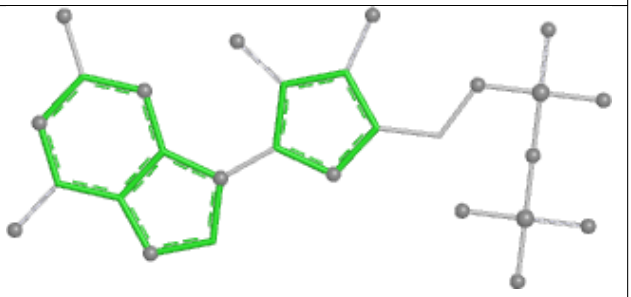
Bond lengths



Bond angles

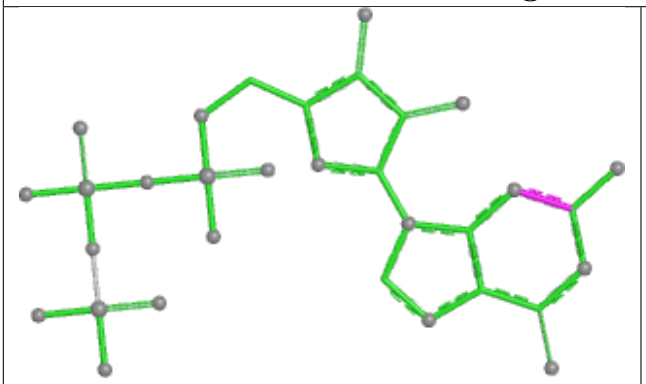


Torsions

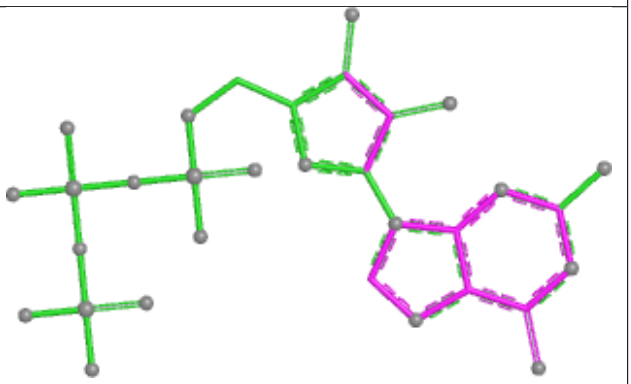


Rings

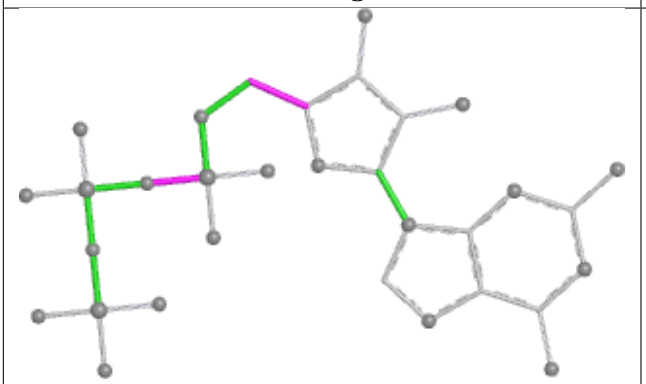
Ligand GTP II 501



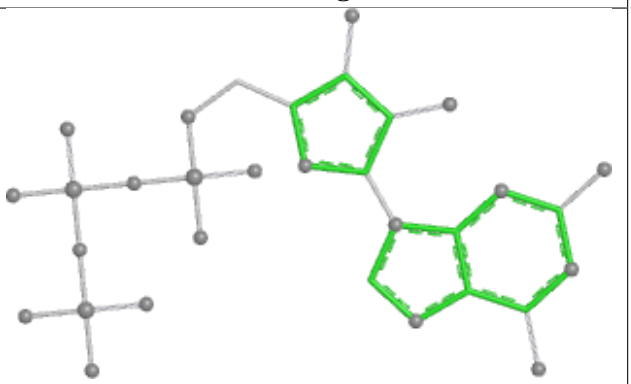
Bond lengths



Bond angles

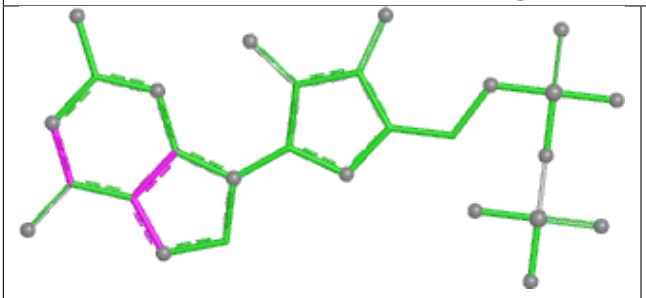


Torsions

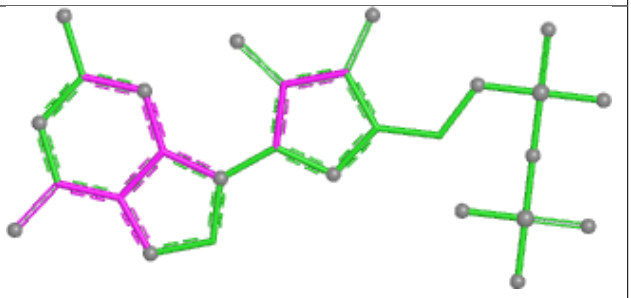


Rings

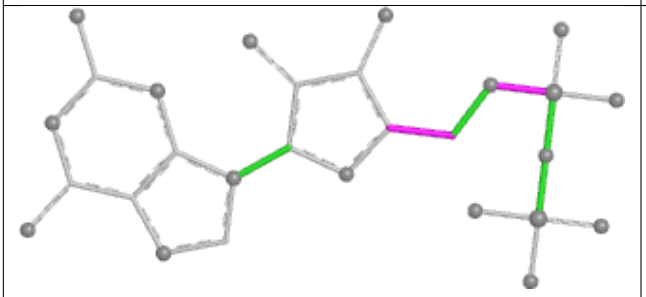
Ligand GDP OJ 500



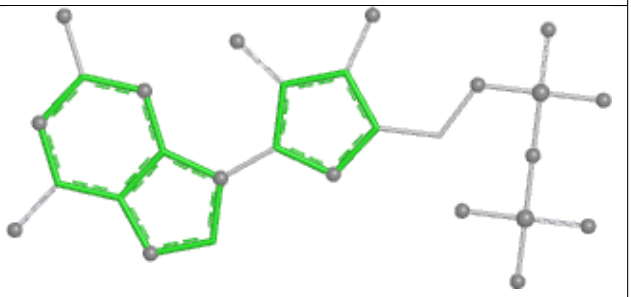
Bond lengths



Bond angles

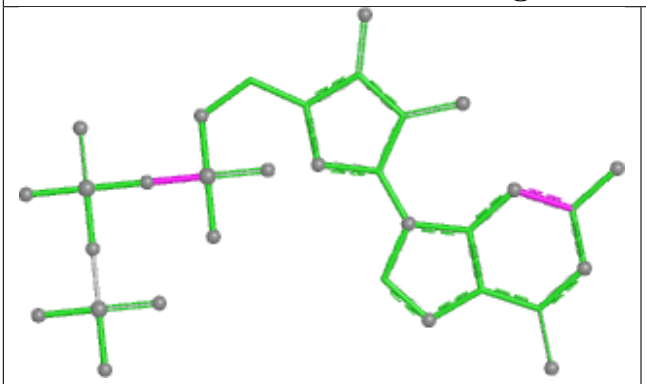


Torsions

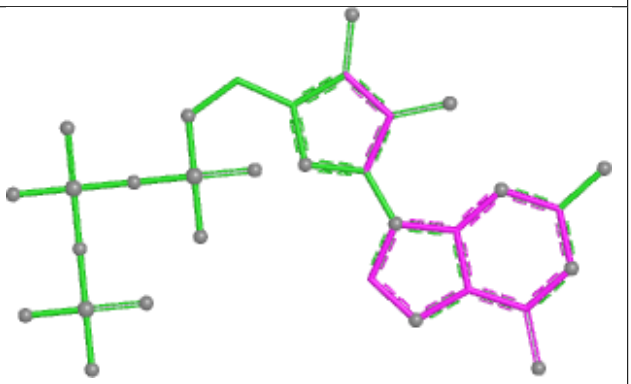


Rings

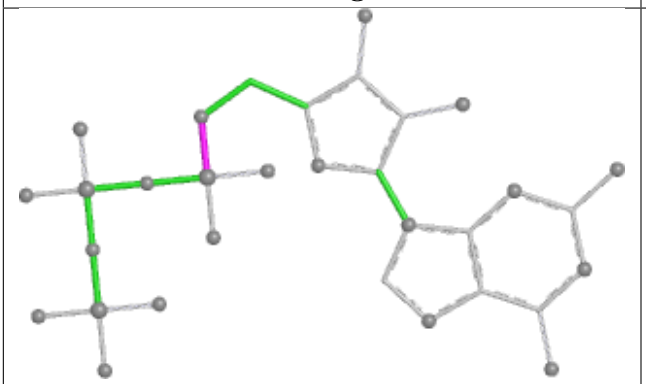
Ligand GTP LB 501



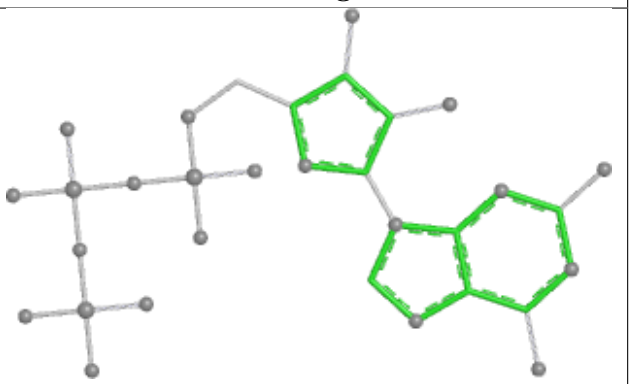
Bond lengths



Bond angles

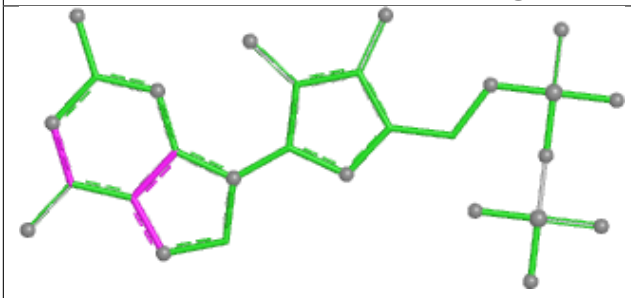


Torsions

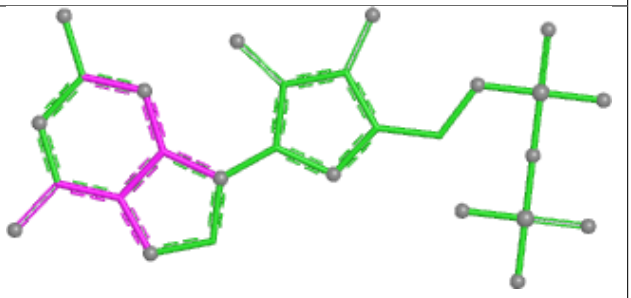


Rings

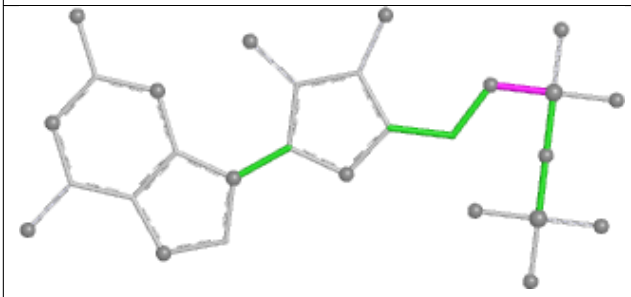
Ligand GDP PT 500



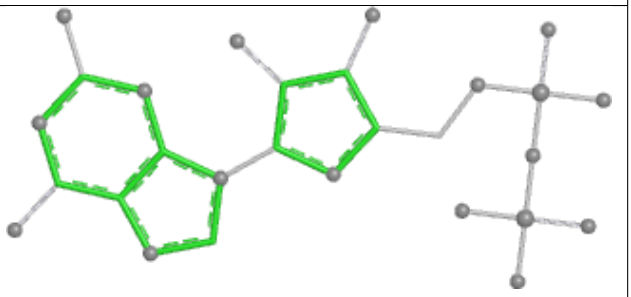
Bond lengths



Bond angles

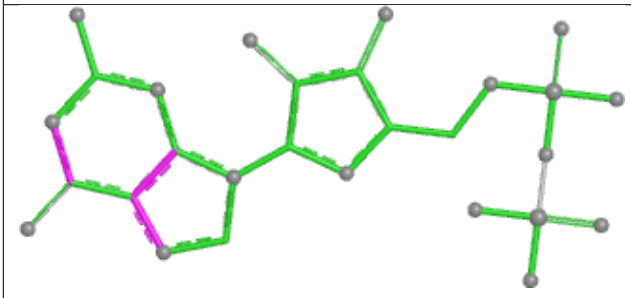


Torsions

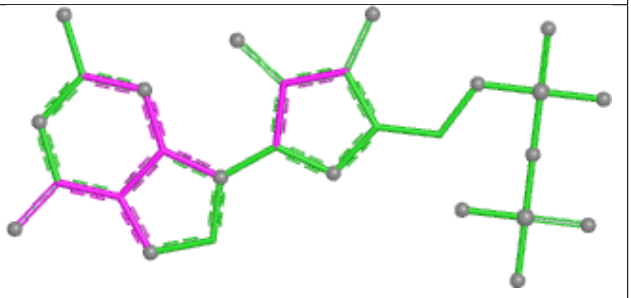


Rings

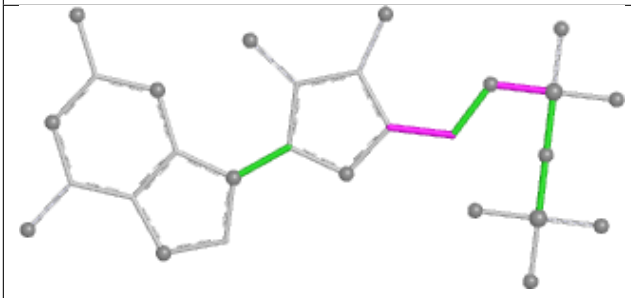
Ligand GDP CI 500



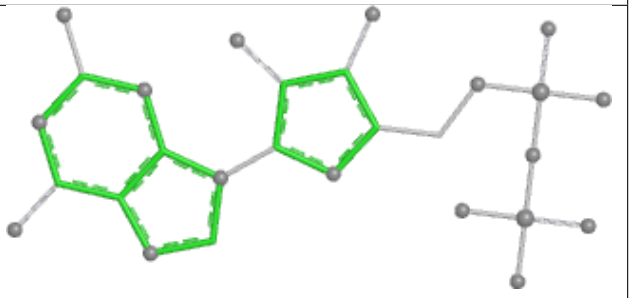
Bond lengths



Bond angles

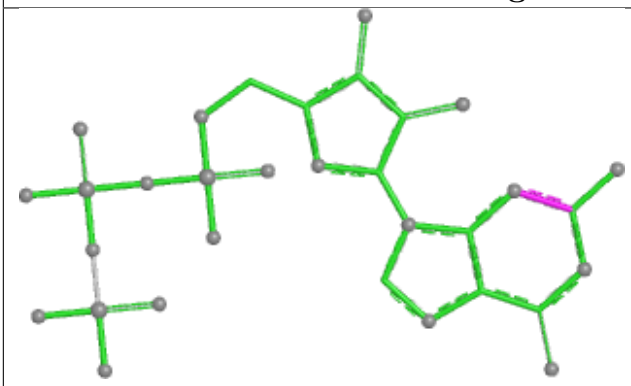


Torsions

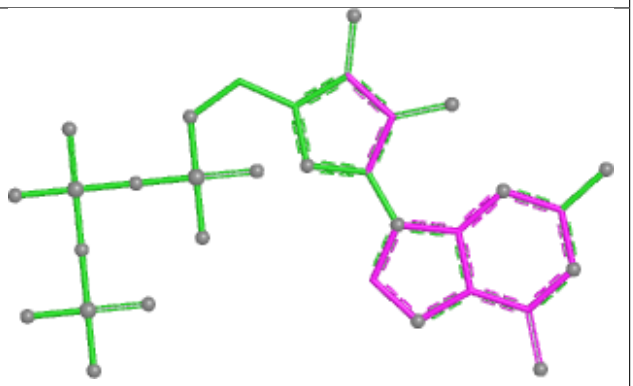


Rings

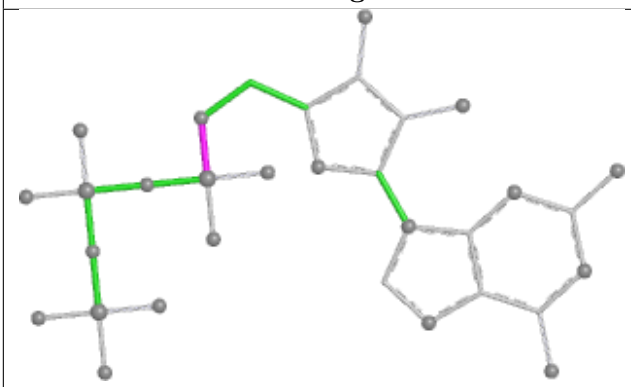
Ligand GTP UO 501



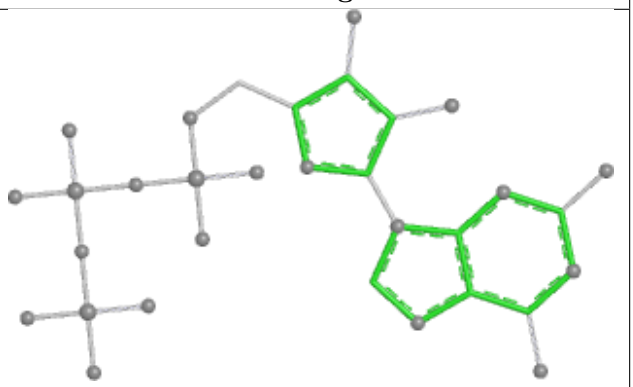
Bond lengths



Bond angles

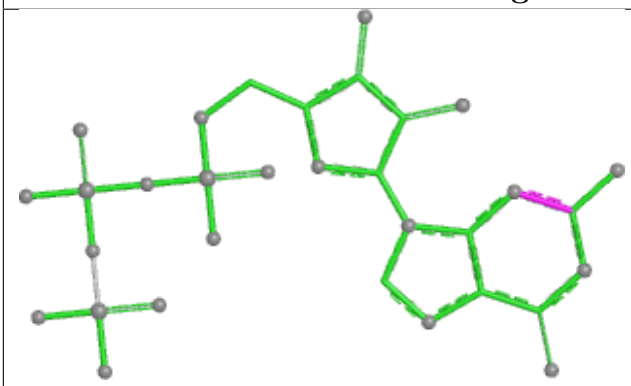


Torsions

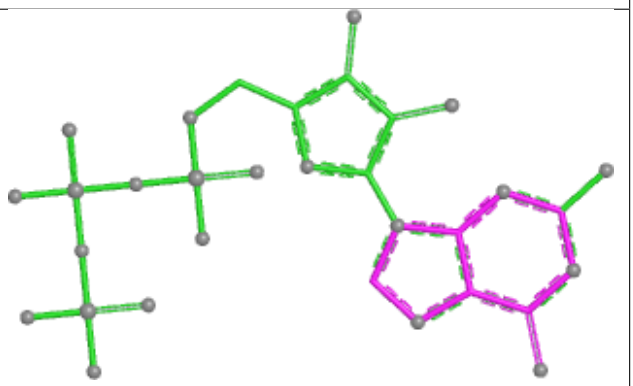


Rings

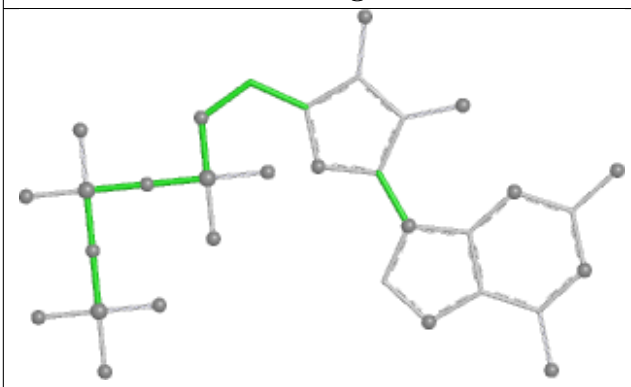
Ligand GTP PA 501



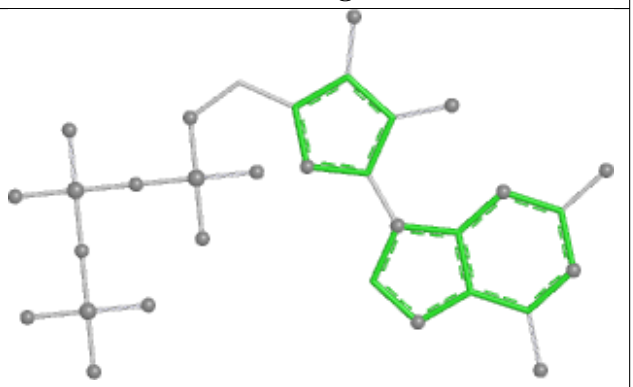
Bond lengths



Bond angles

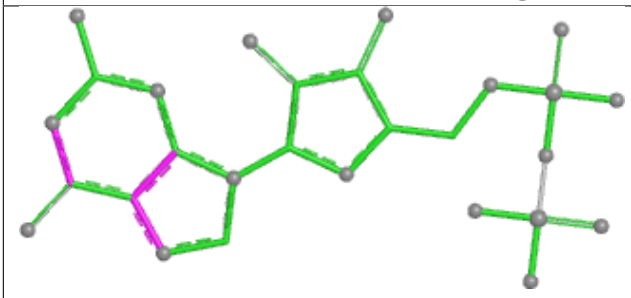


Torsions

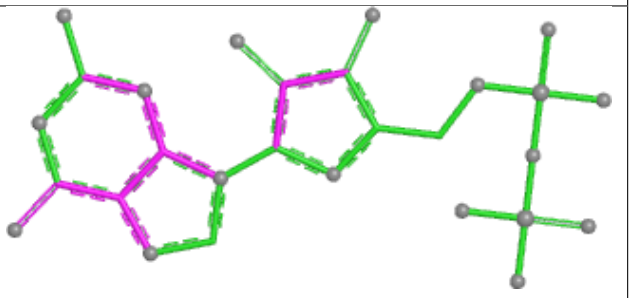


Rings

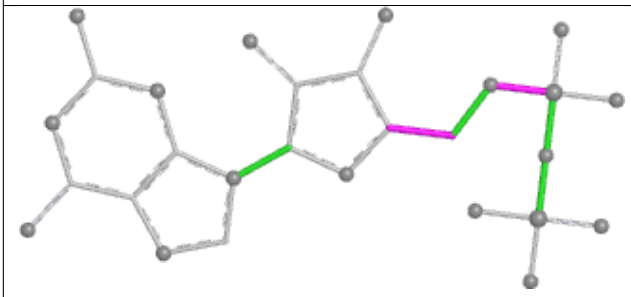
Ligand GDP IH 500



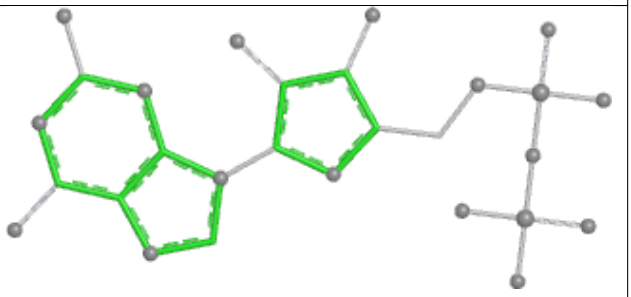
Bond lengths



Bond angles

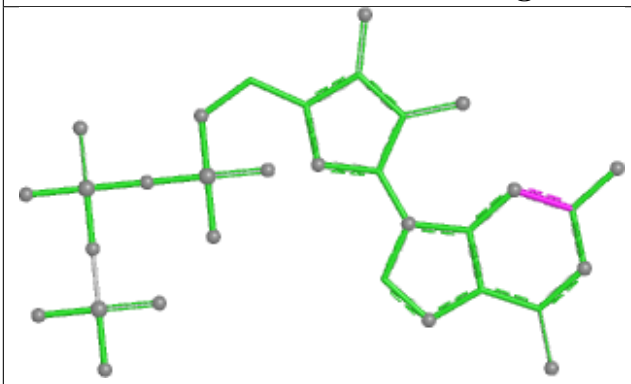


Torsions

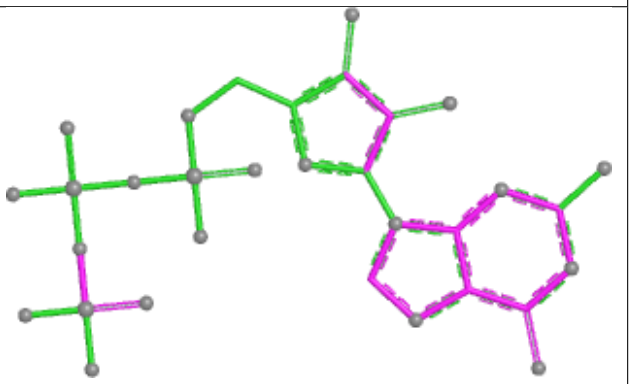


Rings

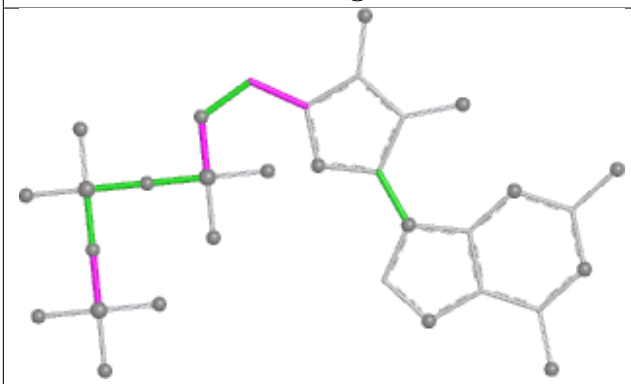
Ligand GTP SS 501



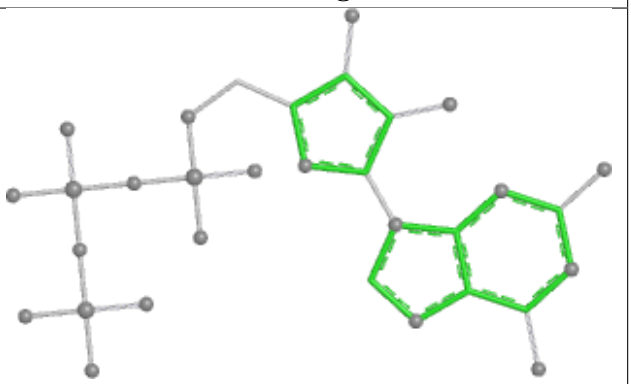
Bond lengths



Bond angles

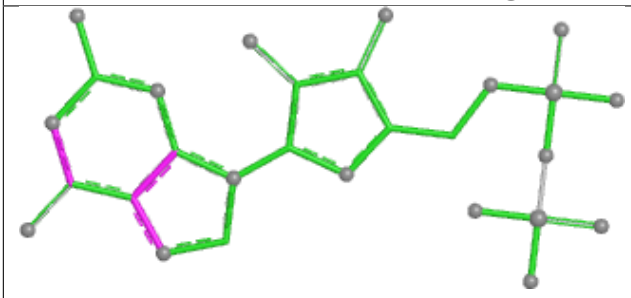


Torsions

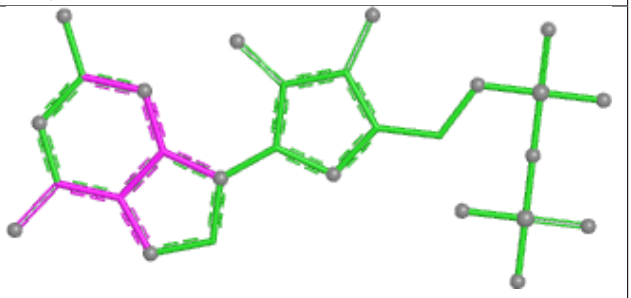


Rings

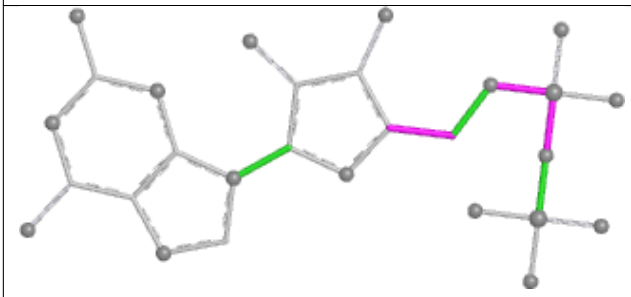
Ligand GDP QW 500



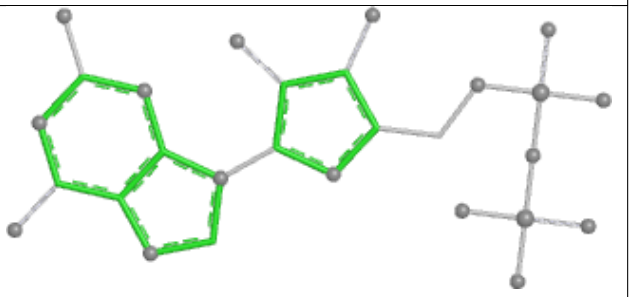
Bond lengths



Bond angles

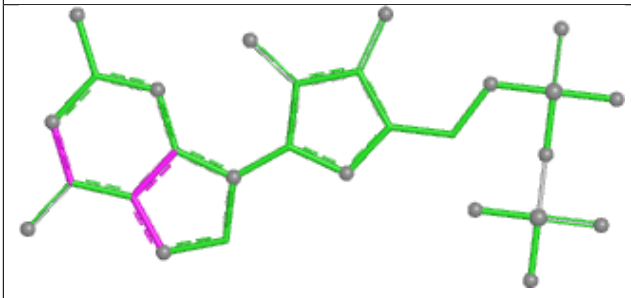


Torsions

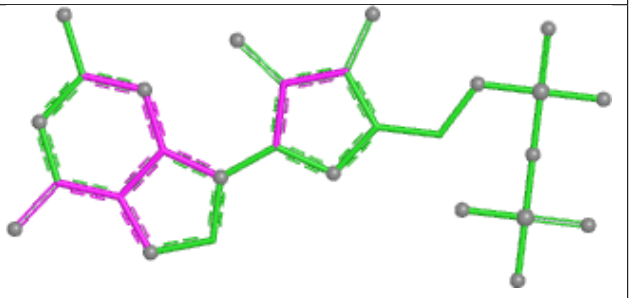


Rings

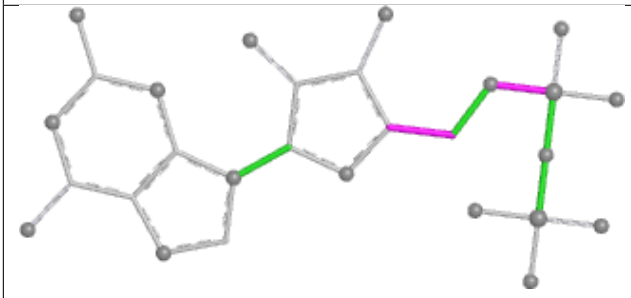
Ligand GDP NH 500



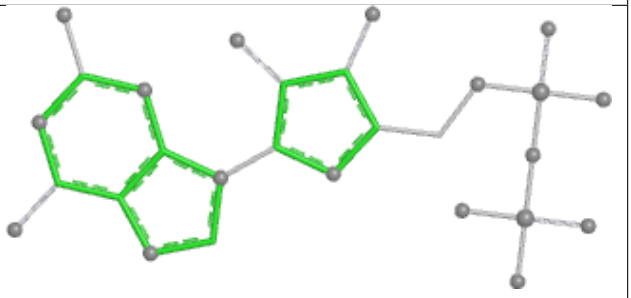
Bond lengths



Bond angles

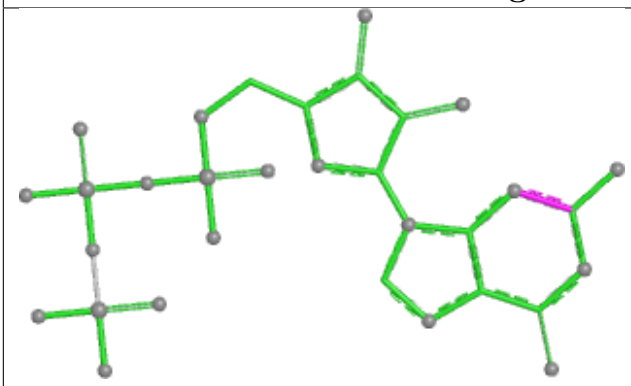


Torsions

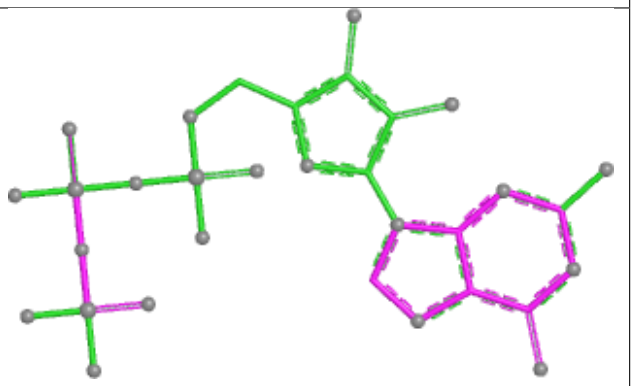


Rings

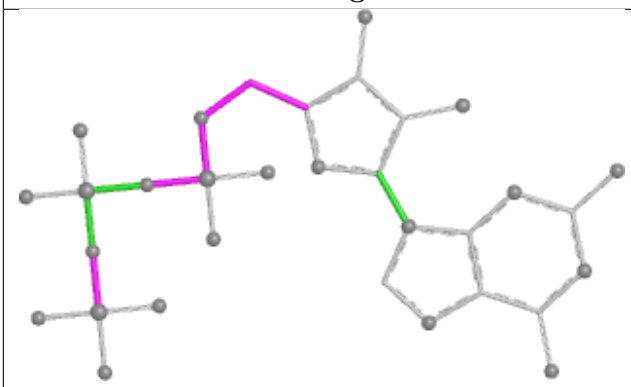
Ligand GTP DX 501



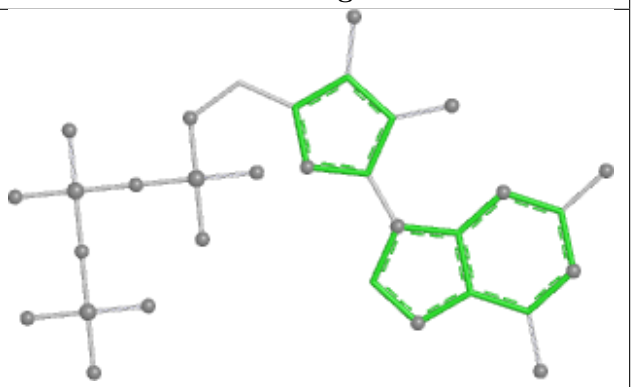
Bond lengths



Bond angles

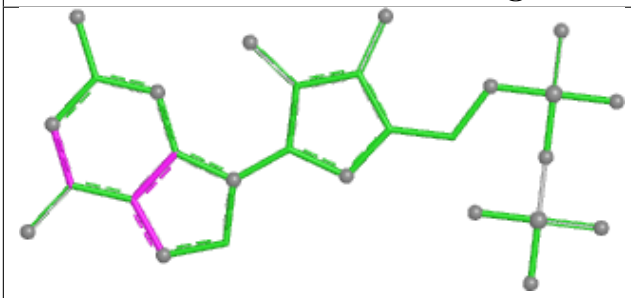


Torsions

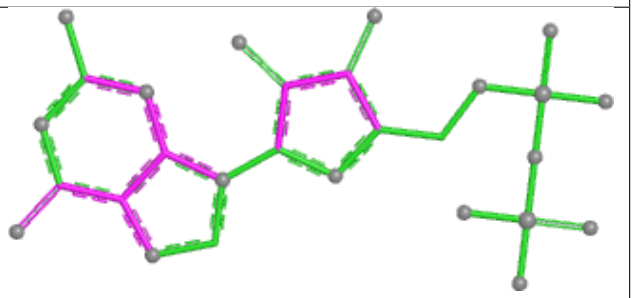


Rings

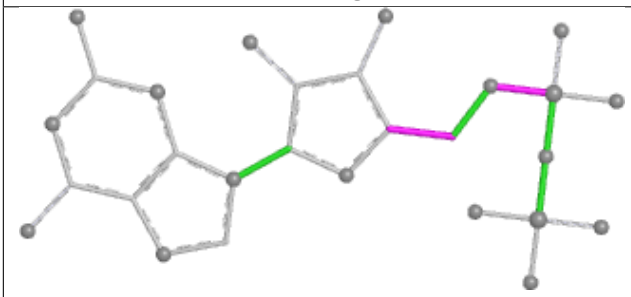
Ligand GDP AD 500



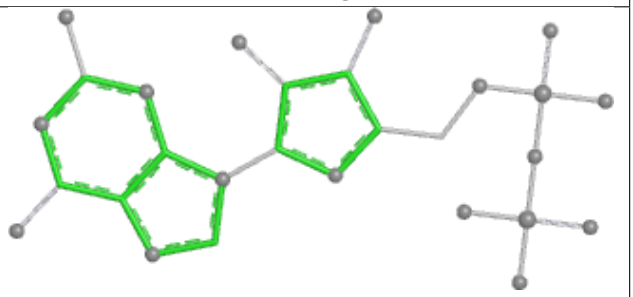
Bond lengths



Bond angles

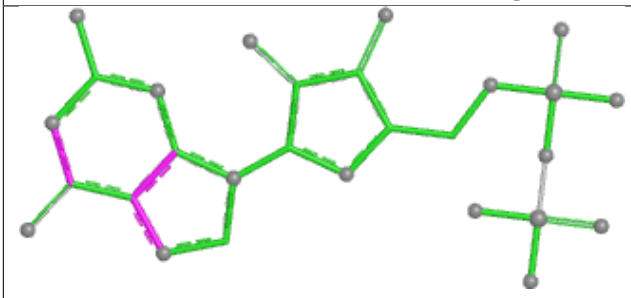


Torsions

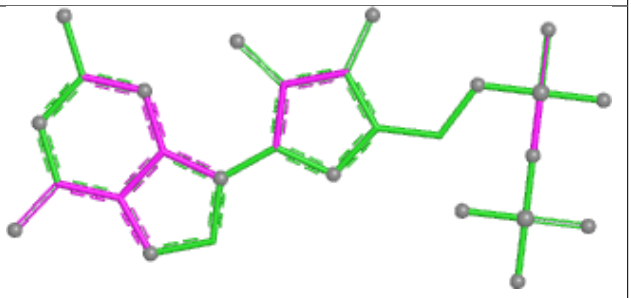


Rings

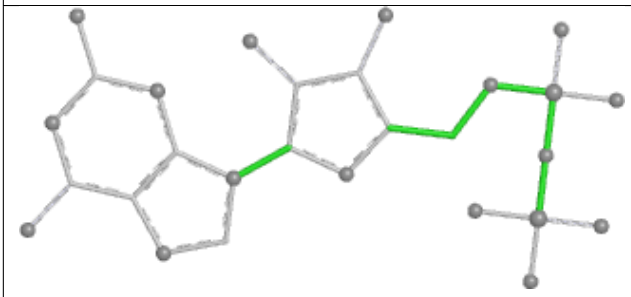
Ligand GDP NP 500



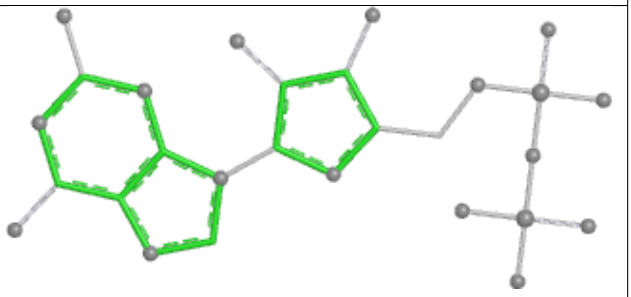
Bond lengths



Bond angles

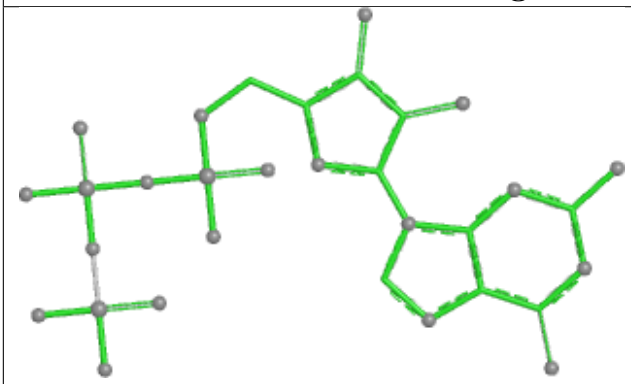


Torsions

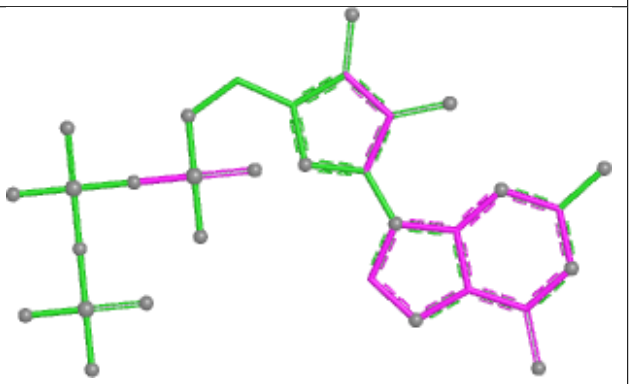


Rings

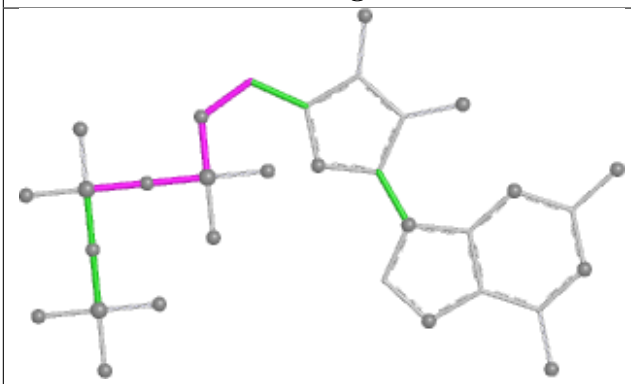
Ligand GTP EG 501



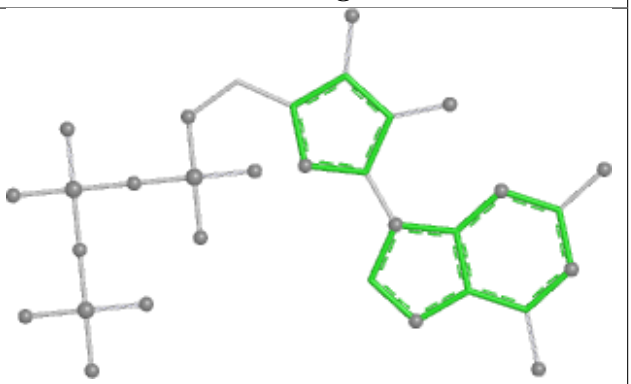
Bond lengths



Bond angles

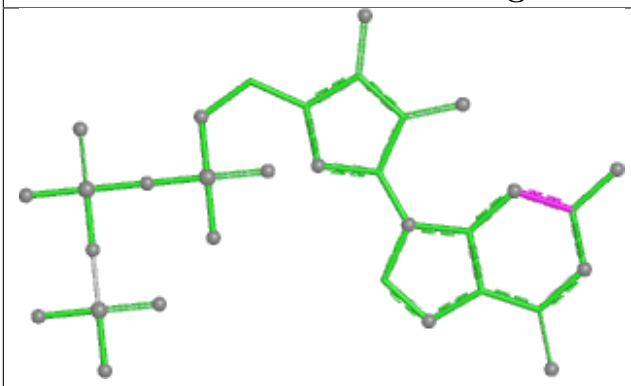


Torsions

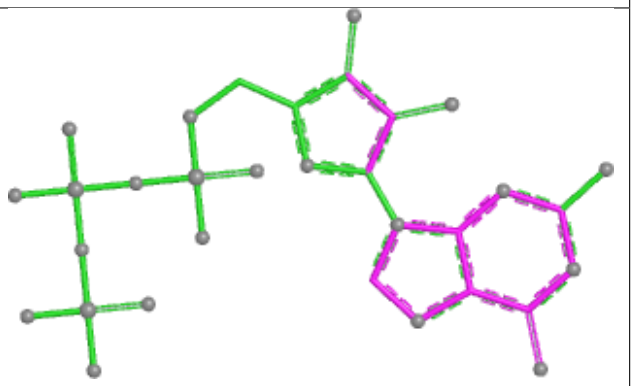


Rings

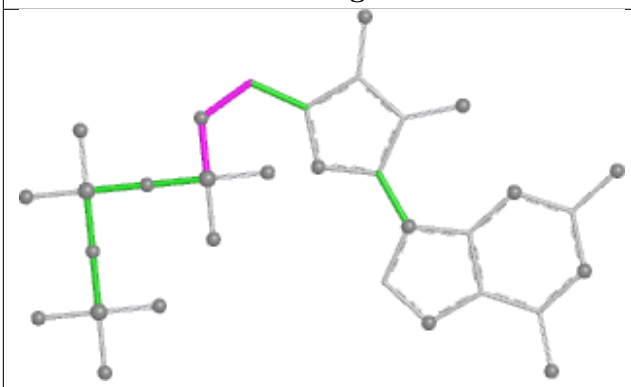
Ligand GTP HK 501



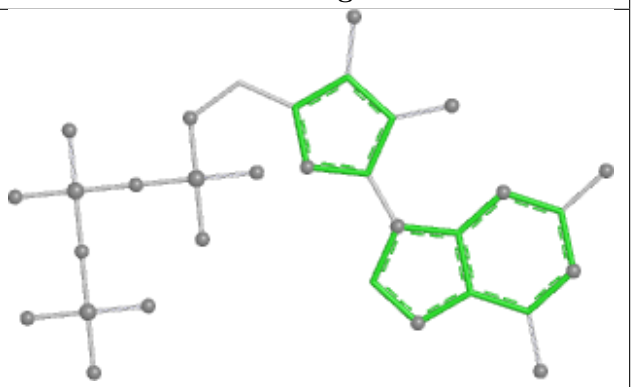
Bond lengths



Bond angles

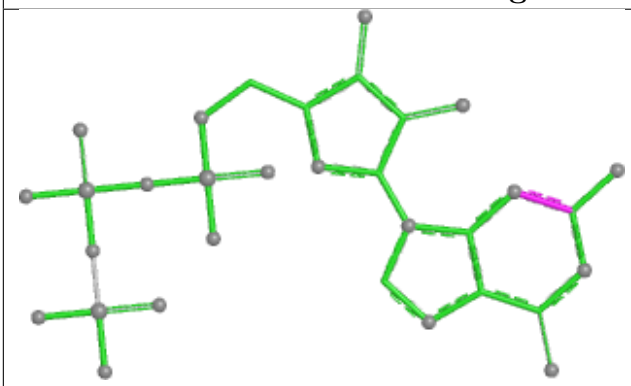


Torsions

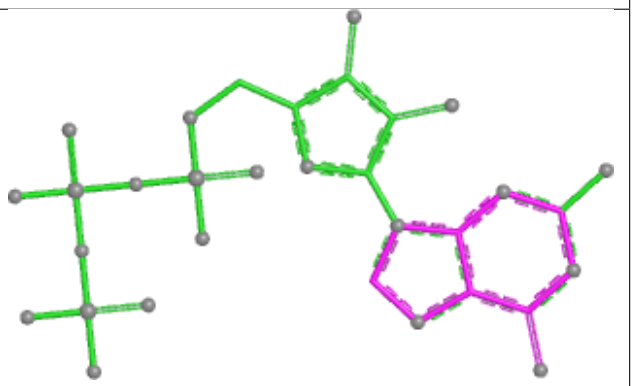


Rings

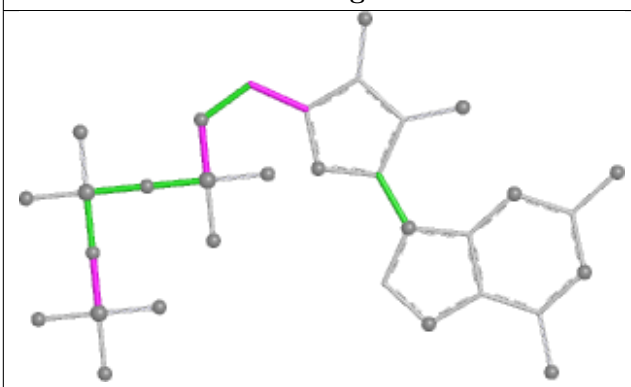
Ligand GTP CO 501



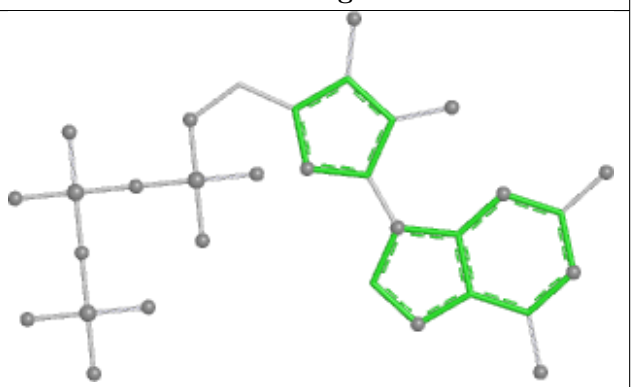
Bond lengths



Bond angles

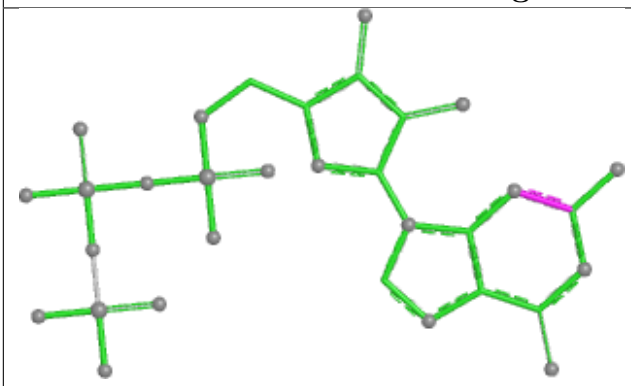


Torsions

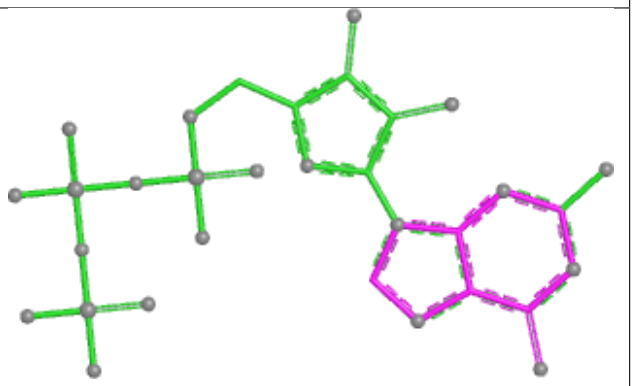


Rings

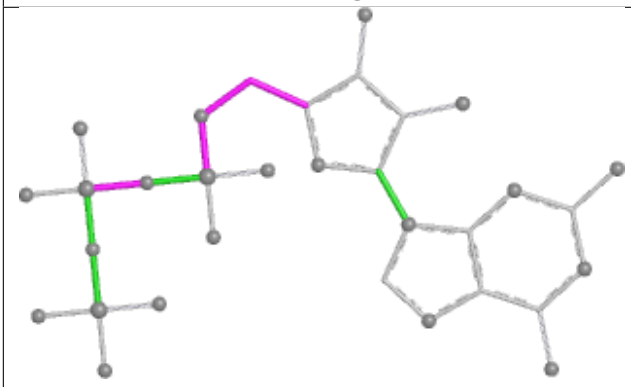
Ligand GTP AS 501



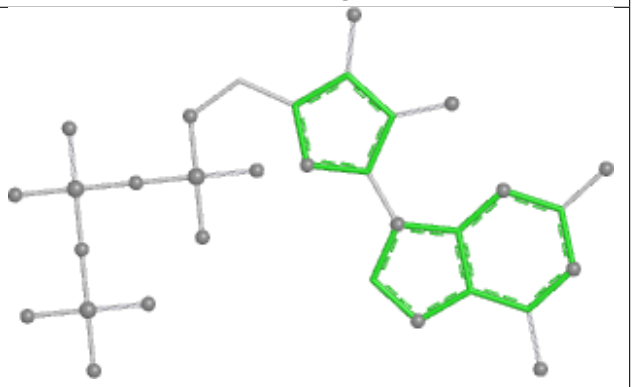
Bond lengths



Bond angles

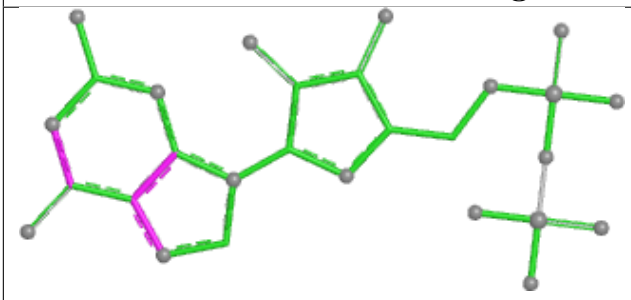


Torsions

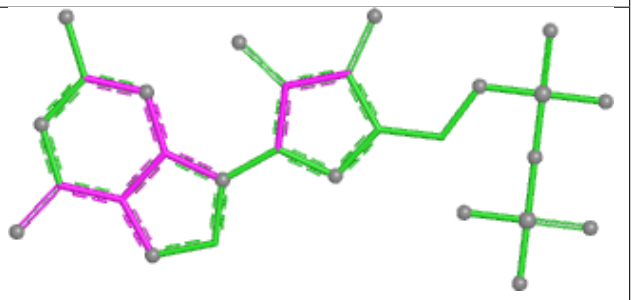


Rings

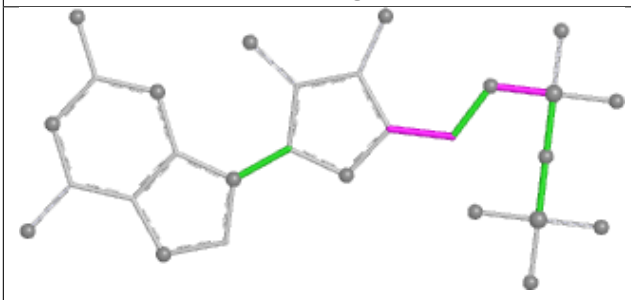
Ligand GDP SN 501



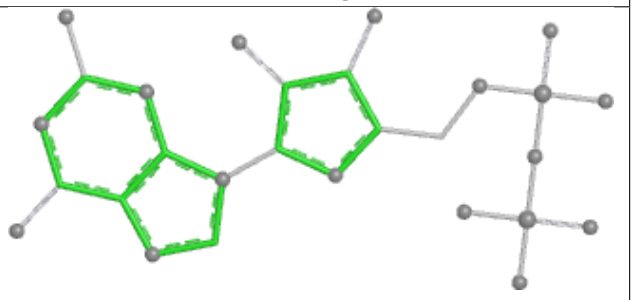
Bond lengths



Bond angles

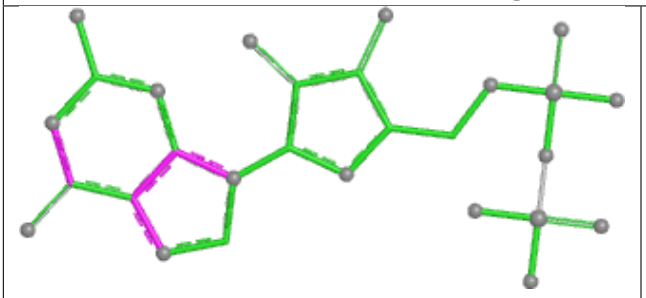


Torsions

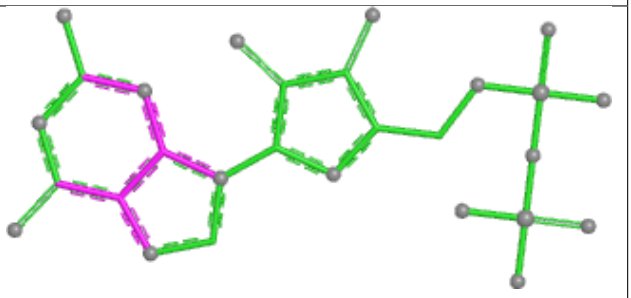


Rings

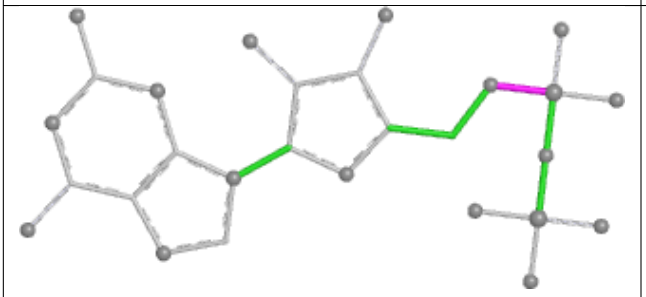
Ligand GDP BV 500



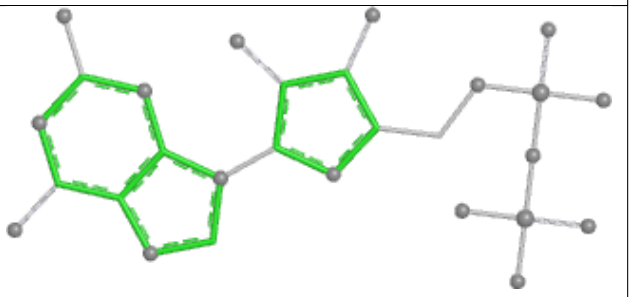
Bond lengths



Bond angles

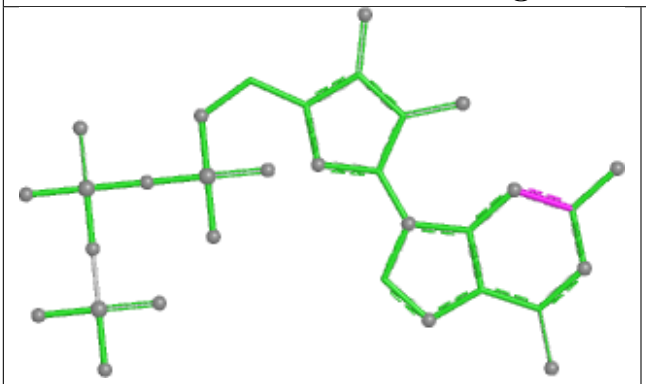


Torsions

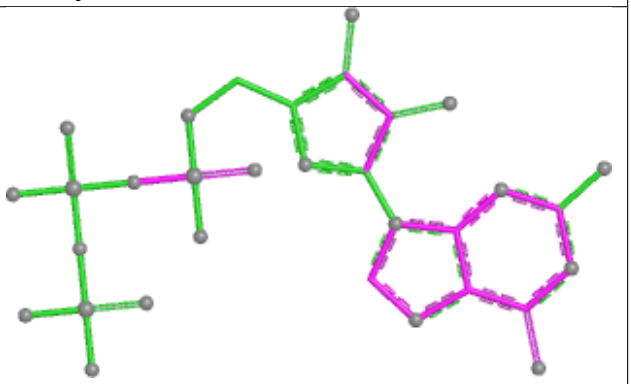


Rings

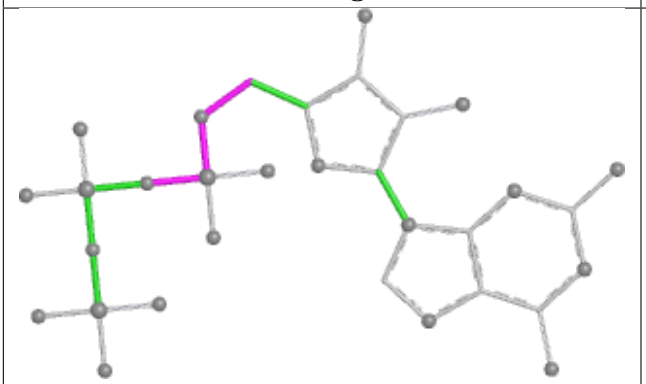
Ligand GTP SQ 501



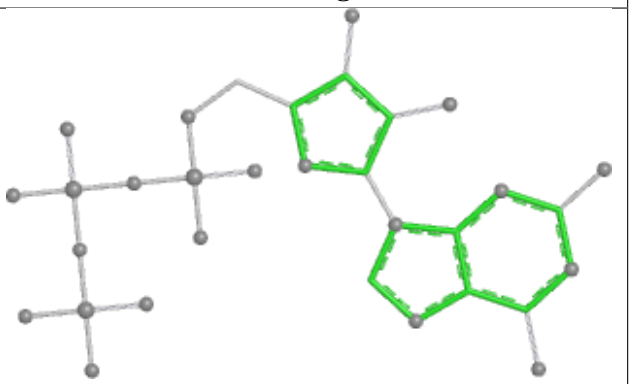
Bond lengths



Bond angles

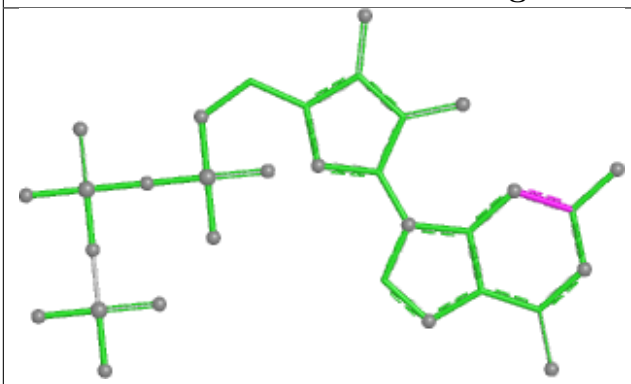


Torsions

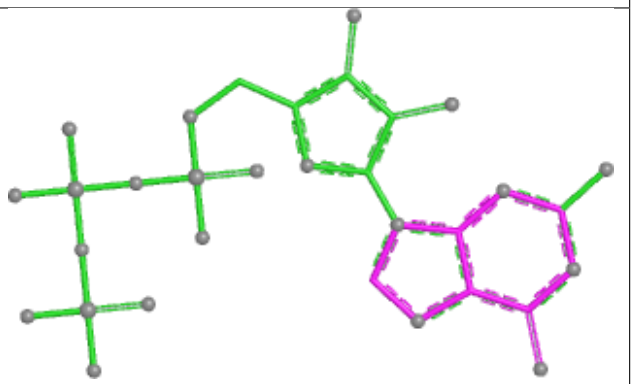


Rings

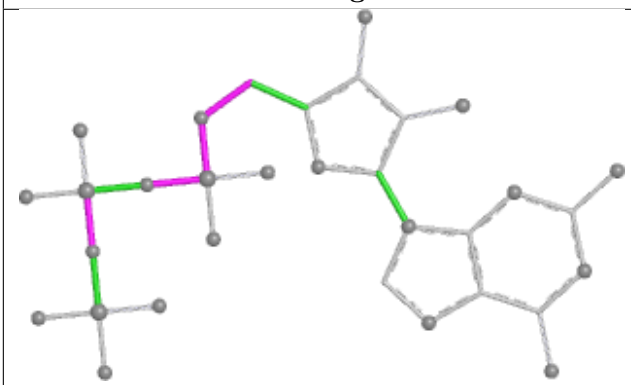
Ligand GTP OY 501



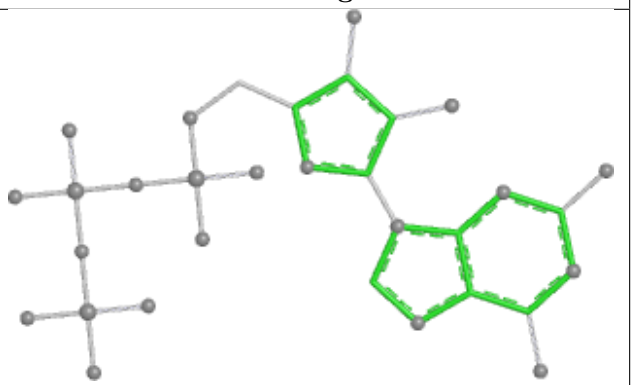
Bond lengths



Bond angles

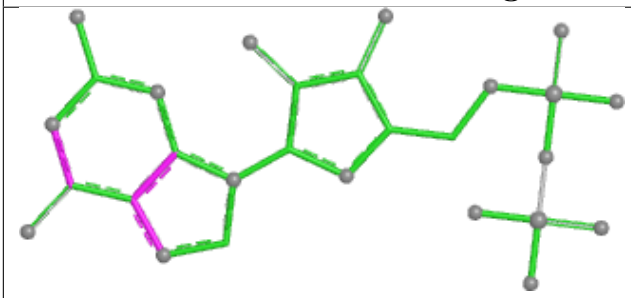


Torsions

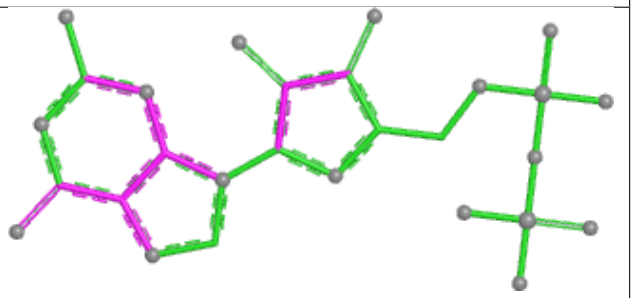


Rings

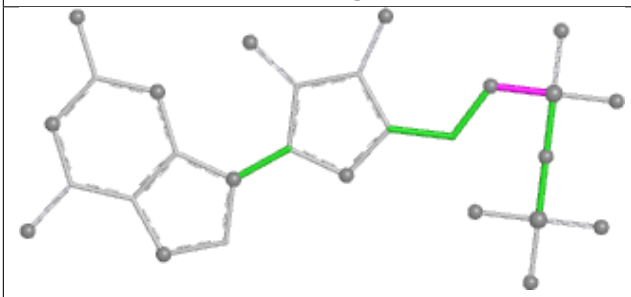
Ligand GDP WR 501



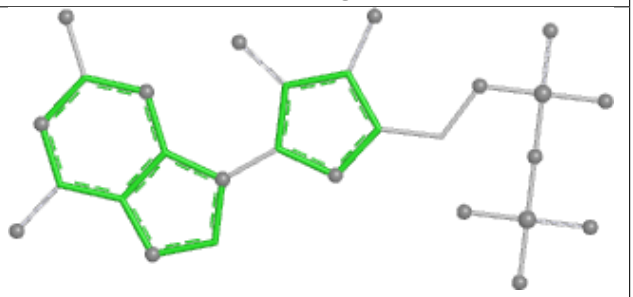
Bond lengths



Bond angles

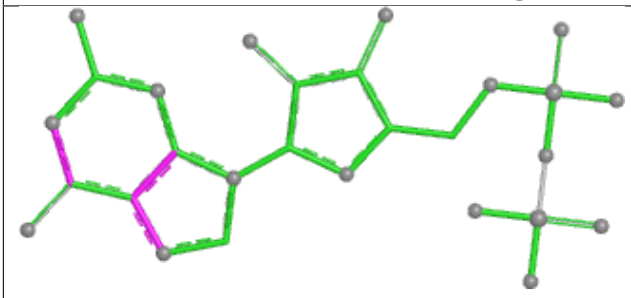


Torsions

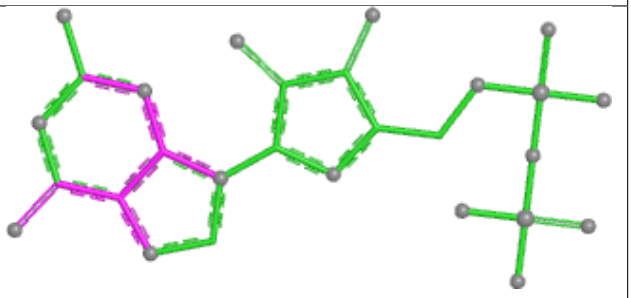


Rings

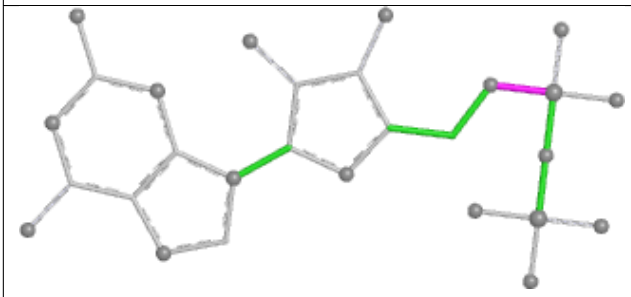
Ligand GDP LC 500



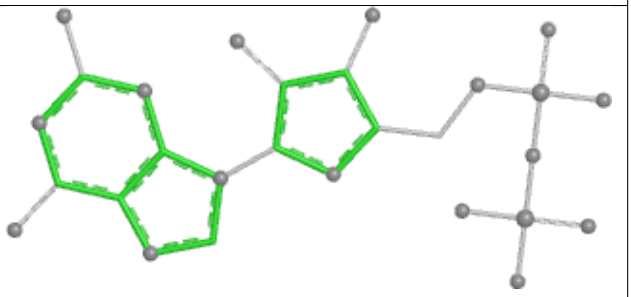
Bond lengths



Bond angles

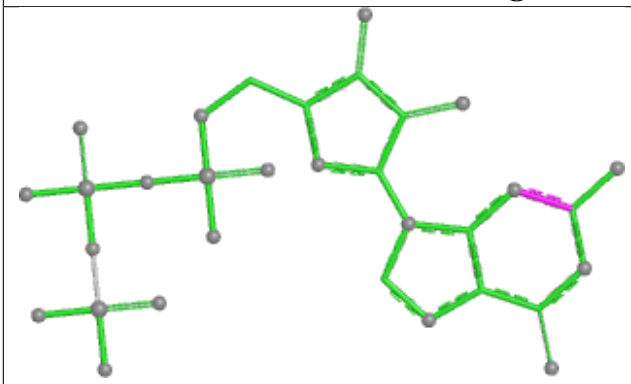


Torsions

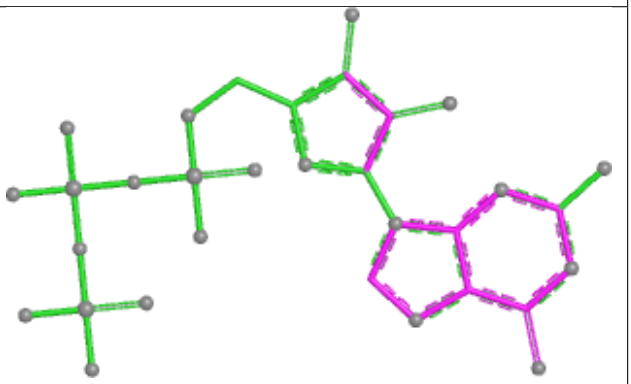


Rings

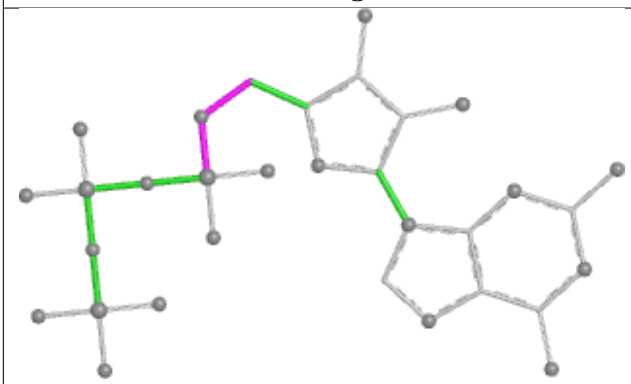
Ligand GTP HA 501



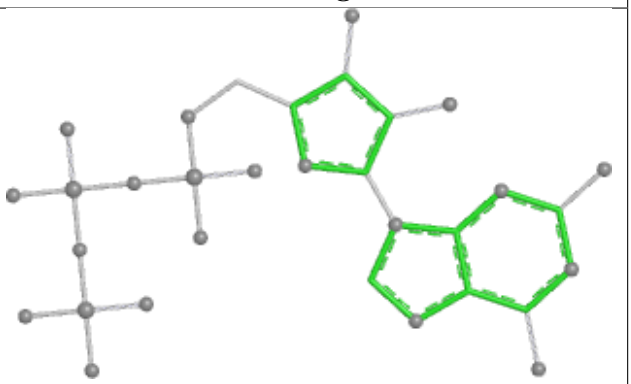
Bond lengths



Bond angles

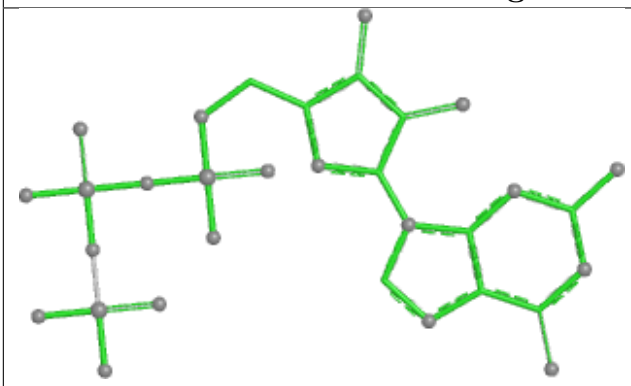


Torsions

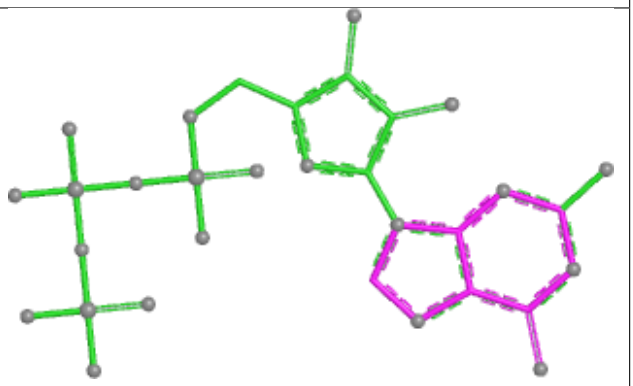


Rings

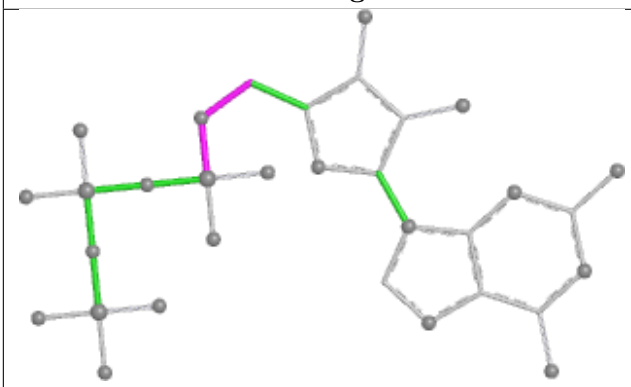
Ligand GTP FM 501



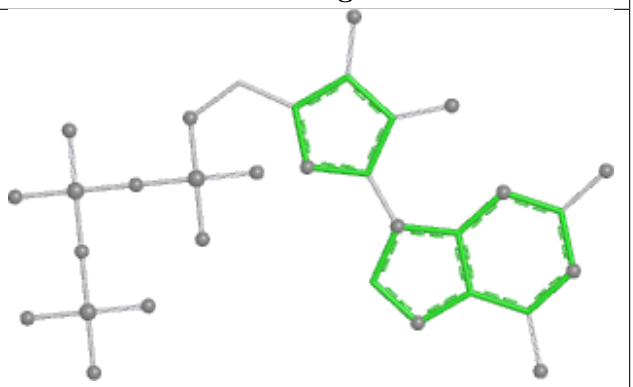
Bond lengths



Bond angles

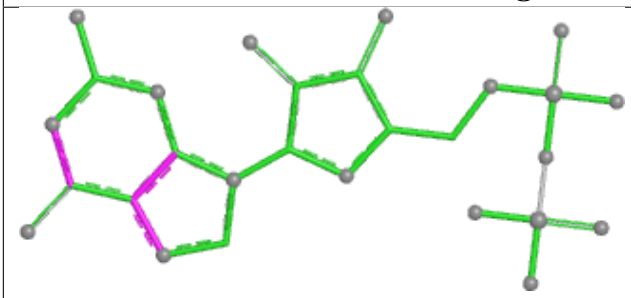


Torsions

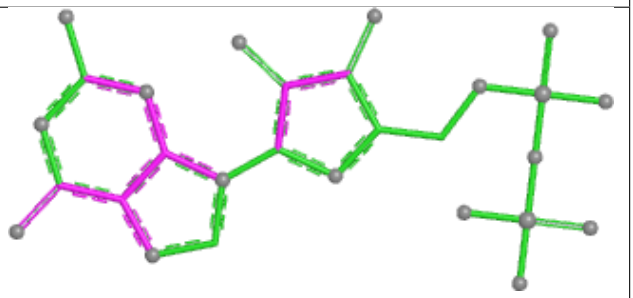


Rings

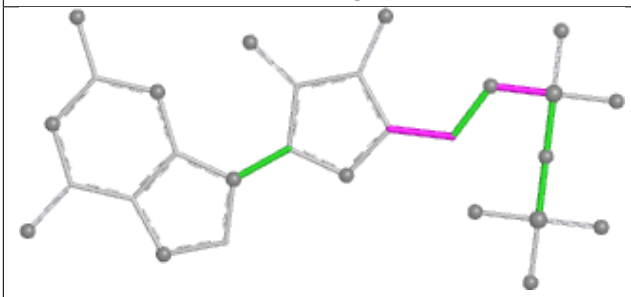
Ligand GDP SJ 501



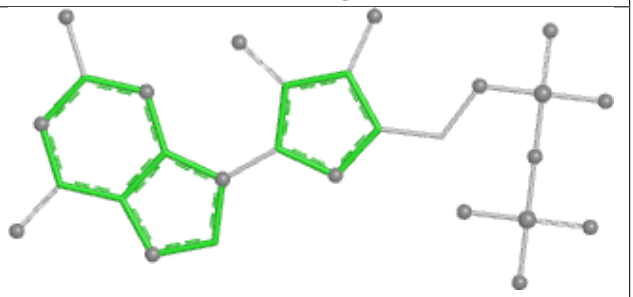
Bond lengths



Bond angles

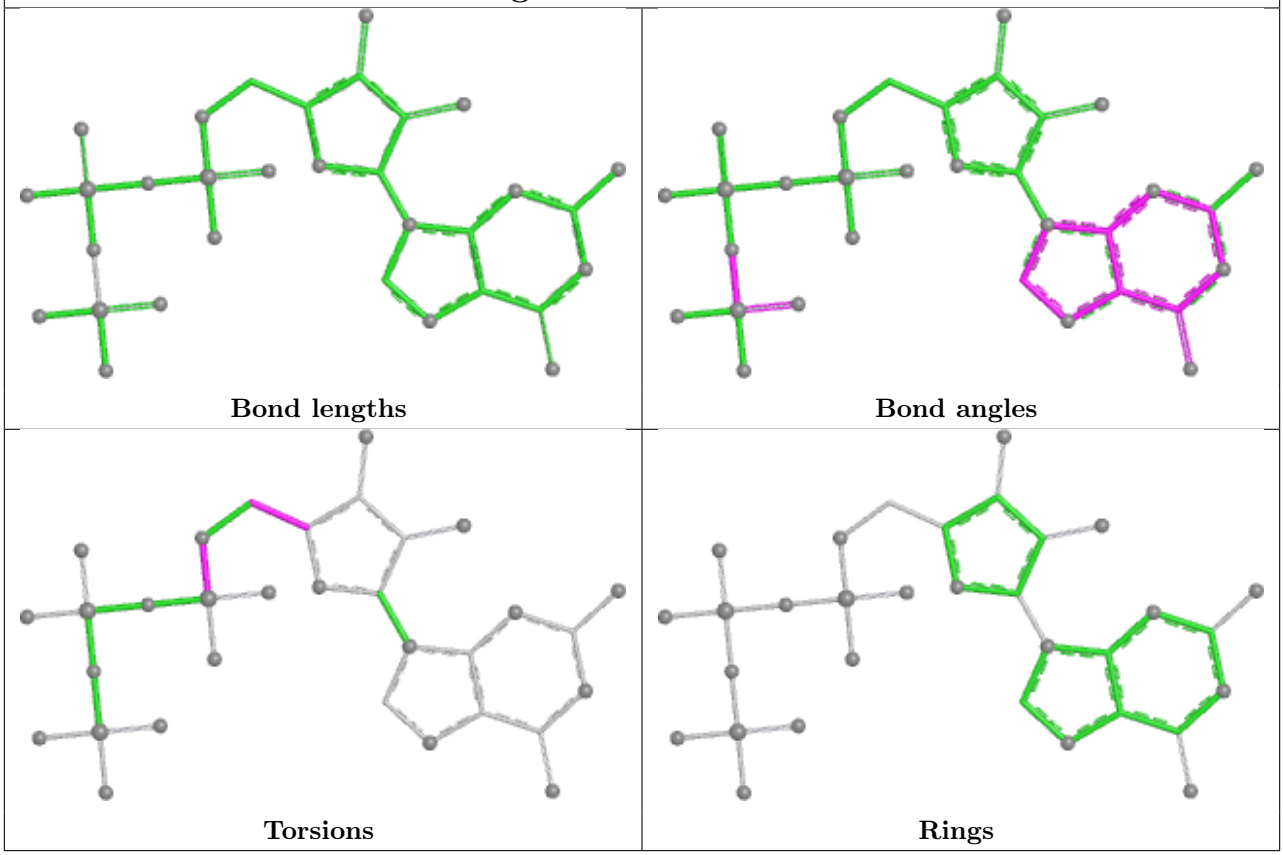


Torsions

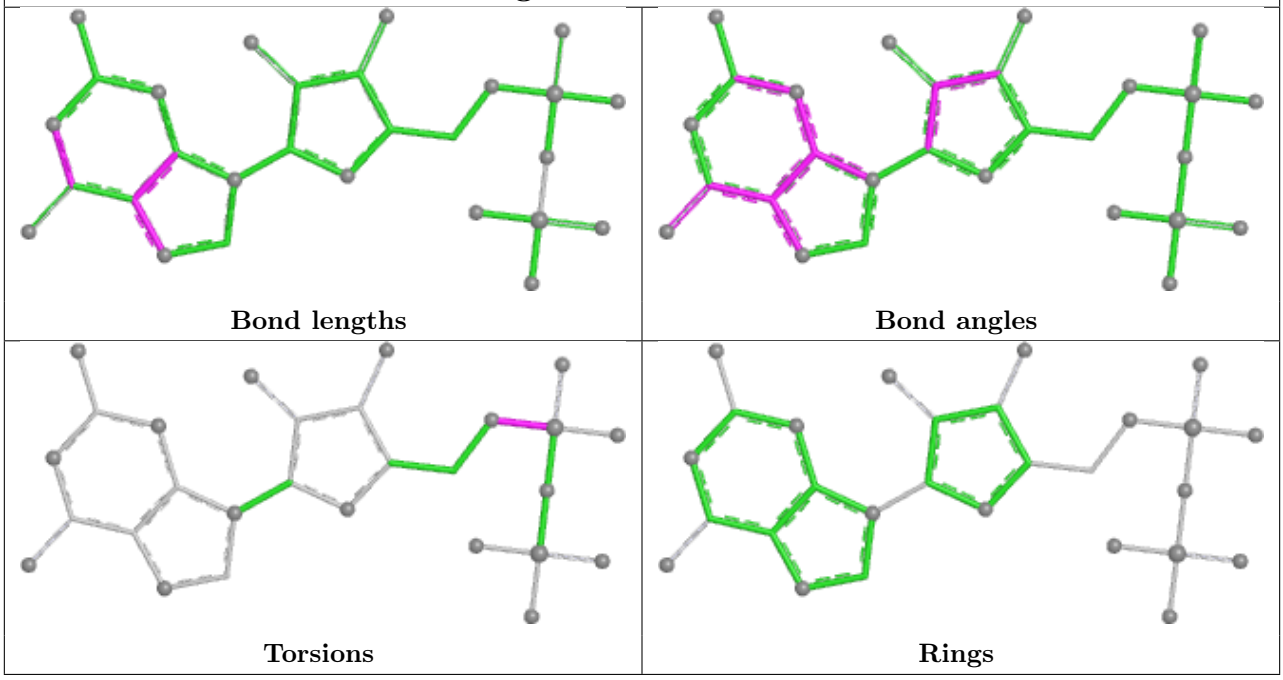


Rings

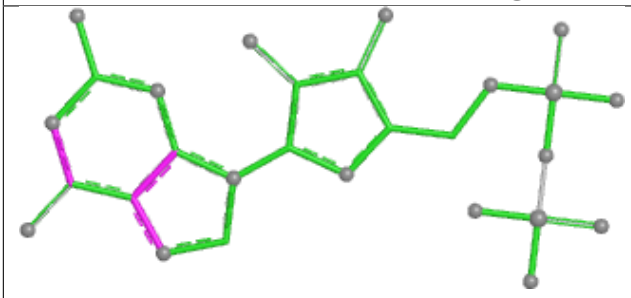
Ligand GTP EV 501



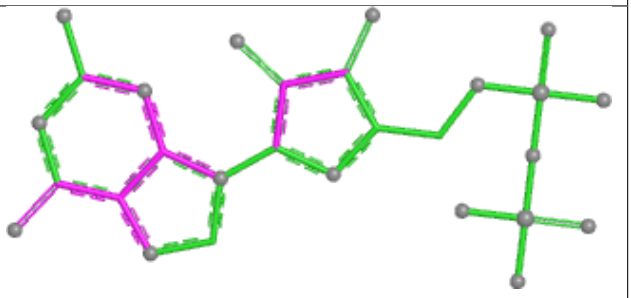
Ligand GDP IV 500



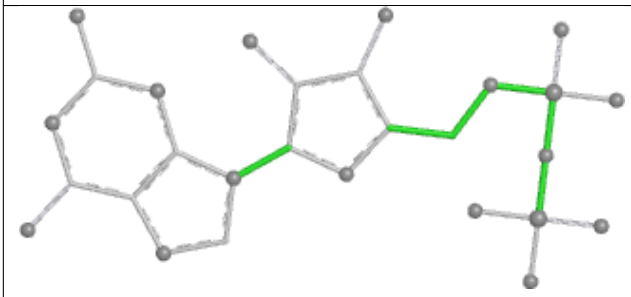
Ligand GDP TX 500



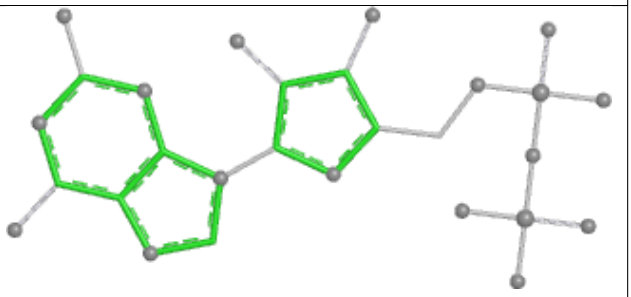
Bond lengths



Bond angles

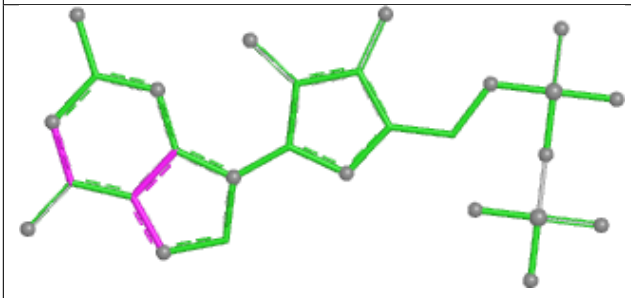


Torsions

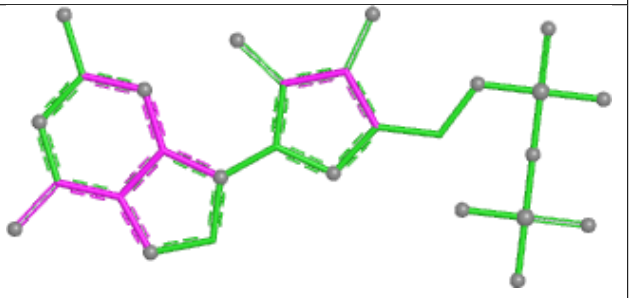


Rings

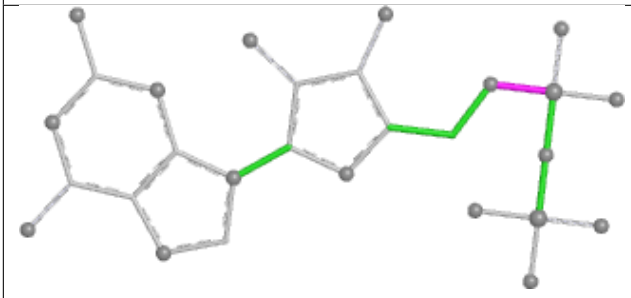
Ligand GDP CG 500



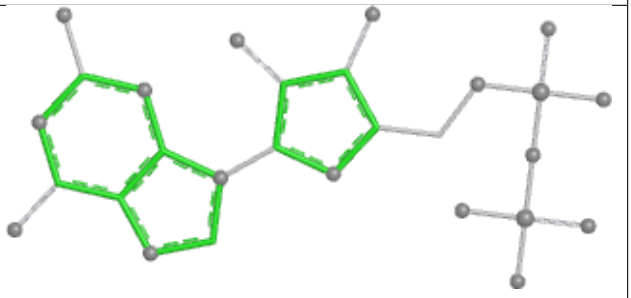
Bond lengths



Bond angles

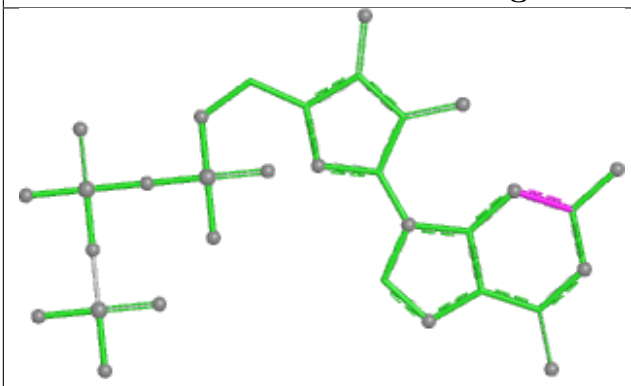


Torsions

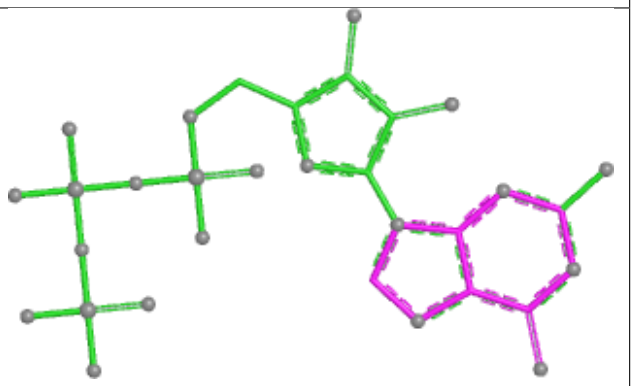


Rings

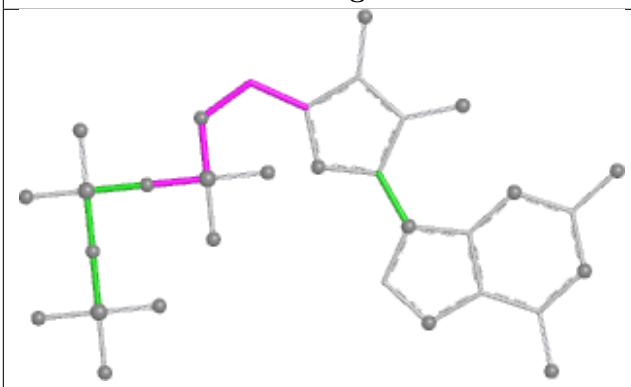
Ligand GTP AY 501



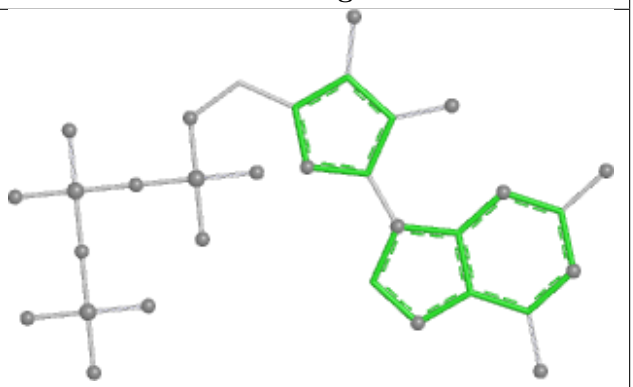
Bond lengths



Bond angles

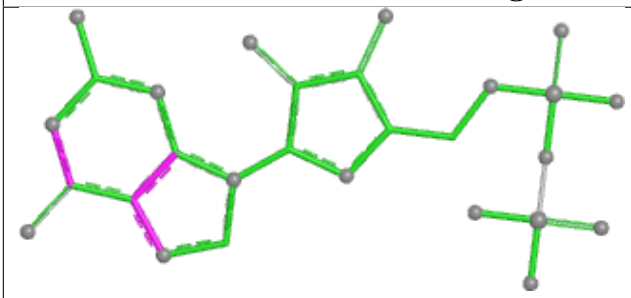


Torsions

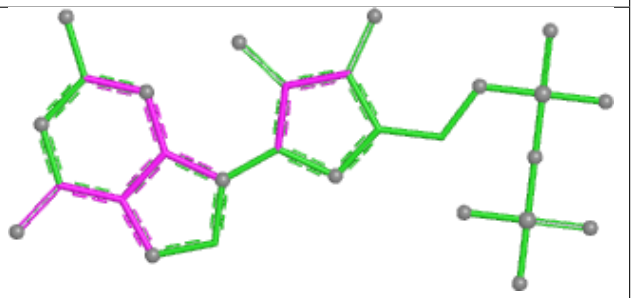


Rings

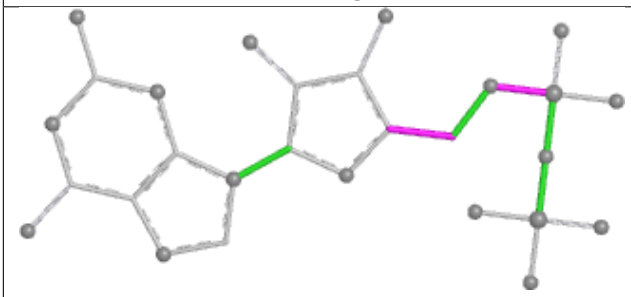
Ligand GDP NB 500



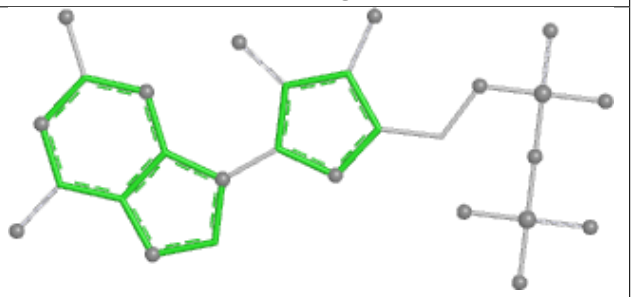
Bond lengths



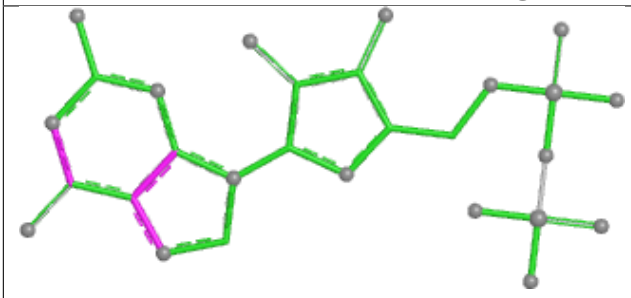
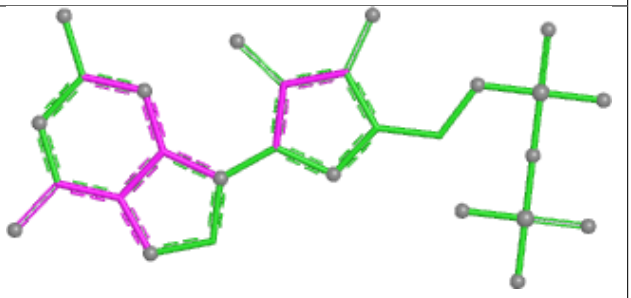
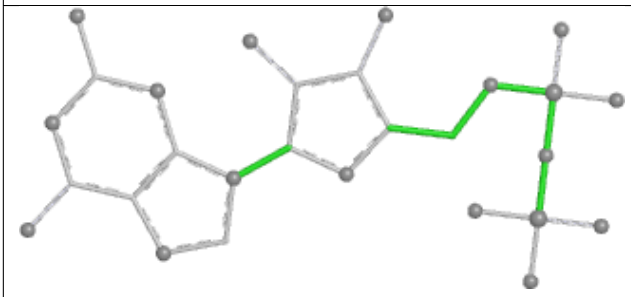
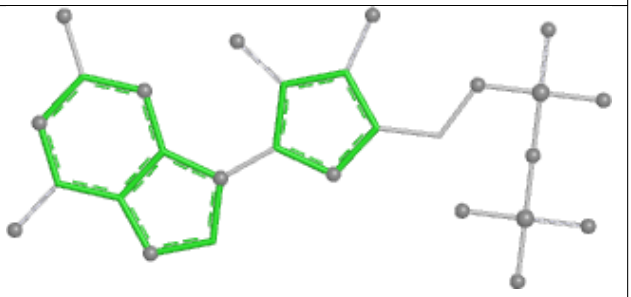
Bond angles

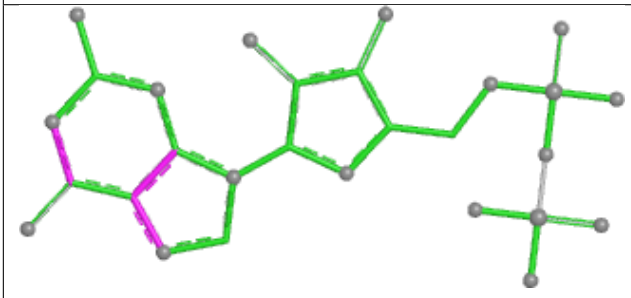
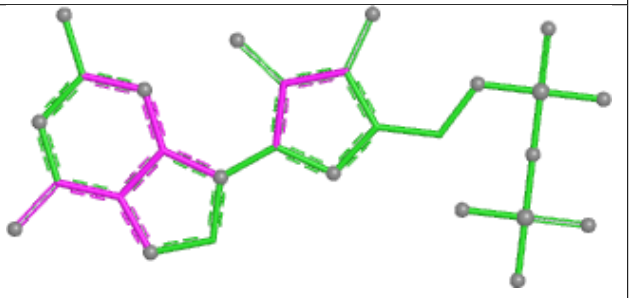
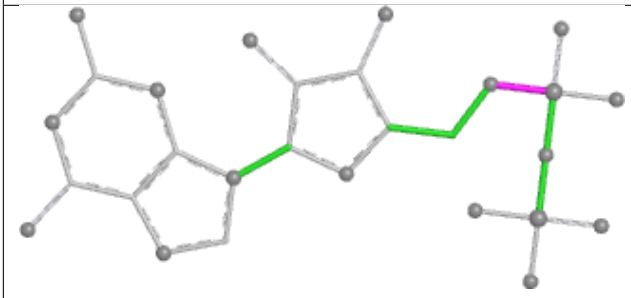
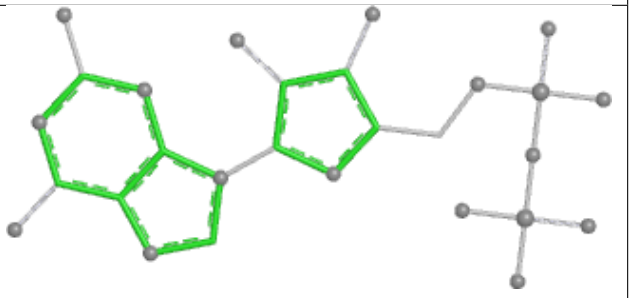


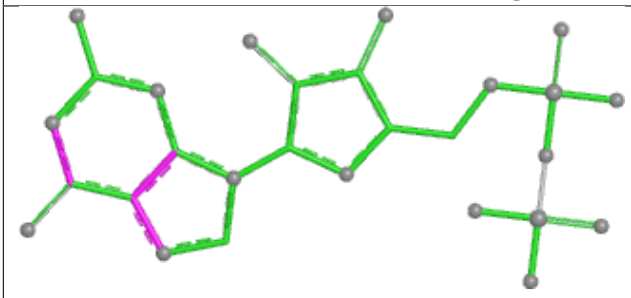
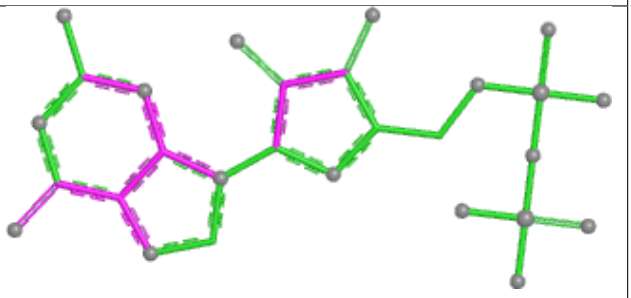
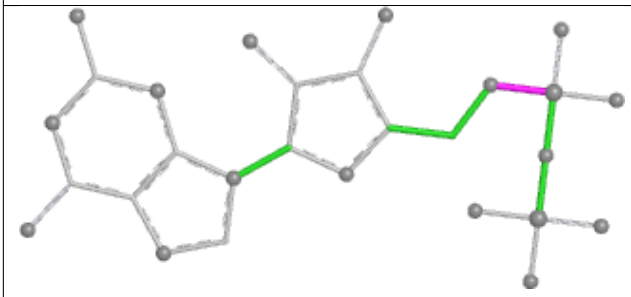
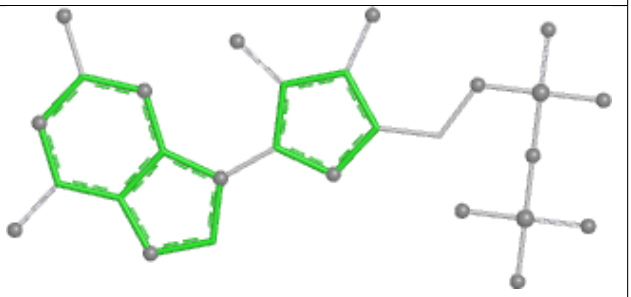
Torsions

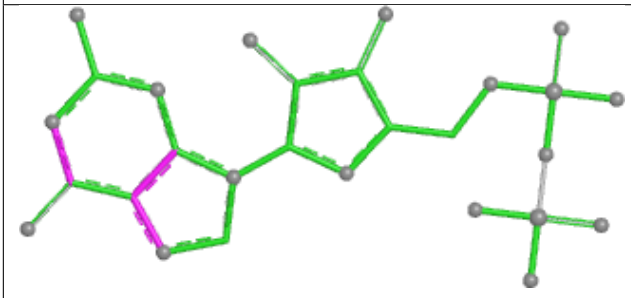
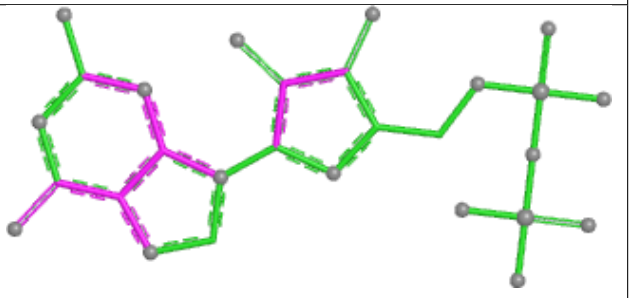
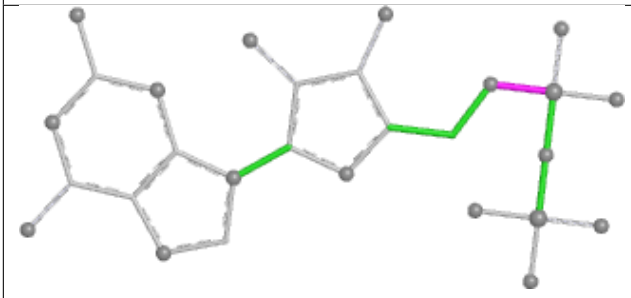
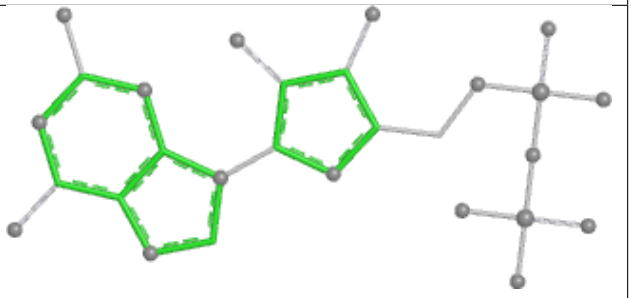


Rings

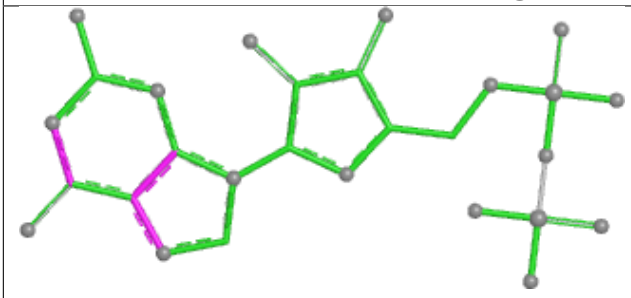
Ligand GDP IX 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP TN 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

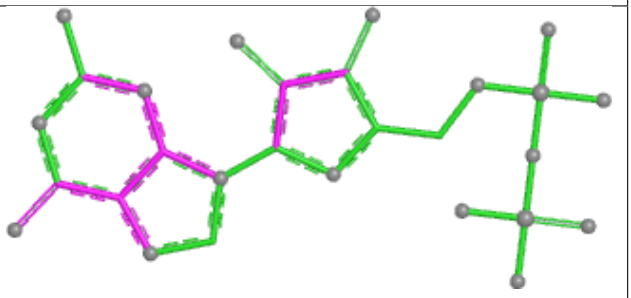
Ligand GDP HT 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP WJ 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

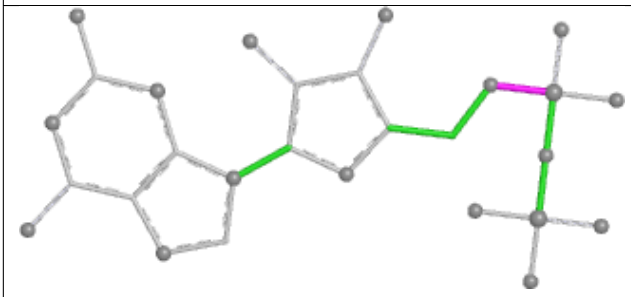
Ligand GDP FP 500



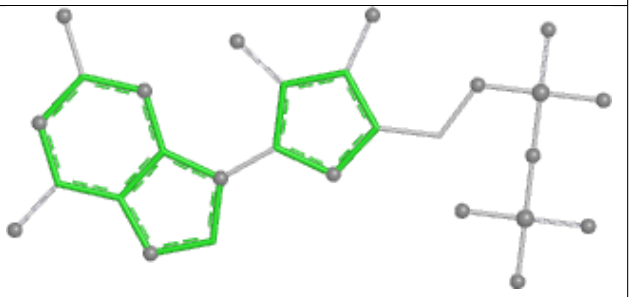
Bond lengths



Bond angles

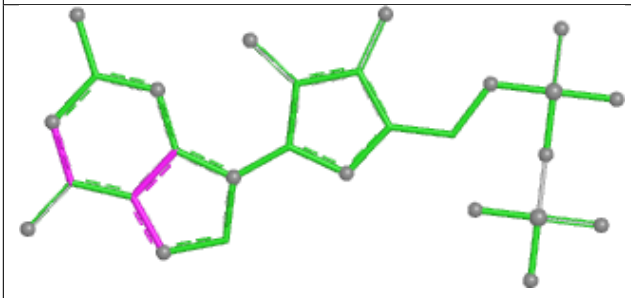


Torsions

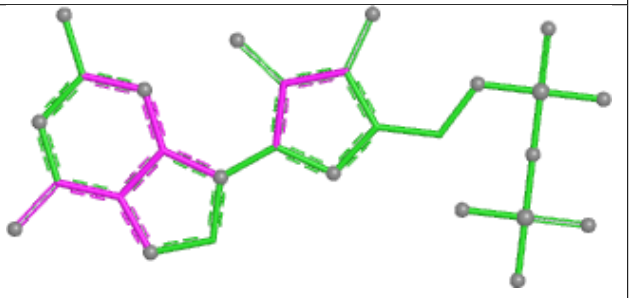


Rings

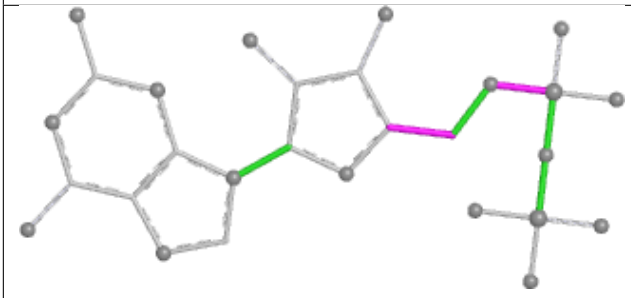
Ligand GDP LI 500



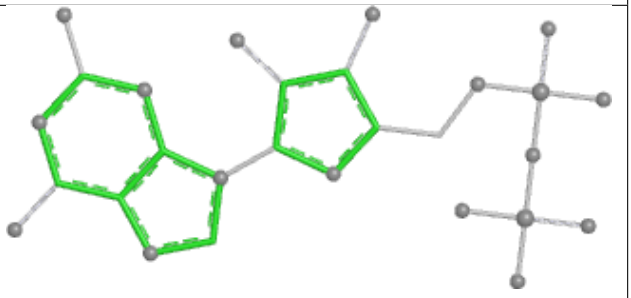
Bond lengths



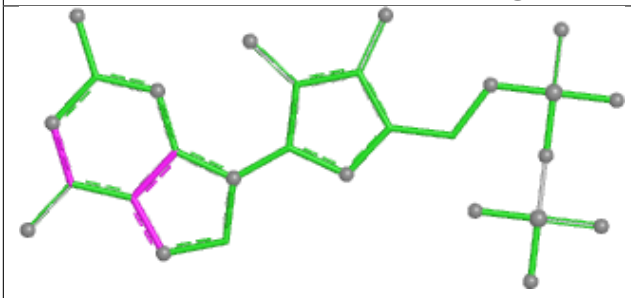
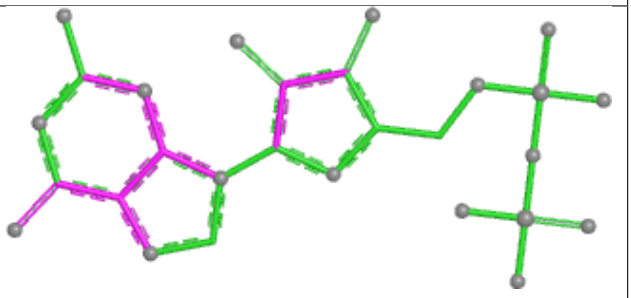
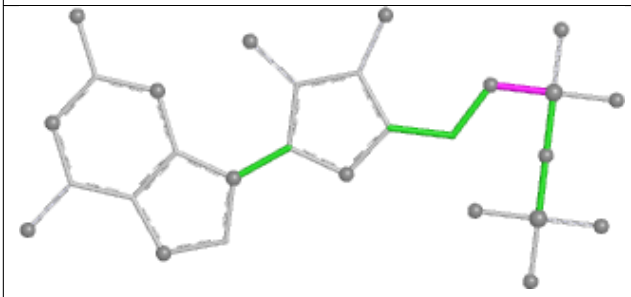
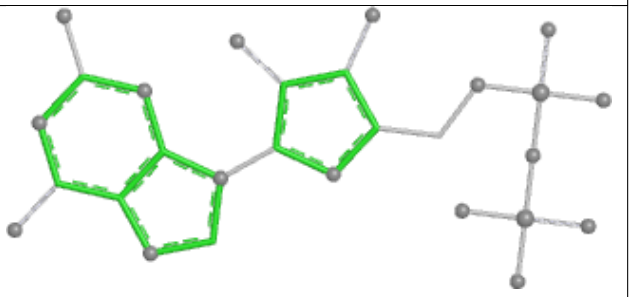
Bond angles

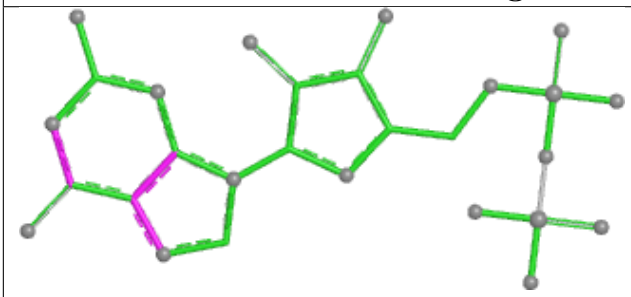
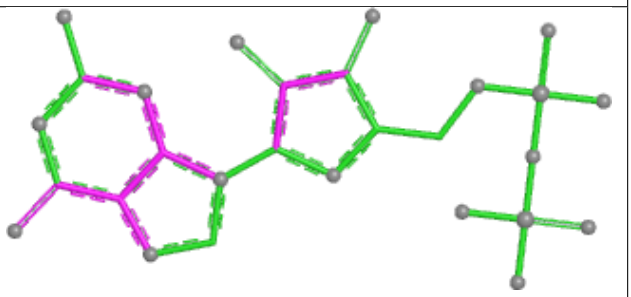
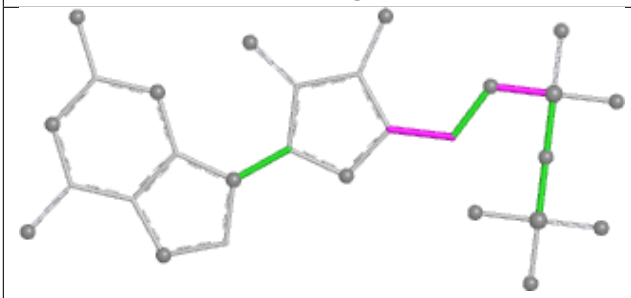
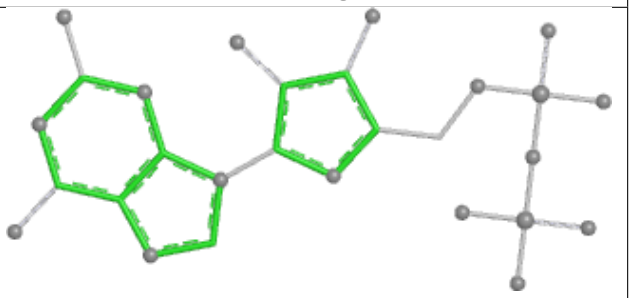


Torsions

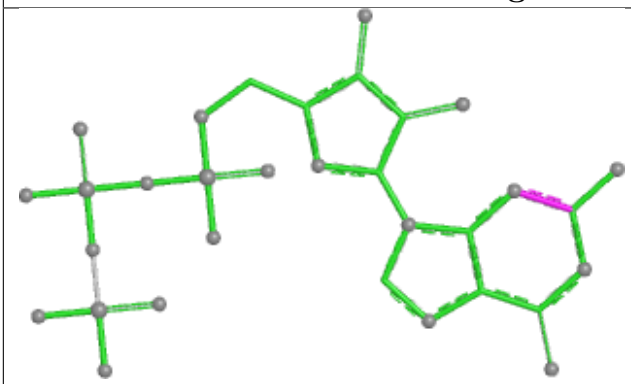


Rings

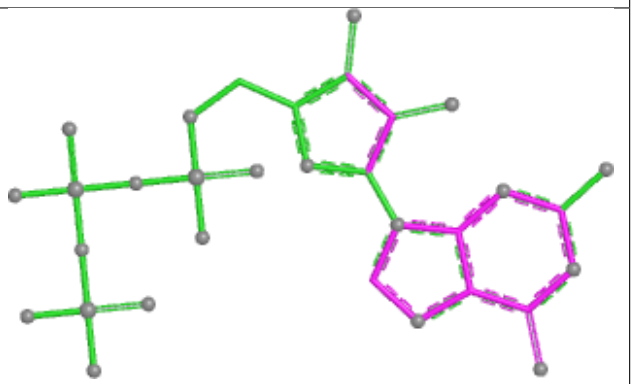
Ligand GDP BT 500	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand GDP GD 500	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

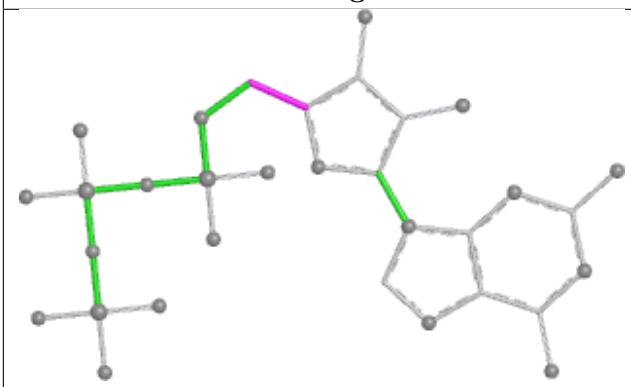
Ligand GTP HU 501



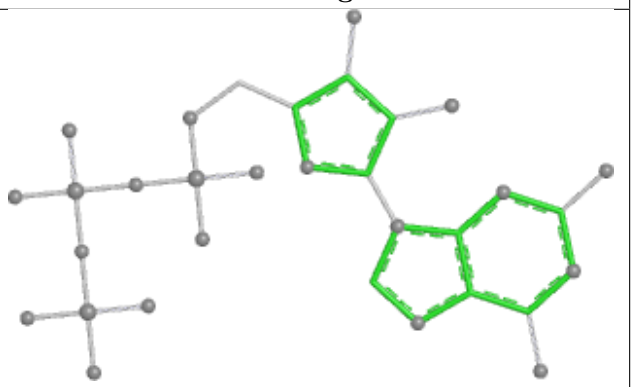
Bond lengths



Bond angles

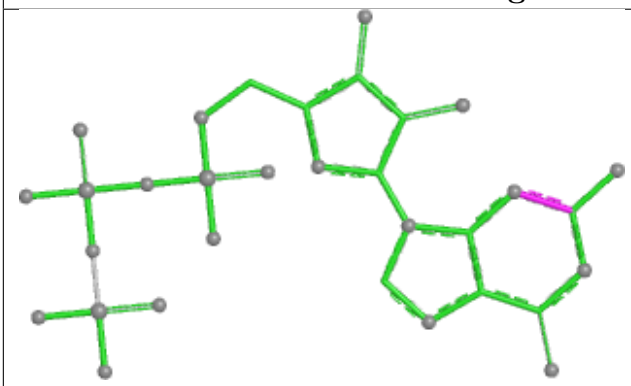


Torsions

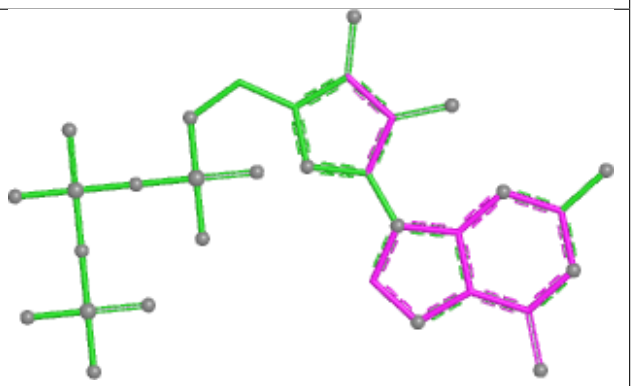


Rings

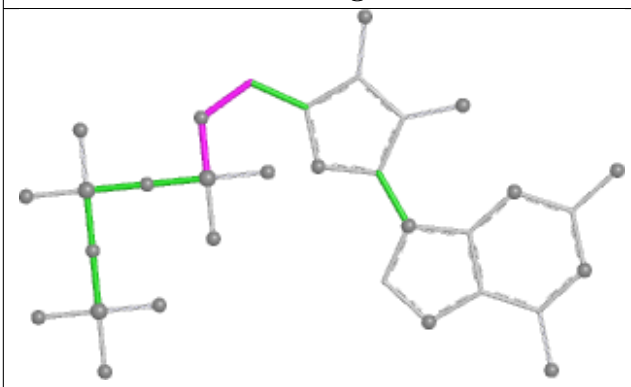
Ligand GTP HY 501



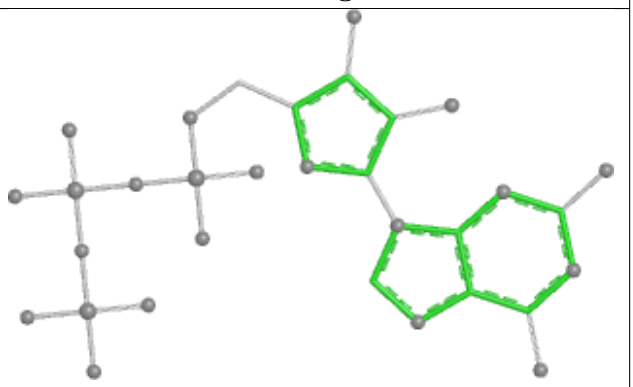
Bond lengths



Bond angles

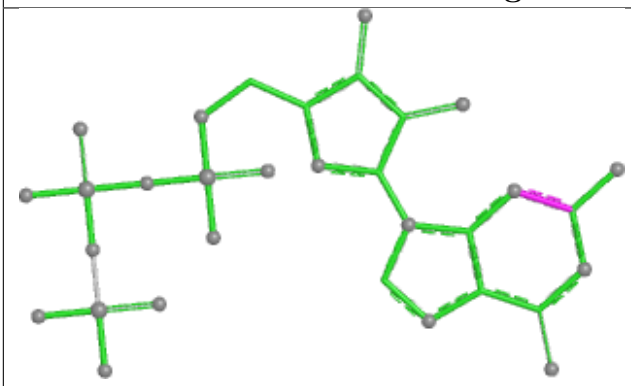


Torsions

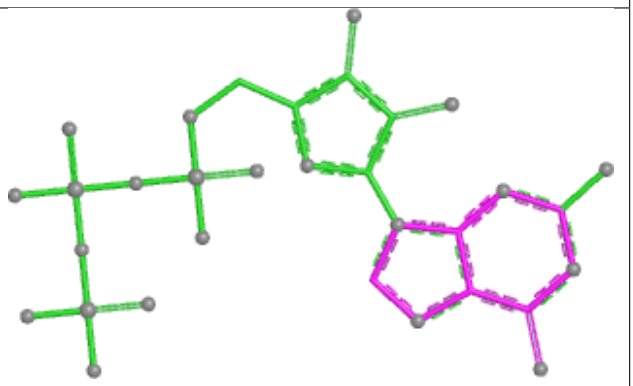


Rings

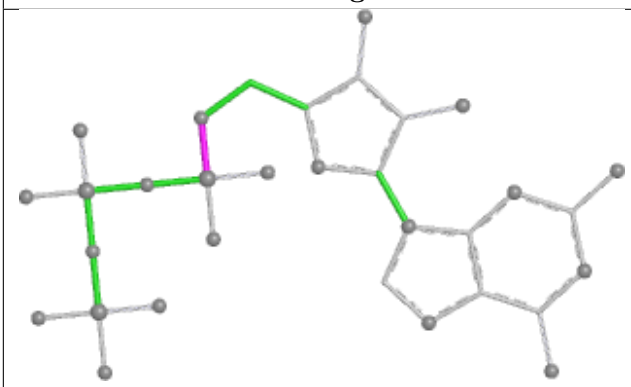
Ligand GTP BW 501



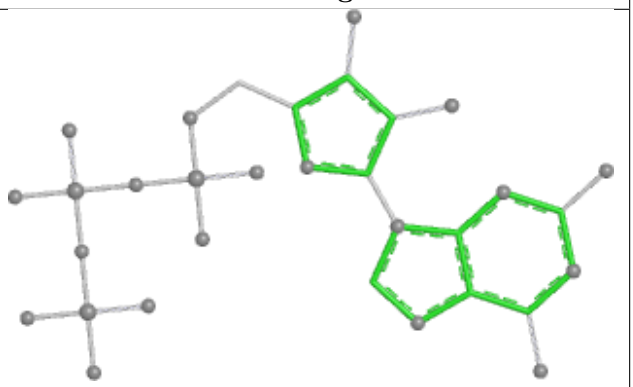
Bond lengths



Bond angles

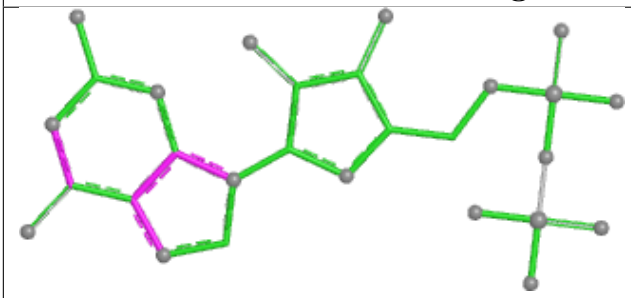


Torsions

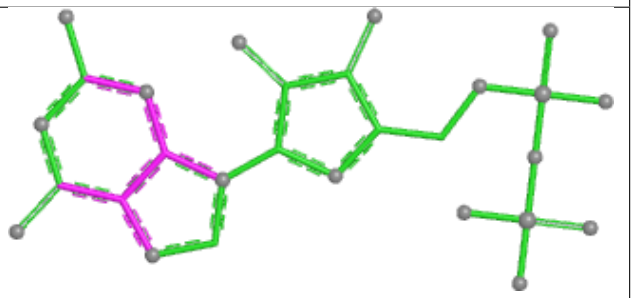


Rings

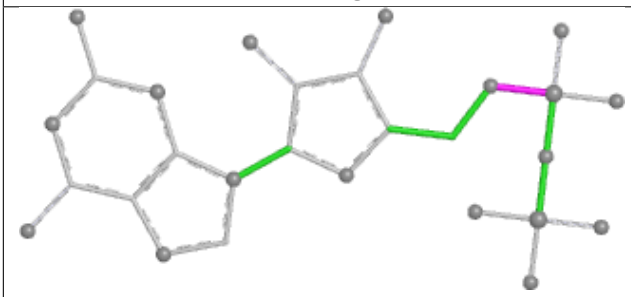
Ligand GDP ET 500



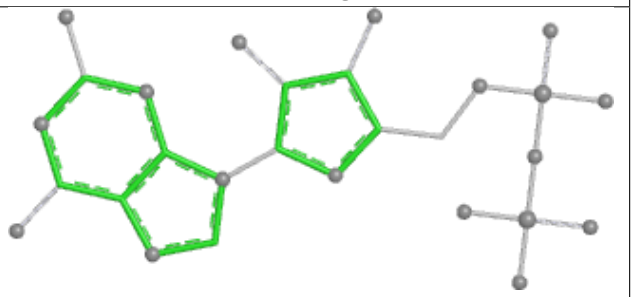
Bond lengths



Bond angles

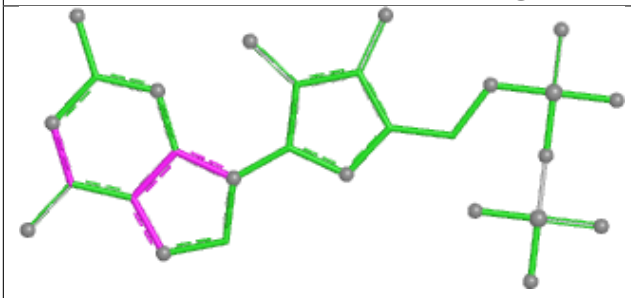


Torsions

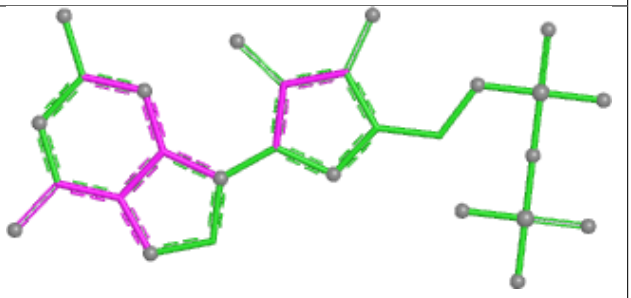


Rings

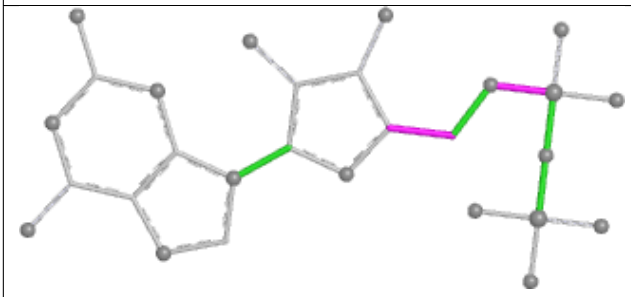
Ligand GDP BJ 500



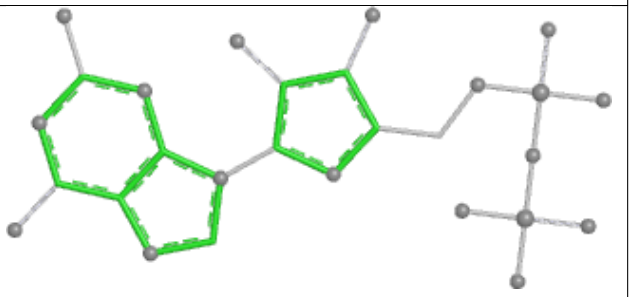
Bond lengths



Bond angles

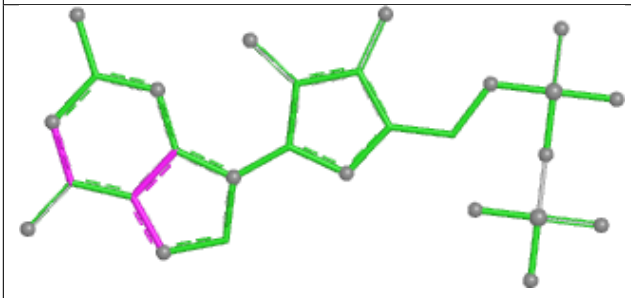


Torsions

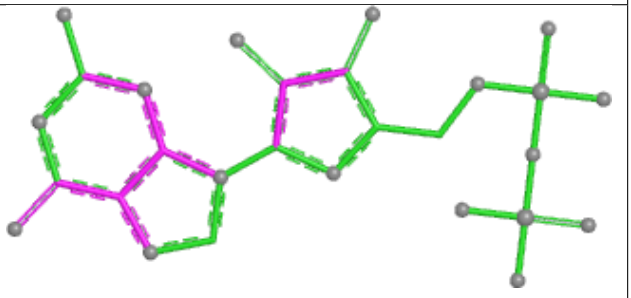


Rings

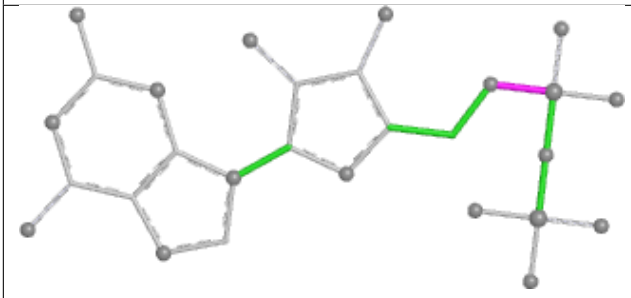
Ligand GDP KO 500



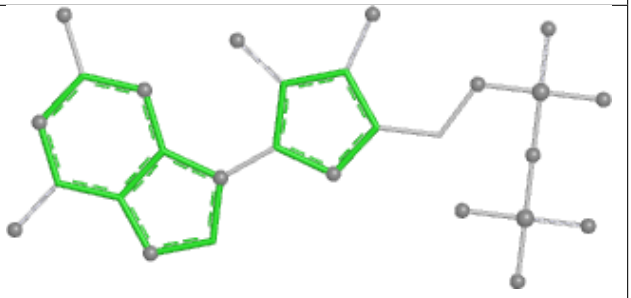
Bond lengths



Bond angles

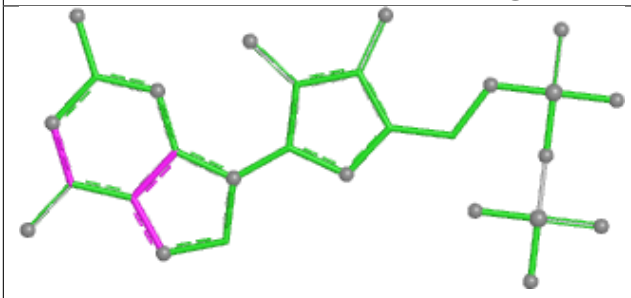


Torsions

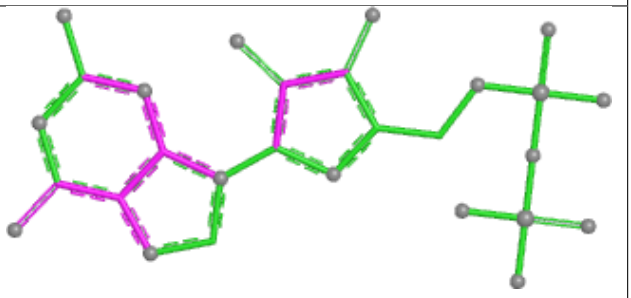


Rings

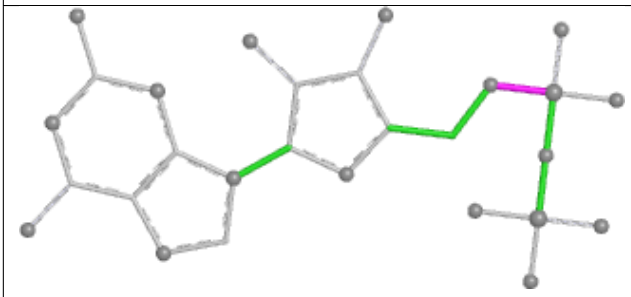
Ligand GDP HV 500



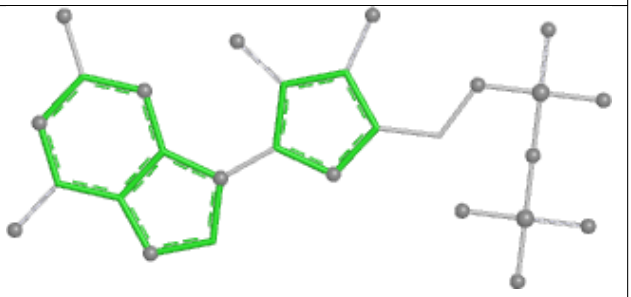
Bond lengths



Bond angles

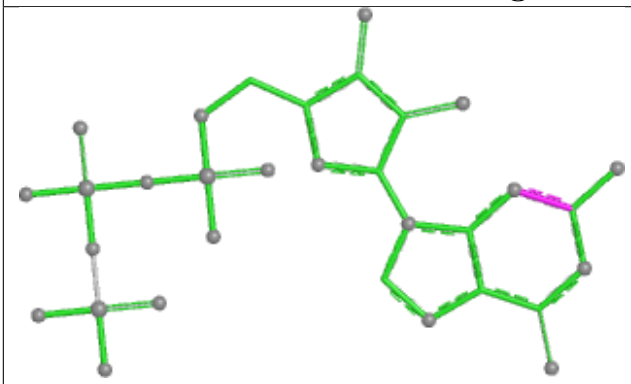


Torsions

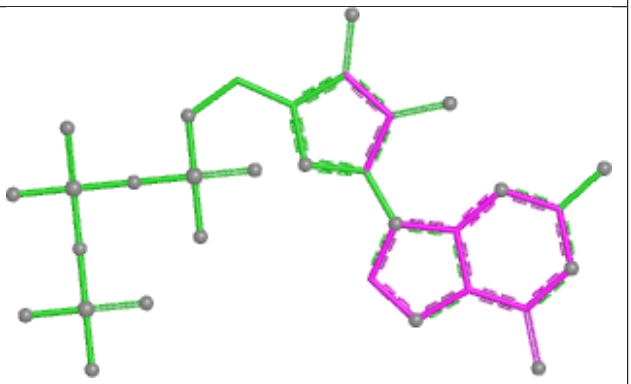


Rings

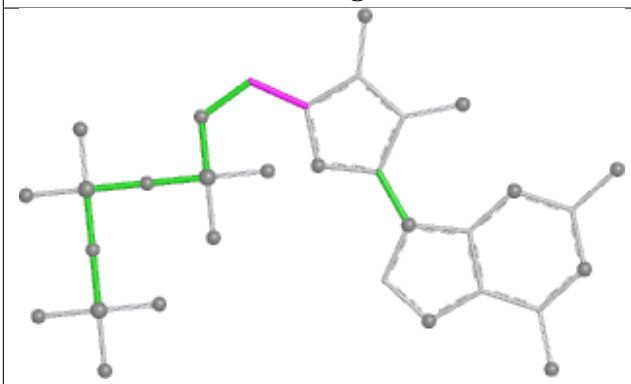
Ligand GTP OC 501



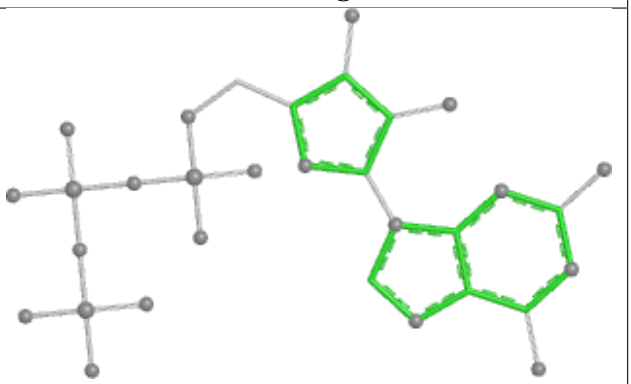
Bond lengths



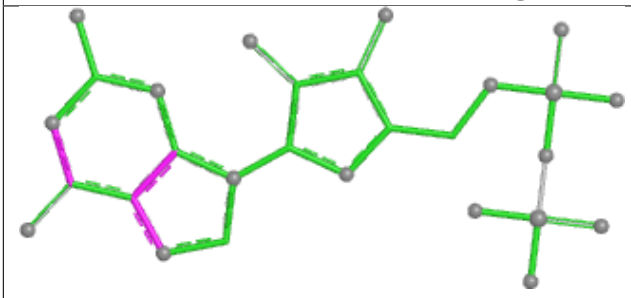
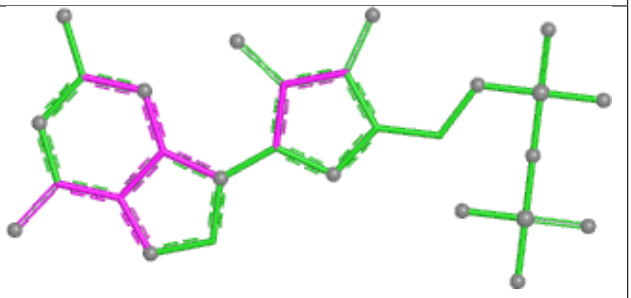
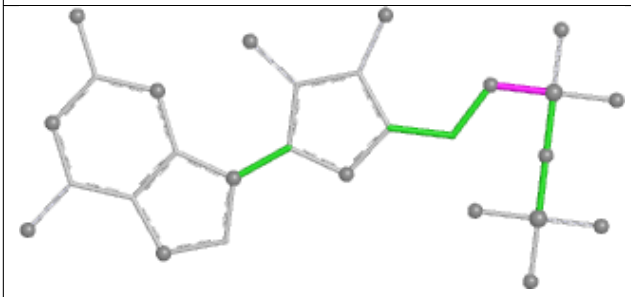
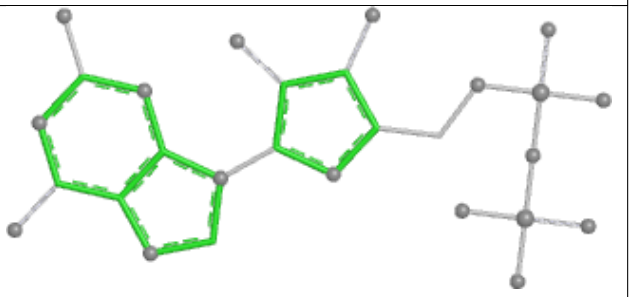
Bond angles

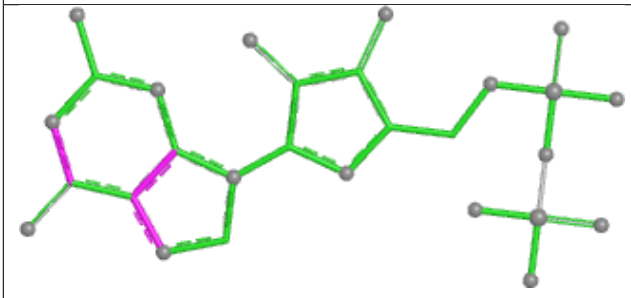
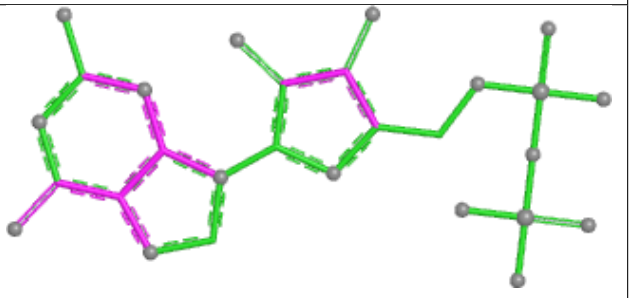
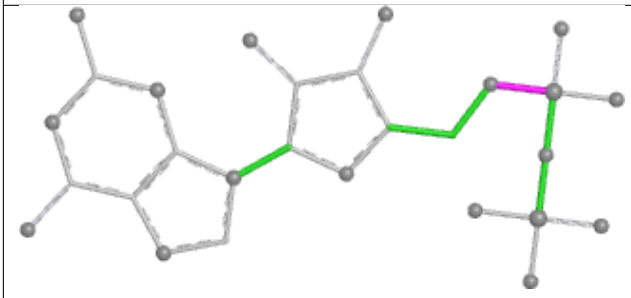
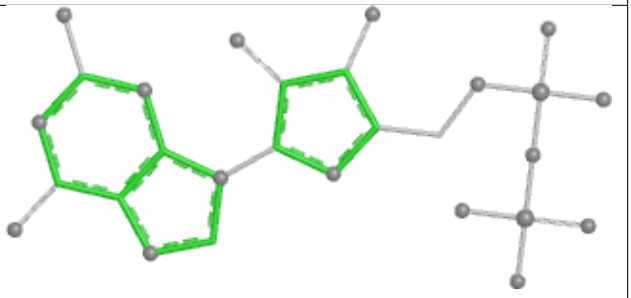


Torsions

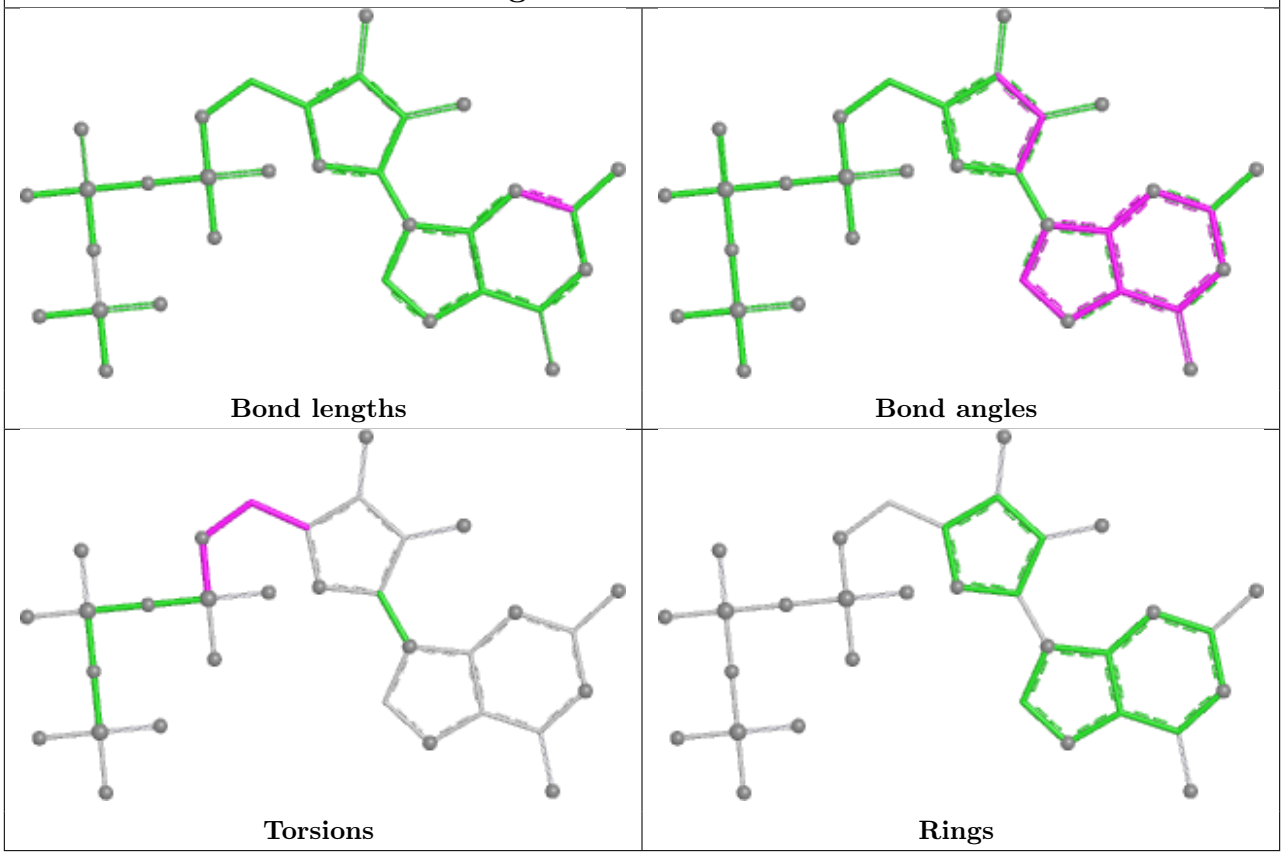


Rings

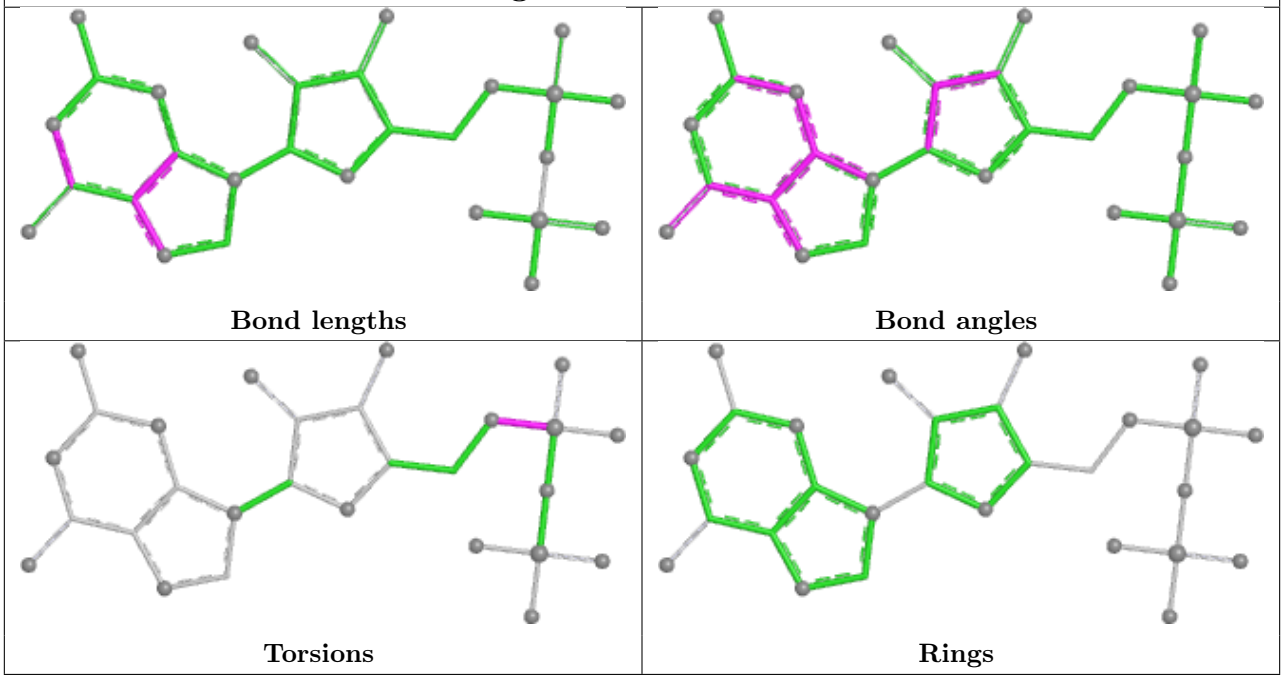
Ligand GDP LE 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP RA 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

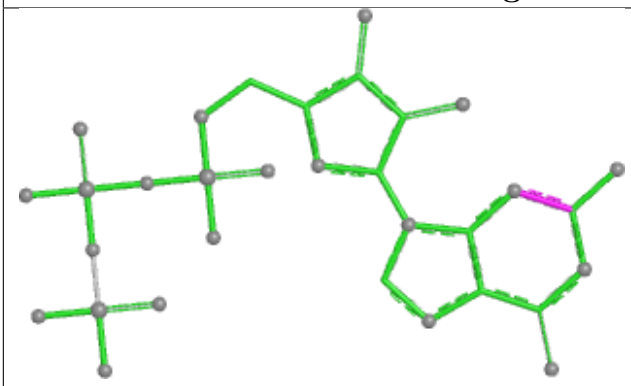
Ligand GTP NK 501



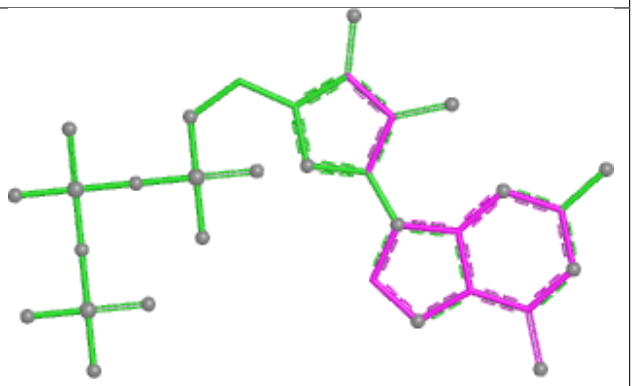
Ligand GDP TP 500



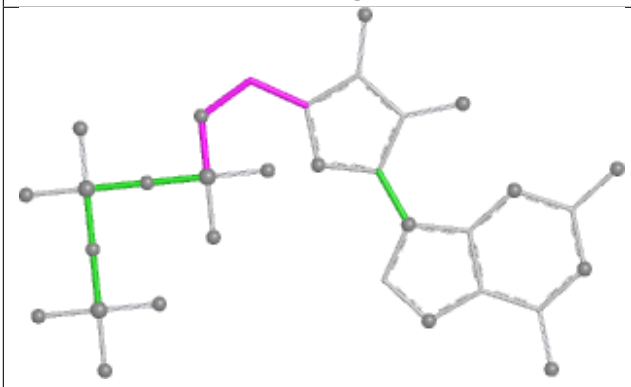
Ligand GTP NW 501



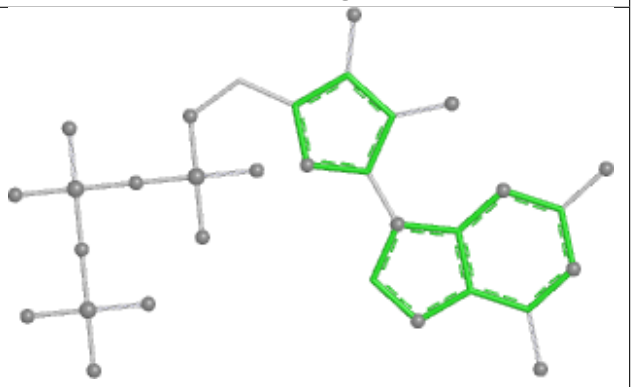
Bond lengths



Bond angles

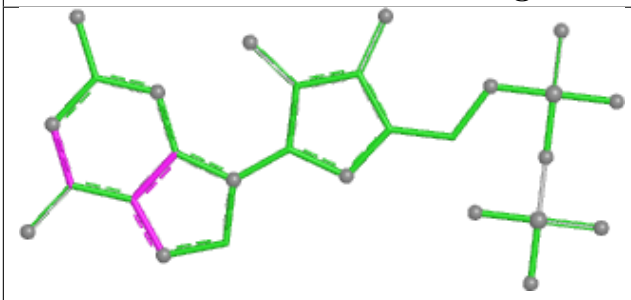


Torsions

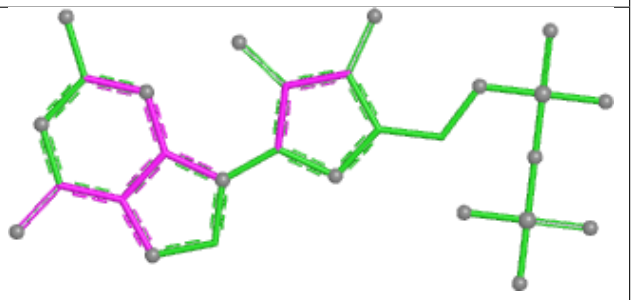


Rings

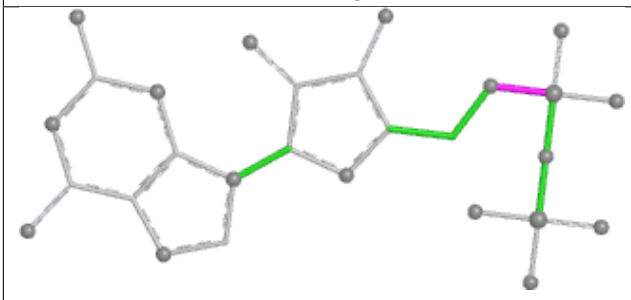
Ligand GDP EJ 500



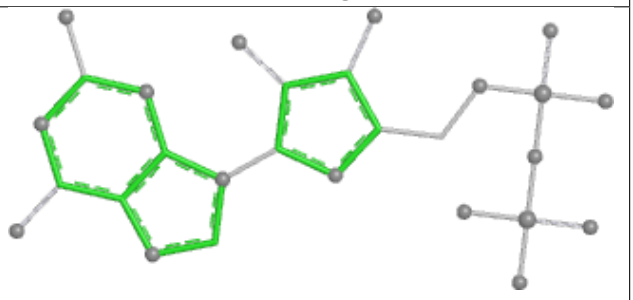
Bond lengths



Bond angles

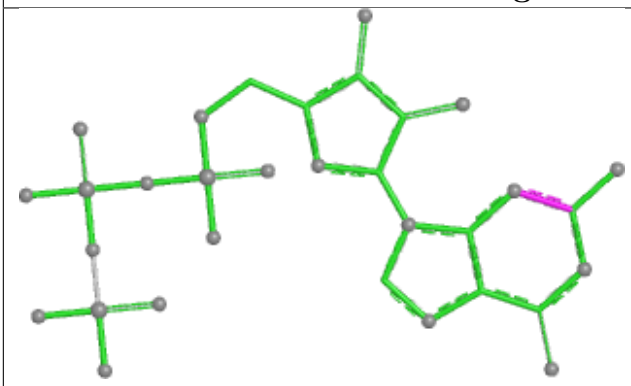


Torsions

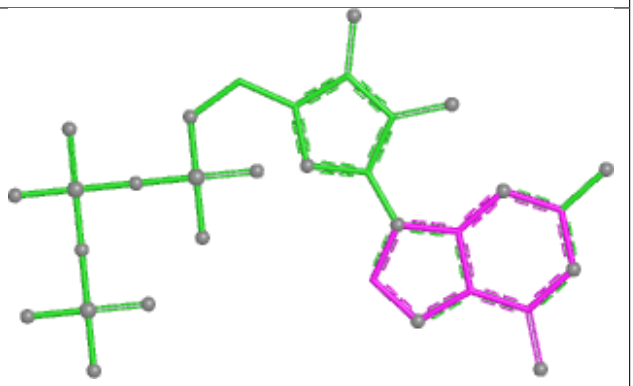


Rings

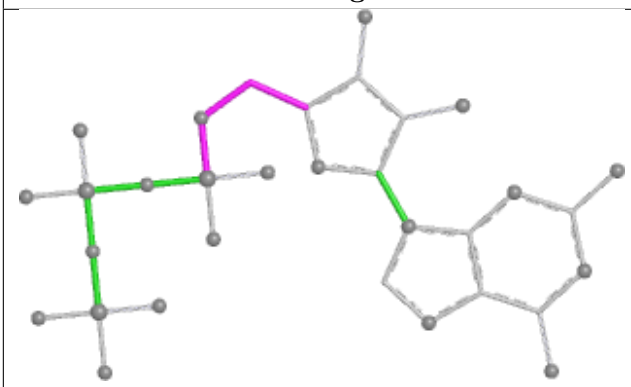
Ligand GTP PS 501



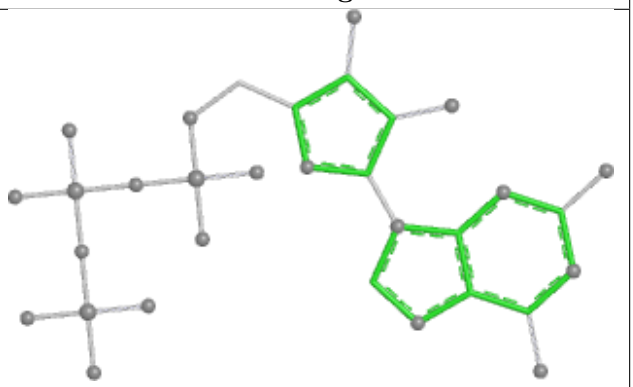
Bond lengths



Bond angles

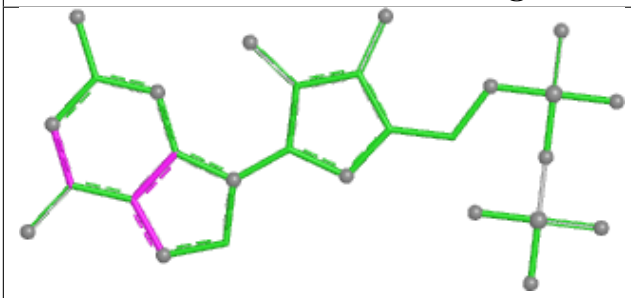


Torsions

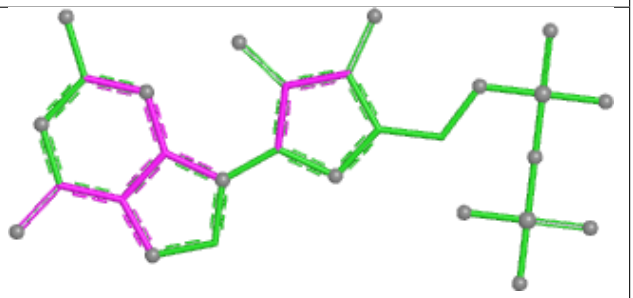


Rings

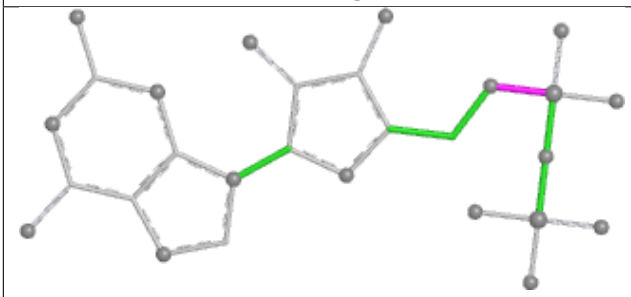
Ligand GDP PN 500



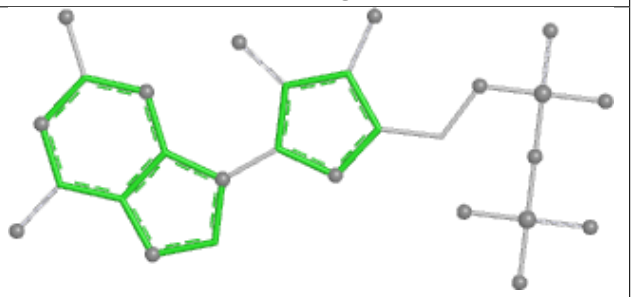
Bond lengths



Bond angles

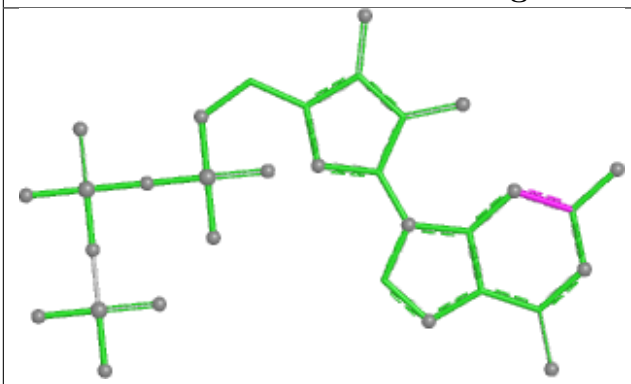


Torsions

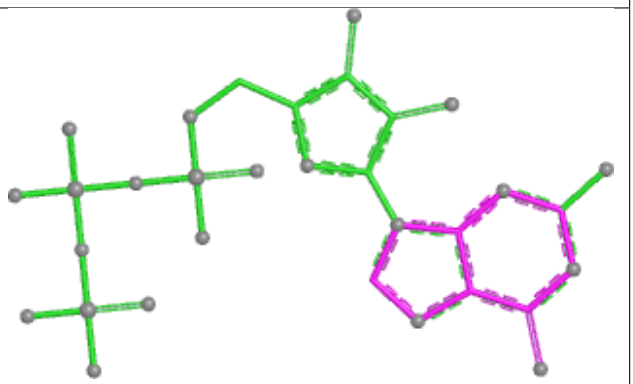


Rings

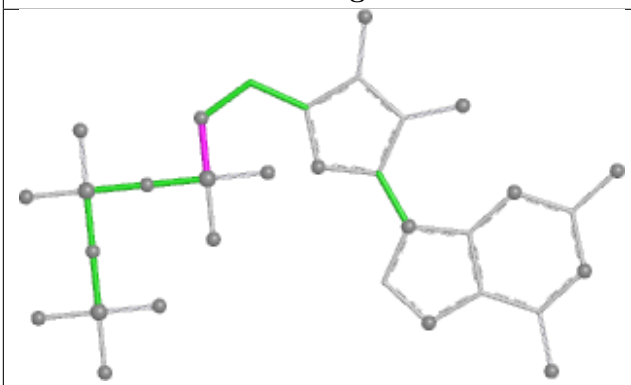
Ligand GTP WI 501



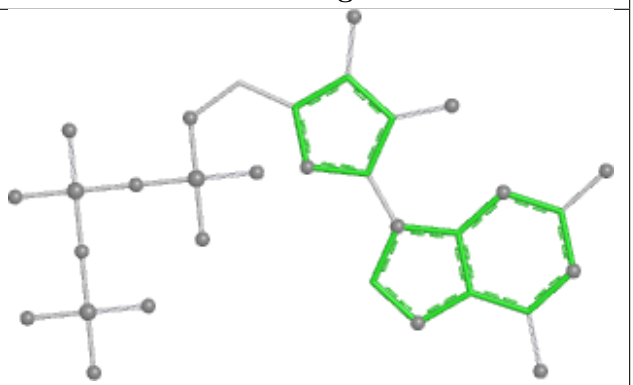
Bond lengths



Bond angles

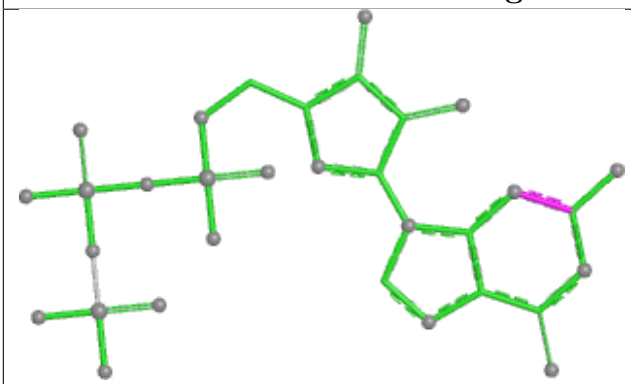


Torsions

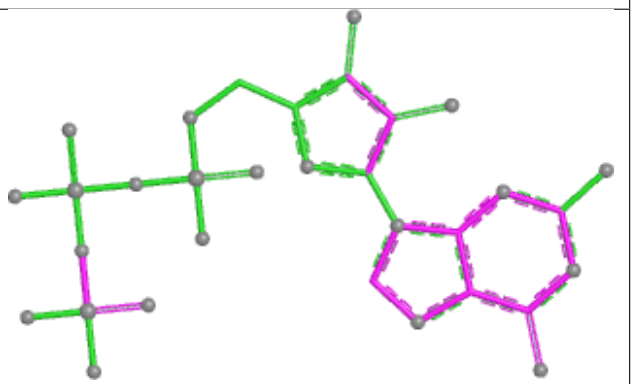


Rings

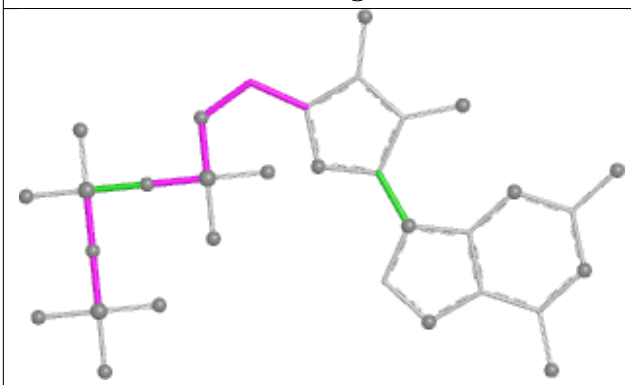
Ligand GTP WE 501



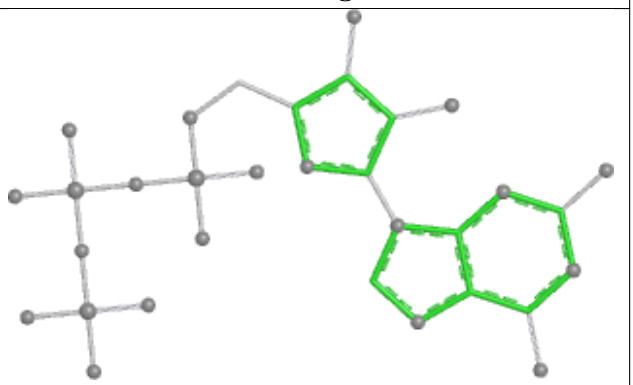
Bond lengths



Bond angles

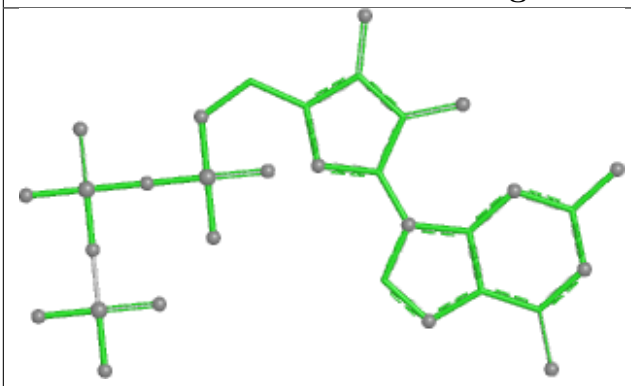


Torsions

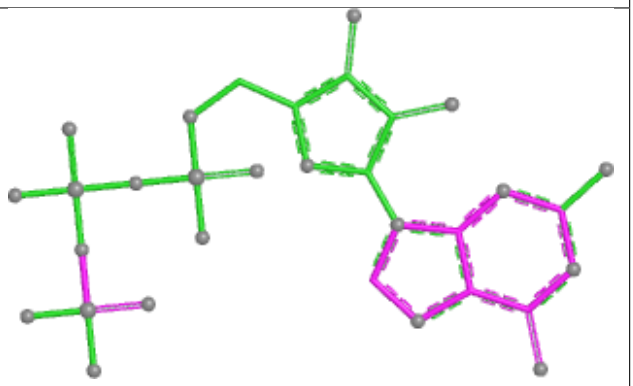


Rings

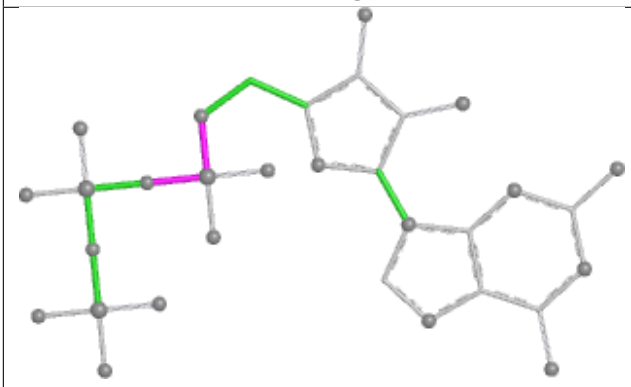
Ligand GTP BO 501



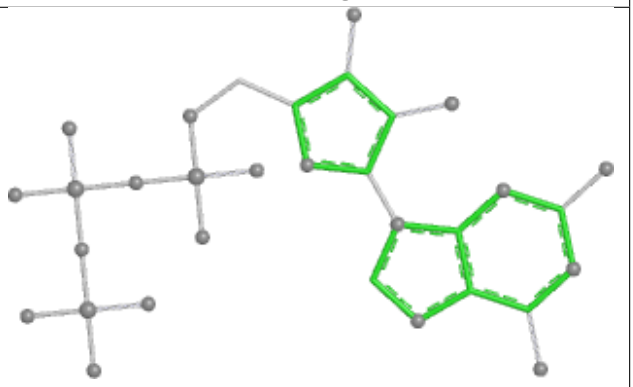
Bond lengths



Bond angles

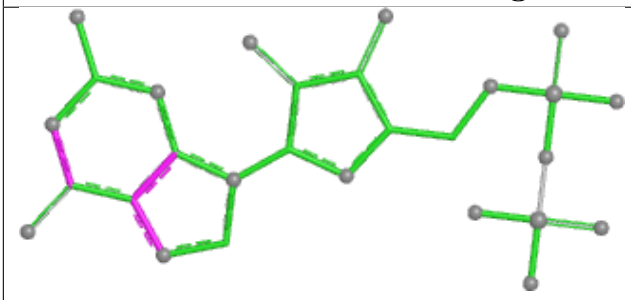


Torsions

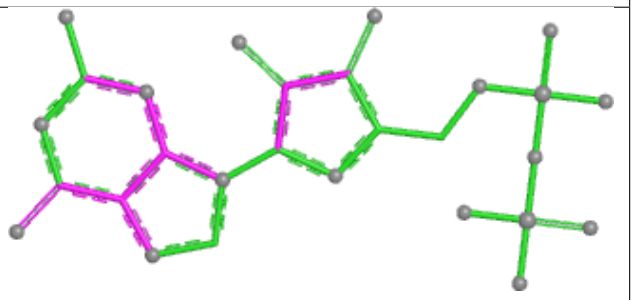


Rings

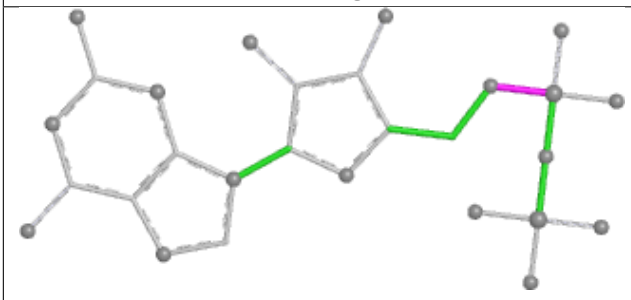
Ligand GDP HL 501



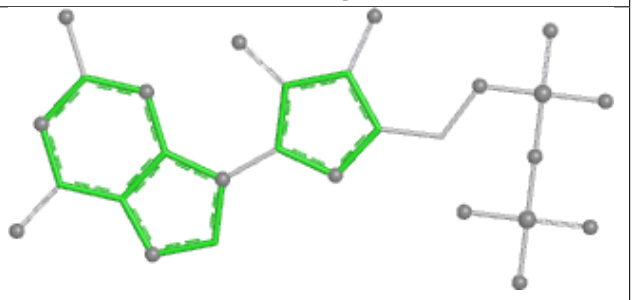
Bond lengths



Bond angles

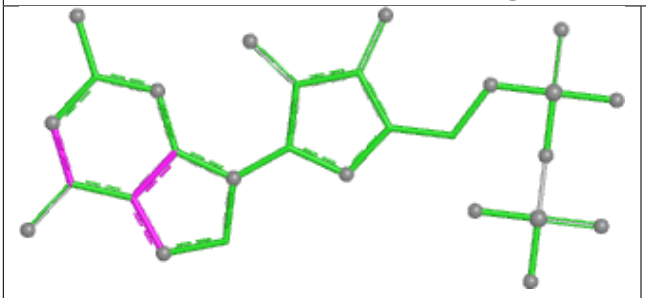


Torsions

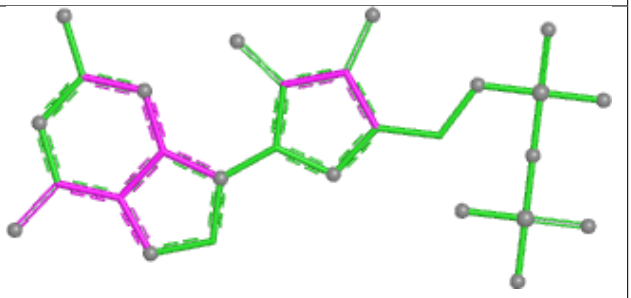


Rings

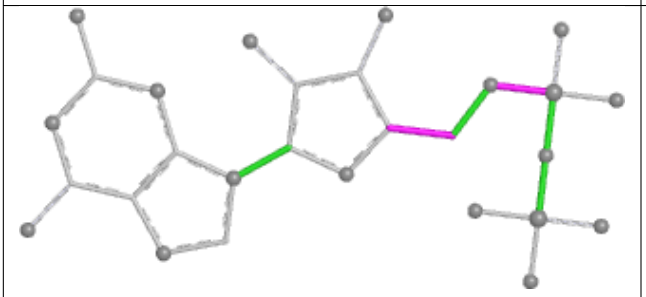
Ligand GDP MR 500



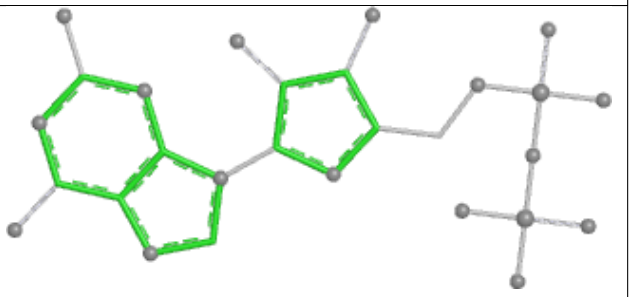
Bond lengths



Bond angles

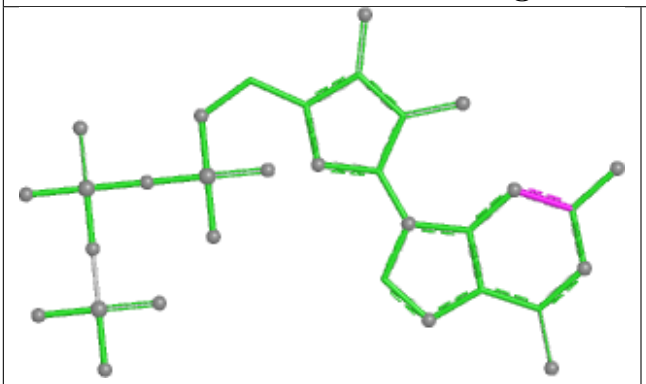


Torsions

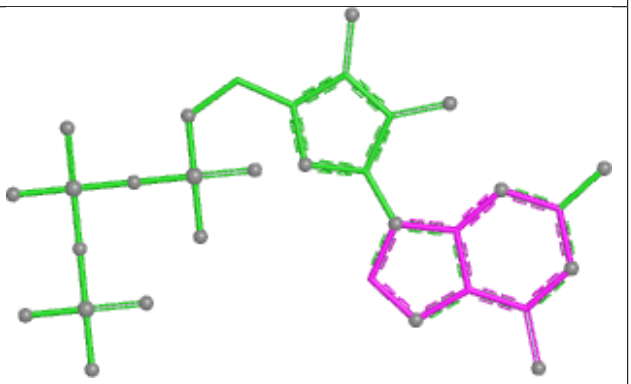


Rings

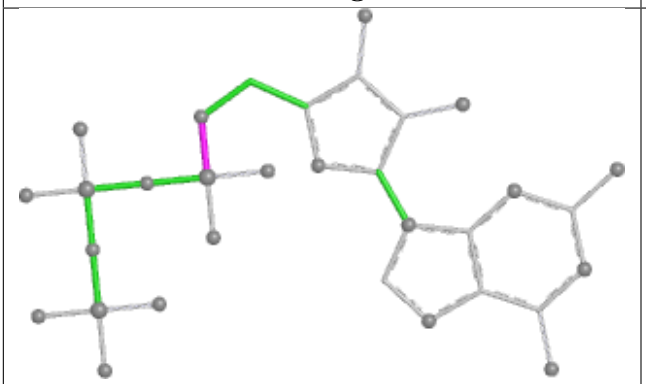
Ligand GTP CJ 501



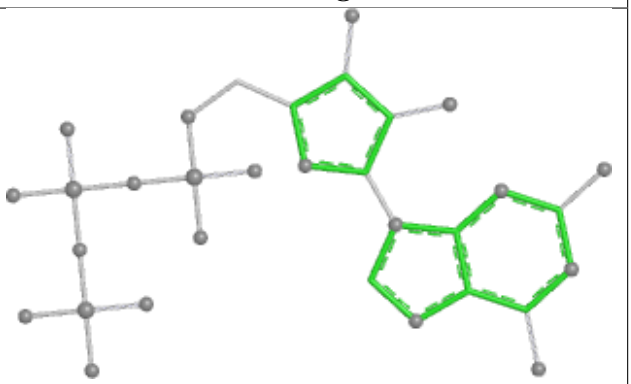
Bond lengths



Bond angles

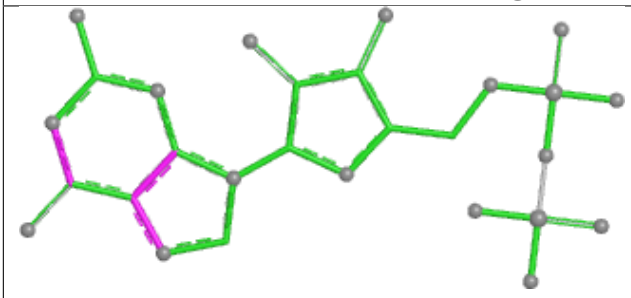


Torsions

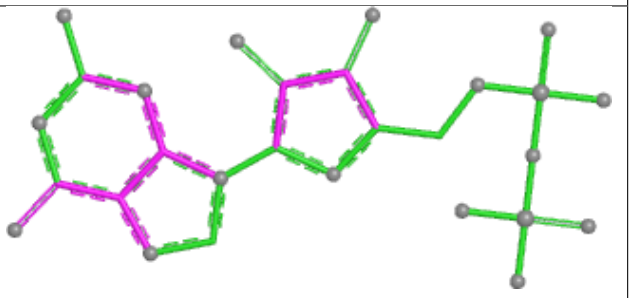


Rings

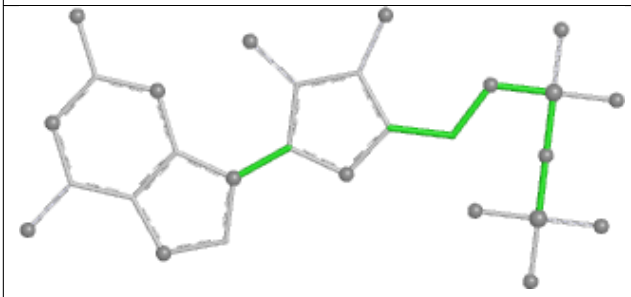
Ligand GDP FN 500



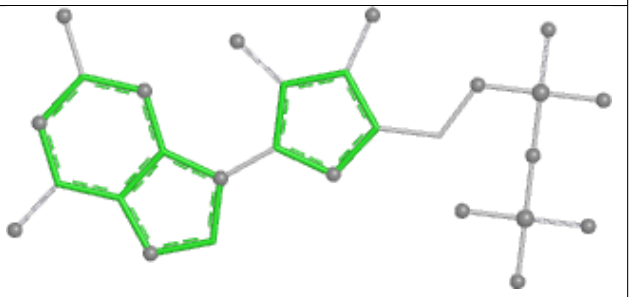
Bond lengths



Bond angles

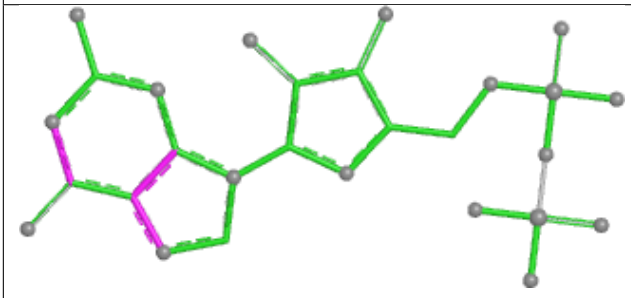


Torsions

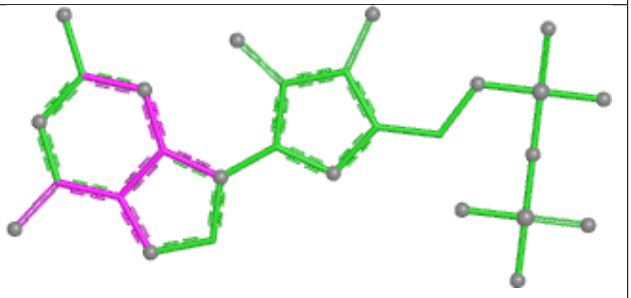


Rings

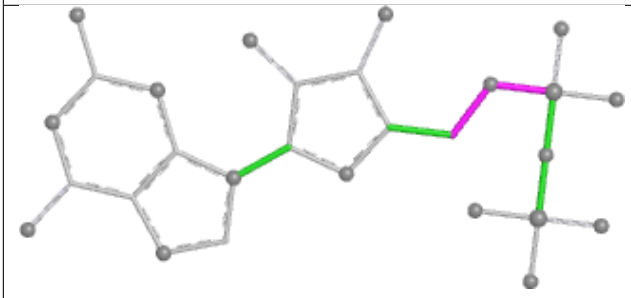
Ligand GDP GH 500



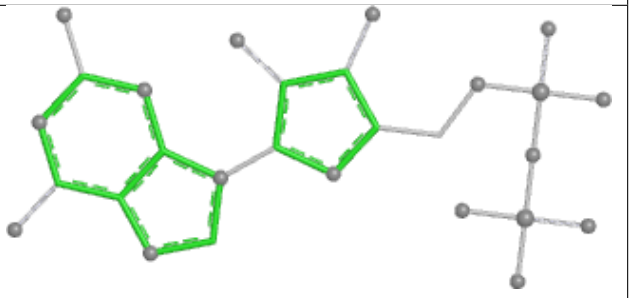
Bond lengths



Bond angles

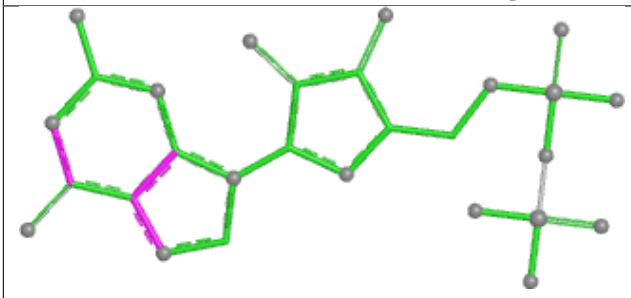


Torsions

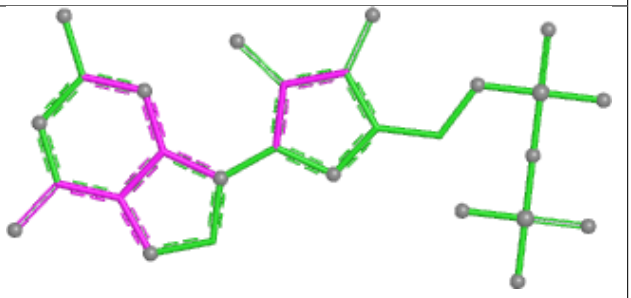


Rings

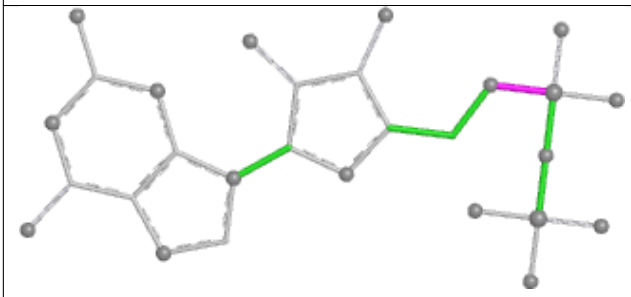
Ligand GDP MX 500



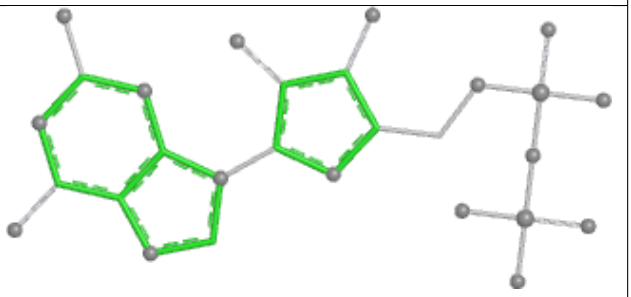
Bond lengths



Bond angles

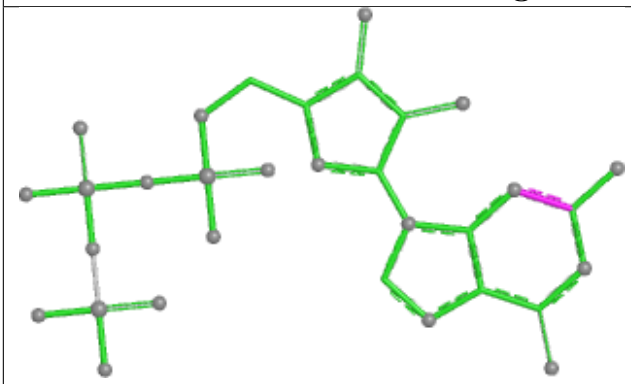


Torsions

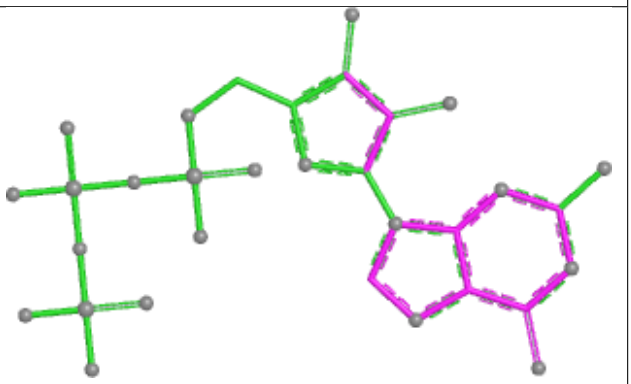


Rings

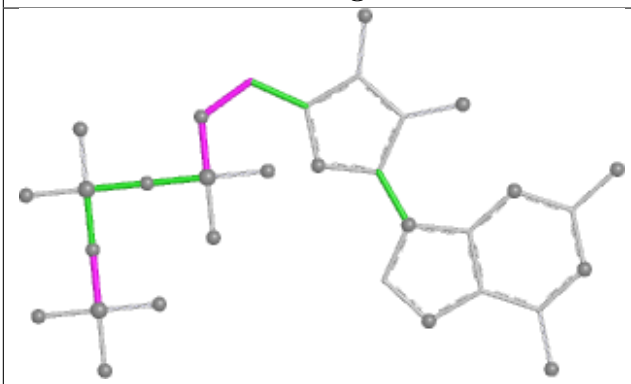
Ligand GTP FE 501



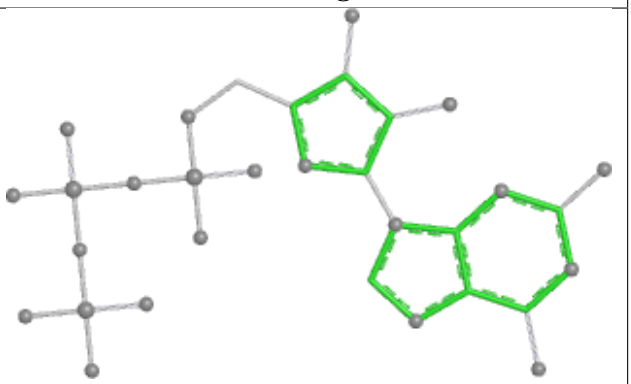
Bond lengths



Bond angles

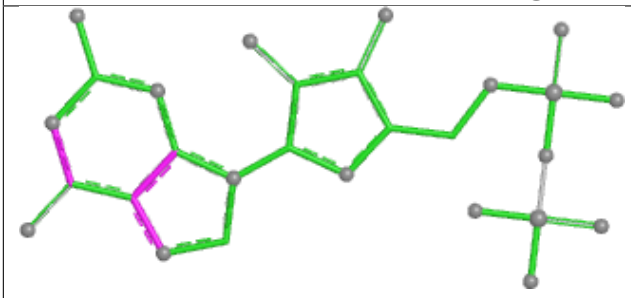


Torsions

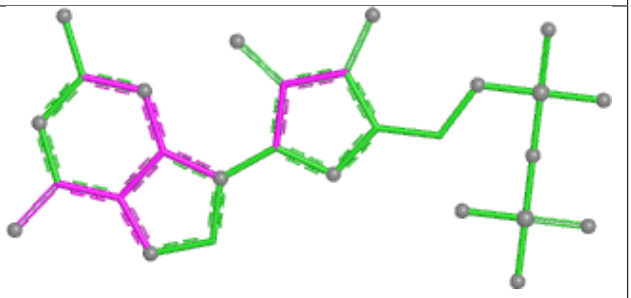


Rings

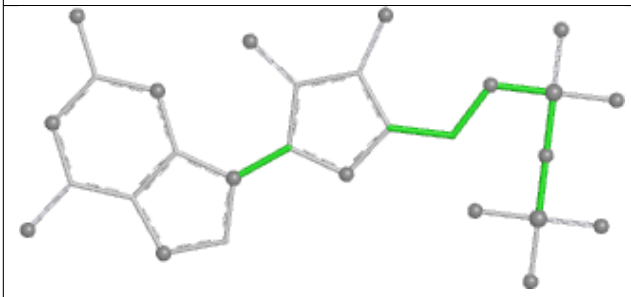
Ligand GDP I 501



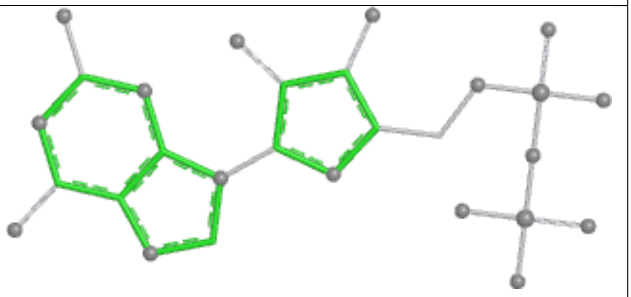
Bond lengths



Bond angles

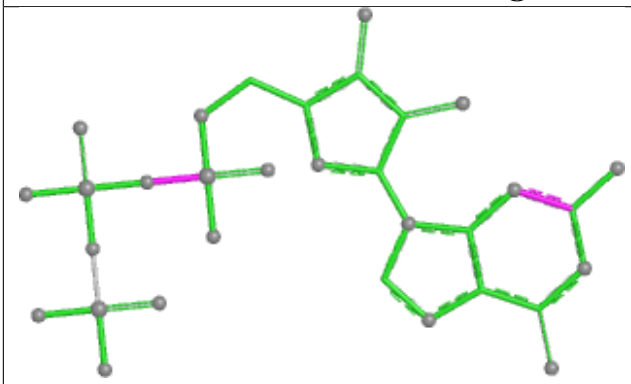


Torsions

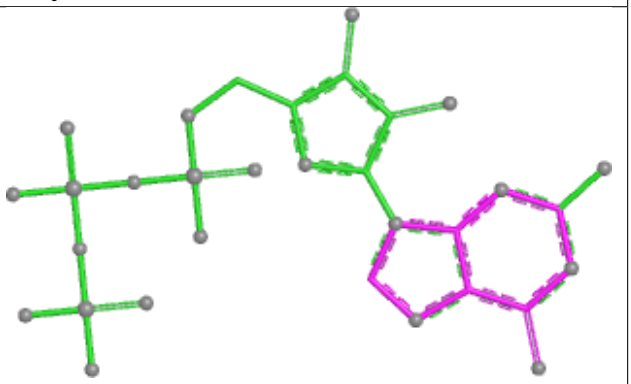


Rings

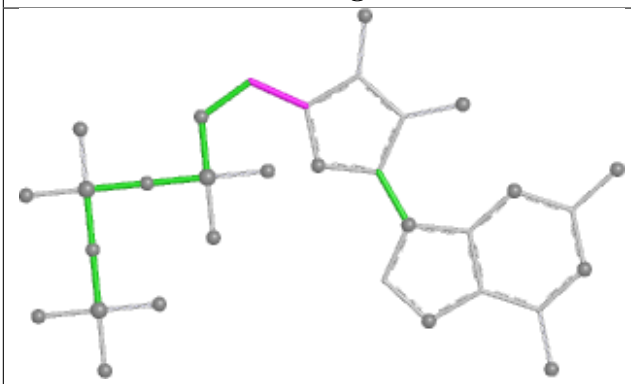
Ligand GTP QN 501



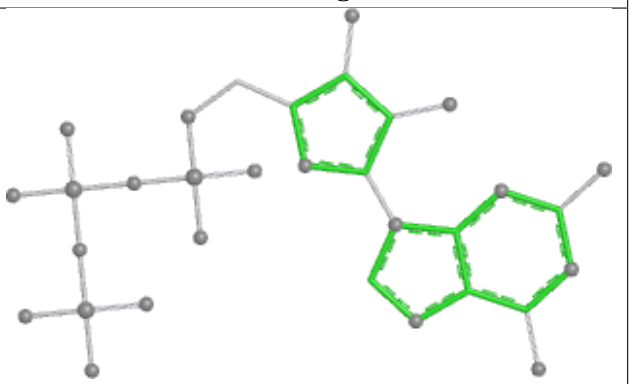
Bond lengths



Bond angles

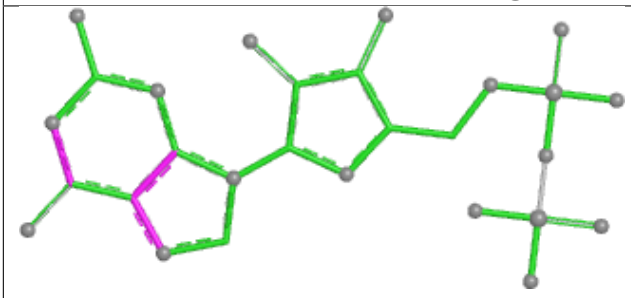


Torsions

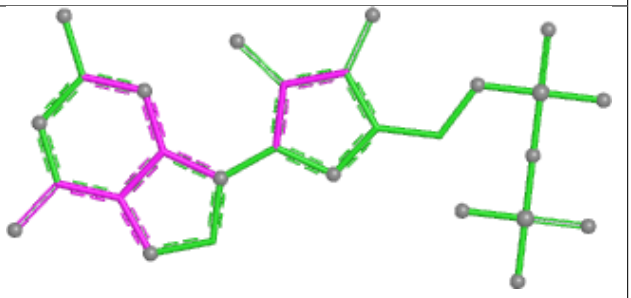


Rings

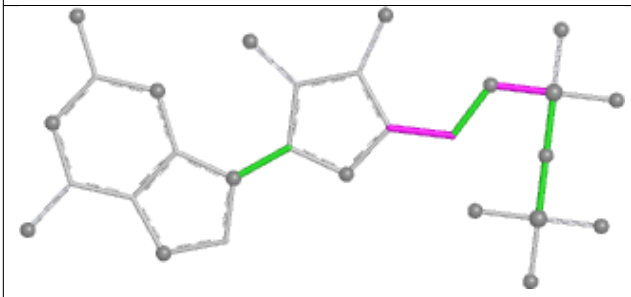
Ligand GDP KY 500



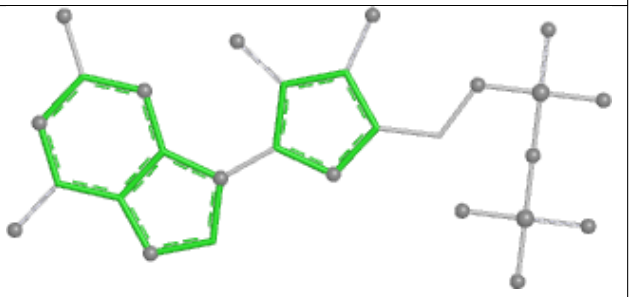
Bond lengths



Bond angles

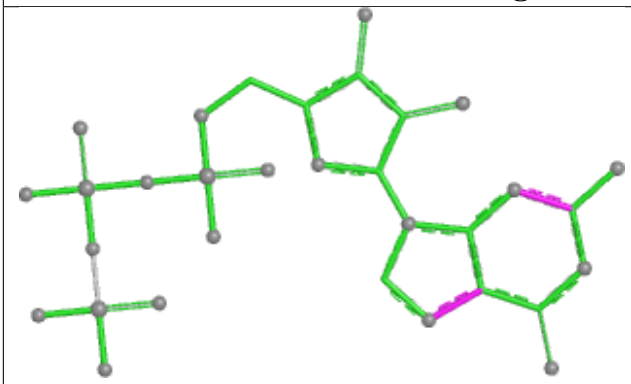


Torsions

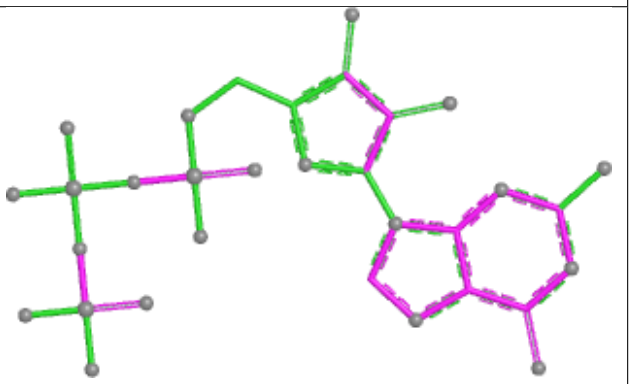


Rings

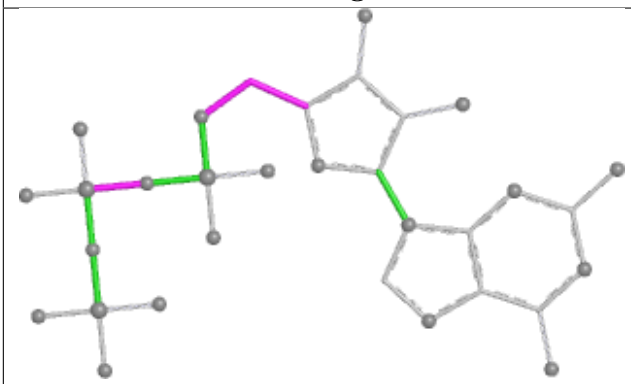
Ligand GTP FT 503



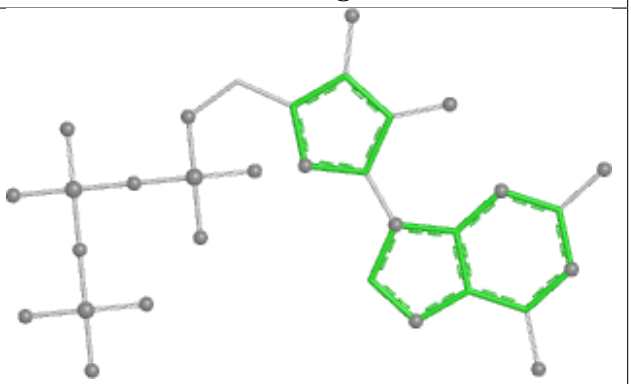
Bond lengths



Bond angles

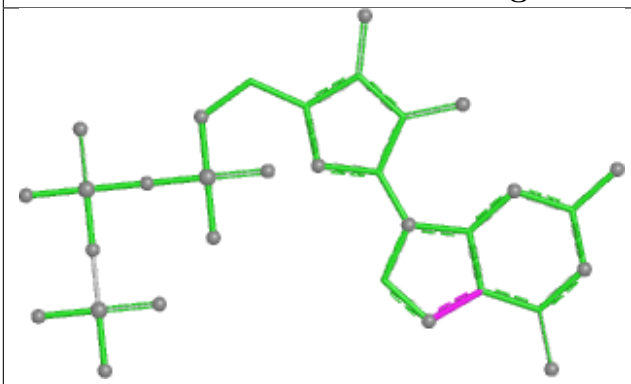


Torsions

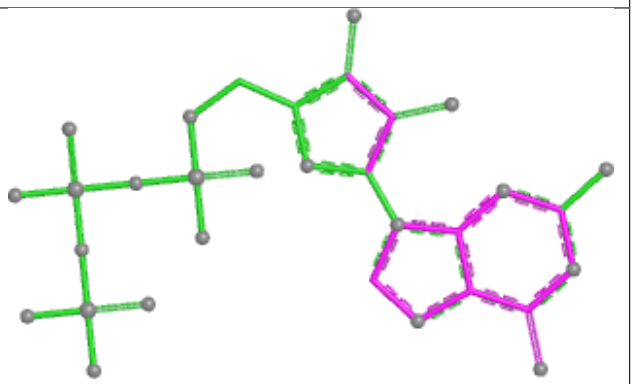


Rings

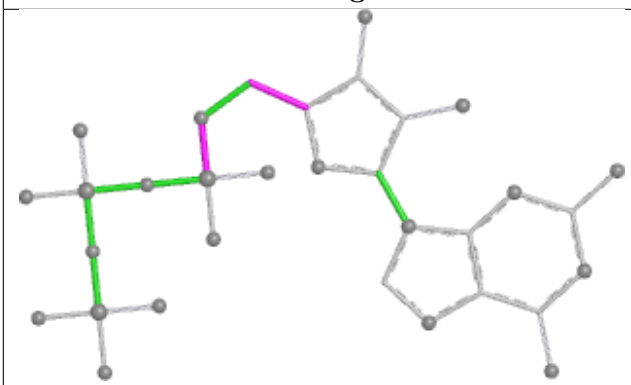
Ligand GTP EU 501



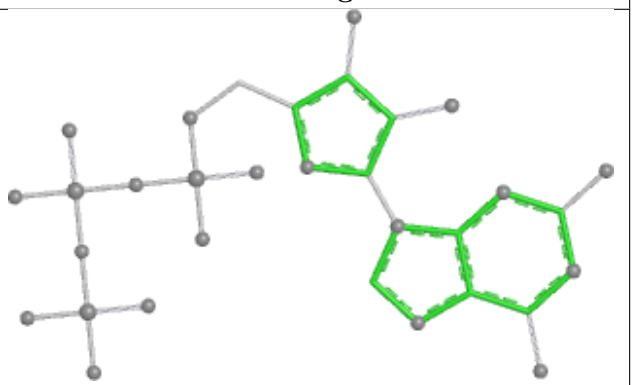
Bond lengths



Bond angles

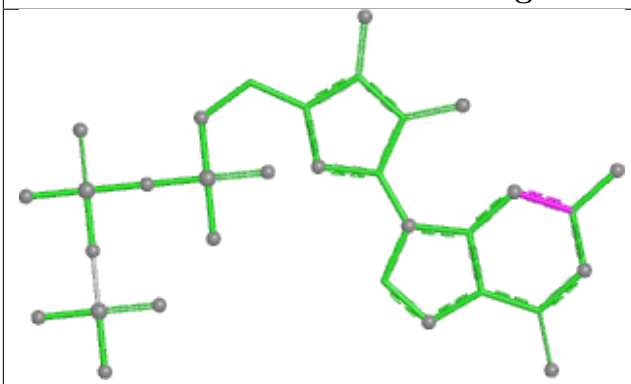


Torsions

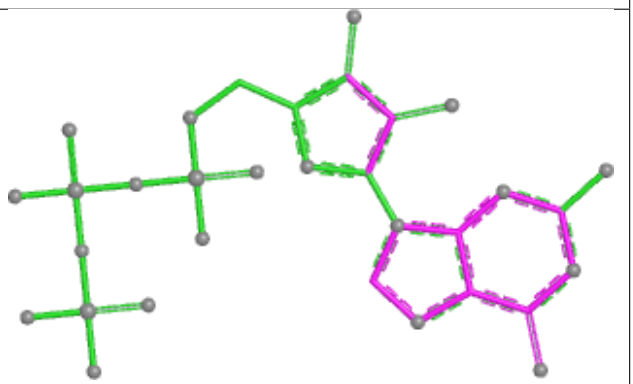


Rings

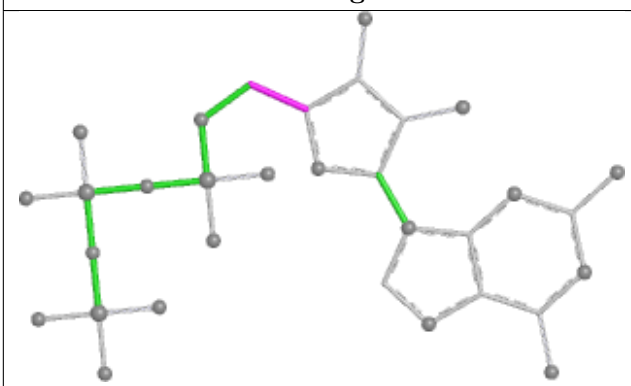
Ligand GTP HI 501



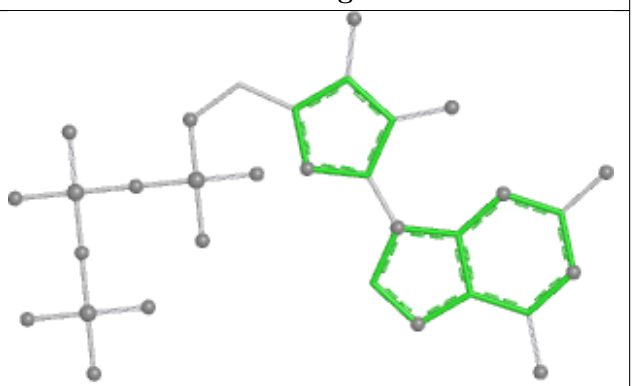
Bond lengths



Bond angles

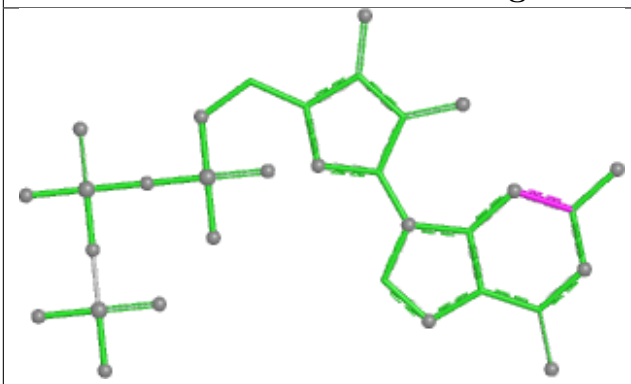


Torsions

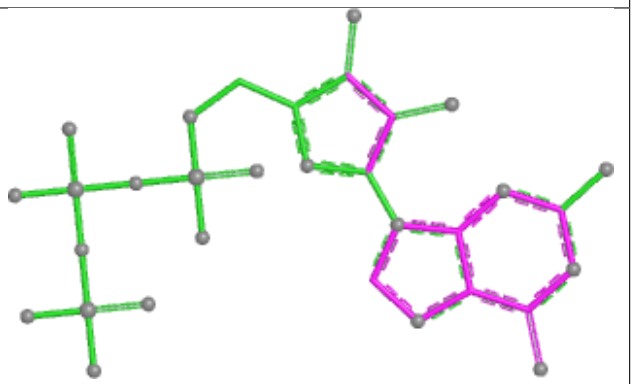


Rings

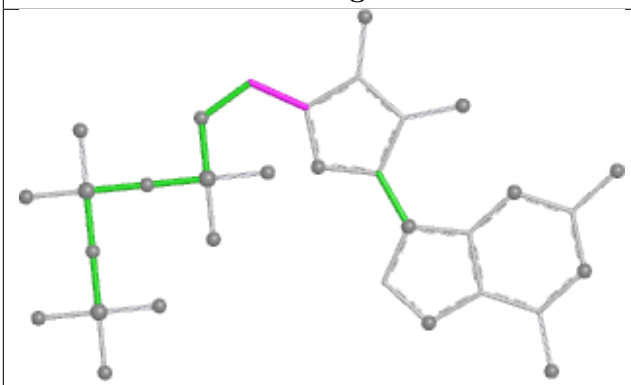
Ligand GTP OO 501



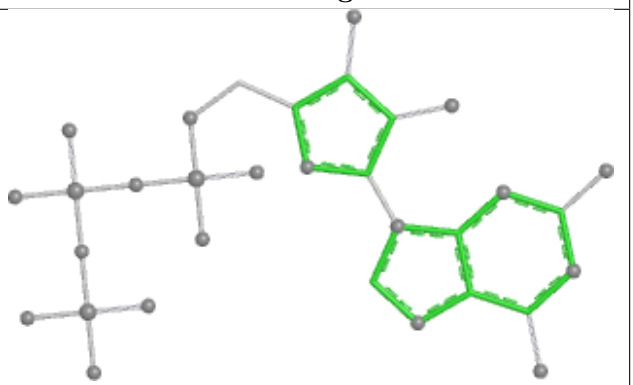
Bond lengths



Bond angles

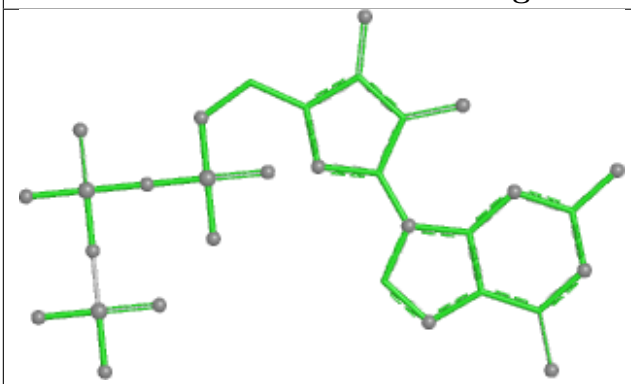


Torsions

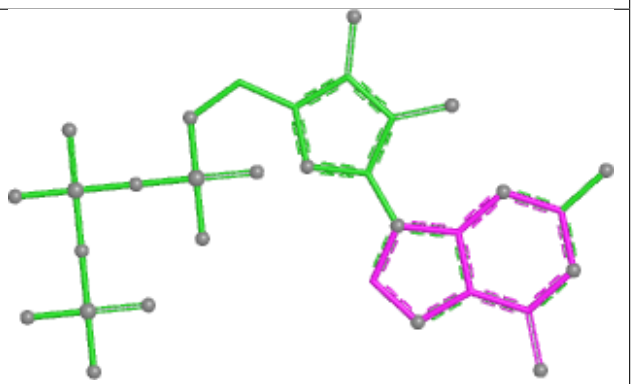


Rings

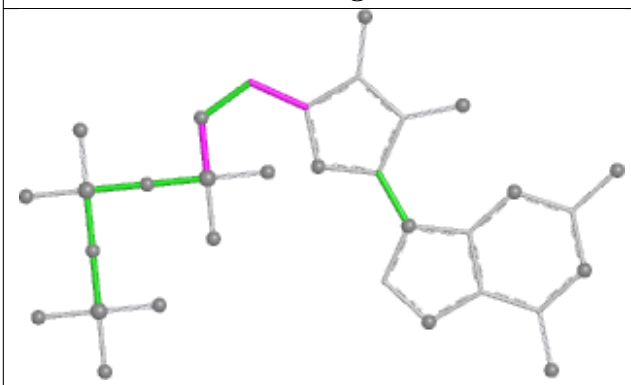
Ligand GTP DJ 501



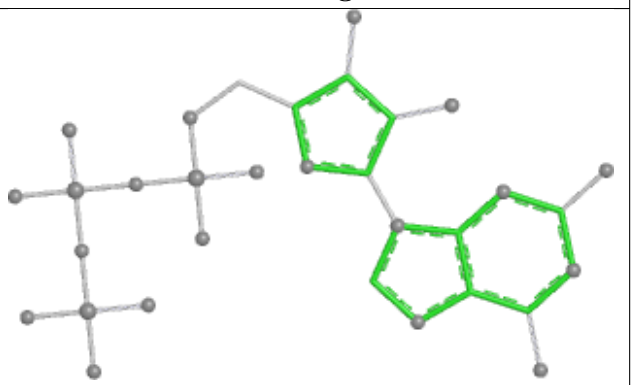
Bond lengths



Bond angles

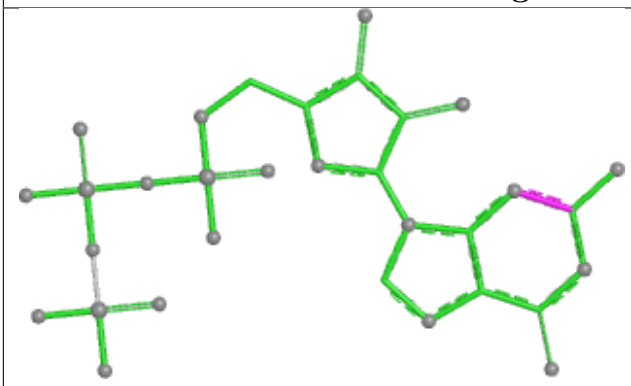


Torsions

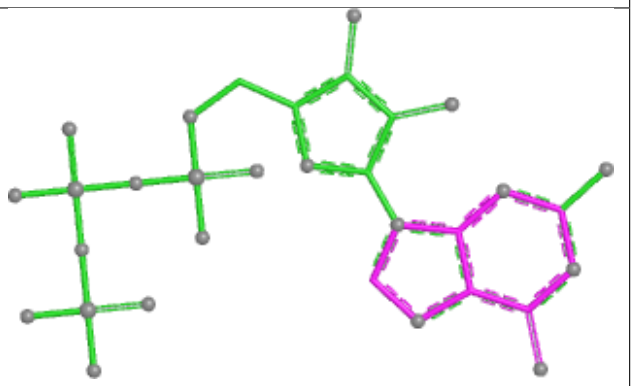


Rings

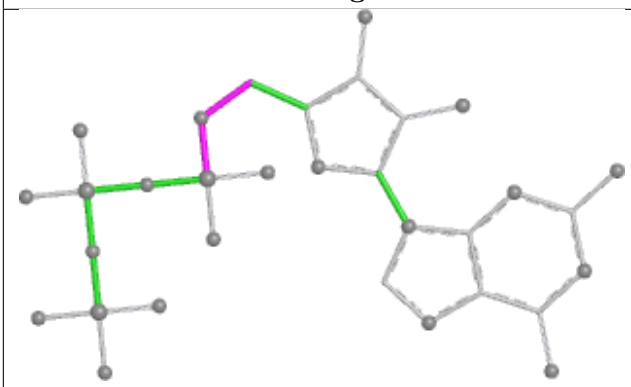
Ligand GTP HS 501



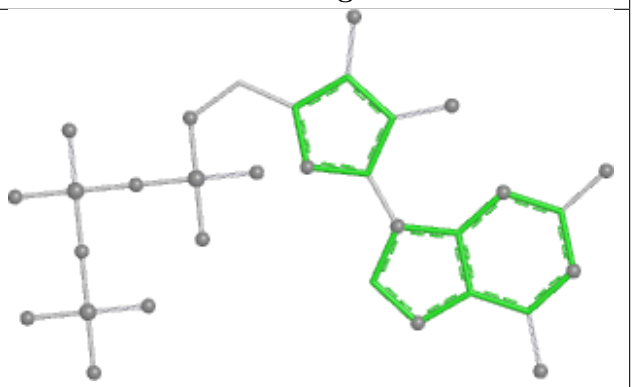
Bond lengths



Bond angles

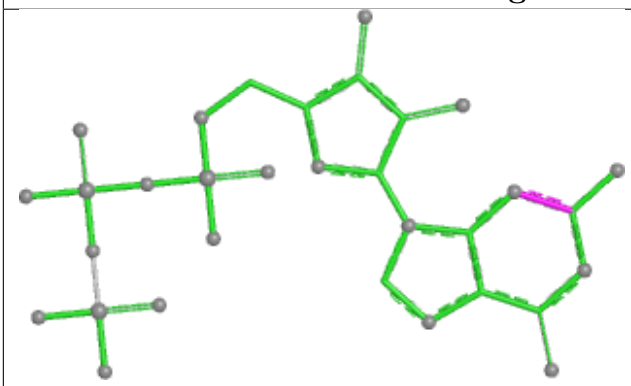


Torsions

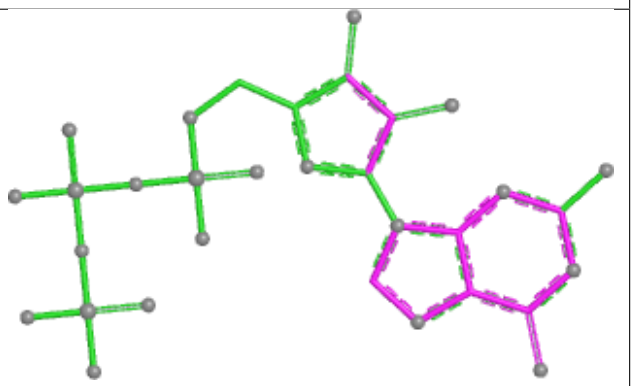


Rings

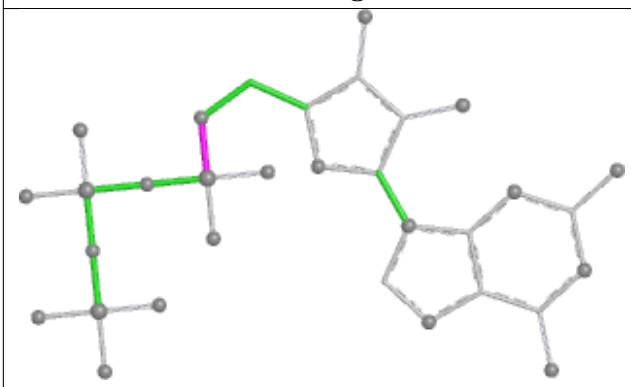
Ligand GTP NC 501



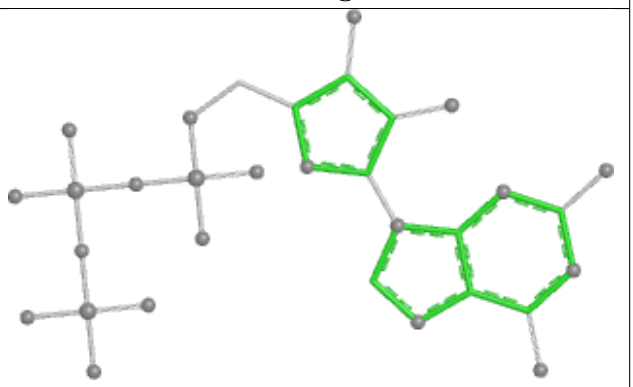
Bond lengths



Bond angles

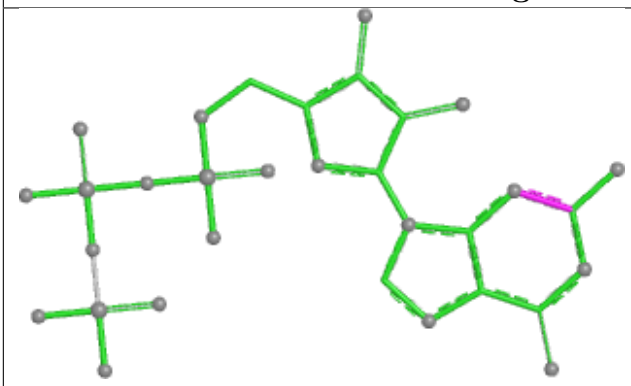


Torsions

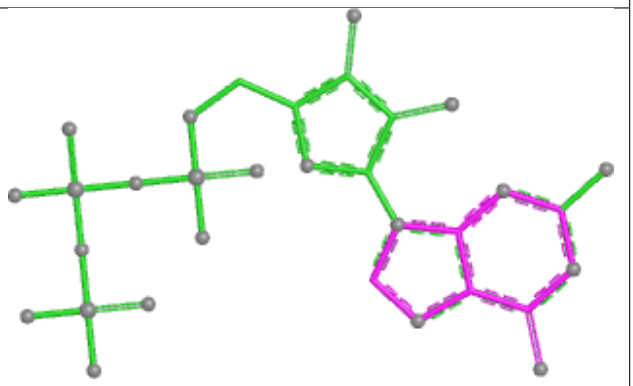


Rings

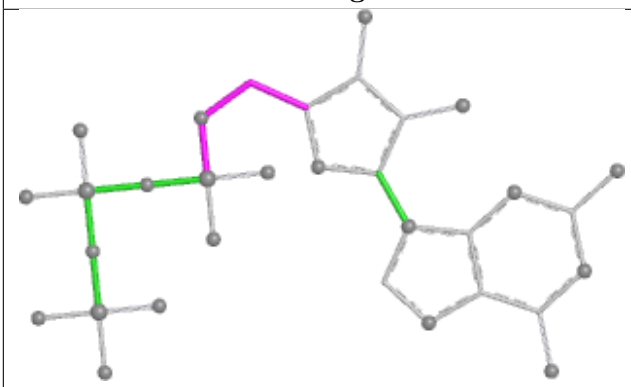
Ligand GTP SO 501



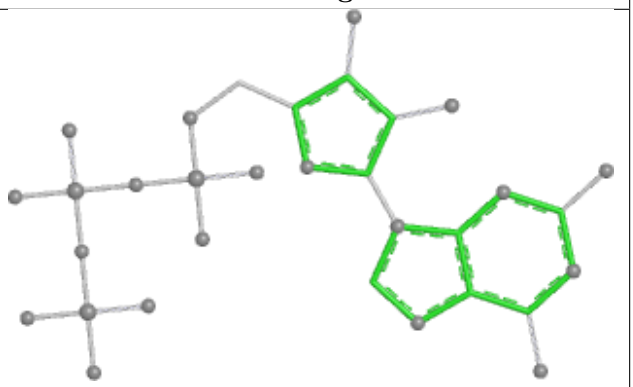
Bond lengths



Bond angles

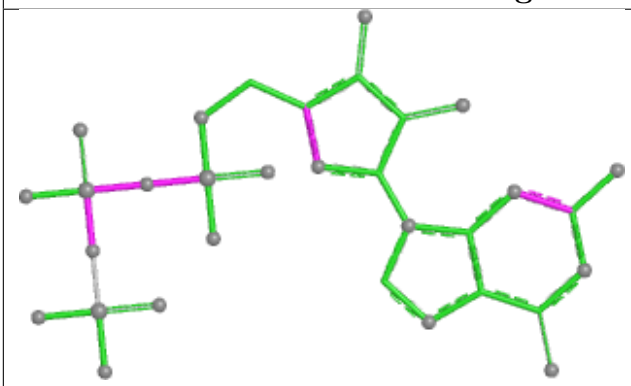


Torsions

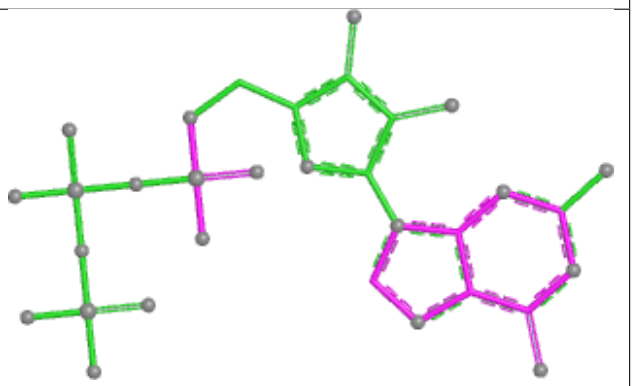


Rings

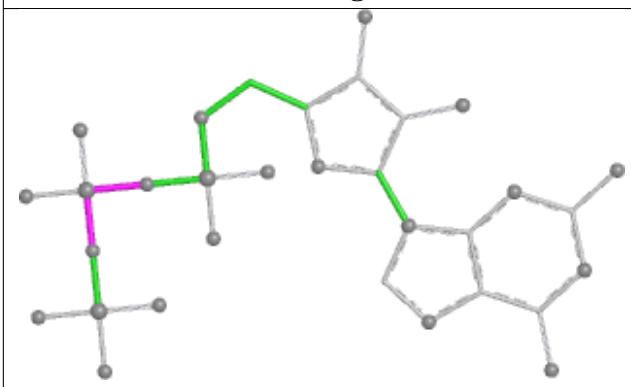
Ligand GTP IK 501



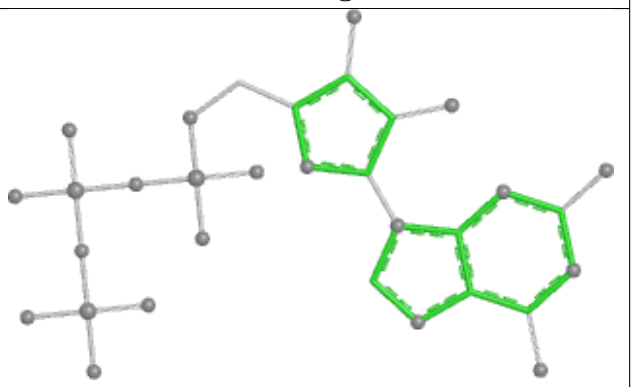
Bond lengths



Bond angles

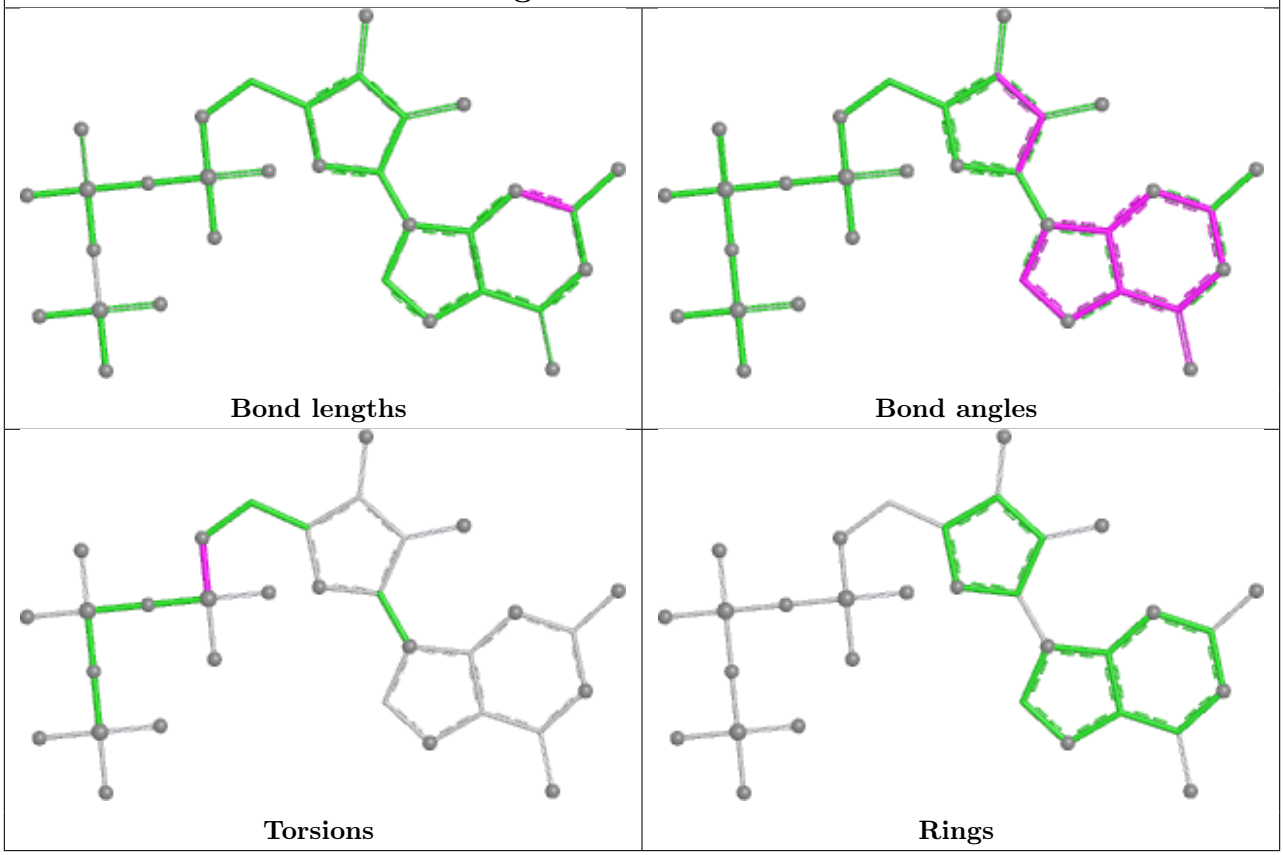


Torsions

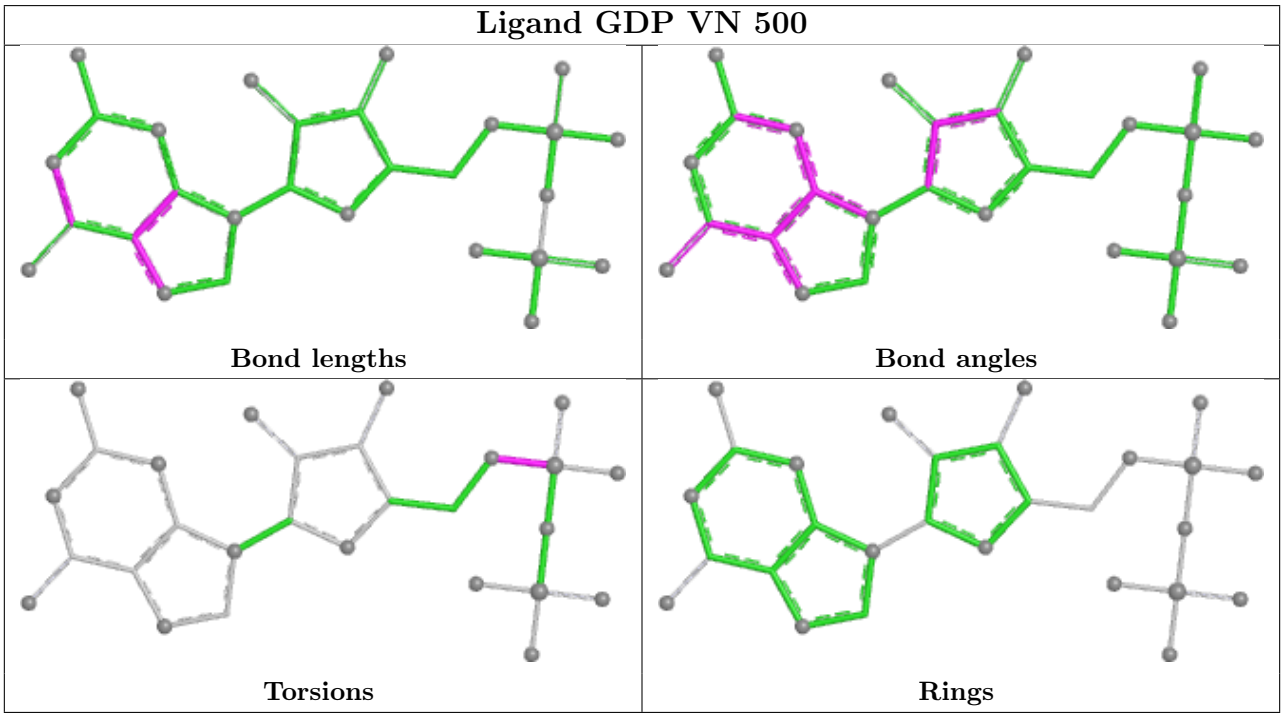


Rings

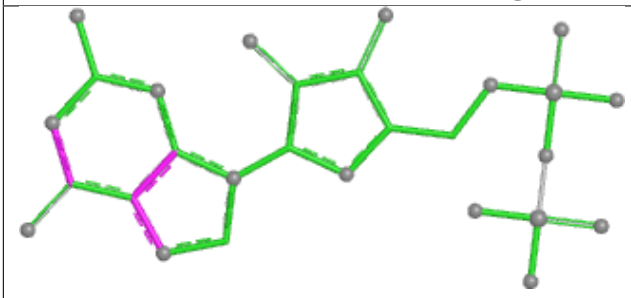
Ligand GTP JV 501



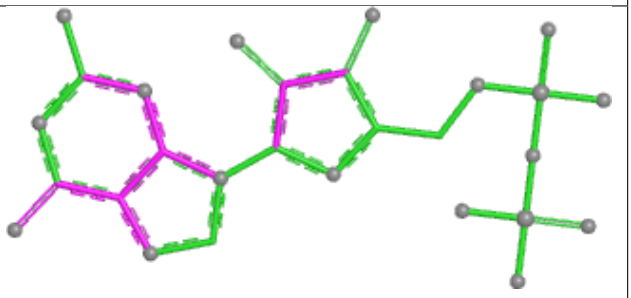
Ligand GDP VN 500



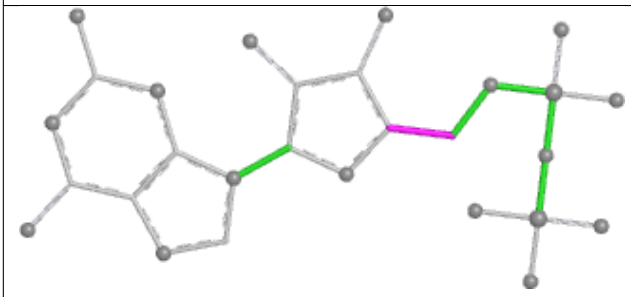
Ligand GDP HF 500



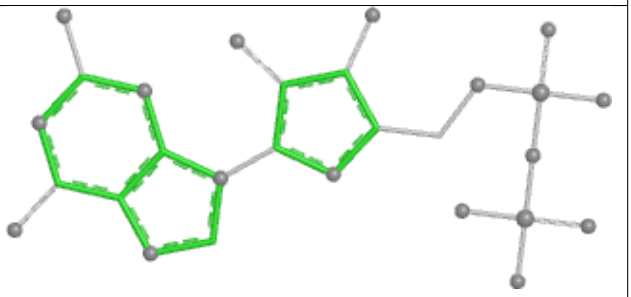
Bond lengths



Bond angles

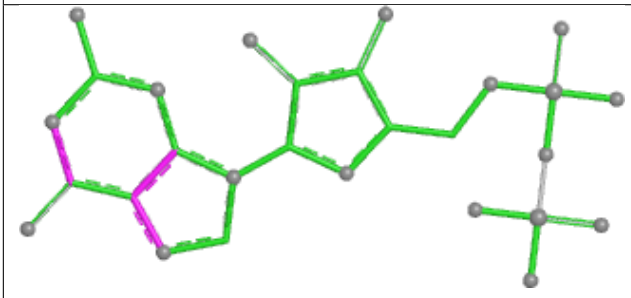


Torsions

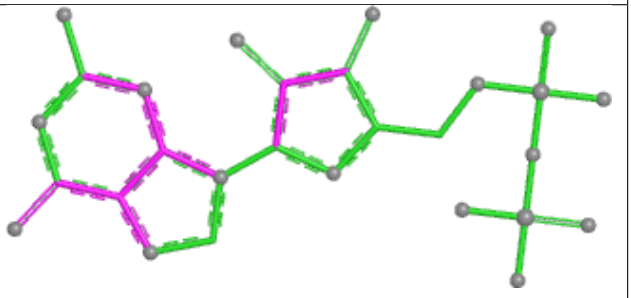


Rings

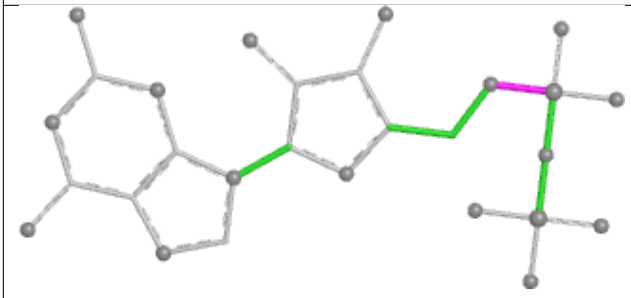
Ligand GDP RS 500



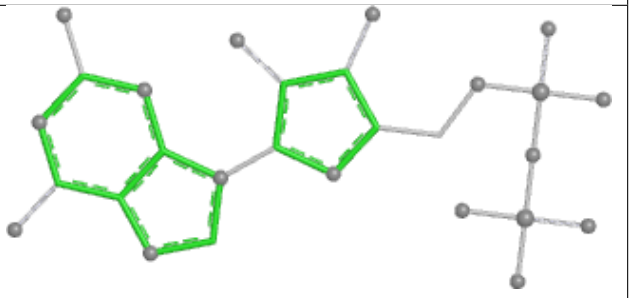
Bond lengths



Bond angles

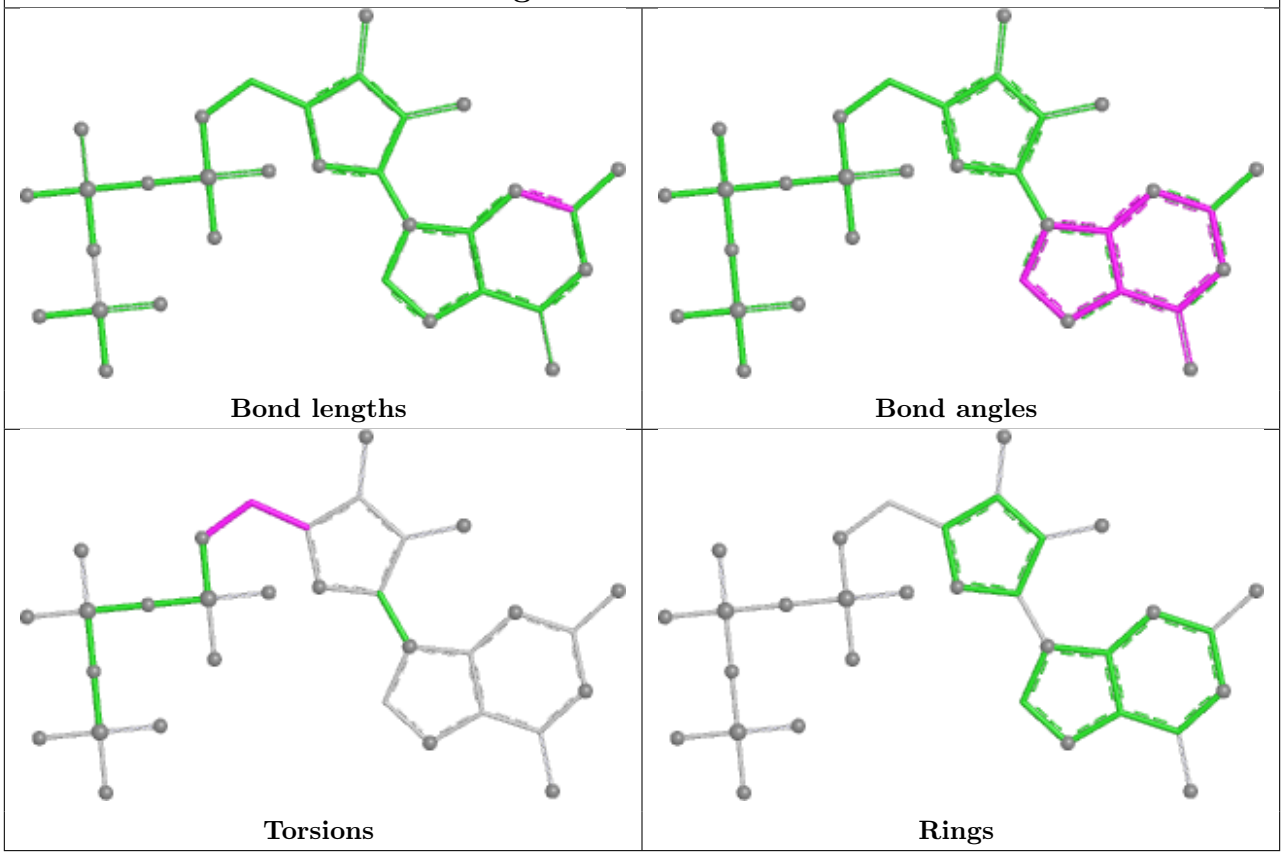


Torsions

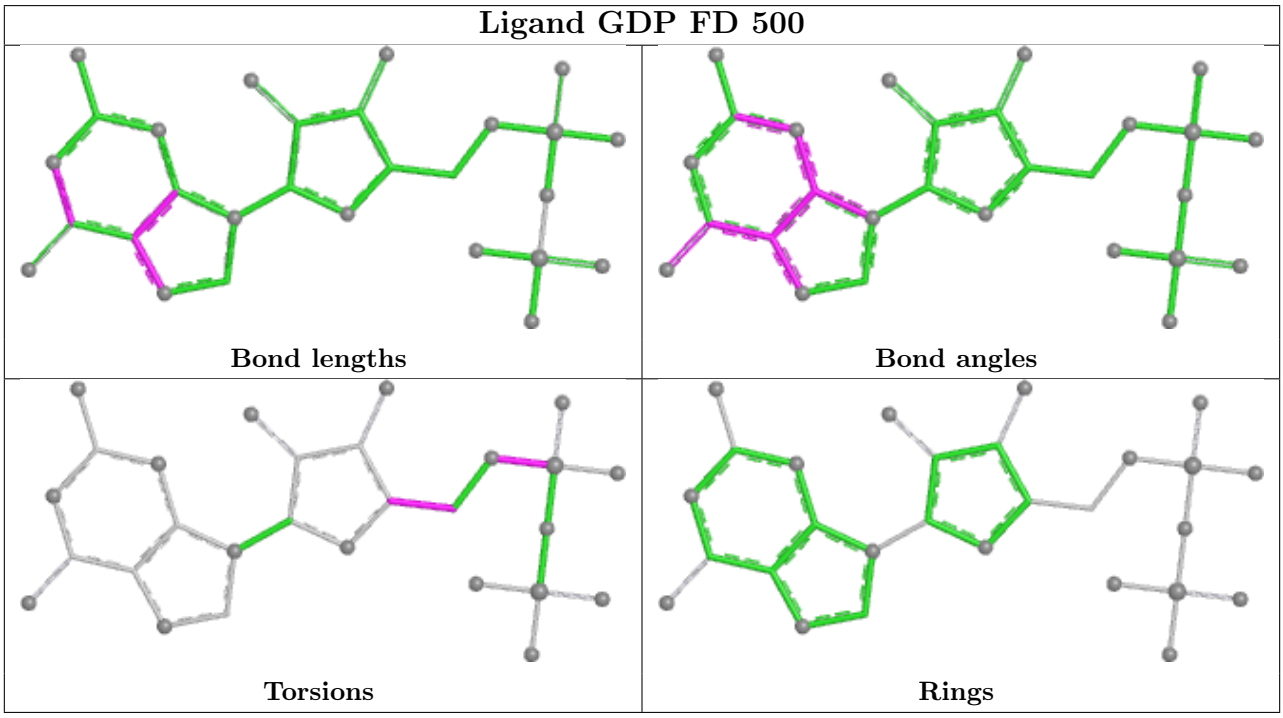


Rings

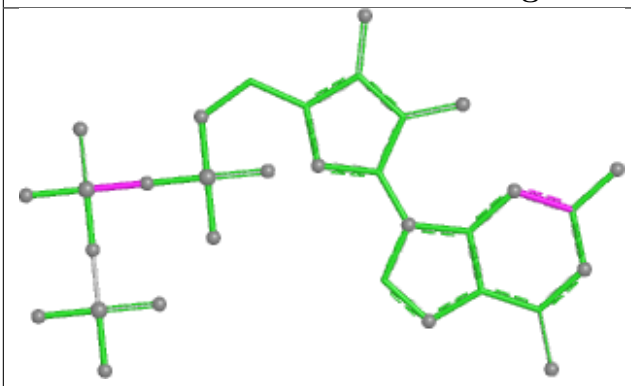
Ligand GTP JK 501



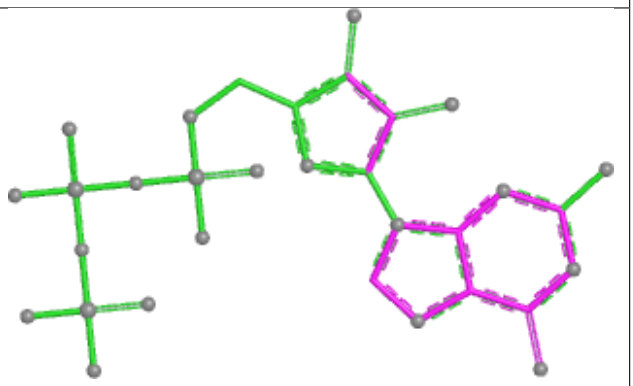
Ligand GDP FD 500



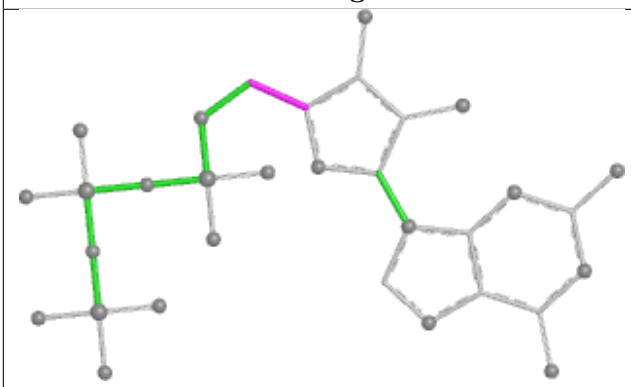
Ligand GTP K 501



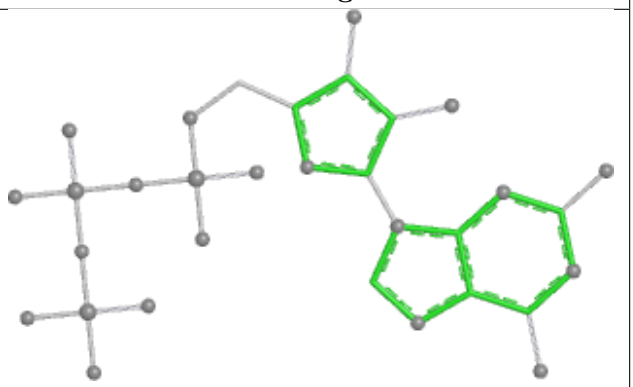
Bond lengths



Bond angles

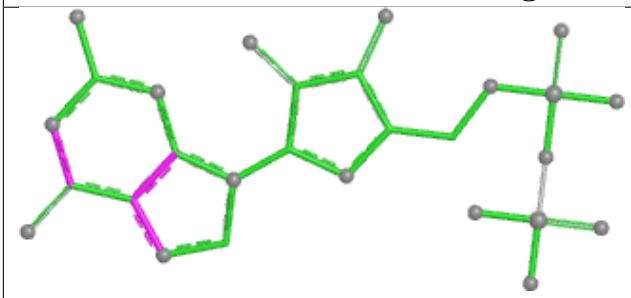


Torsions

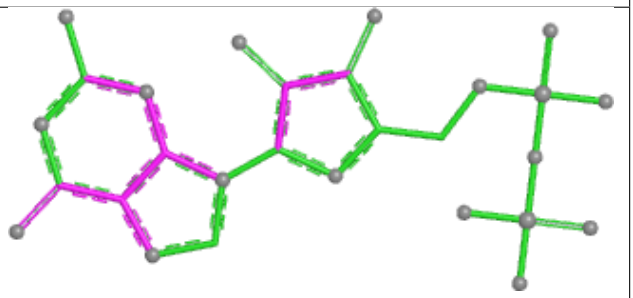


Rings

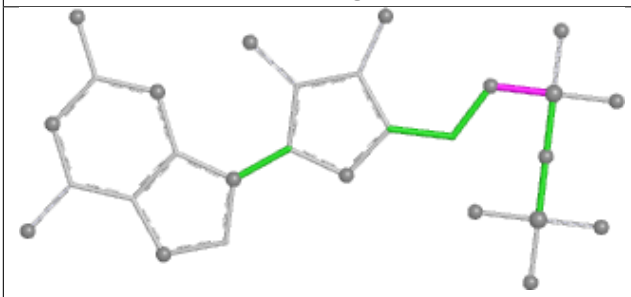
Ligand GDP H 500



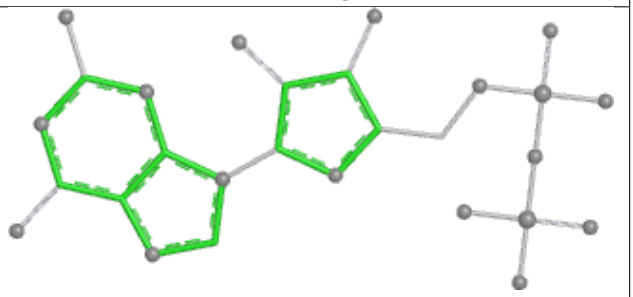
Bond lengths



Bond angles

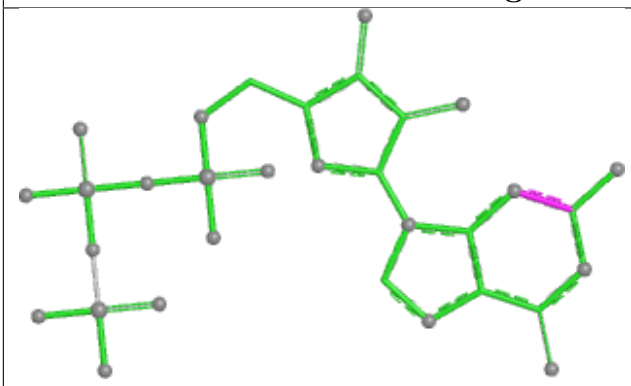


Torsions

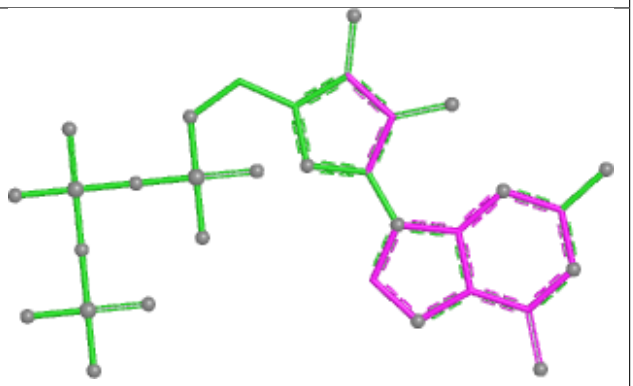


Rings

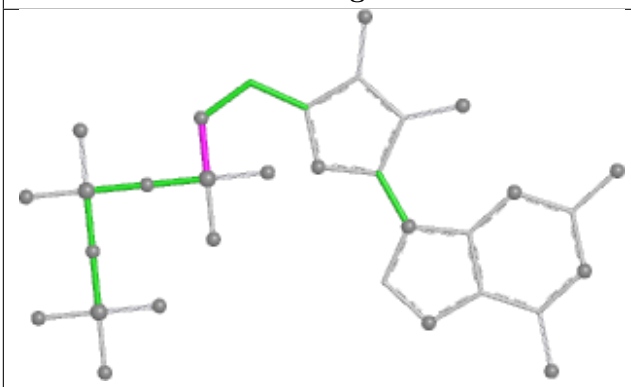
Ligand GTP MY 501



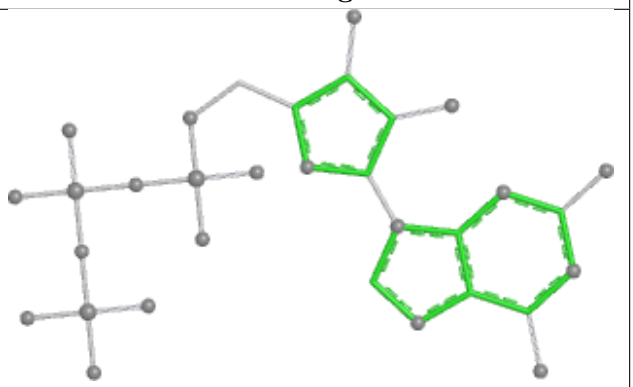
Bond lengths



Bond angles

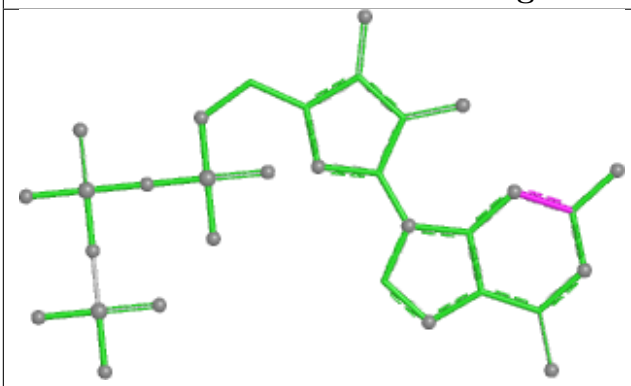


Torsions

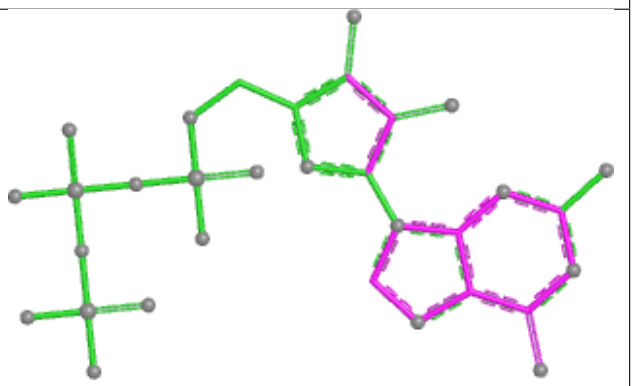


Rings

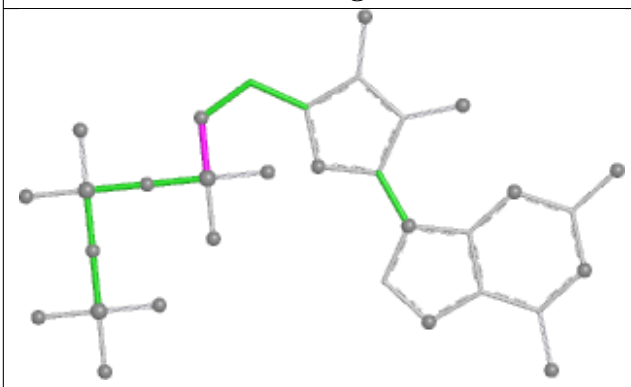
Ligand GTP JJ 501



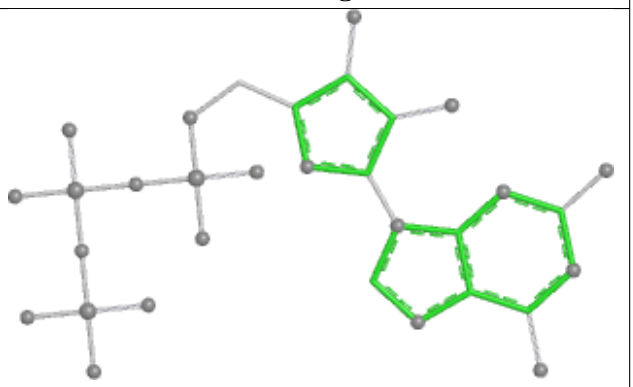
Bond lengths



Bond angles

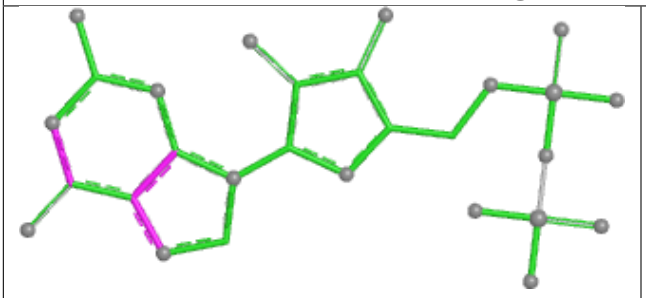


Torsions

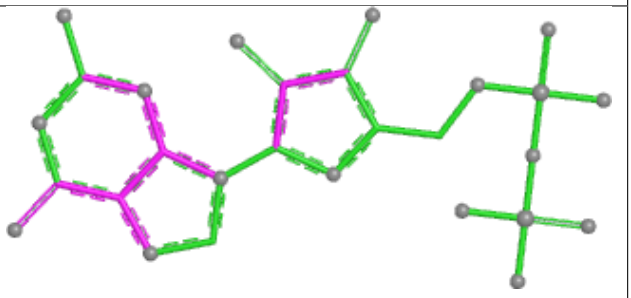


Rings

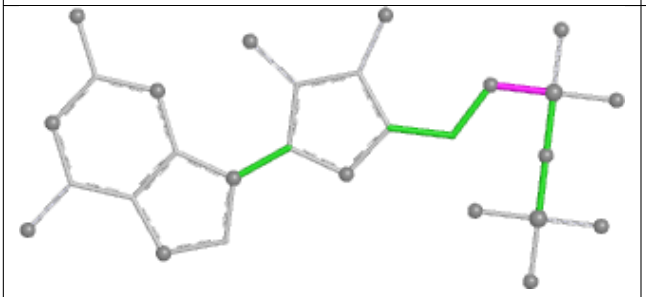
Ligand GDP AJ 500



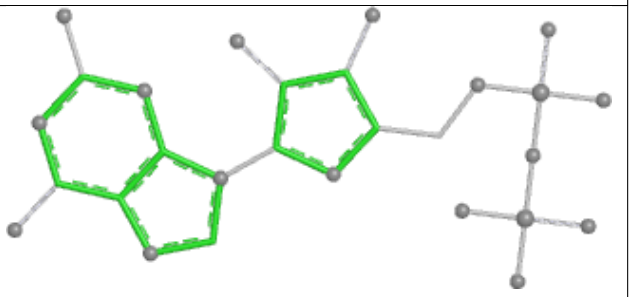
Bond lengths



Bond angles

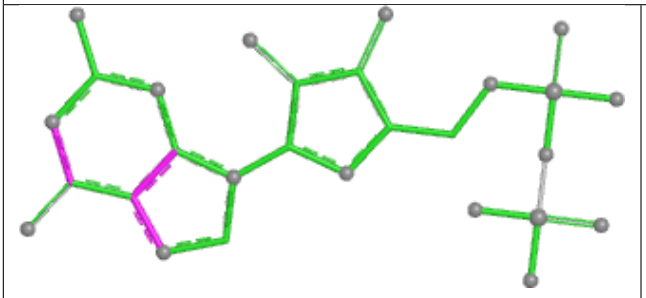


Torsions

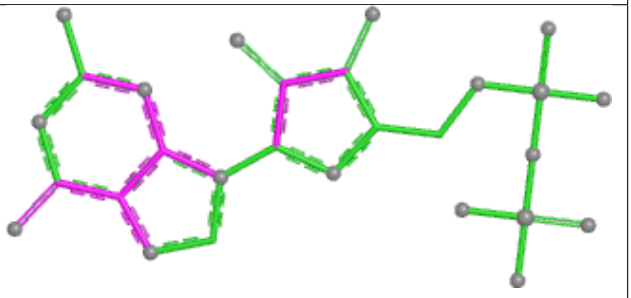


Rings

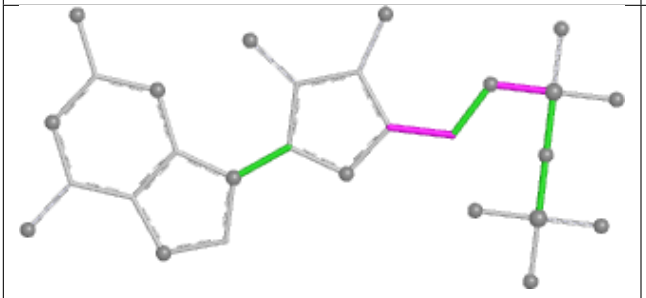
Ligand GDP CE 500



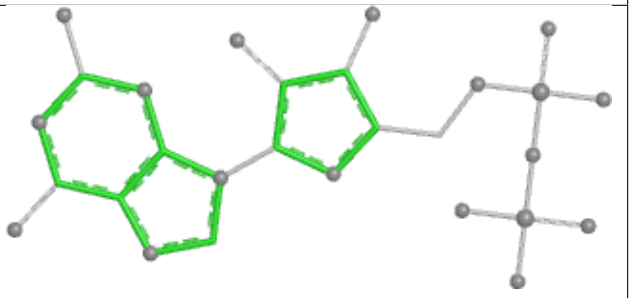
Bond lengths



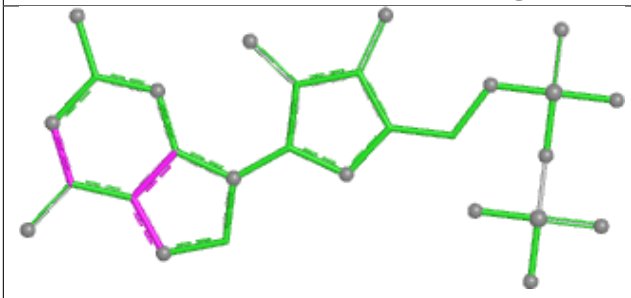
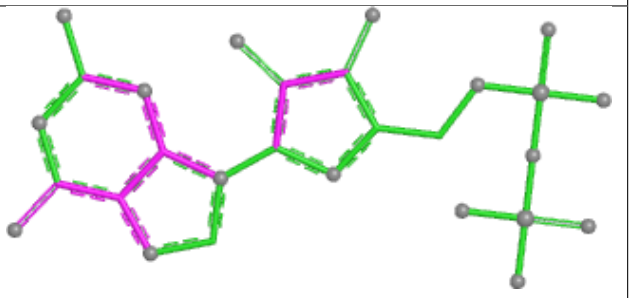
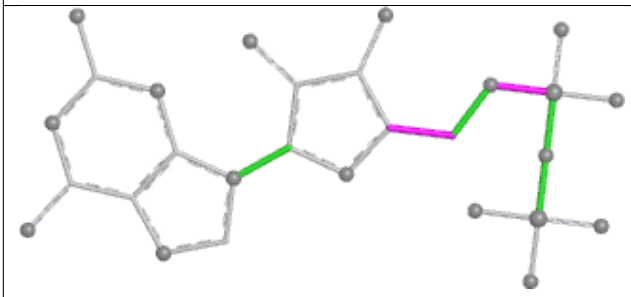
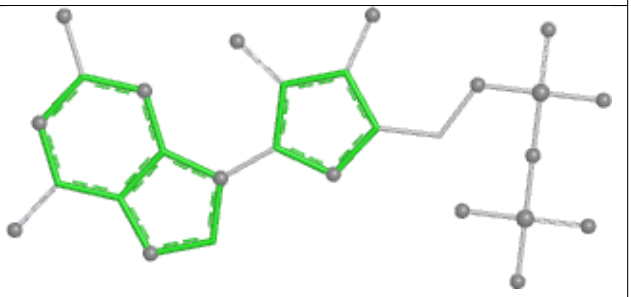
Bond angles

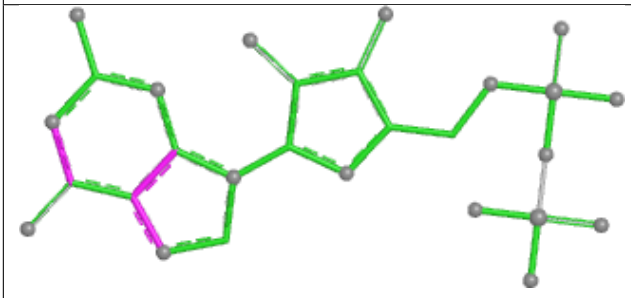
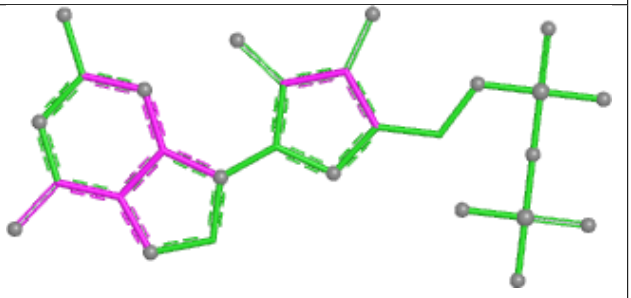
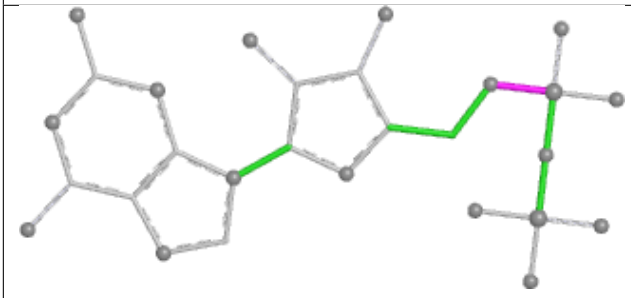
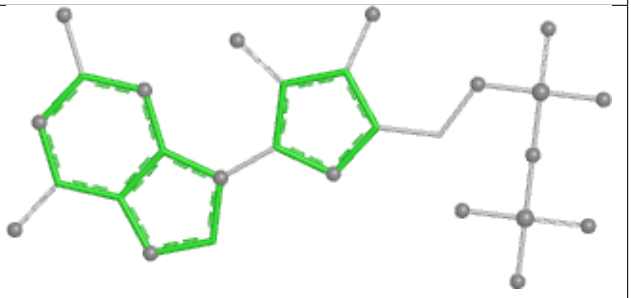


Torsions

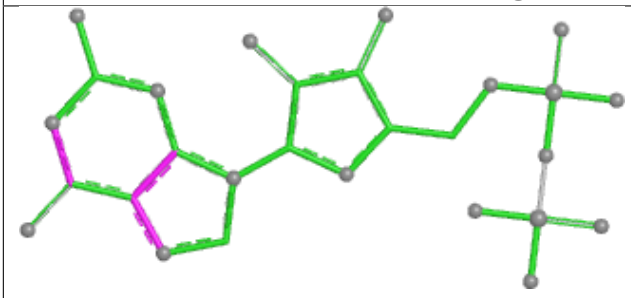


Rings

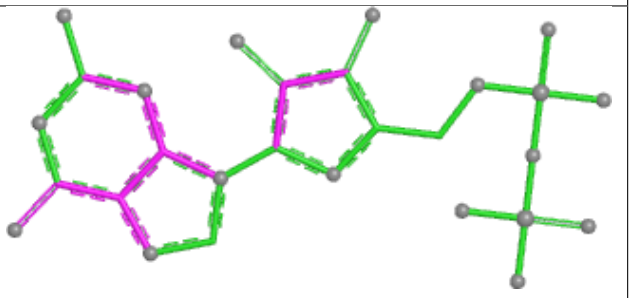
Ligand GDP SH 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP BH 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

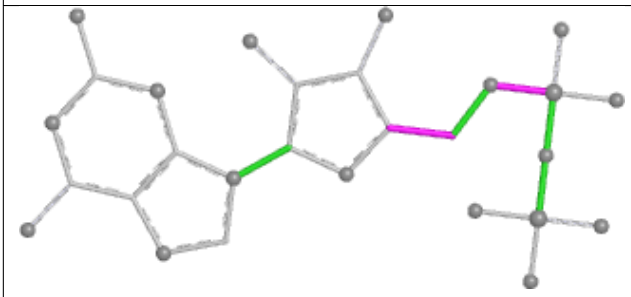
Ligand GDP FX 500



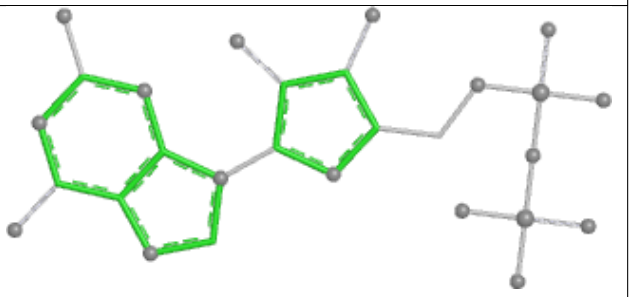
Bond lengths



Bond angles

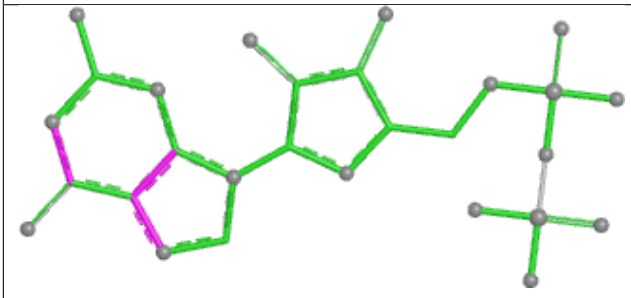


Torsions

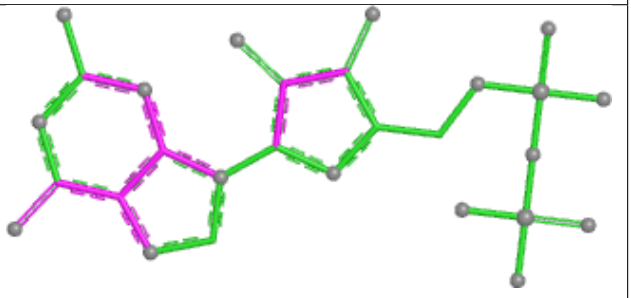


Rings

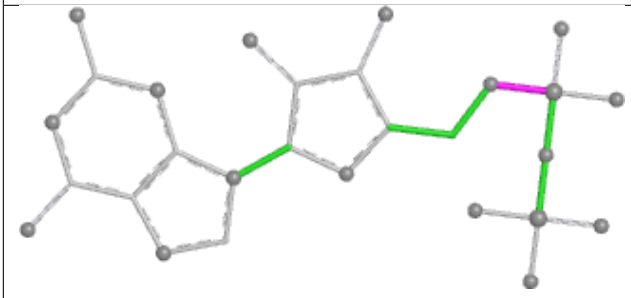
Ligand GDP AP 500



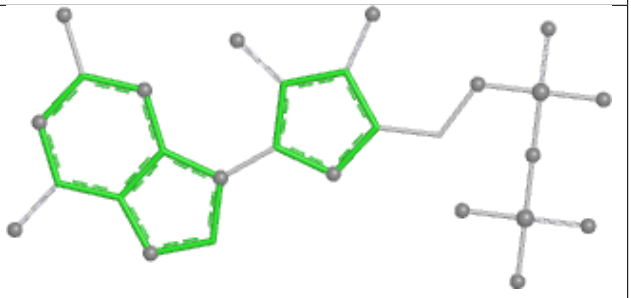
Bond lengths



Bond angles

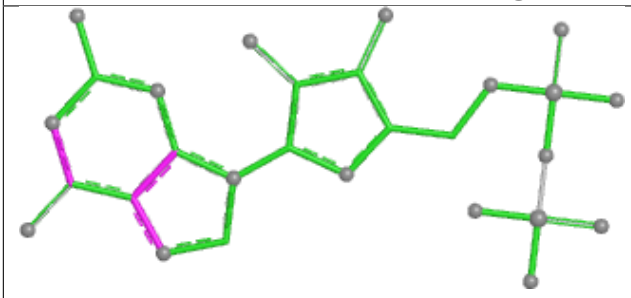


Torsions

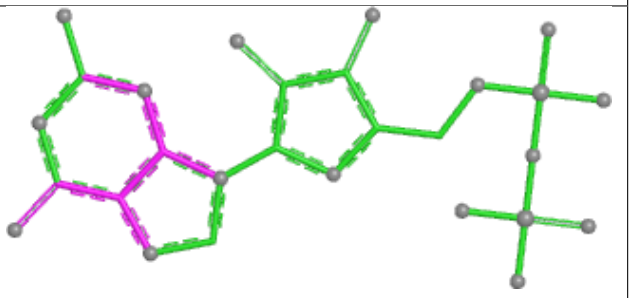


Rings

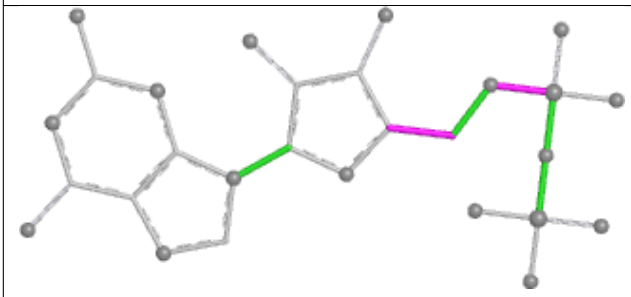
Ligand GDP LO 500



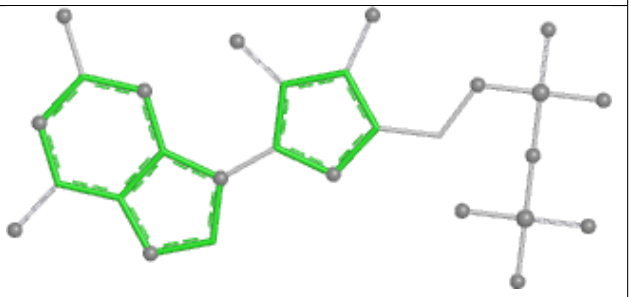
Bond lengths



Bond angles

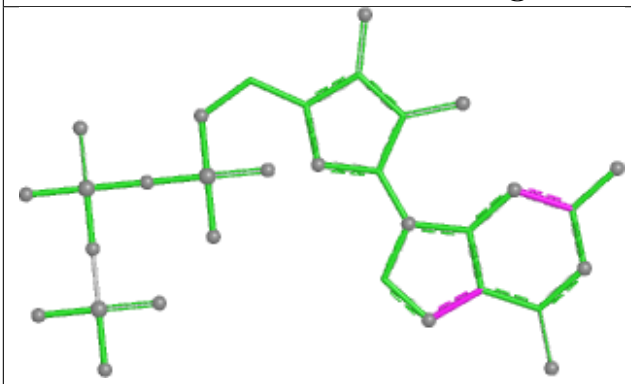


Torsions

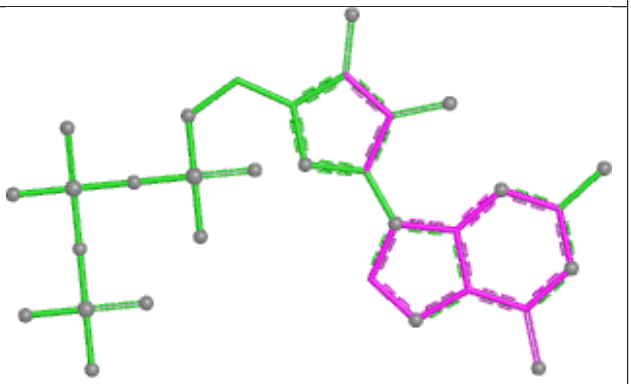


Rings

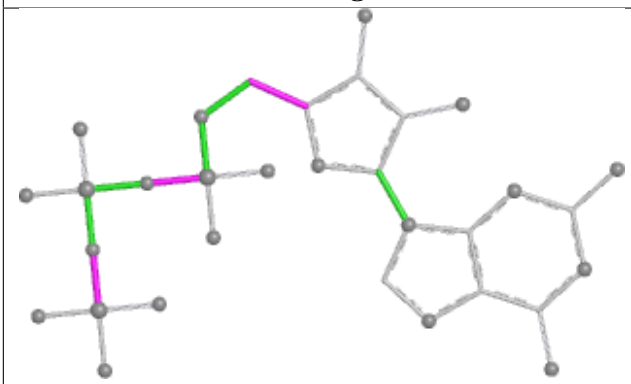
Ligand GTP CH 501



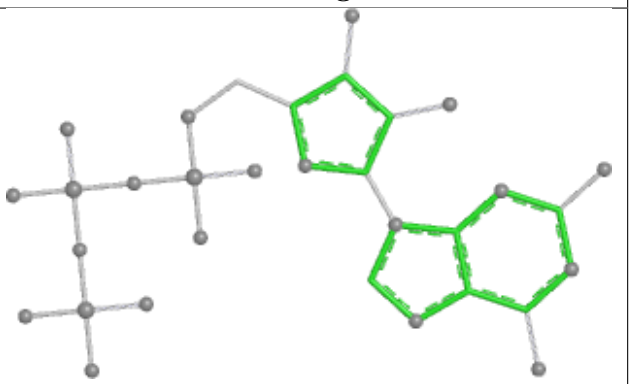
Bond lengths



Bond angles

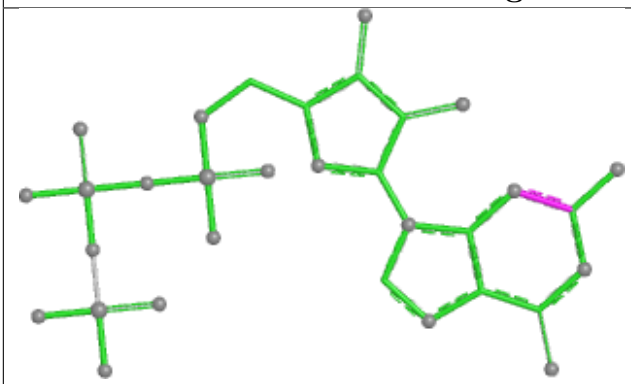


Torsions

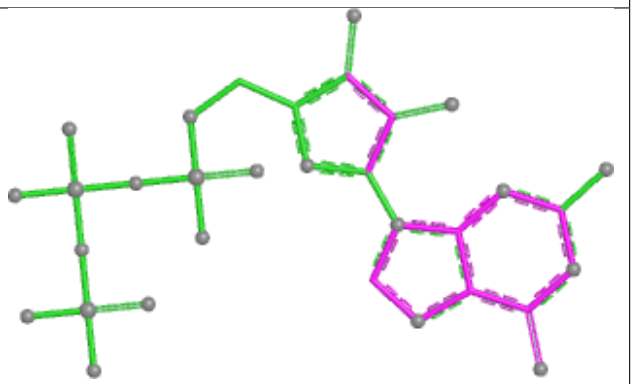


Rings

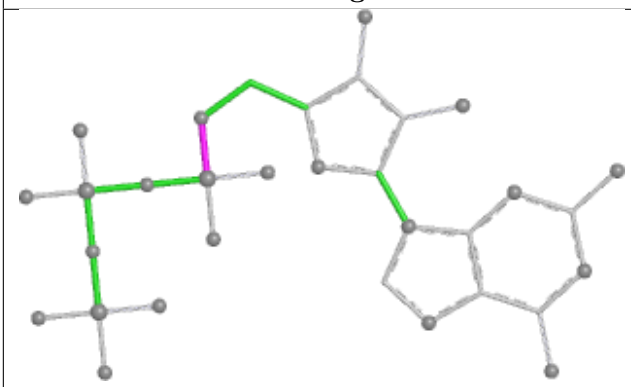
Ligand GTP WA 501



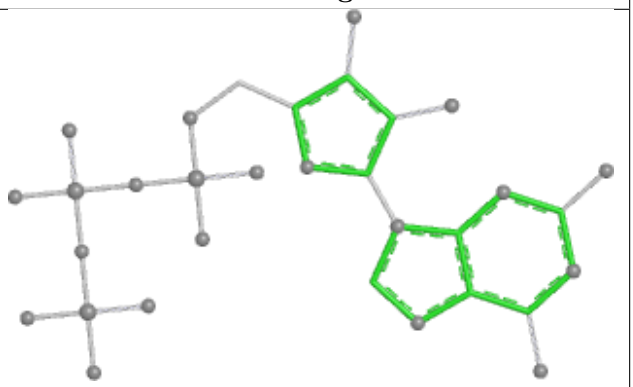
Bond lengths



Bond angles

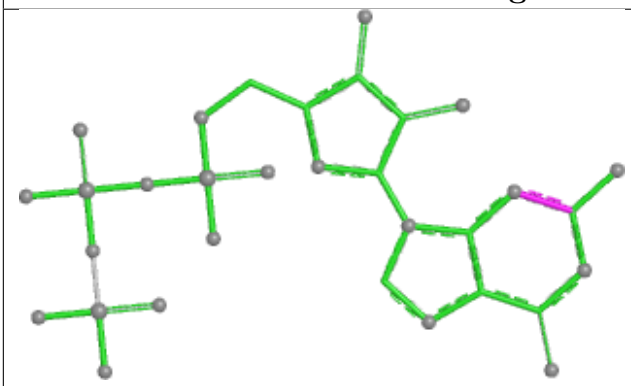


Torsions

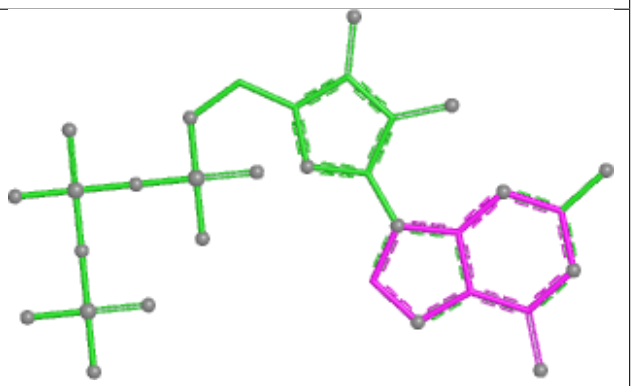


Rings

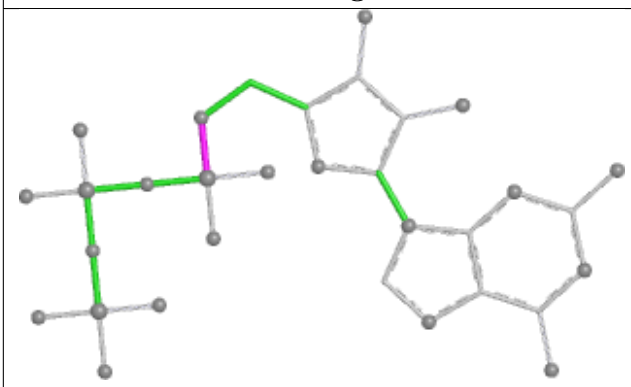
Ligand GTP DV 501



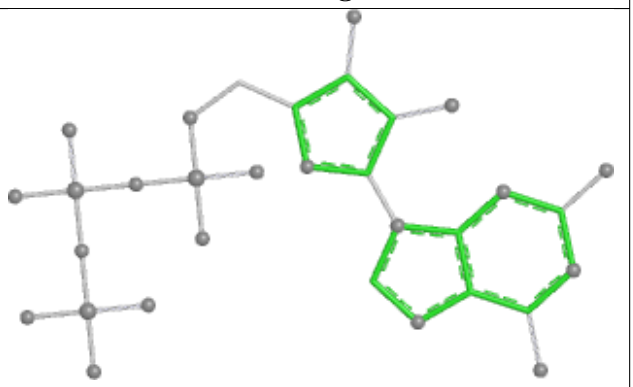
Bond lengths



Bond angles

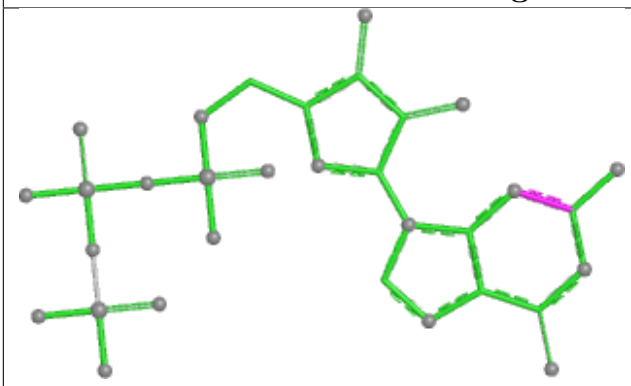


Torsions

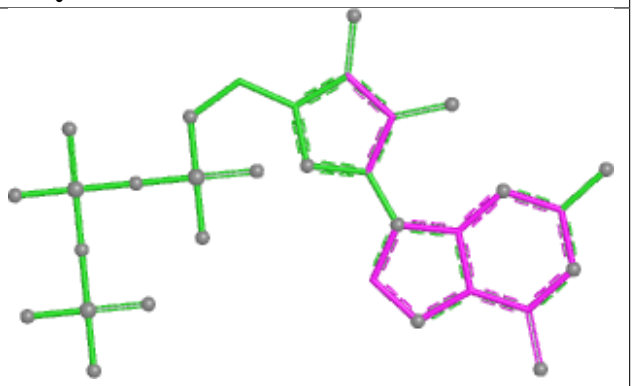


Rings

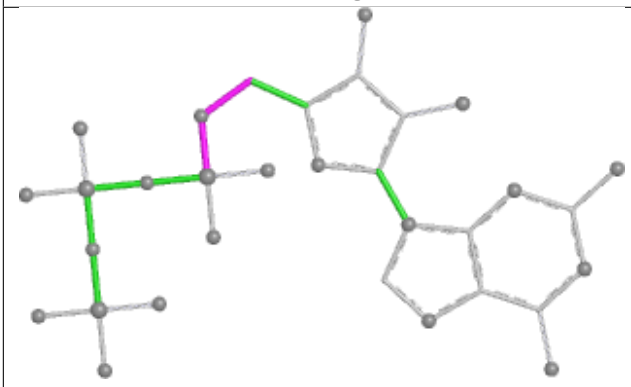
Ligand GTP QF 501



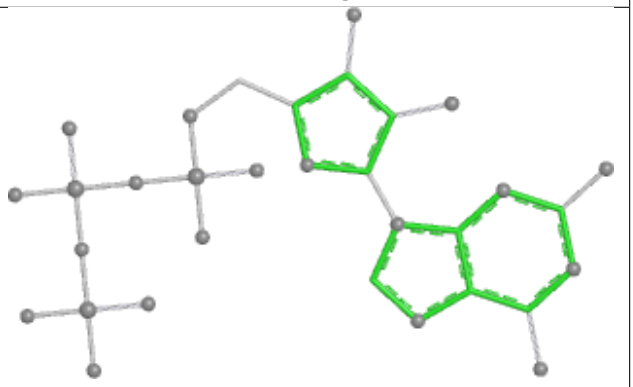
Bond lengths



Bond angles

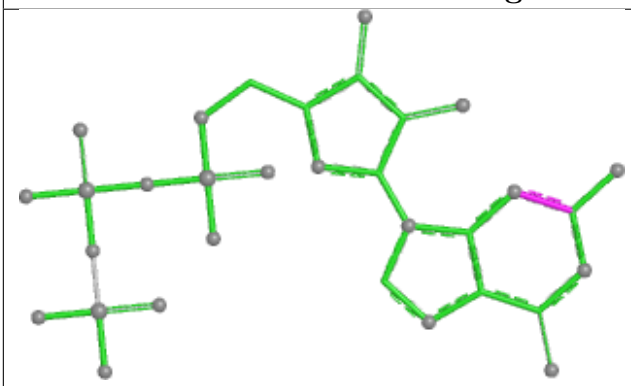


Torsions

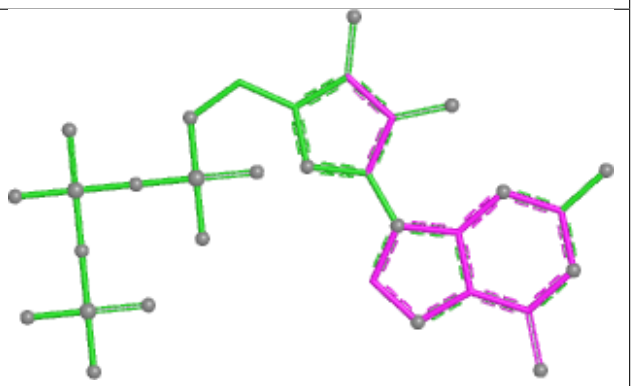


Rings

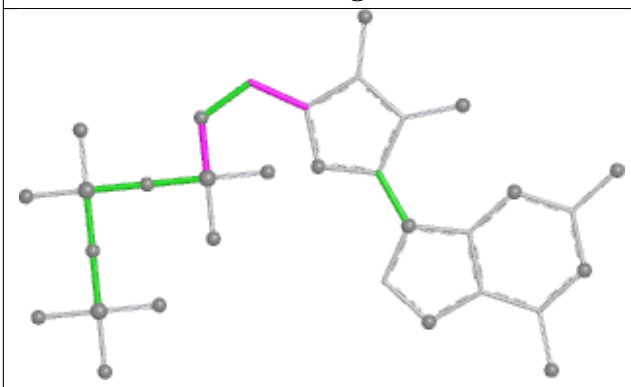
Ligand GTP VM 501



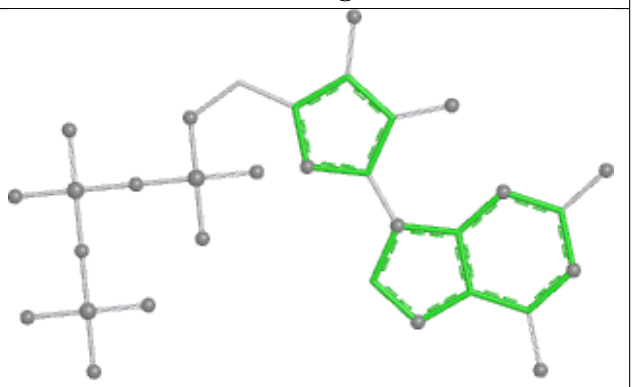
Bond lengths



Bond angles

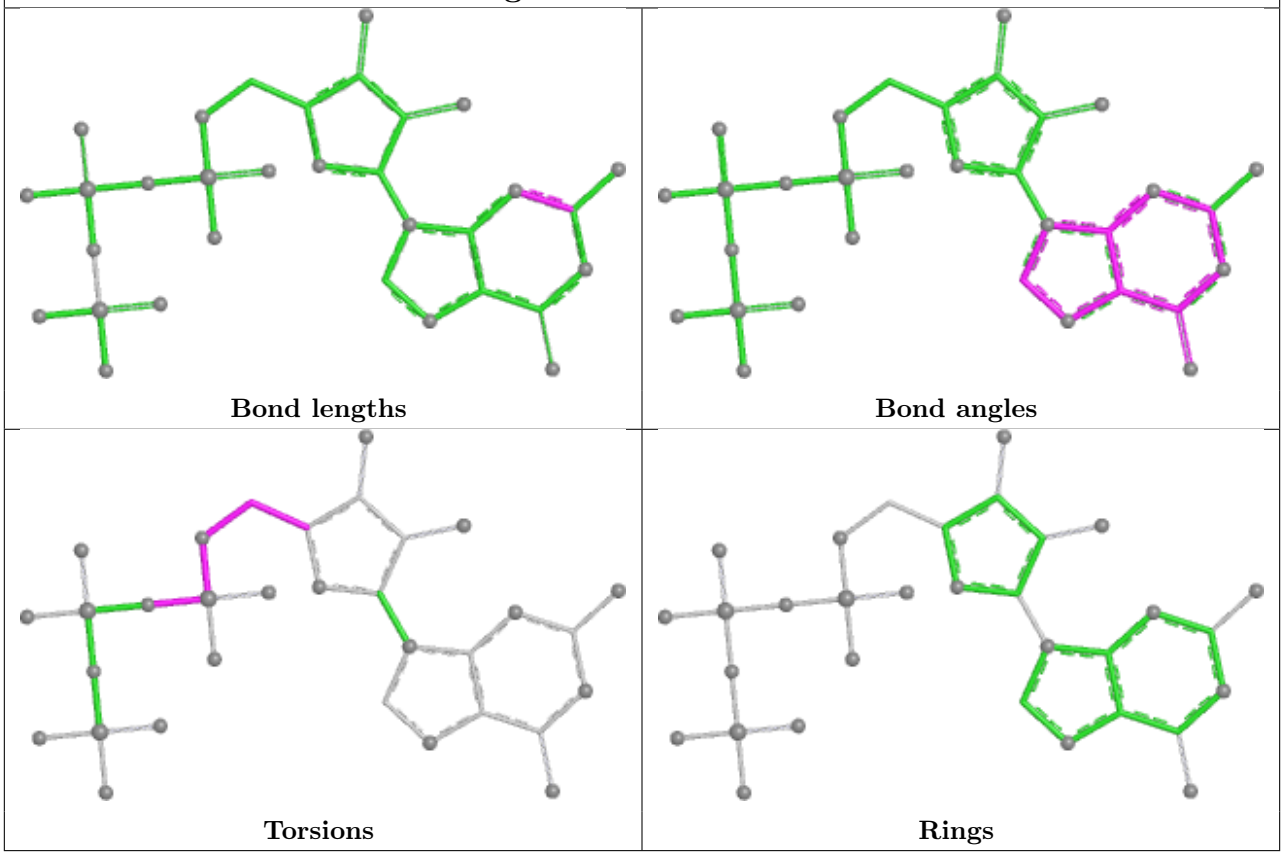


Torsions

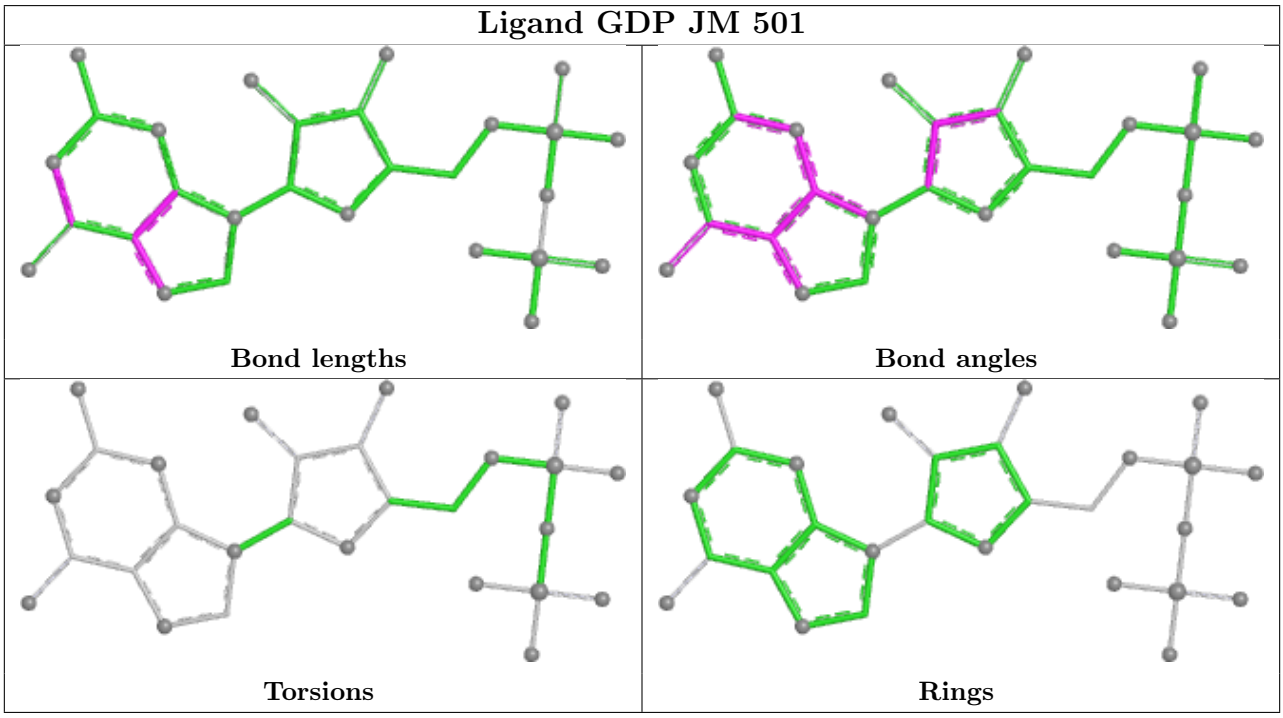


Rings

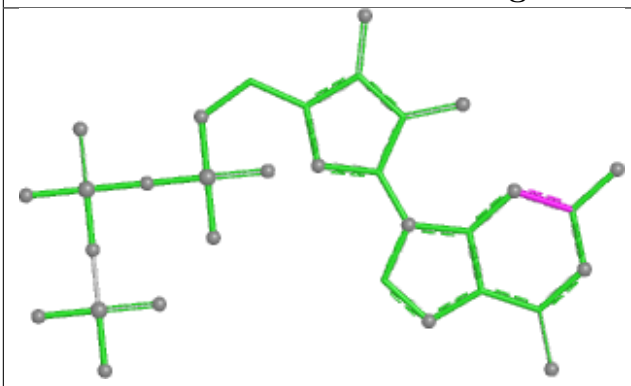
Ligand GTP UW 501



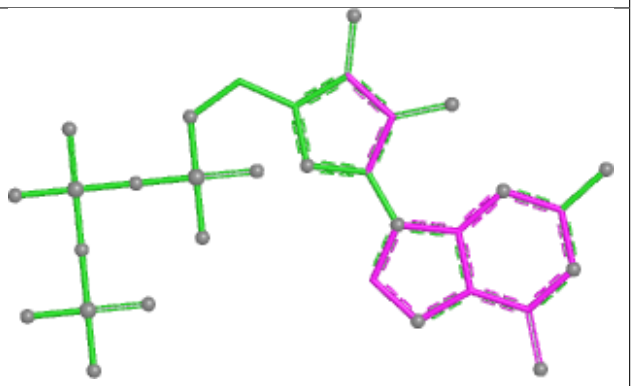
Ligand GDP JM 501



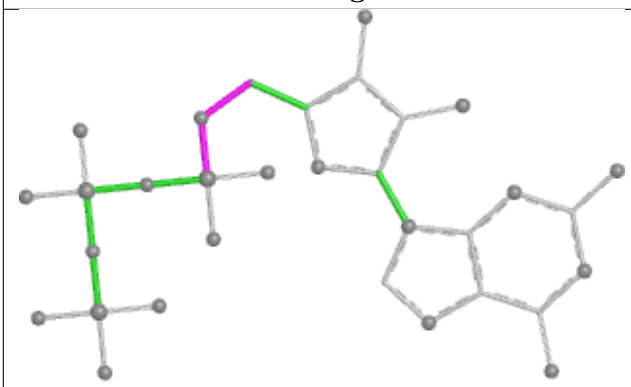
Ligand GTP AO 501



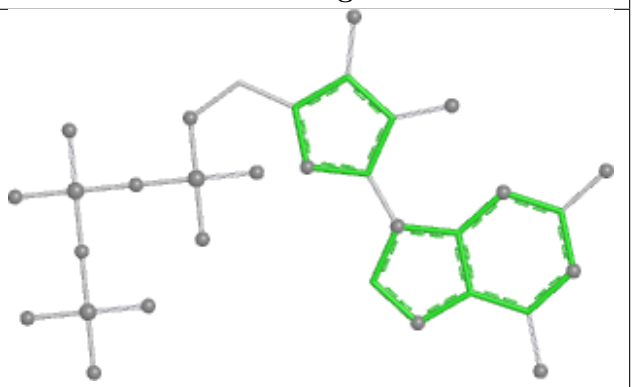
Bond lengths



Bond angles

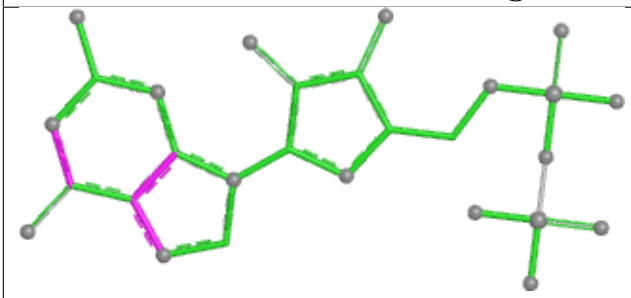


Torsions

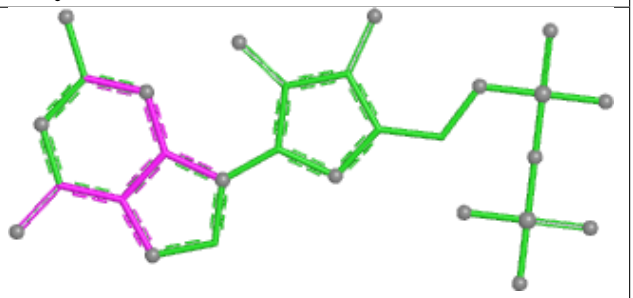


Rings

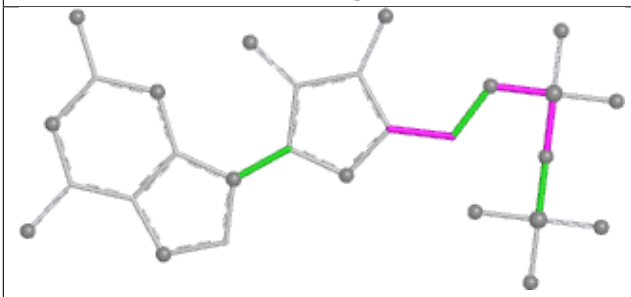
Ligand GDP QK 500



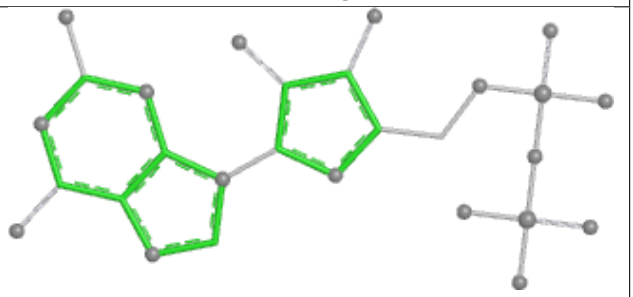
Bond lengths



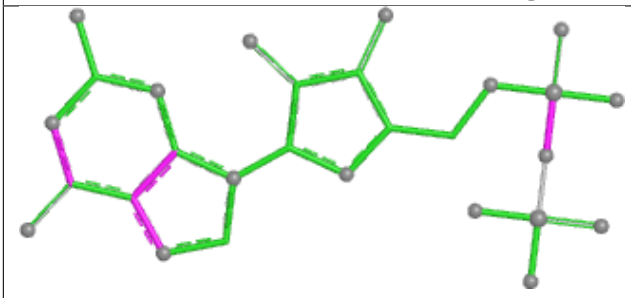
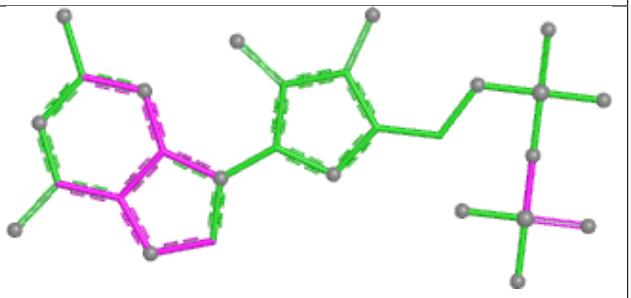
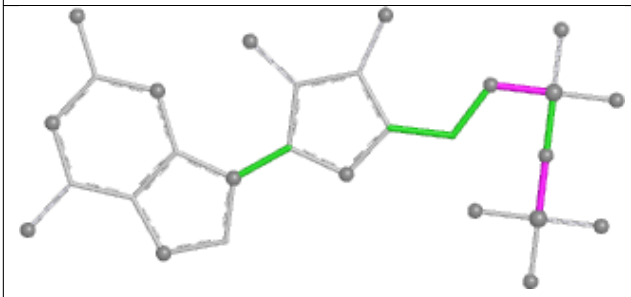
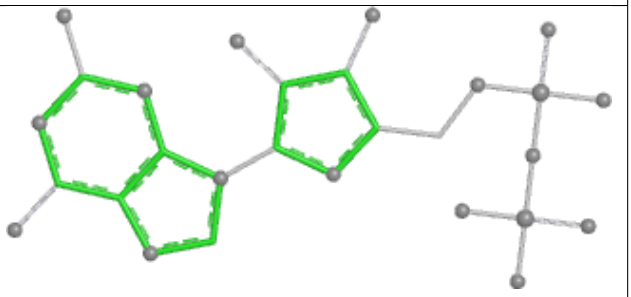
Bond angles

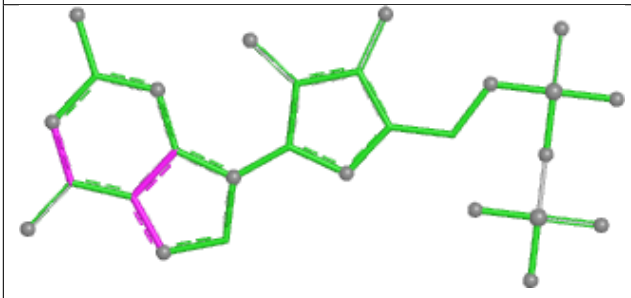
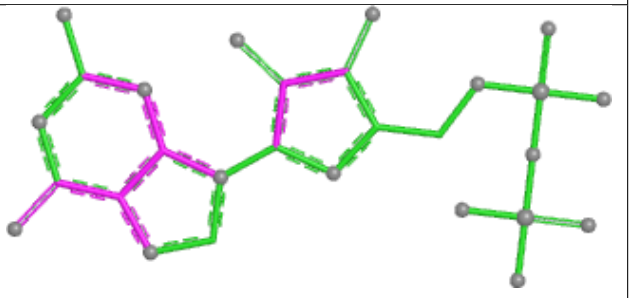
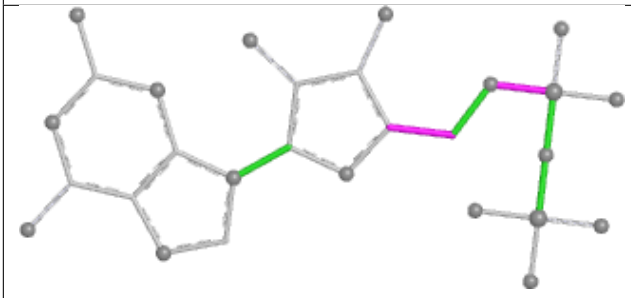
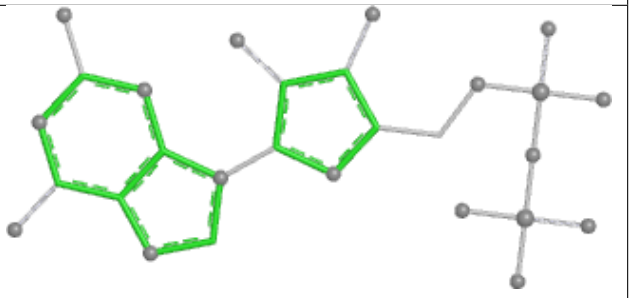


Torsions

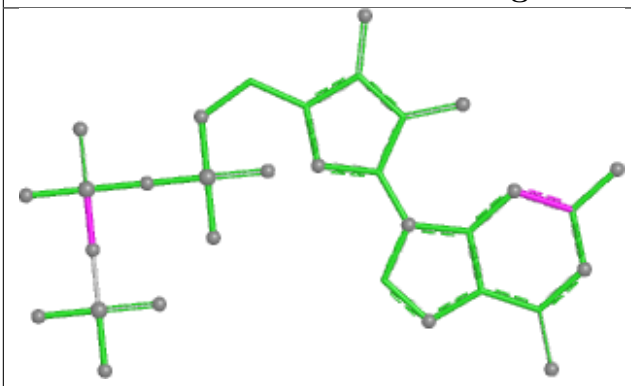


Rings

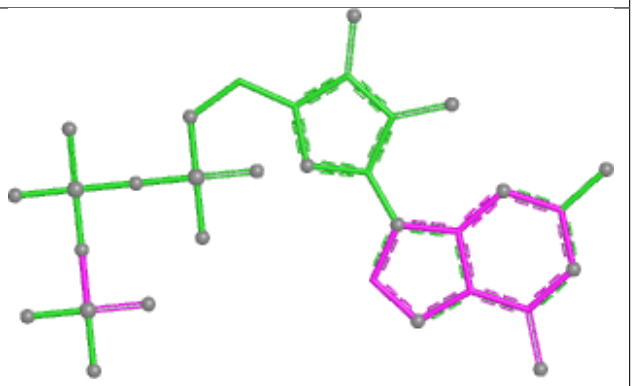
Ligand GDP E 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP ST 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

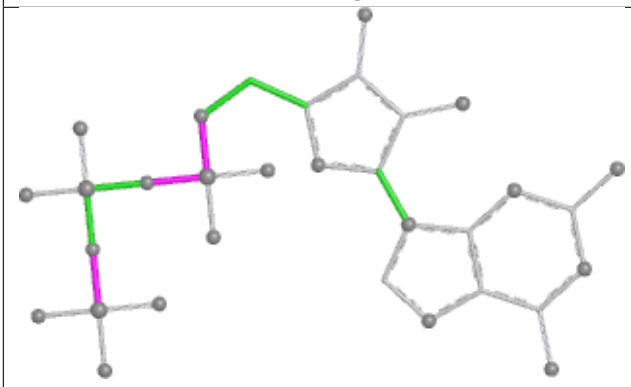
Ligand GTP CE 501



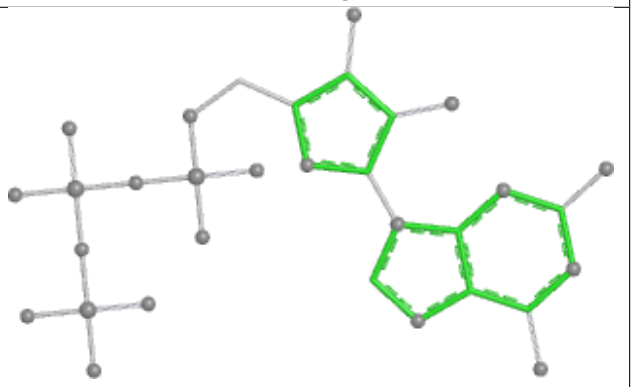
Bond lengths



Bond angles

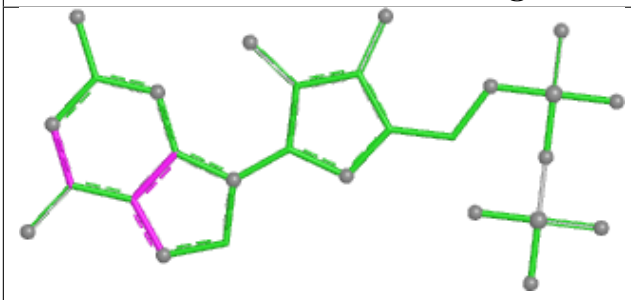


Torsions

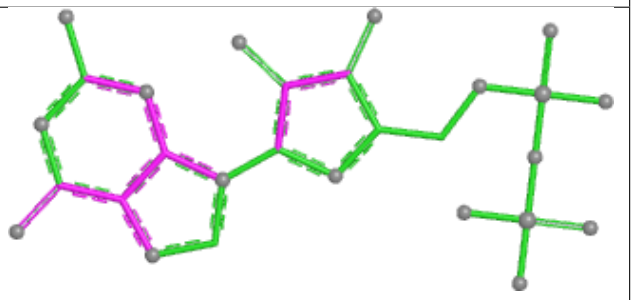


Rings

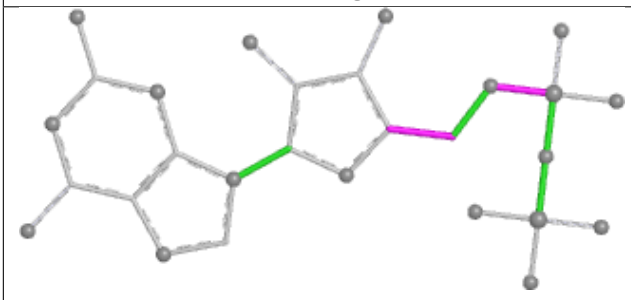
Ligand GDP PD 500



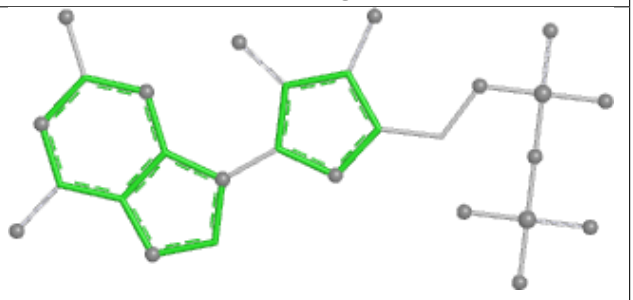
Bond lengths



Bond angles

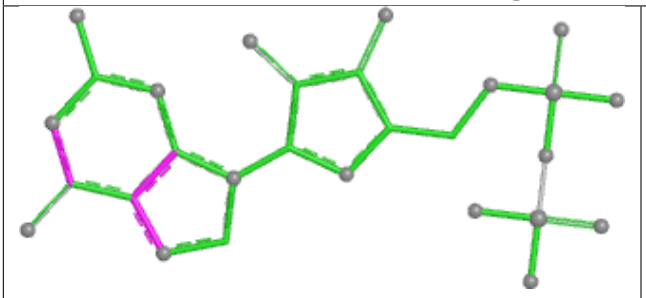


Torsions

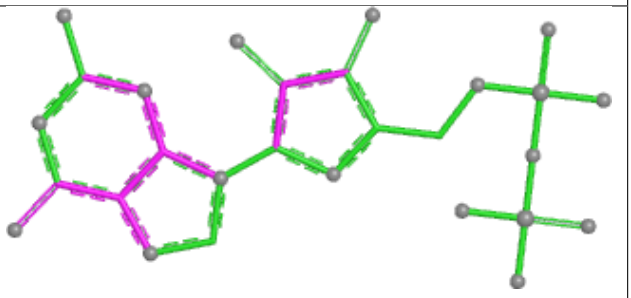


Rings

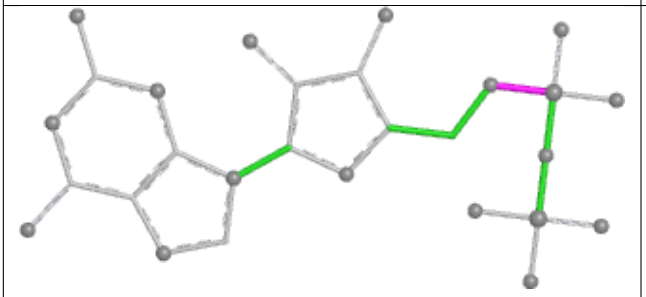
Ligand GDP OR 500



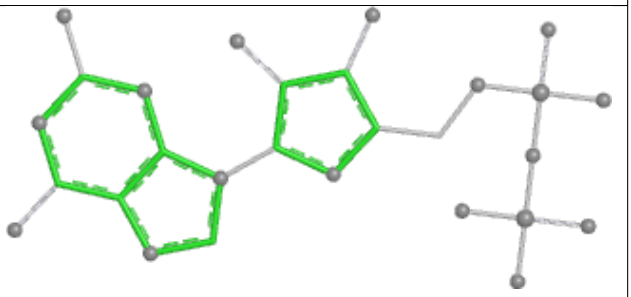
Bond lengths



Bond angles

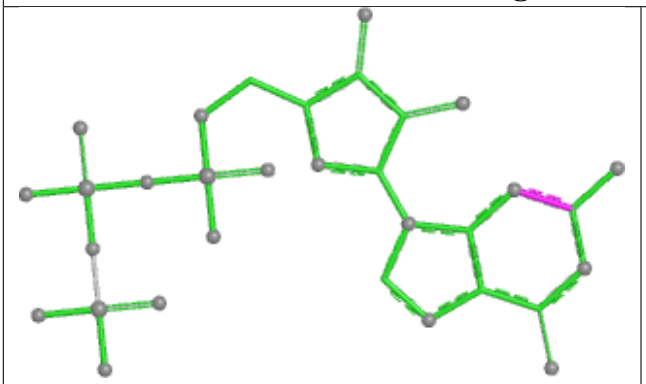


Torsions

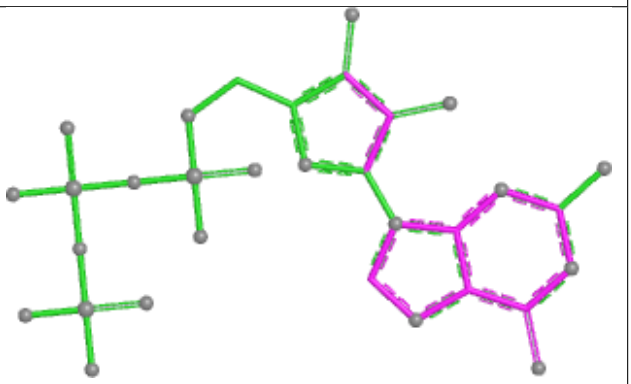


Rings

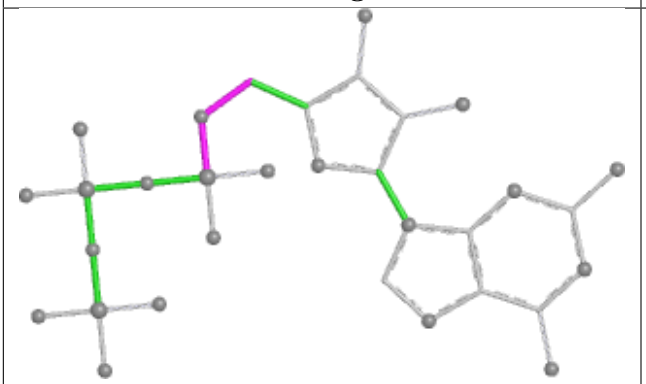
Ligand GTP SA 501



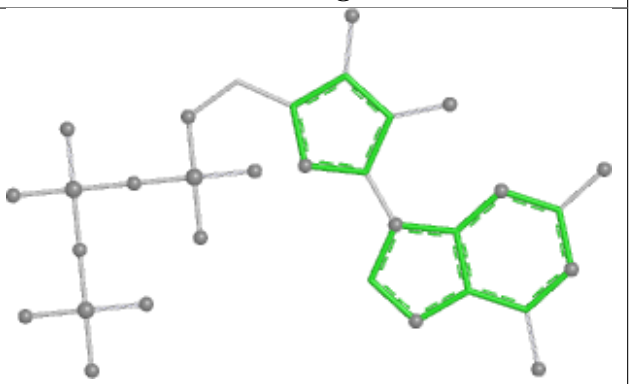
Bond lengths



Bond angles

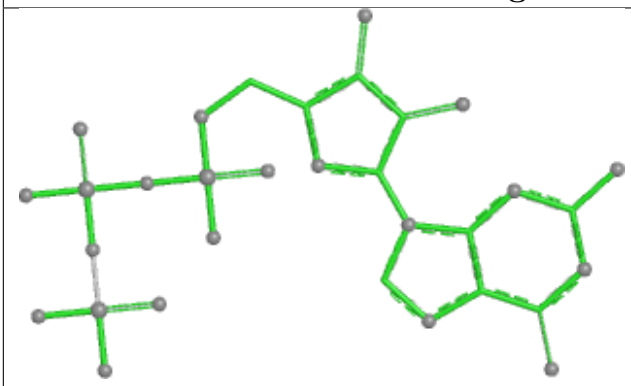


Torsions

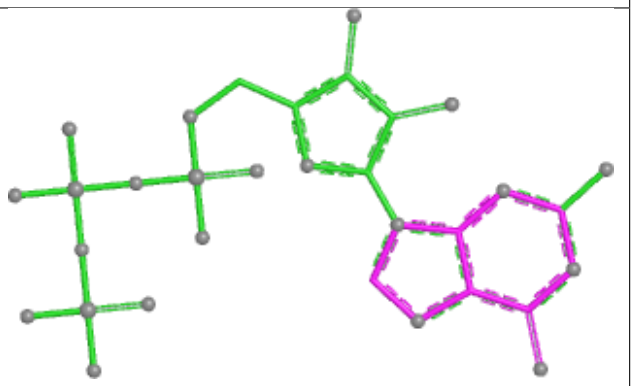


Rings

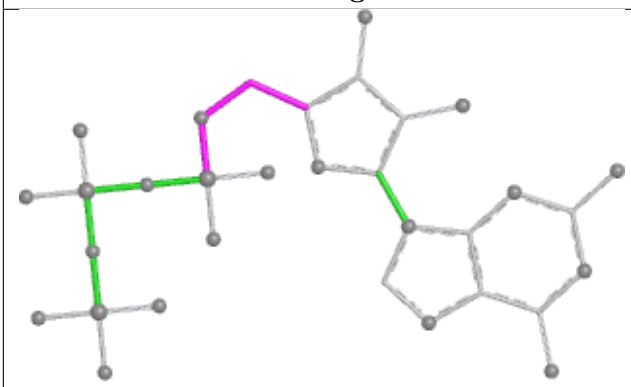
Ligand GTP AG 501



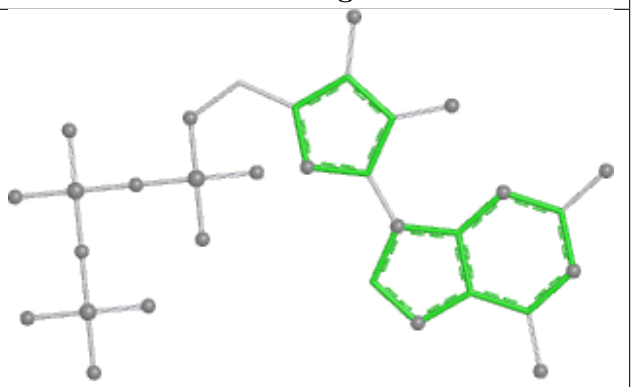
Bond lengths



Bond angles

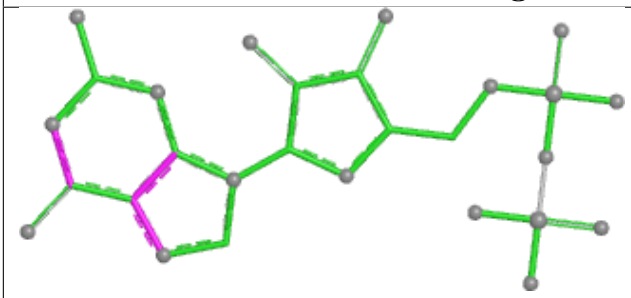


Torsions

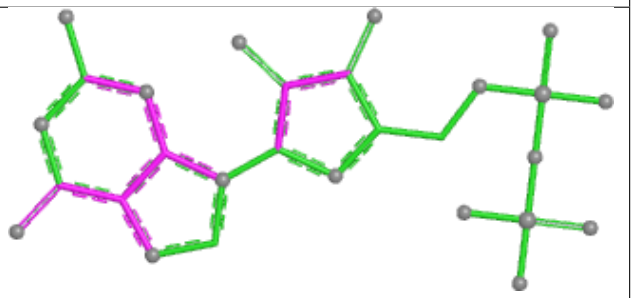


Rings

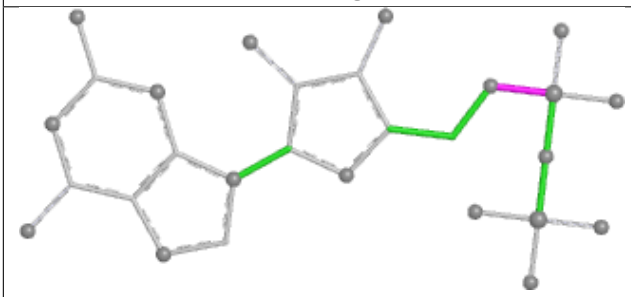
Ligand GDP OF 500



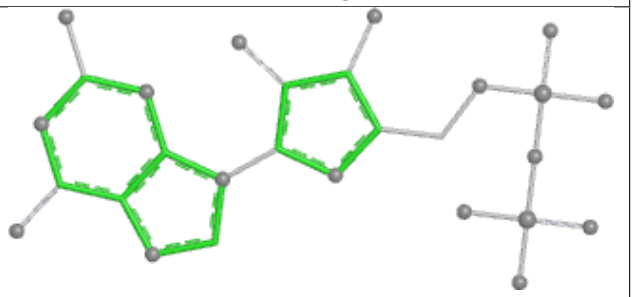
Bond lengths



Bond angles

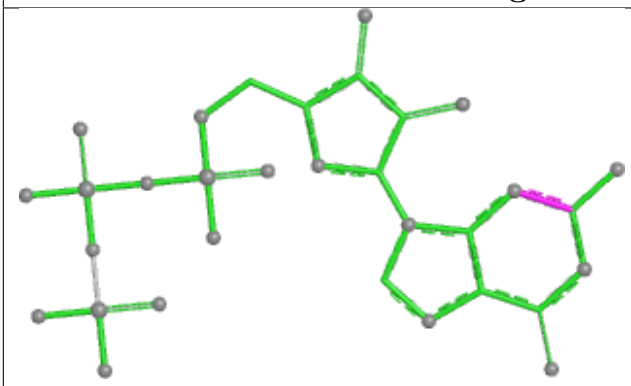


Torsions

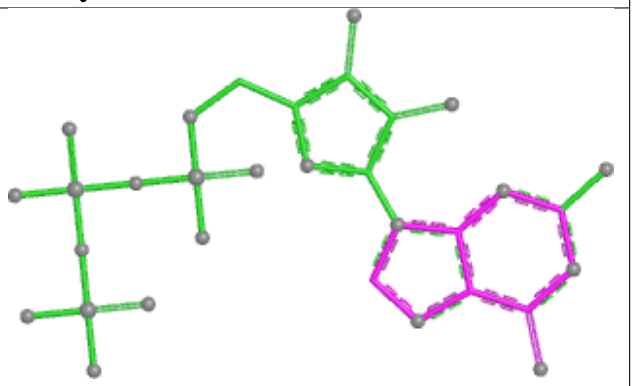


Rings

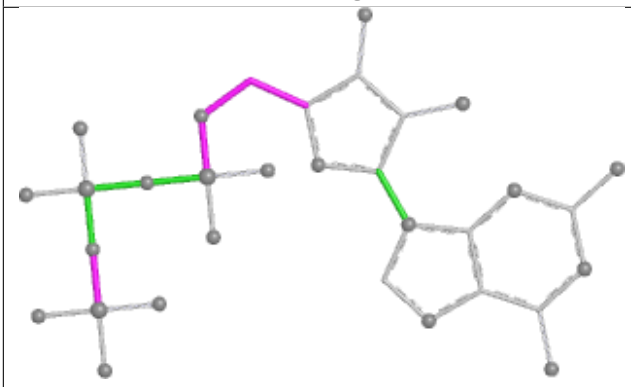
Ligand GTP BQ 501



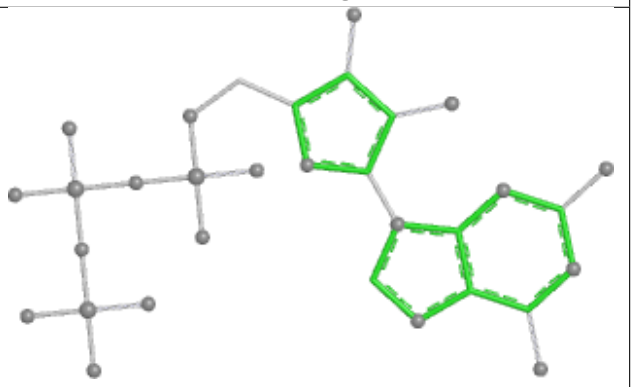
Bond lengths



Bond angles

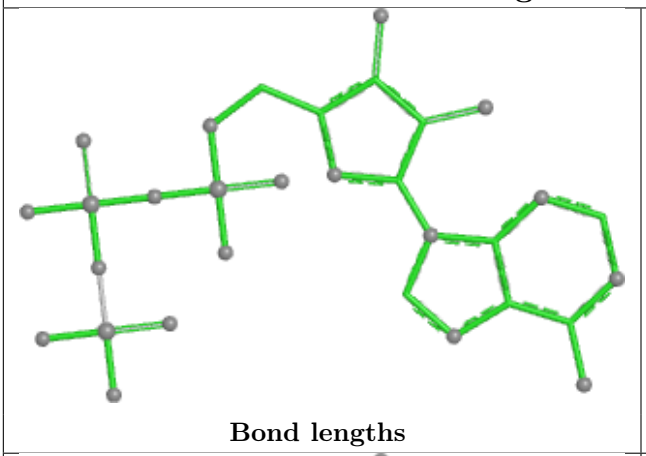


Torsions

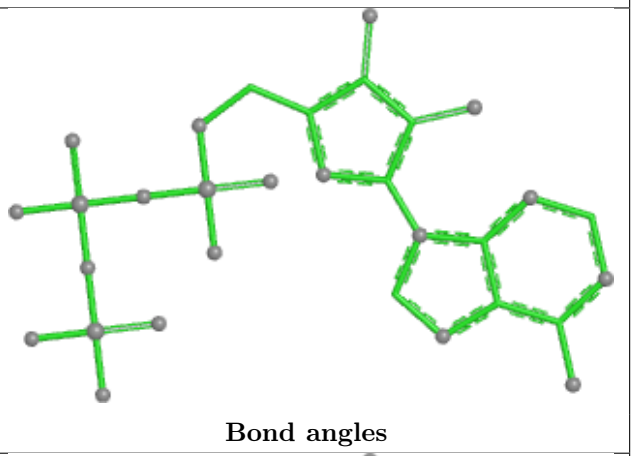


Rings

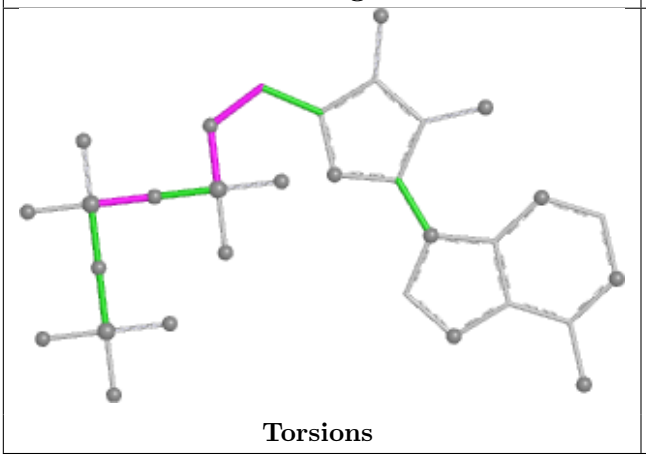
Ligand ATP 7A 402



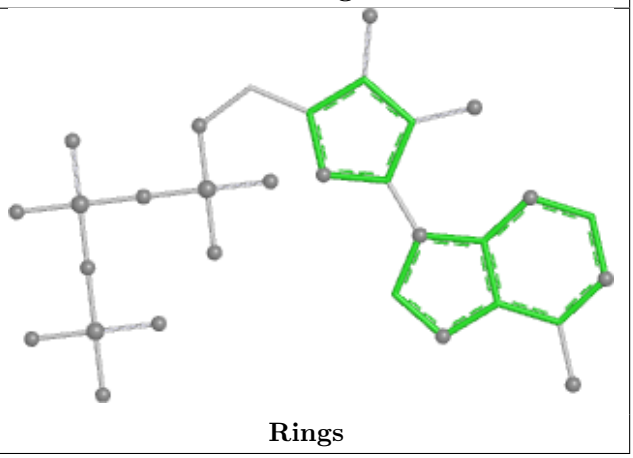
Bond lengths



Bond angles

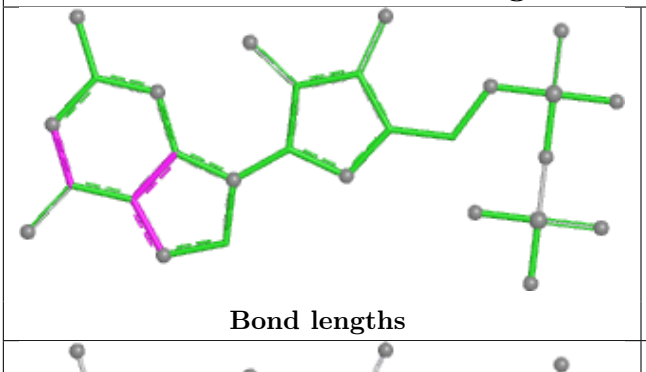


Torsions

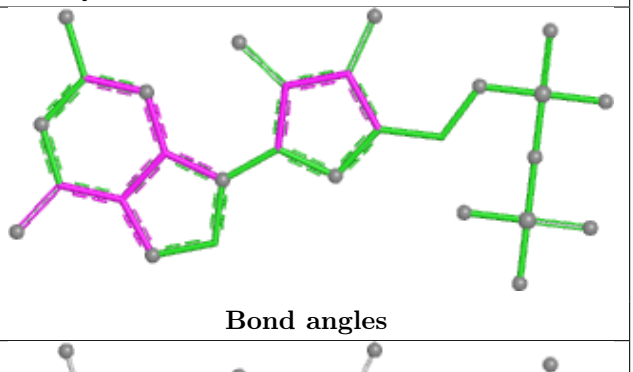


Rings

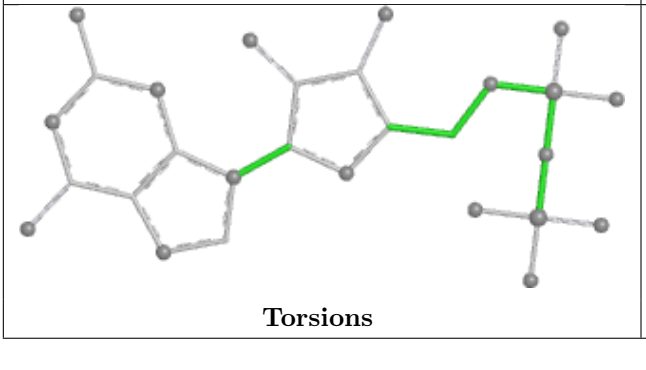
Ligand GDP RQ 500



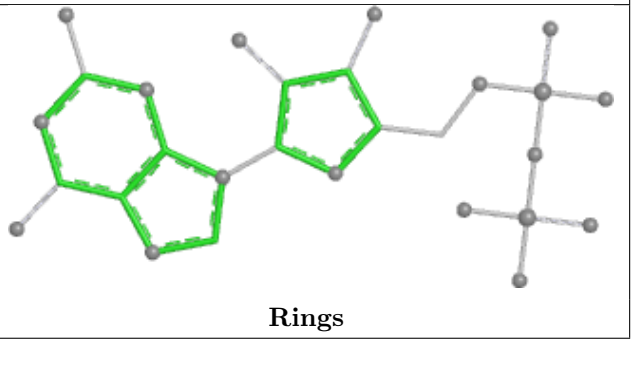
Bond lengths



Bond angles

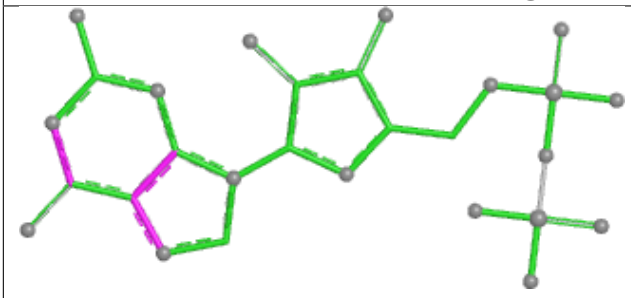


Torsions

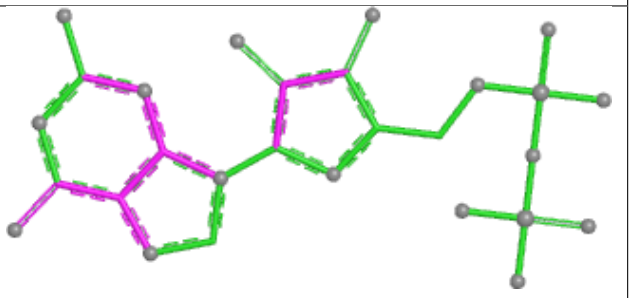


Rings

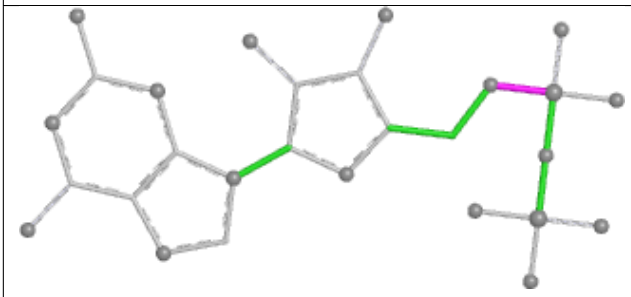
Ligand GDP T 501



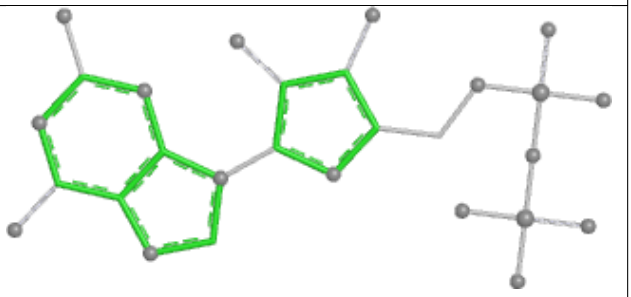
Bond lengths



Bond angles

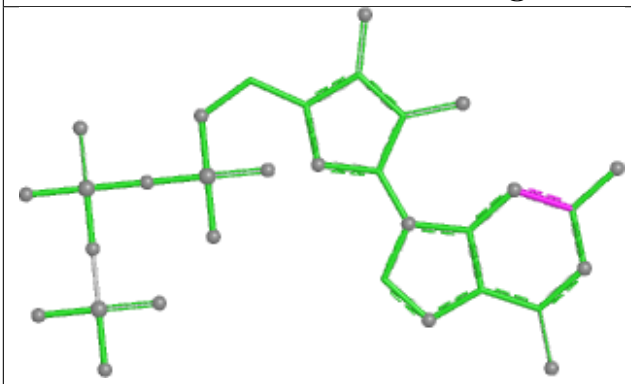


Torsions

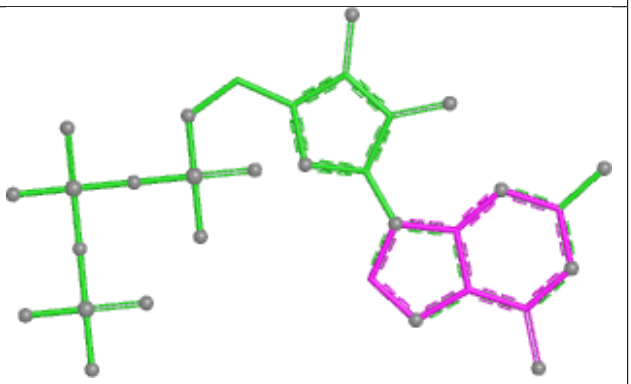


Rings

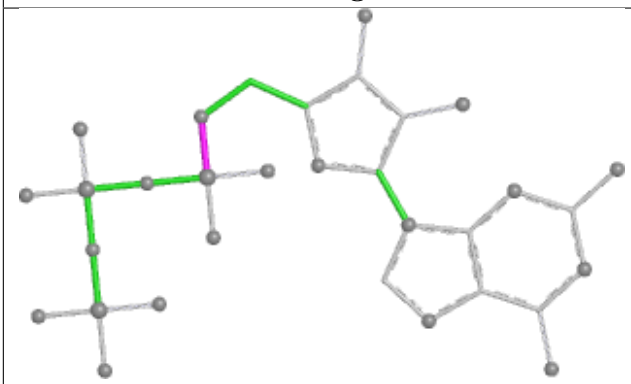
Ligand GTP RN 501



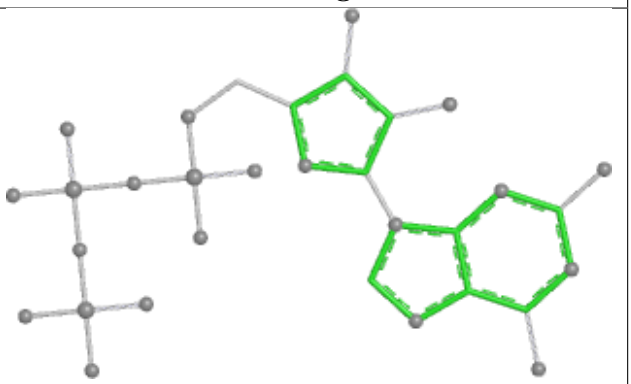
Bond lengths



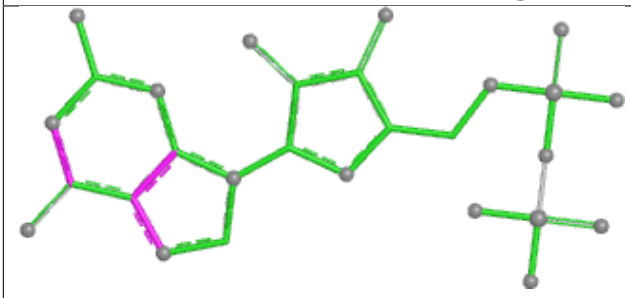
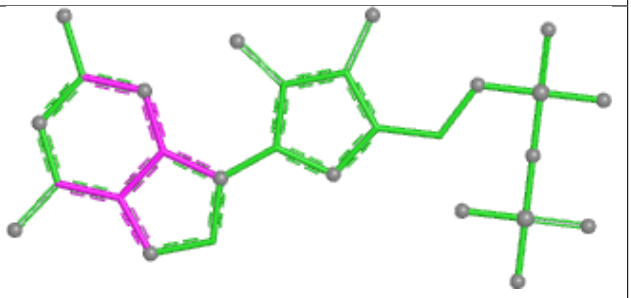
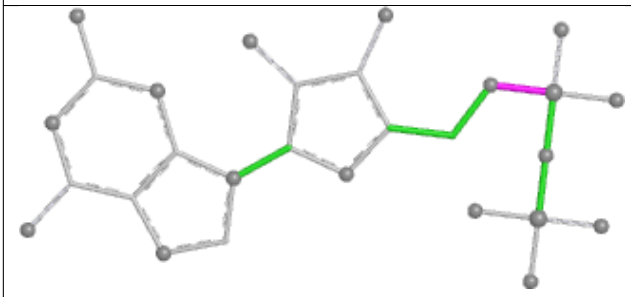
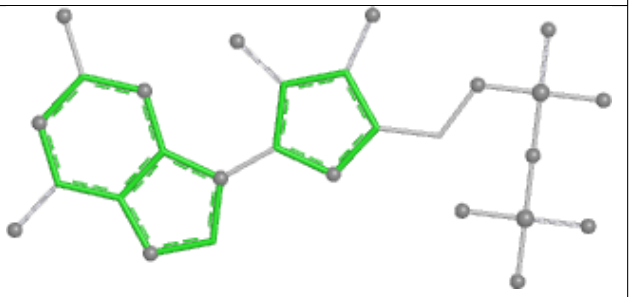
Bond angles

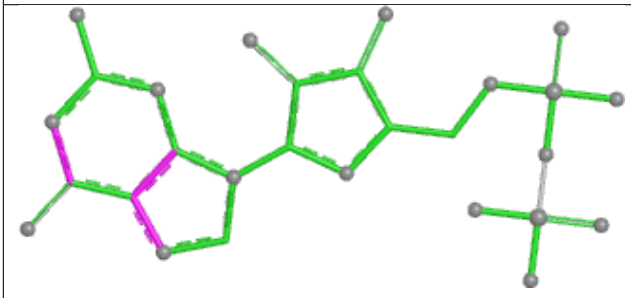
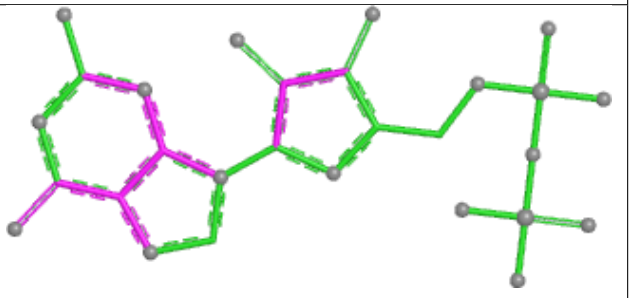
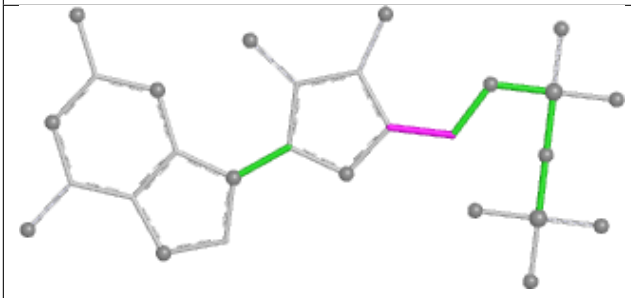
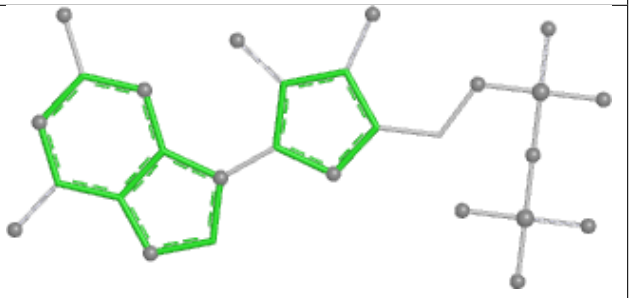


Torsions

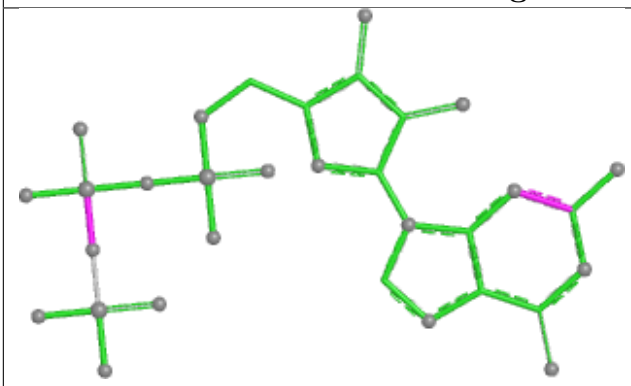


Rings

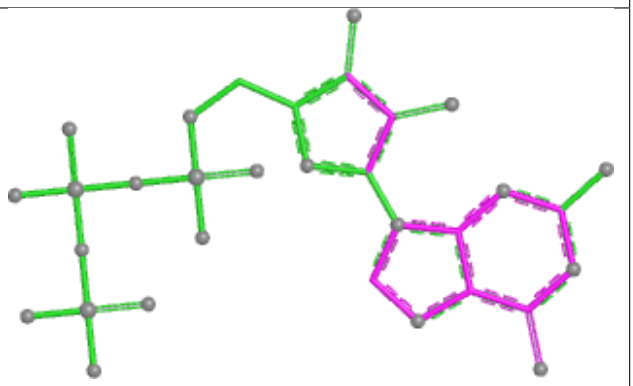
Ligand GDP EL 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP LM 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

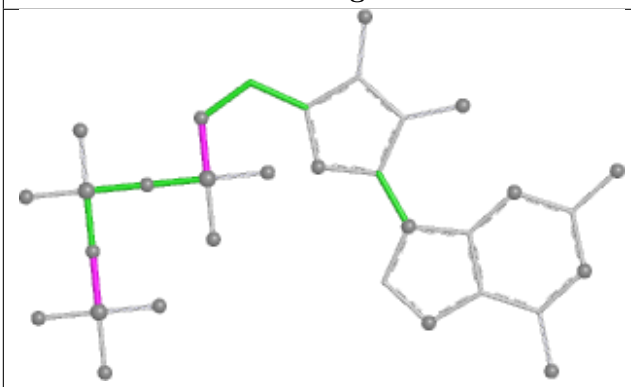
Ligand GTP VC 501



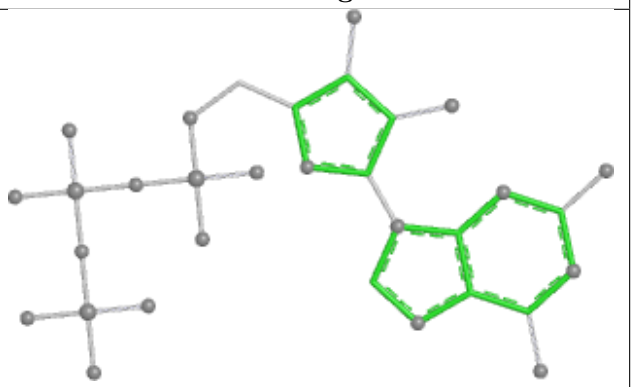
Bond lengths



Bond angles

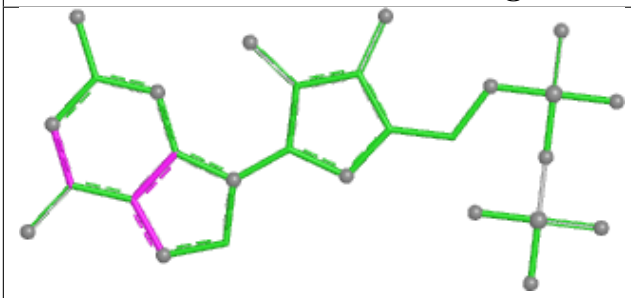


Torsions

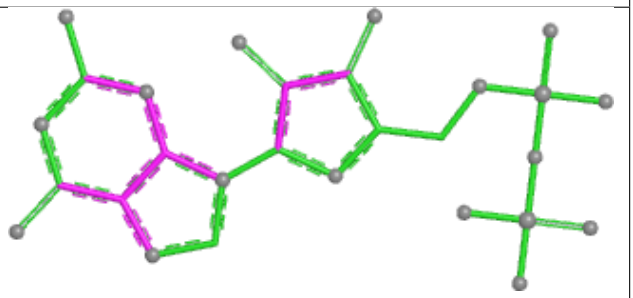


Rings

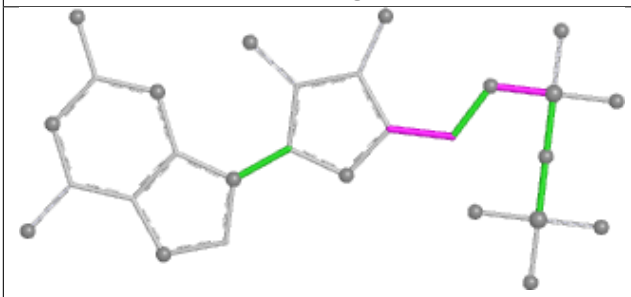
Ligand GDP MB 500



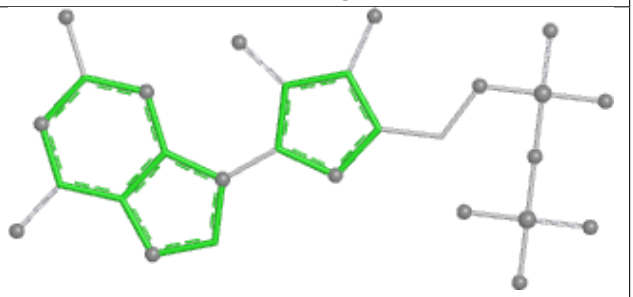
Bond lengths



Bond angles

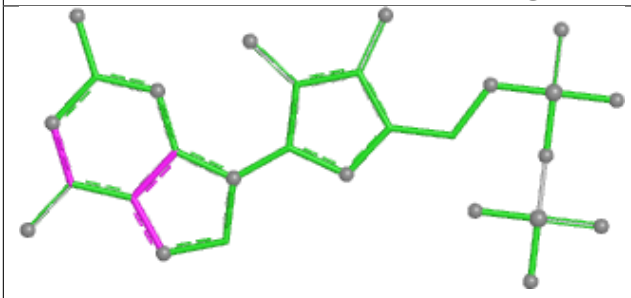


Torsions

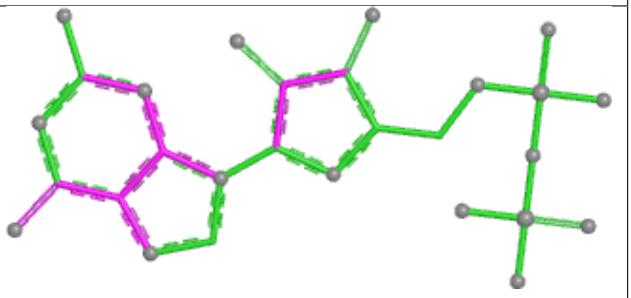


Rings

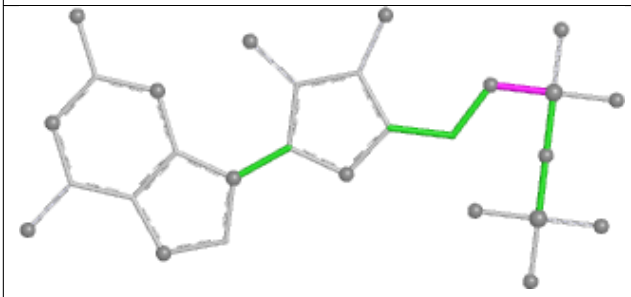
Ligand GDP S 500



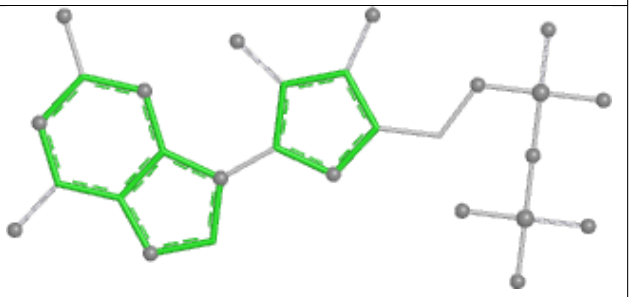
Bond lengths



Bond angles

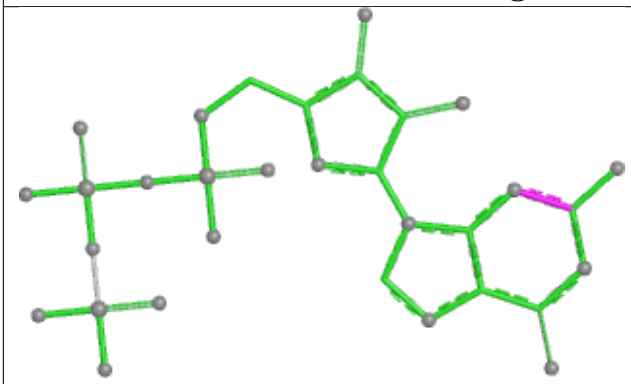


Torsions

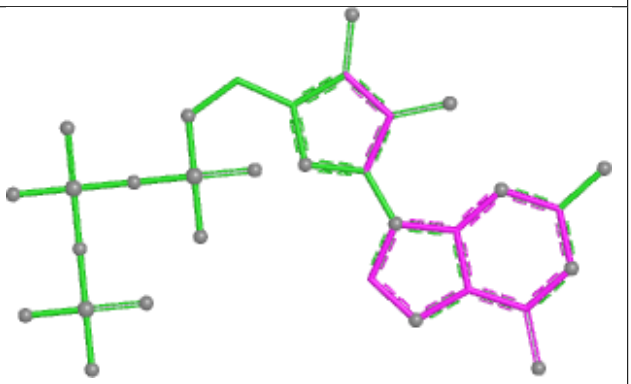


Rings

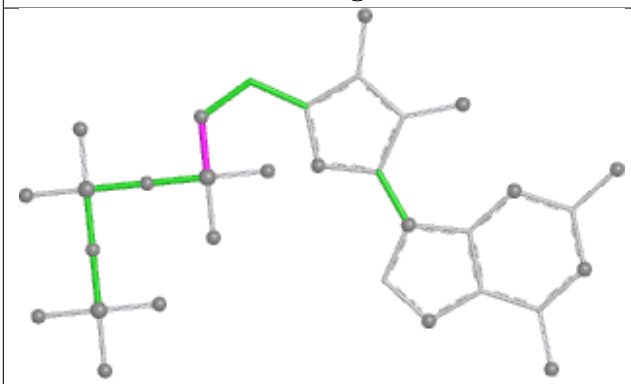
Ligand GTP CV 501



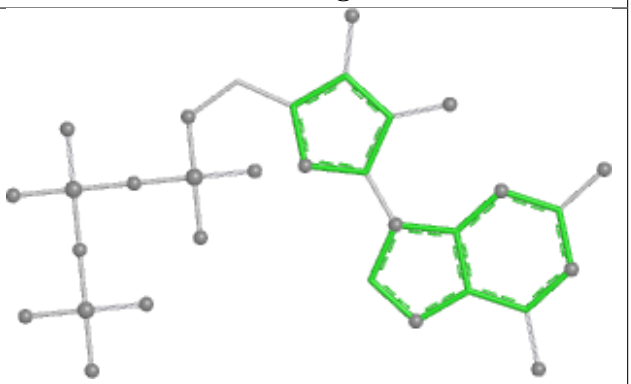
Bond lengths



Bond angles

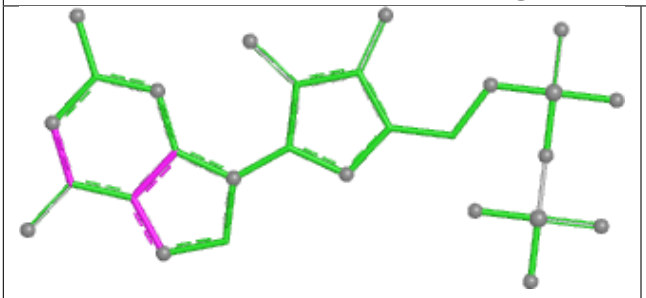


Torsions

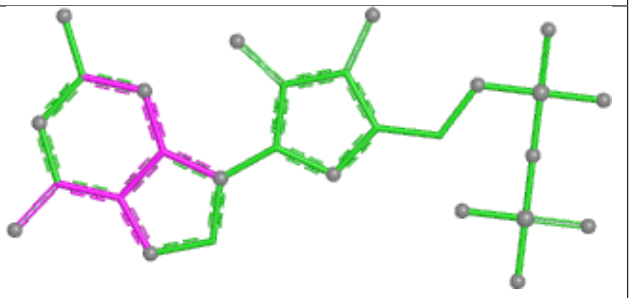


Rings

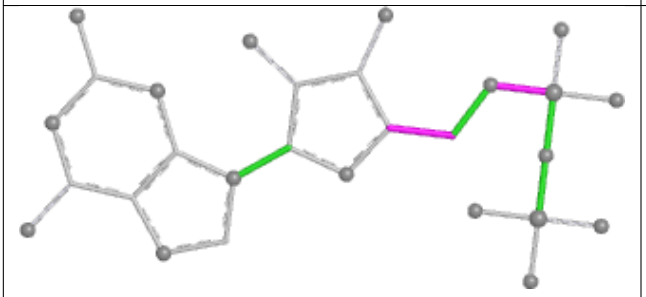
Ligand GDP SP 500



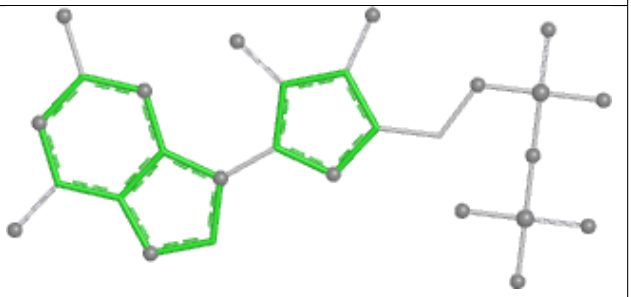
Bond lengths



Bond angles

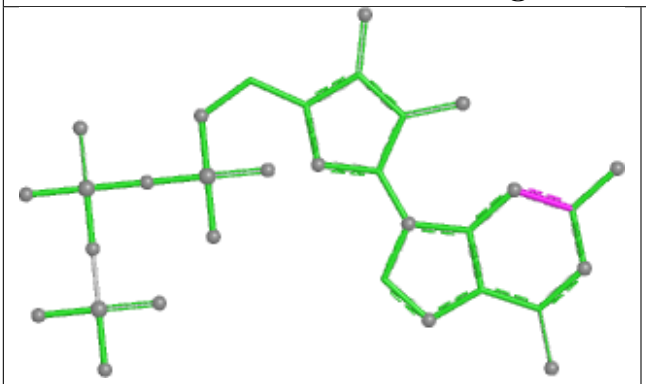


Torsions

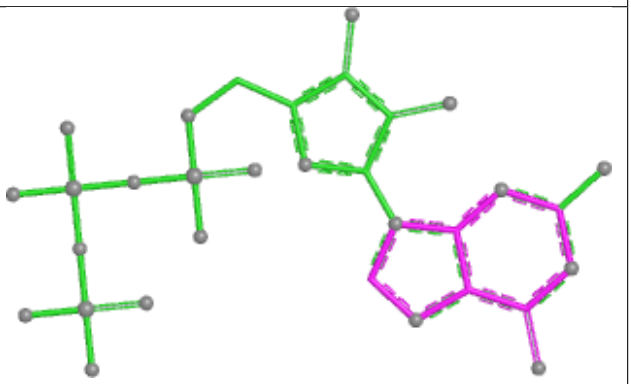


Rings

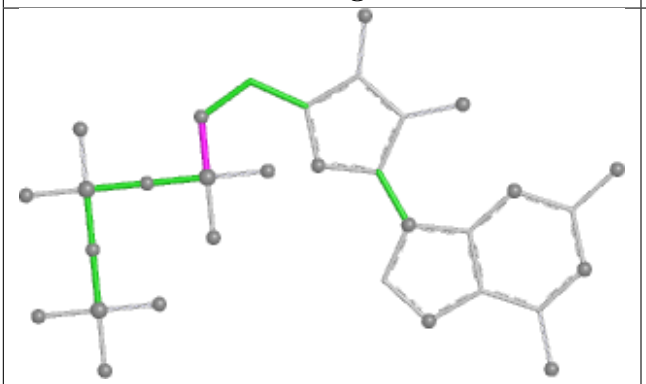
Ligand GTP BA 501



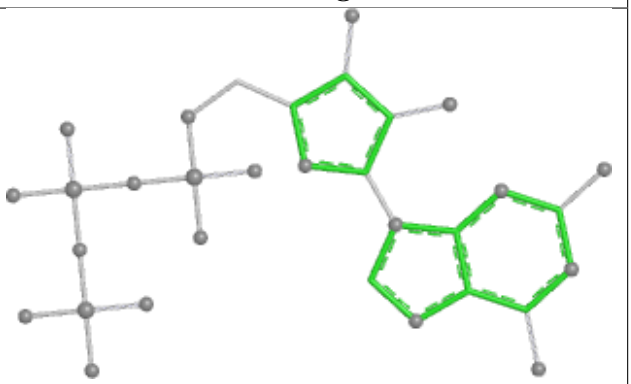
Bond lengths



Bond angles

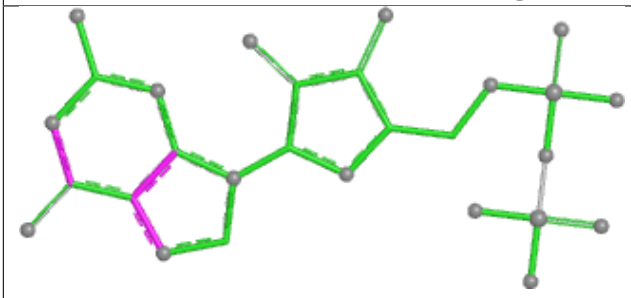


Torsions

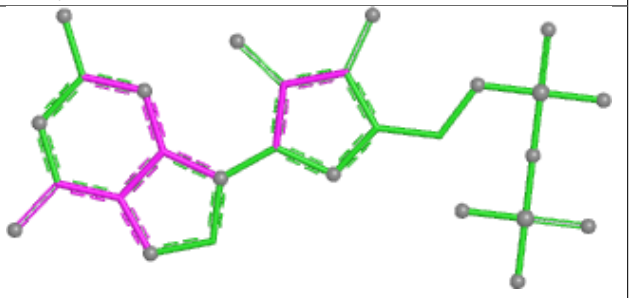


Rings

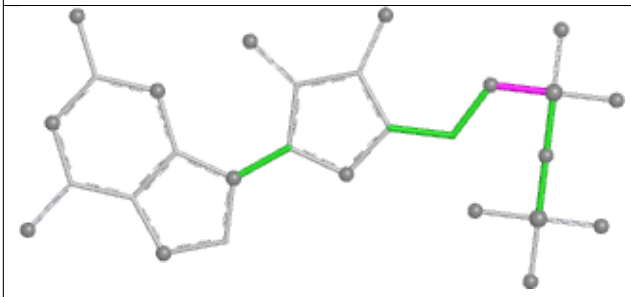
Ligand GDP QS 500



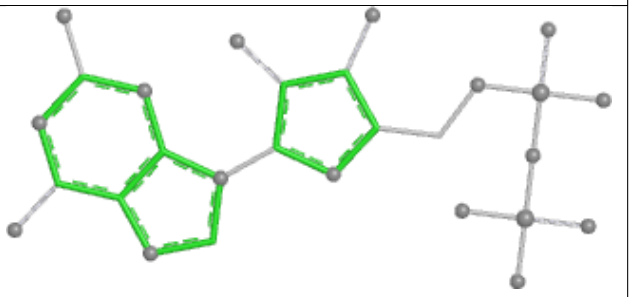
Bond lengths



Bond angles

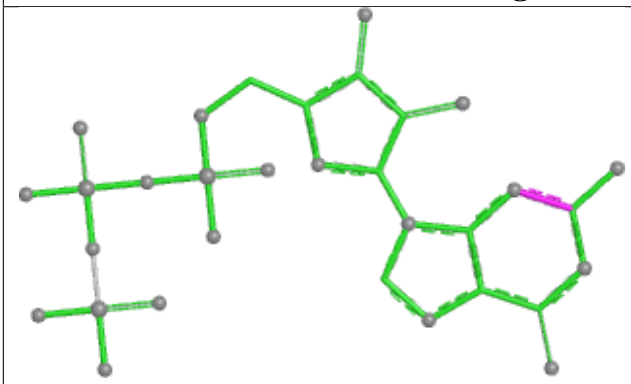


Torsions

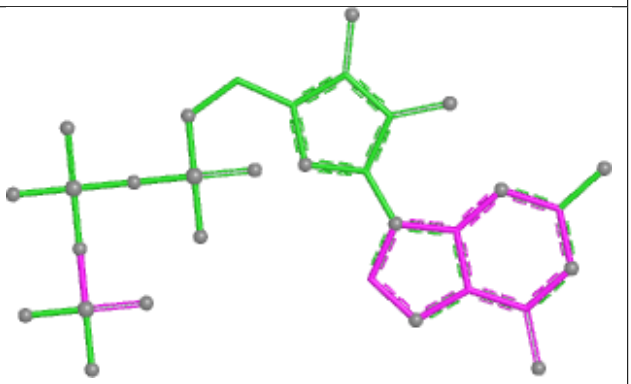


Rings

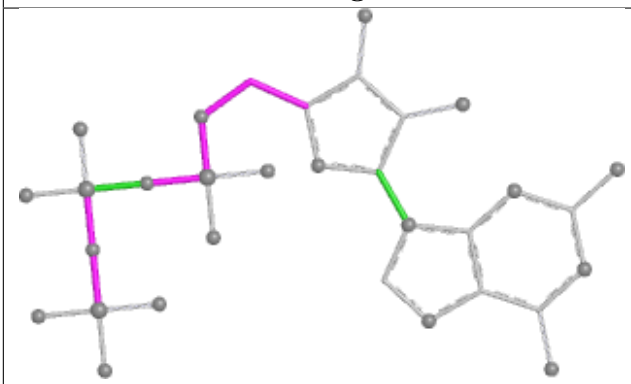
Ligand GTP RL 501



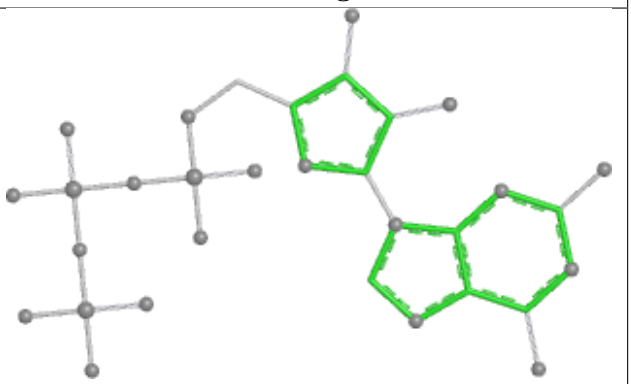
Bond lengths



Bond angles

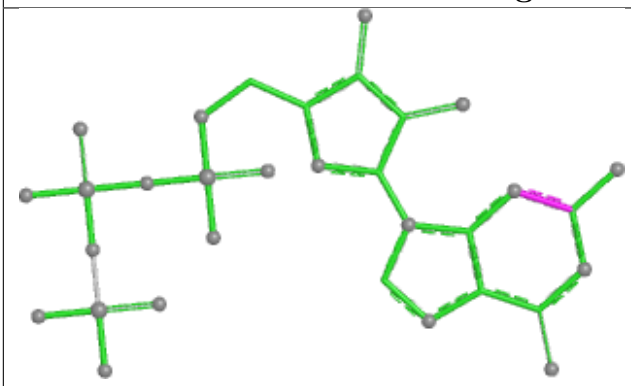


Torsions

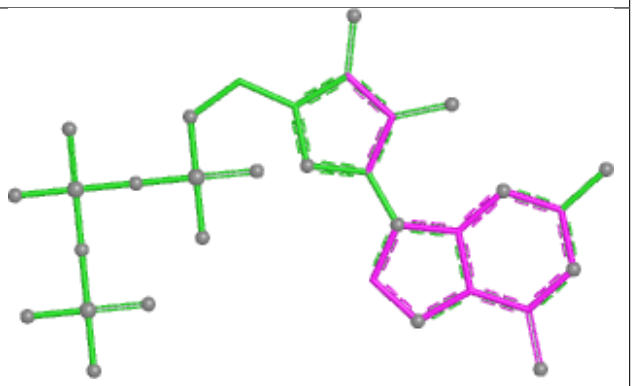


Rings

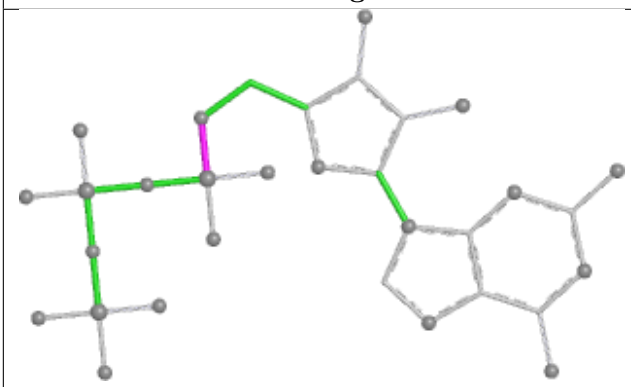
Ligand GTP UI 501



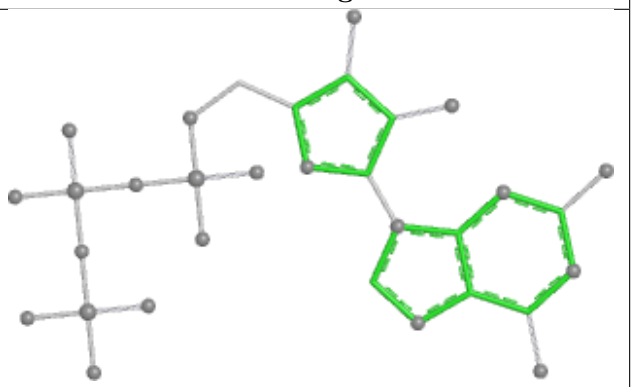
Bond lengths



Bond angles

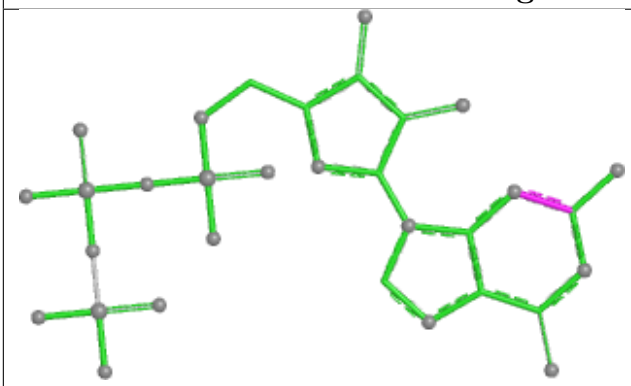


Torsions

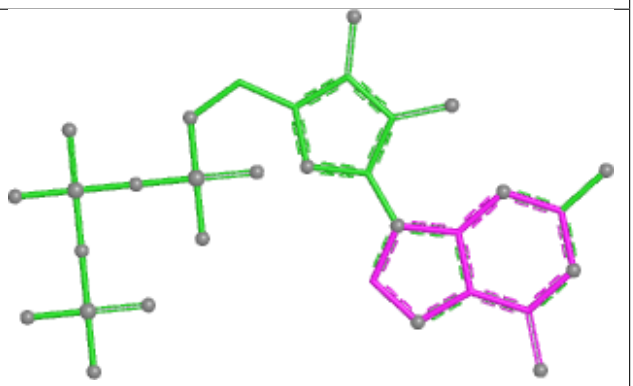


Rings

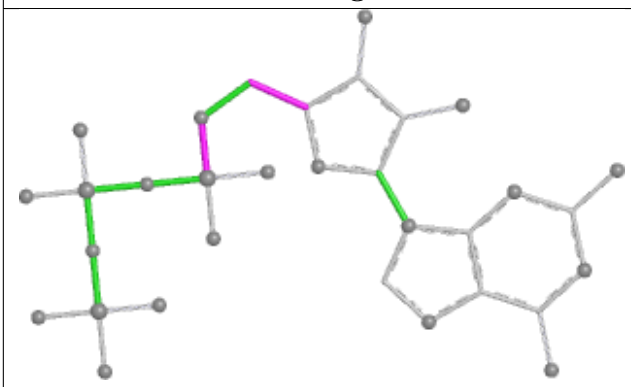
Ligand GTP PI 501



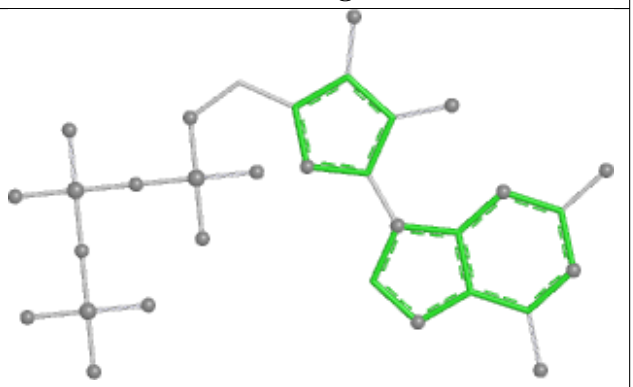
Bond lengths



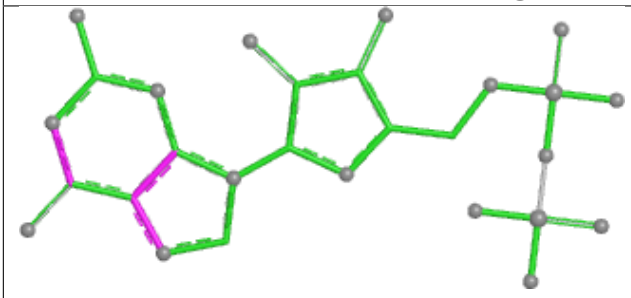
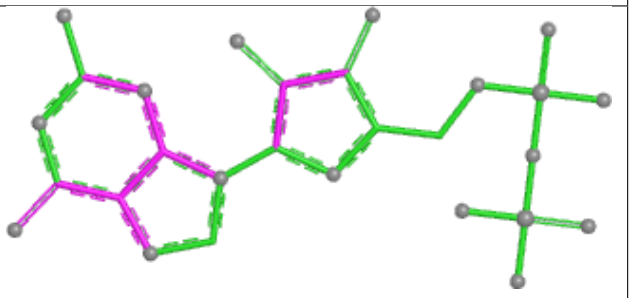
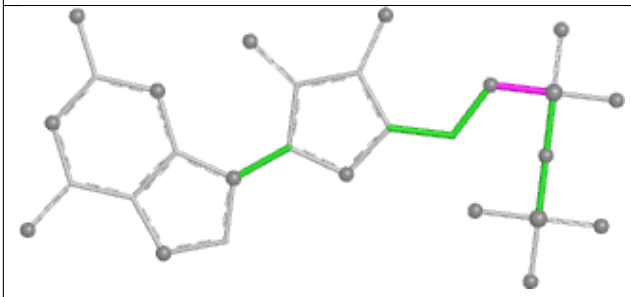
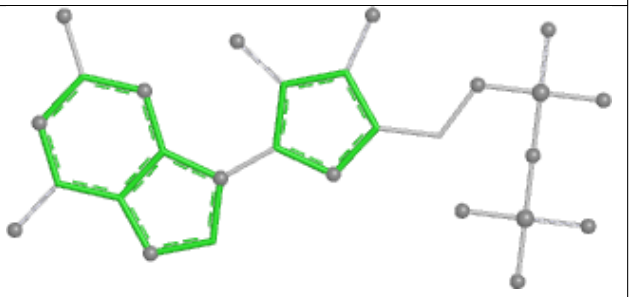
Bond angles

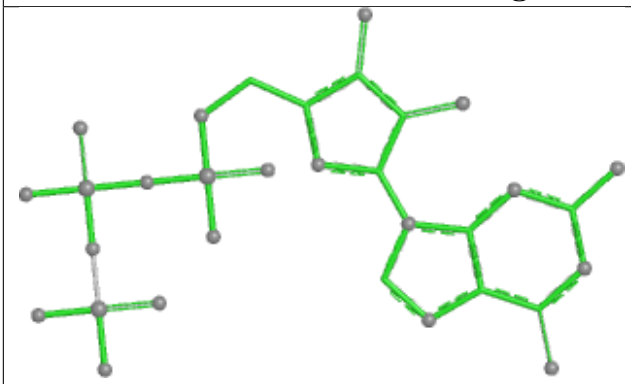
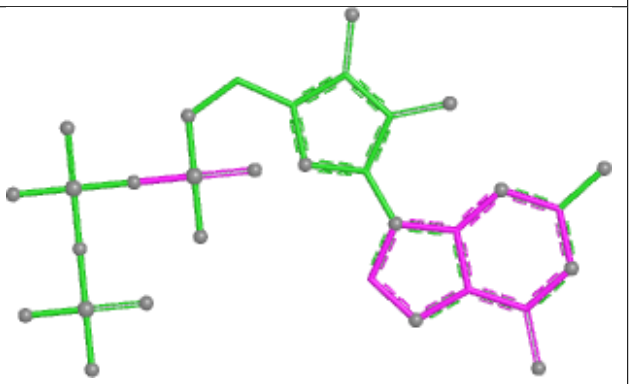
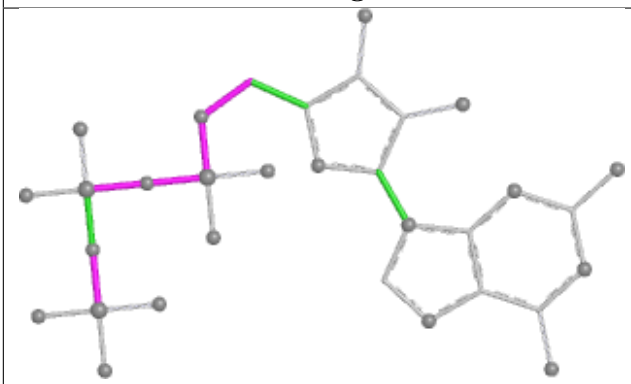
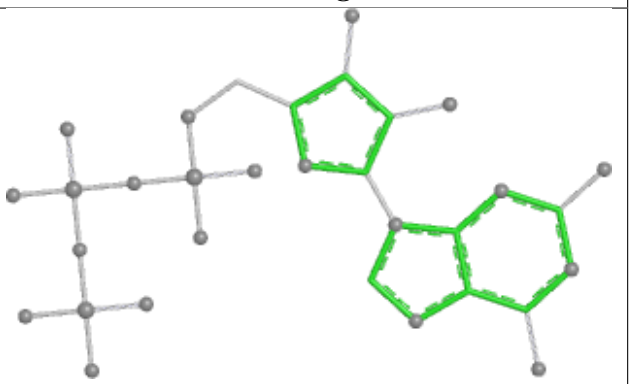


Torsions

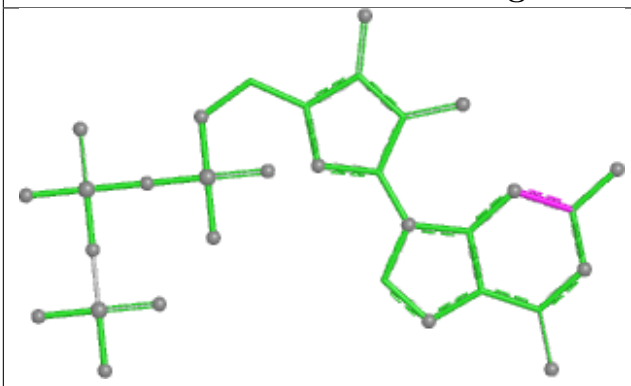


Rings

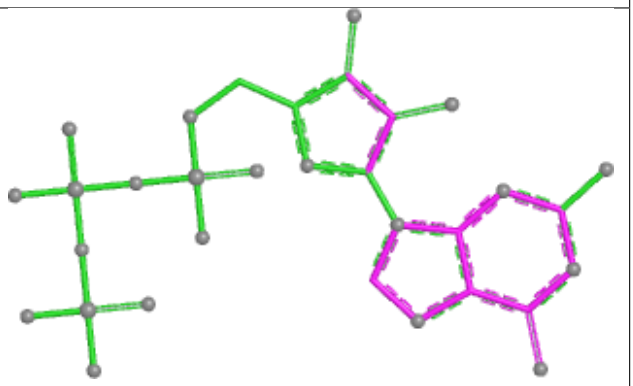
Ligand GDP UJ 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP GL 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

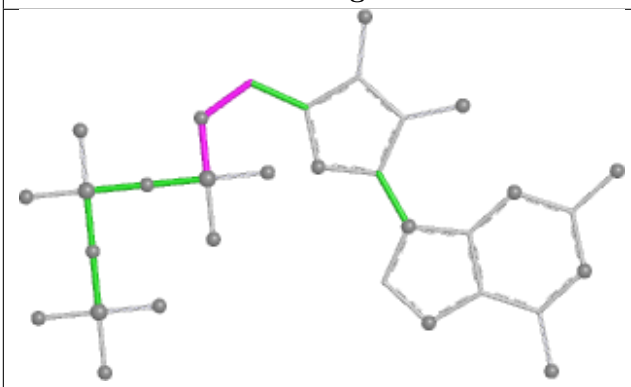
Ligand GTP OG 501



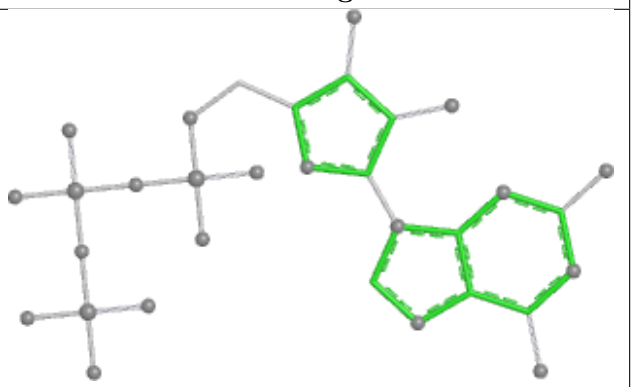
Bond lengths



Bond angles

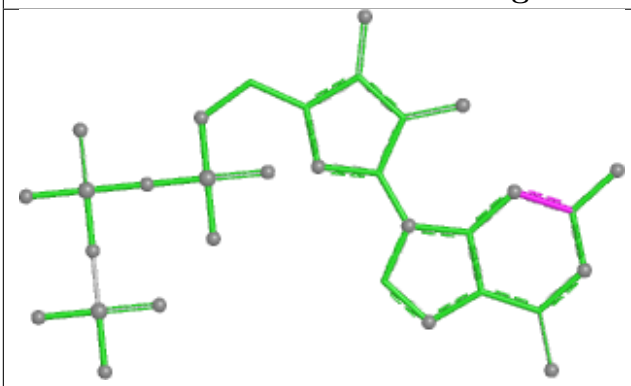


Torsions

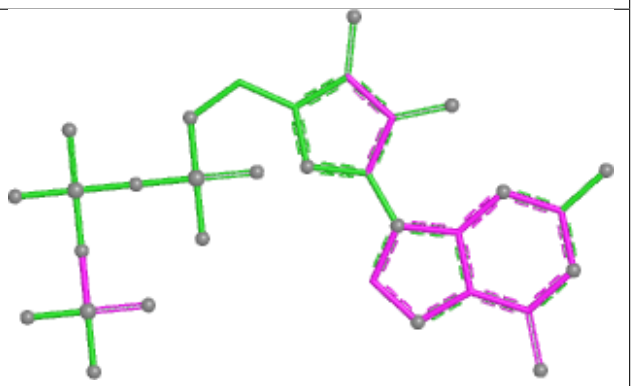


Rings

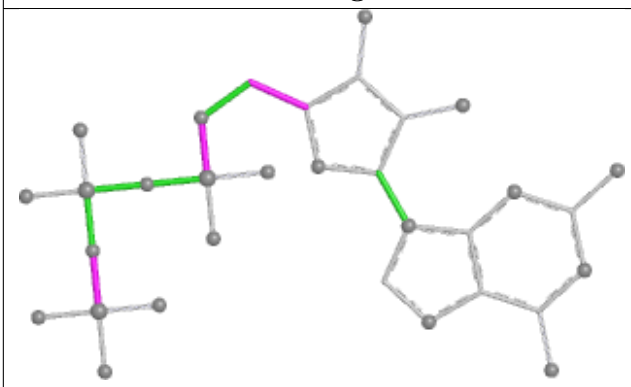
Ligand GTP SG 501



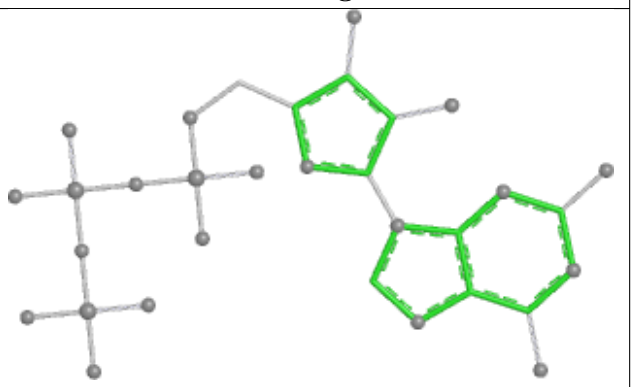
Bond lengths



Bond angles

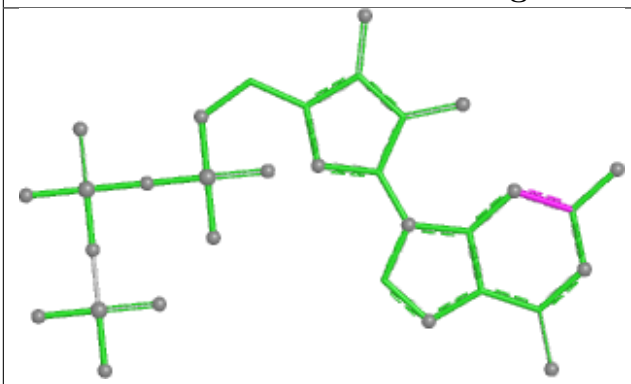


Torsions

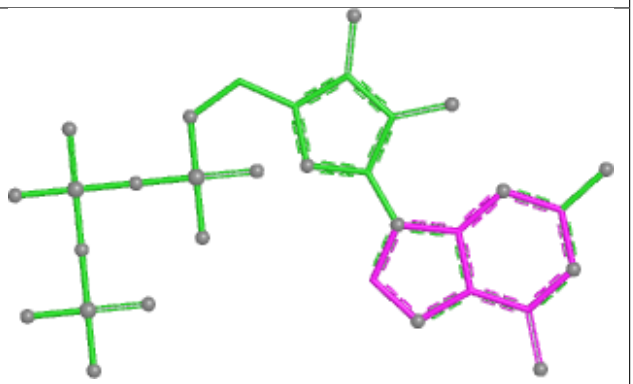


Rings

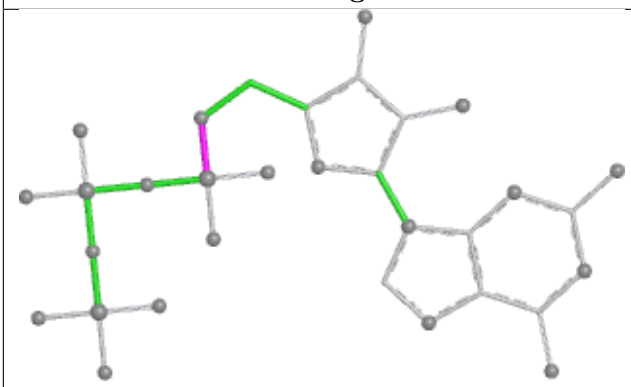
Ligand GTP PO 501



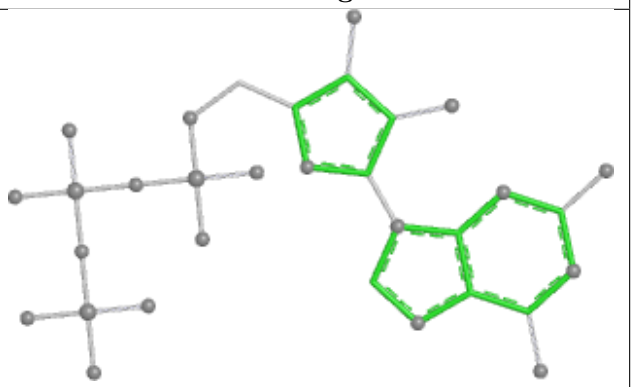
Bond lengths



Bond angles

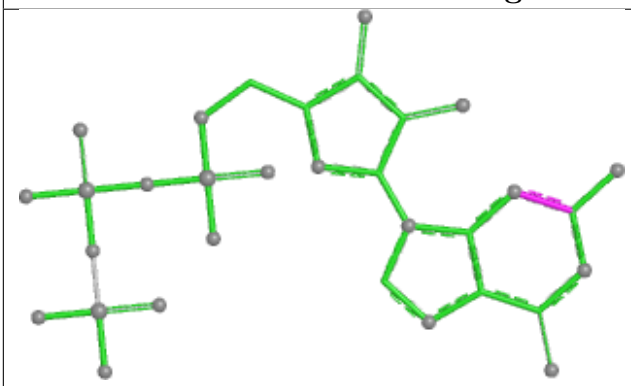


Torsions

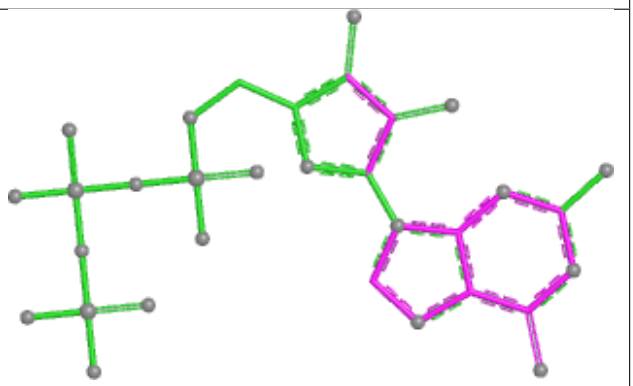


Rings

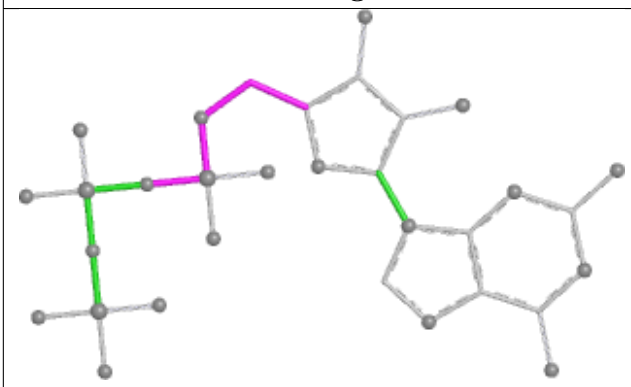
Ligand GTP TW 501



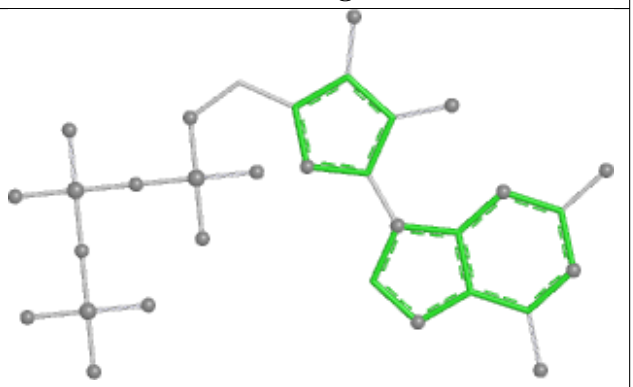
Bond lengths



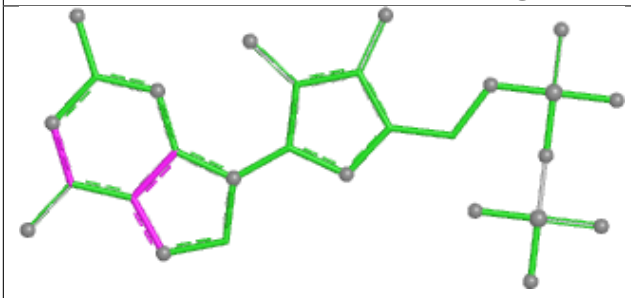
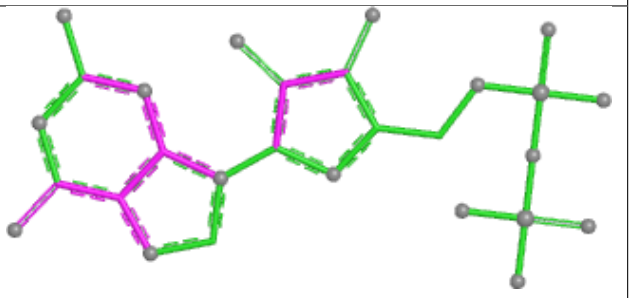
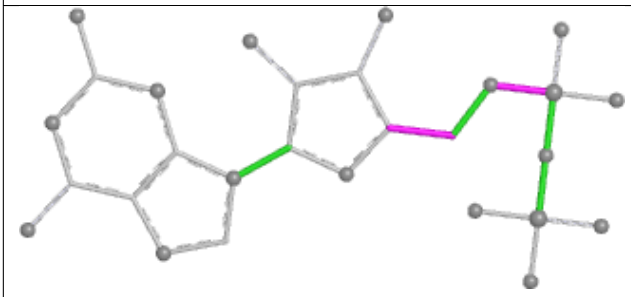
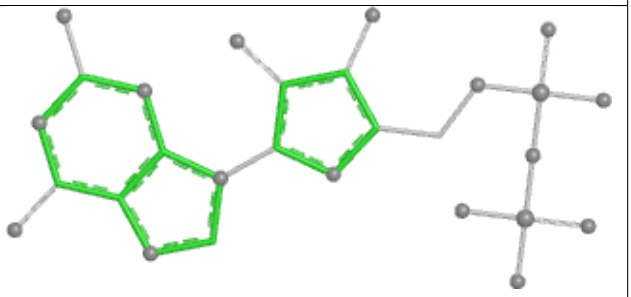
Bond angles

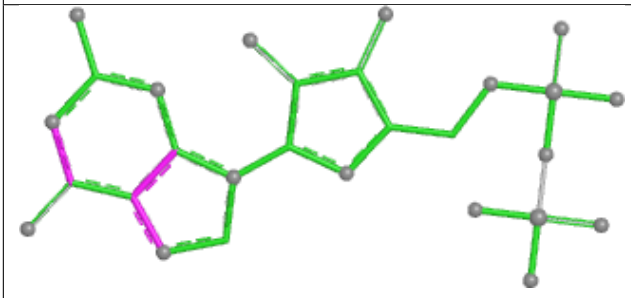
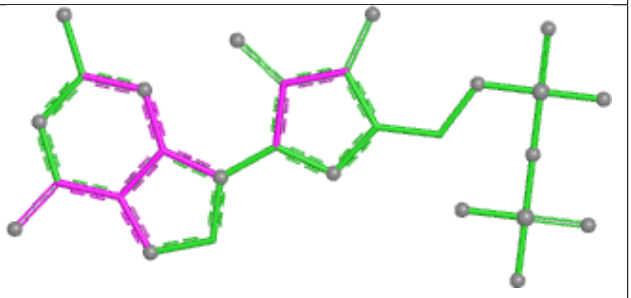
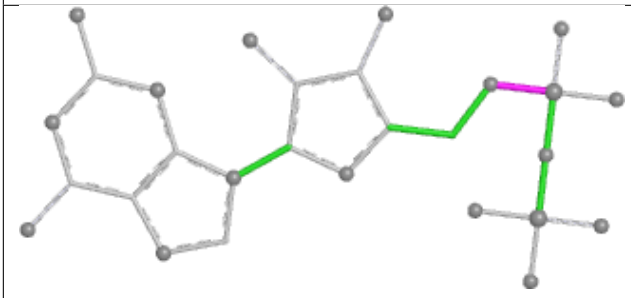
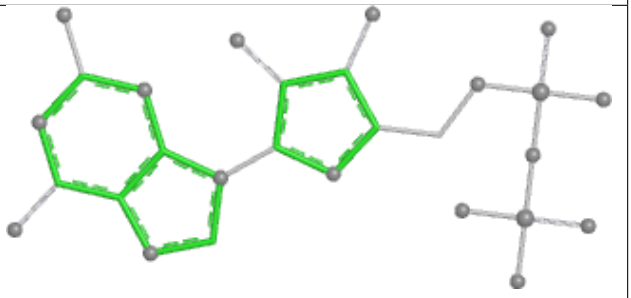


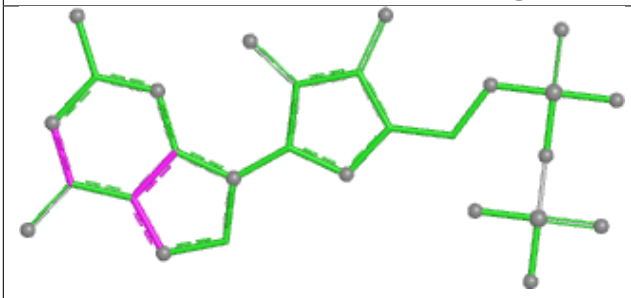
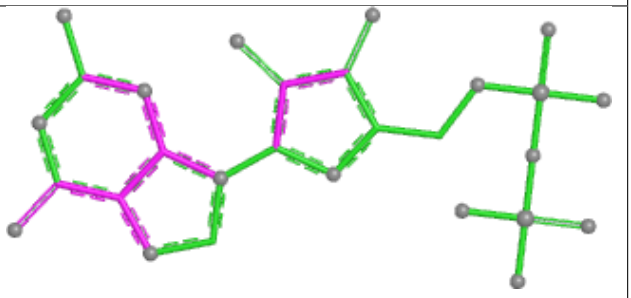
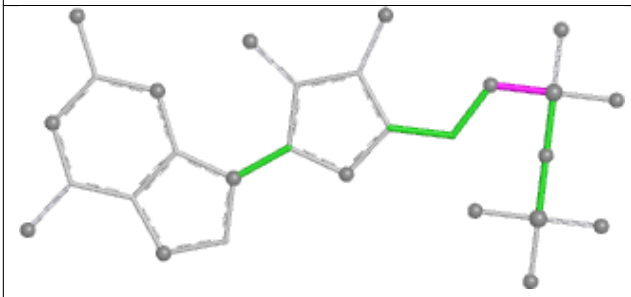
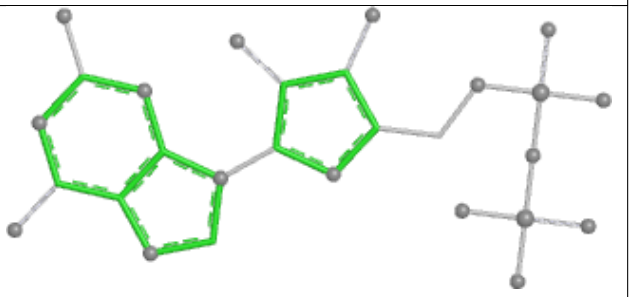
Torsions

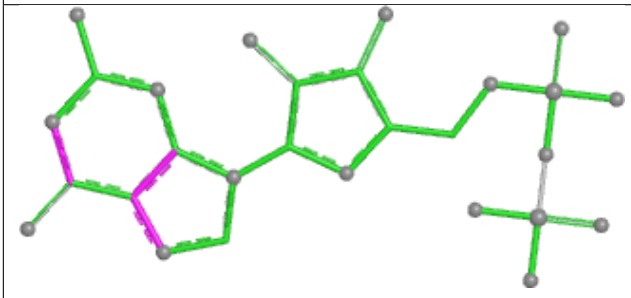
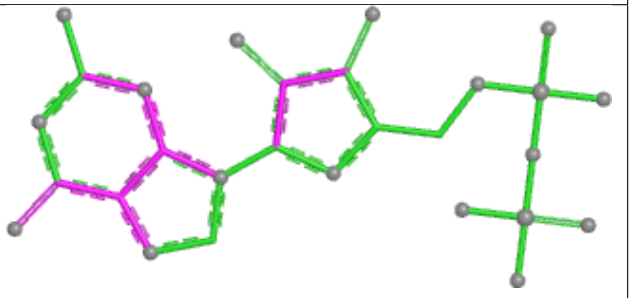
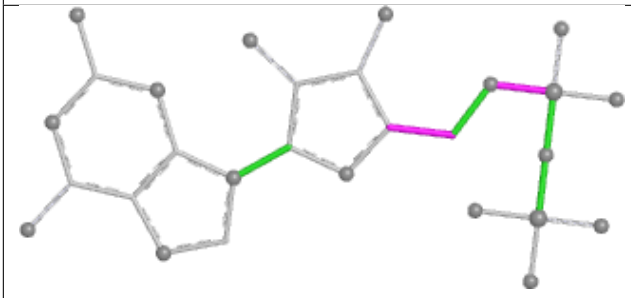
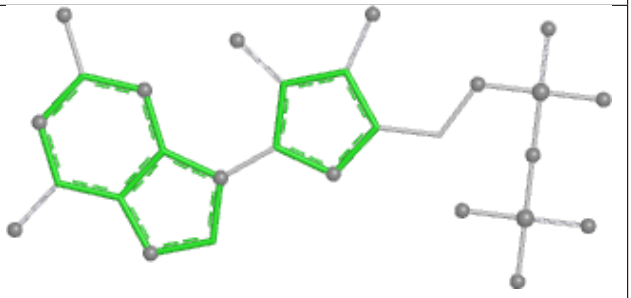


Rings

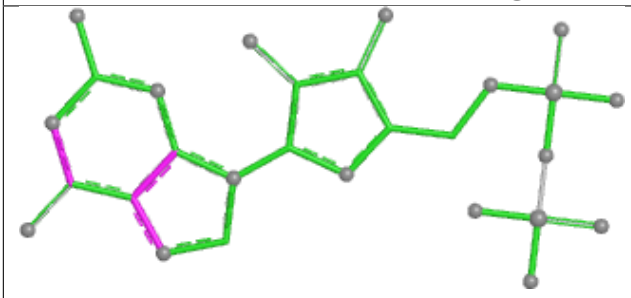
Ligand GDP IN 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP WF 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

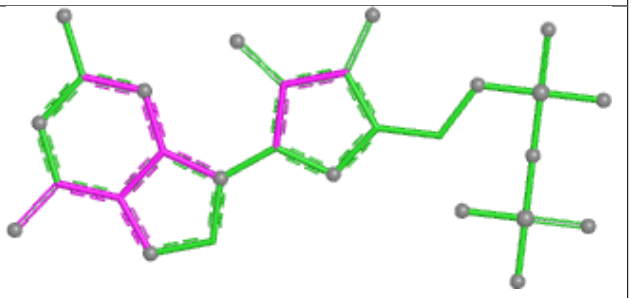
Ligand GDP KS 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP M 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

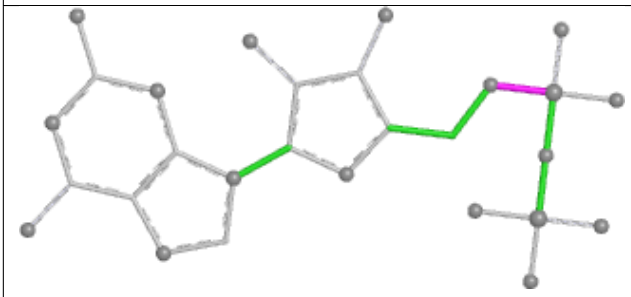
Ligand GDP VT 500



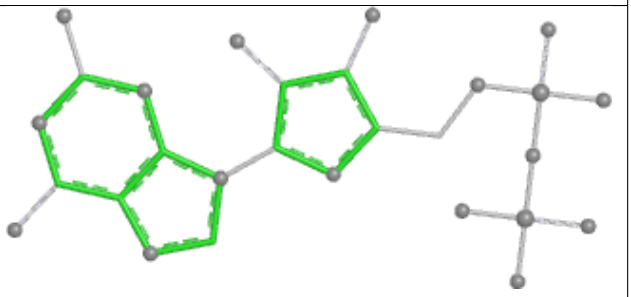
Bond lengths



Bond angles

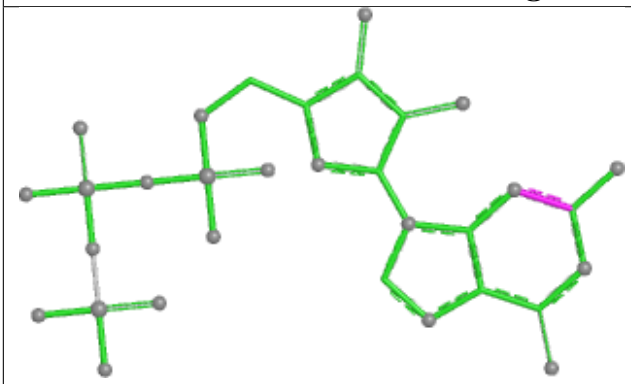


Torsions

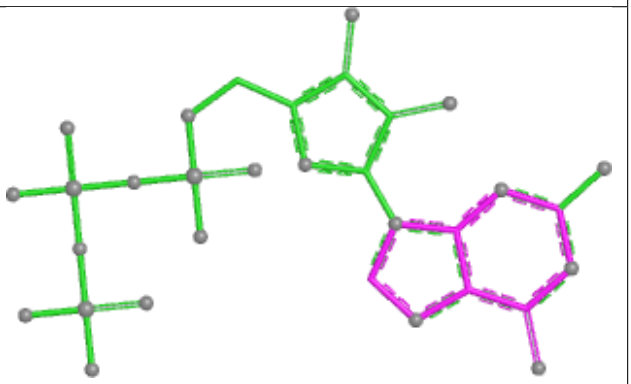


Rings

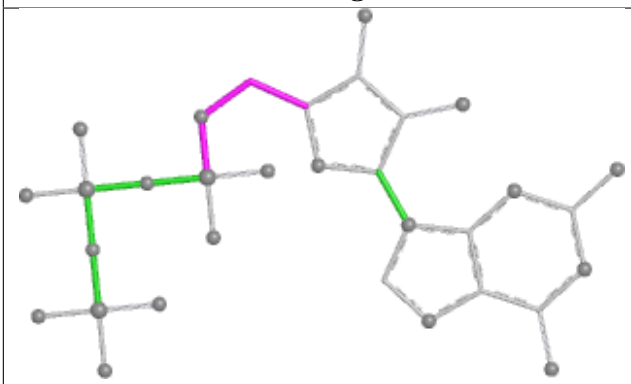
Ligand GTP L 501



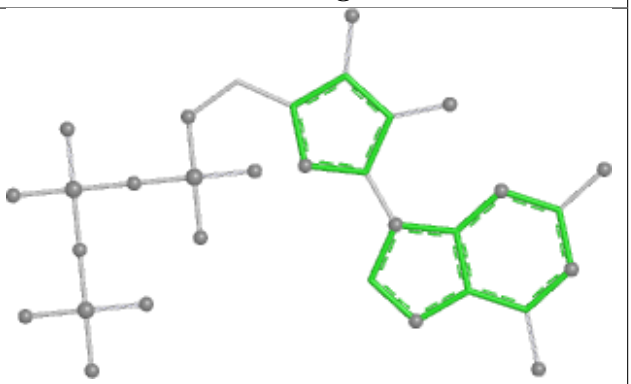
Bond lengths



Bond angles

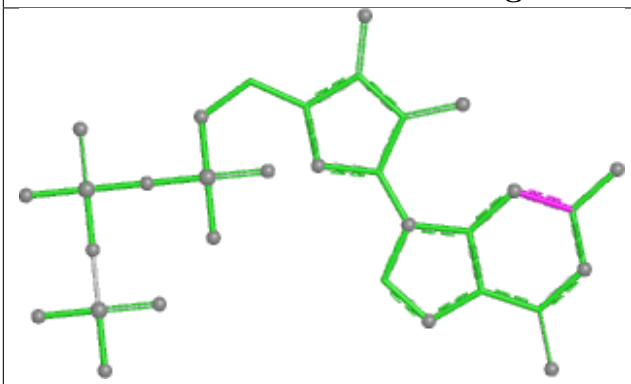


Torsions

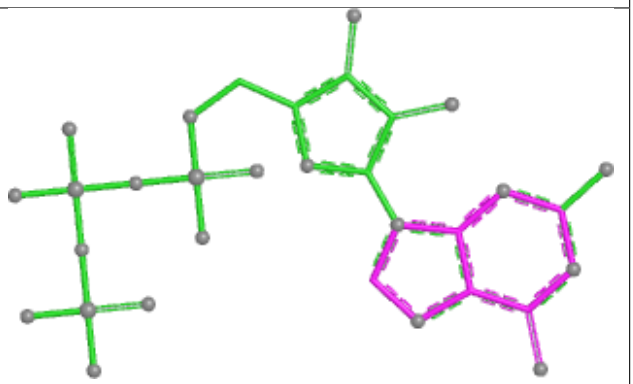


Rings

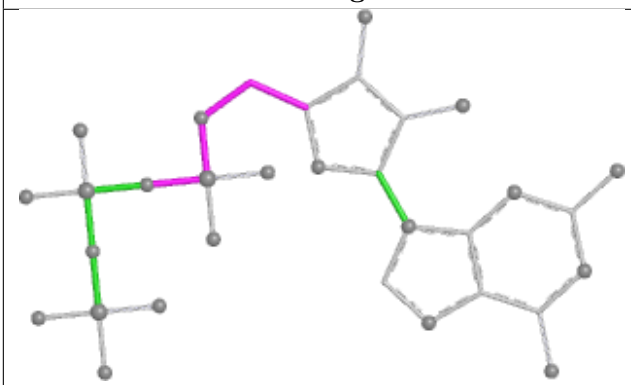
Ligand GTP MV 501



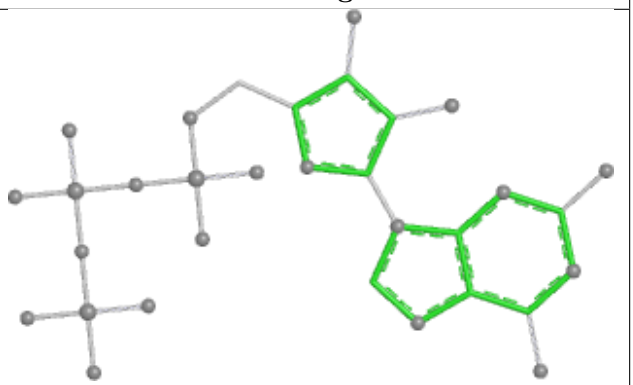
Bond lengths



Bond angles

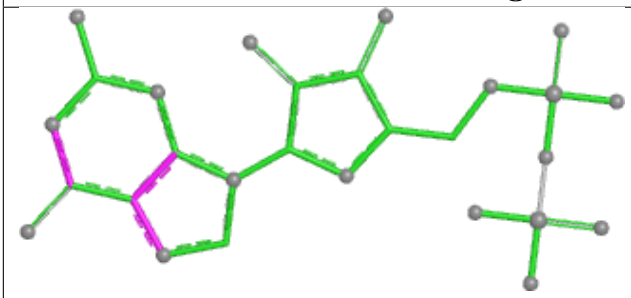


Torsions

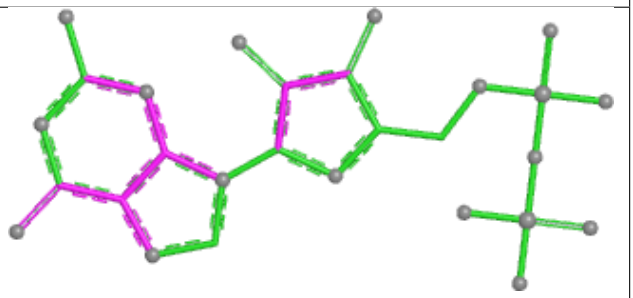


Rings

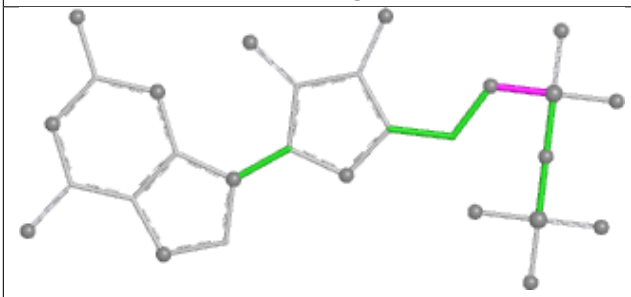
Ligand GDP LW 500



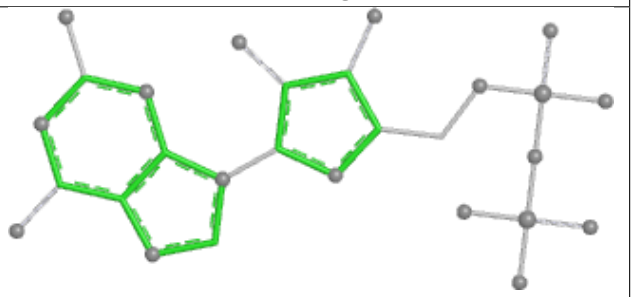
Bond lengths



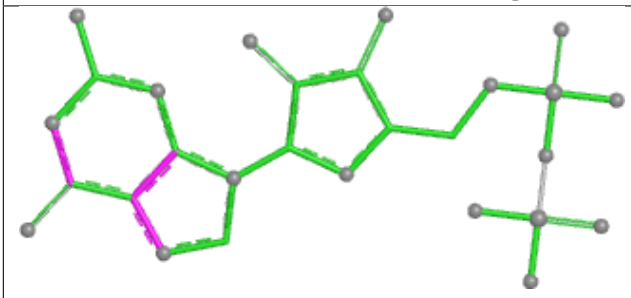
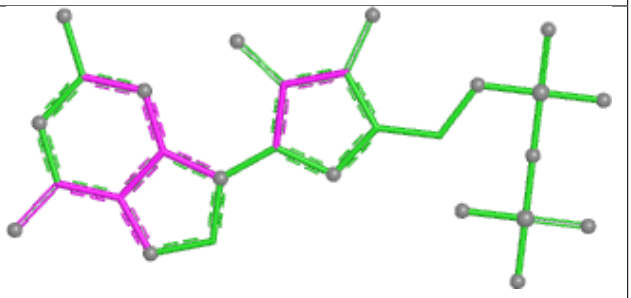
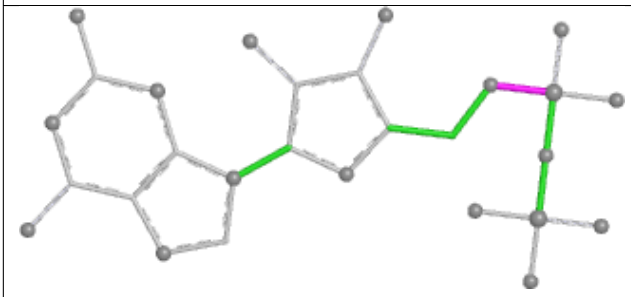
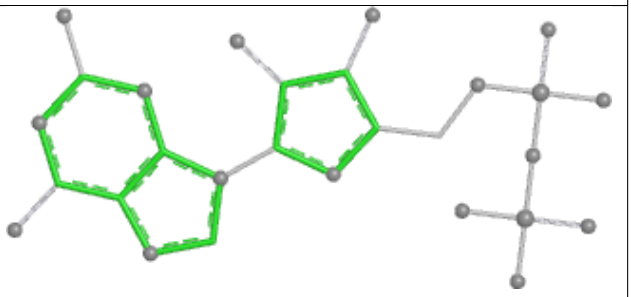
Bond angles

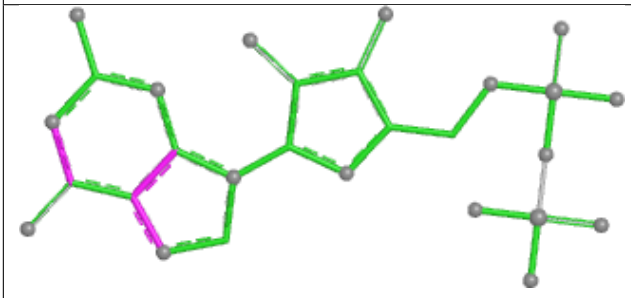
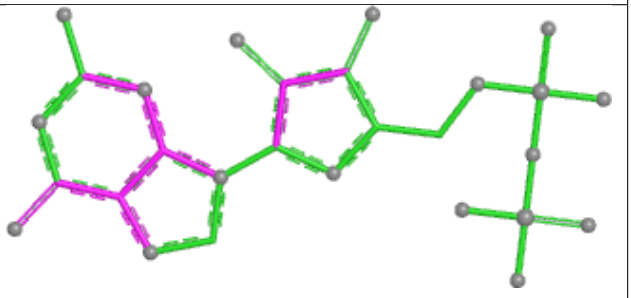
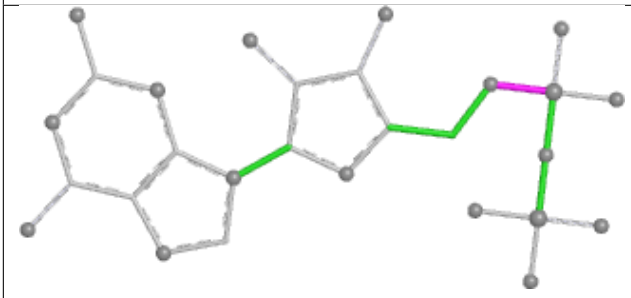
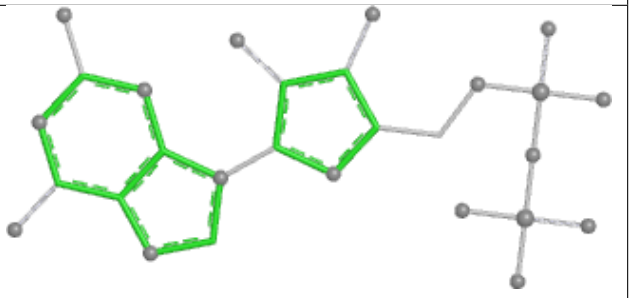


Torsions

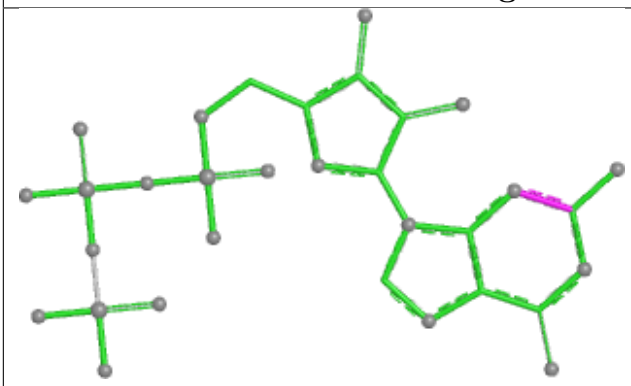


Rings

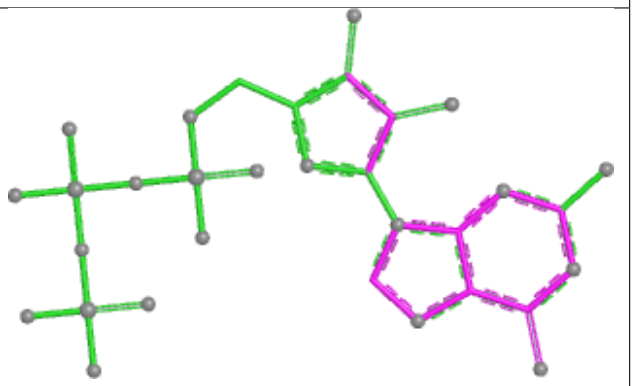
Ligand GDP DK 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP ID 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

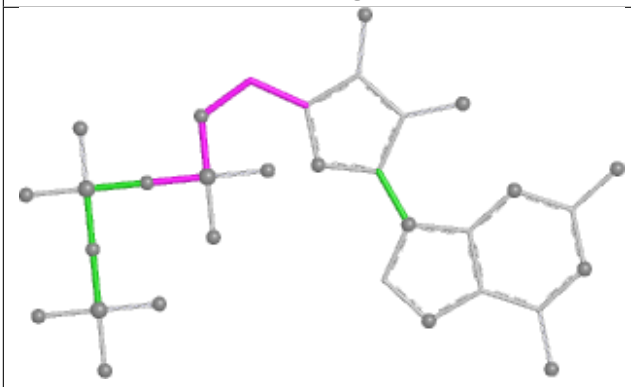
Ligand GTP WW 501



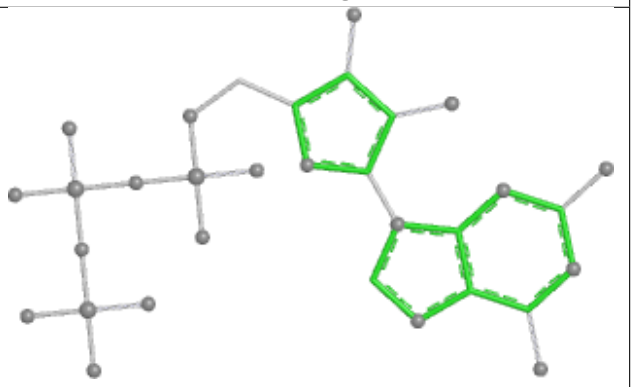
Bond lengths



Bond angles

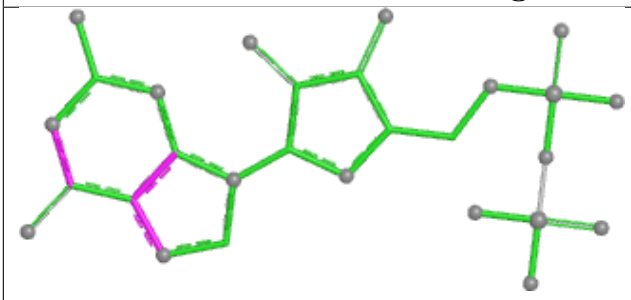


Torsions

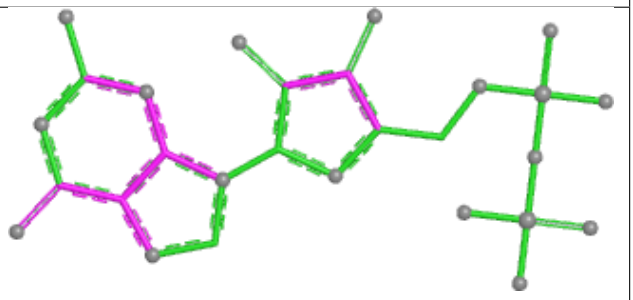


Rings

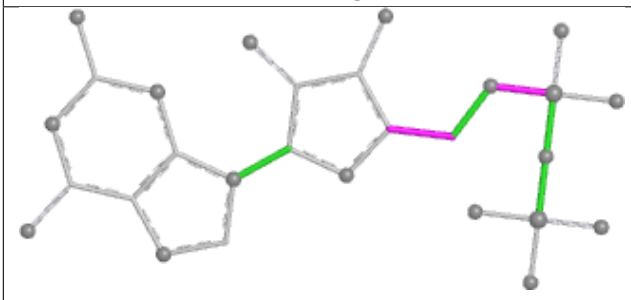
Ligand GDP AT 500



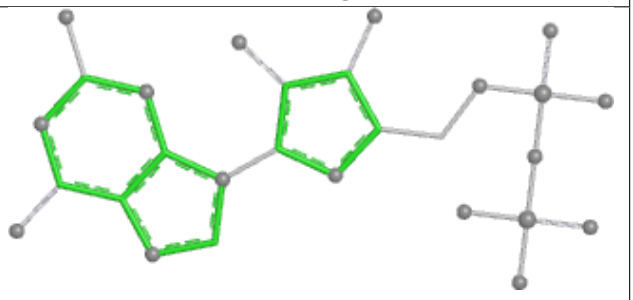
Bond lengths



Bond angles

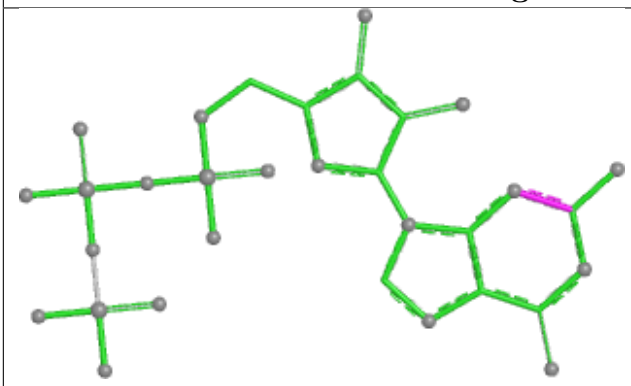


Torsions

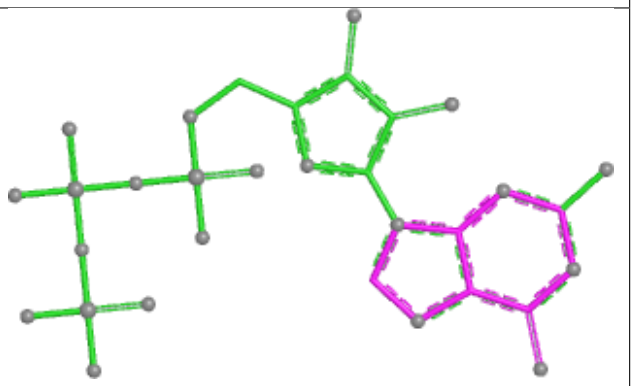


Rings

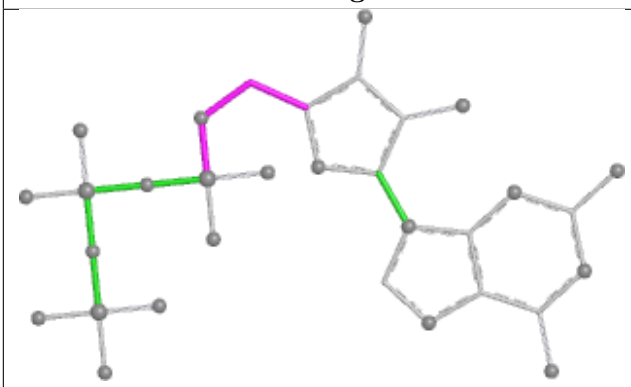
Ligand GTP LX 501



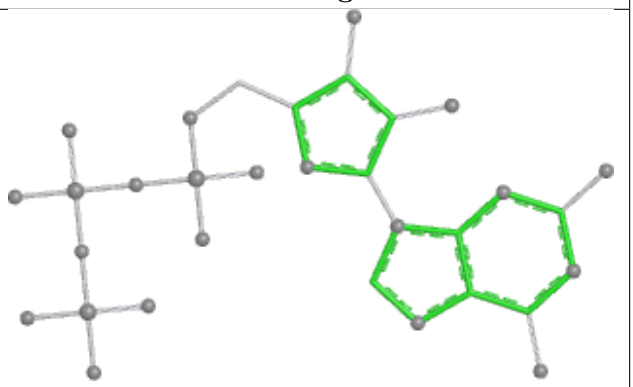
Bond lengths



Bond angles

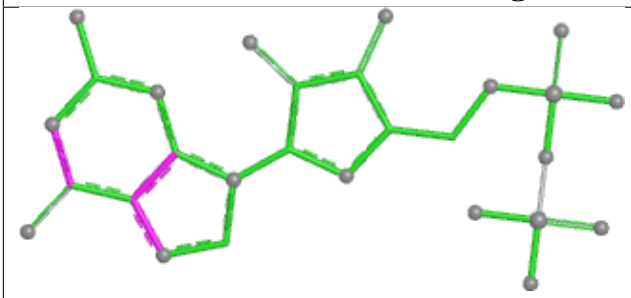


Torsions

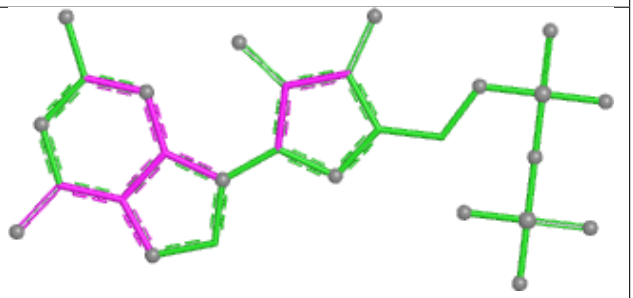


Rings

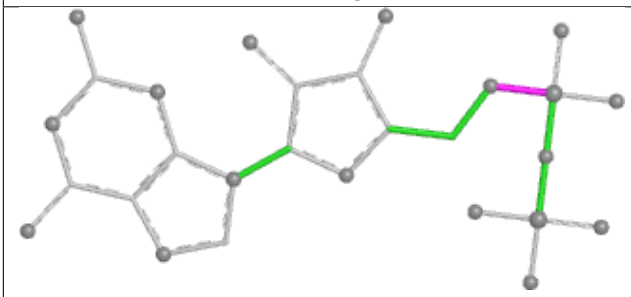
Ligand GDP ER 500



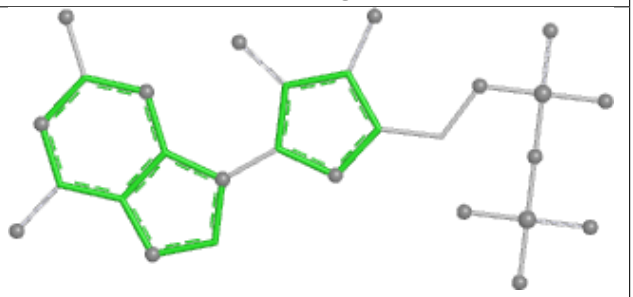
Bond lengths



Bond angles

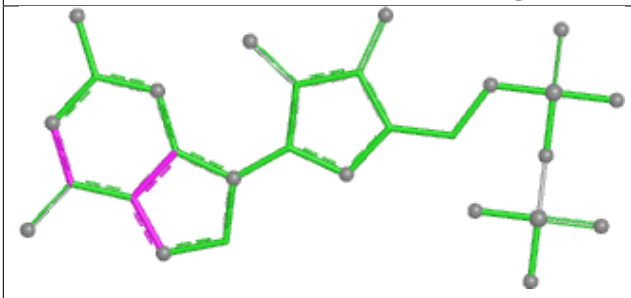


Torsions

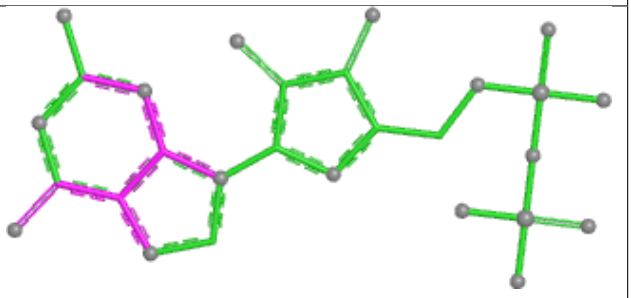


Rings

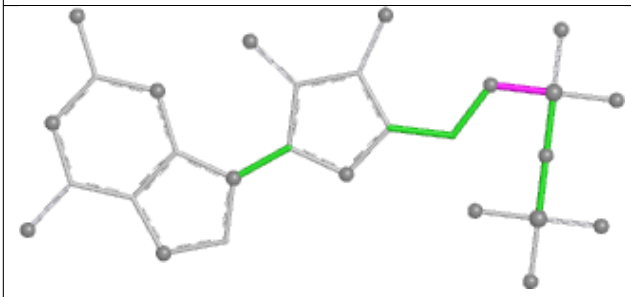
Ligand GDP VL 500



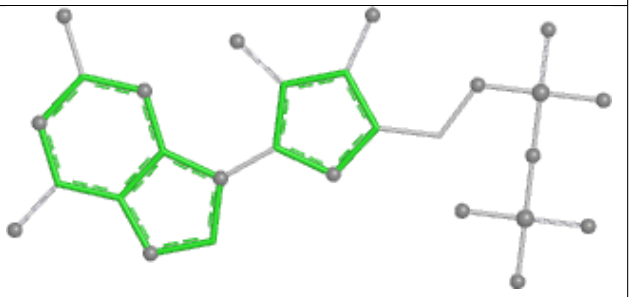
Bond lengths



Bond angles

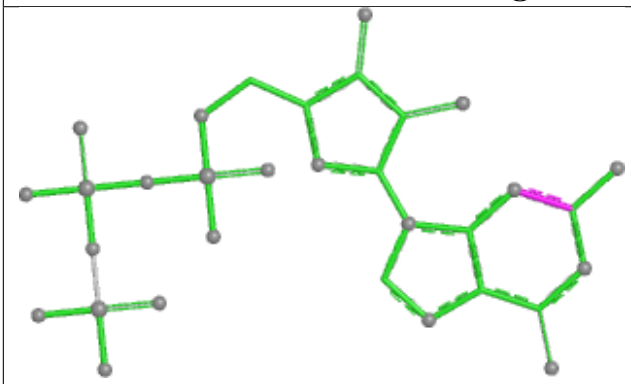


Torsions

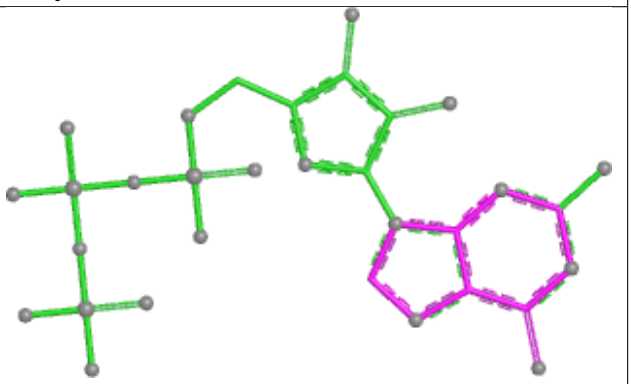


Rings

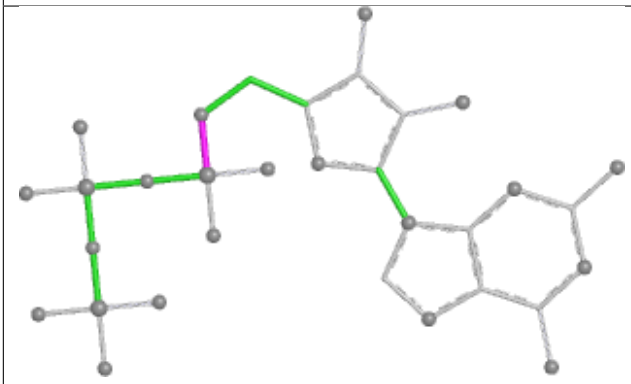
Ligand GTP QL 501



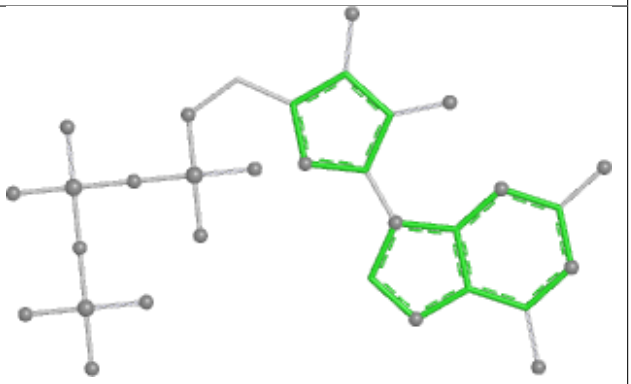
Bond lengths



Bond angles

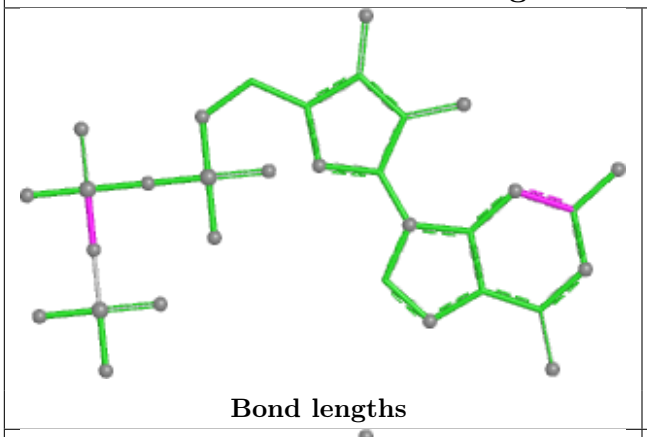


Torsions

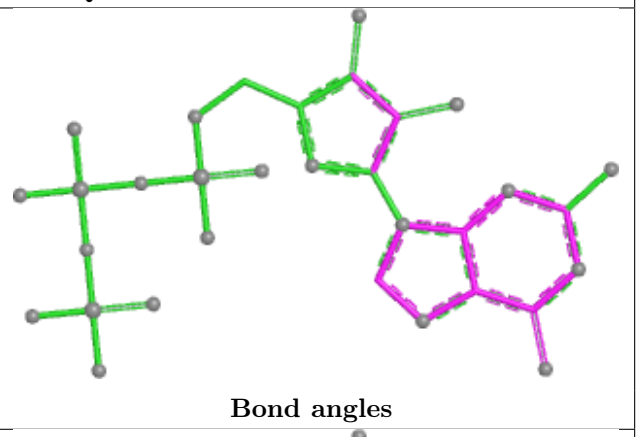


Rings

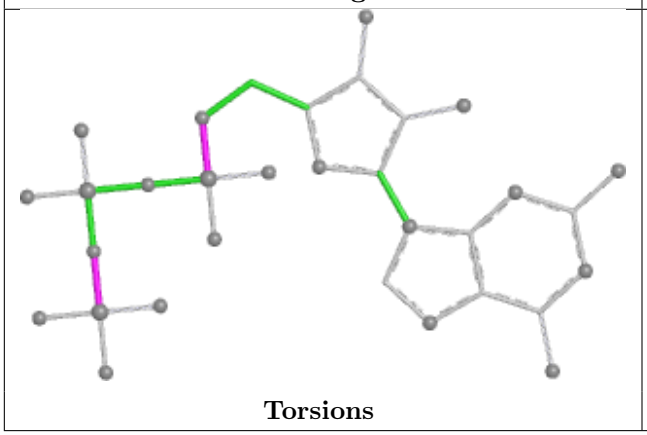
Ligand GTP NQ 501



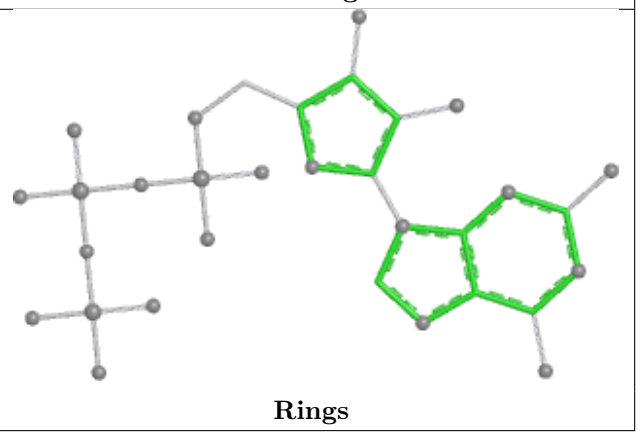
Bond lengths



Bond angles

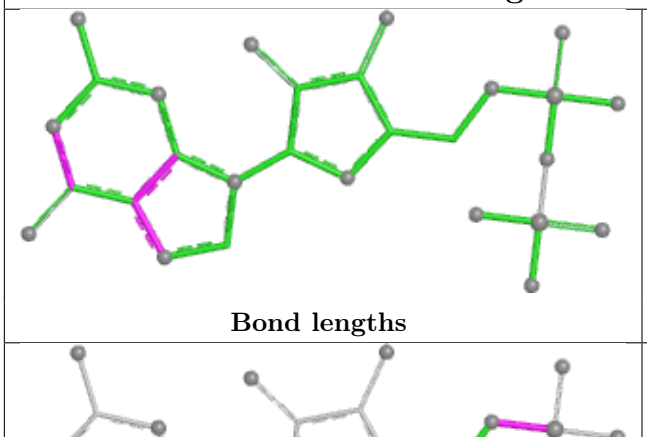


Torsions

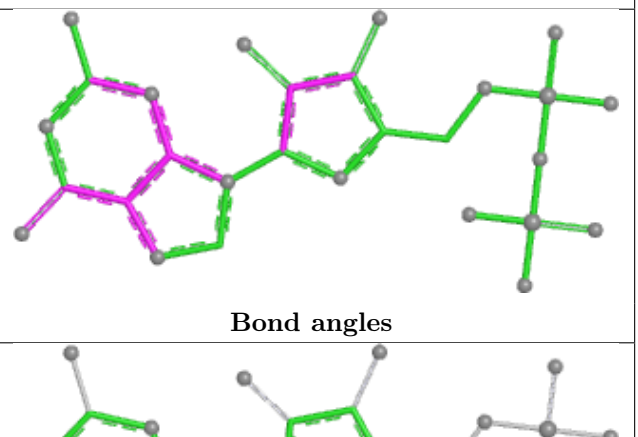


Rings

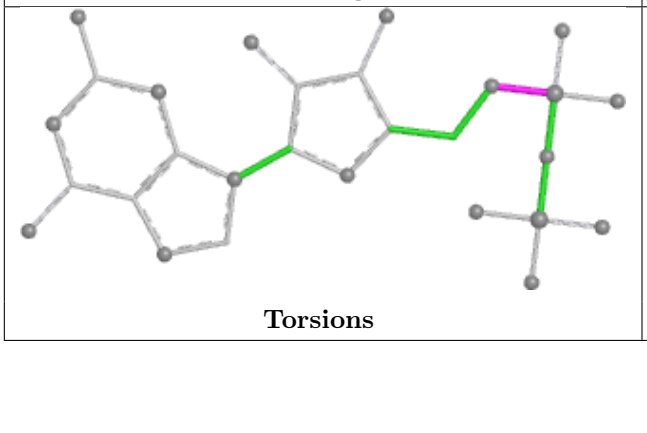
Ligand GDP WL 500



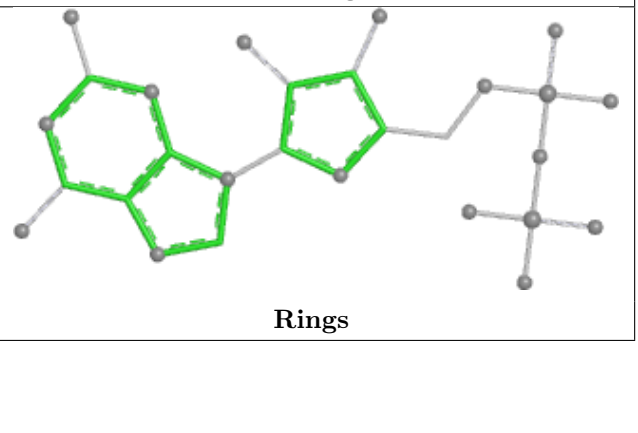
Bond lengths



Bond angles

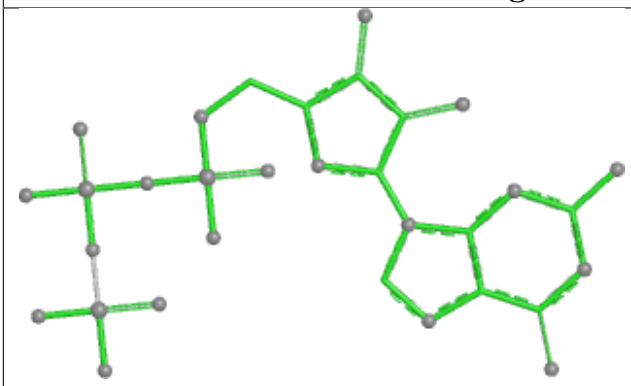


Torsions

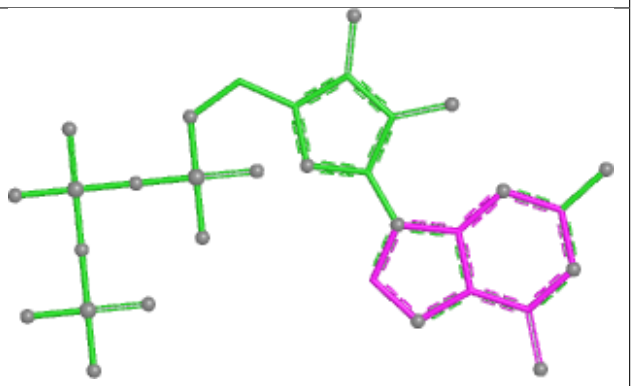


Rings

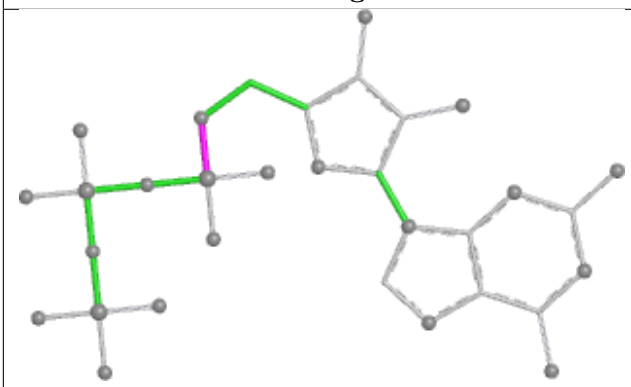
Ligand GTP CN 501



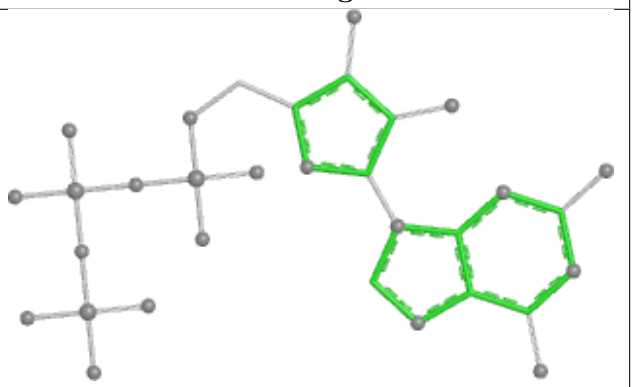
Bond lengths



Bond angles

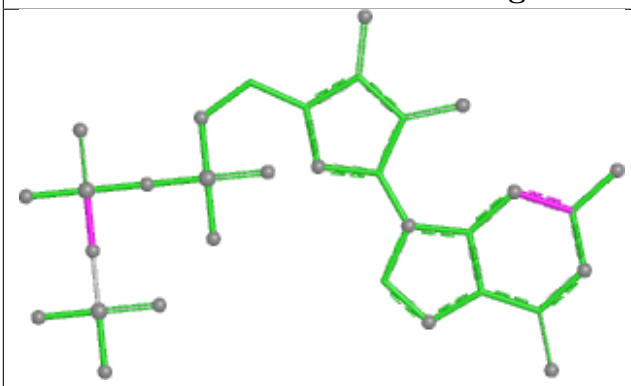


Torsions

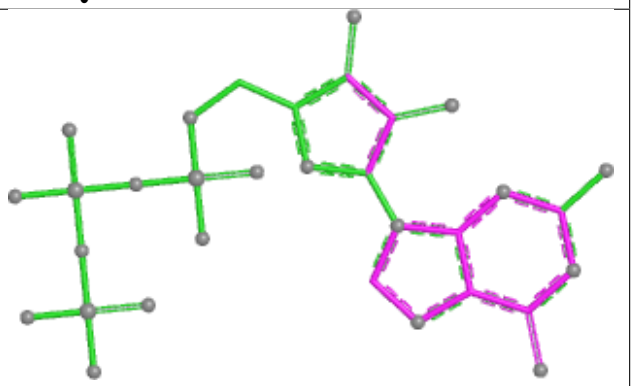


Rings

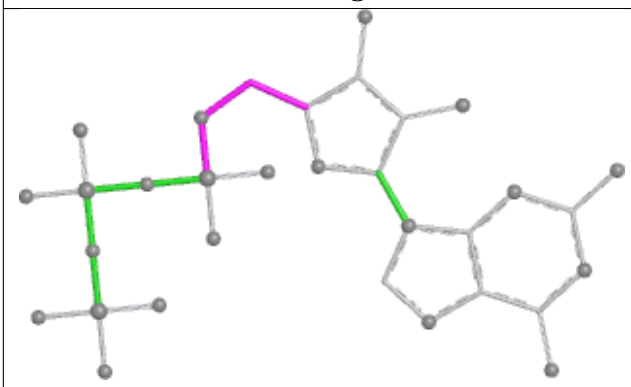
Ligand GTP DQ 501



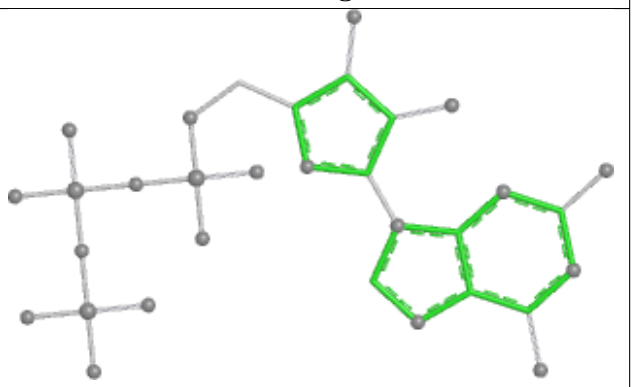
Bond lengths



Bond angles

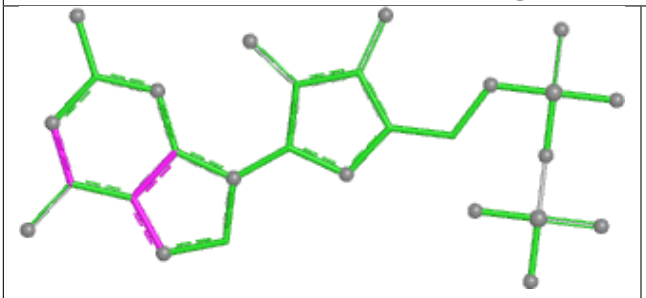


Torsions

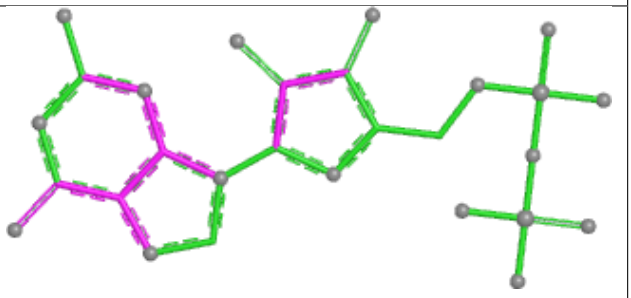


Rings

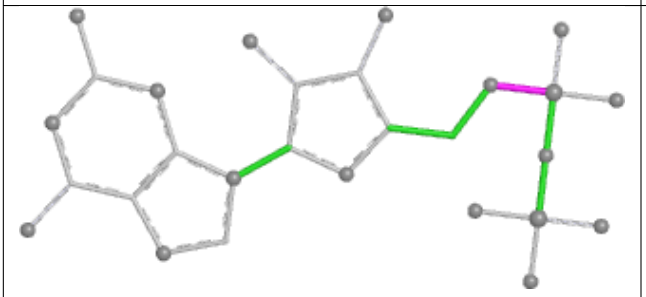
Ligand GDP PL 501



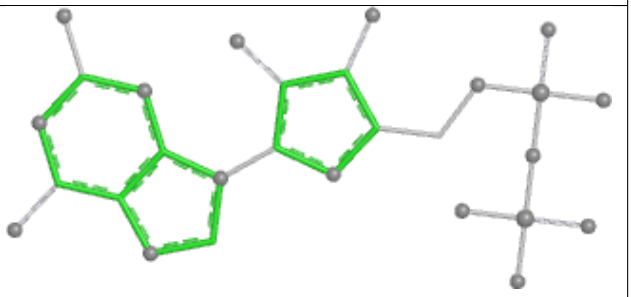
Bond lengths



Bond angles

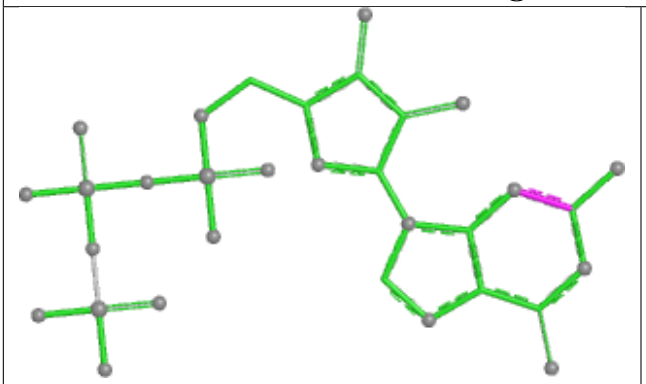


Torsions

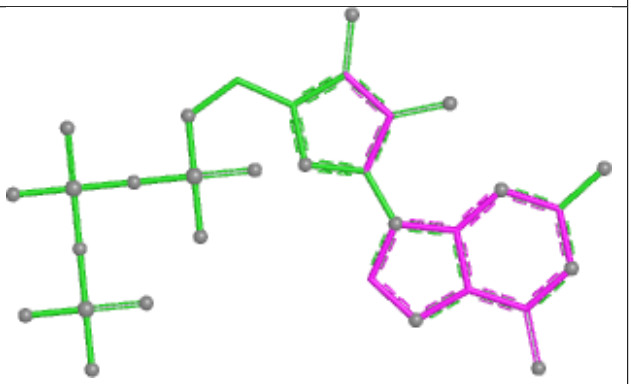


Rings

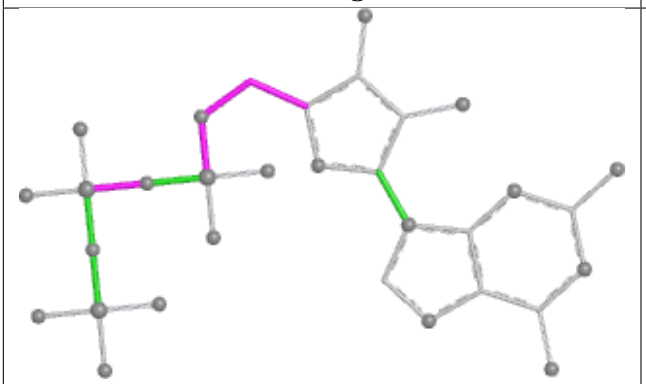
Ligand GTP OK 501



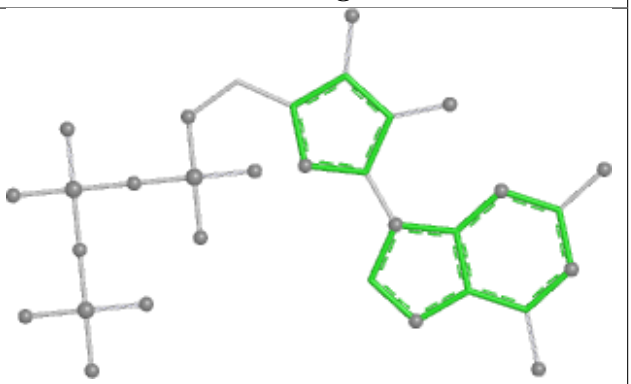
Bond lengths



Bond angles

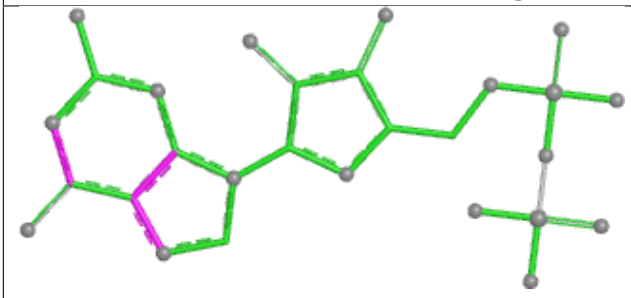


Torsions

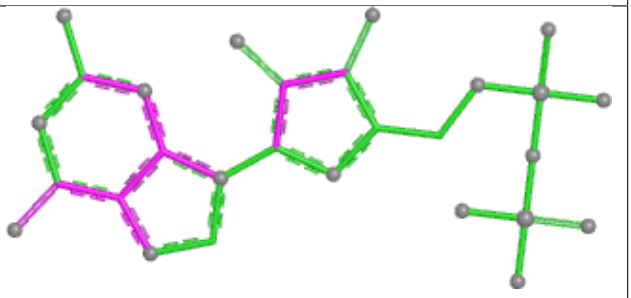


Rings

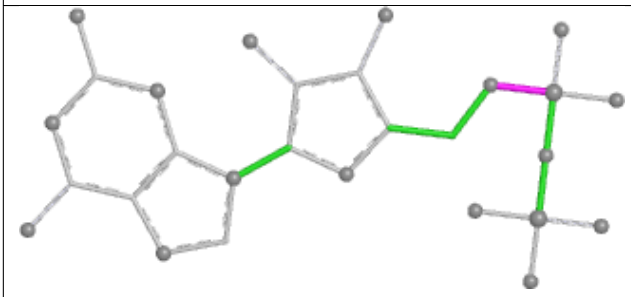
Ligand GDP LK 500



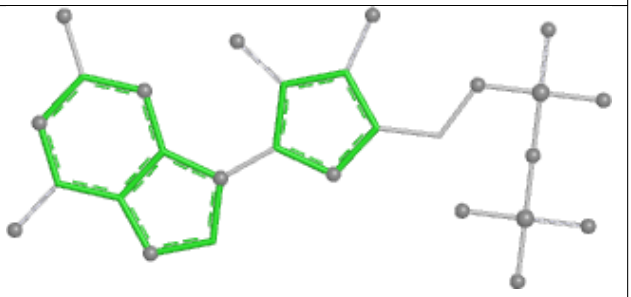
Bond lengths



Bond angles

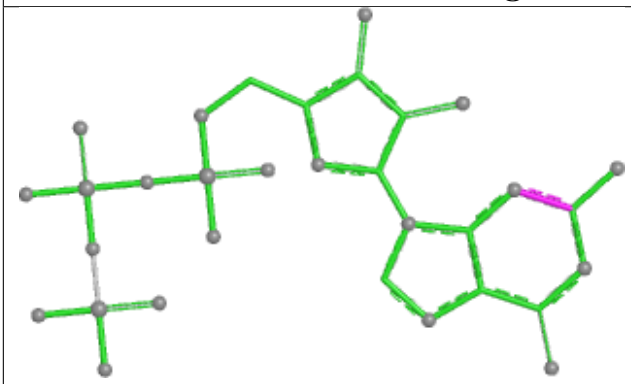


Torsions

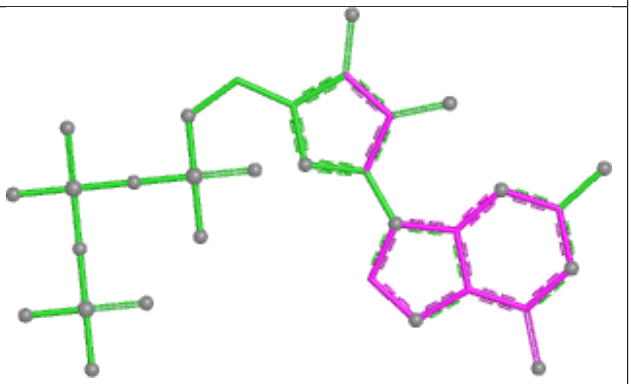


Rings

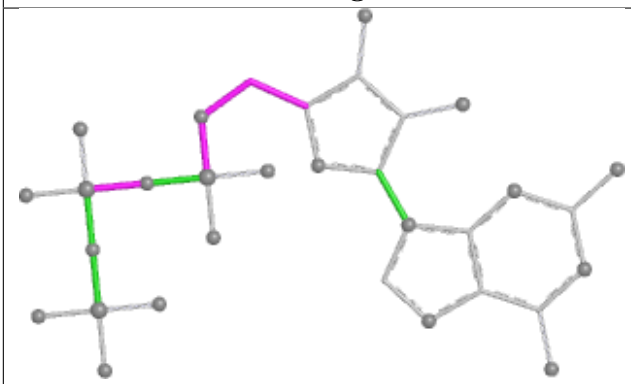
Ligand GTP OW 501



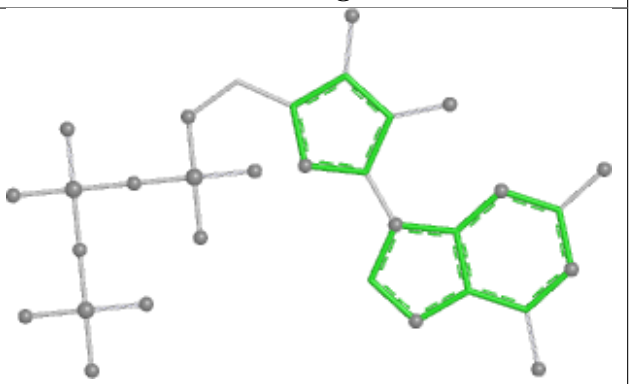
Bond lengths



Bond angles

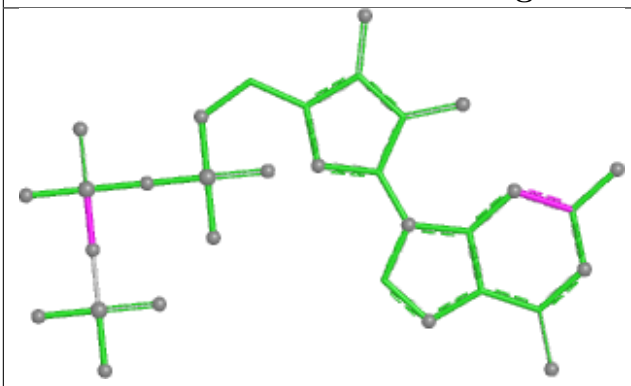


Torsions

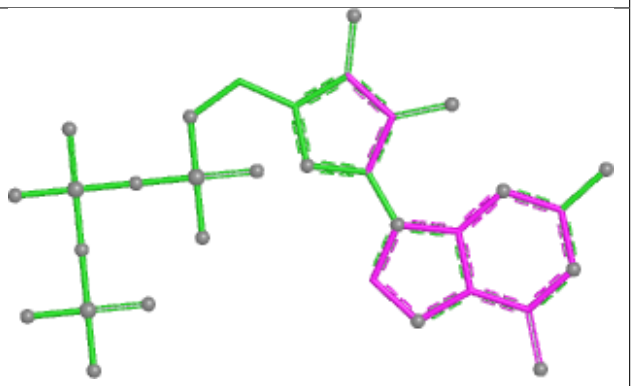


Rings

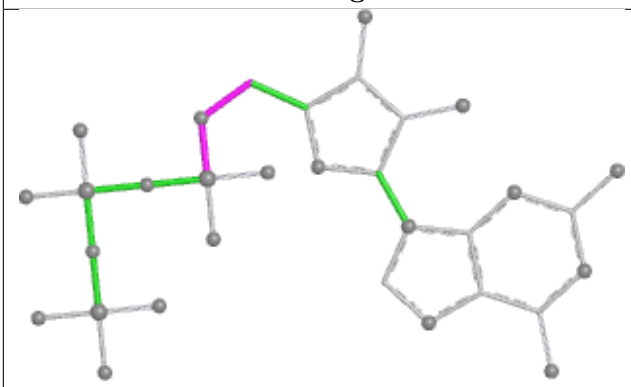
Ligand GTP IO 501



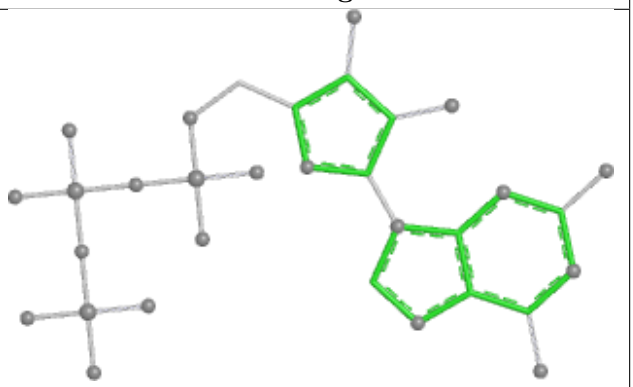
Bond lengths



Bond angles

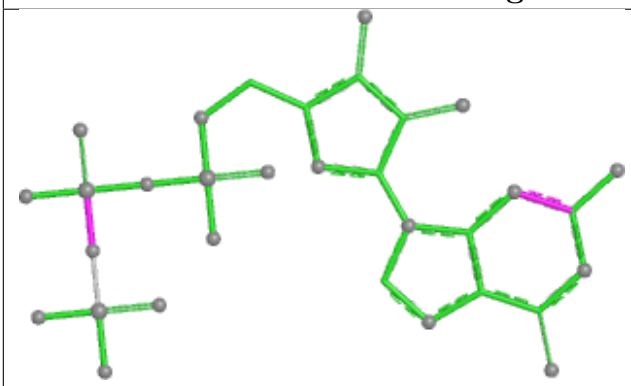


Torsions

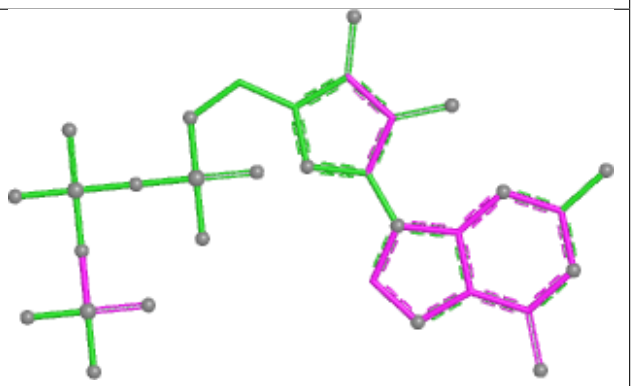


Rings

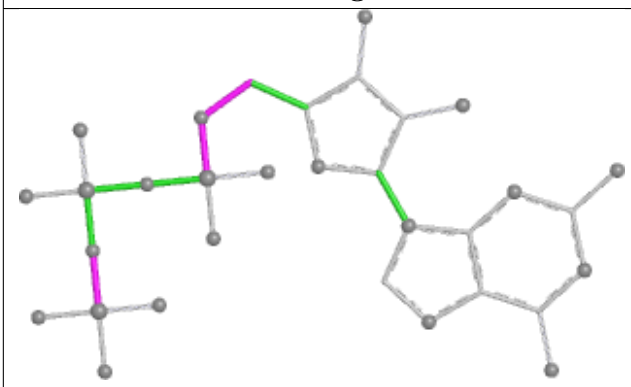
Ligand GTP TM 501



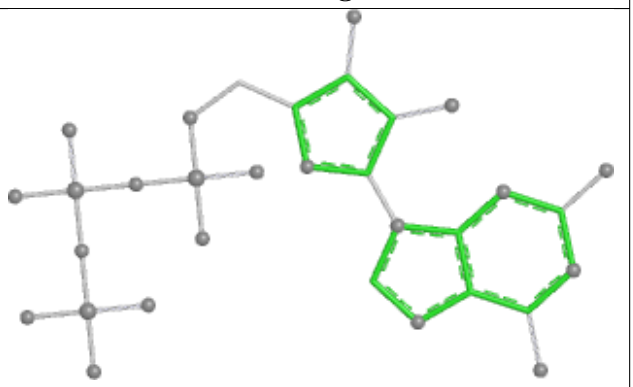
Bond lengths



Bond angles

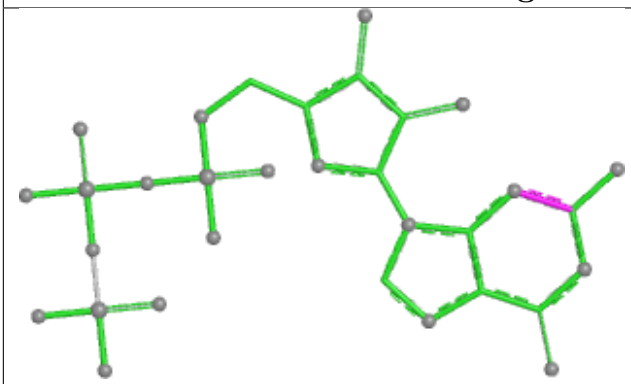


Torsions

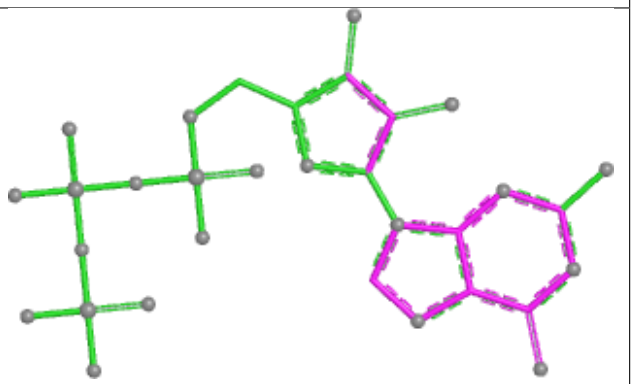


Rings

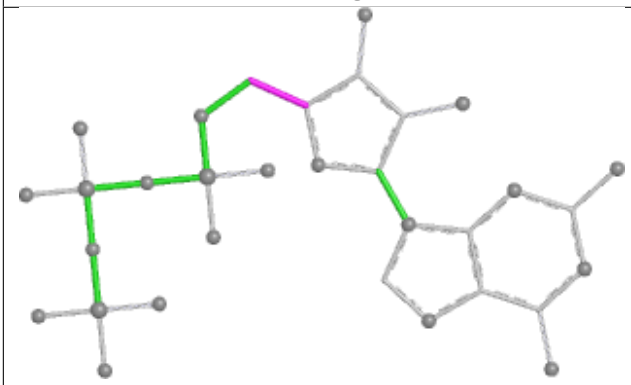
Ligand GTP IE 501



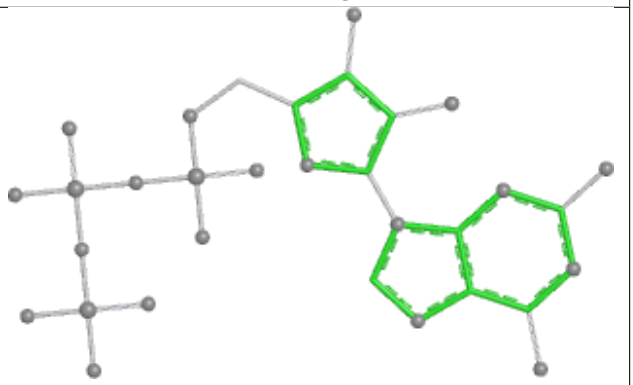
Bond lengths



Bond angles

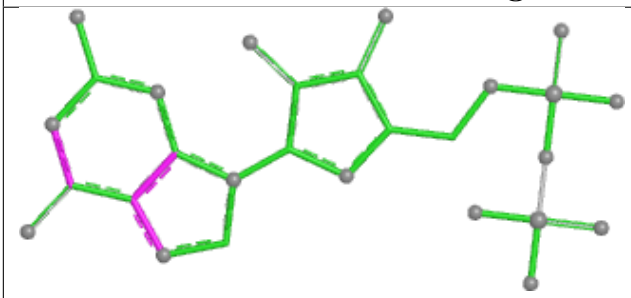


Torsions

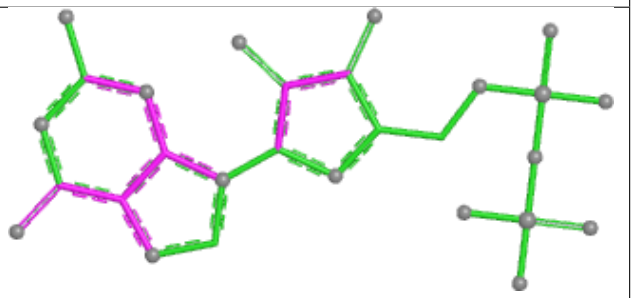


Rings

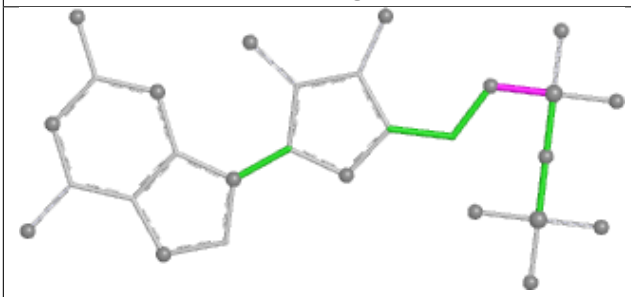
Ligand GDP DU 500



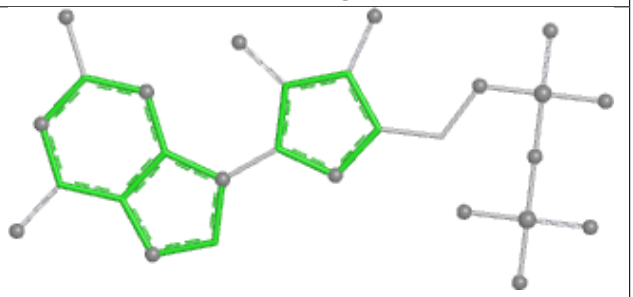
Bond lengths



Bond angles

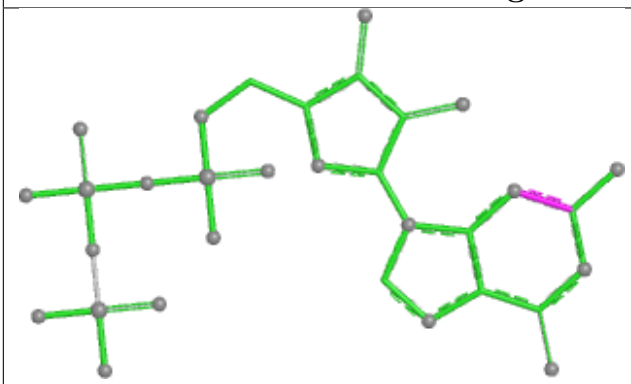


Torsions

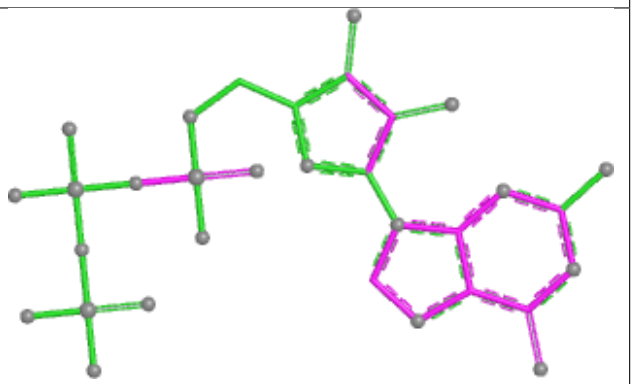


Rings

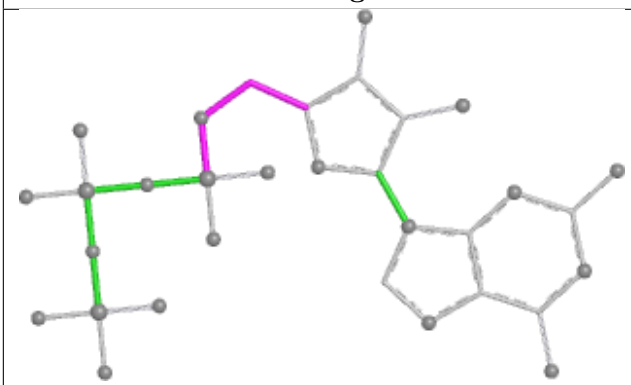
Ligand GTP GG 501



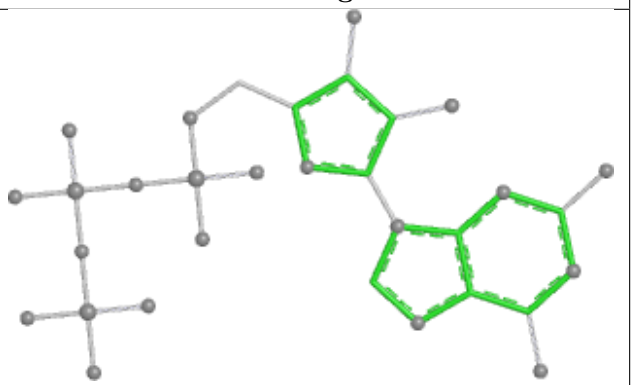
Bond lengths



Bond angles

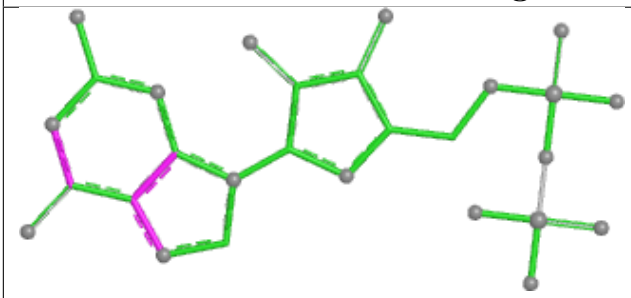


Torsions

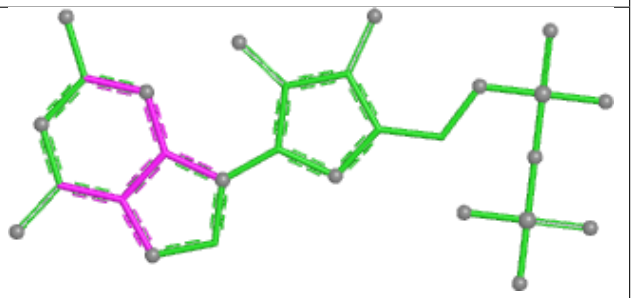


Rings

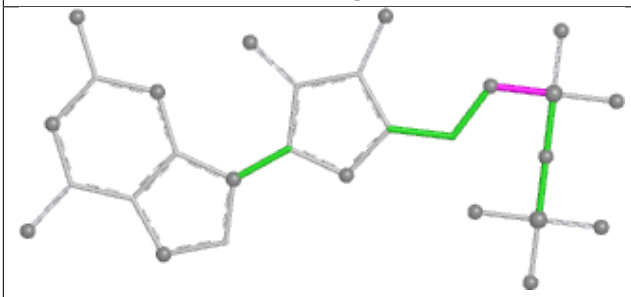
Ligand GDP CS 500



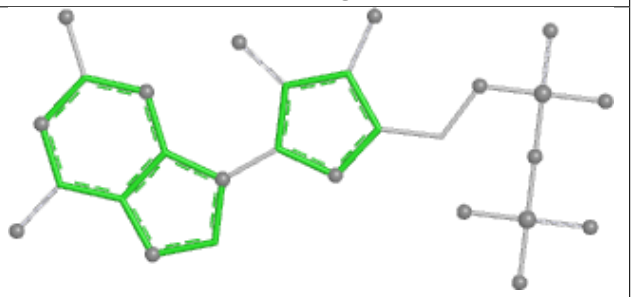
Bond lengths



Bond angles

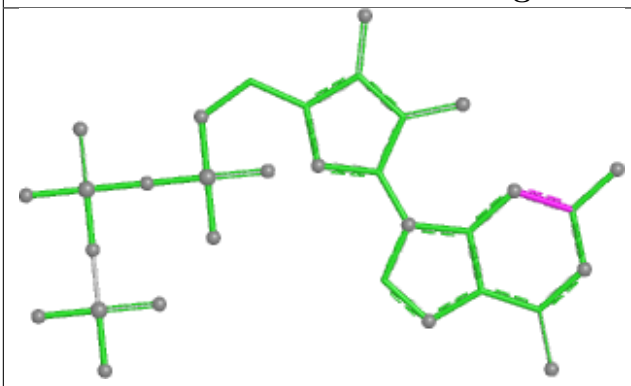


Torsions

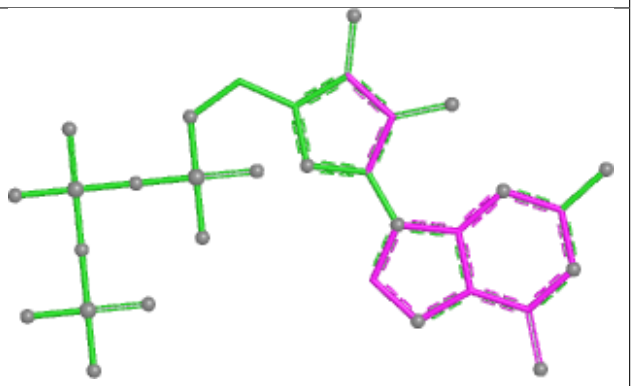


Rings

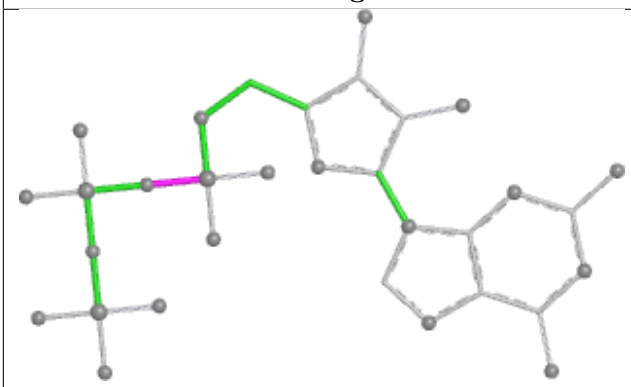
Ligand GTP TS 501



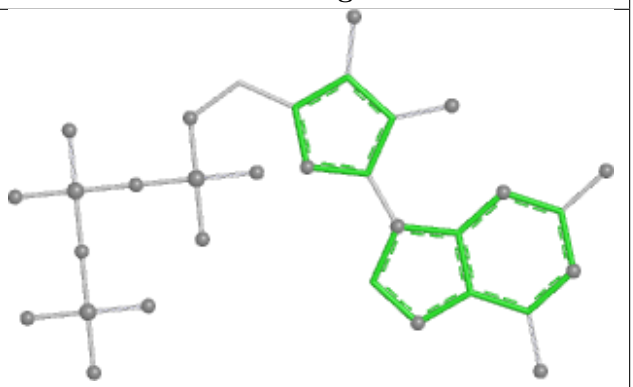
Bond lengths



Bond angles

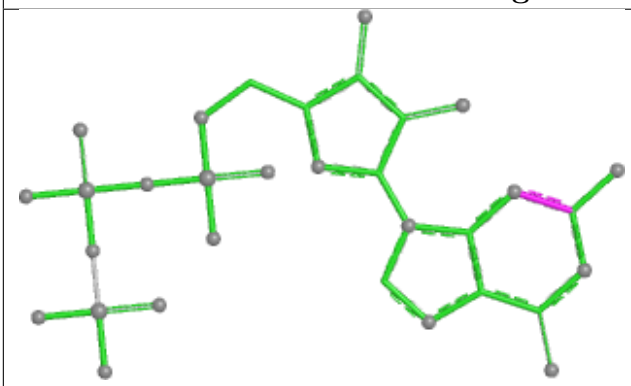


Torsions

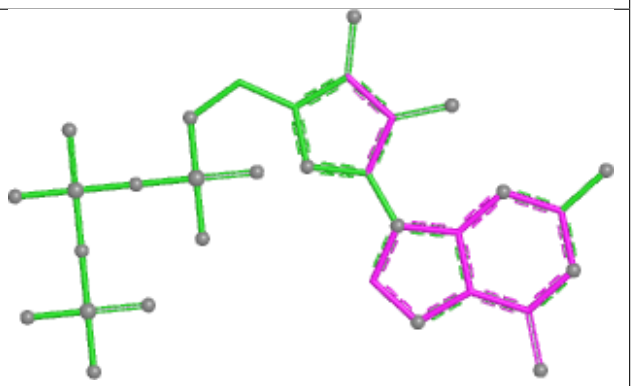


Rings

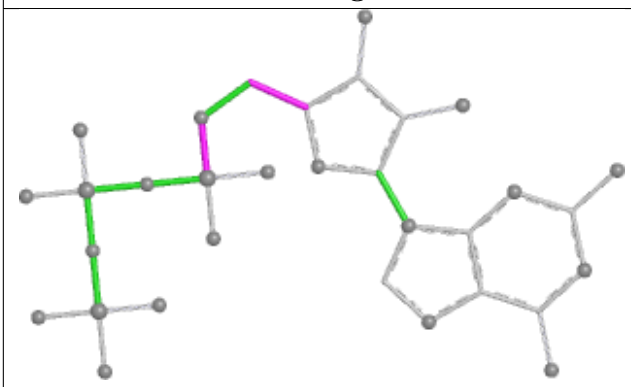
Ligand GTP US 501



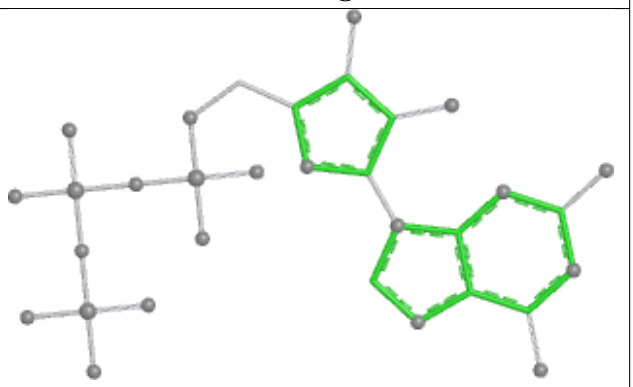
Bond lengths



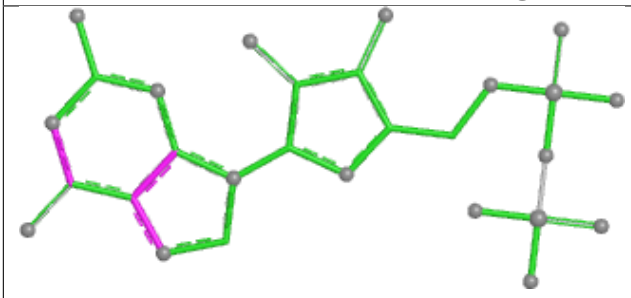
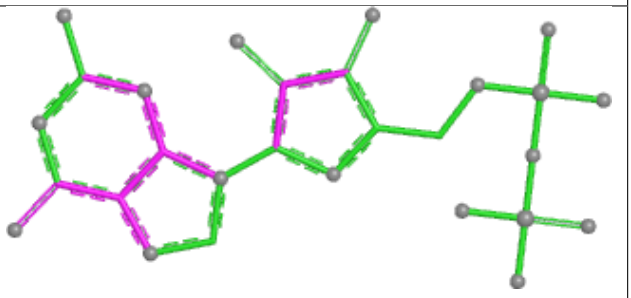
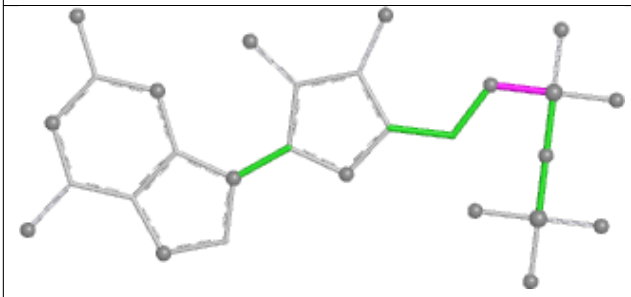
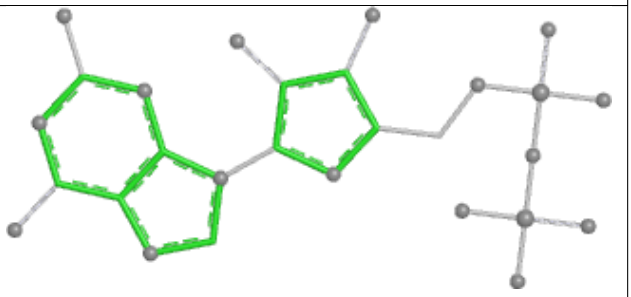
Bond angles

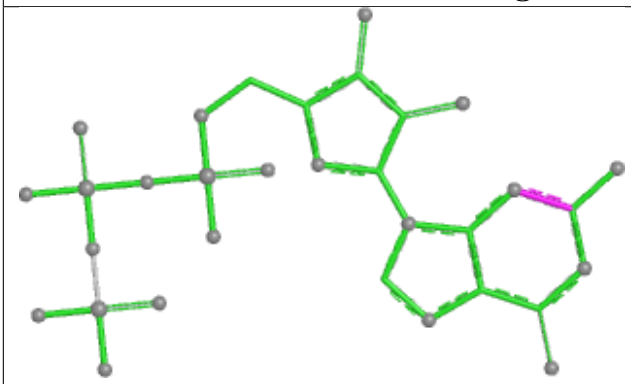
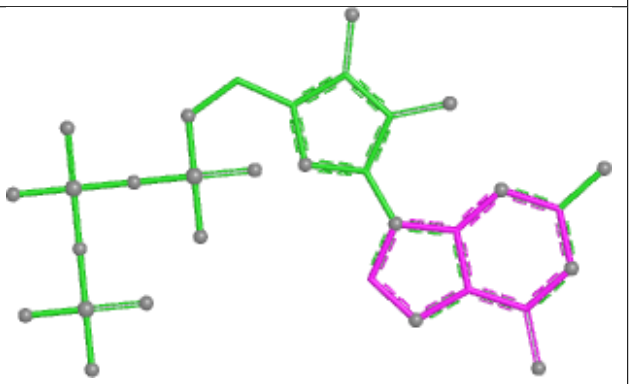
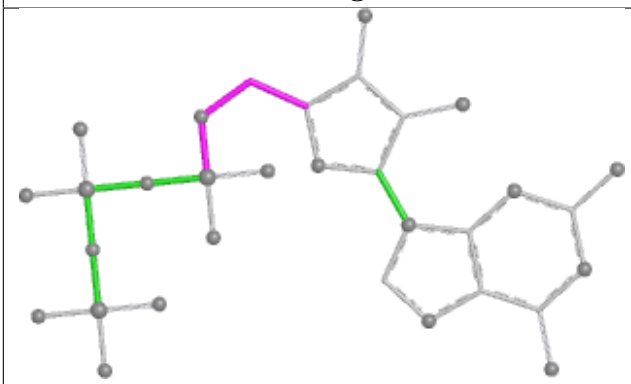
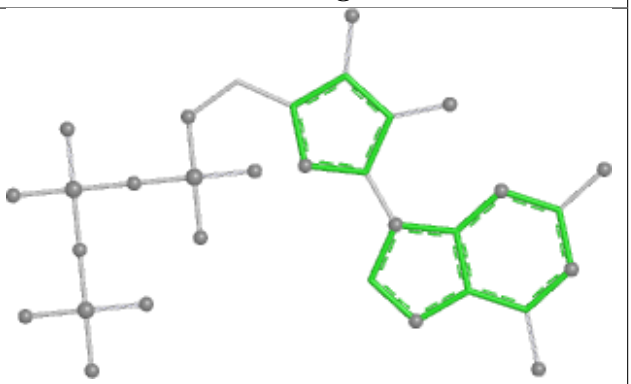


Torsions

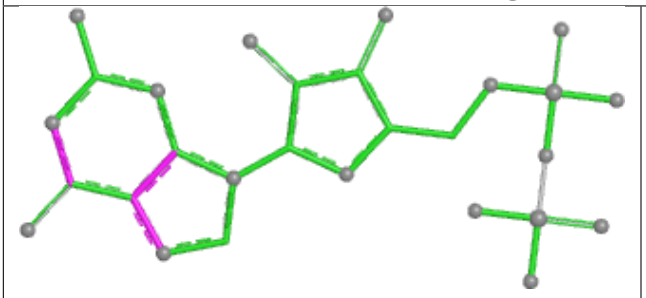


Rings

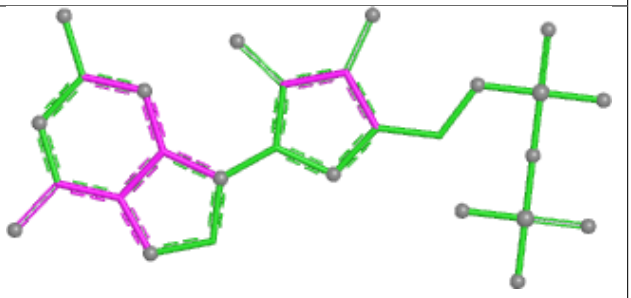
Ligand GDP SL 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP LL 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

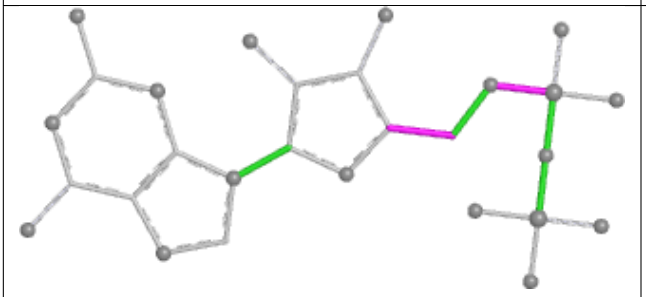
Ligand GDP MV 500



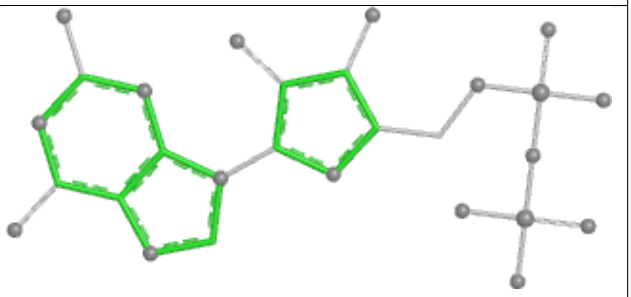
Bond lengths



Bond angles

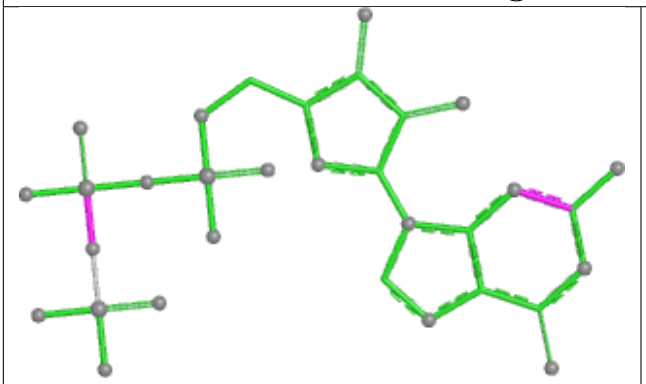


Torsions

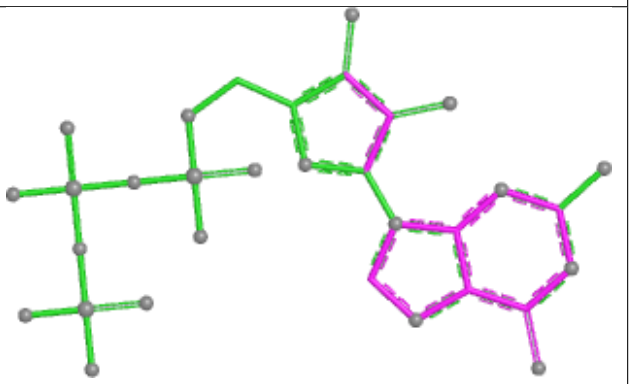


Rings

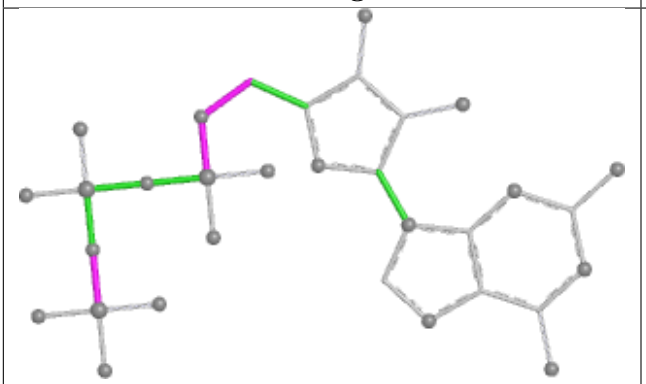
Ligand GTP HN 503



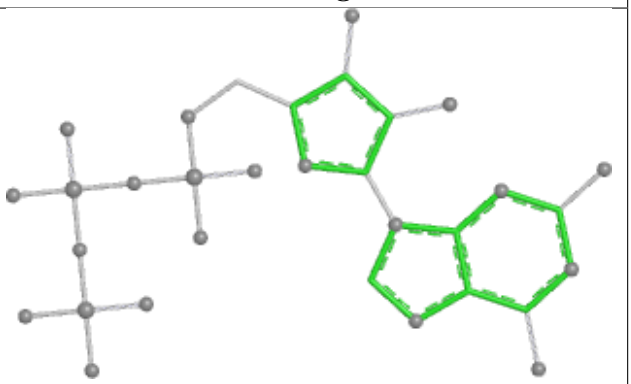
Bond lengths



Bond angles

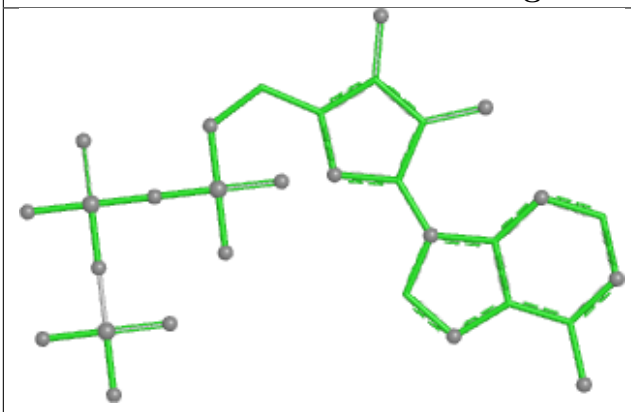


Torsions

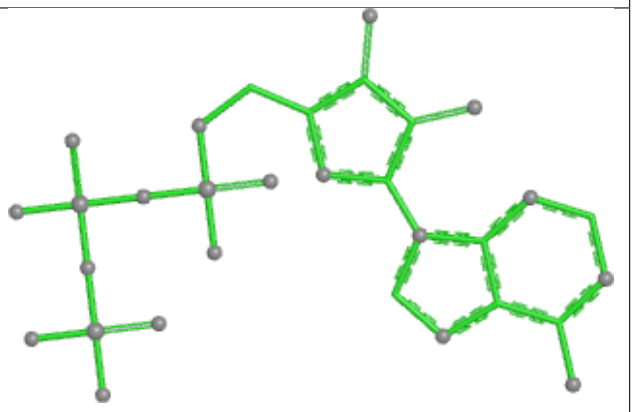


Rings

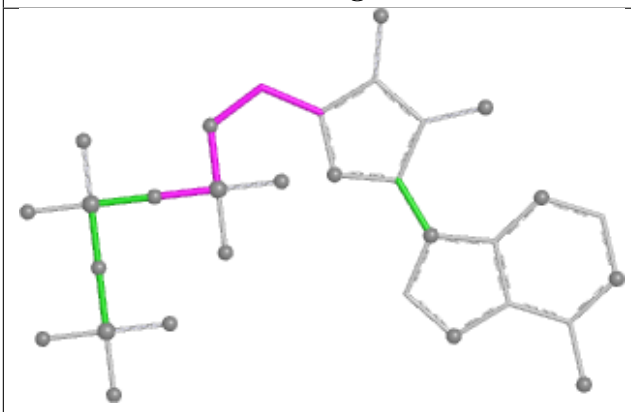
Ligand ATP 6l 400



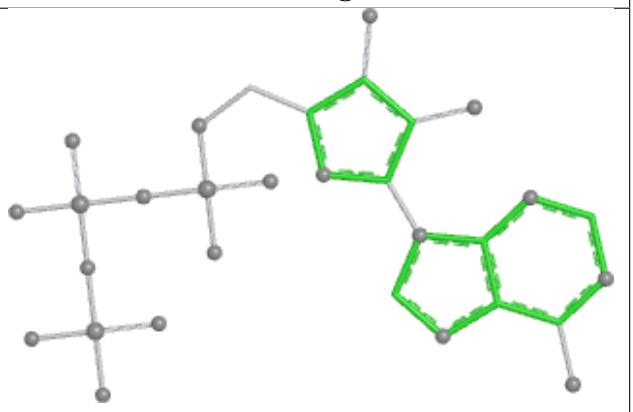
Bond lengths



Bond angles

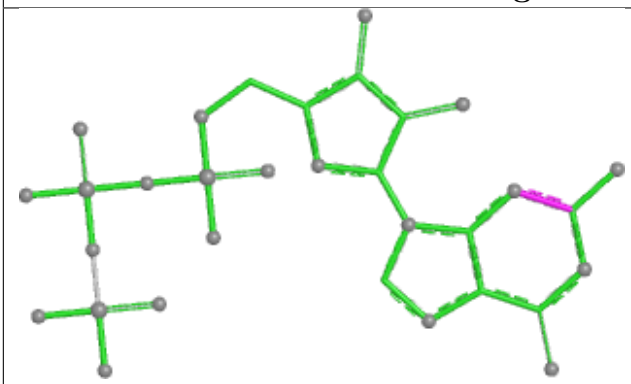


Torsions

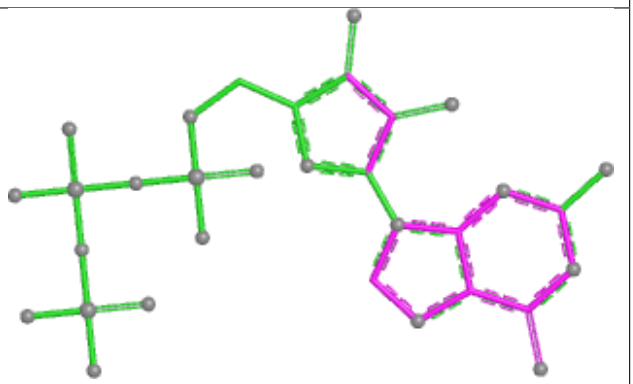


Rings

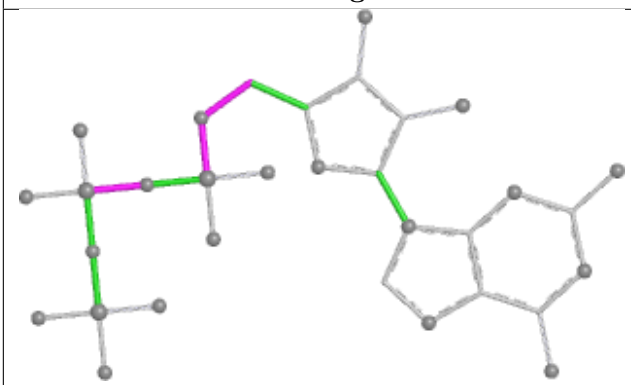
Ligand GTP LV 501



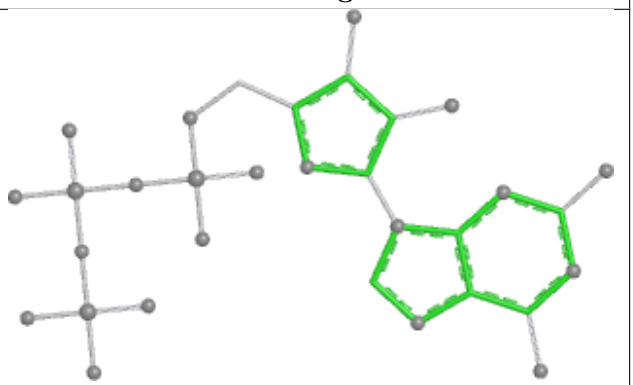
Bond lengths



Bond angles

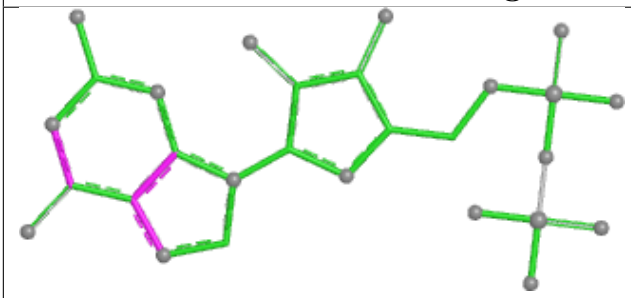


Torsions

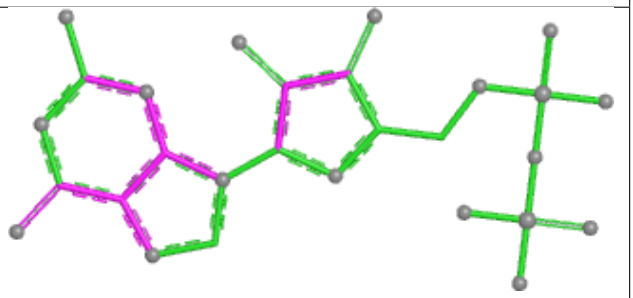


Rings

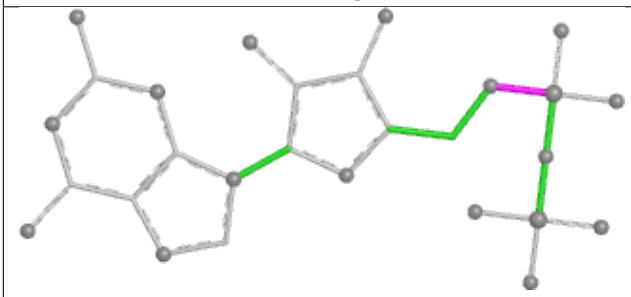
Ligand GDP DM 500



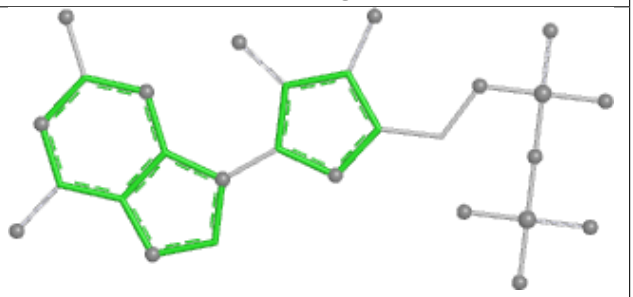
Bond lengths



Bond angles

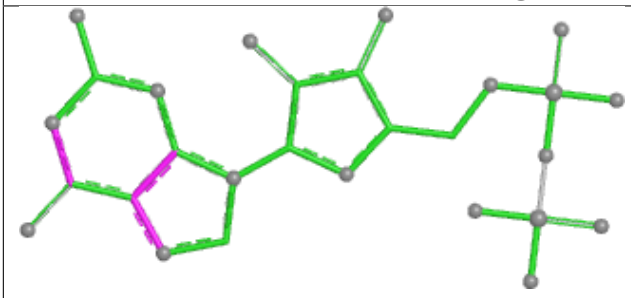


Torsions

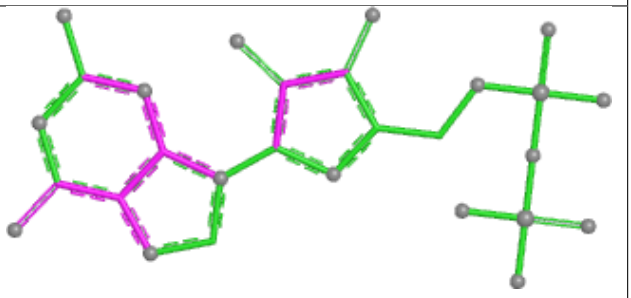


Rings

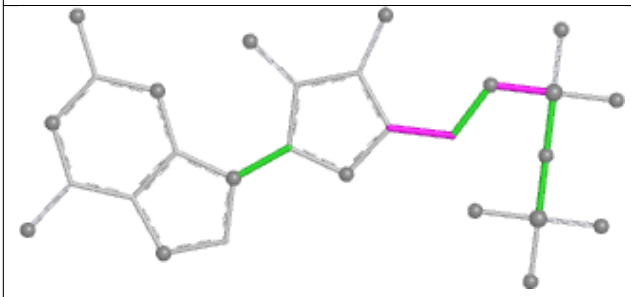
Ligand GDP JC 500



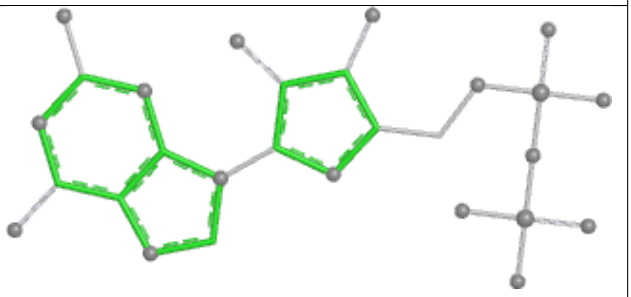
Bond lengths



Bond angles

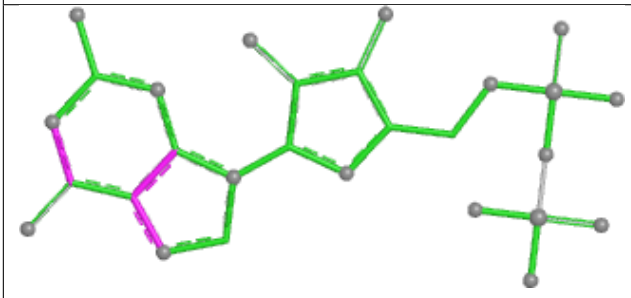


Torsions

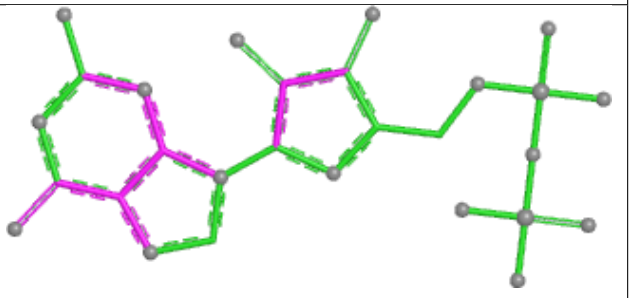


Rings

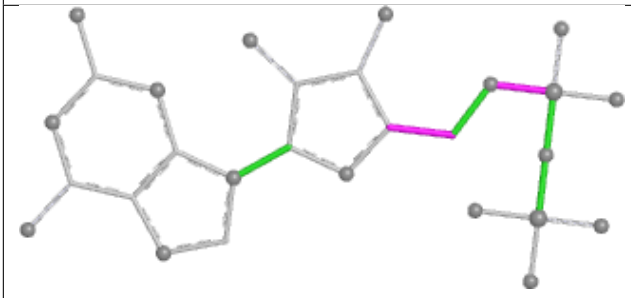
Ligand GDP KA 500



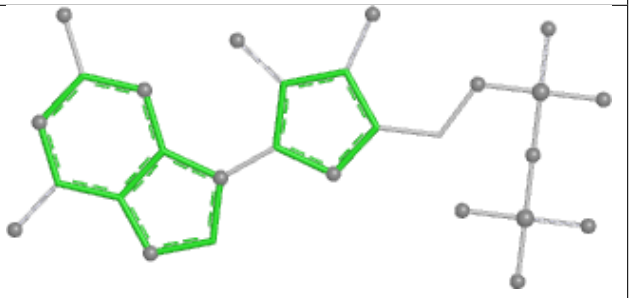
Bond lengths



Bond angles

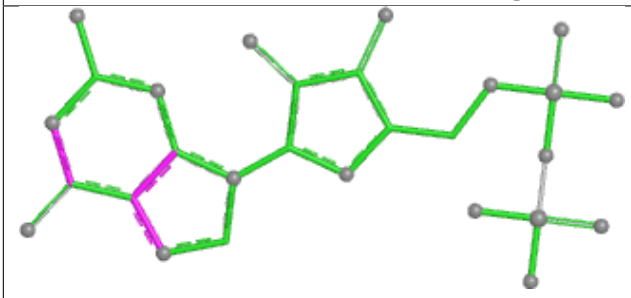


Torsions

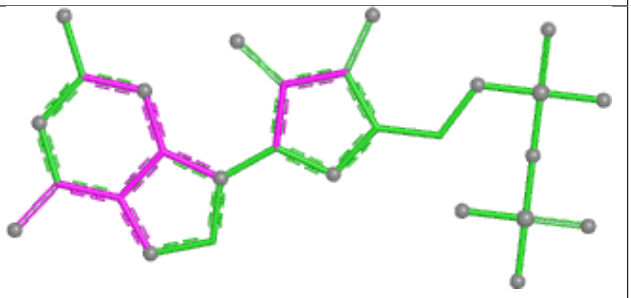


Rings

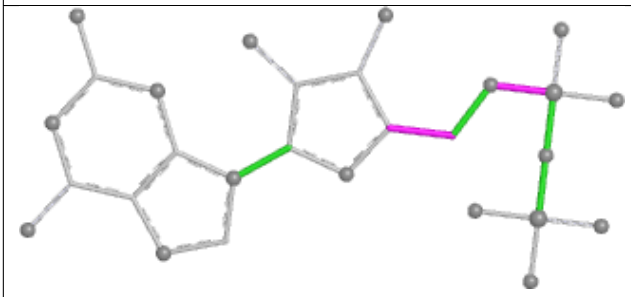
Ligand GDP HP 501



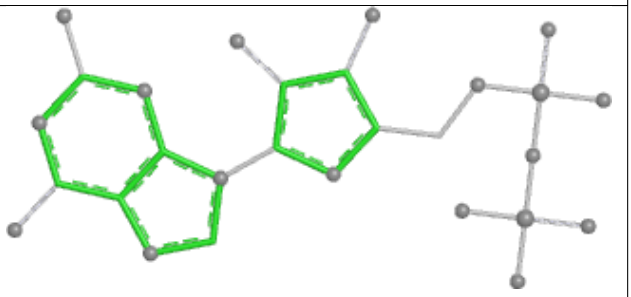
Bond lengths



Bond angles

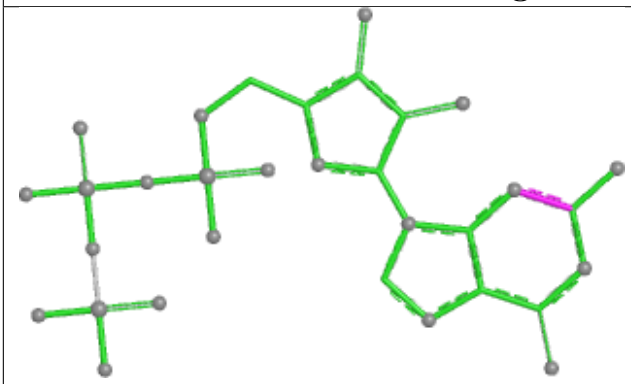


Torsions

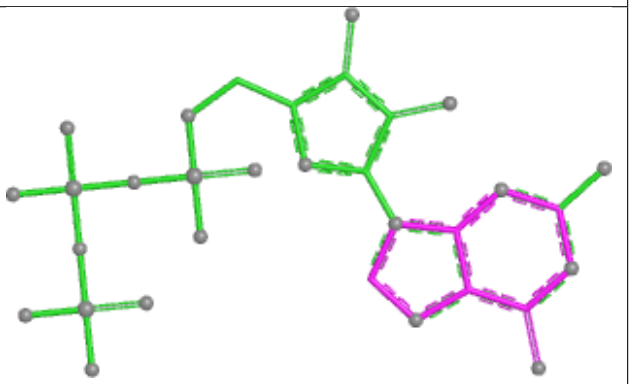


Rings

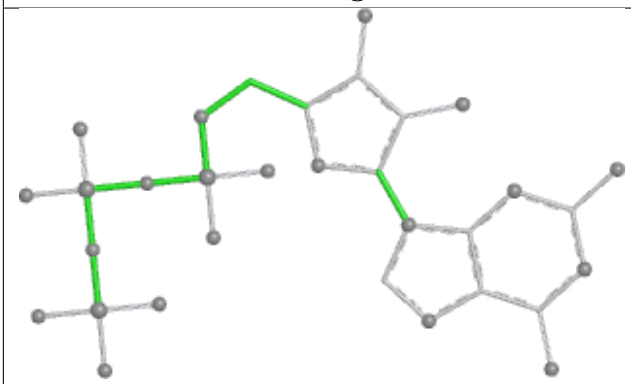
Ligand GTP PE 501



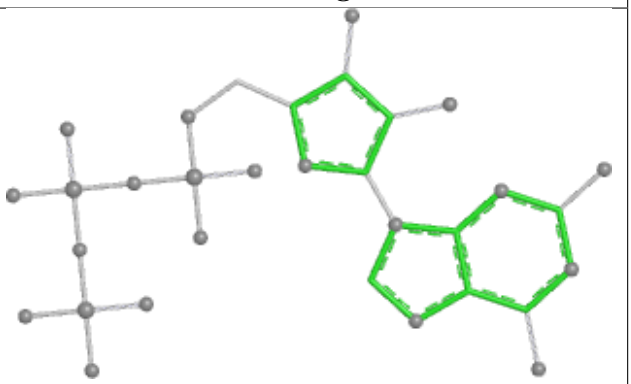
Bond lengths



Bond angles

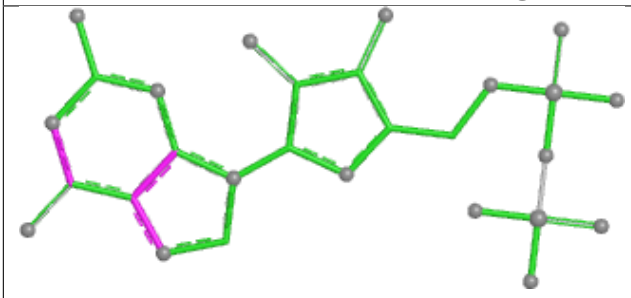


Torsions

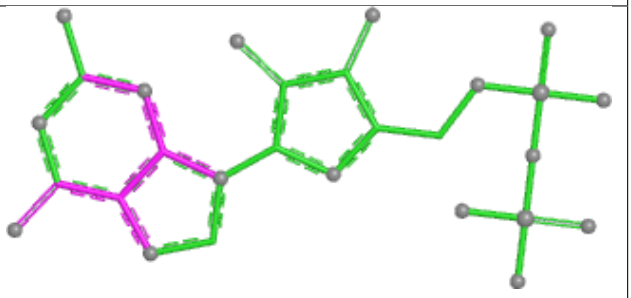


Rings

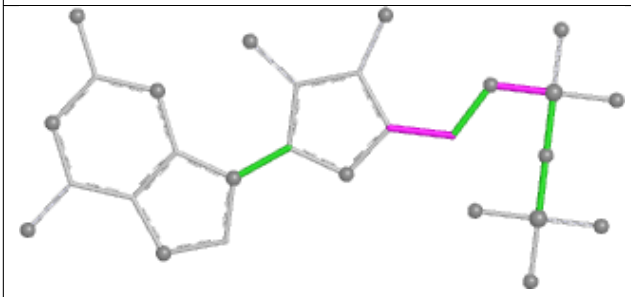
Ligand GDP LS 500



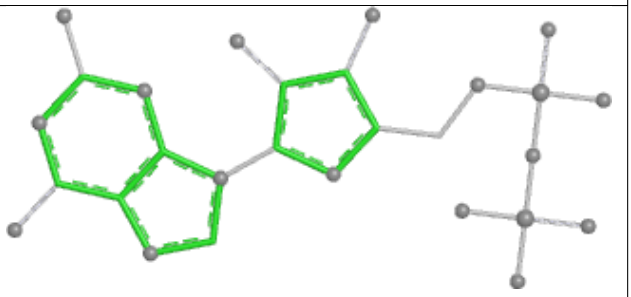
Bond lengths



Bond angles

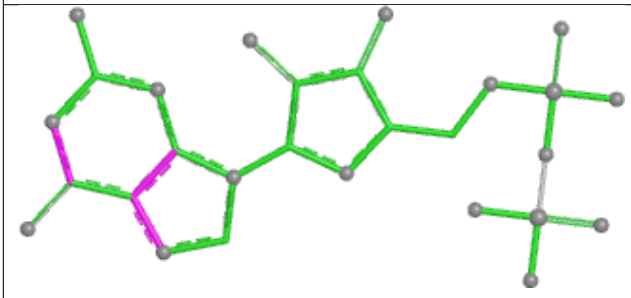


Torsions

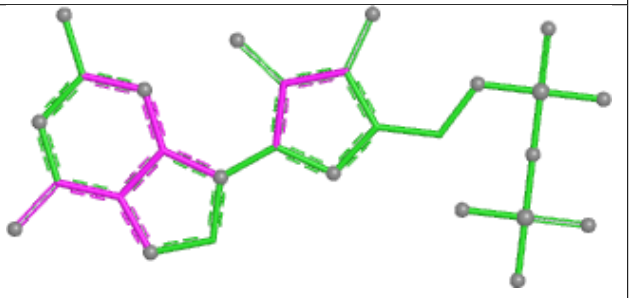


Rings

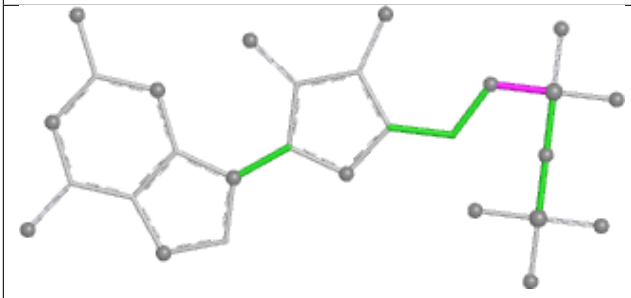
Ligand GDP JQ 500



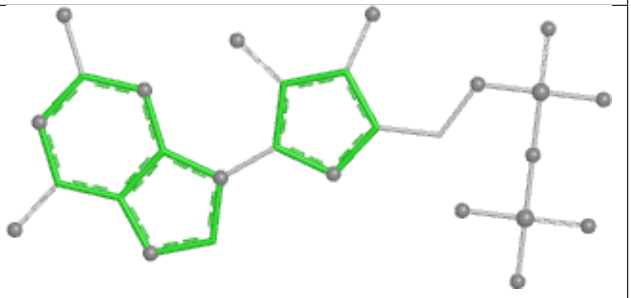
Bond lengths



Bond angles

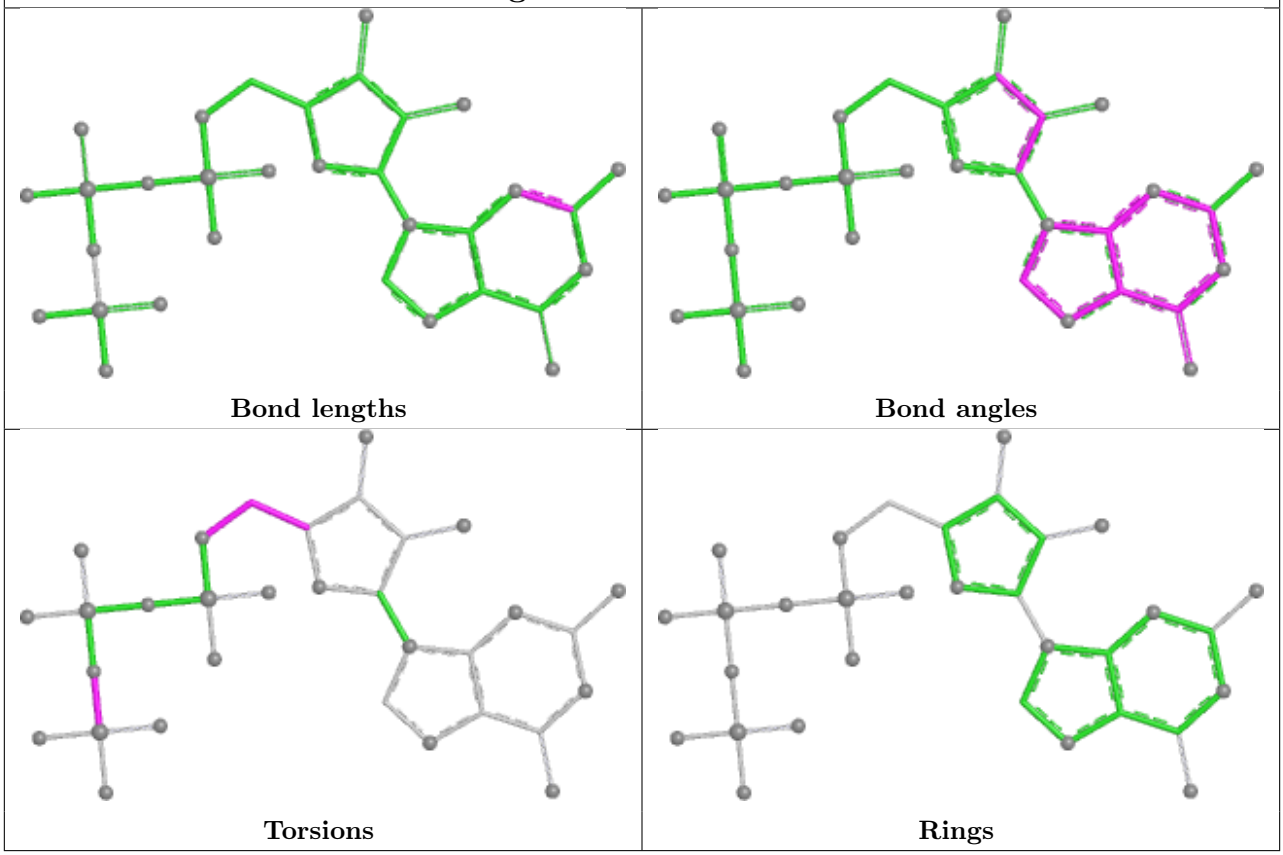


Torsions

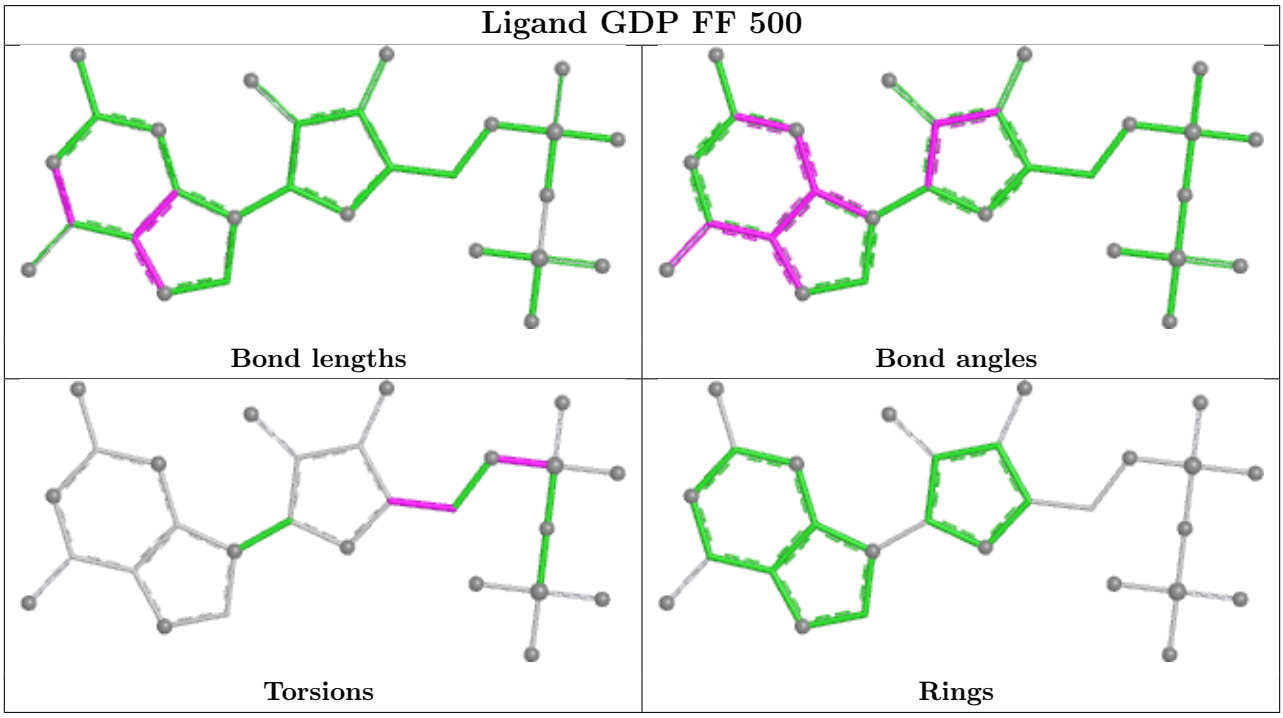


Rings

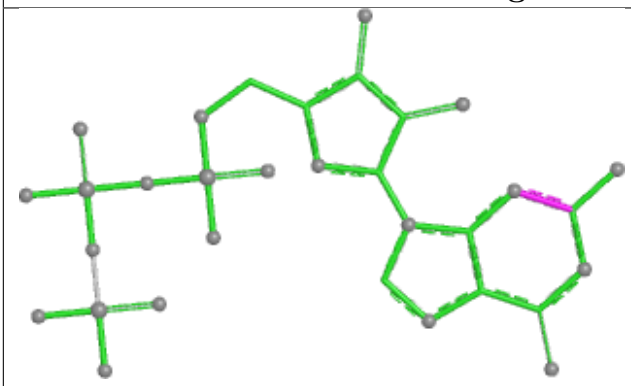
Ligand GTP KH 501



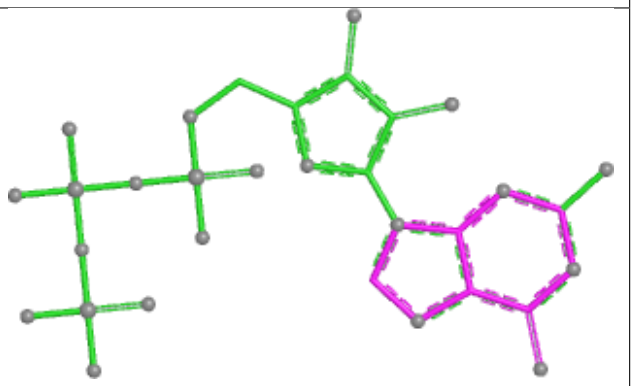
Ligand GDP FF 500



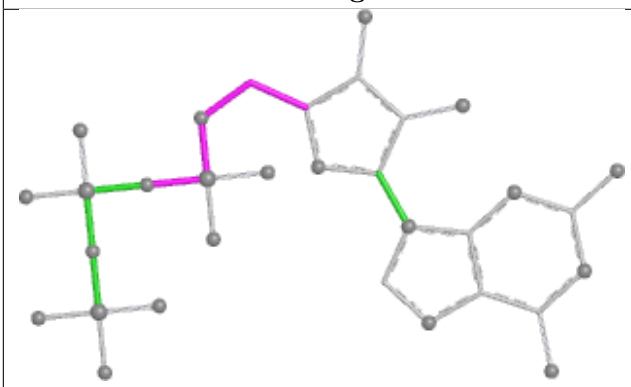
Ligand GTP UK 501



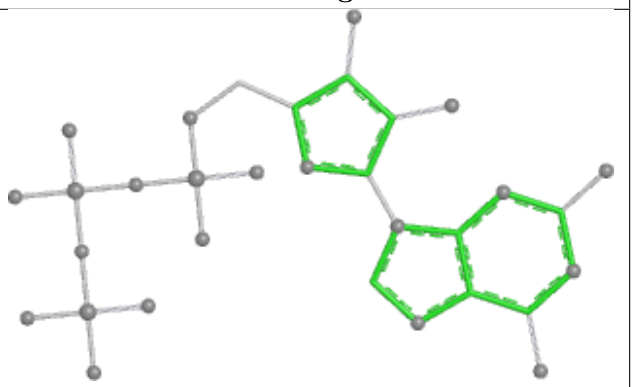
Bond lengths



Bond angles

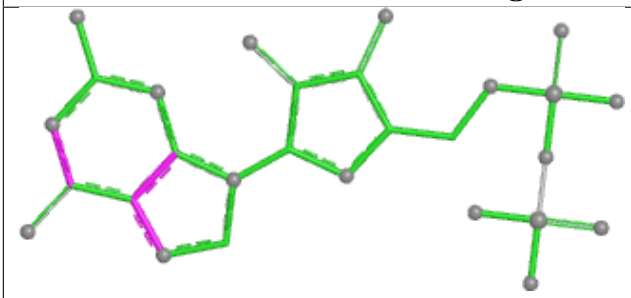


Torsions

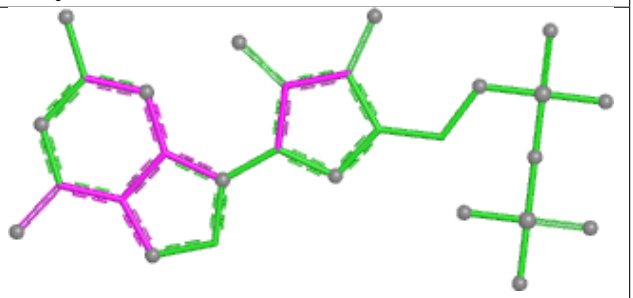


Rings

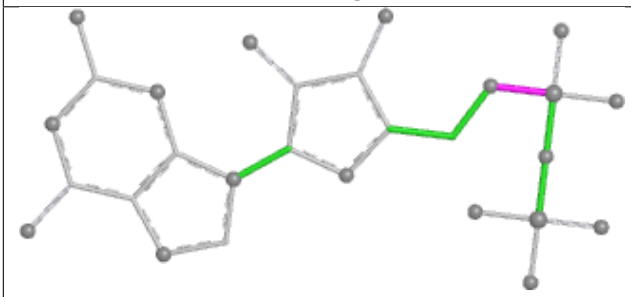
Ligand GDP QA 500



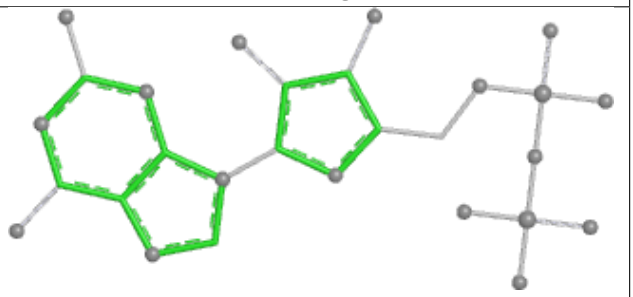
Bond lengths



Bond angles

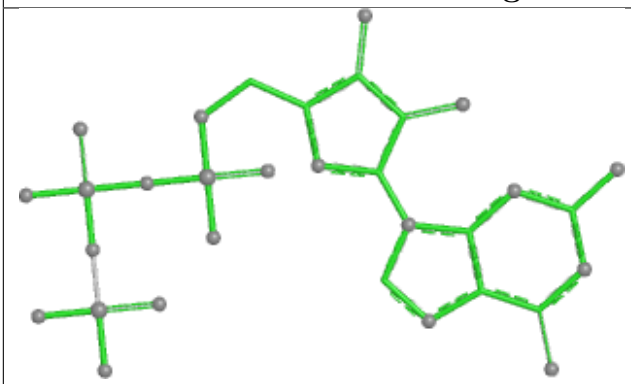


Torsions

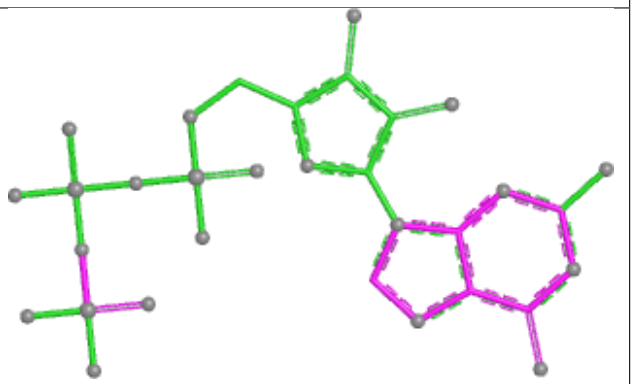


Rings

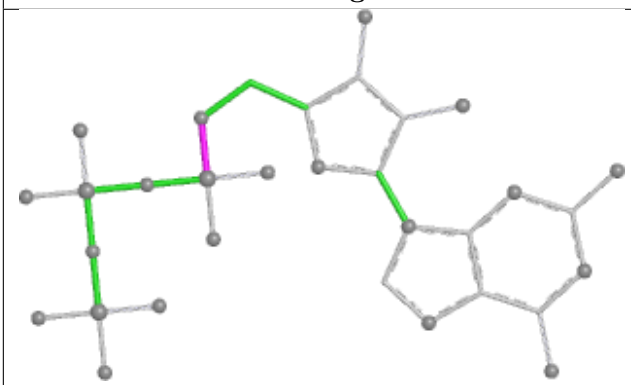
Ligand GTP GW 501



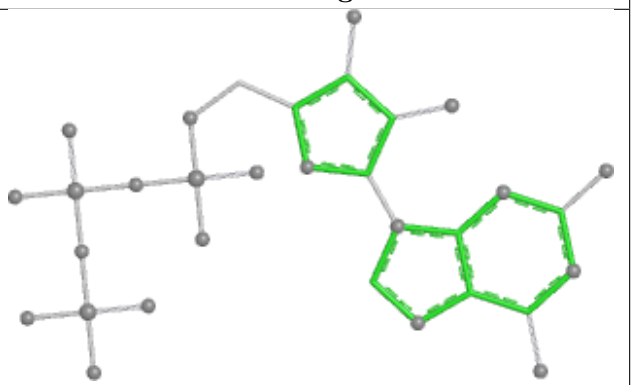
Bond lengths



Bond angles

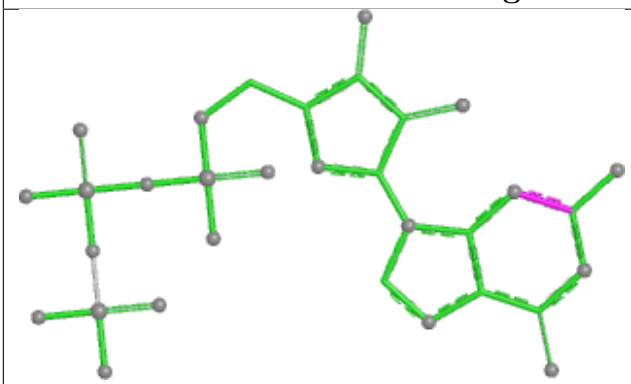


Torsions

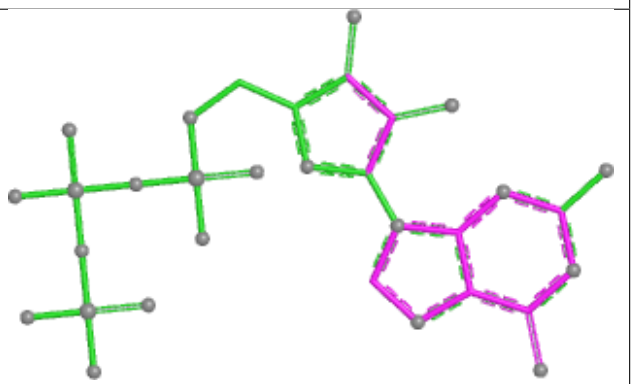


Rings

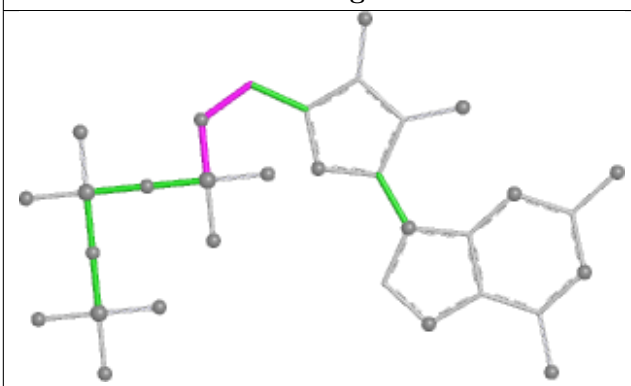
Ligand GTP HW 501



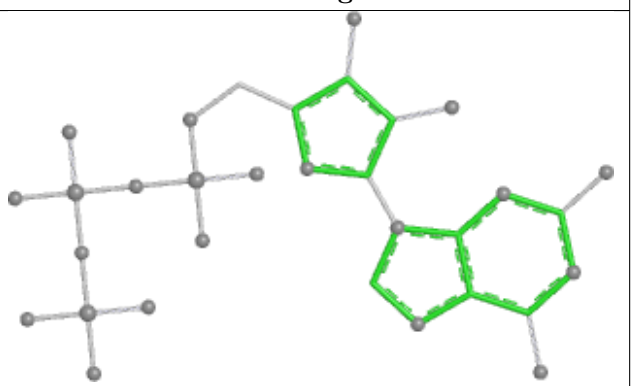
Bond lengths



Bond angles

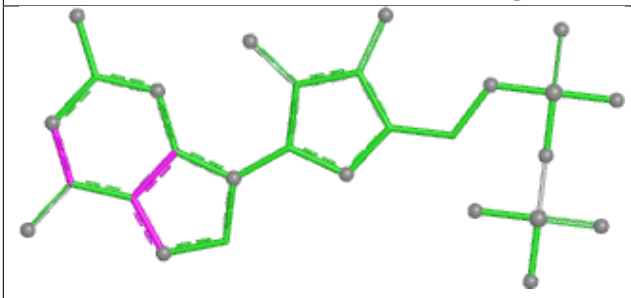


Torsions

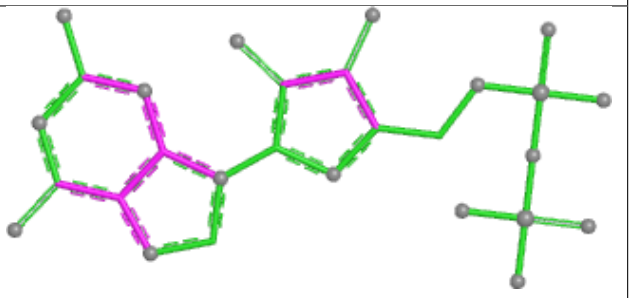


Rings

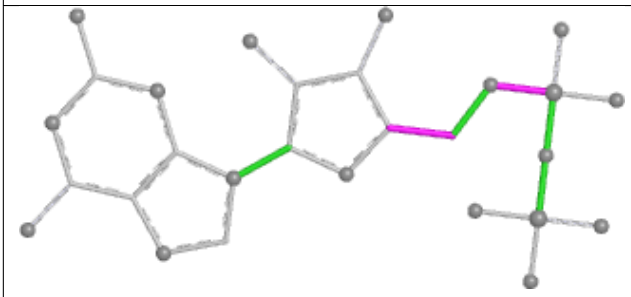
Ligand GDP CC 500



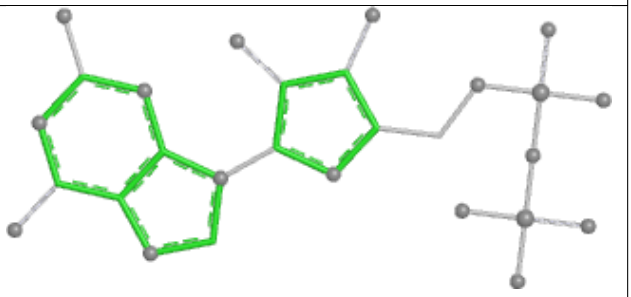
Bond lengths



Bond angles

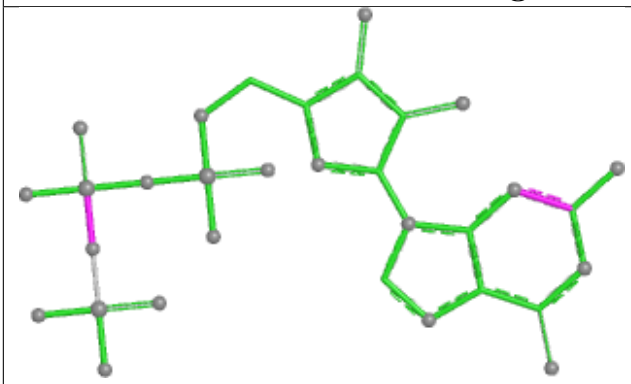


Torsions

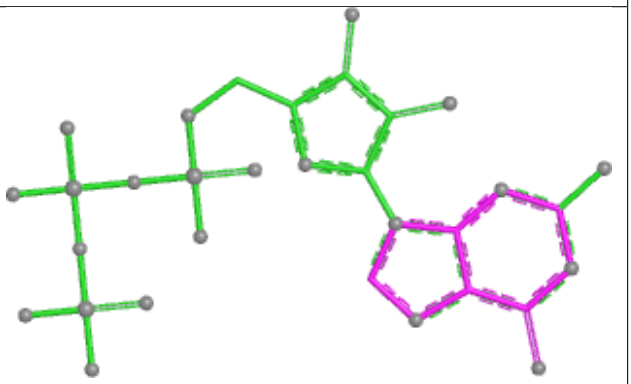


Rings

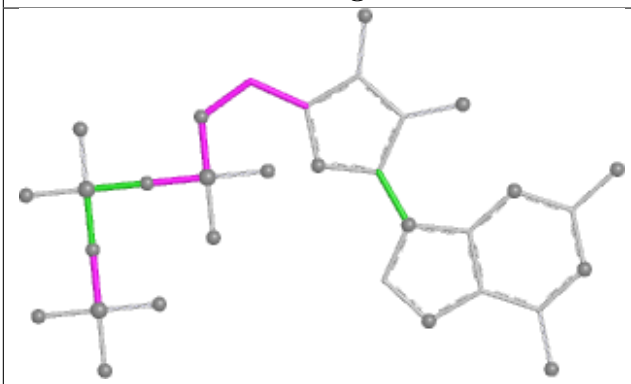
Ligand GTP RO 501



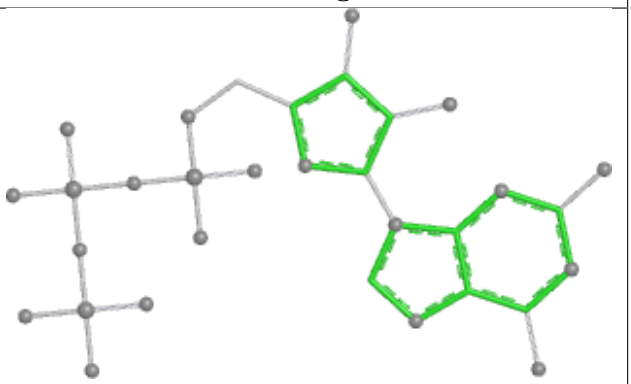
Bond lengths



Bond angles

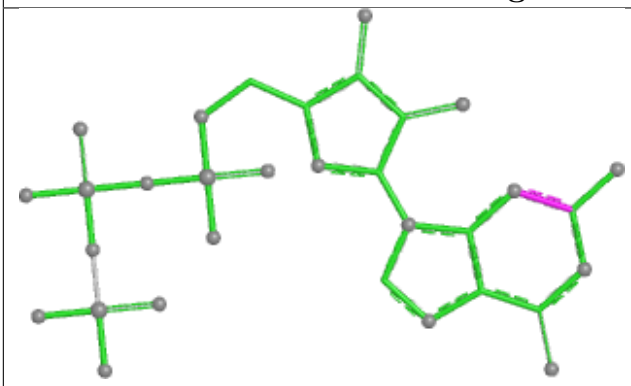


Torsions

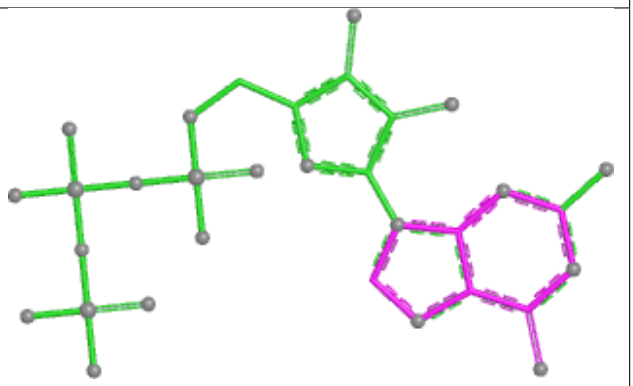


Rings

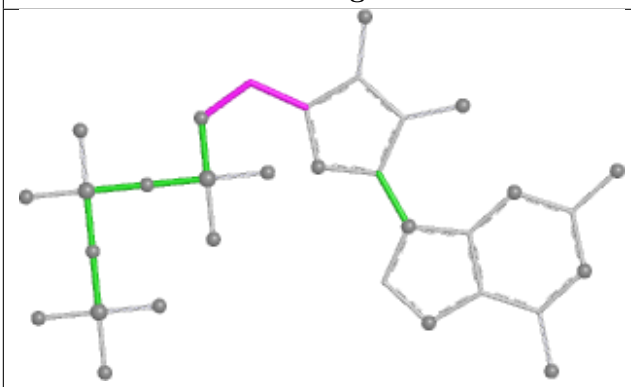
Ligand GTP JW 501



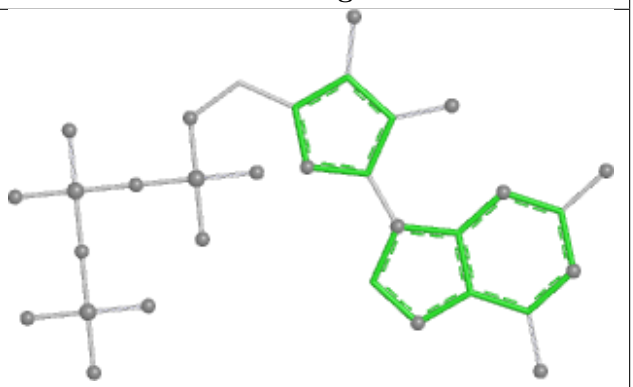
Bond lengths



Bond angles

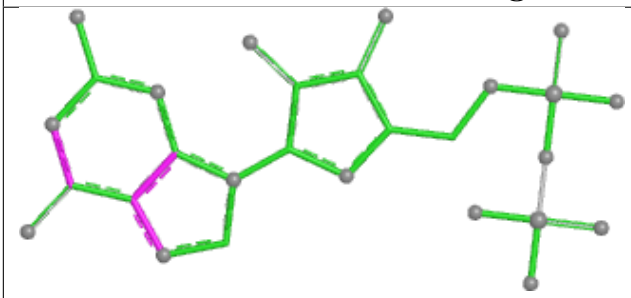


Torsions

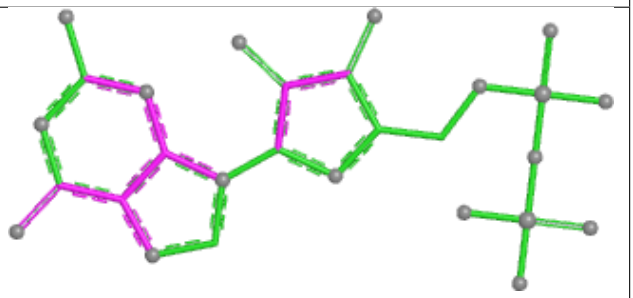


Rings

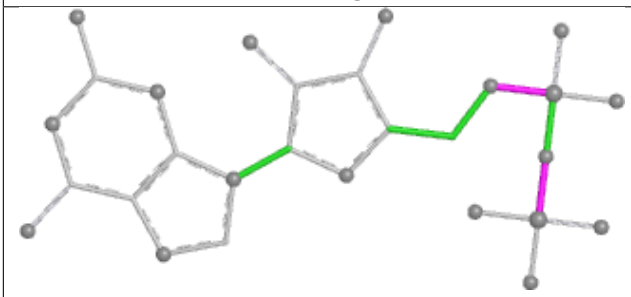
Ligand GDP CY 500



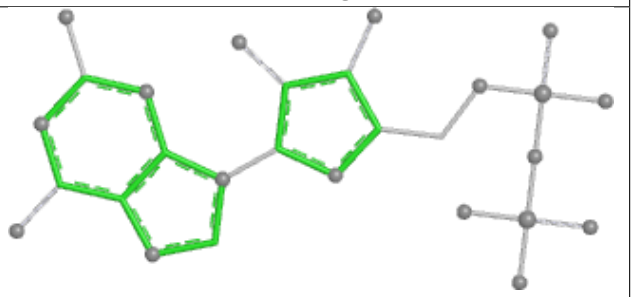
Bond lengths



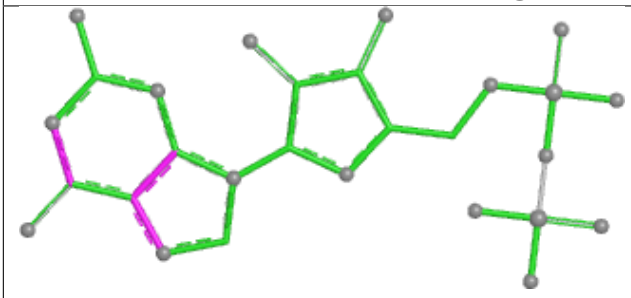
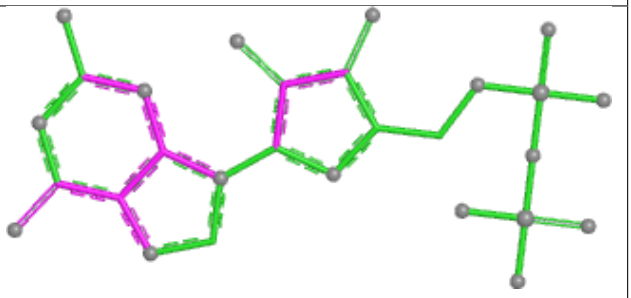
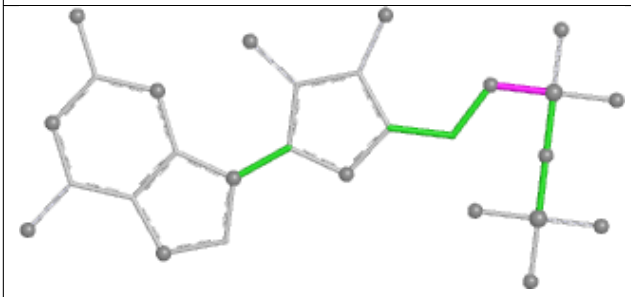
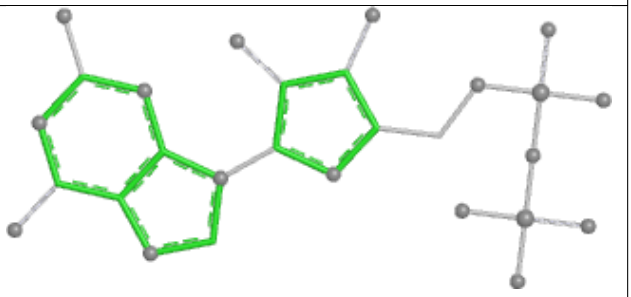
Bond angles

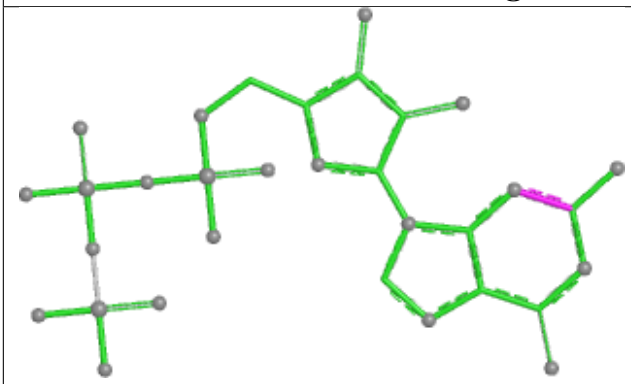
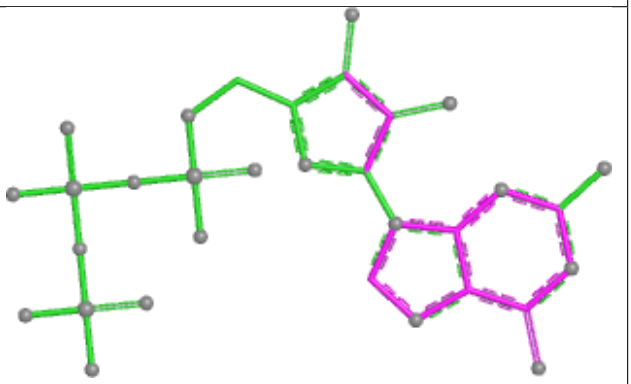
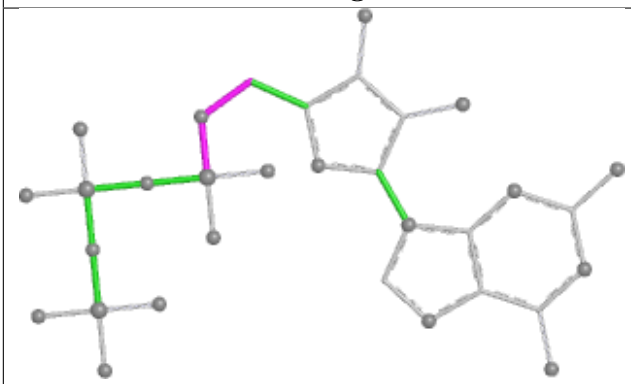
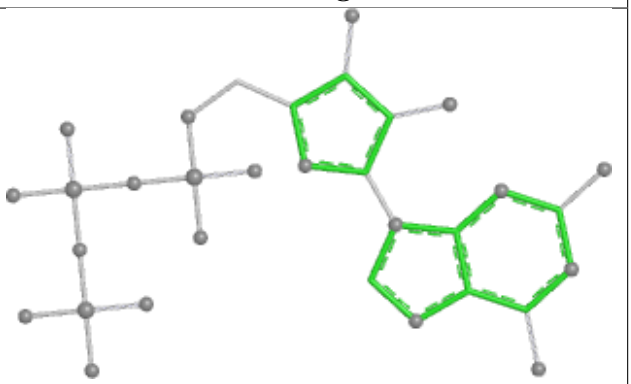


Torsions

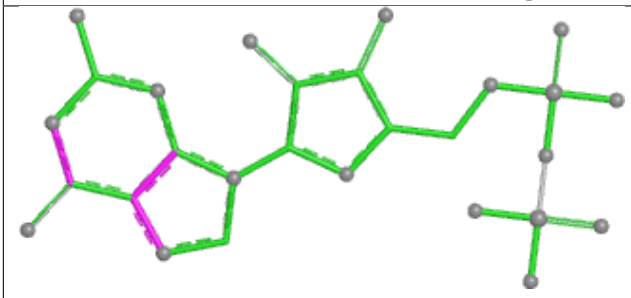


Rings

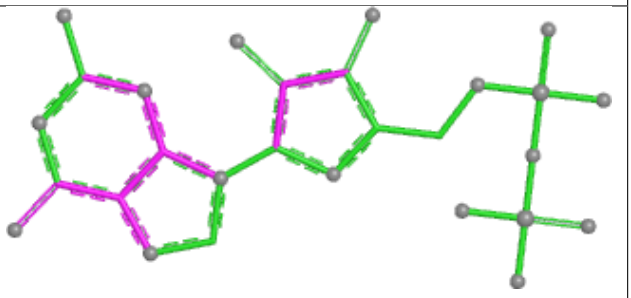
Ligand GDP JK 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP HM 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

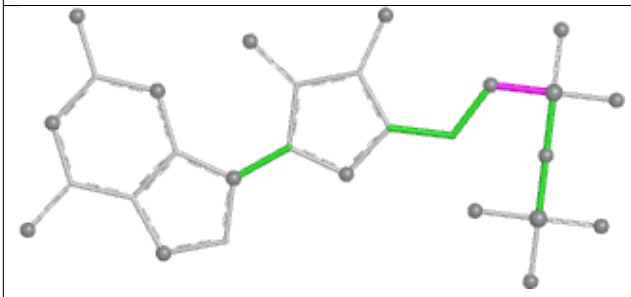
Ligand GDP N 500



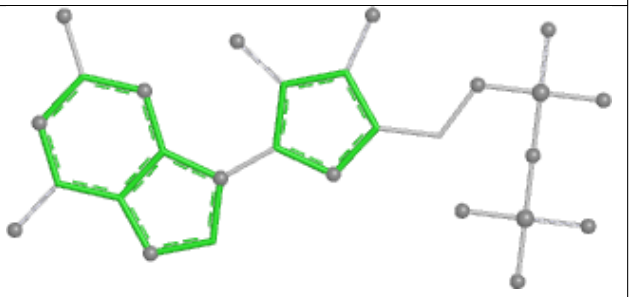
Bond lengths



Bond angles

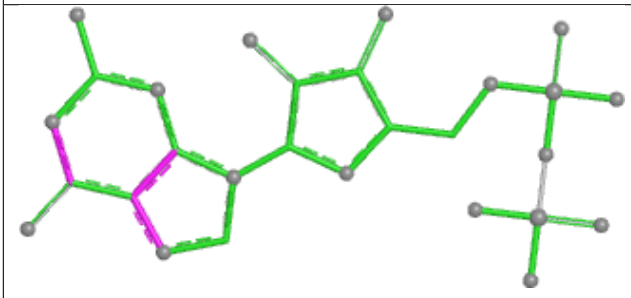


Torsions

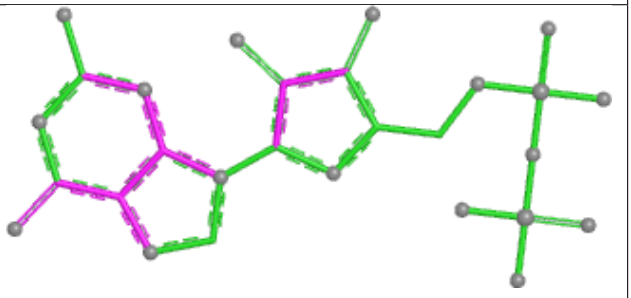


Rings

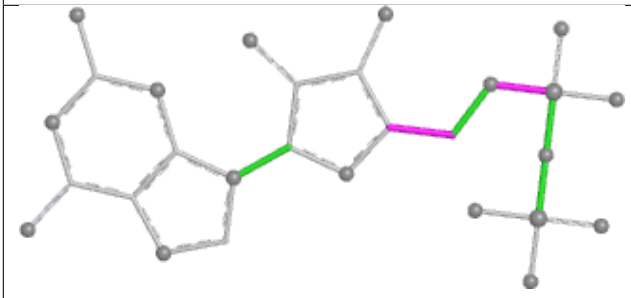
Ligand GDP CW 500



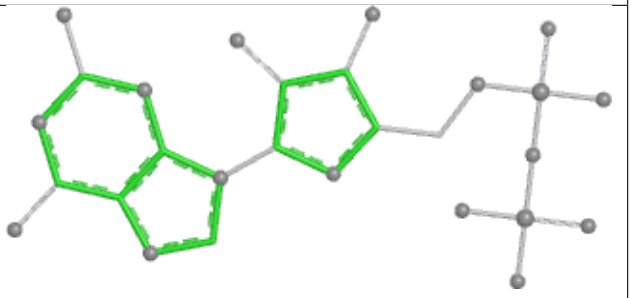
Bond lengths



Bond angles

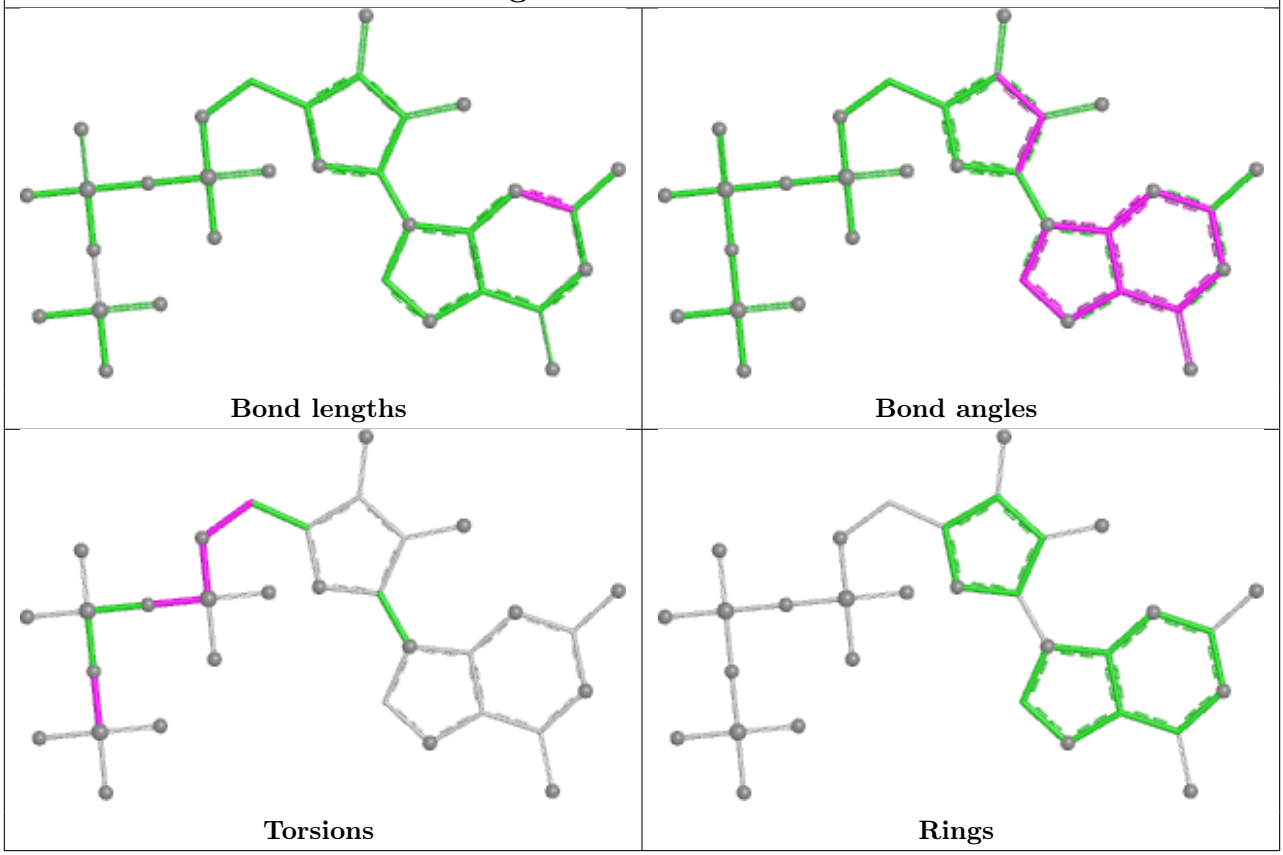


Torsions

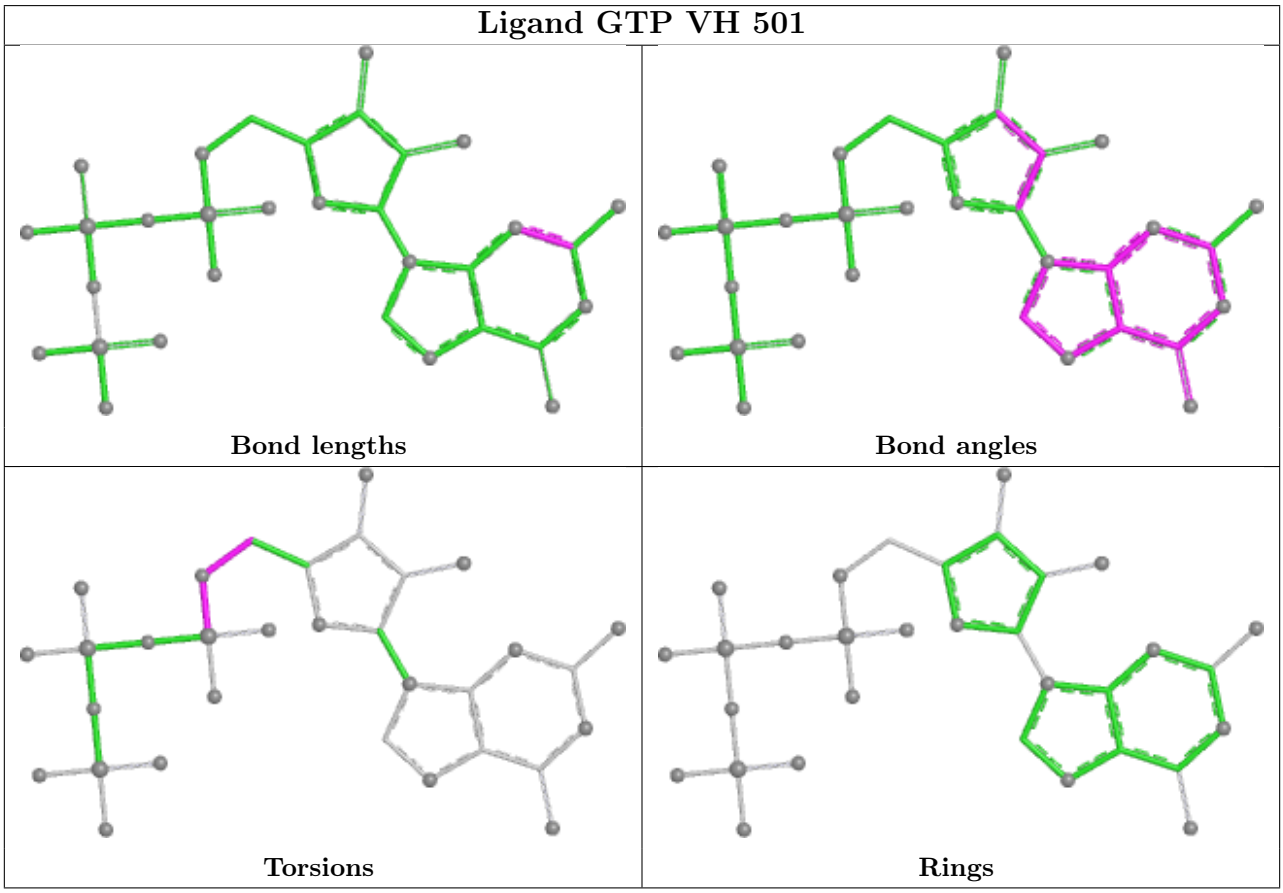


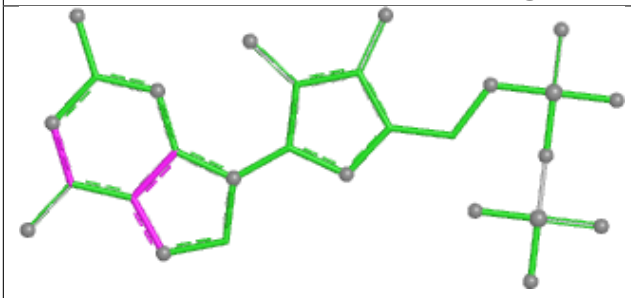
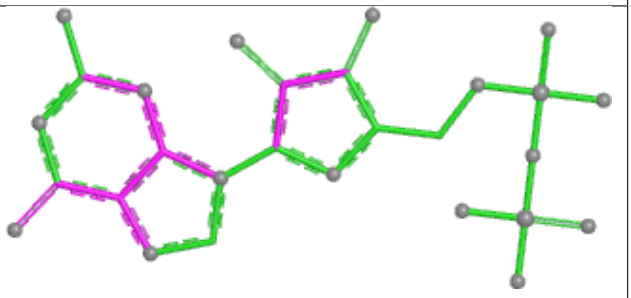
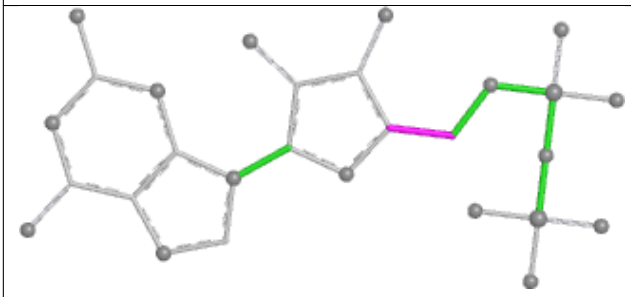
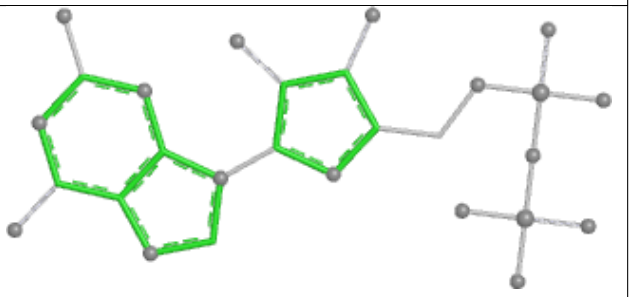
Rings

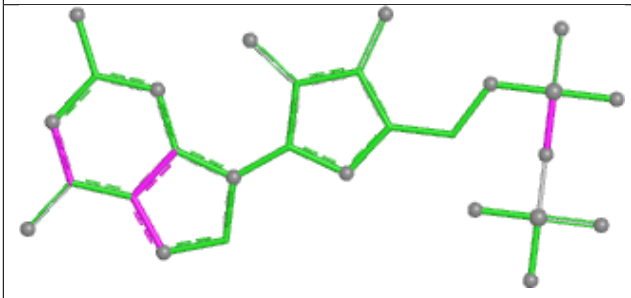
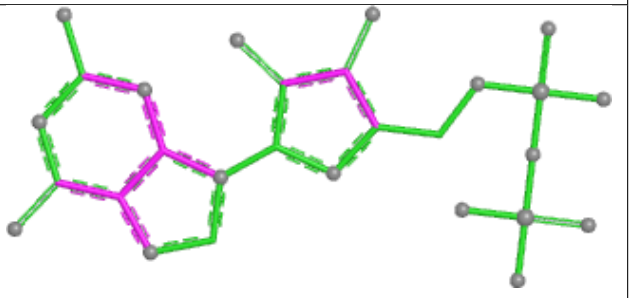
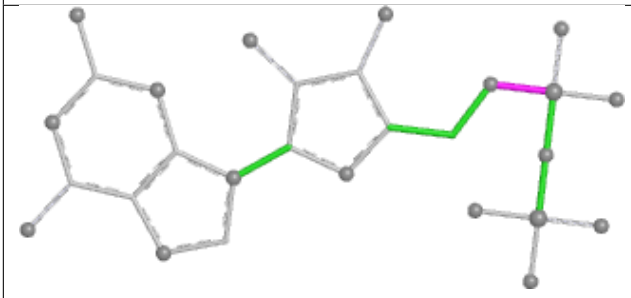
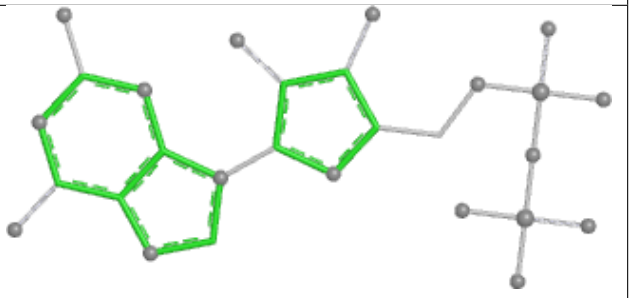
Ligand GTP UA 501



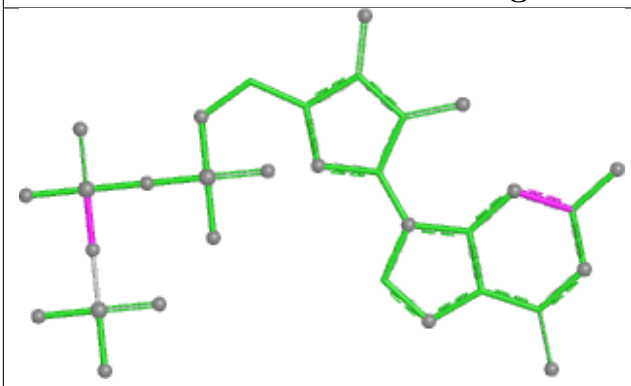
Ligand GTP VH 501



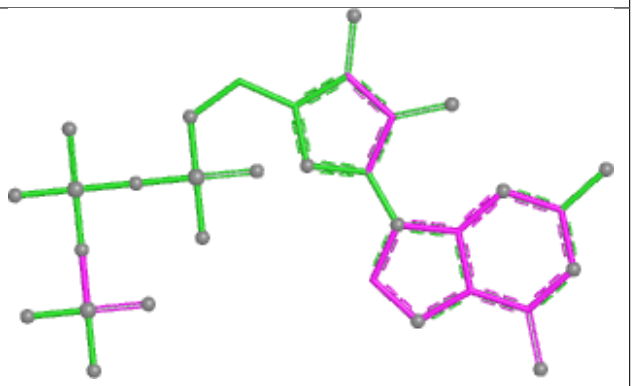
Ligand GDP A 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP EX 500	
	
Bond lengths	Bond angles
	
Torsions	Rings

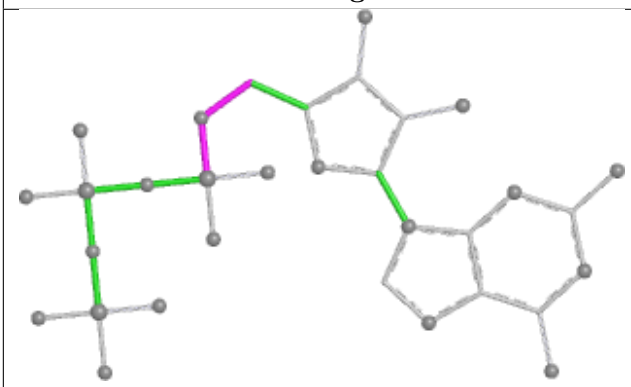
Ligand GTP OP 503



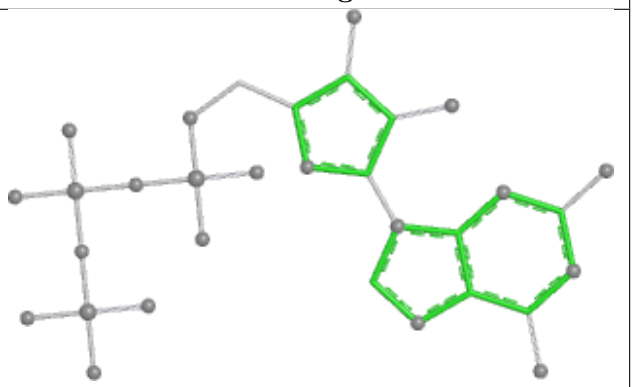
Bond lengths



Bond angles

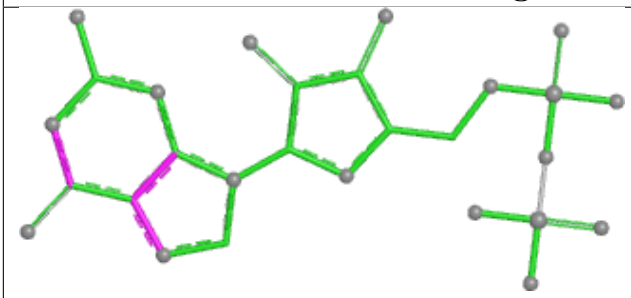


Torsions

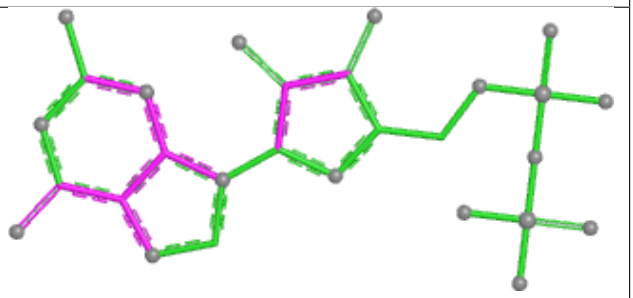


Rings

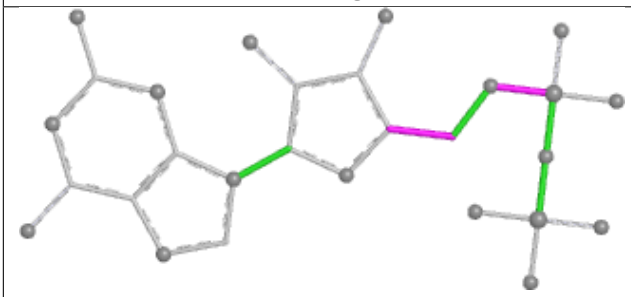
Ligand GDP FL 500



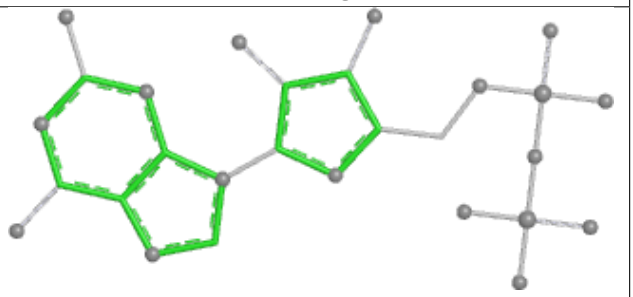
Bond lengths



Bond angles

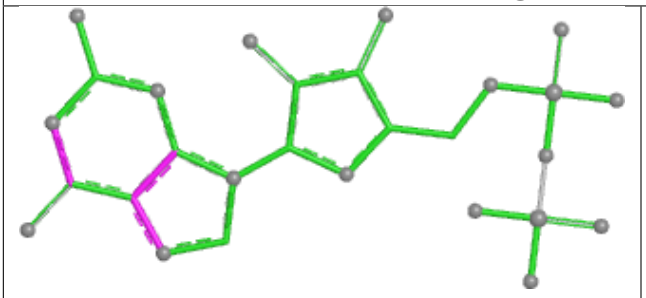


Torsions

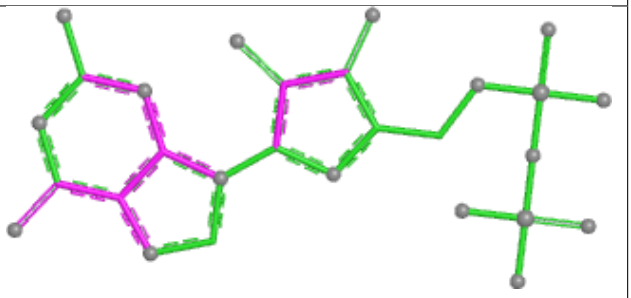


Rings

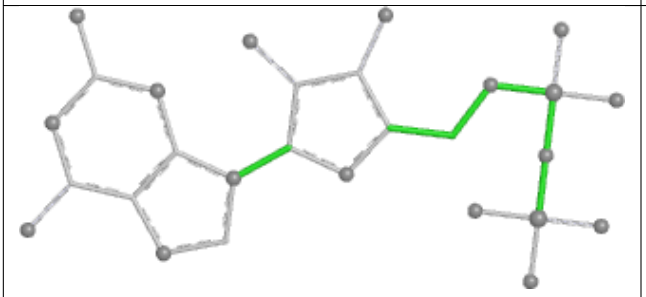
Ligand GDP JY 501



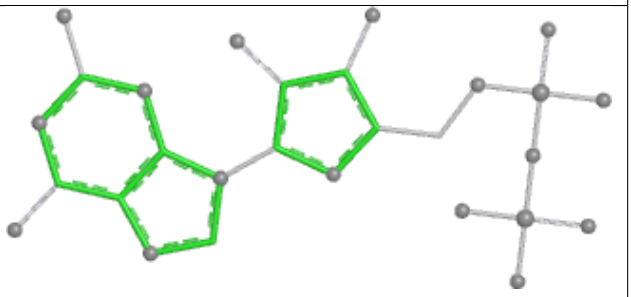
Bond lengths



Bond angles

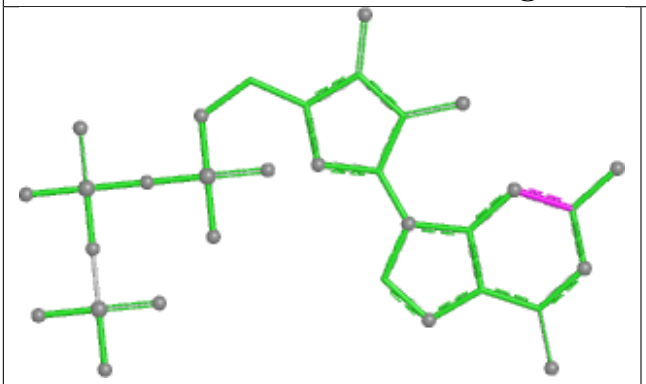


Torsions

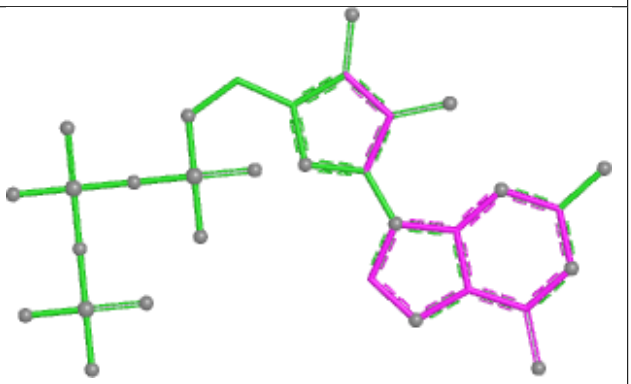


Rings

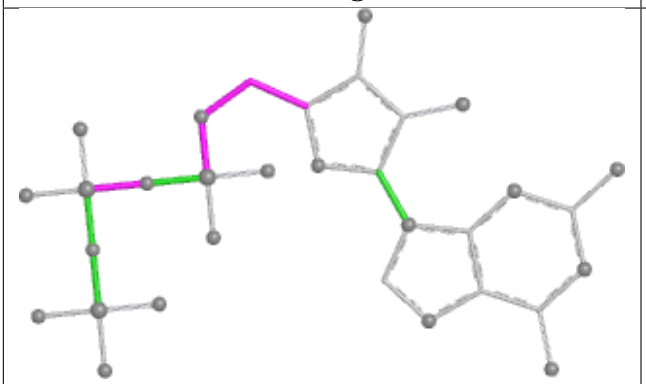
Ligand GTP IS 501



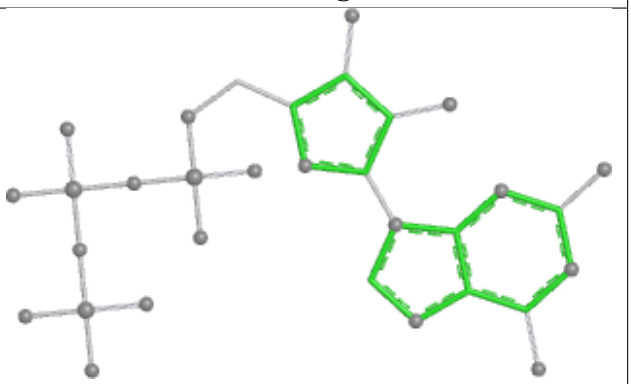
Bond lengths



Bond angles

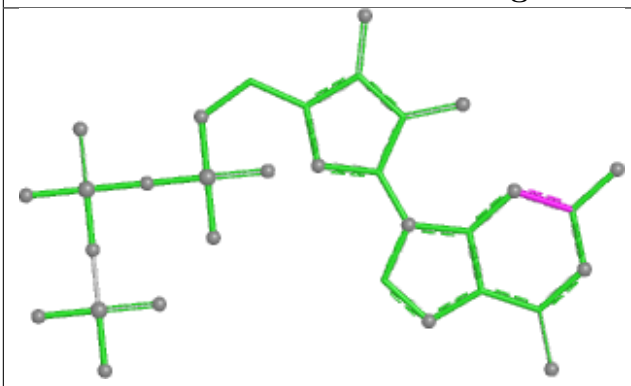


Torsions

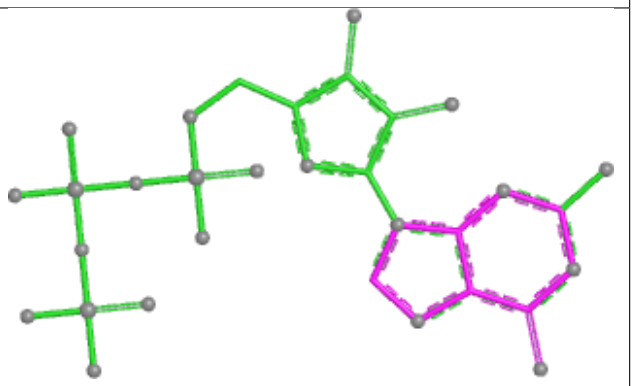


Rings

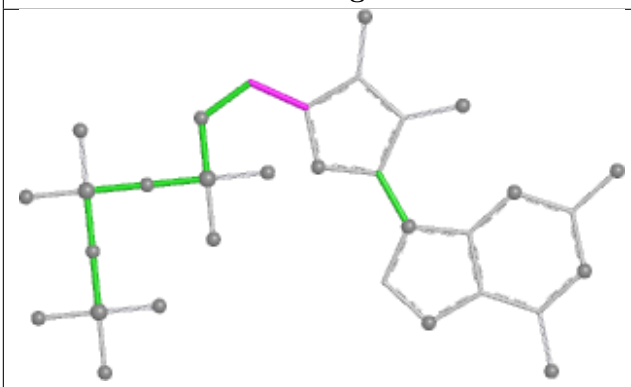
Ligand GTP RV 501



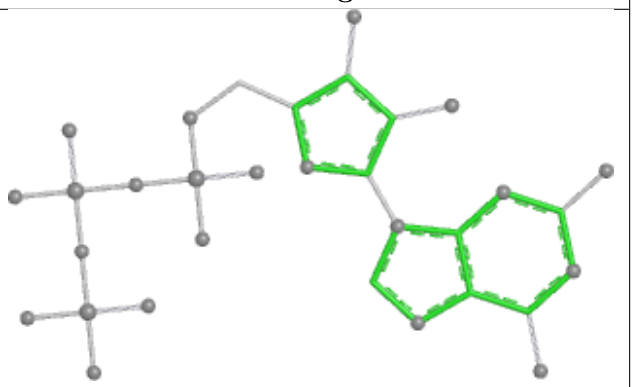
Bond lengths



Bond angles

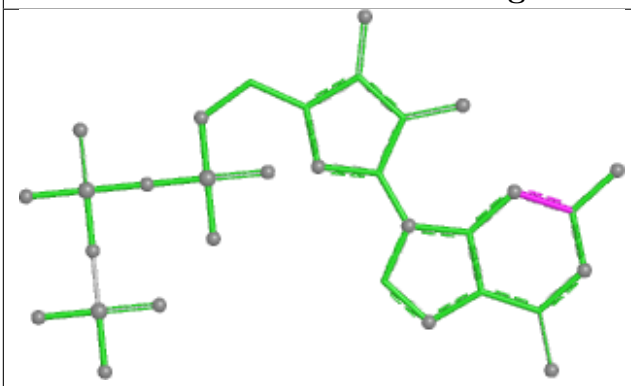


Torsions

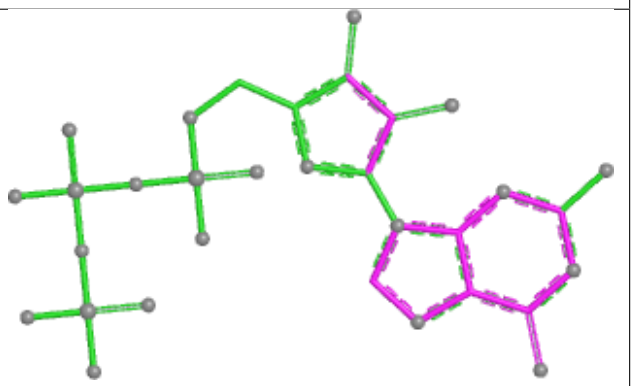


Rings

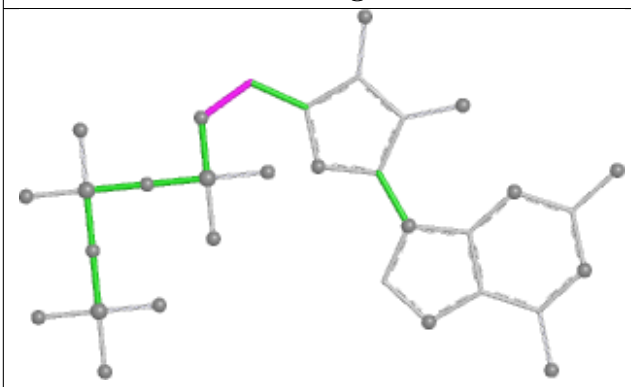
Ligand GTP DH 501



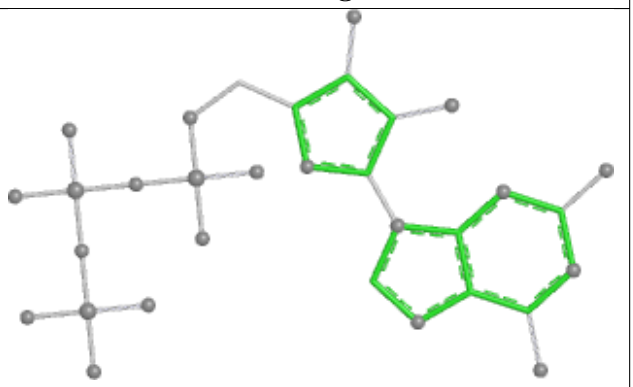
Bond lengths



Bond angles

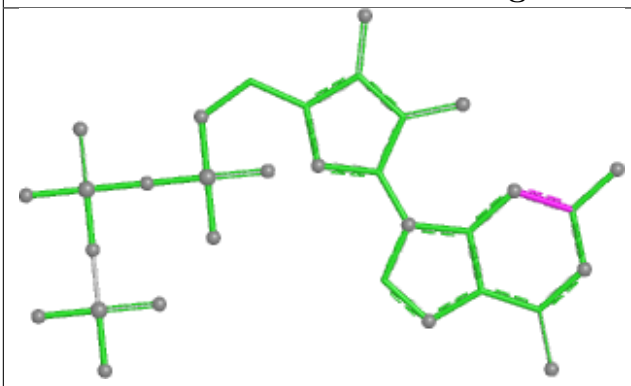


Torsions

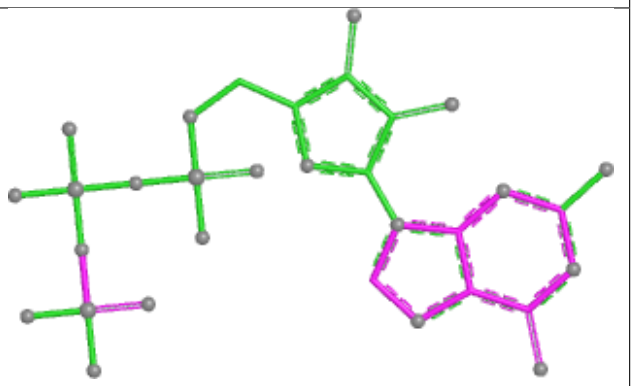


Rings

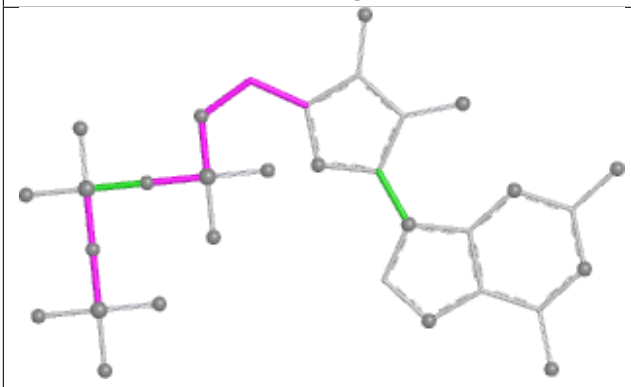
Ligand GTP RX 501



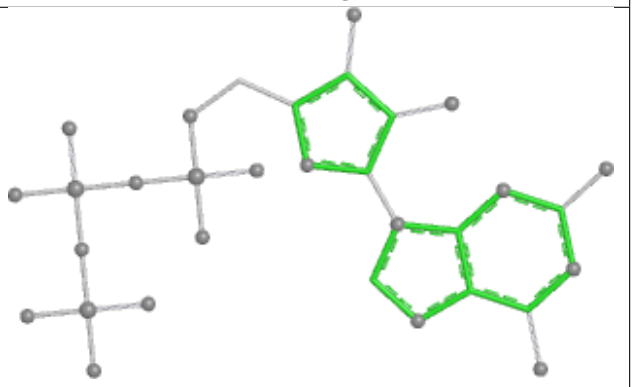
Bond lengths



Bond angles

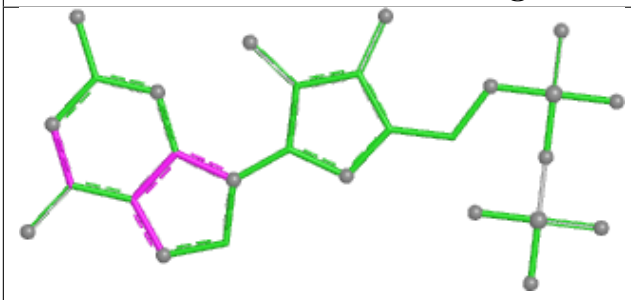


Torsions

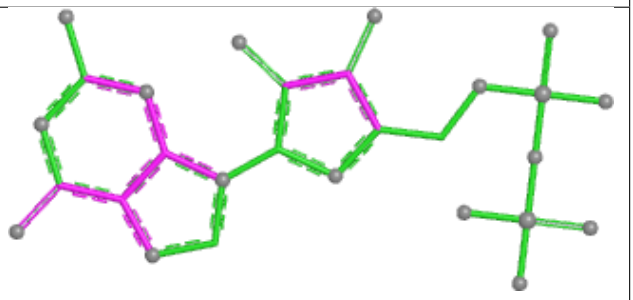


Rings

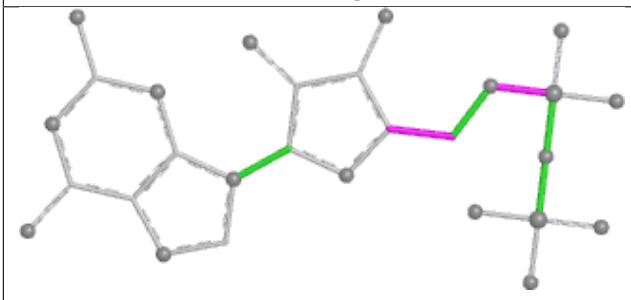
Ligand GDP EV 500



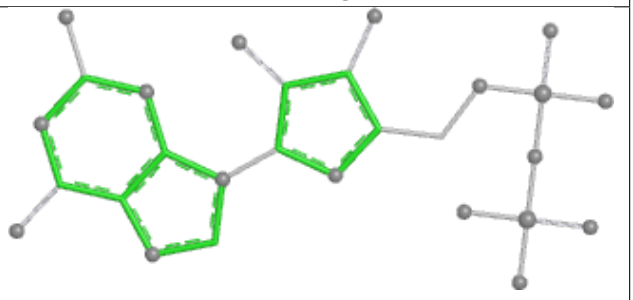
Bond lengths



Bond angles

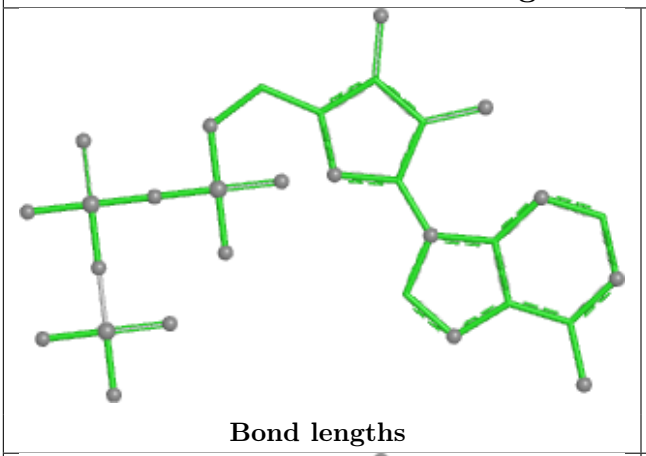


Torsions

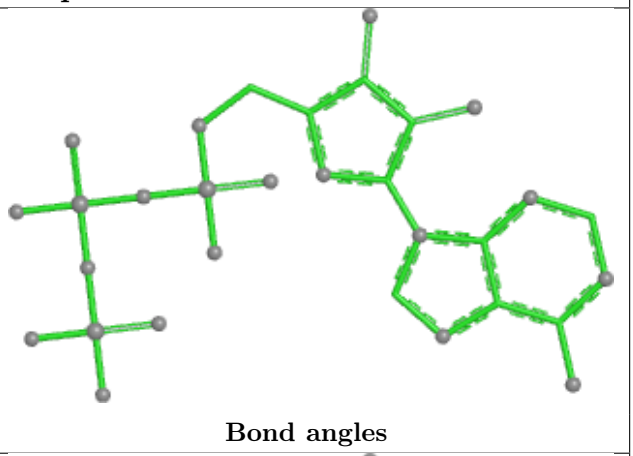


Rings

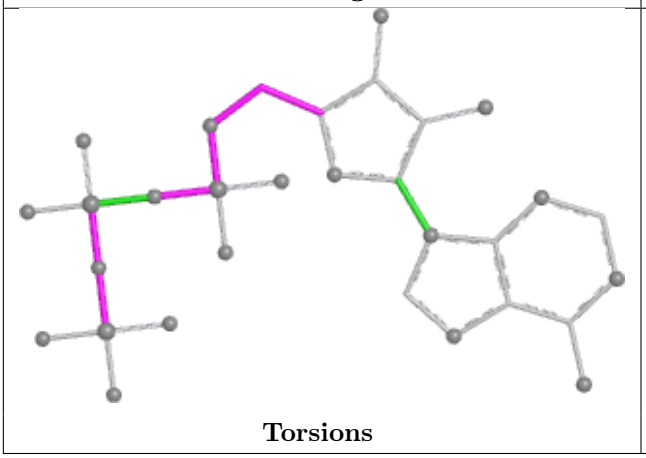
Ligand ATP 6p 500



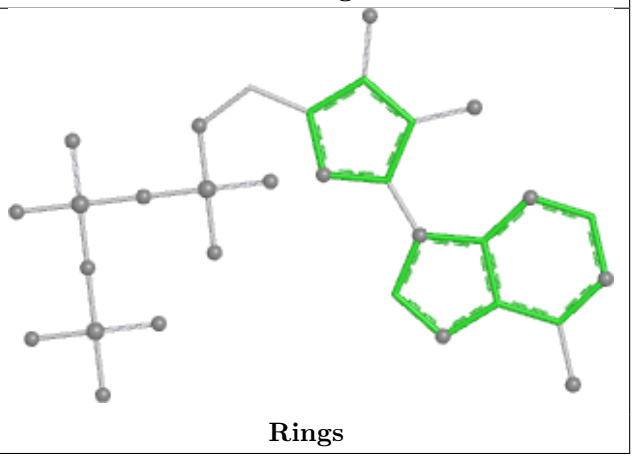
Bond lengths



Bond angles

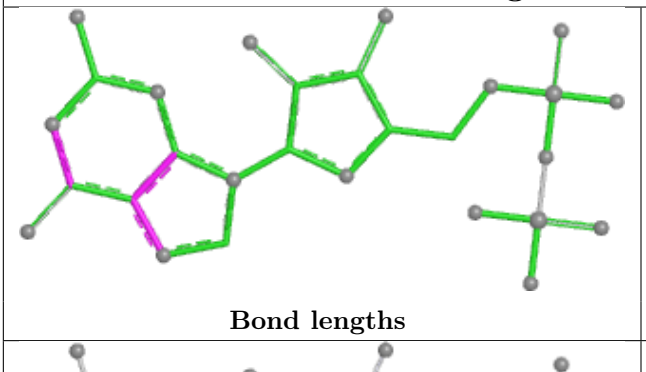


Torsions

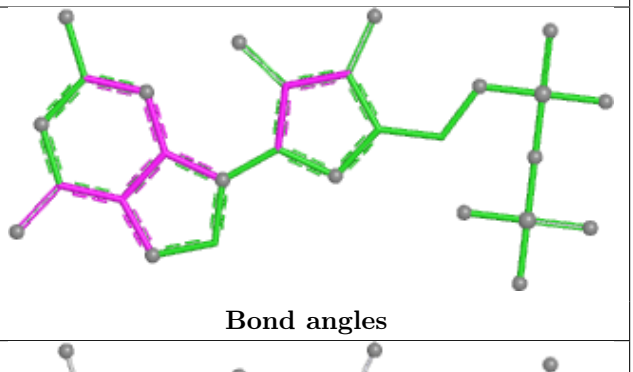


Rings

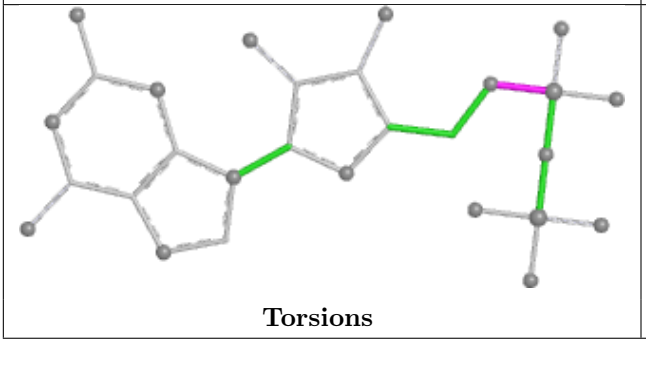
Ligand GDP KK 500



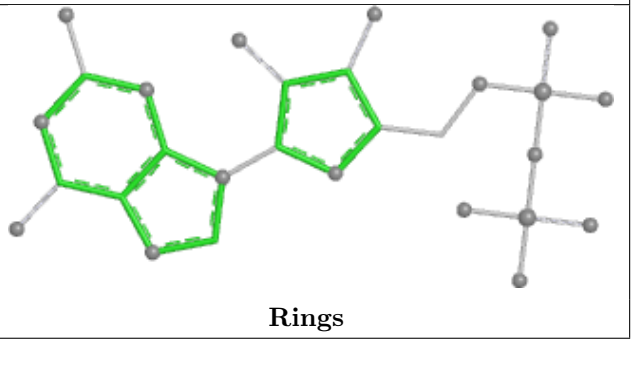
Bond lengths



Bond angles

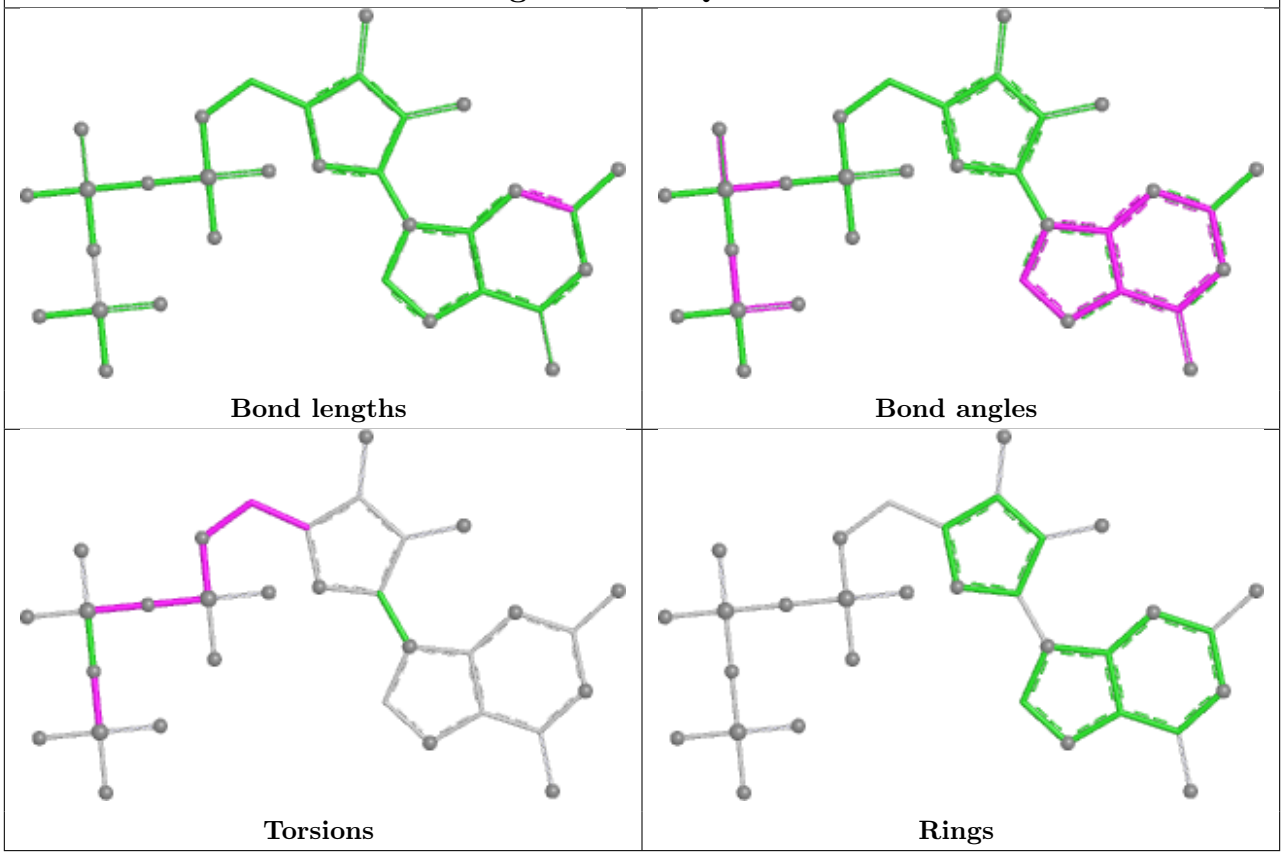


Torsions

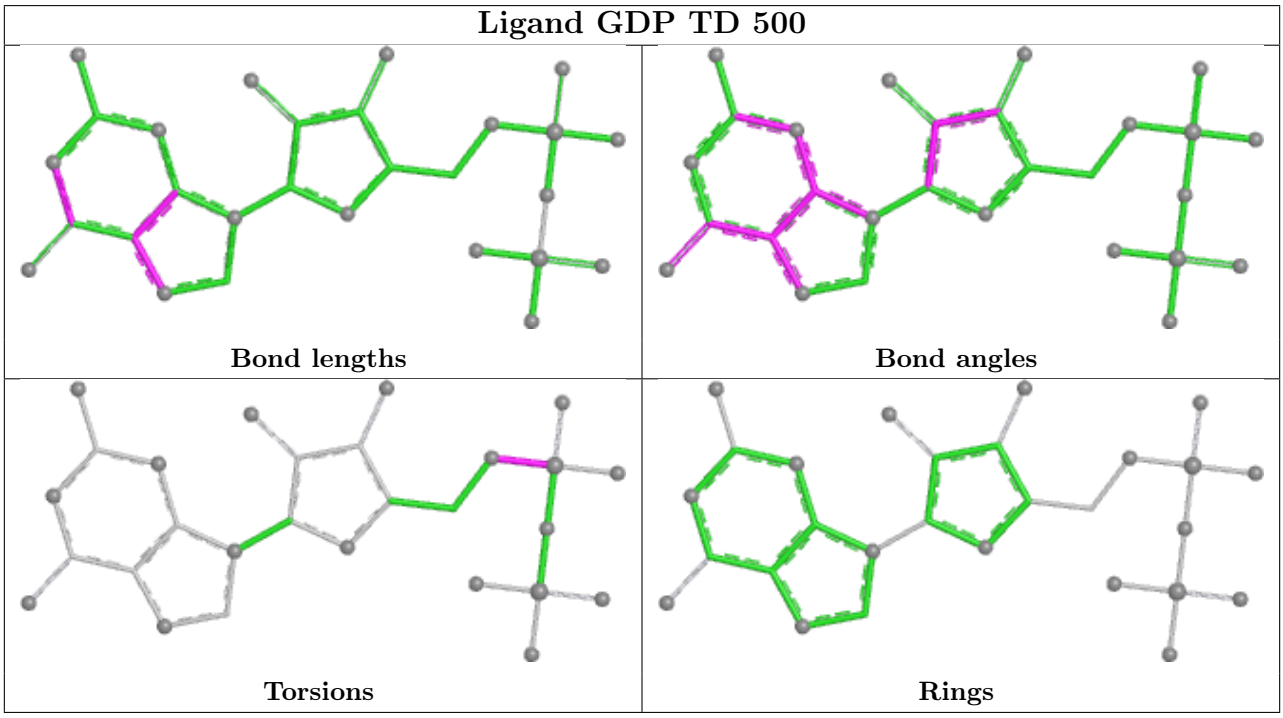


Rings

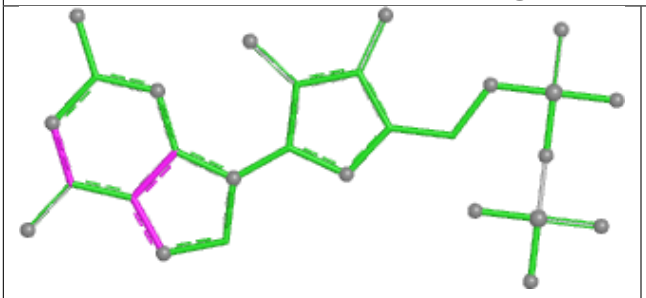
Ligand GTP QH 501



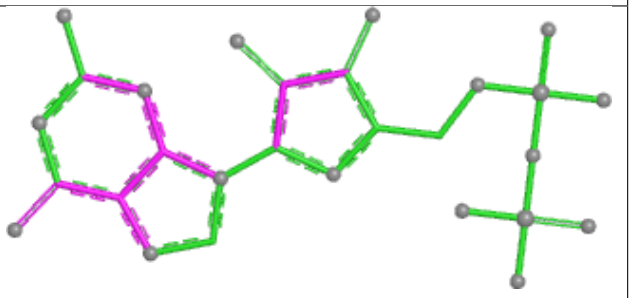
Ligand GDP TD 500



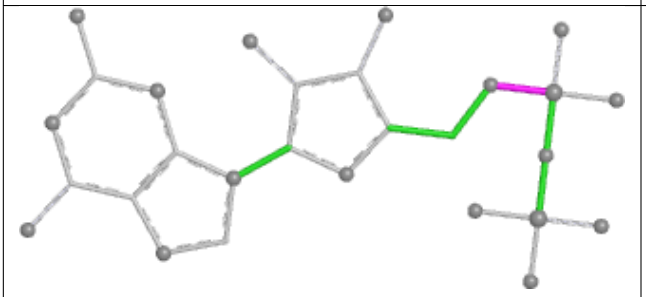
Ligand GDP SR 500



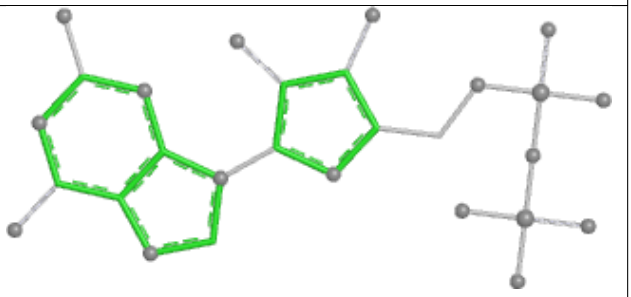
Bond lengths



Bond angles

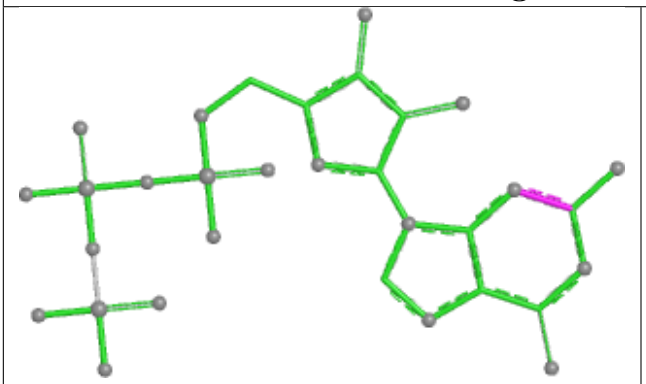


Torsions

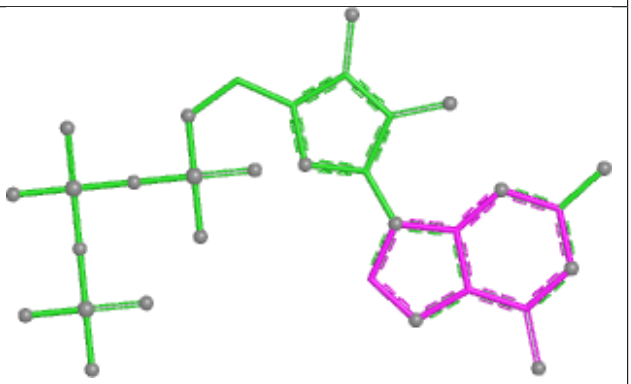


Rings

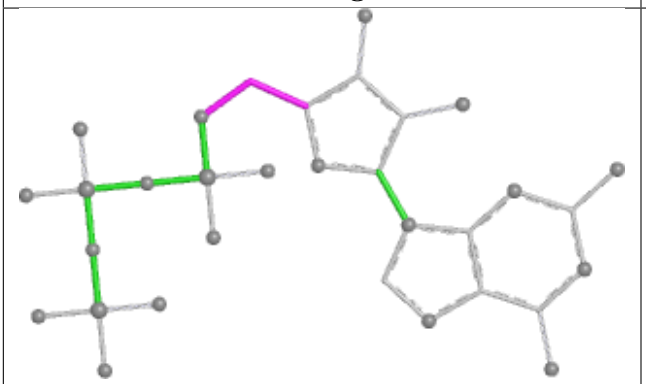
Ligand GTP KZ 501



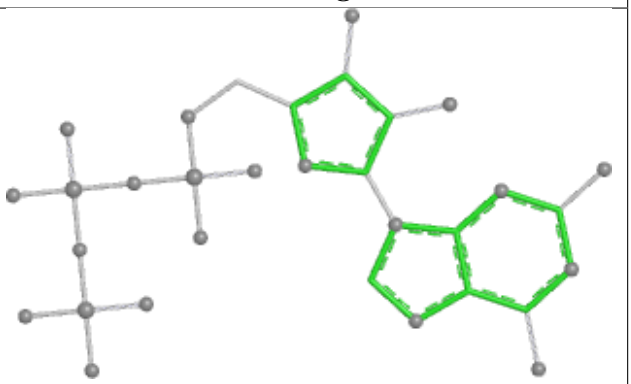
Bond lengths



Bond angles

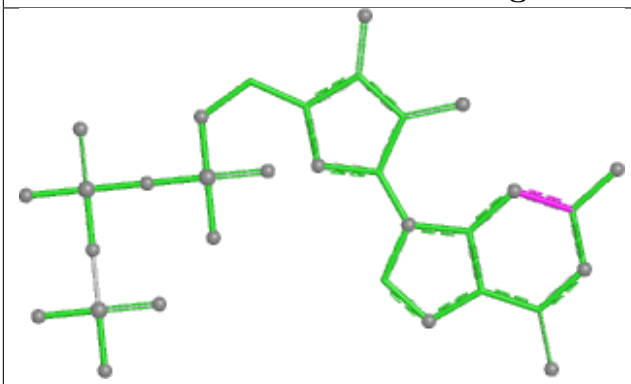


Torsions

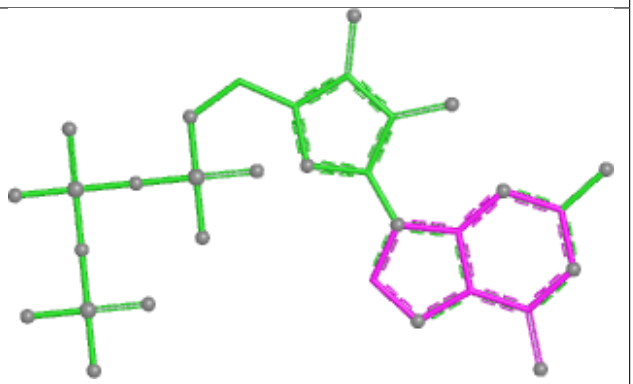


Rings

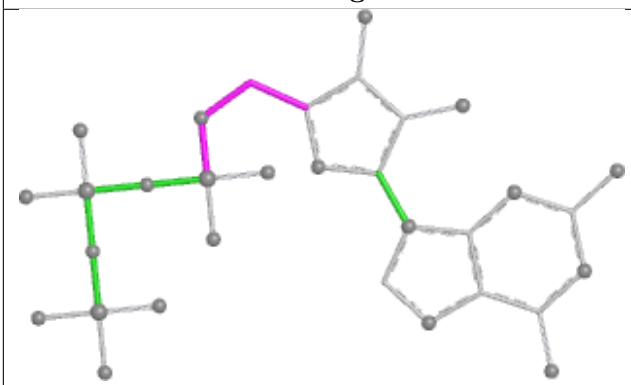
Ligand GTP PG 501



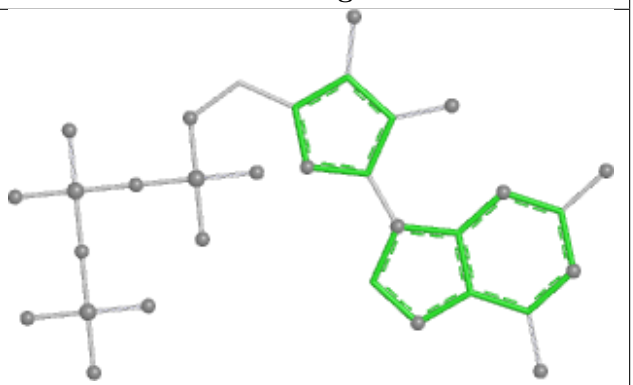
Bond lengths



Bond angles

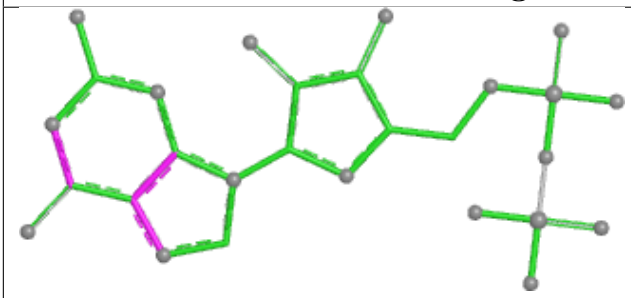


Torsions

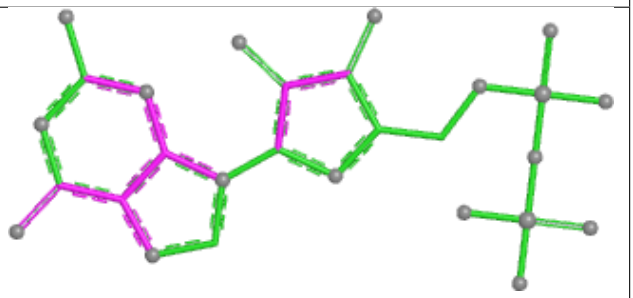


Rings

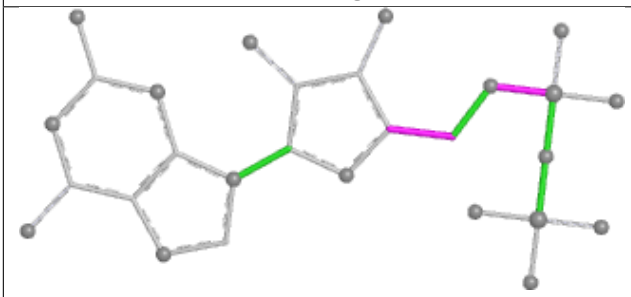
Ligand GDP LA 500



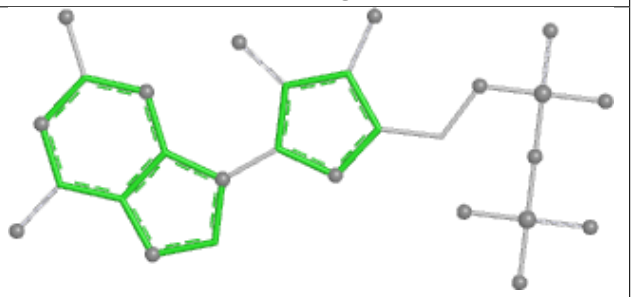
Bond lengths



Bond angles

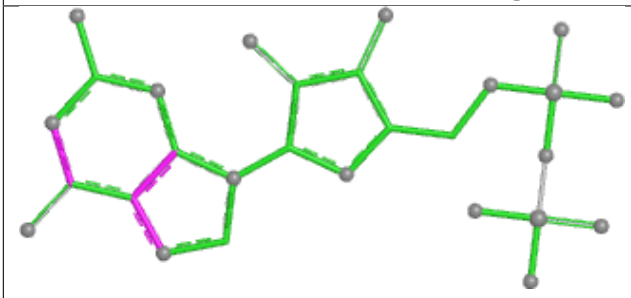


Torsions

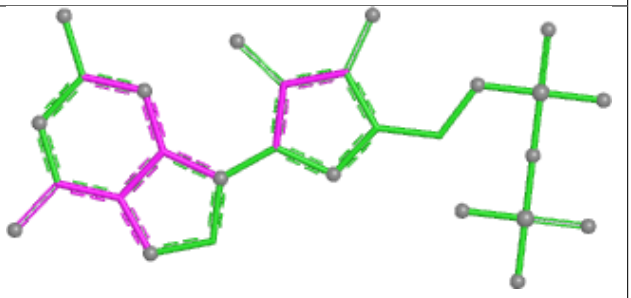


Rings

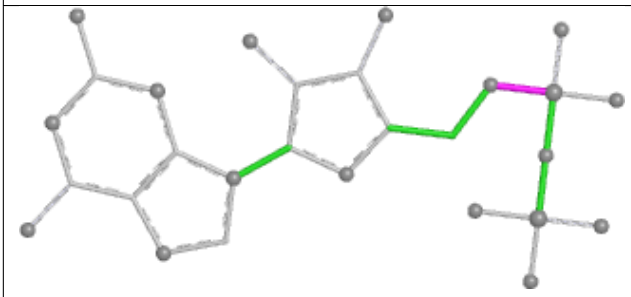
Ligand GDP RO 500



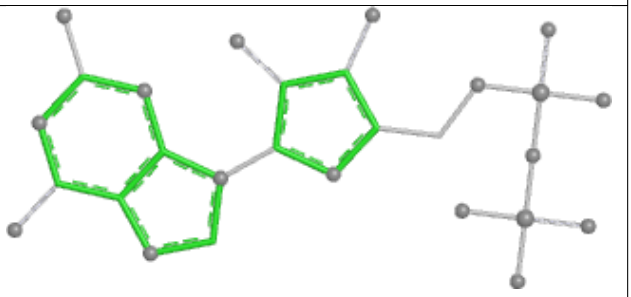
Bond lengths



Bond angles

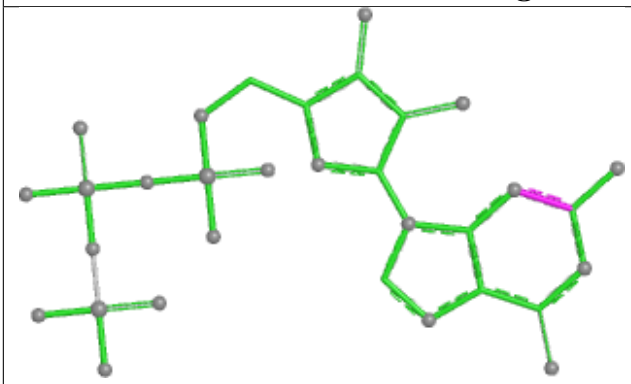


Torsions

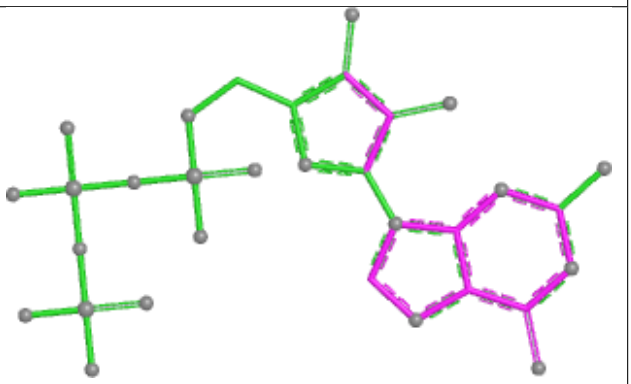


Rings

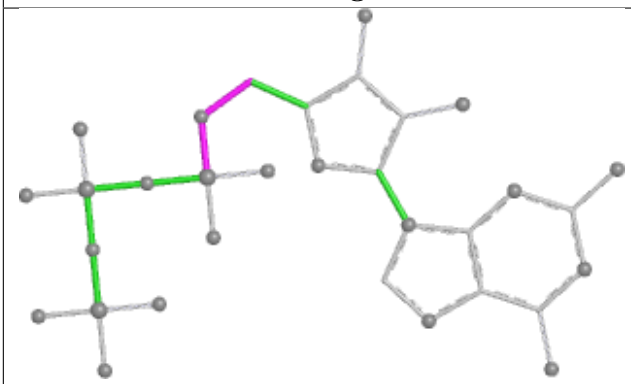
Ligand GTP JZ 501



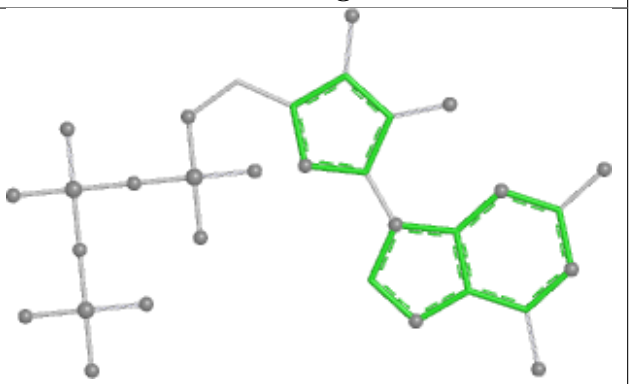
Bond lengths



Bond angles

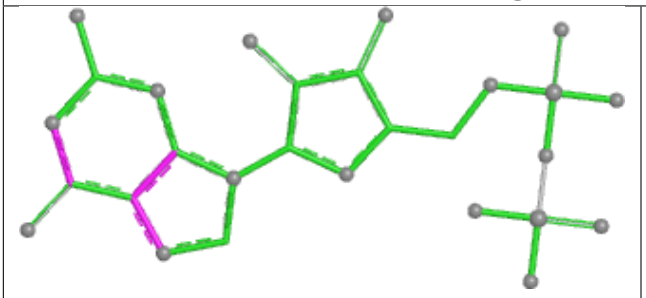


Torsions

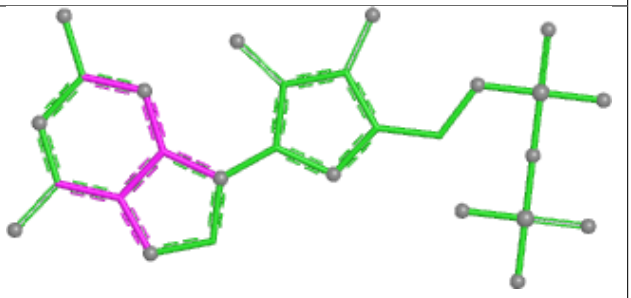


Rings

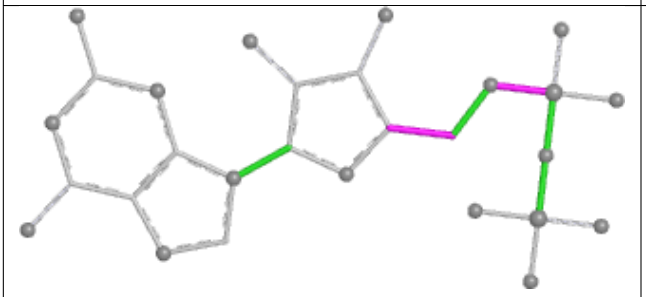
Ligand GDP DE 500



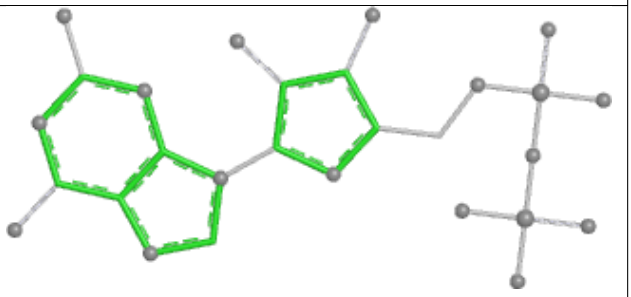
Bond lengths



Bond angles

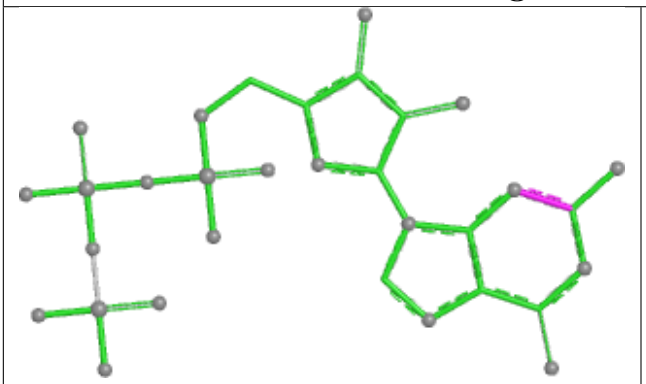


Torsions

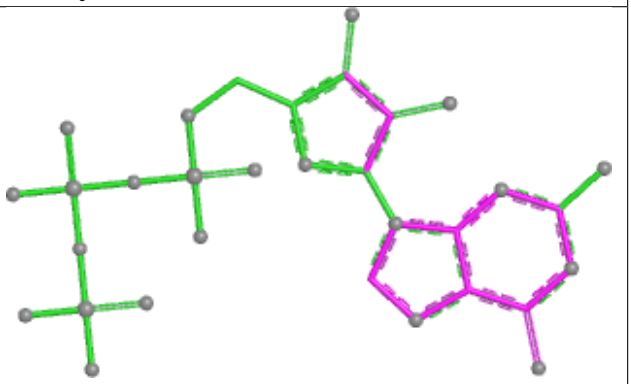


Rings

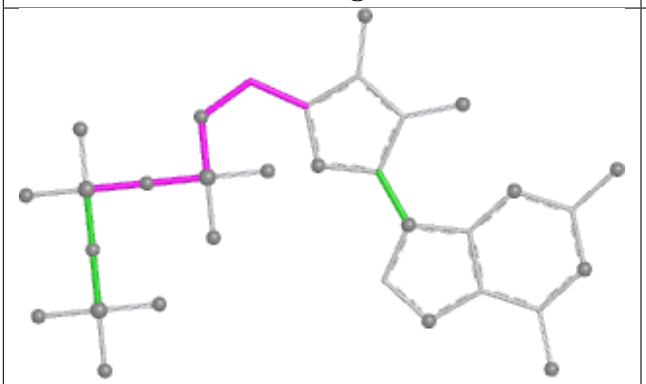
Ligand GTP UQ 501



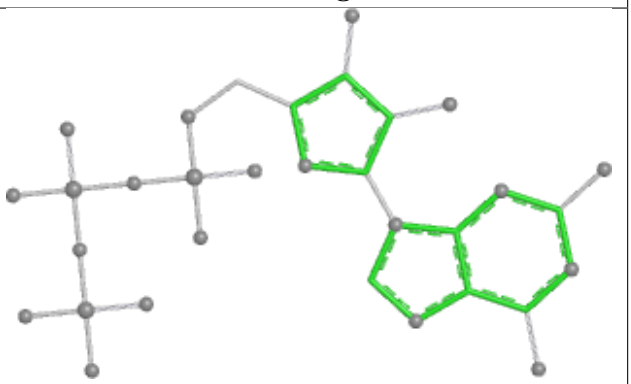
Bond lengths



Bond angles

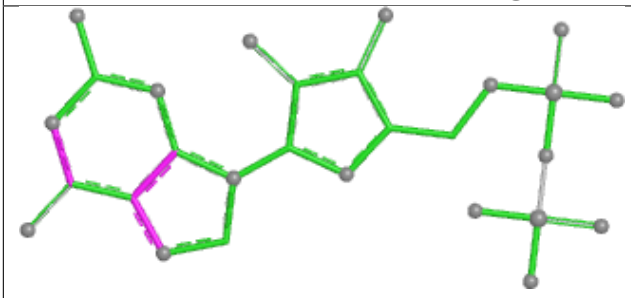


Torsions

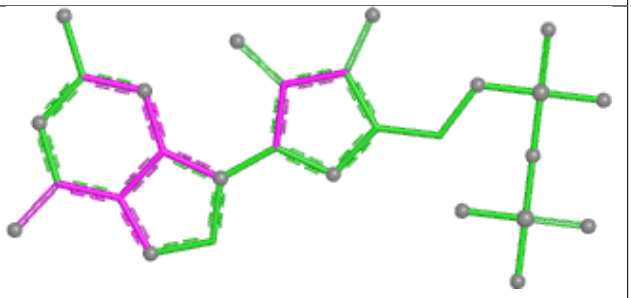


Rings

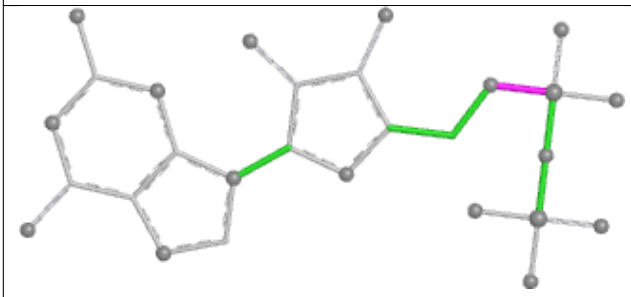
Ligand GDP RG 500



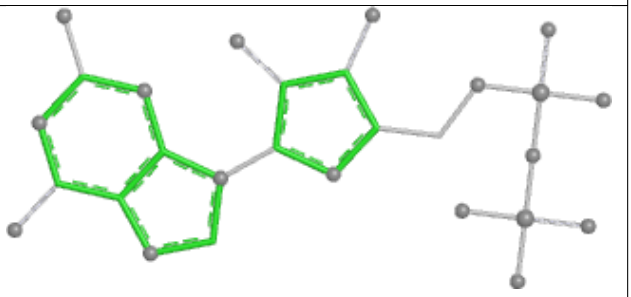
Bond lengths



Bond angles

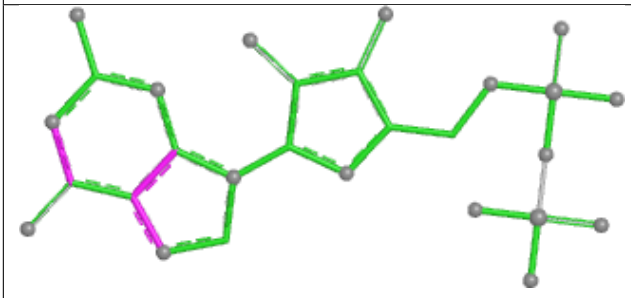


Torsions

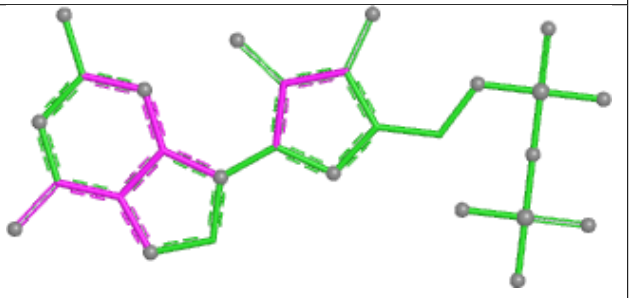


Rings

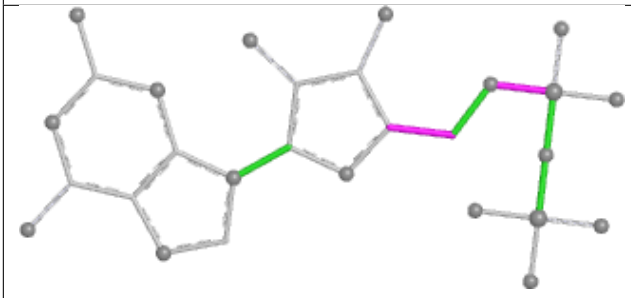
Ligand GDP OB 500



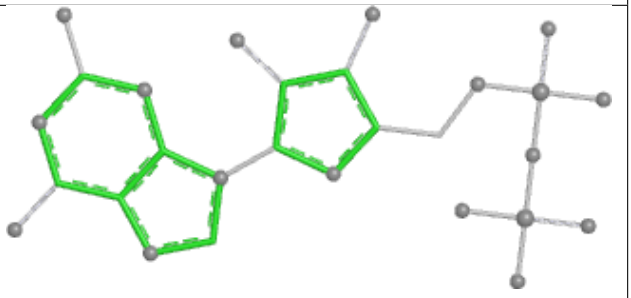
Bond lengths



Bond angles

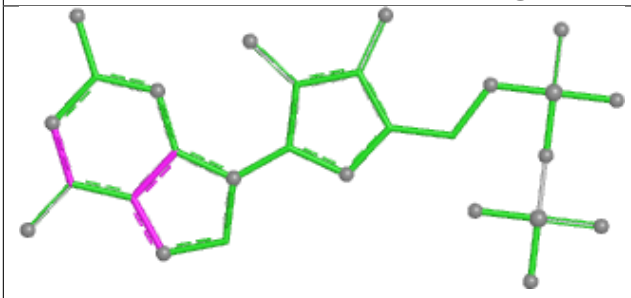


Torsions

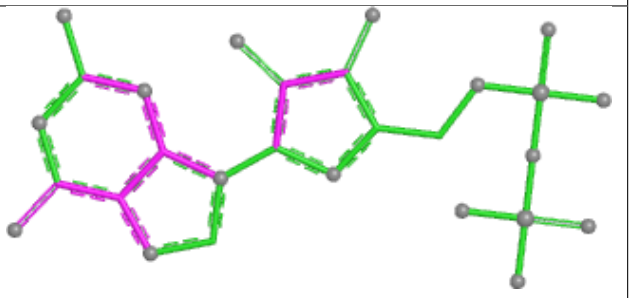


Rings

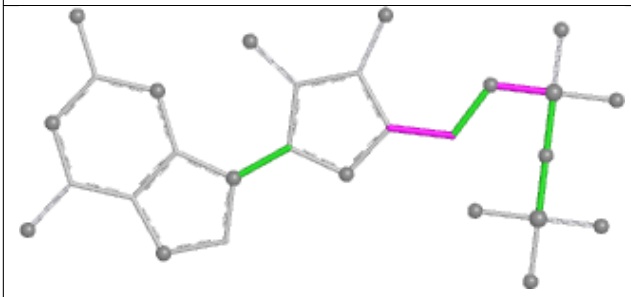
Ligand GDP JO 500



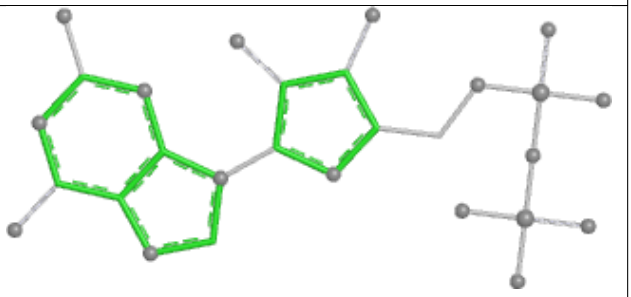
Bond lengths



Bond angles

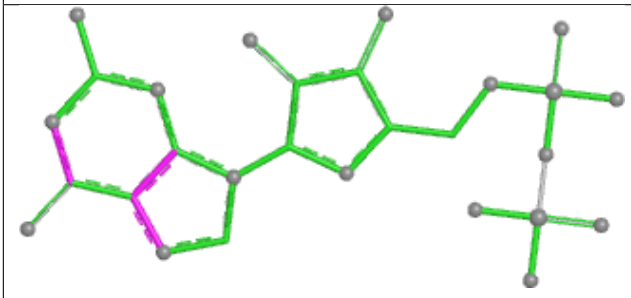


Torsions

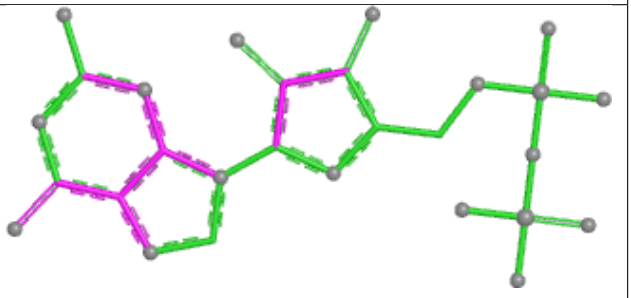


Rings

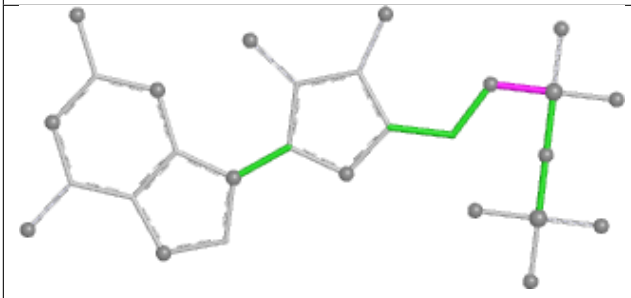
Ligand GDP NJ 501



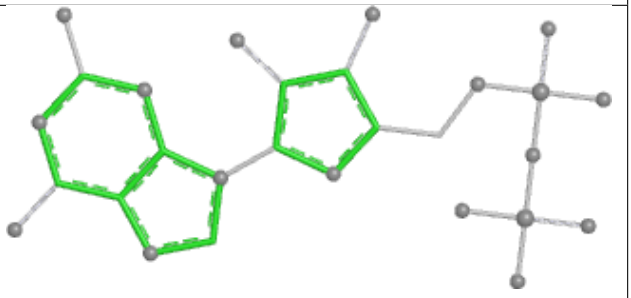
Bond lengths



Bond angles

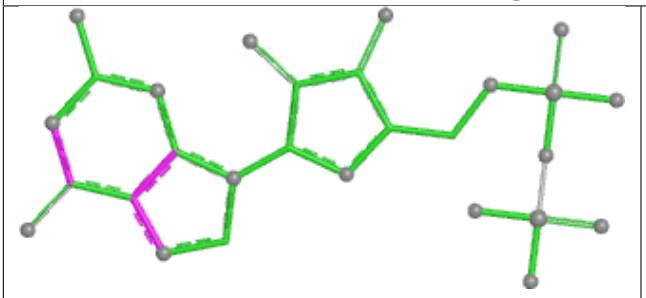


Torsions

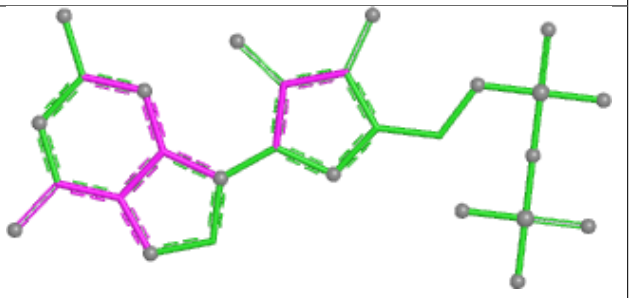


Rings

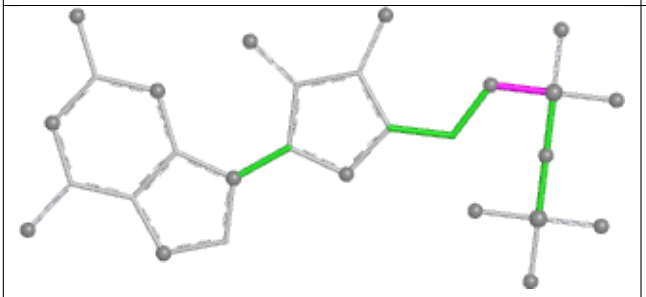
Ligand GDP GT 501



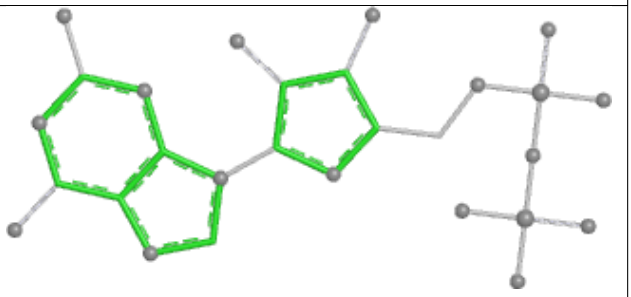
Bond lengths



Bond angles

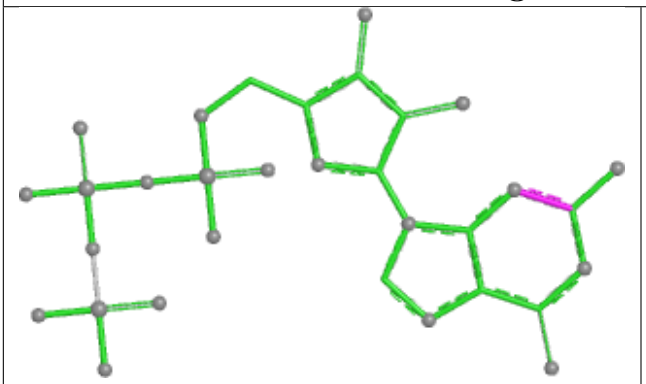


Torsions

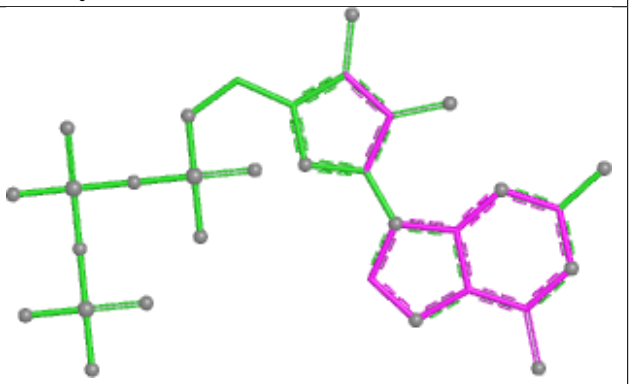


Rings

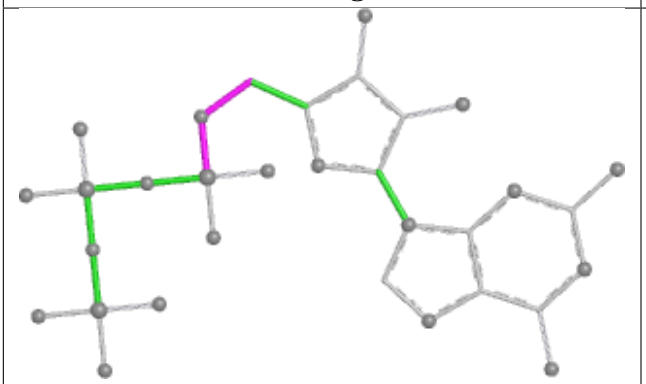
Ligand GTP HQ 501



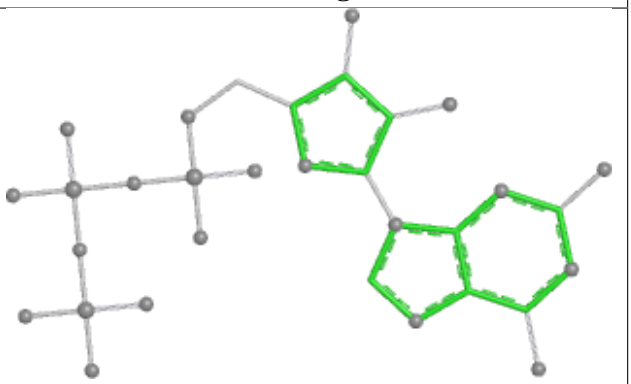
Bond lengths



Bond angles

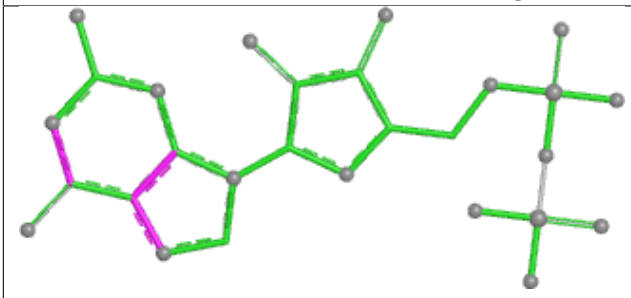


Torsions

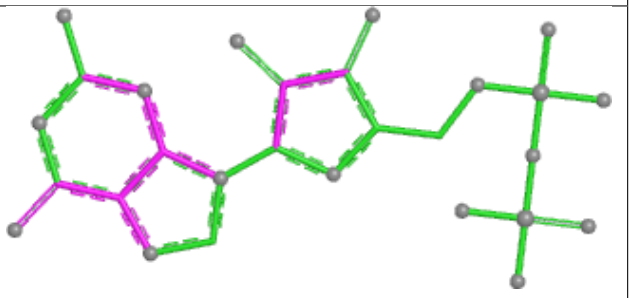


Rings

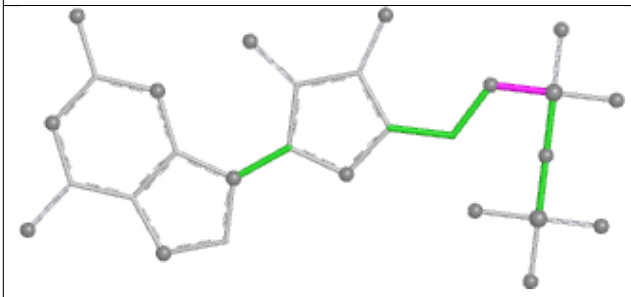
Ligand GDP UF 500



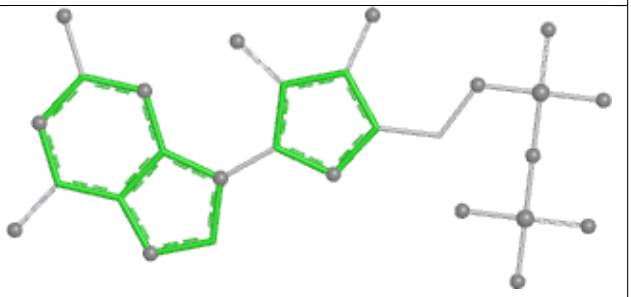
Bond lengths



Bond angles

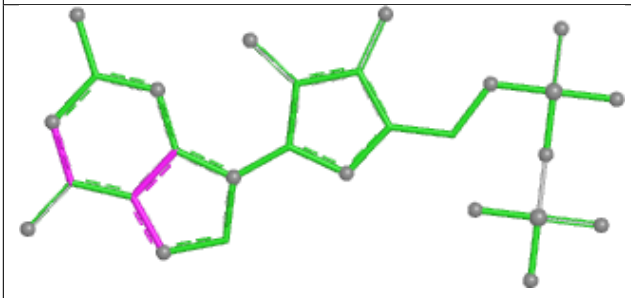


Torsions

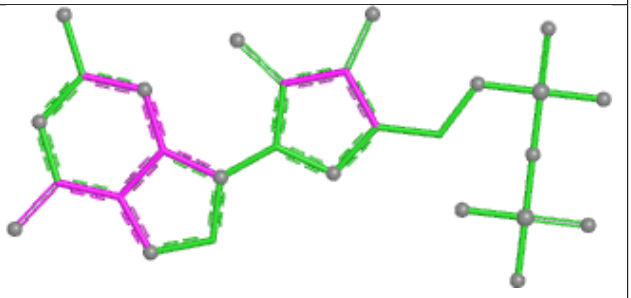


Rings

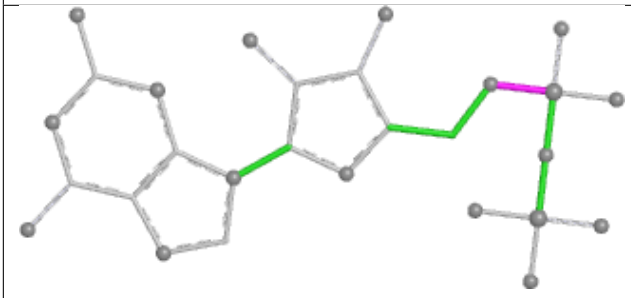
Ligand GDP DI 500



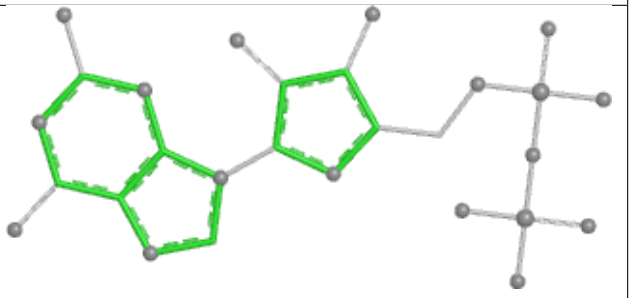
Bond lengths



Bond angles

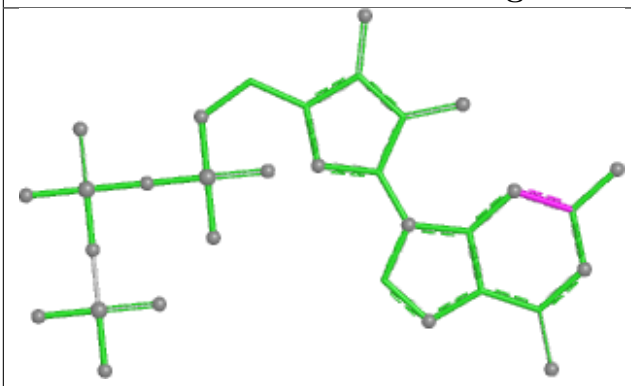


Torsions

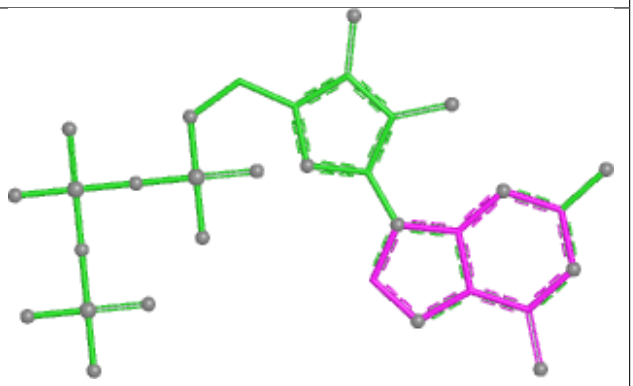


Rings

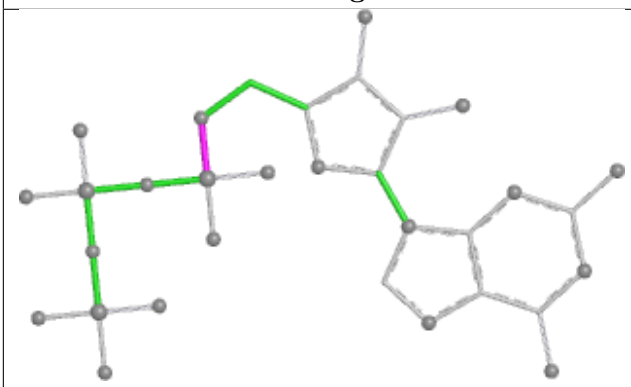
Ligand GTP PM 501



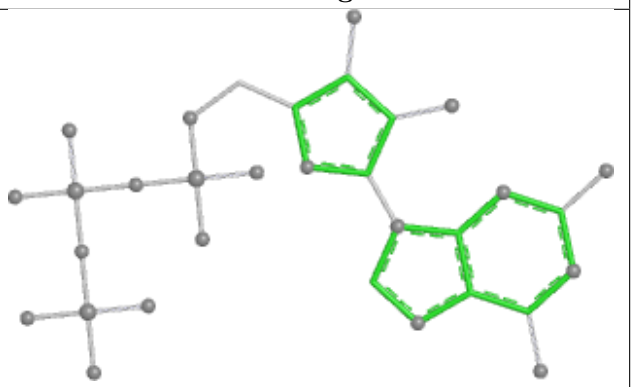
Bond lengths



Bond angles

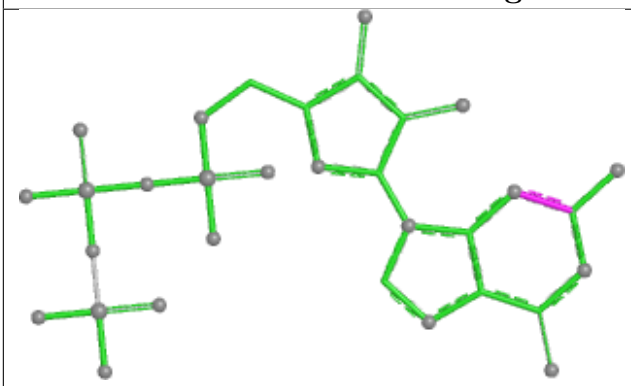


Torsions

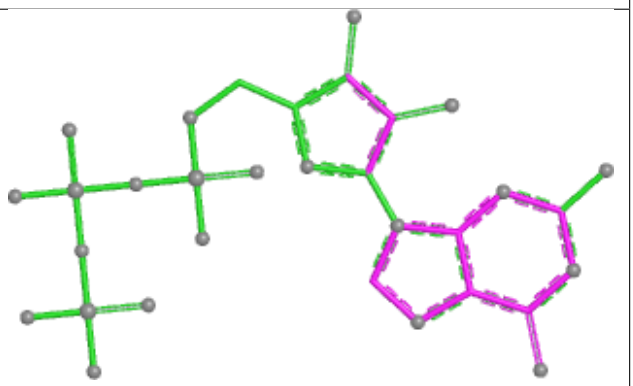


Rings

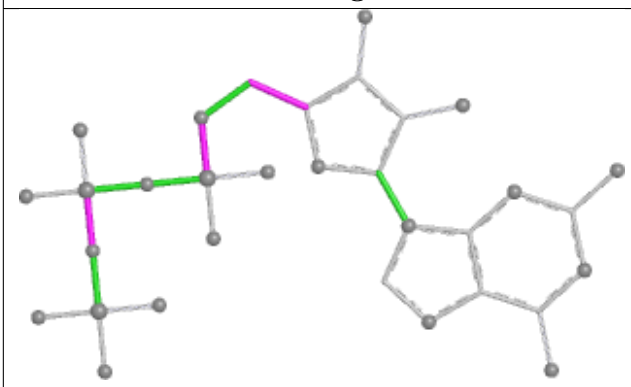
Ligand GTP MG 501



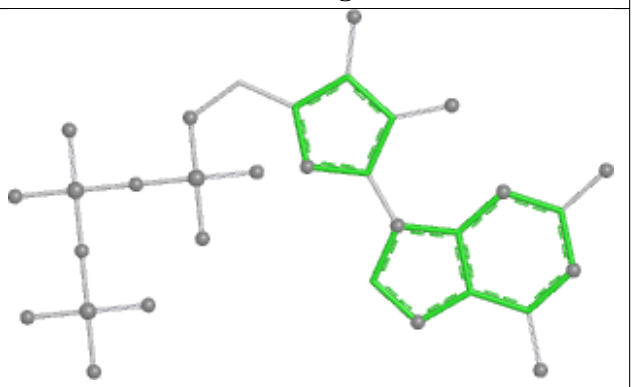
Bond lengths



Bond angles

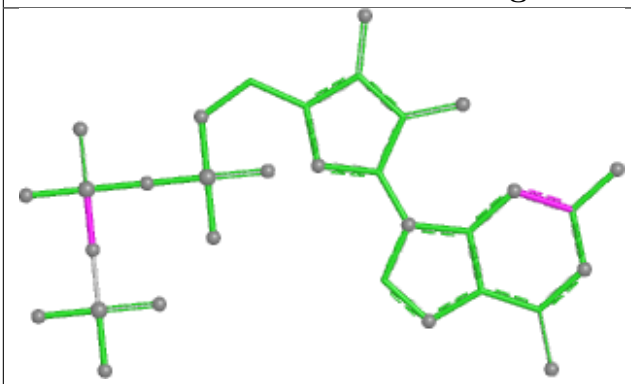


Torsions

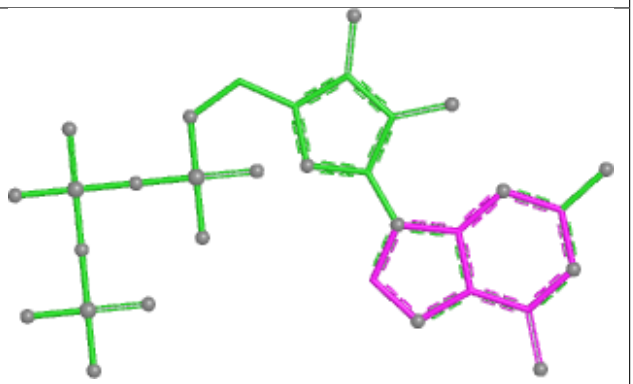


Rings

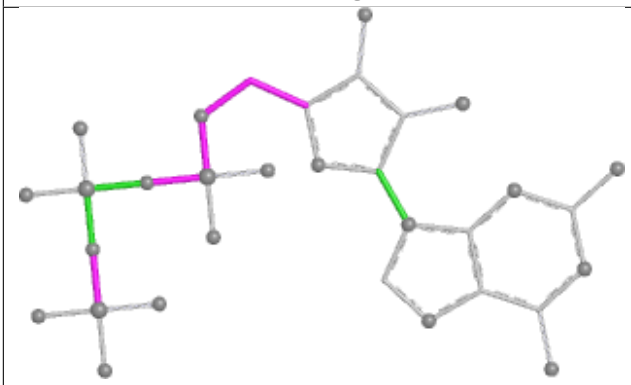
Ligand GTP RC 501



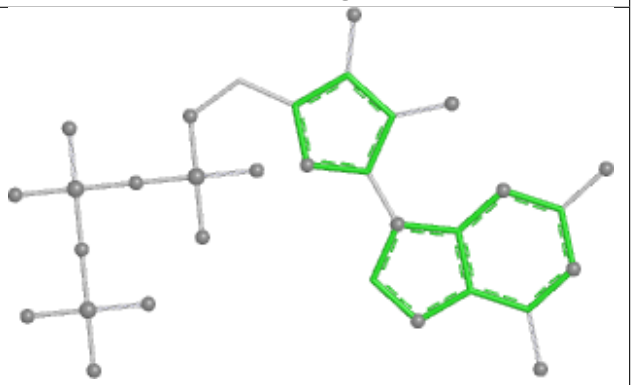
Bond lengths



Bond angles

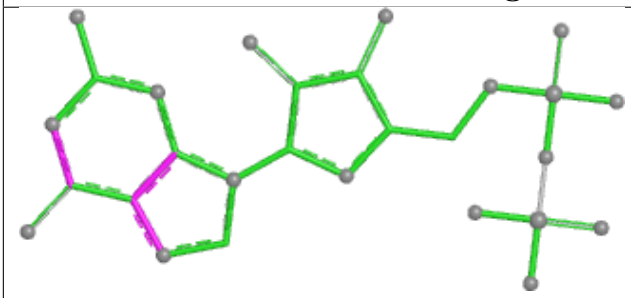


Torsions

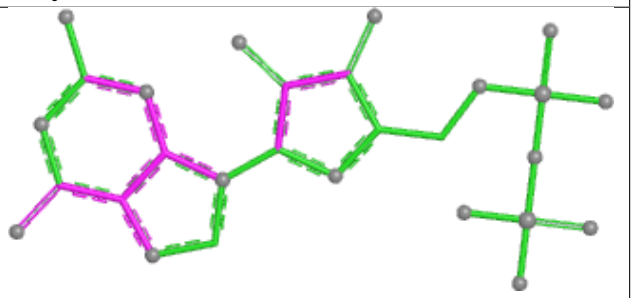


Rings

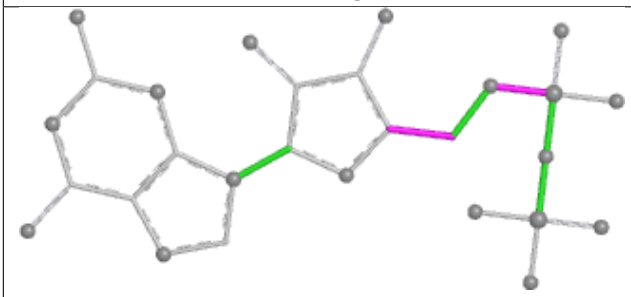
Ligand GDP QM 500



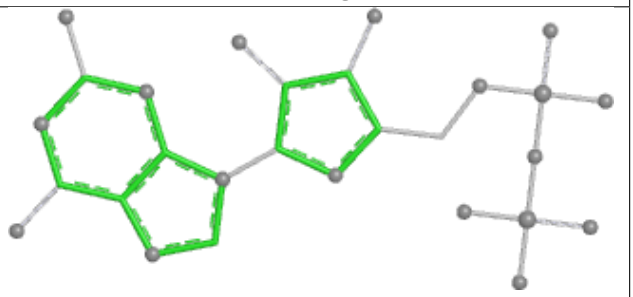
Bond lengths



Bond angles

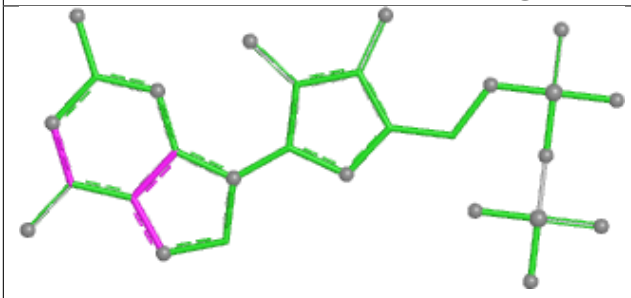


Torsions

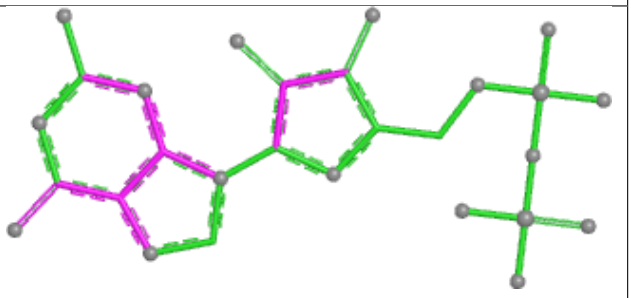


Rings

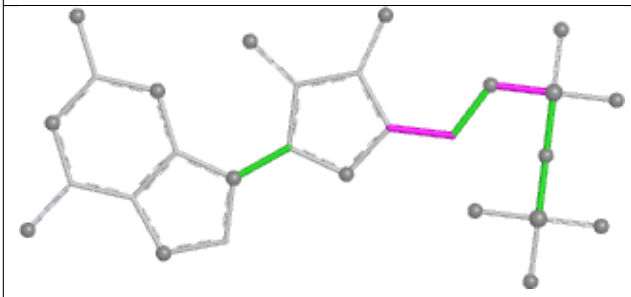
Ligand GDP IF 500



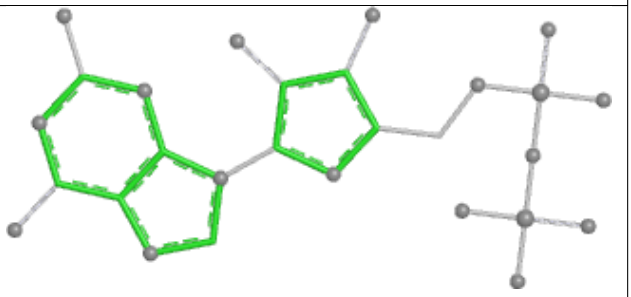
Bond lengths



Bond angles

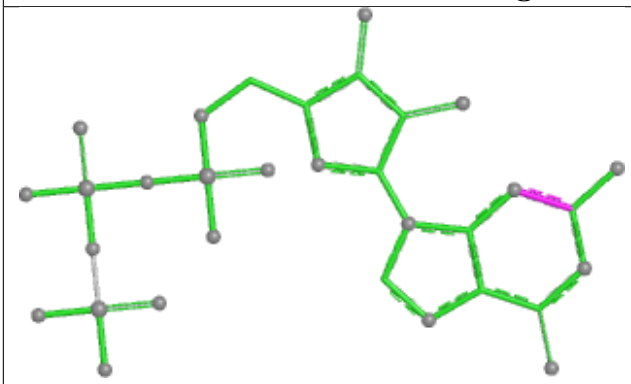


Torsions

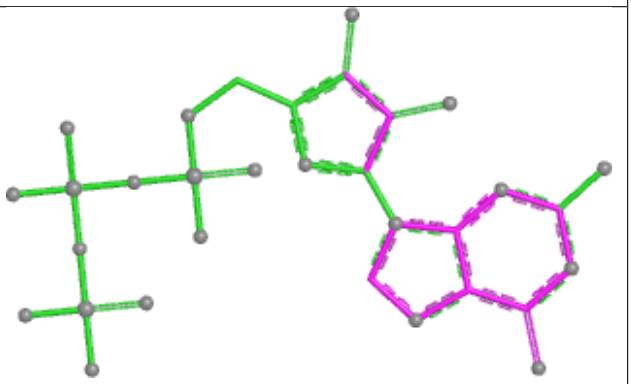


Rings

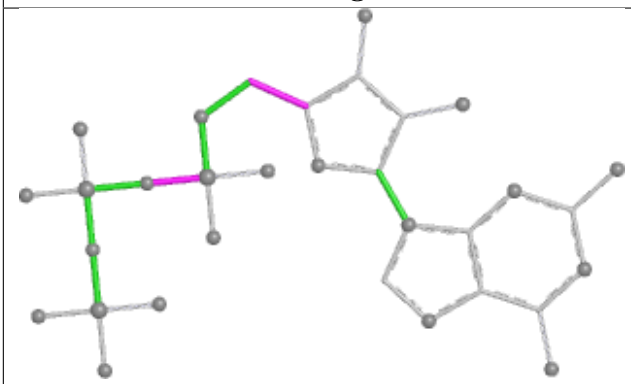
Ligand GTP IU 501



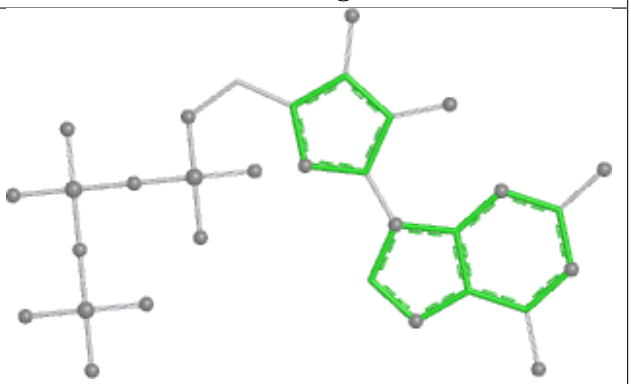
Bond lengths



Bond angles

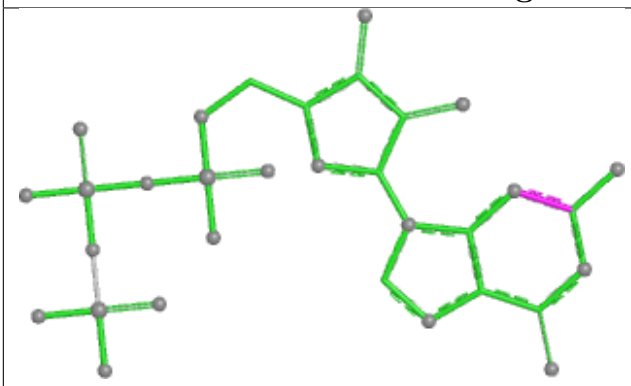


Torsions

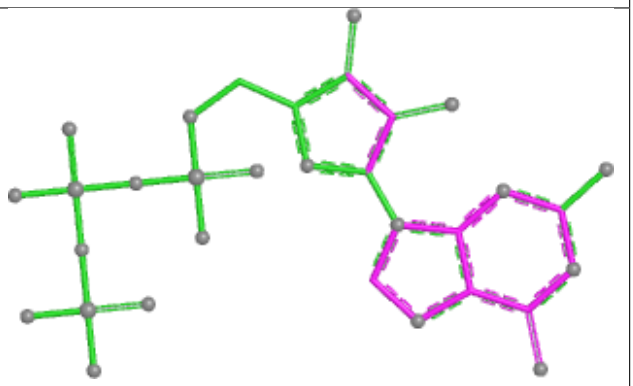


Rings

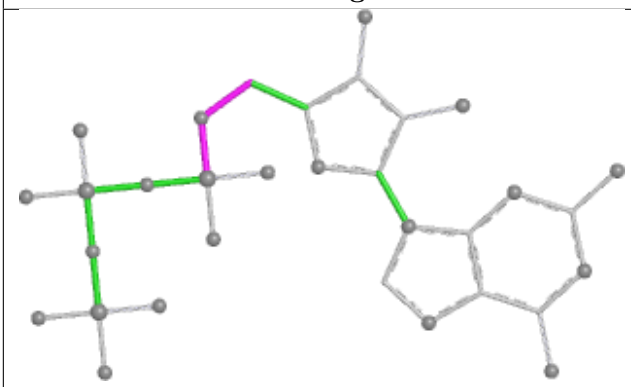
Ligand GTP LJ 501



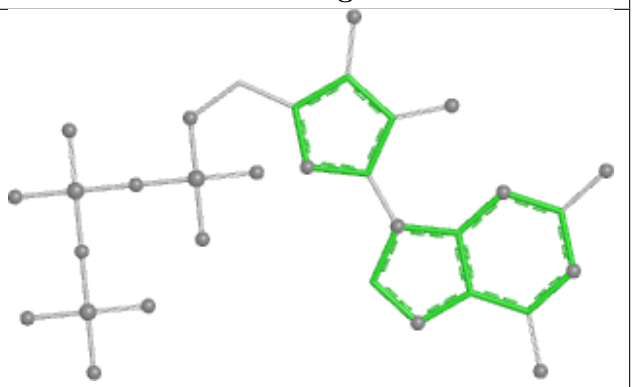
Bond lengths



Bond angles

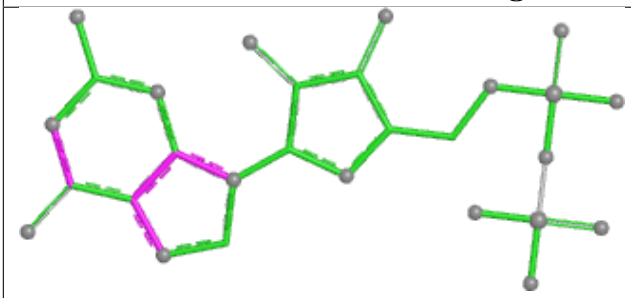


Torsions

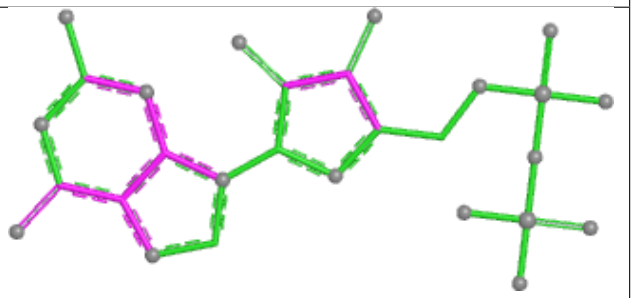


Rings

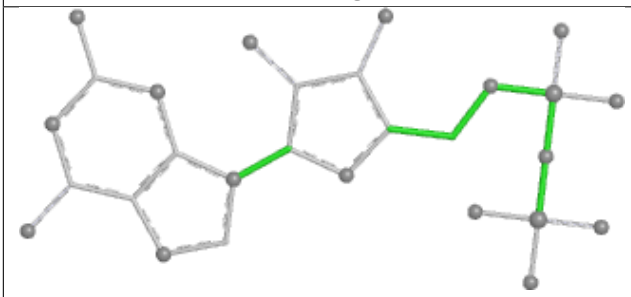
Ligand GDP CU 500



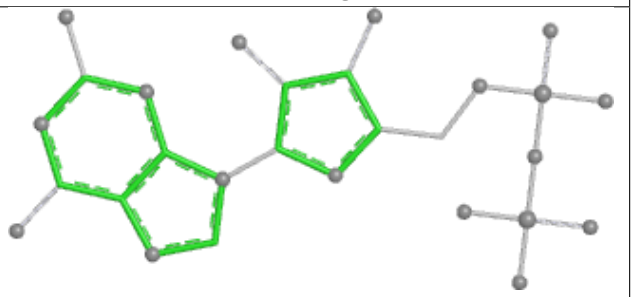
Bond lengths



Bond angles

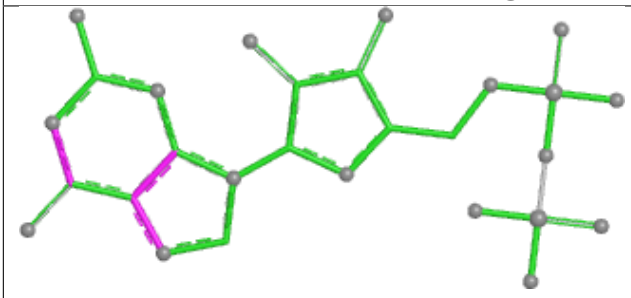


Torsions

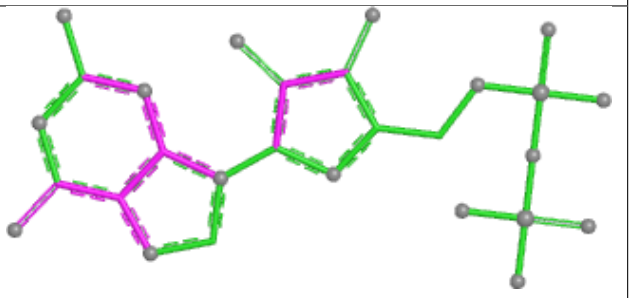


Rings

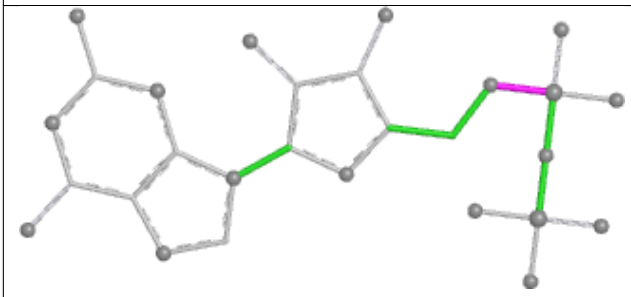
Ligand GDP WN 500



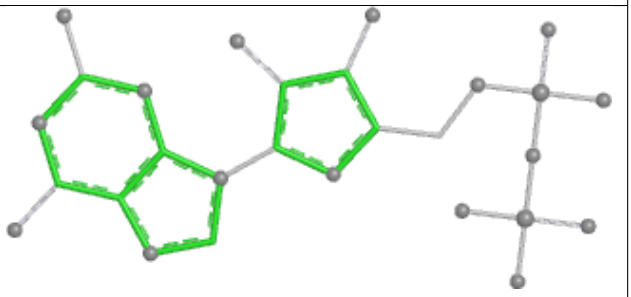
Bond lengths



Bond angles

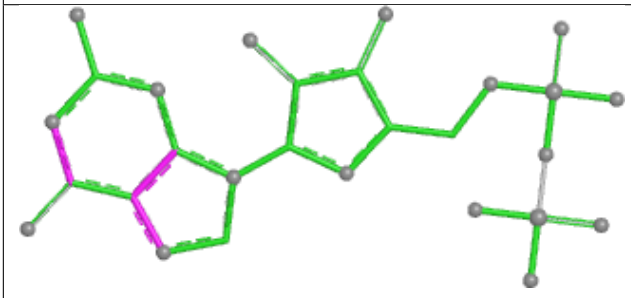


Torsions

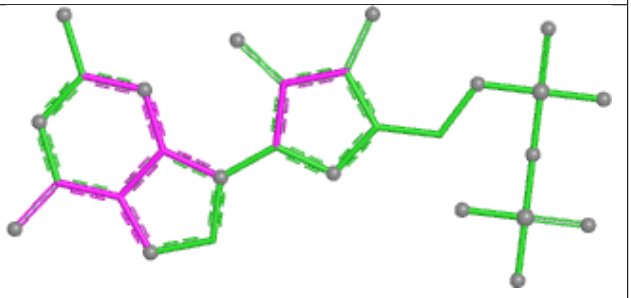


Rings

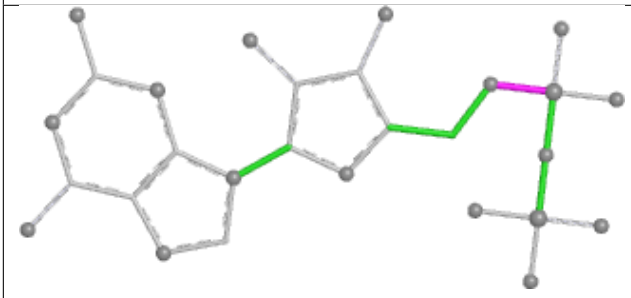
Ligand GDP KC 500



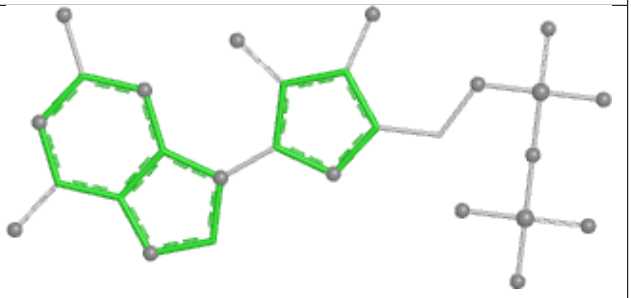
Bond lengths



Bond angles

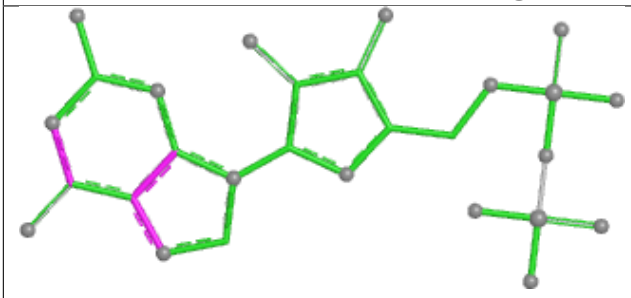


Torsions

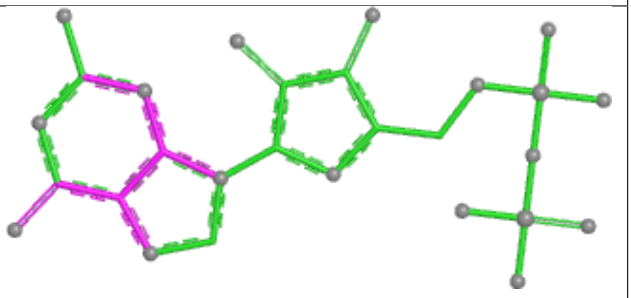


Rings

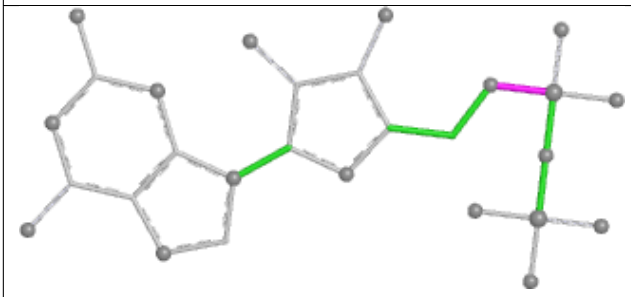
Ligand GDP BF 500



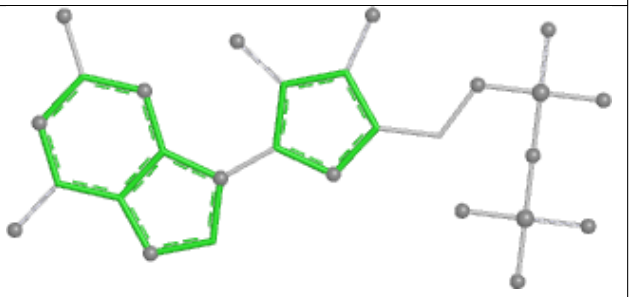
Bond lengths



Bond angles

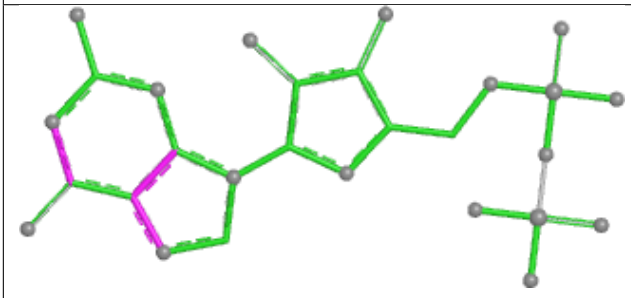


Torsions

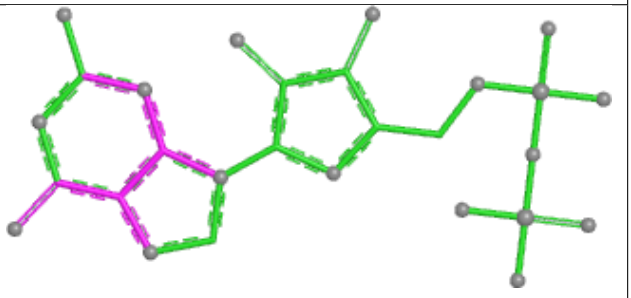


Rings

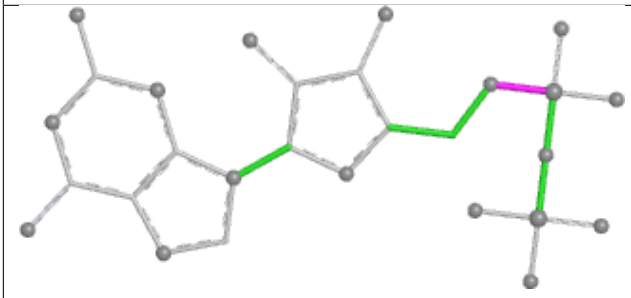
Ligand GDP TV 500



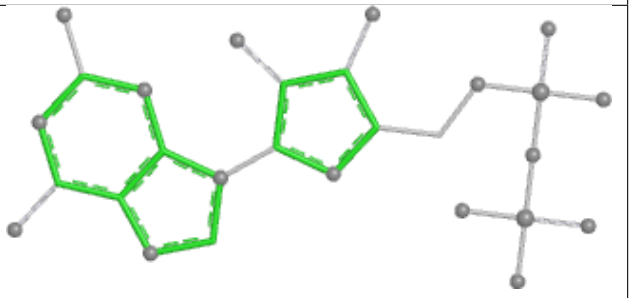
Bond lengths



Bond angles

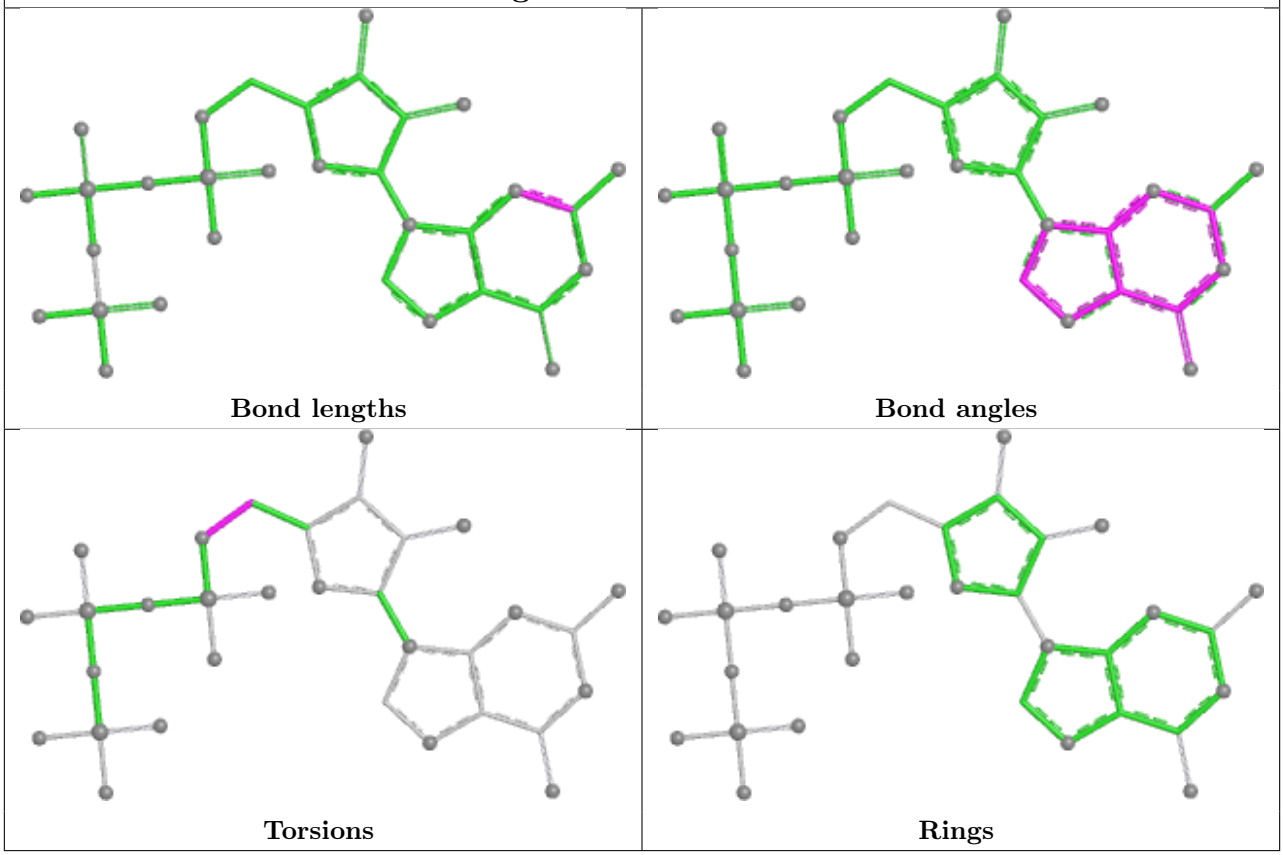


Torsions

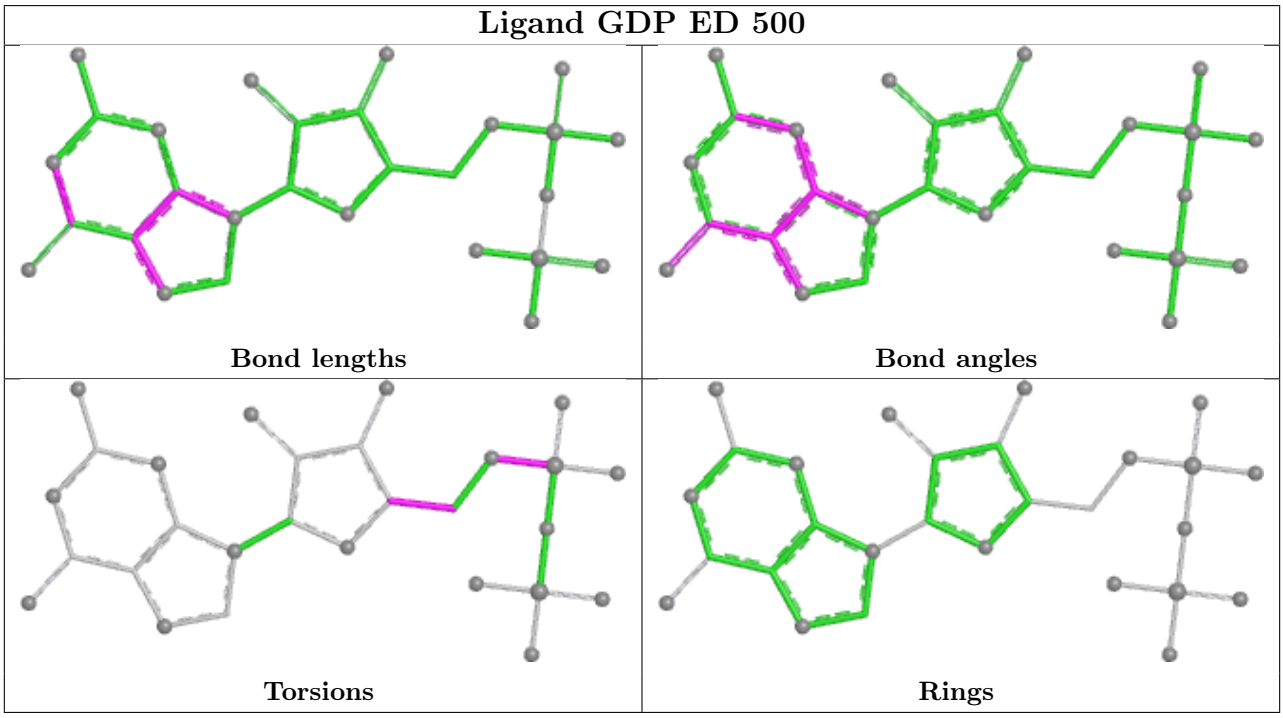


Rings

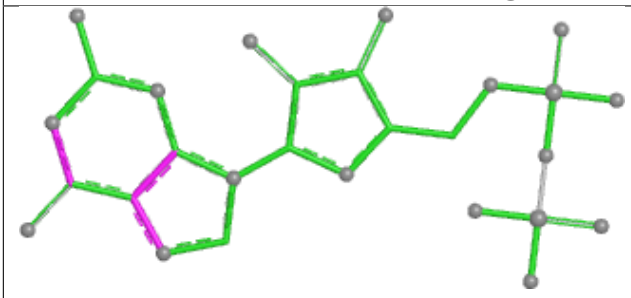
Ligand GTP RF 501



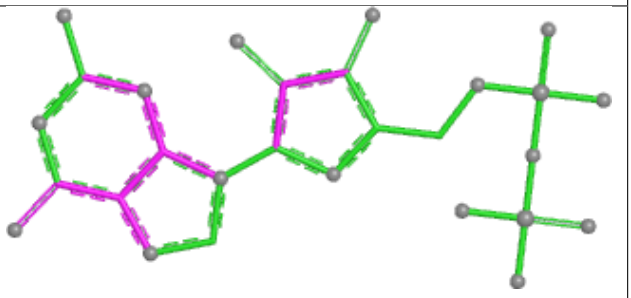
Ligand GDP ED 500



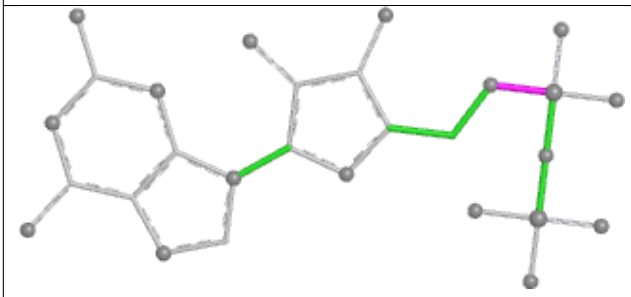
Ligand GDP WD 500



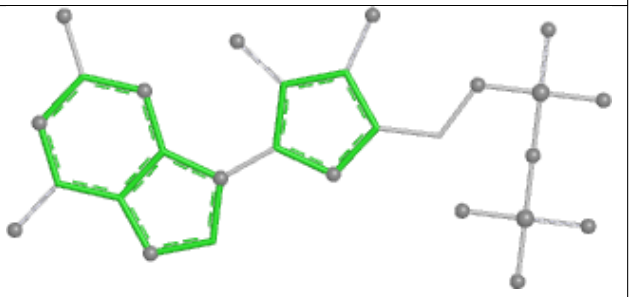
Bond lengths



Bond angles

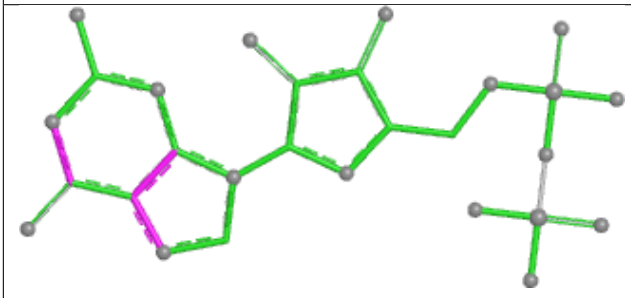


Torsions

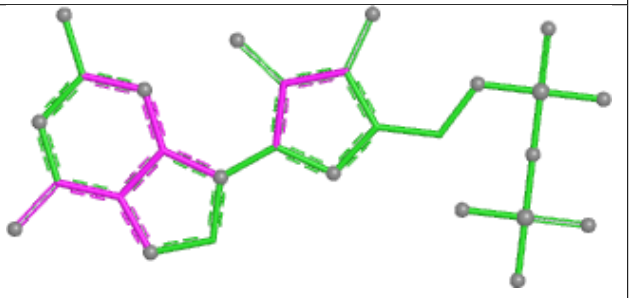


Rings

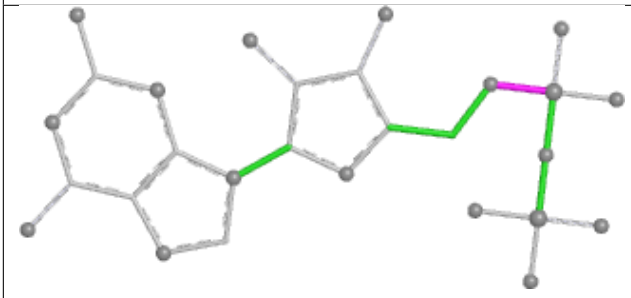
Ligand GDP UN 500



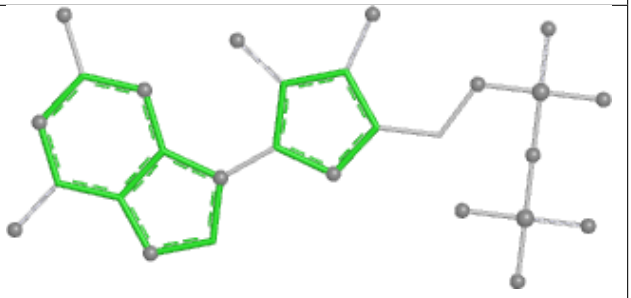
Bond lengths



Bond angles

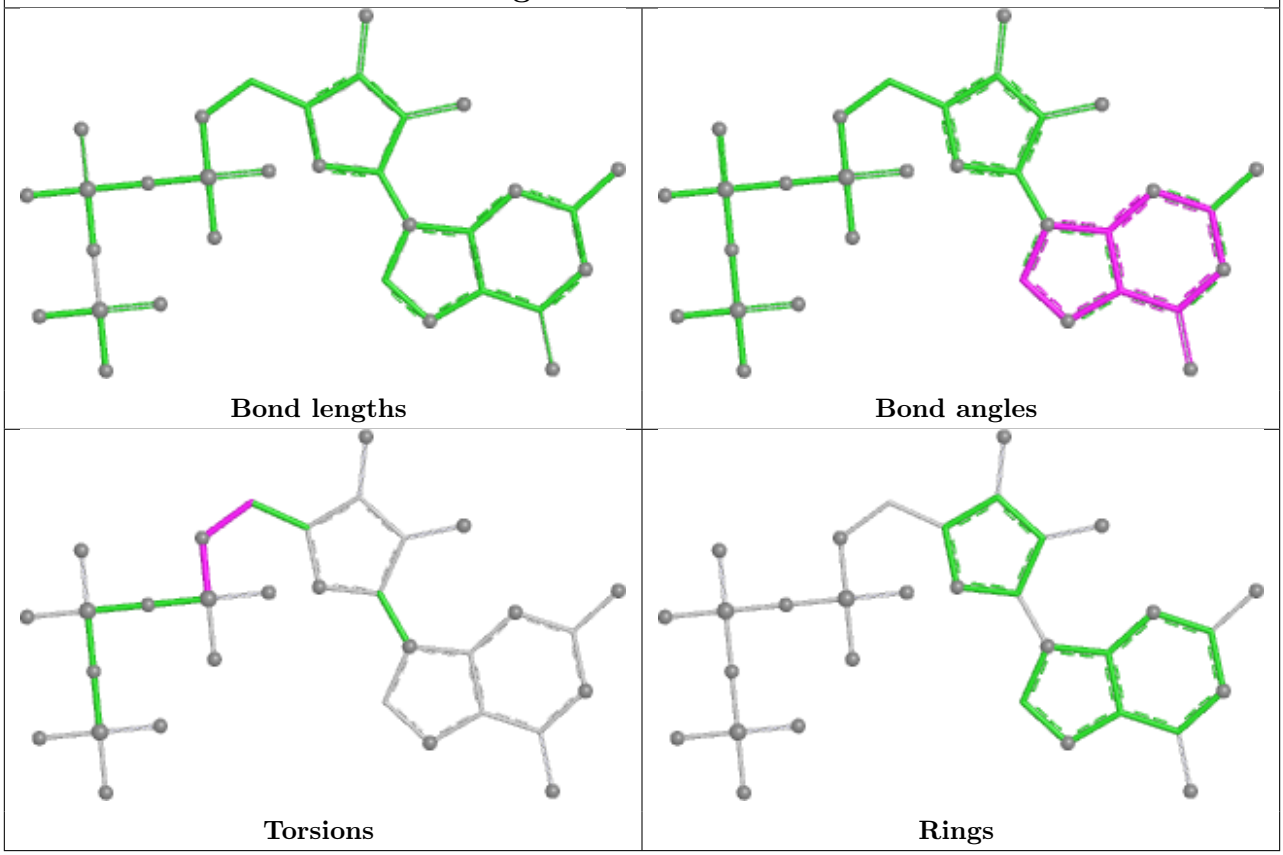


Torsions

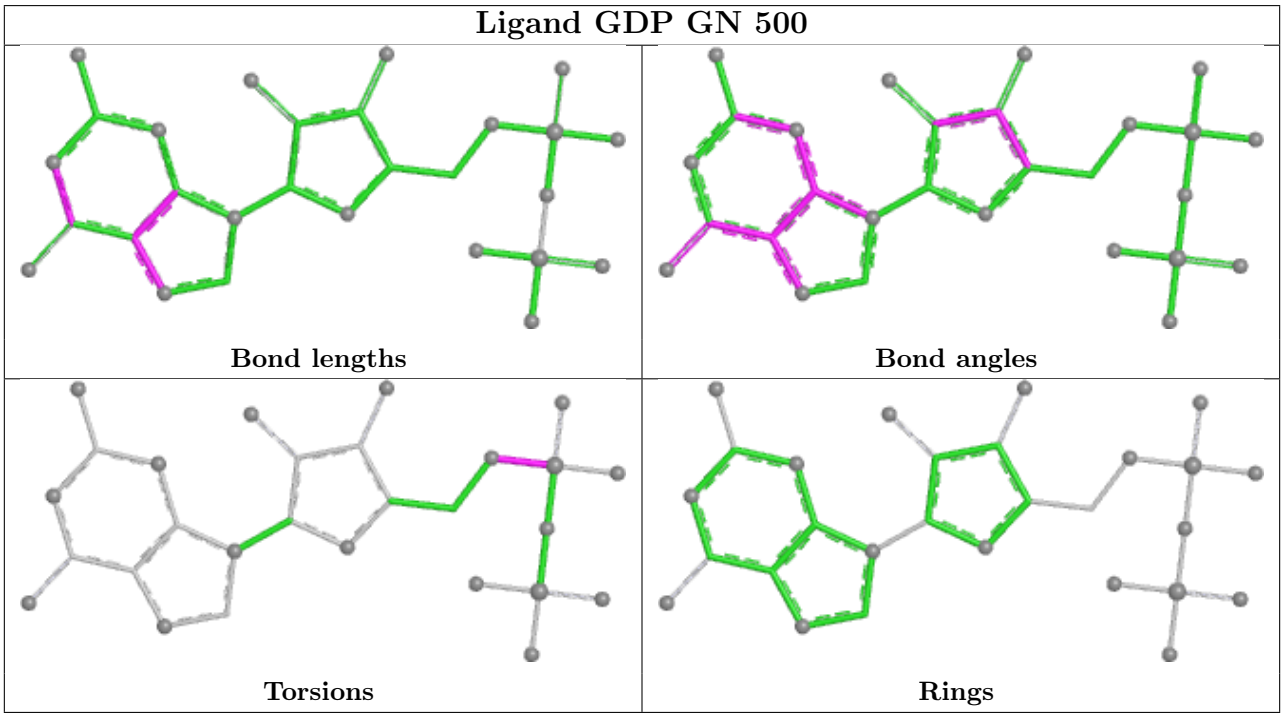


Rings

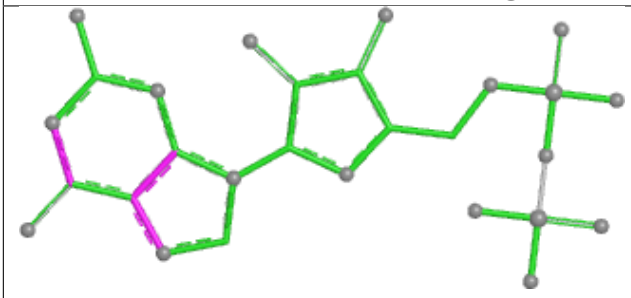
Ligand GTP FC 501



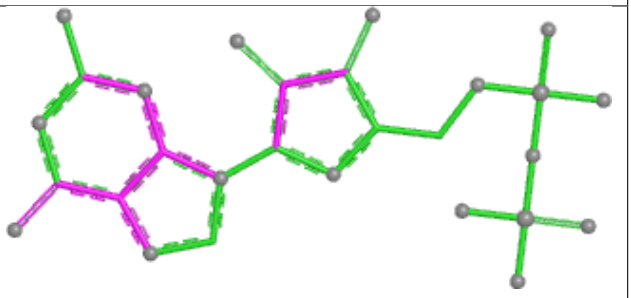
Ligand GDP GN 500



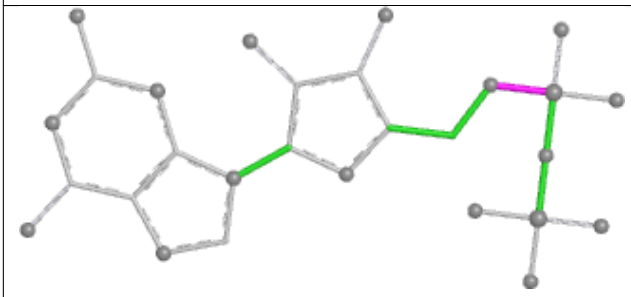
Ligand GDP WX 500



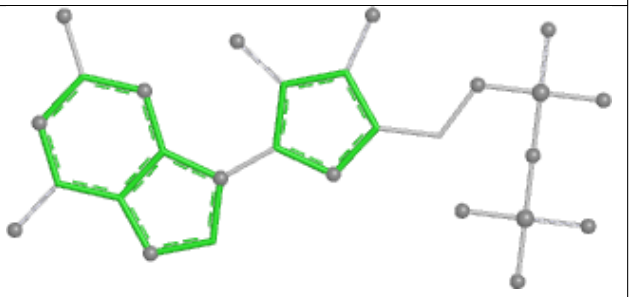
Bond lengths



Bond angles

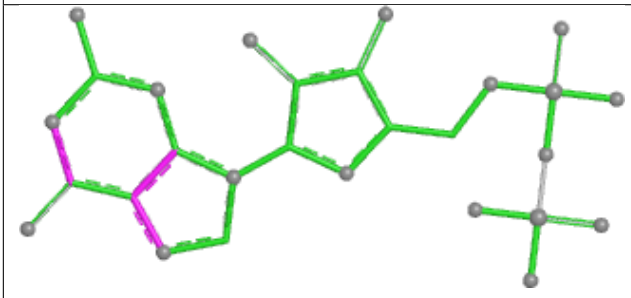


Torsions

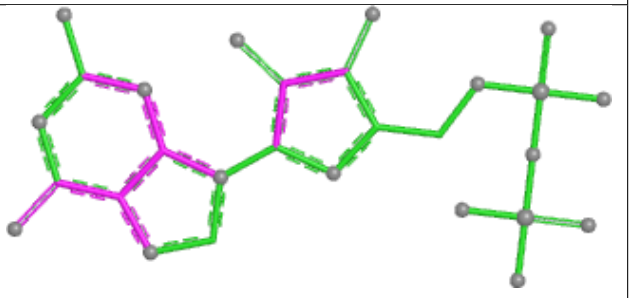


Rings

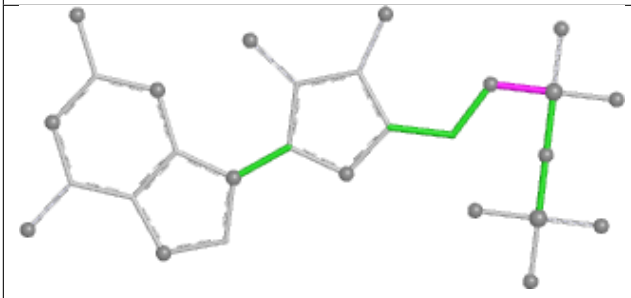
Ligand GDP HH 501



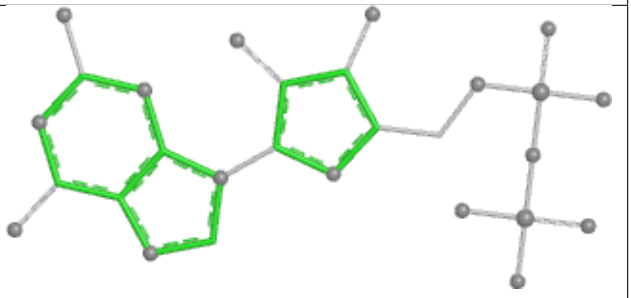
Bond lengths



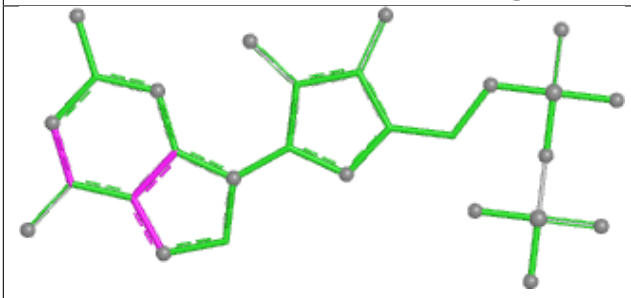
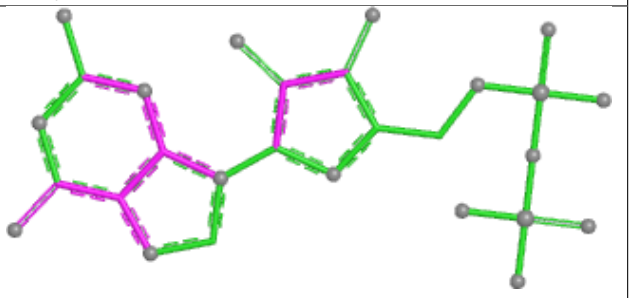
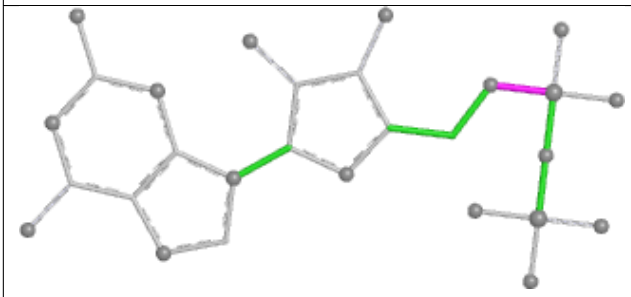
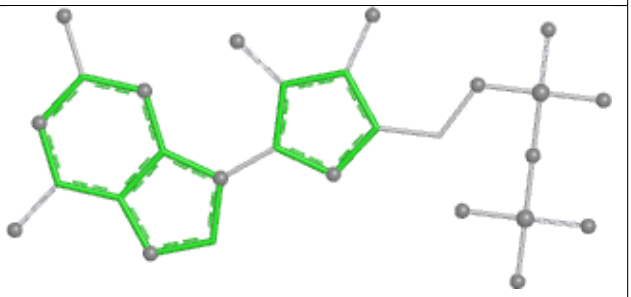
Bond angles

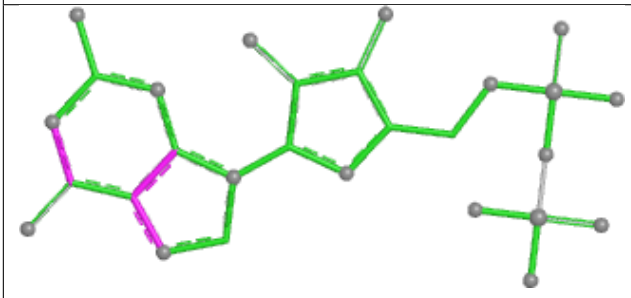
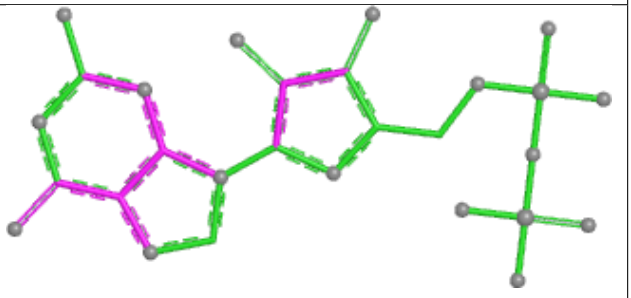
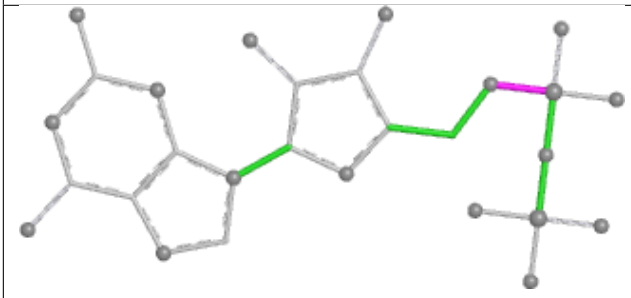
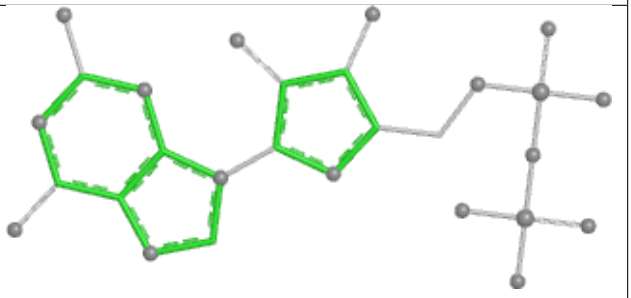


Torsions

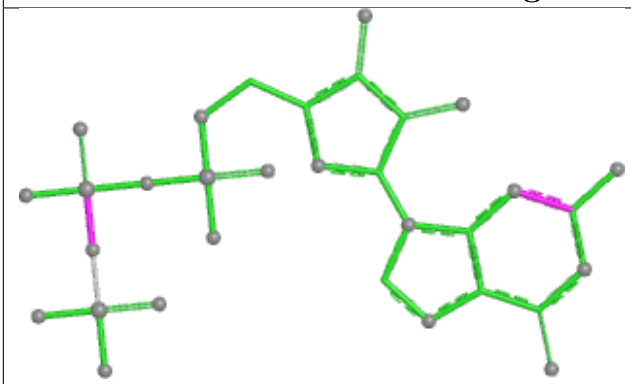


Rings

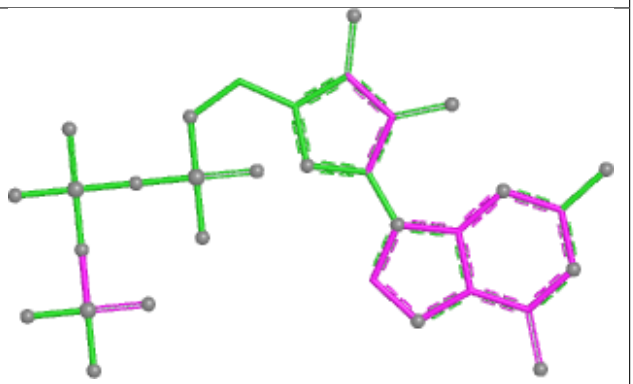
Ligand GDP QC 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP QU 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

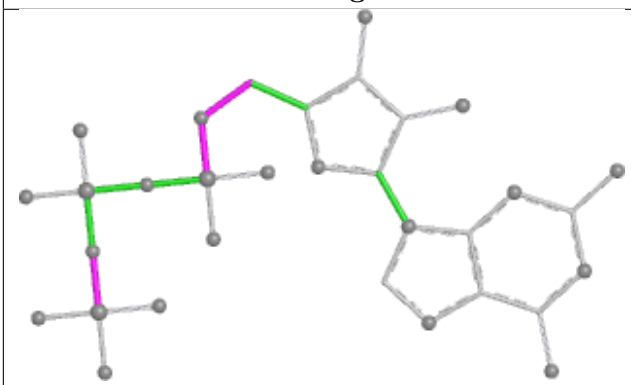
Ligand GTP T 503



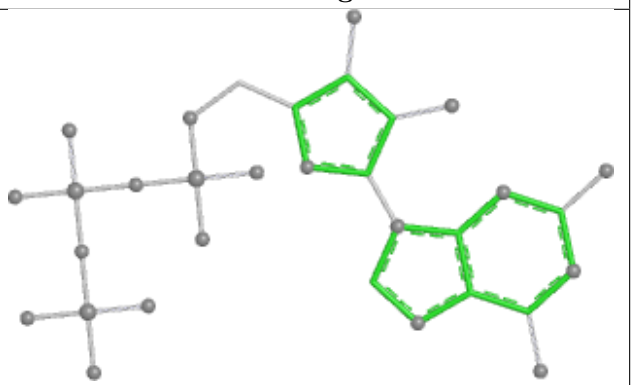
Bond lengths



Bond angles

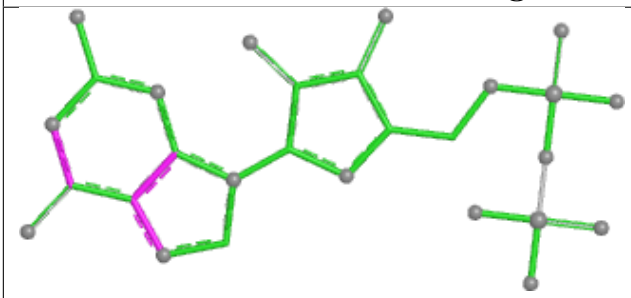


Torsions

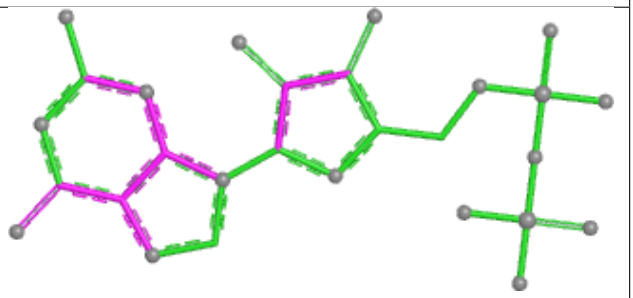


Rings

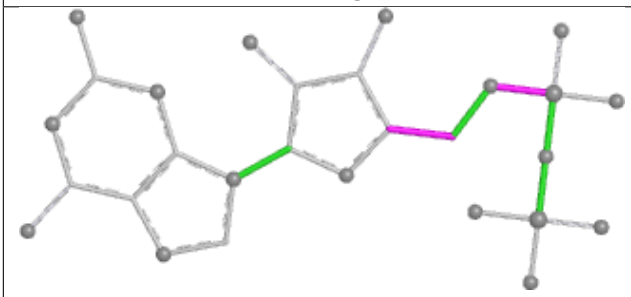
Ligand GDP GP 500



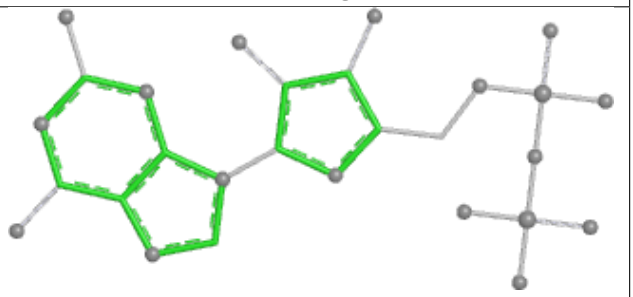
Bond lengths



Bond angles

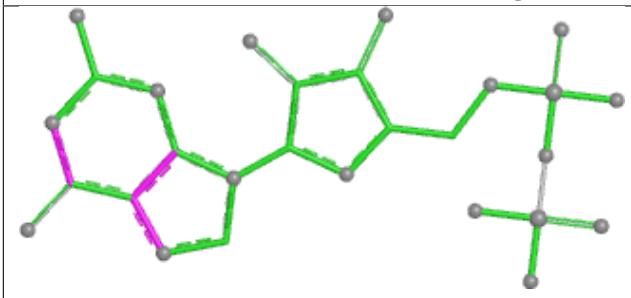


Torsions

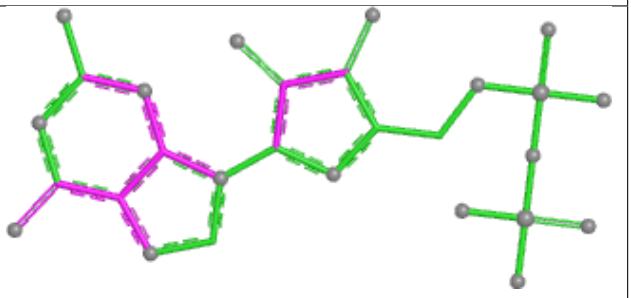


Rings

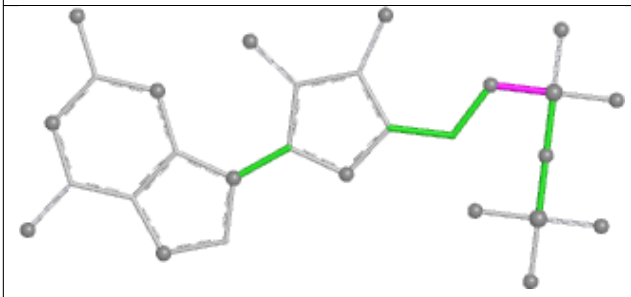
Ligand GDP PB 500



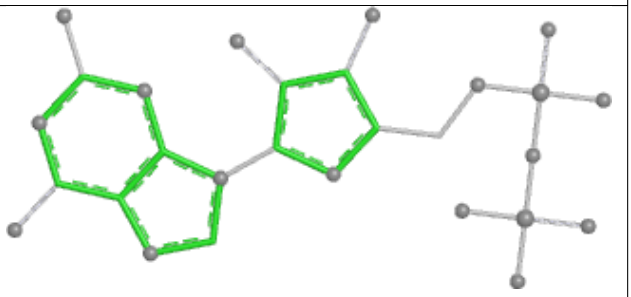
Bond lengths



Bond angles

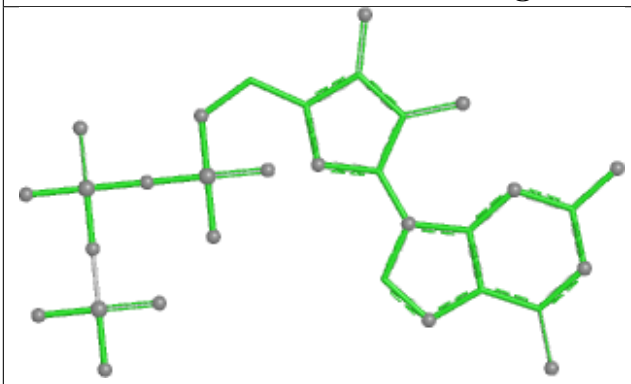


Torsions

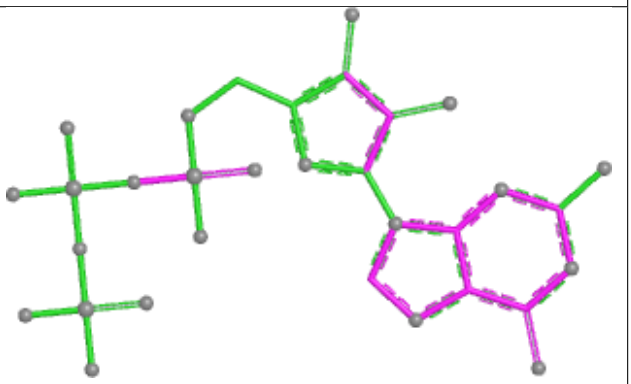


Rings

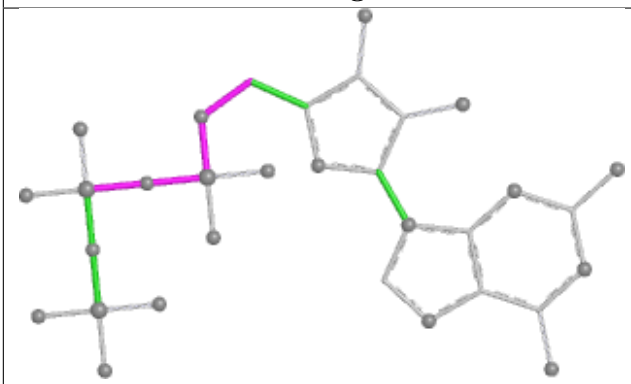
Ligand GTP ES 501



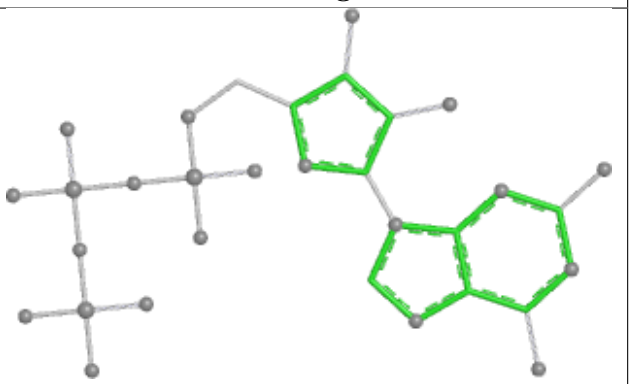
Bond lengths



Bond angles

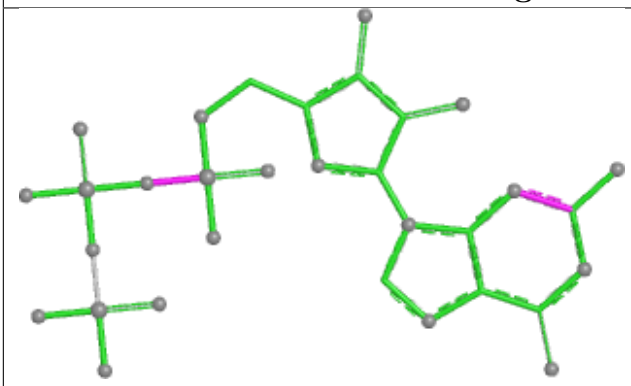


Torsions

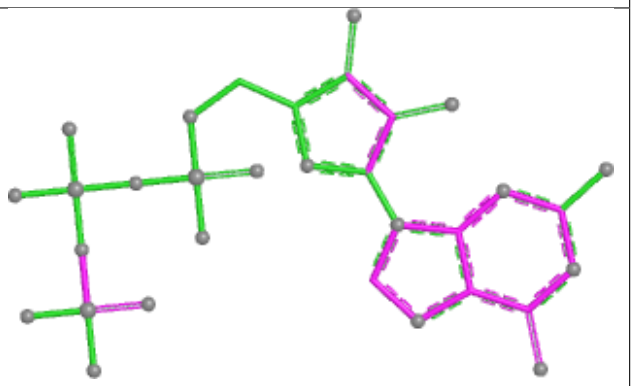


Rings

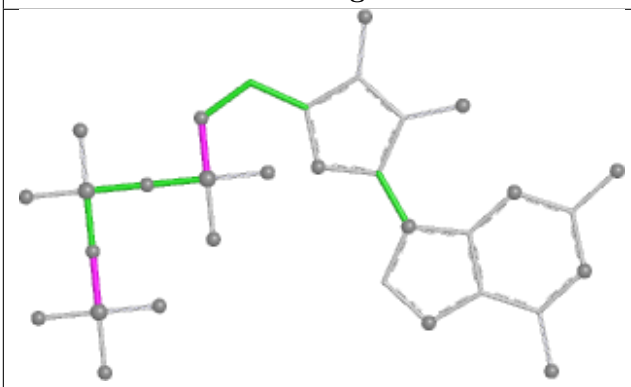
Ligand GTP EJ 501



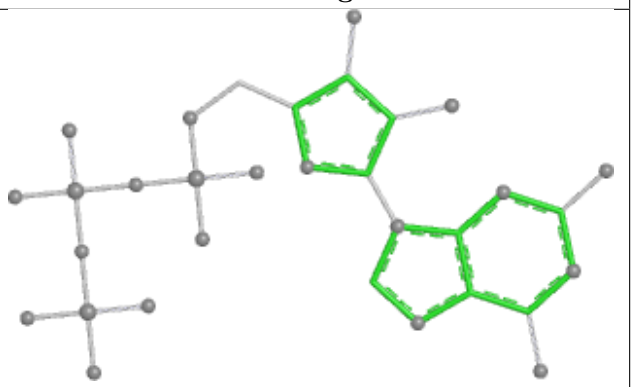
Bond lengths



Bond angles

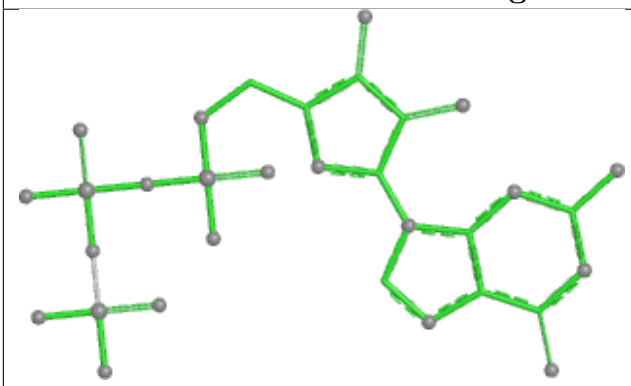


Torsions

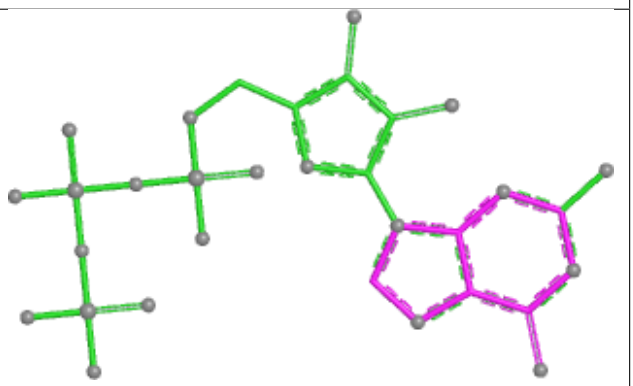


Rings

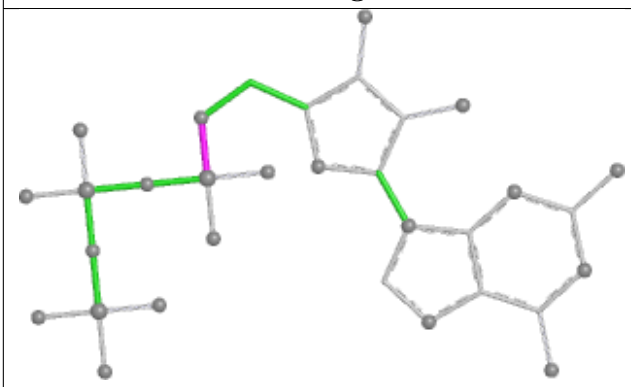
Ligand GTP BK 501



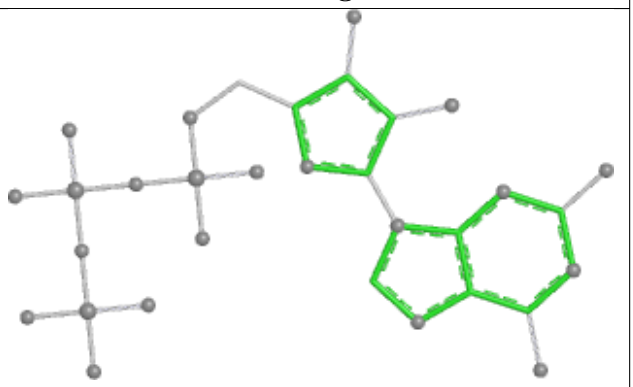
Bond lengths



Bond angles

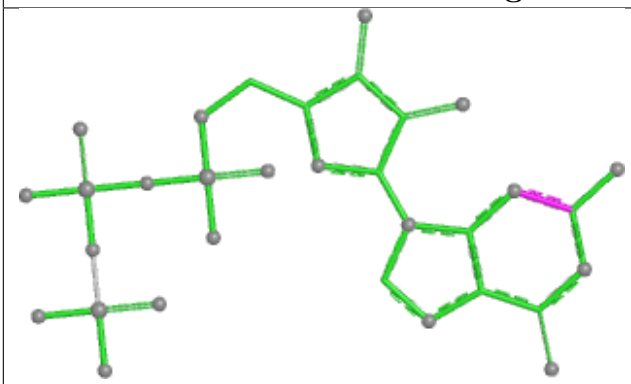


Torsions

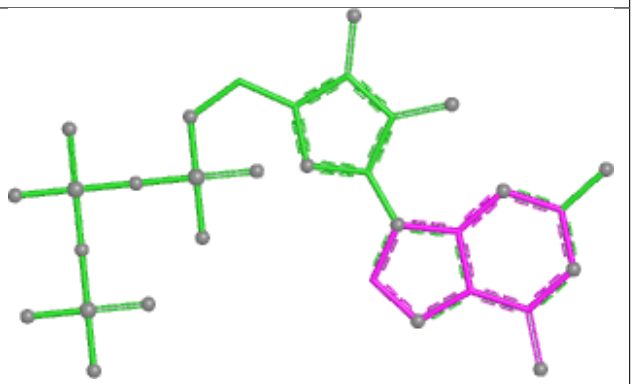


Rings

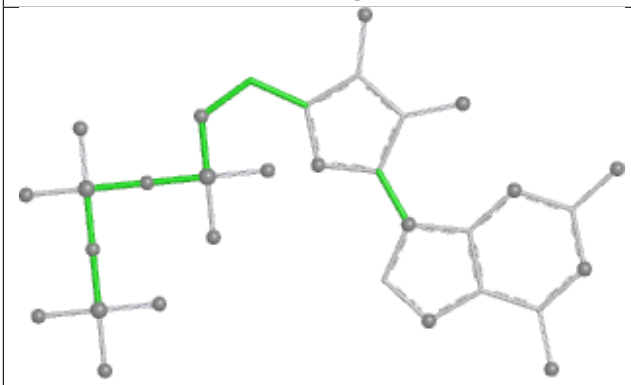
Ligand GTP MA 501



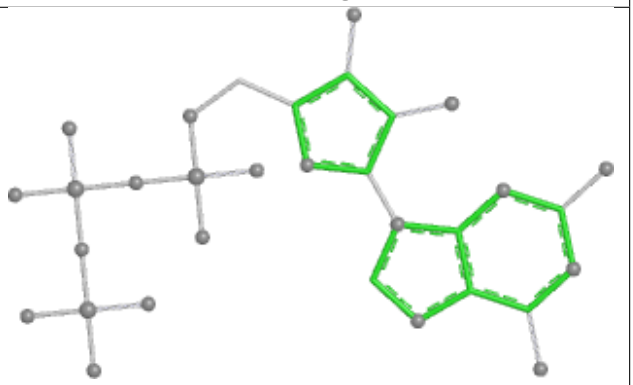
Bond lengths



Bond angles

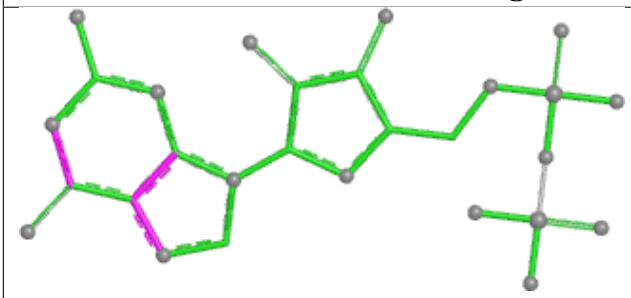


Torsions

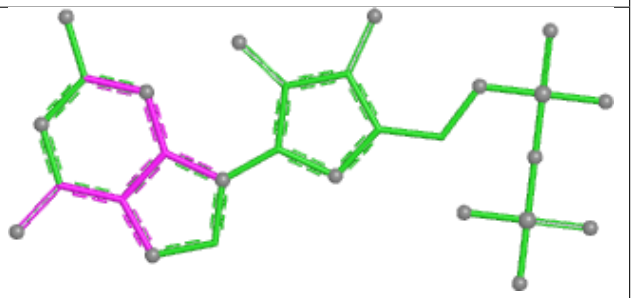


Rings

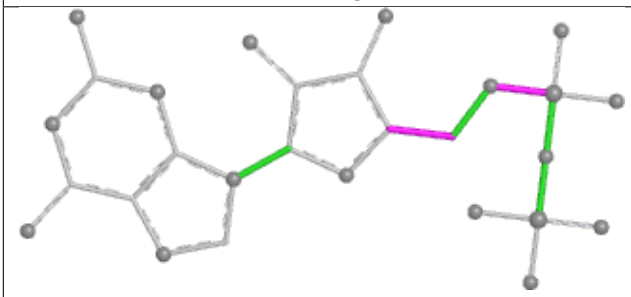
Ligand GDP DC 500



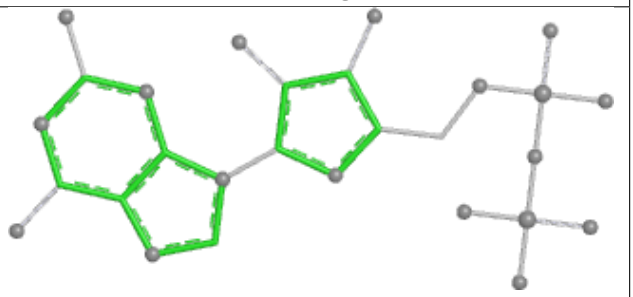
Bond lengths



Bond angles

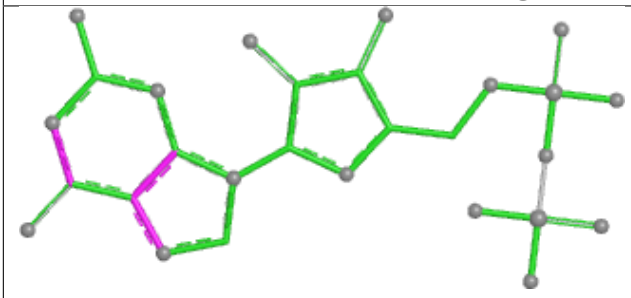


Torsions

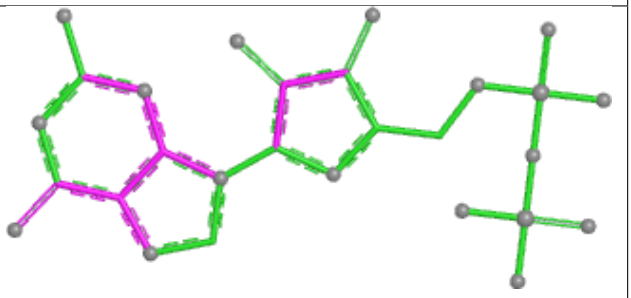


Rings

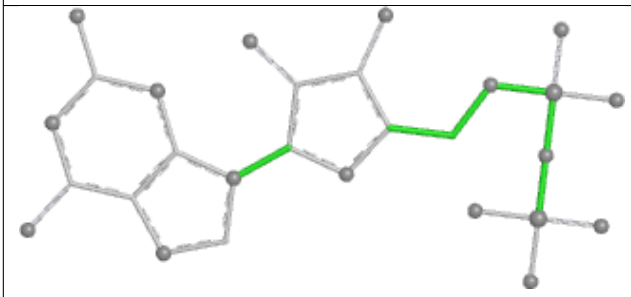
Ligand GDP RI 500



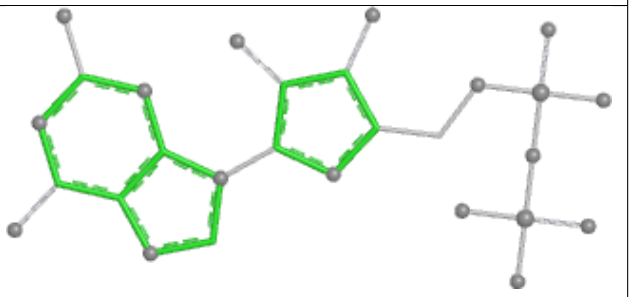
Bond lengths



Bond angles

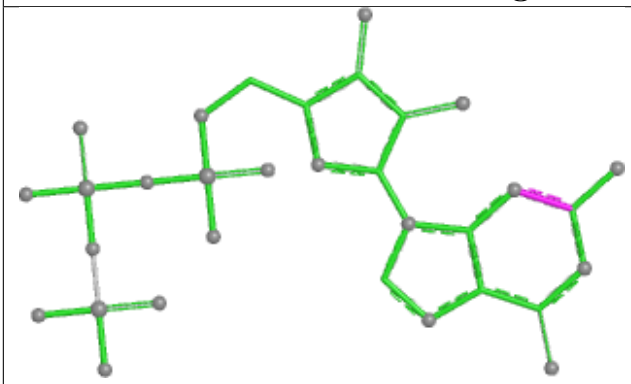


Torsions

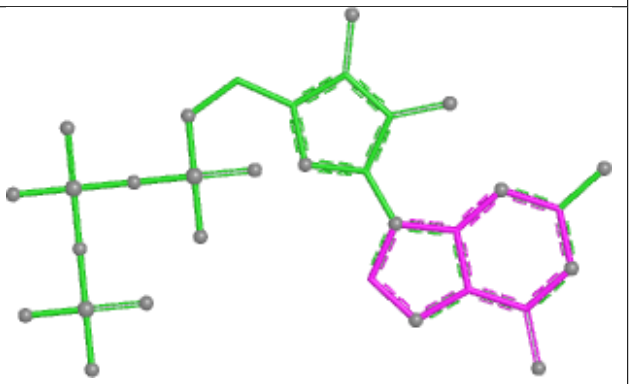


Rings

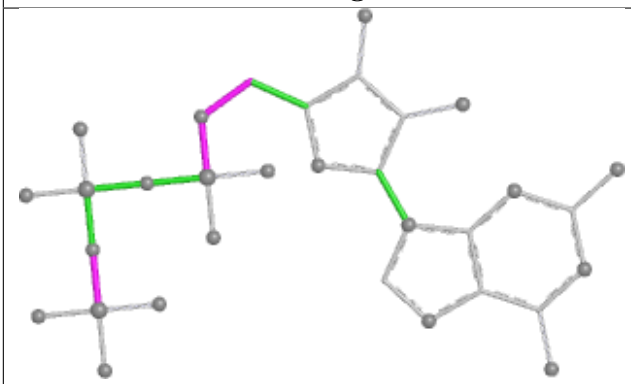
Ligand GTP MI 501



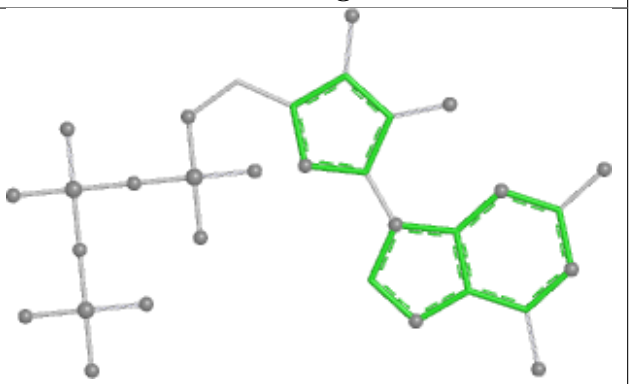
Bond lengths



Bond angles

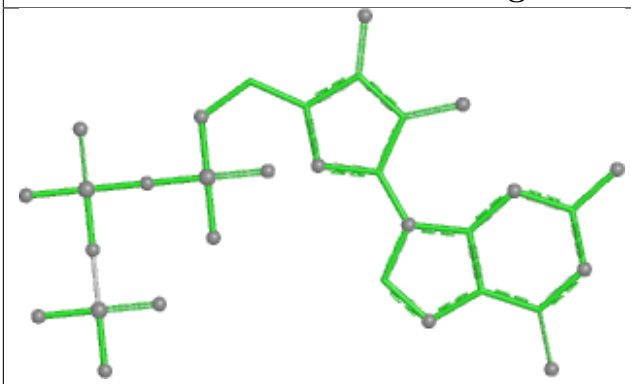


Torsions

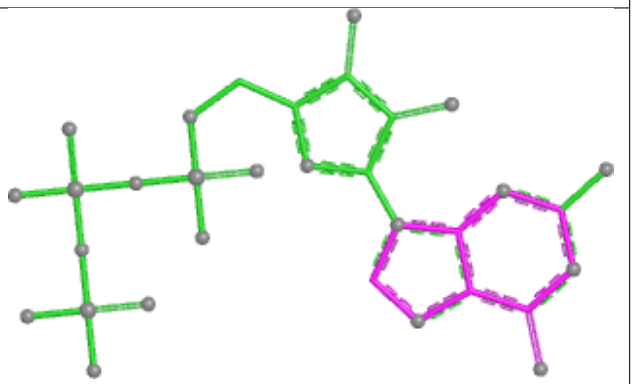


Rings

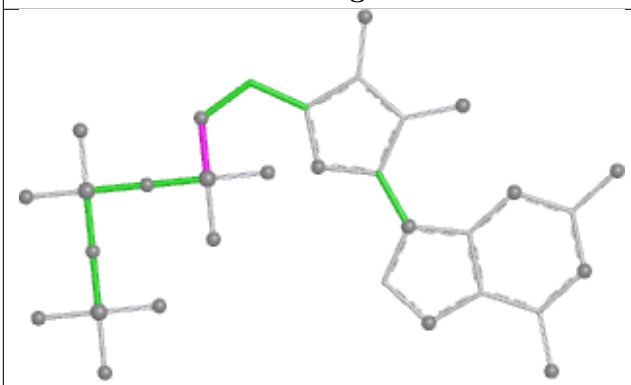
Ligand GTP DN 501



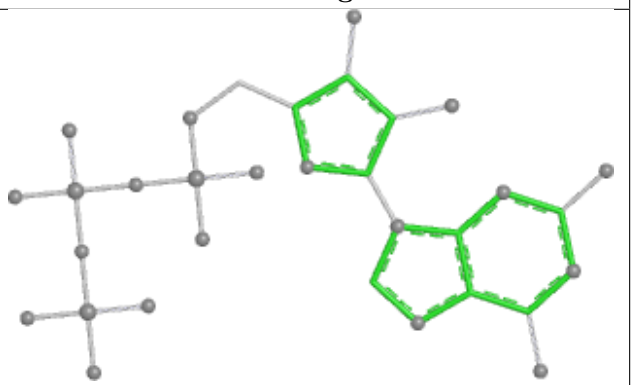
Bond lengths



Bond angles

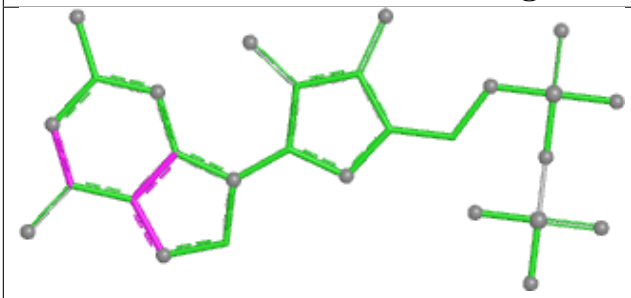


Torsions

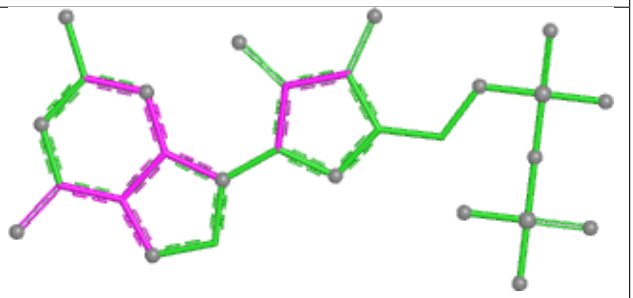


Rings

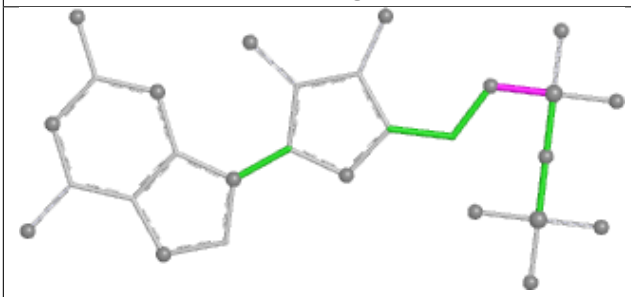
Ligand GDP U 500



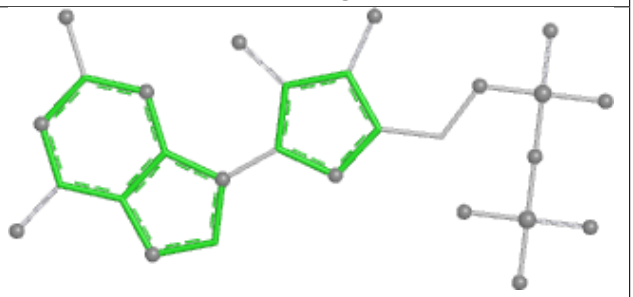
Bond lengths



Bond angles

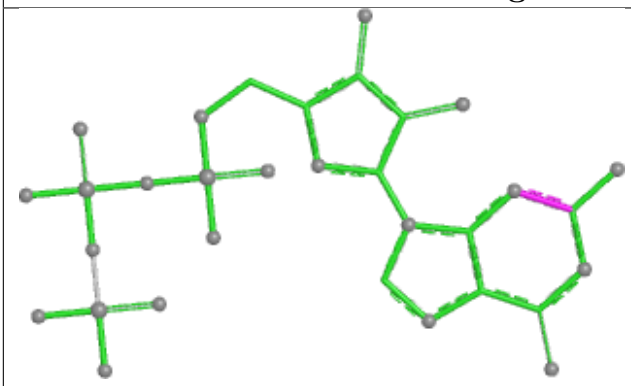


Torsions

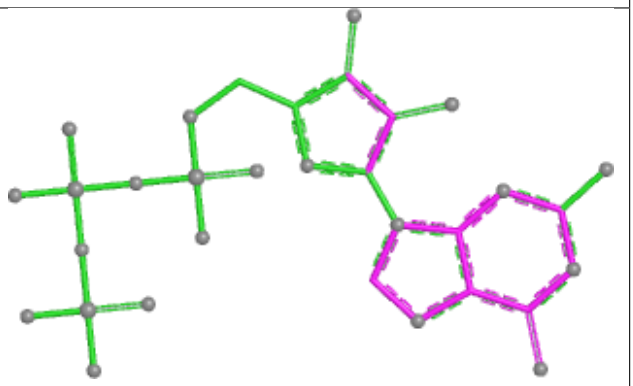


Rings

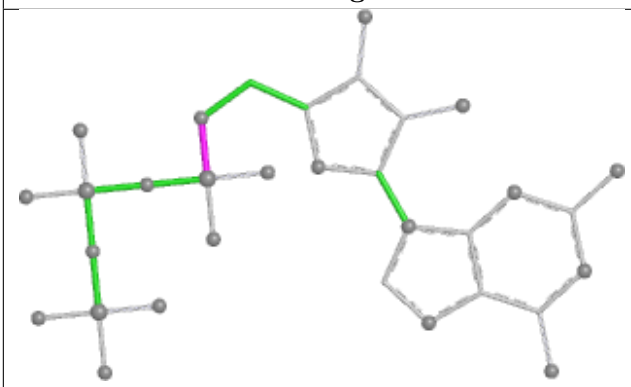
Ligand GTP NO 501



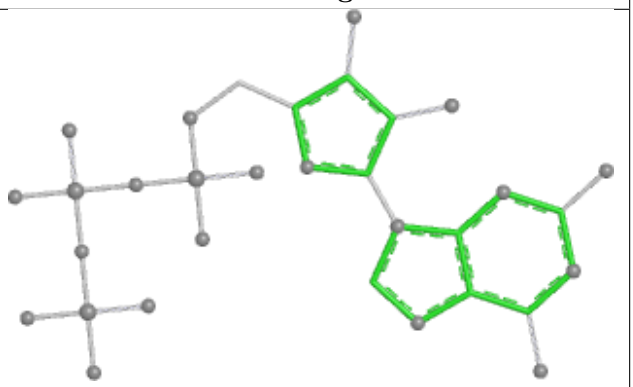
Bond lengths



Bond angles

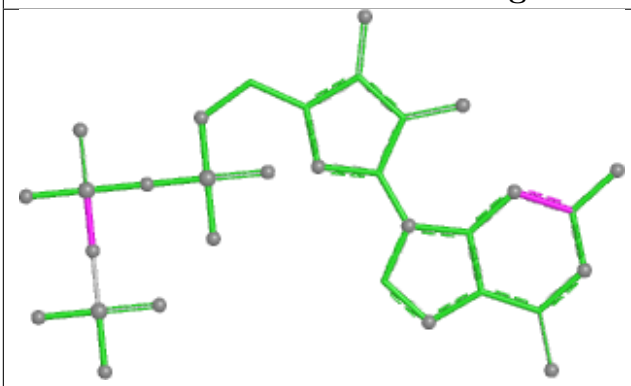


Torsions

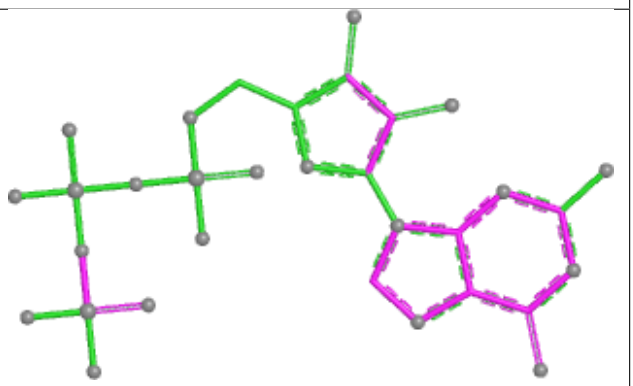


Rings

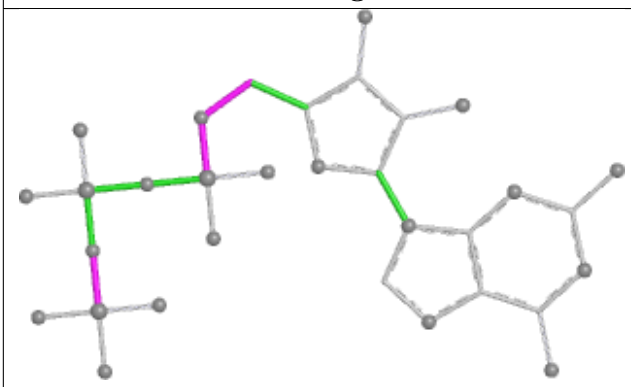
Ligand GTP HB 503



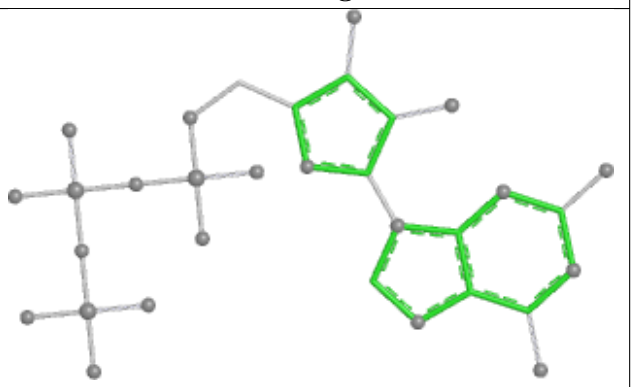
Bond lengths



Bond angles

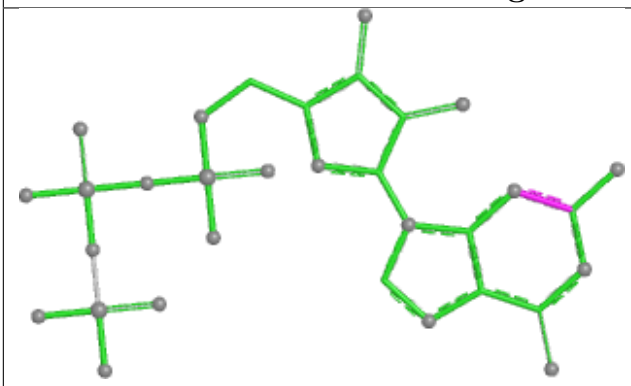


Torsions

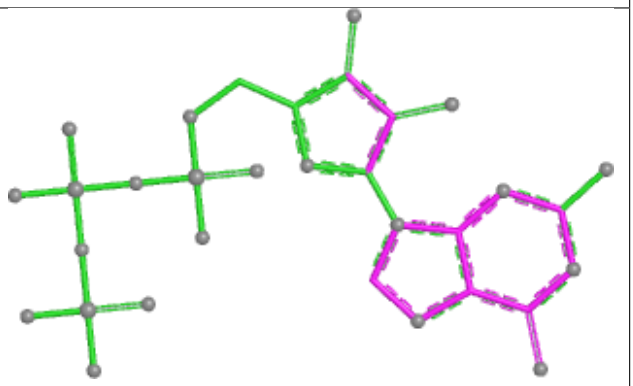


Rings

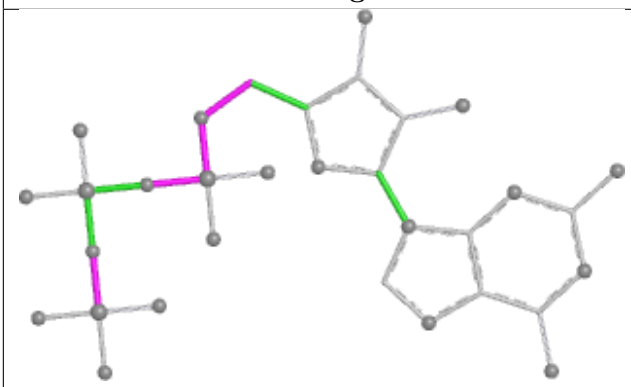
Ligand GTP NA 501



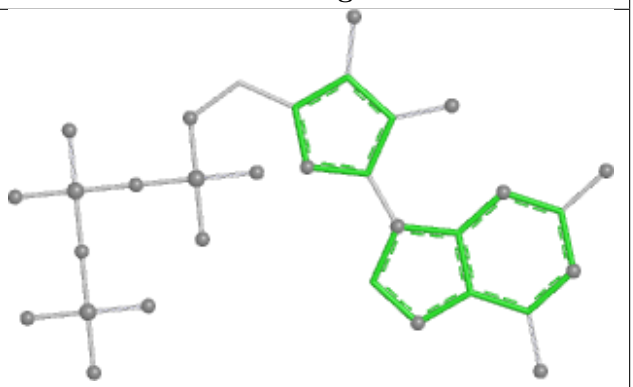
Bond lengths



Bond angles

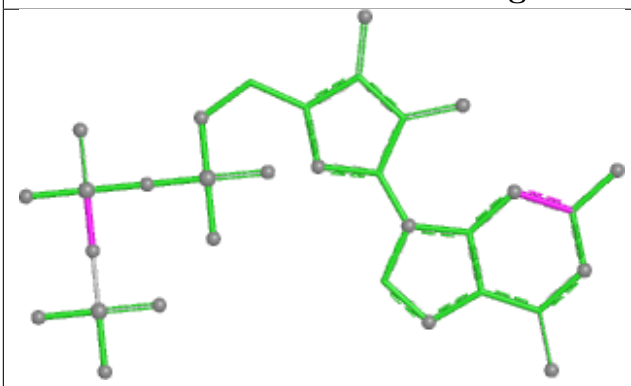


Torsions

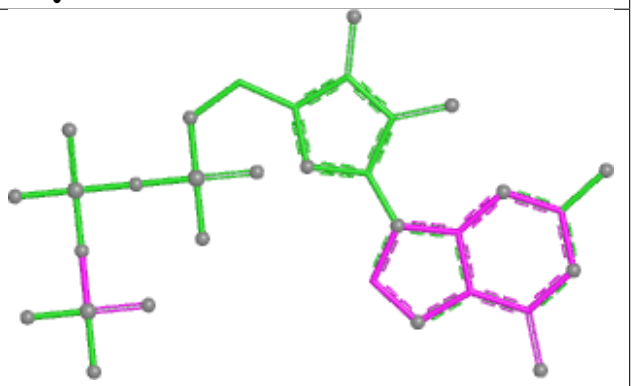


Rings

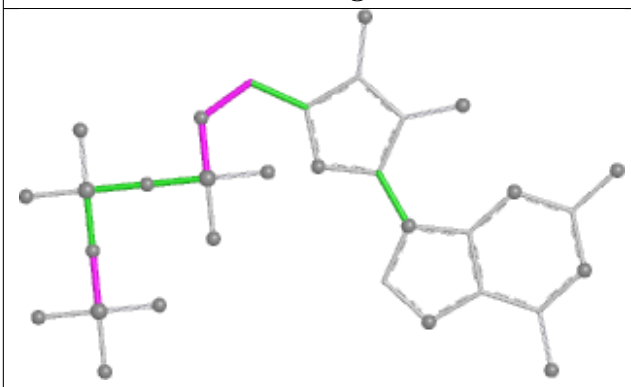
Ligand GTP QO 501



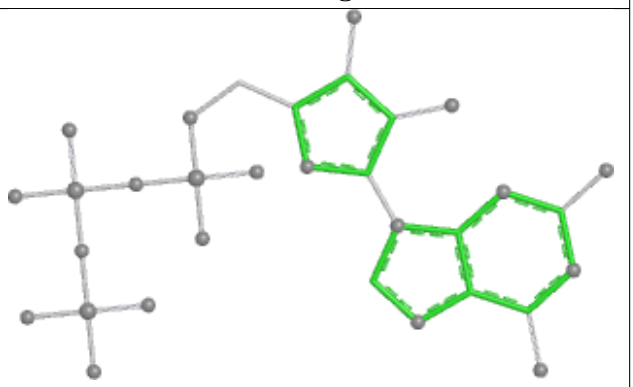
Bond lengths



Bond angles

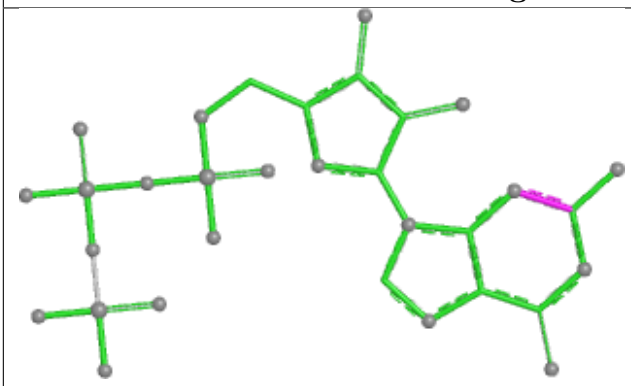


Torsions

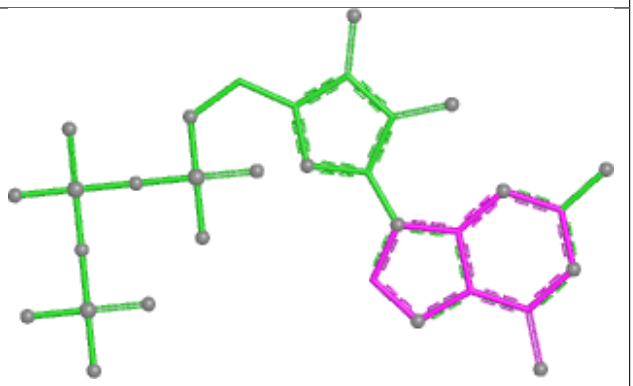


Rings

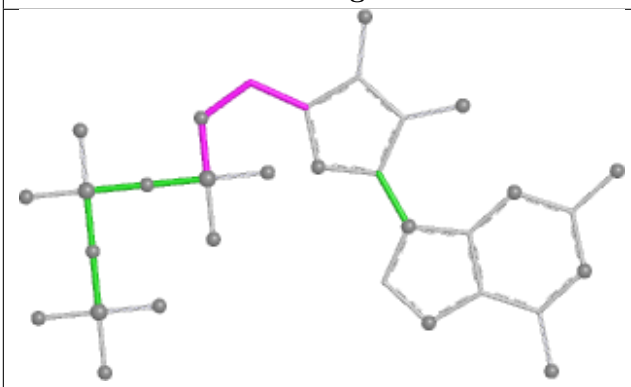
Ligand GTP PK 501



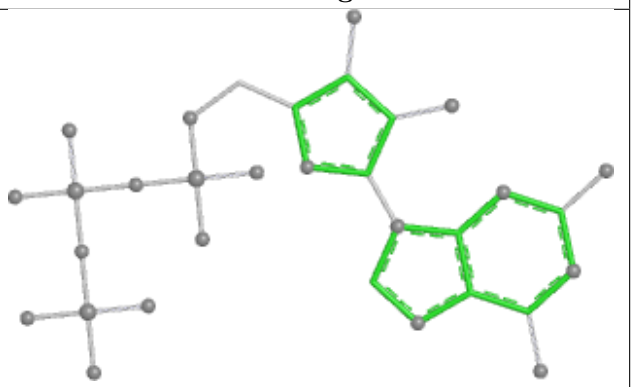
Bond lengths



Bond angles

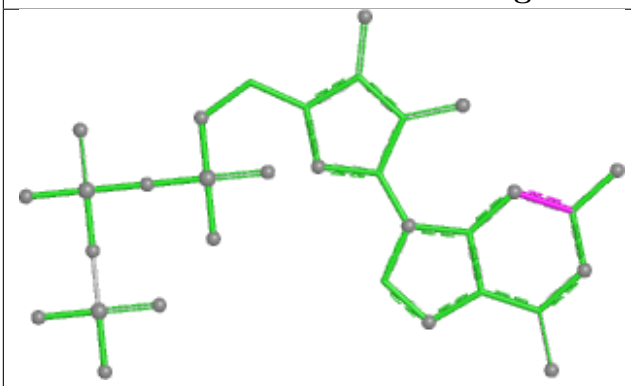


Torsions

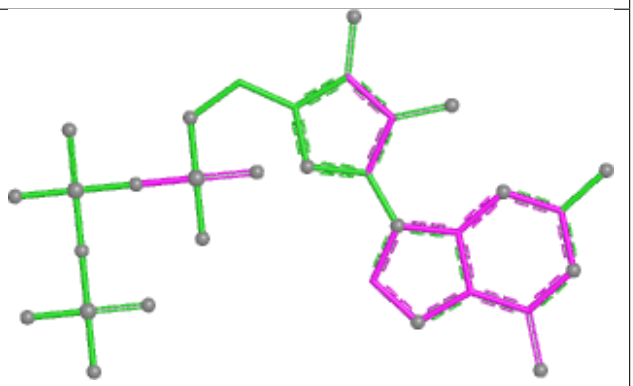


Rings

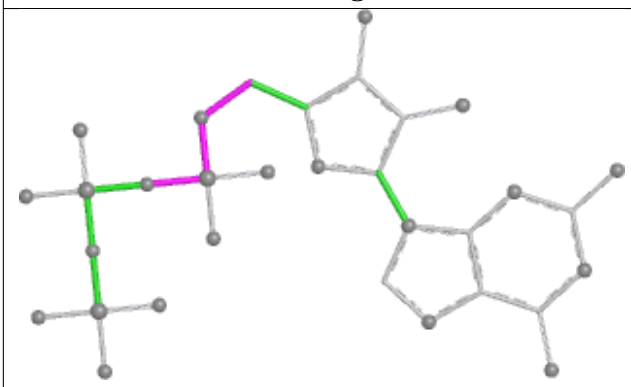
Ligand GTP SE 501



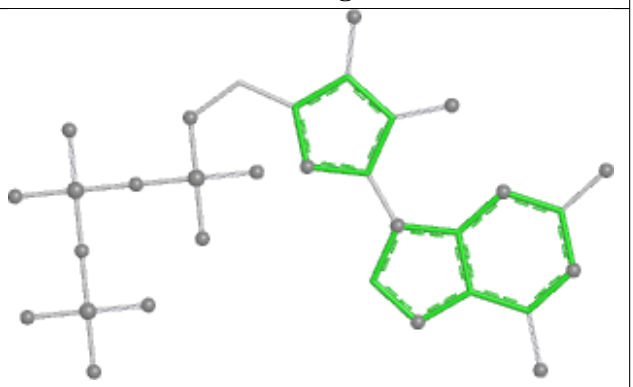
Bond lengths



Bond angles

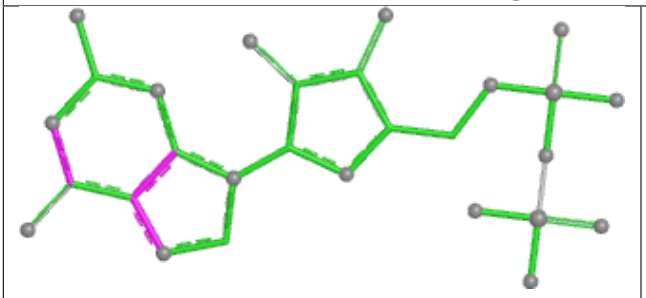


Torsions

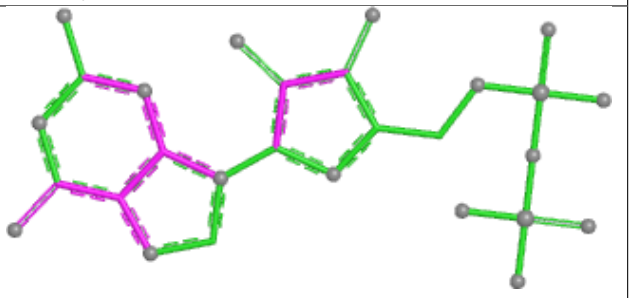


Rings

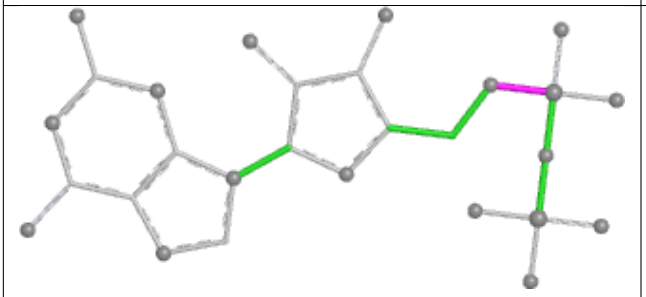
Ligand GDP KQ 500



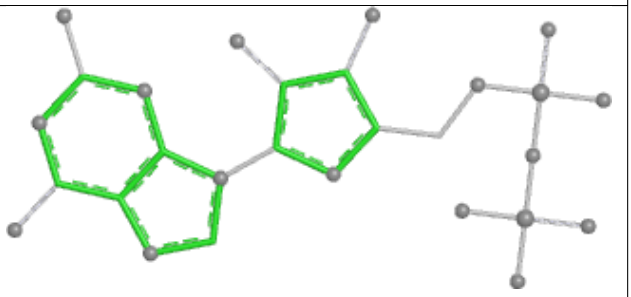
Bond lengths



Bond angles

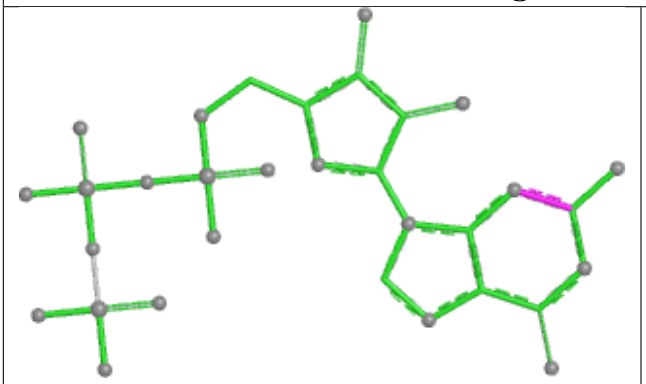


Torsions

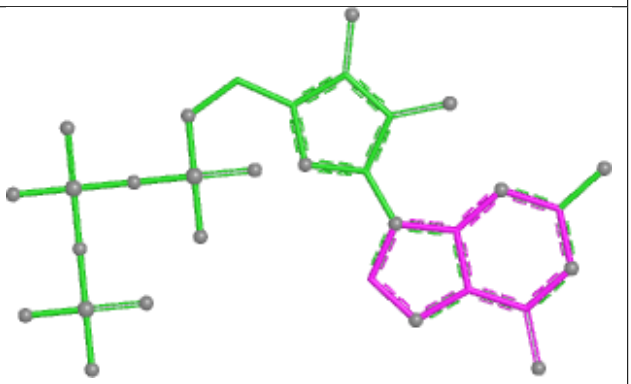


Rings

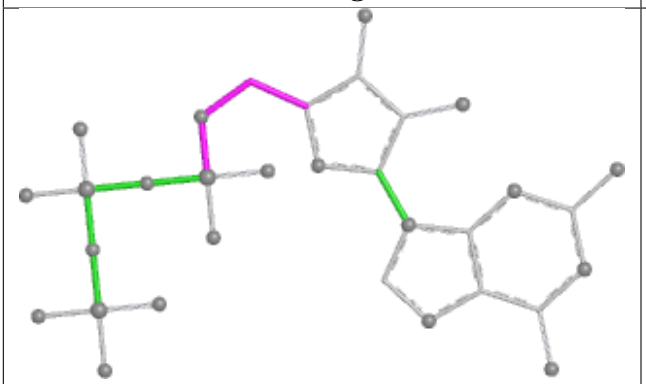
Ligand GTP FV 503



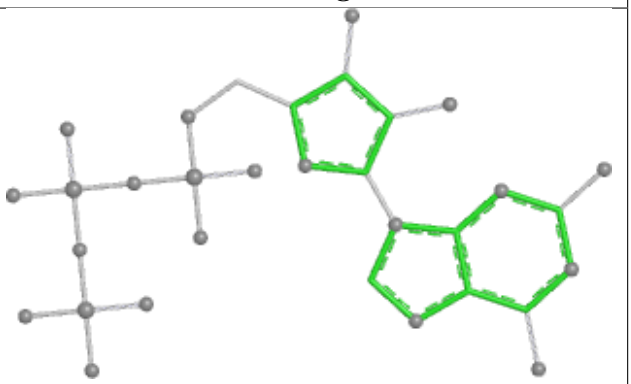
Bond lengths



Bond angles

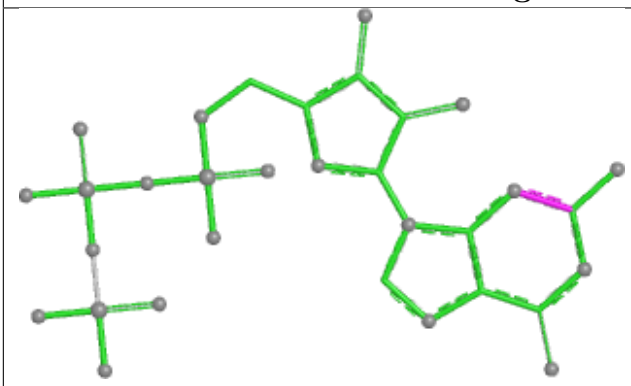


Torsions

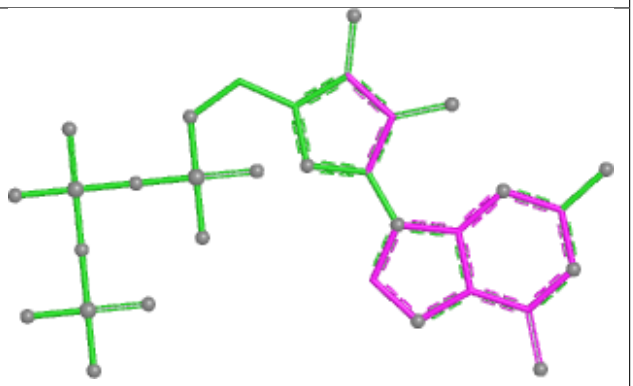


Rings

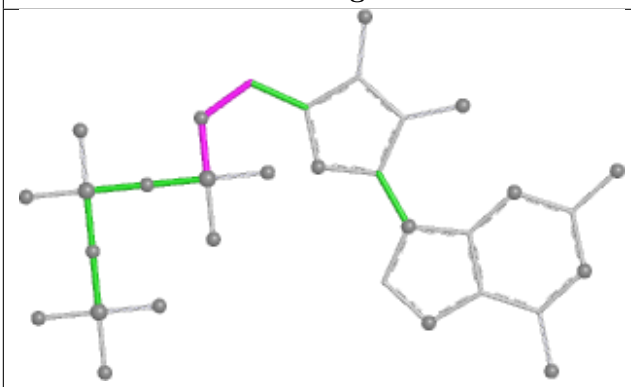
Ligand GTP LF 502



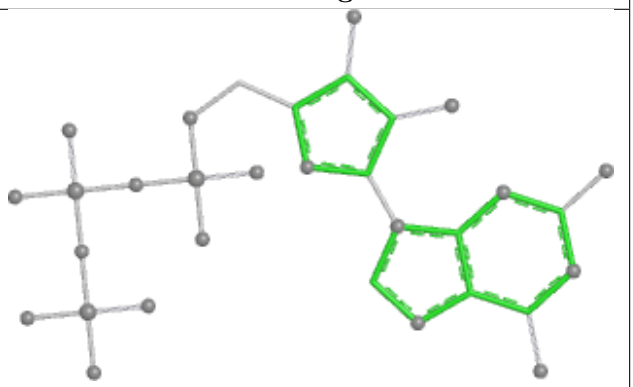
Bond lengths



Bond angles

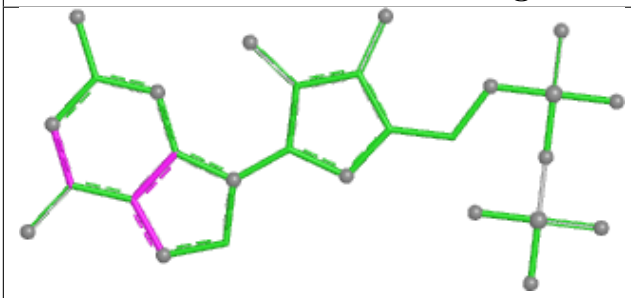


Torsions

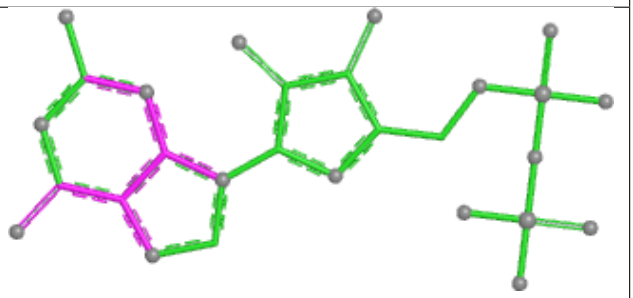


Rings

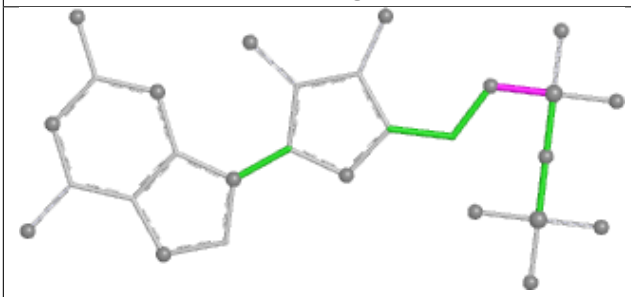
Ligand GDP TJ 500



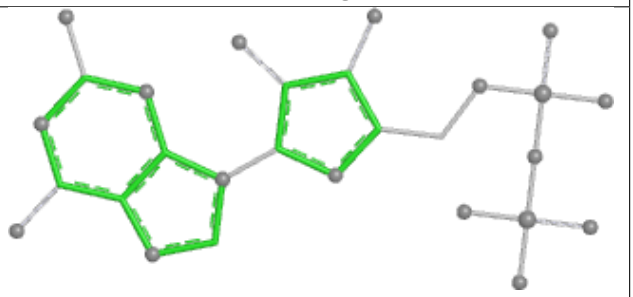
Bond lengths



Bond angles

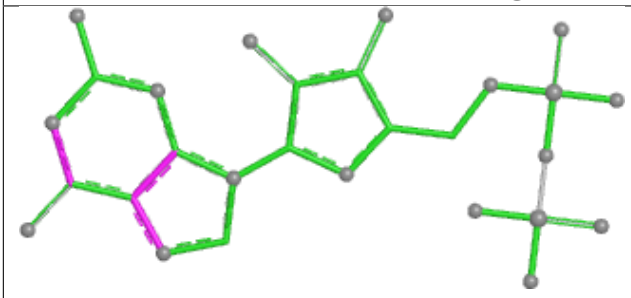


Torsions

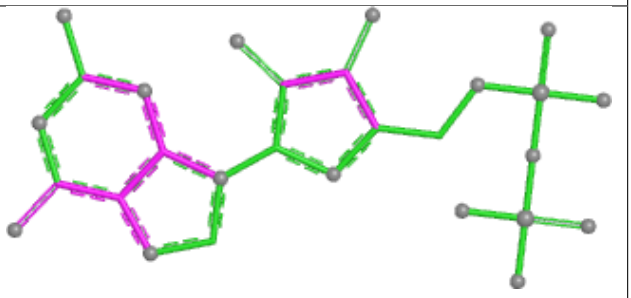


Rings

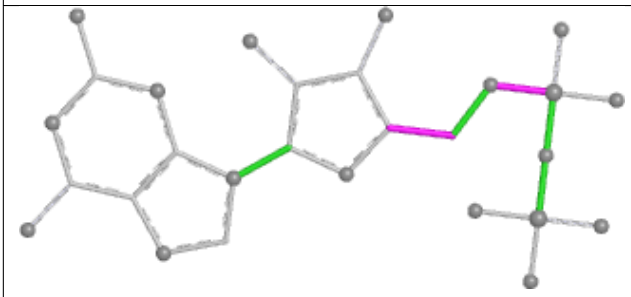
Ligand GDP BR 500



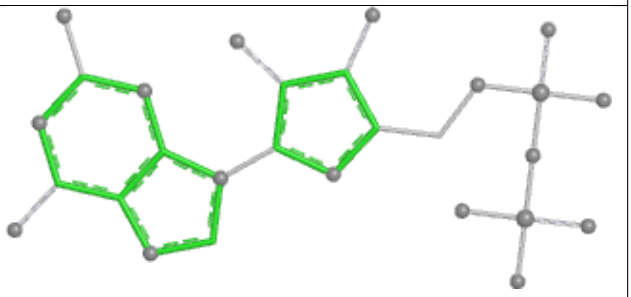
Bond lengths



Bond angles

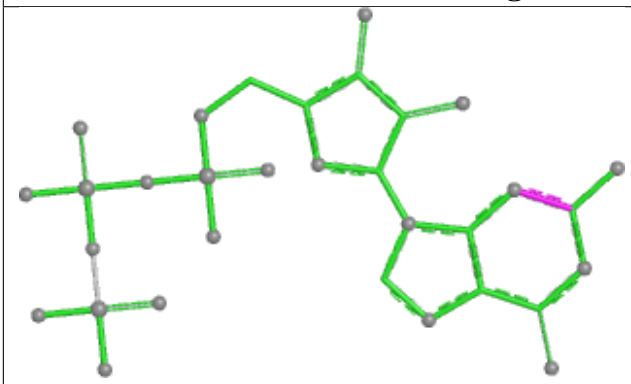


Torsions

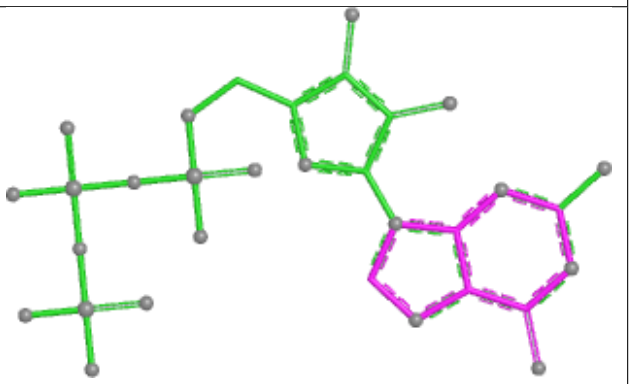


Rings

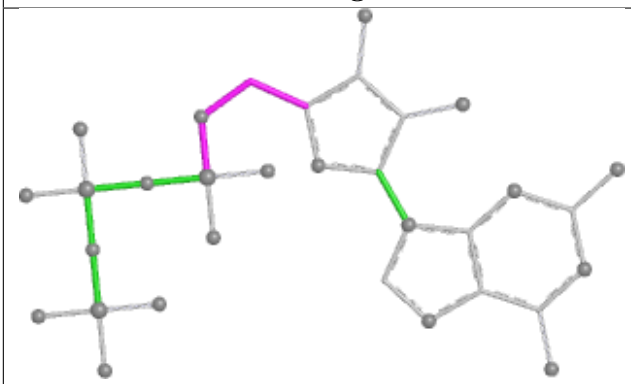
Ligand GTP MC 501



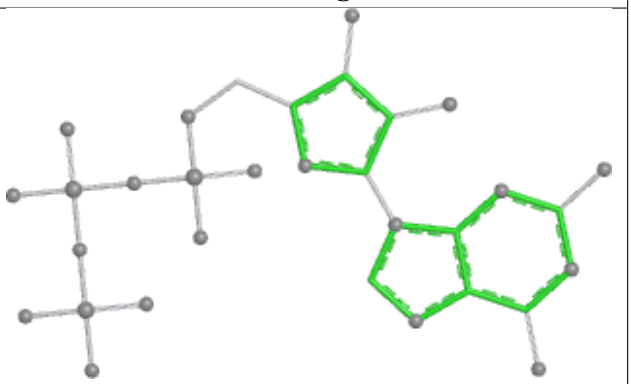
Bond lengths



Bond angles

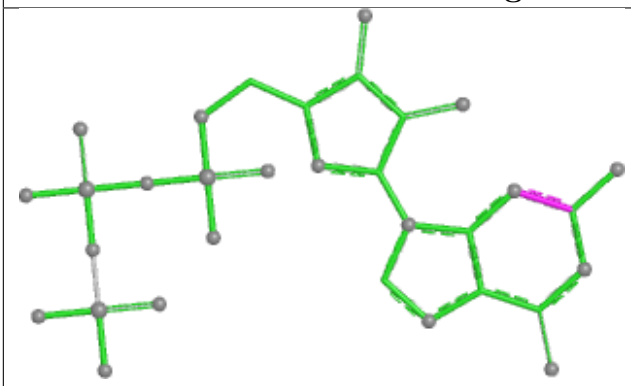


Torsions

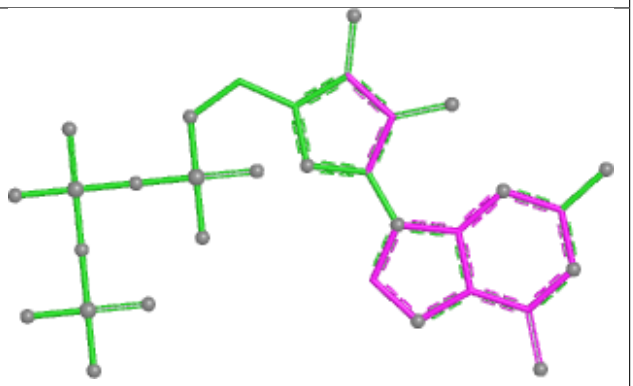


Rings

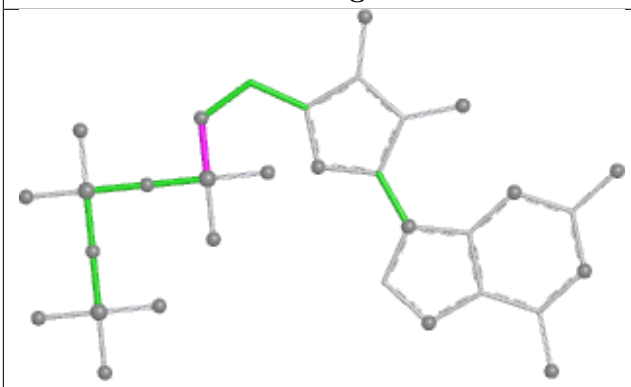
Ligand GTP WC 501



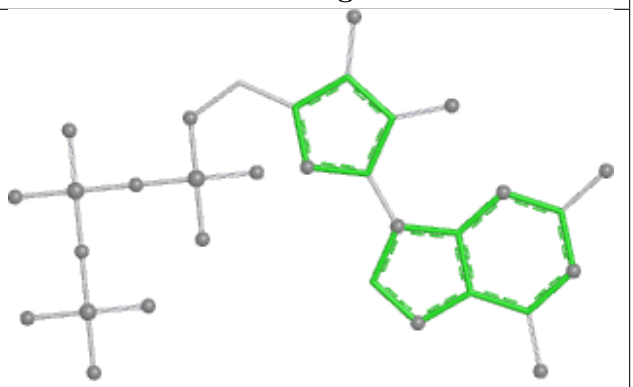
Bond lengths



Bond angles

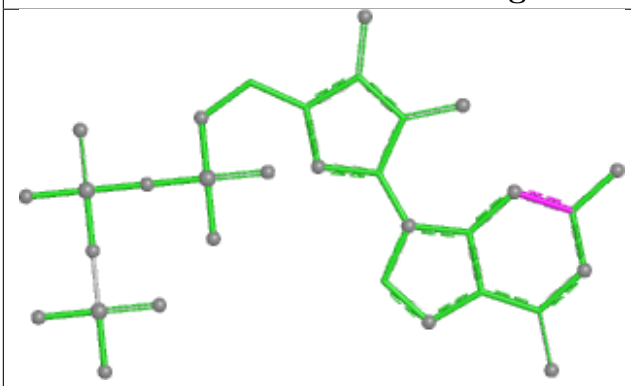


Torsions

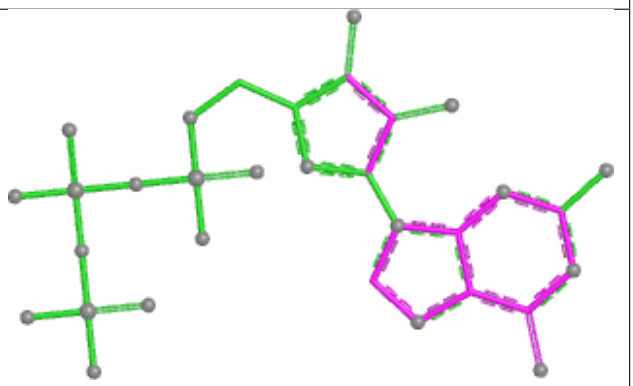


Rings

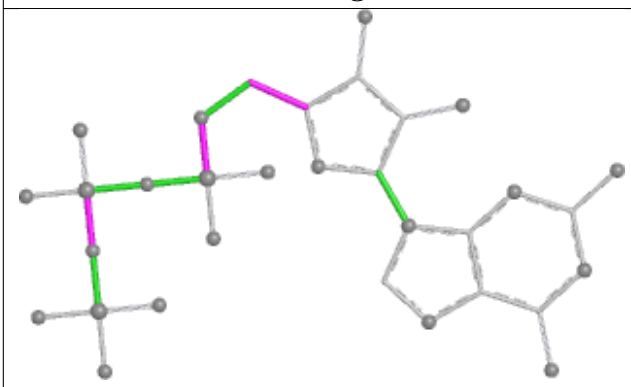
Ligand GTP MS 501



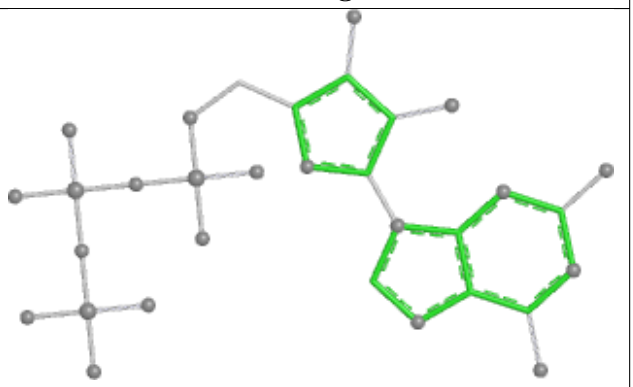
Bond lengths



Bond angles

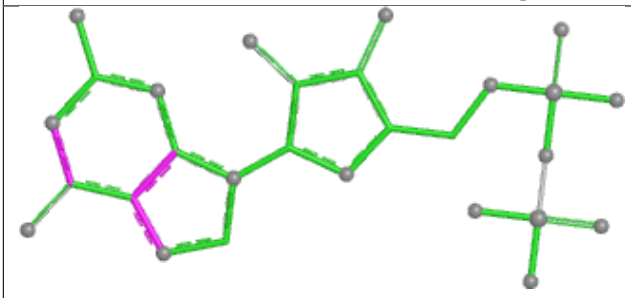


Torsions

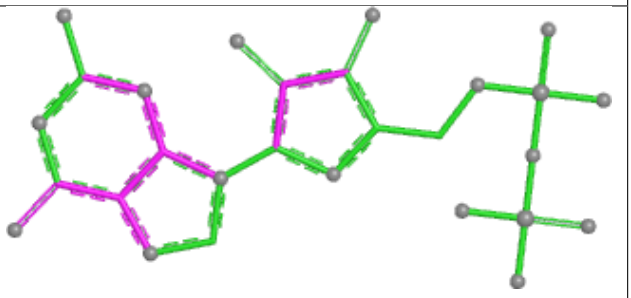


Rings

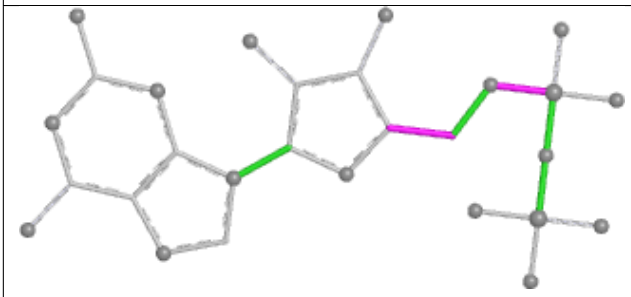
Ligand GDP IR 500



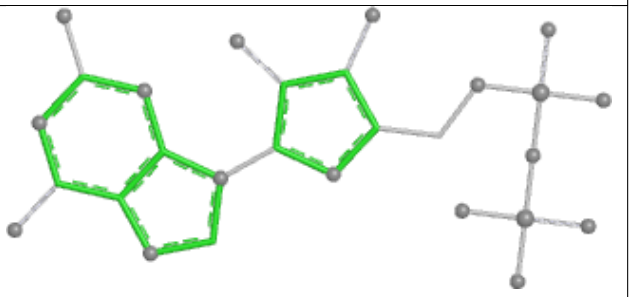
Bond lengths



Bond angles

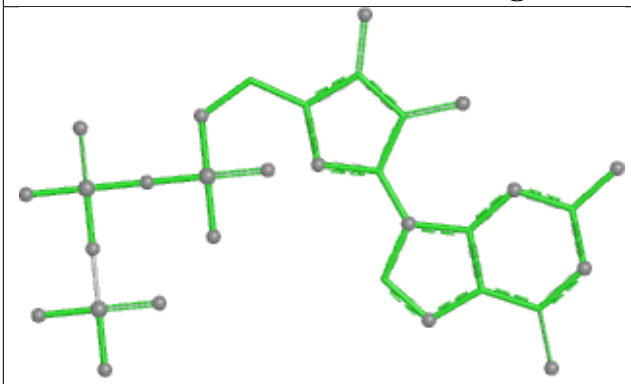


Torsions

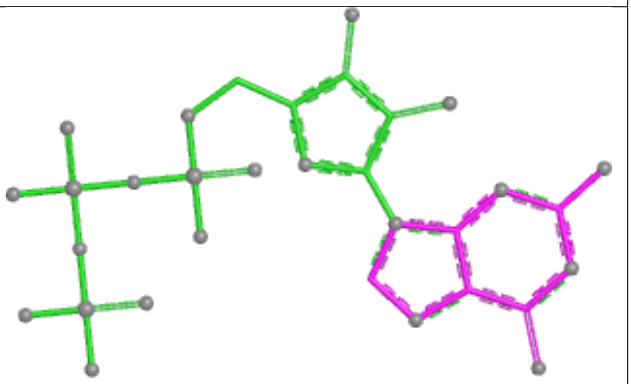


Rings

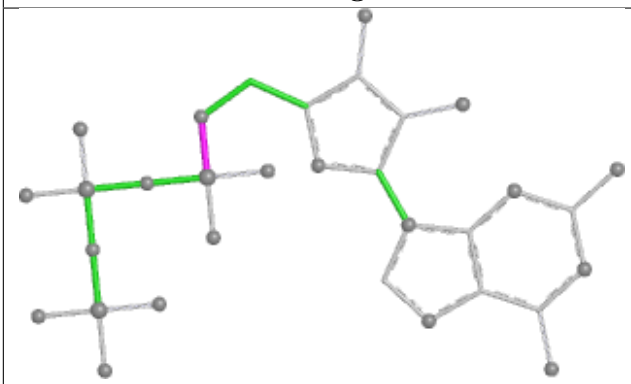
Ligand GTP DD 501



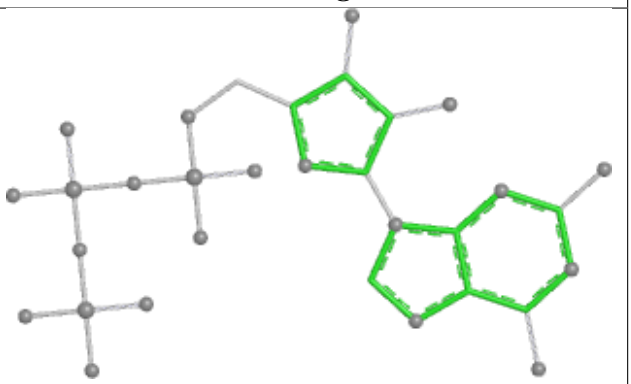
Bond lengths



Bond angles

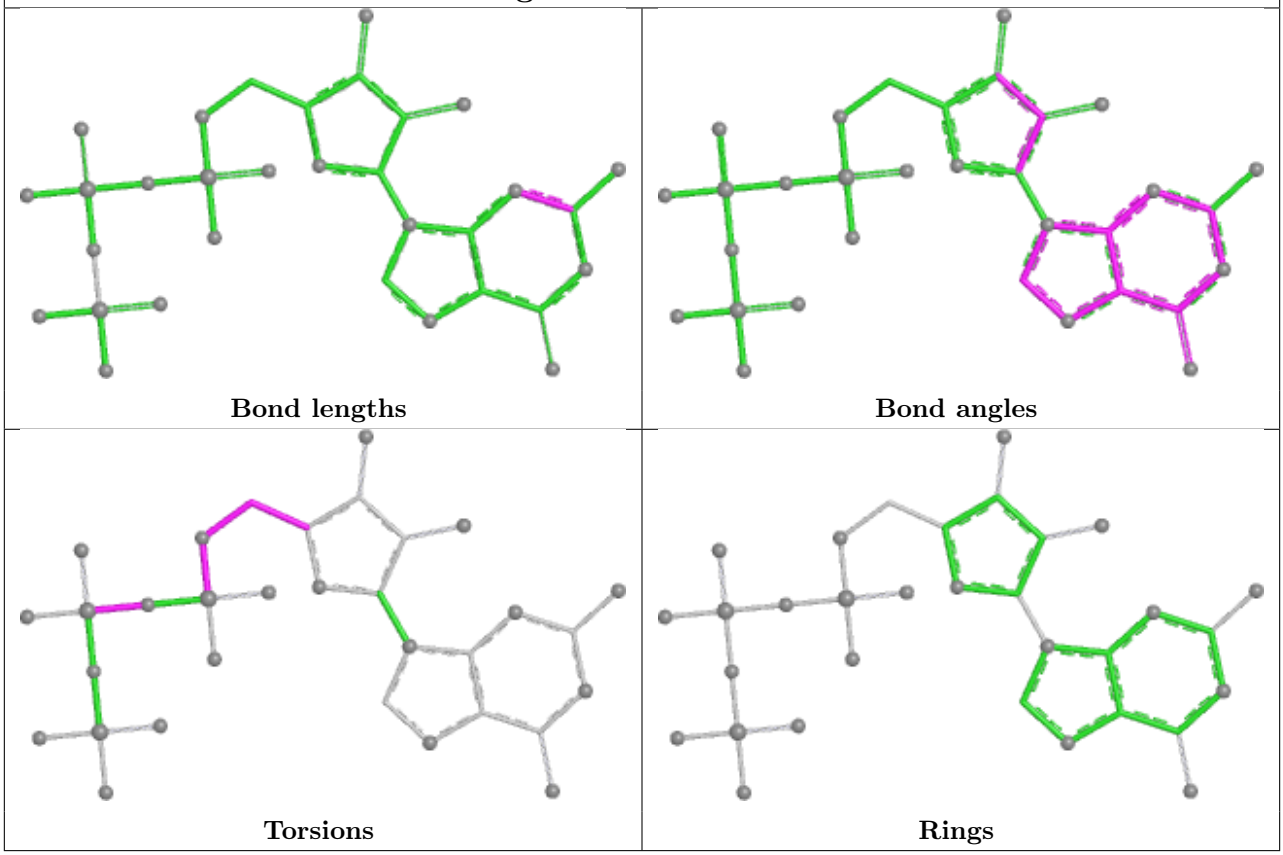


Torsions

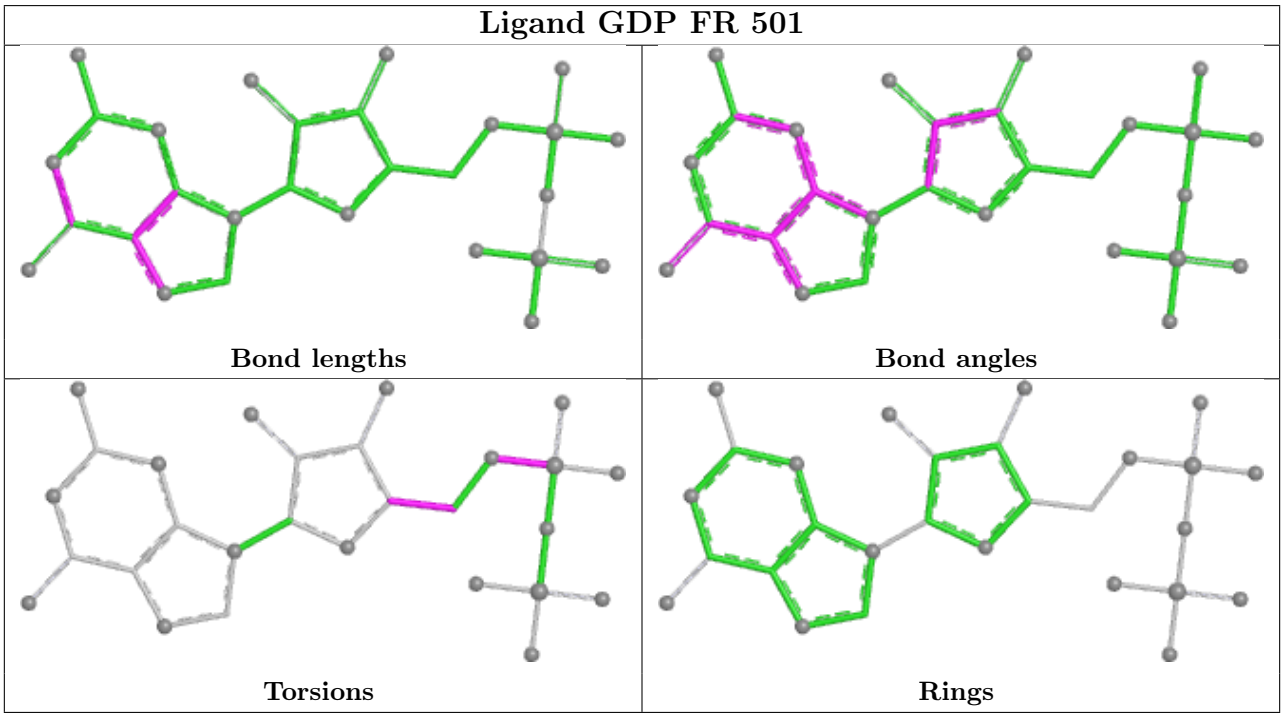


Rings

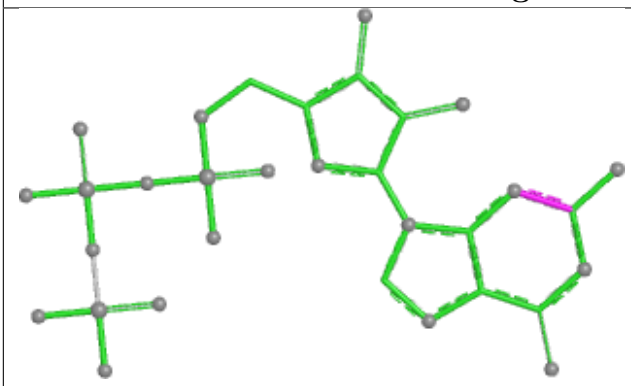
Ligand GTP IG 501



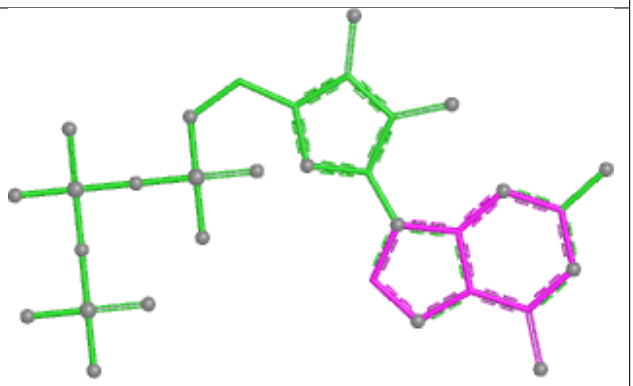
Ligand GDP FR 501



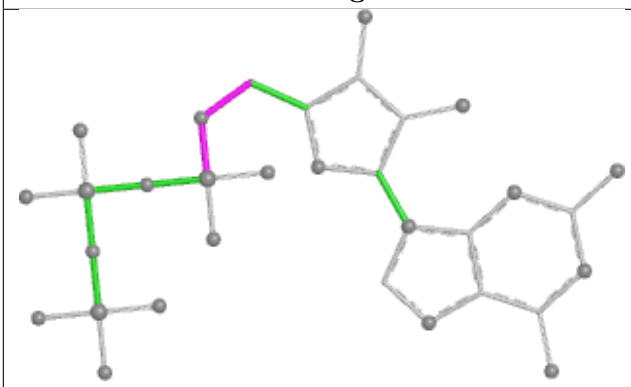
Ligand GTP SU 501



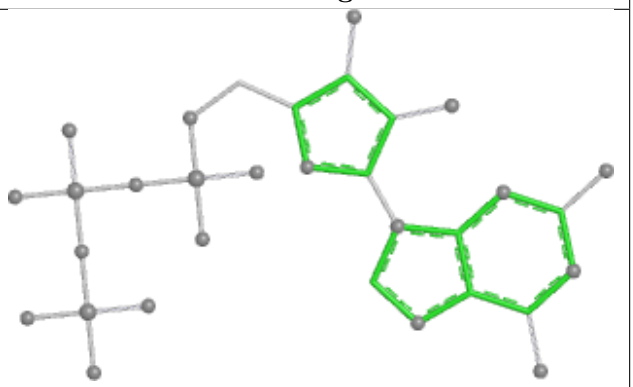
Bond lengths



Bond angles

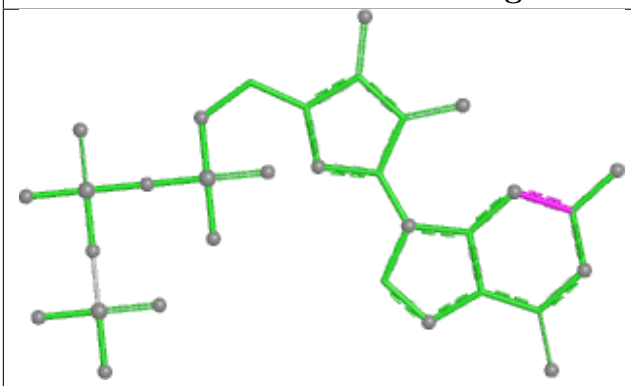


Torsions

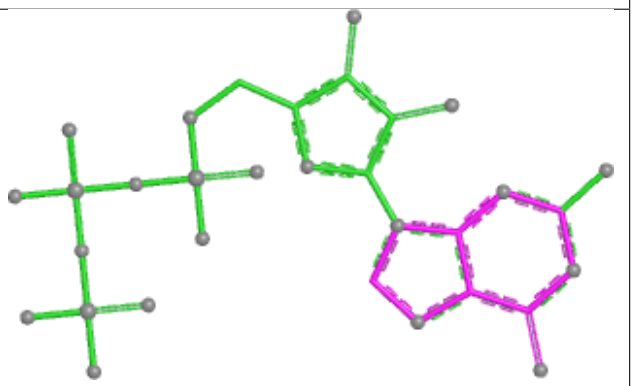


Rings

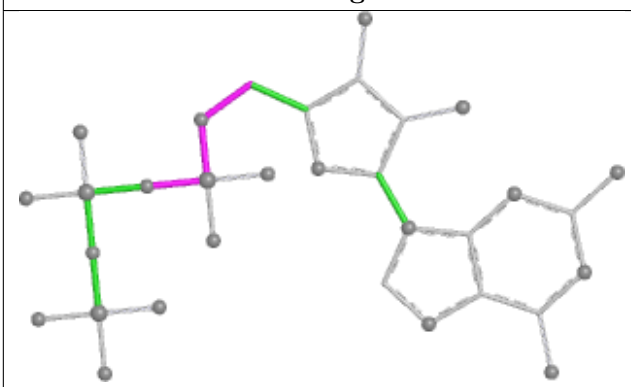
Ligand GTP NM 501



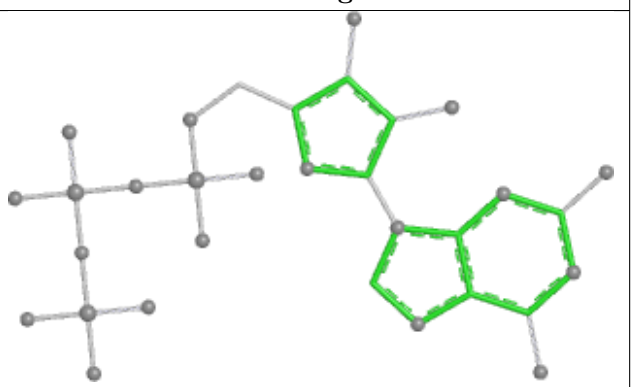
Bond lengths



Bond angles

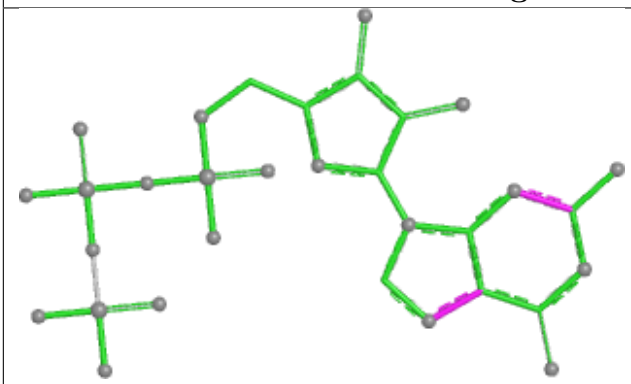


Torsions

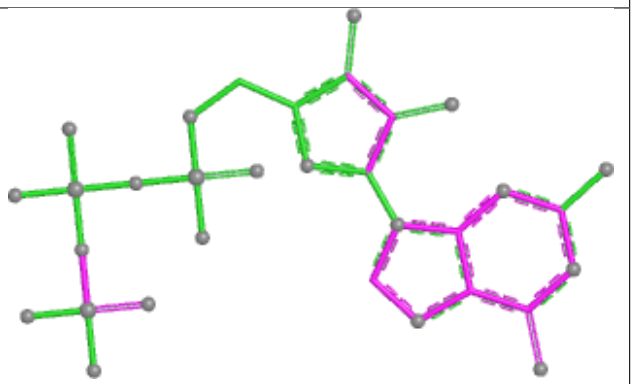


Rings

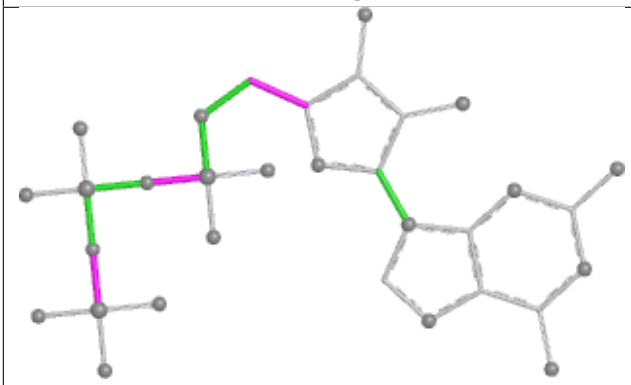
Ligand GTP CT 501



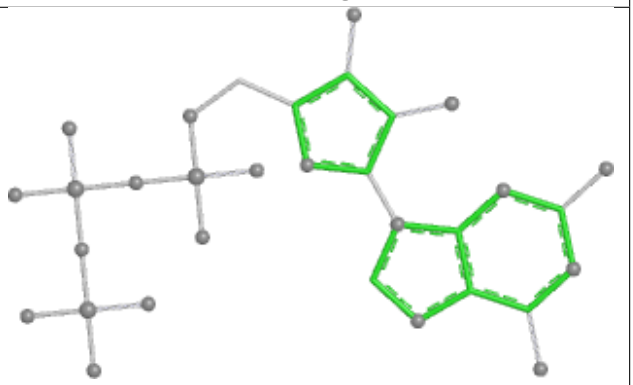
Bond lengths



Bond angles

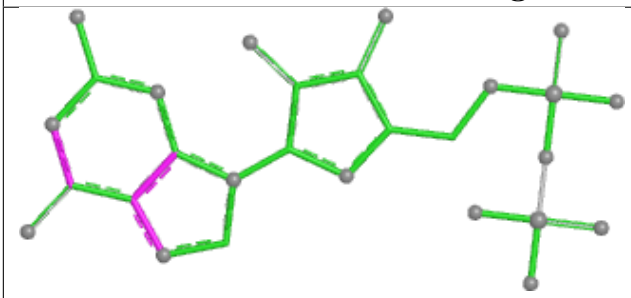


Torsions

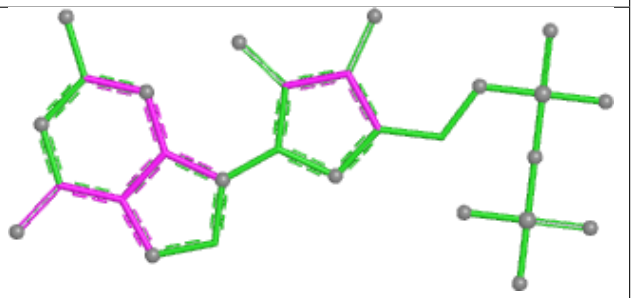


Rings

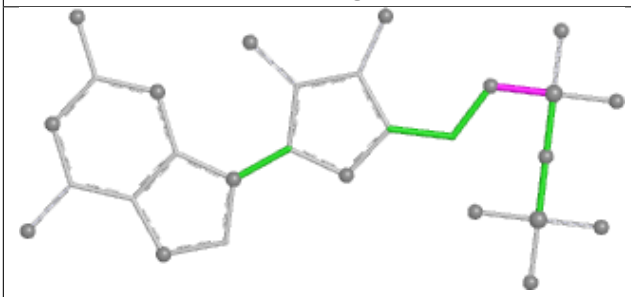
Ligand GDP BP 500



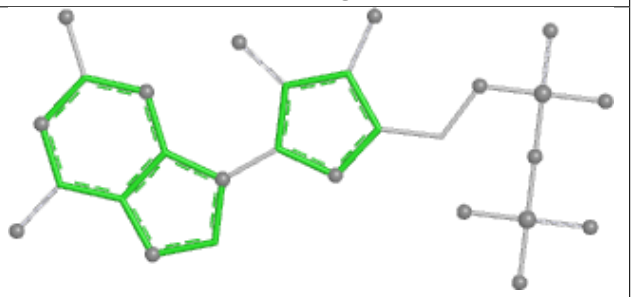
Bond lengths



Bond angles

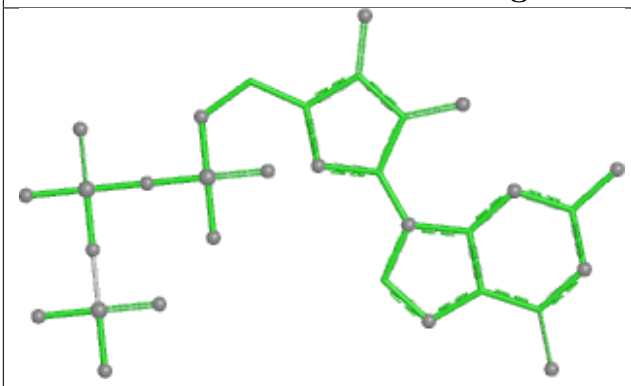


Torsions

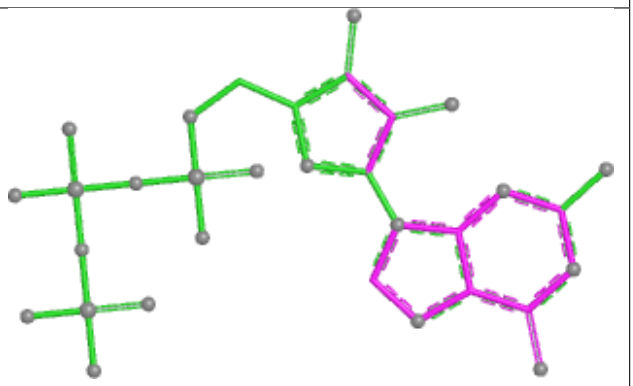


Rings

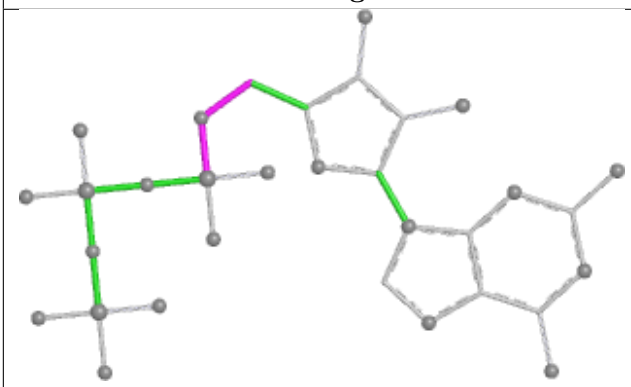
Ligand GTP EO 501



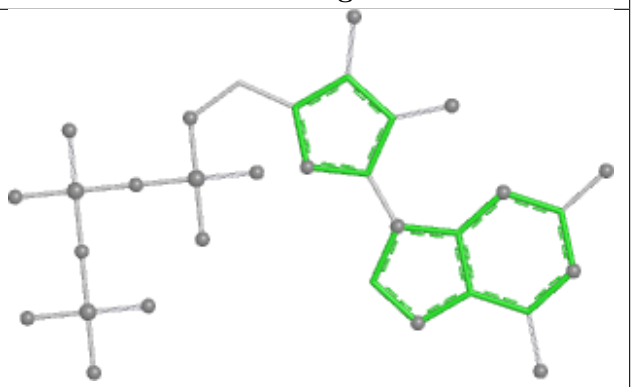
Bond lengths



Bond angles

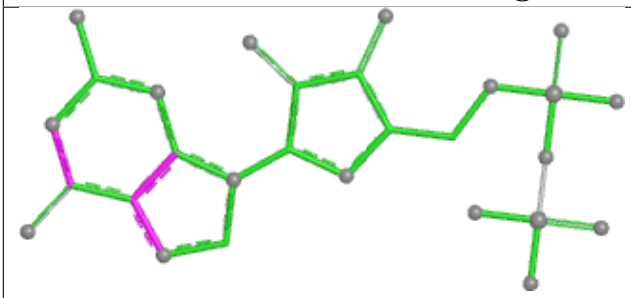


Torsions

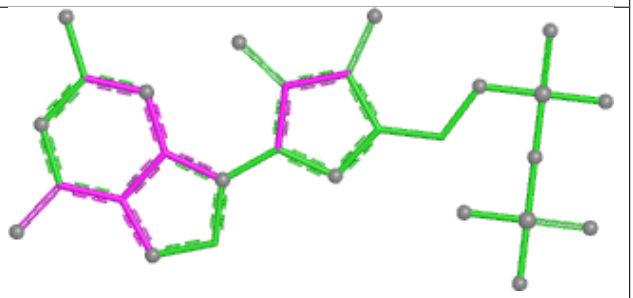


Rings

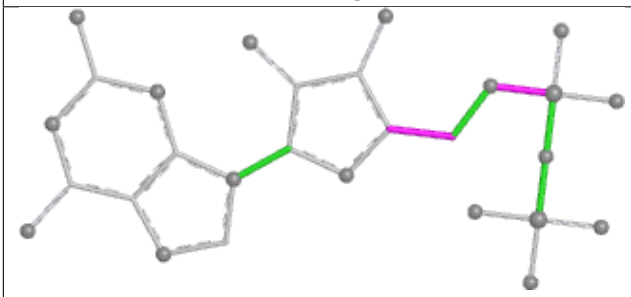
Ligand GDP KI 500



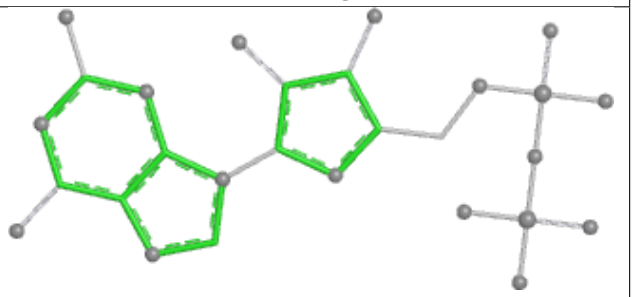
Bond lengths



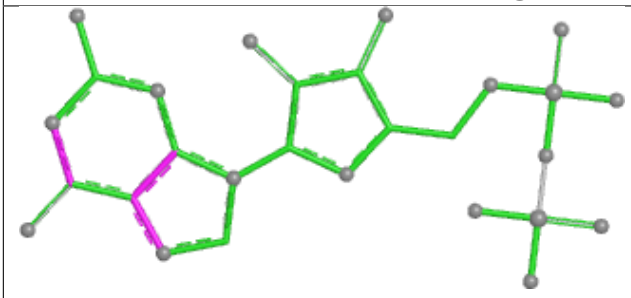
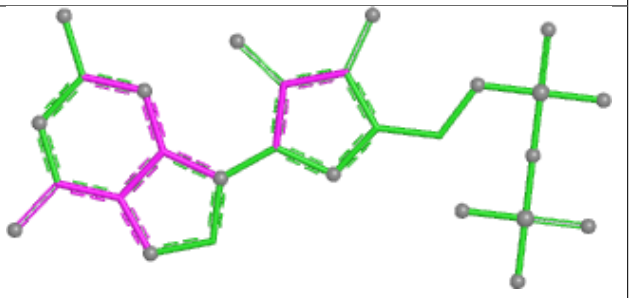
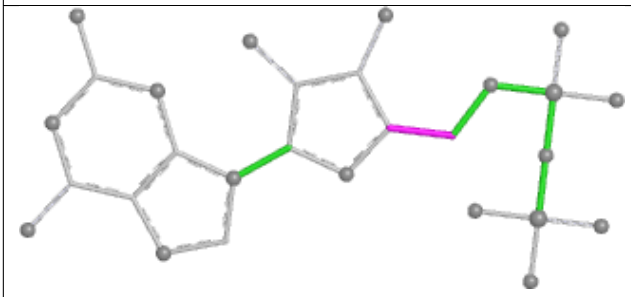
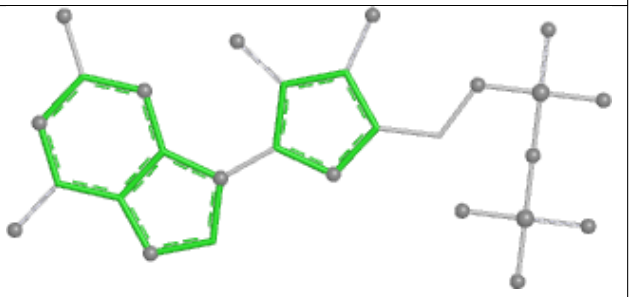
Bond angles

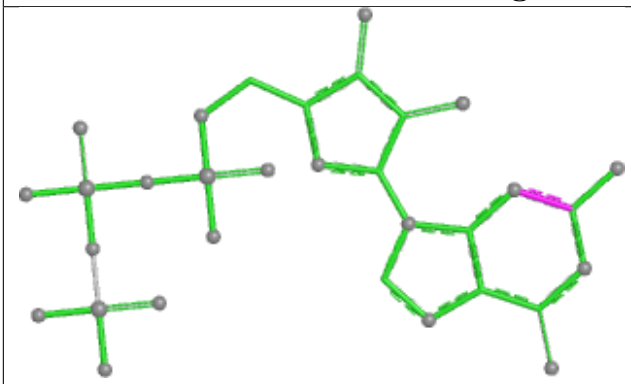
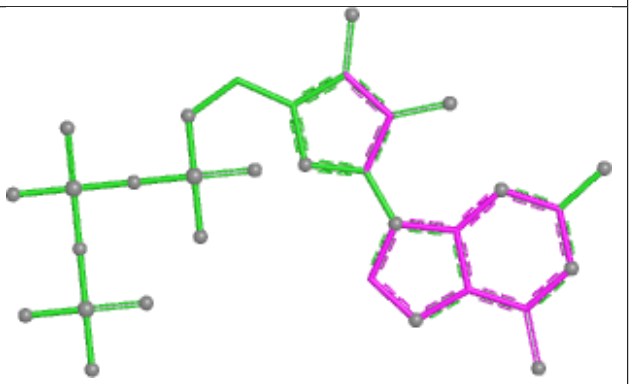
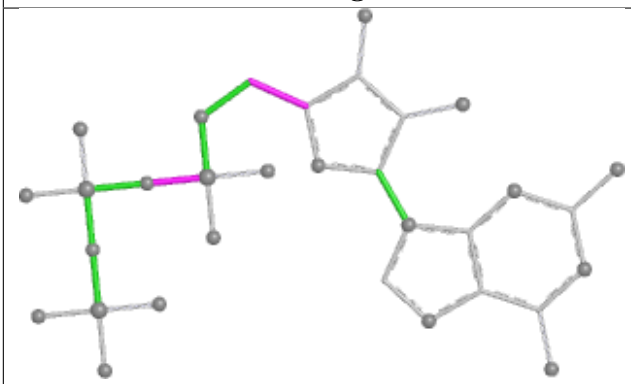
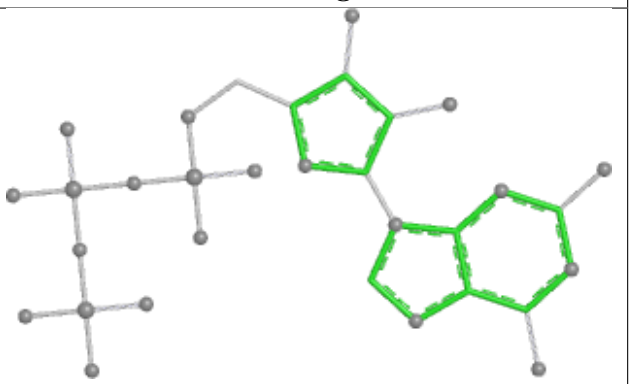


Torsions

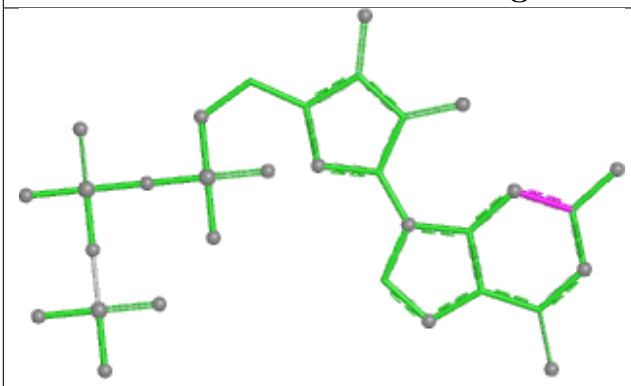


Rings

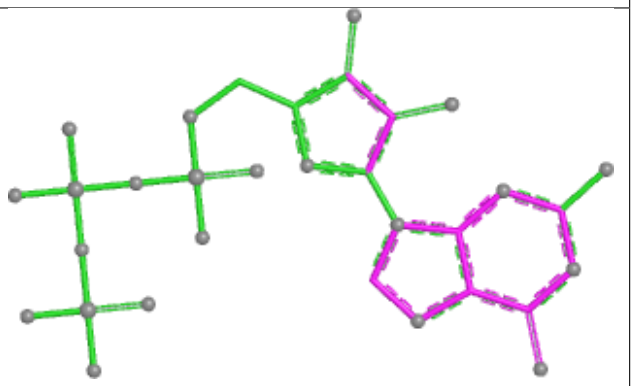
Ligand GDP JG 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP LH 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

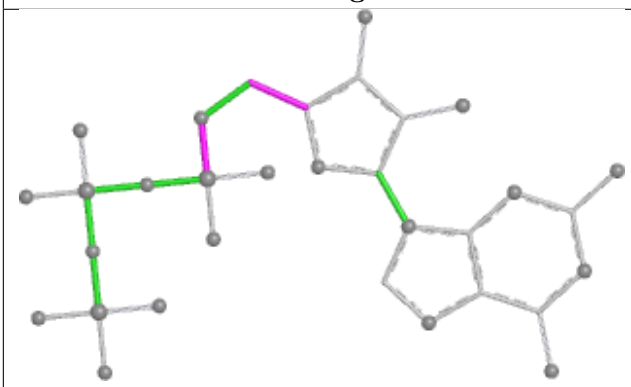
Ligand GTP VA 501



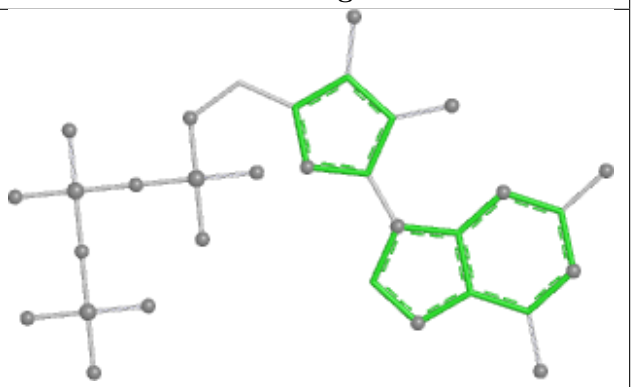
Bond lengths



Bond angles

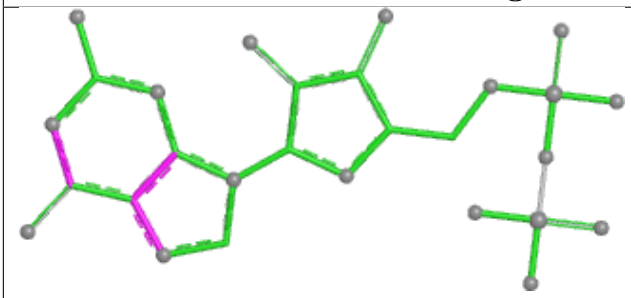


Torsions

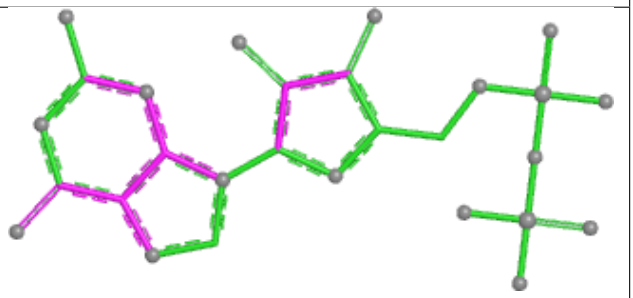


Rings

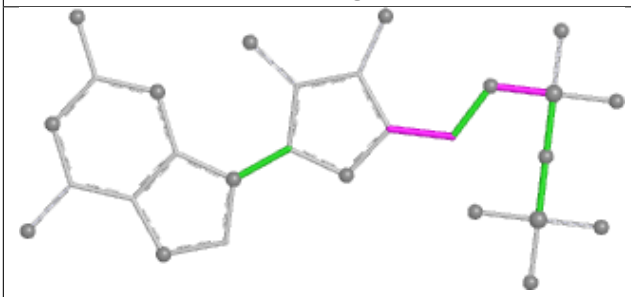
Ligand GDP HD 501



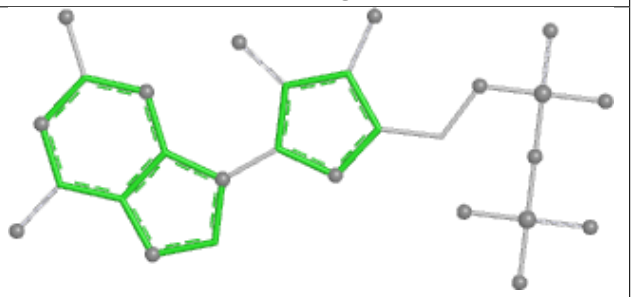
Bond lengths



Bond angles

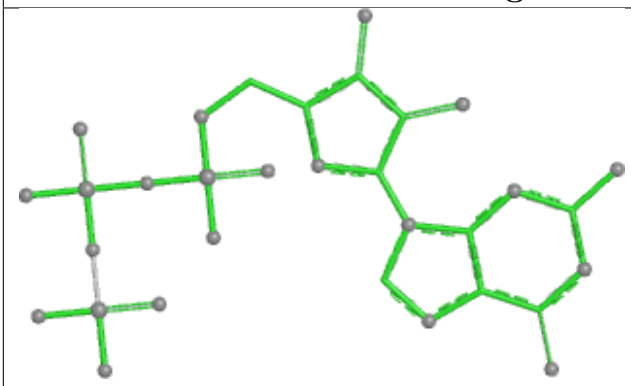


Torsions

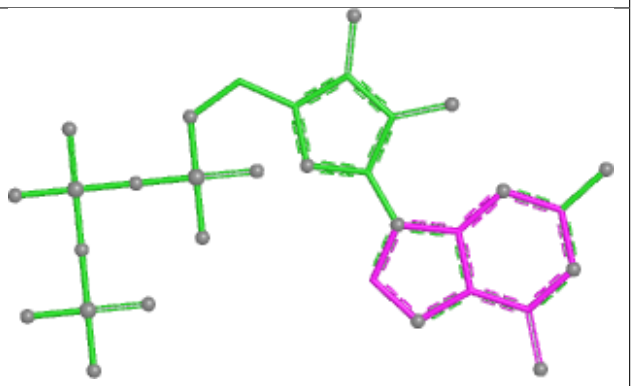


Rings

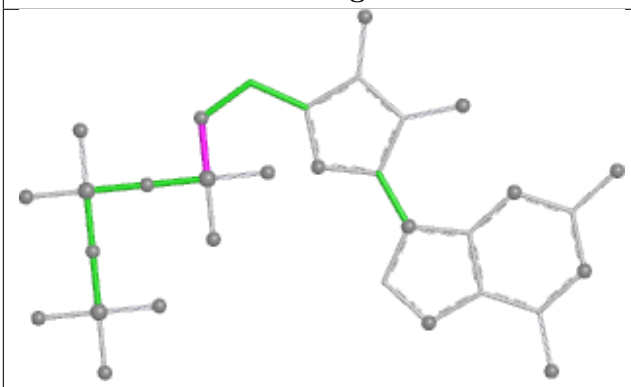
Ligand GTP BM 501



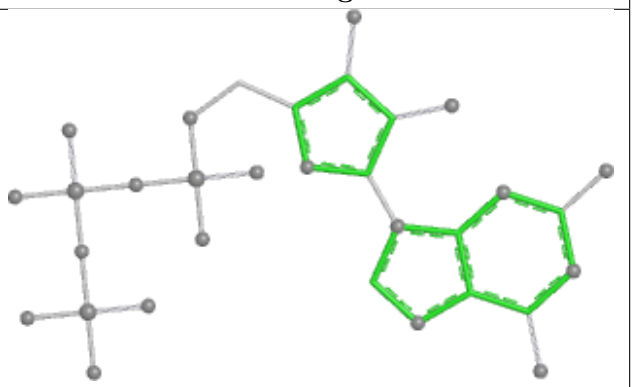
Bond lengths



Bond angles

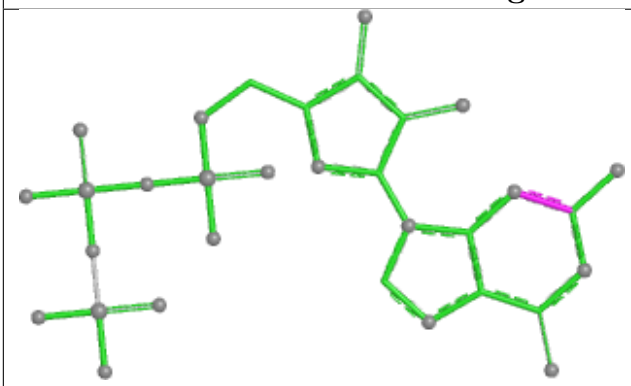


Torsions

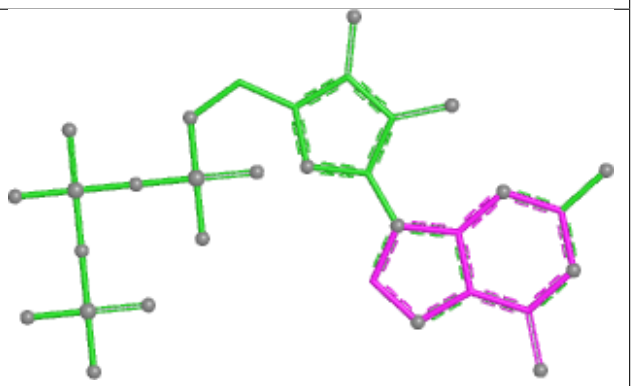


Rings

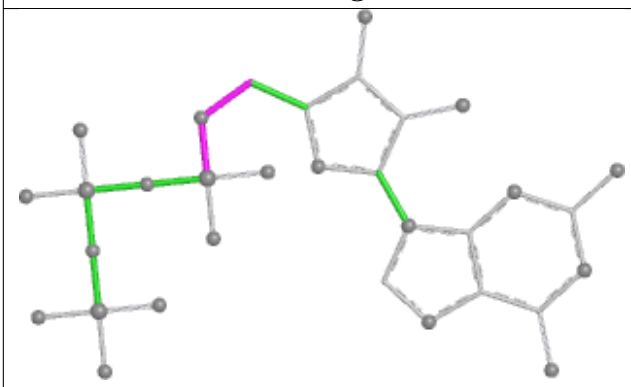
Ligand GTP HG 501



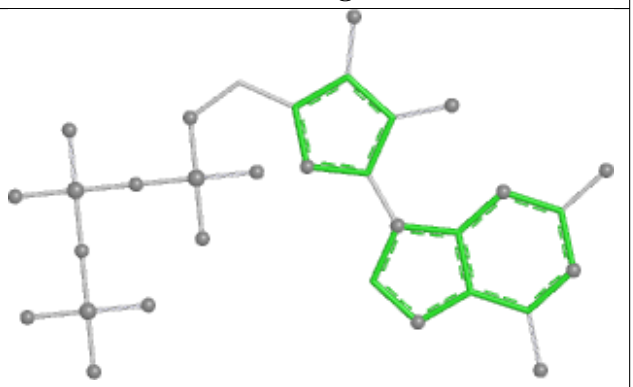
Bond lengths



Bond angles

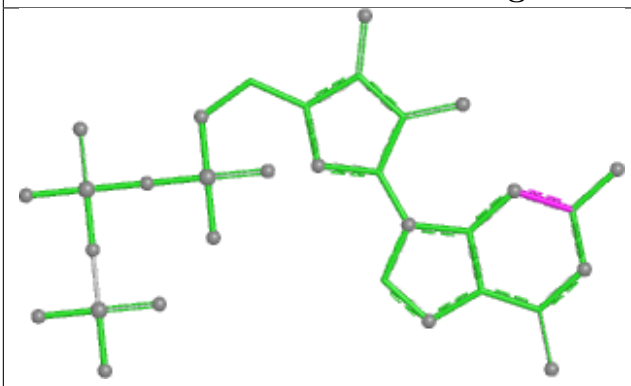


Torsions

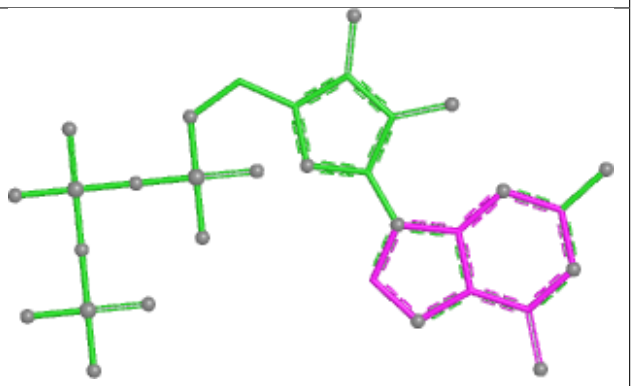


Rings

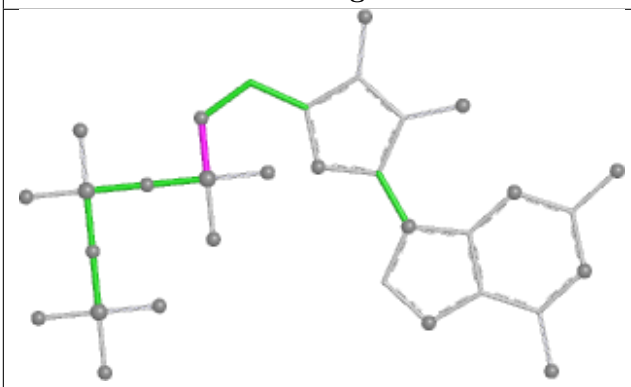
Ligand GTP AK 501



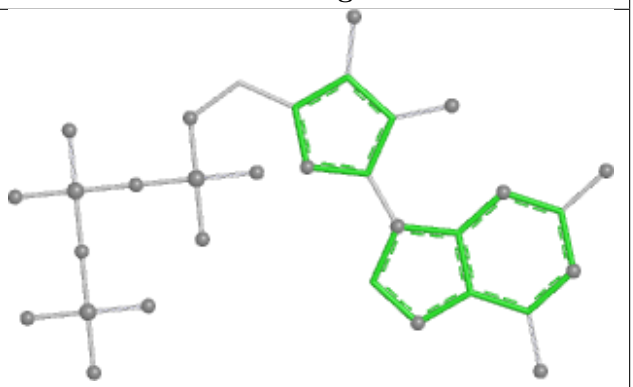
Bond lengths



Bond angles

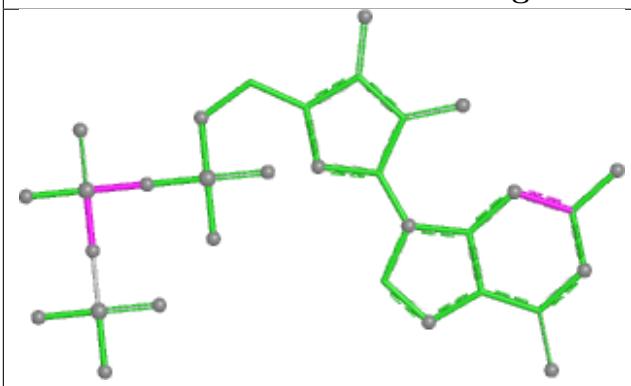


Torsions

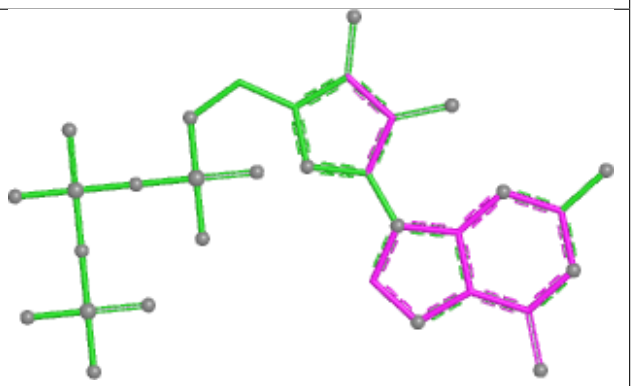


Rings

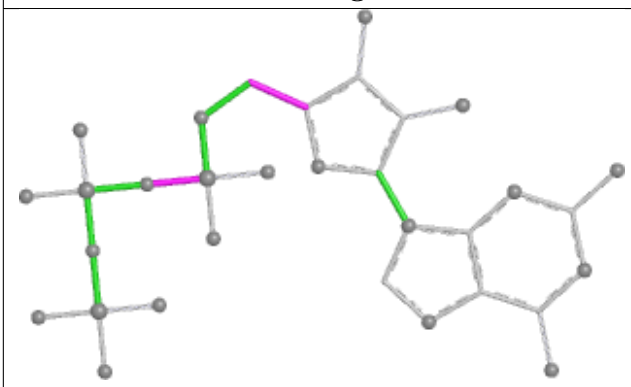
Ligand GTP VS 501



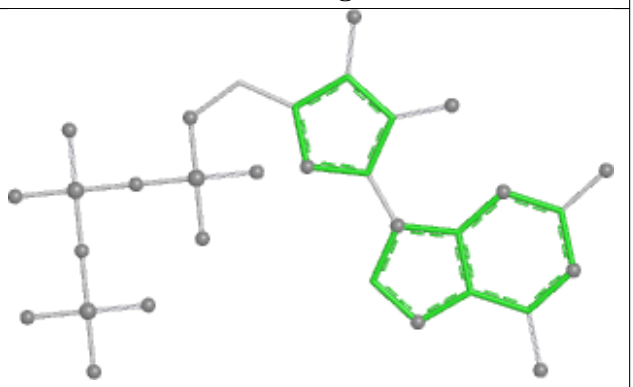
Bond lengths



Bond angles

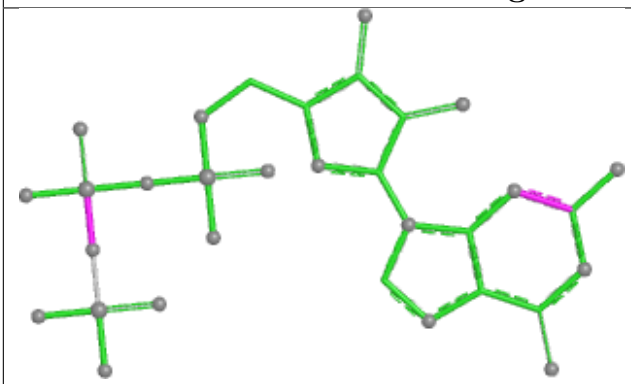


Torsions

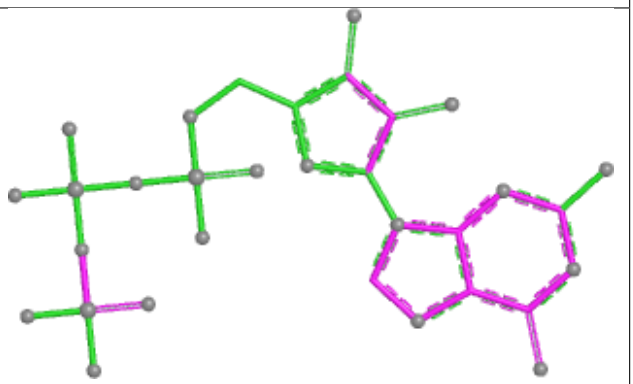


Rings

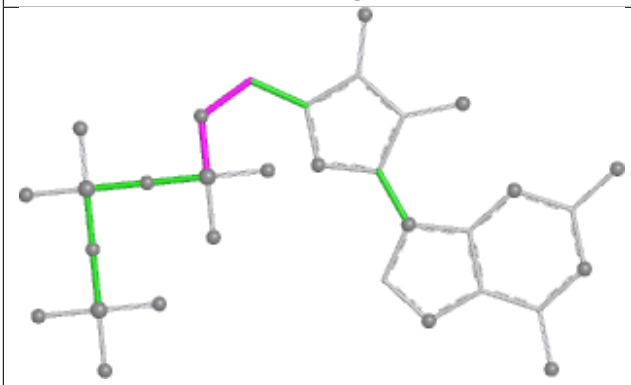
Ligand GTP OD 503



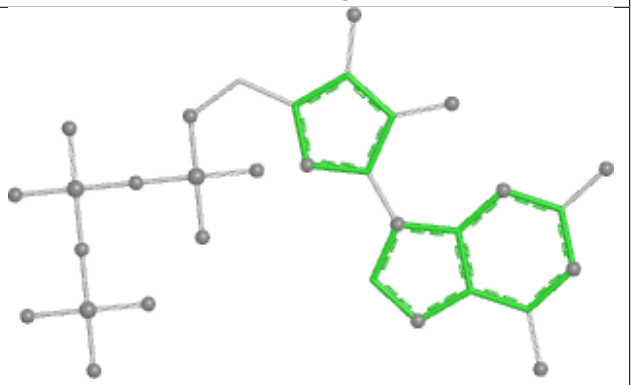
Bond lengths



Bond angles

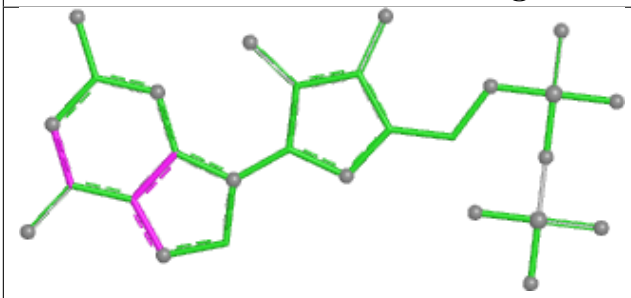


Torsions

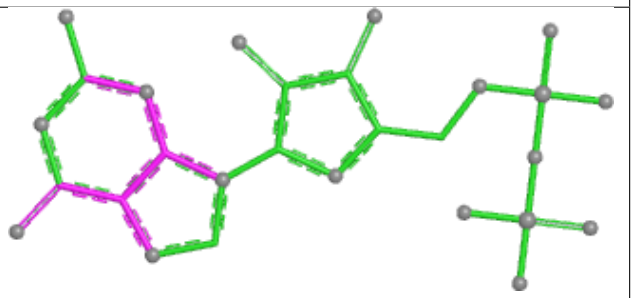


Rings

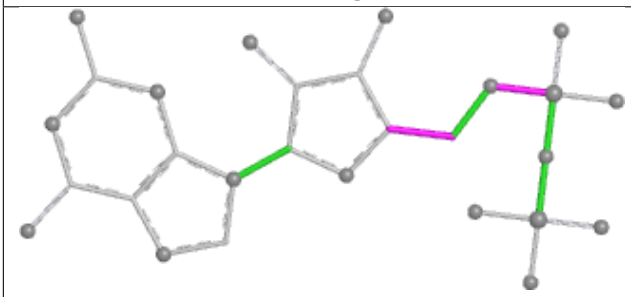
Ligand GDP SD 500



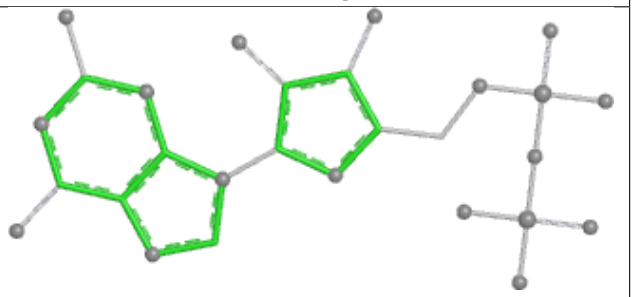
Bond lengths



Bond angles

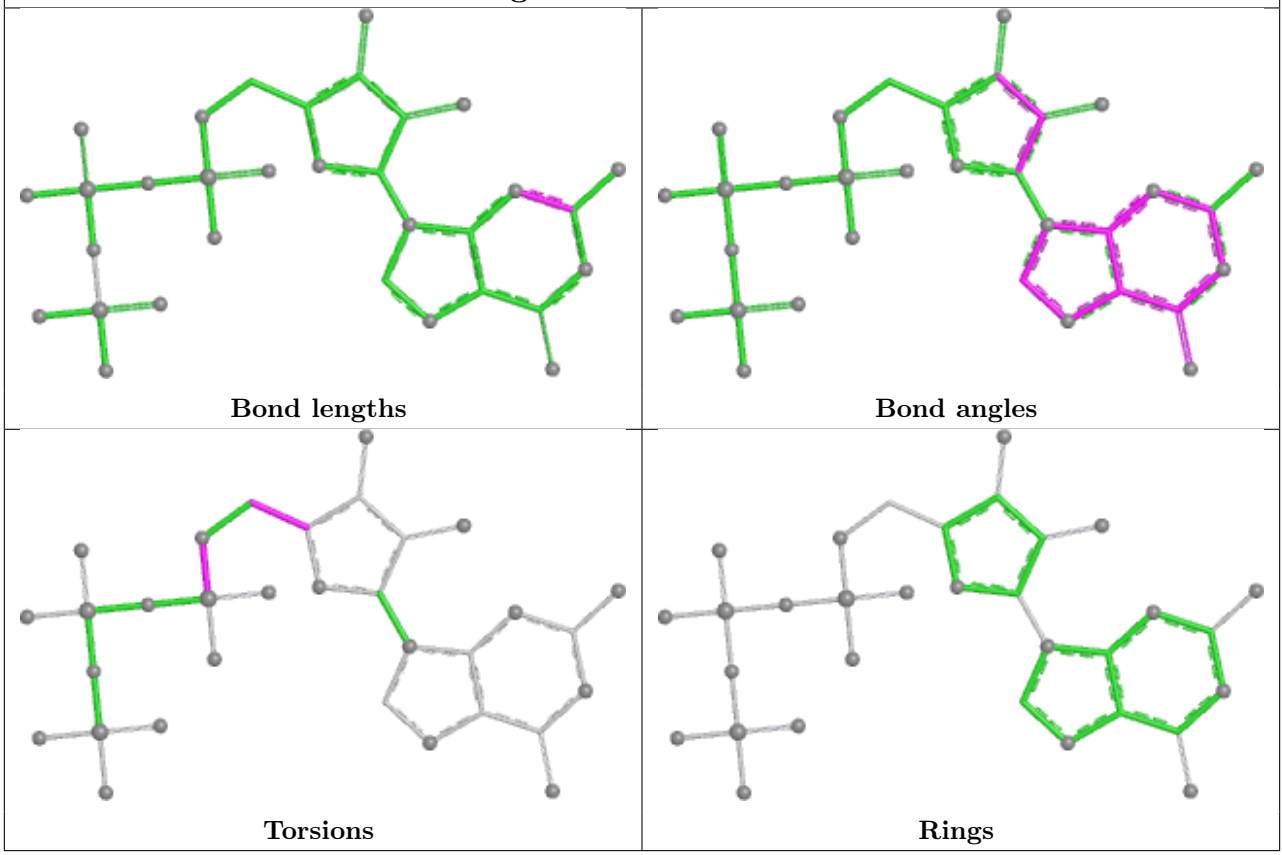


Torsions

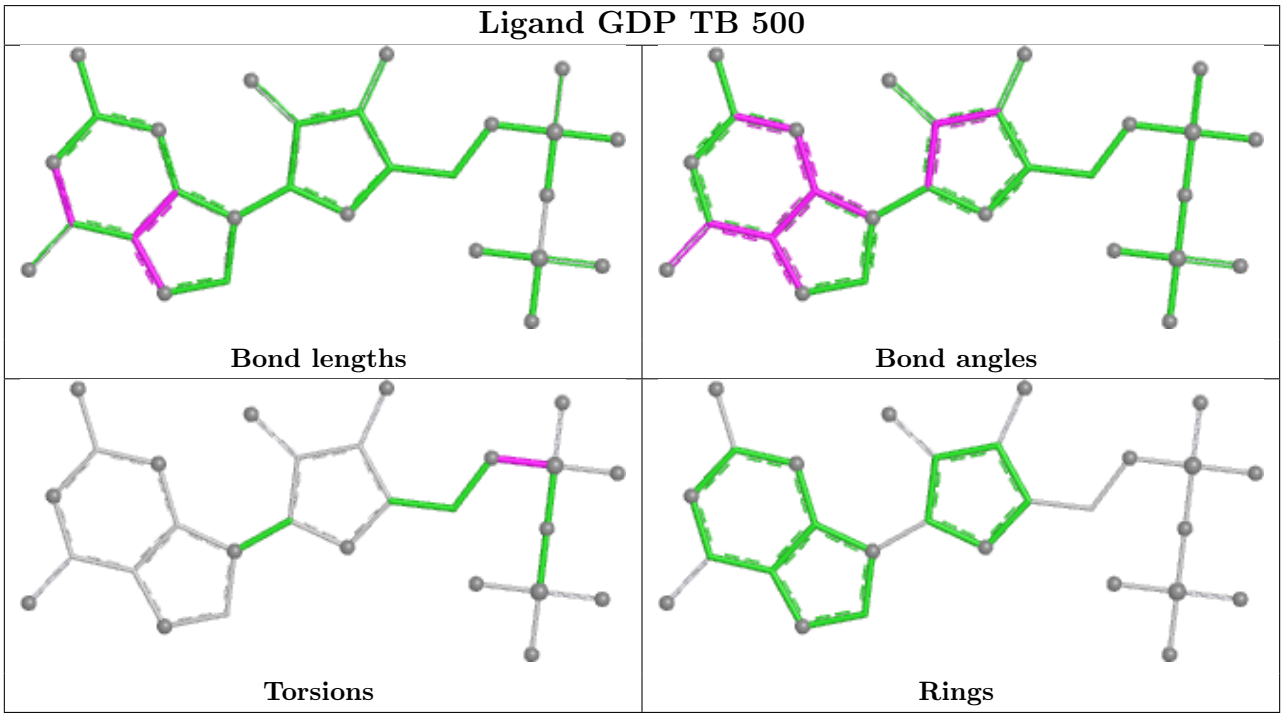


Rings

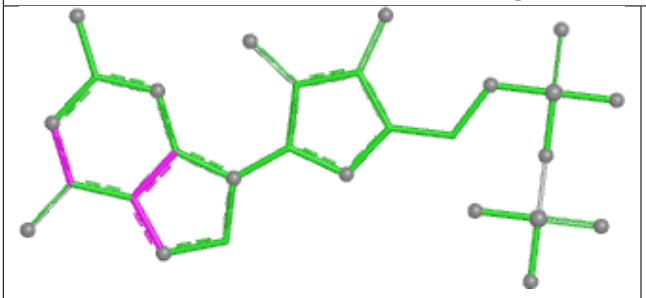
Ligand GTP TU 501



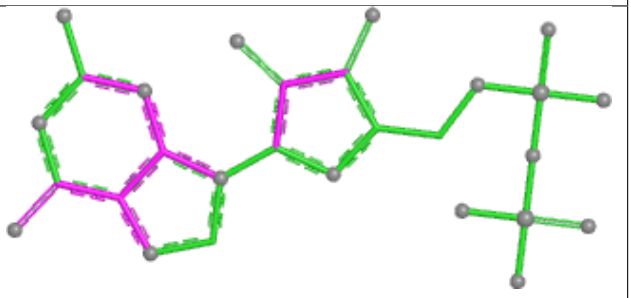
Ligand GDP TB 500



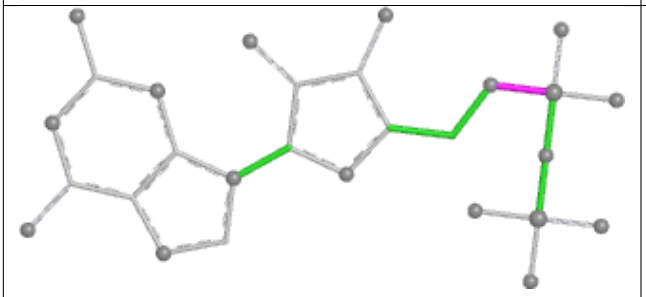
Ligand GDP TT 500



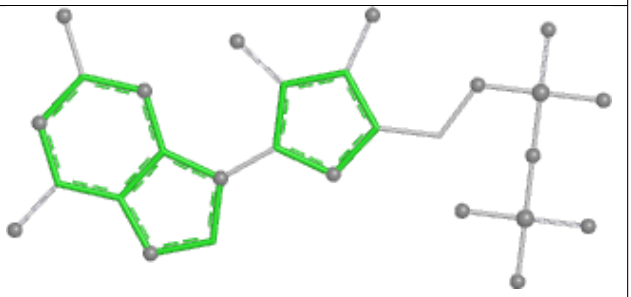
Bond lengths



Bond angles

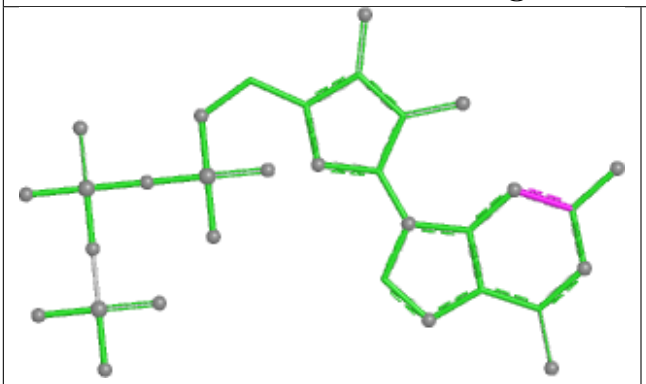


Torsions

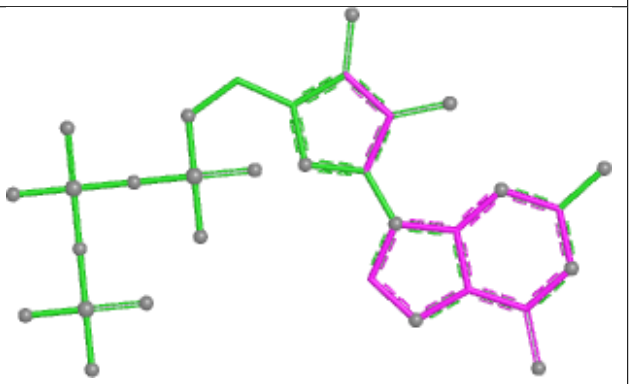


Rings

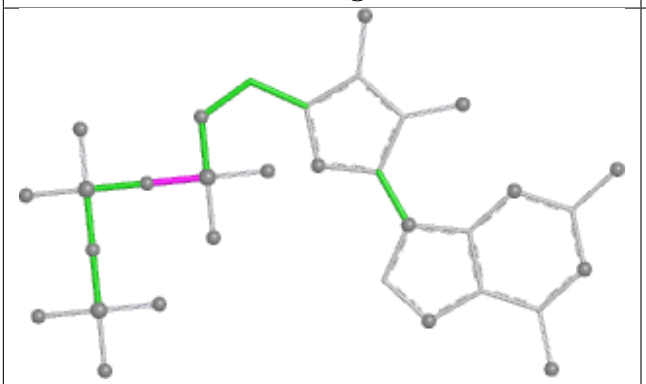
Ligand GTP NU 501



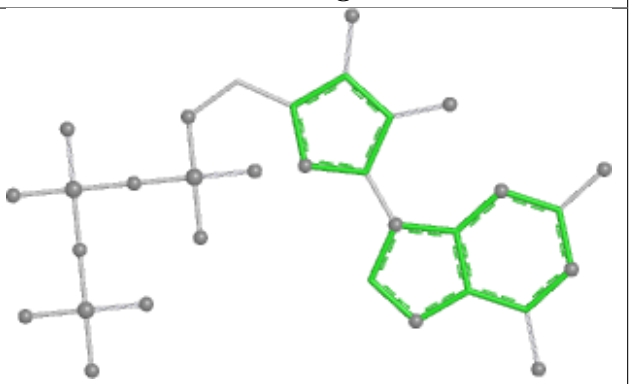
Bond lengths



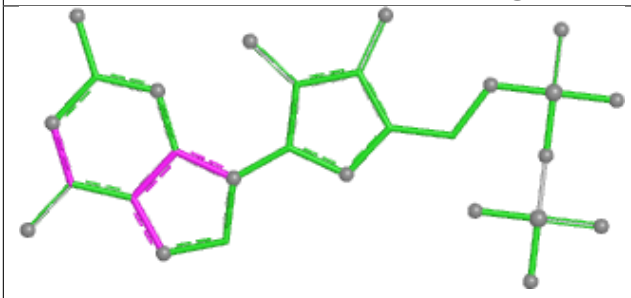
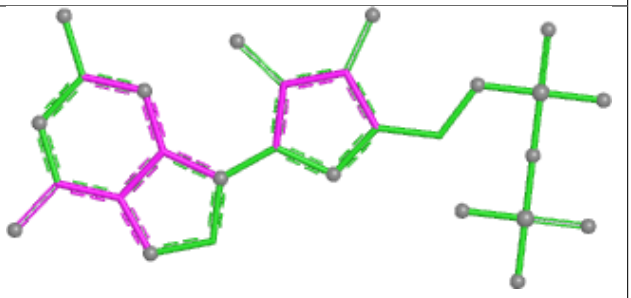
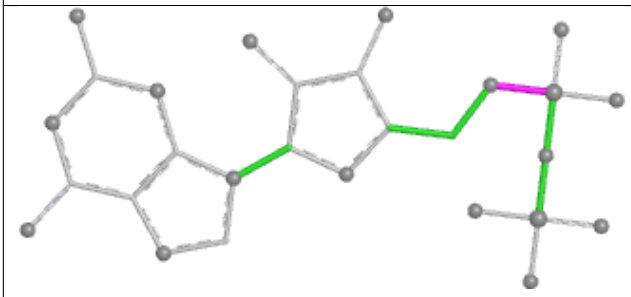
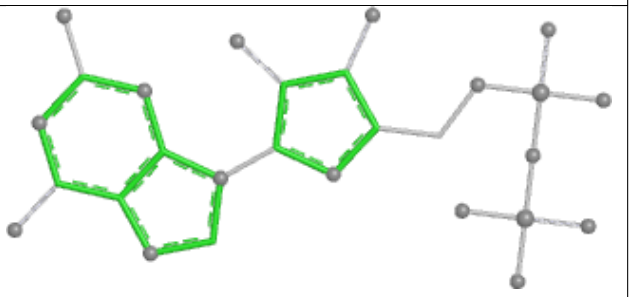
Bond angles

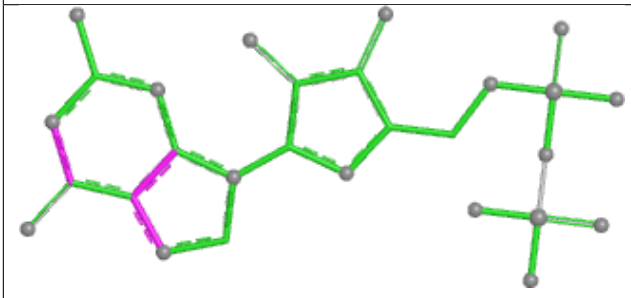
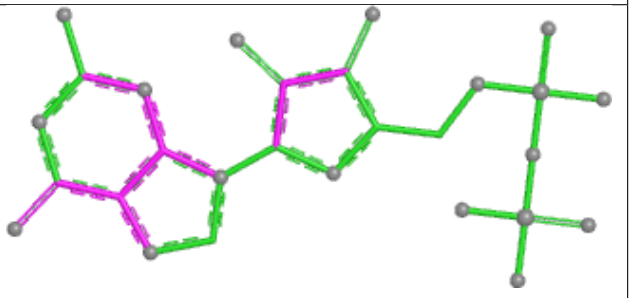
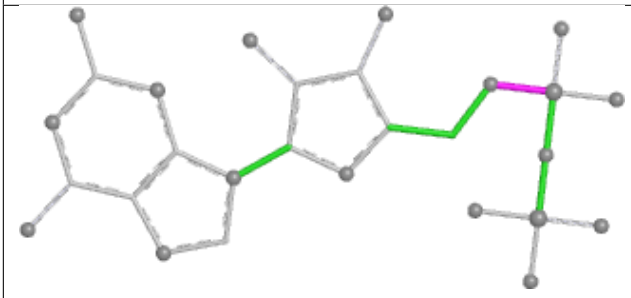
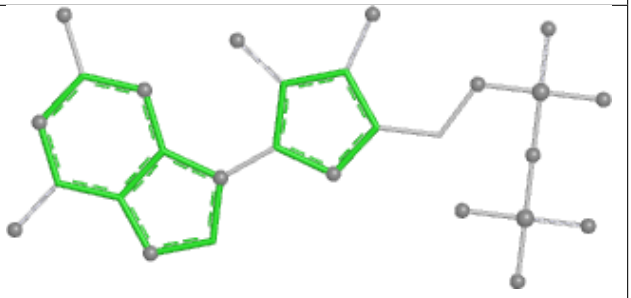


Torsions

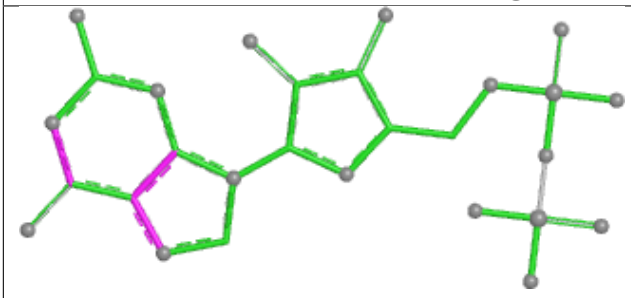


Rings

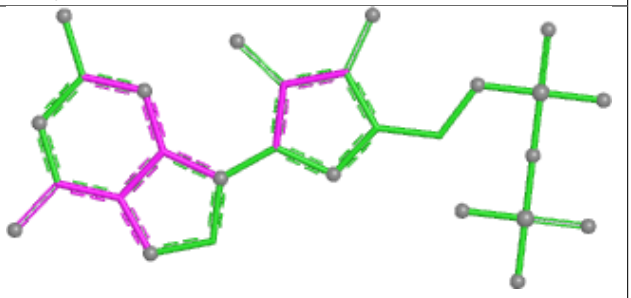
Ligand GDP EH 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP VF 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

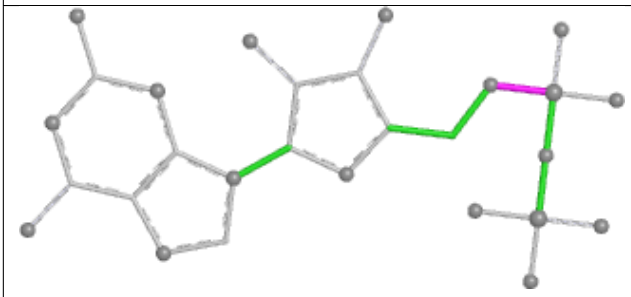
Ligand GDP QO 500



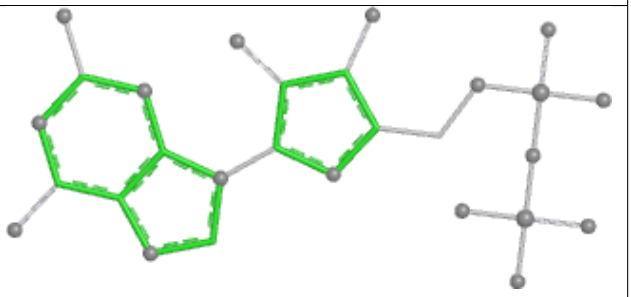
Bond lengths



Bond angles

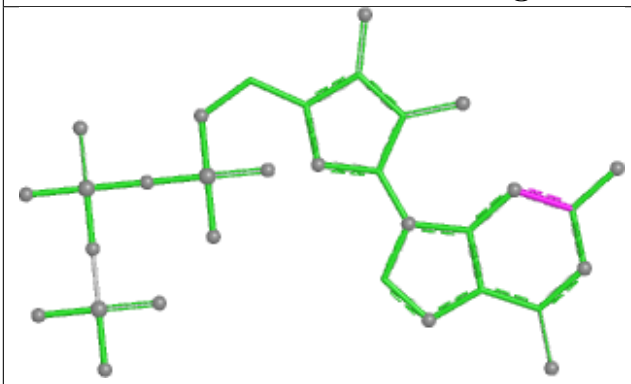


Torsions

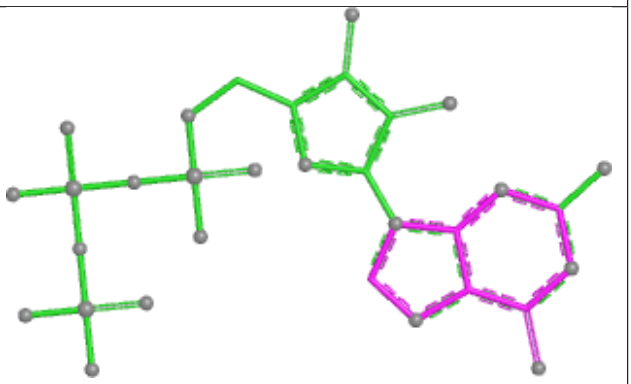


Rings

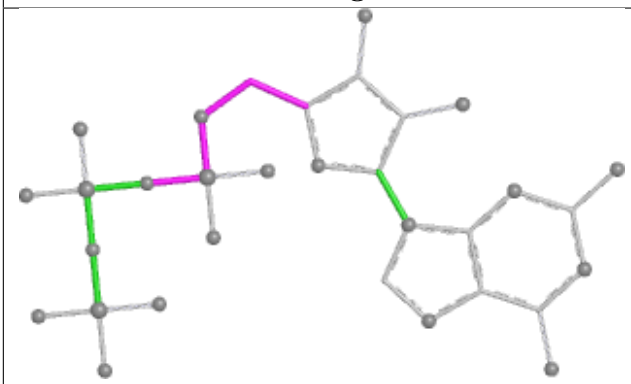
Ligand GTP LP 502



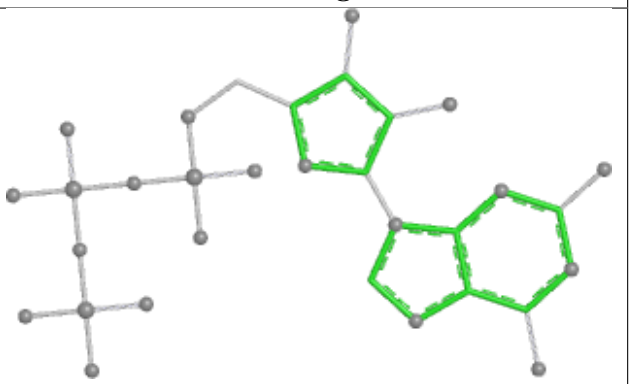
Bond lengths



Bond angles

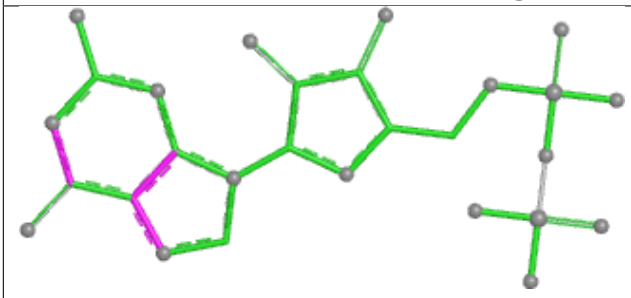


Torsions

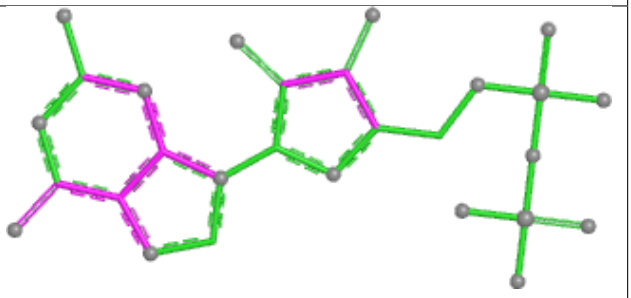


Rings

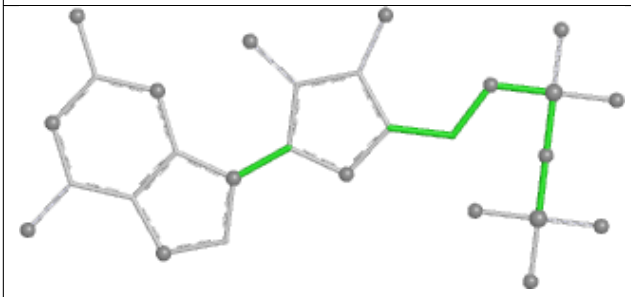
Ligand GDP FB 500



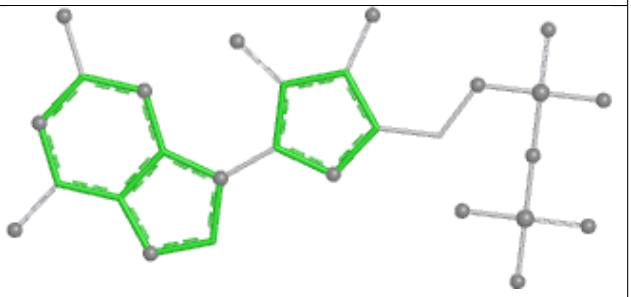
Bond lengths



Bond angles

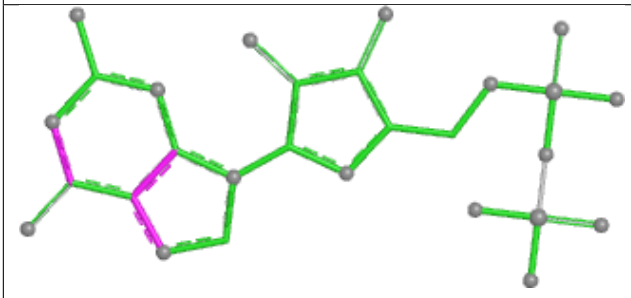


Torsions

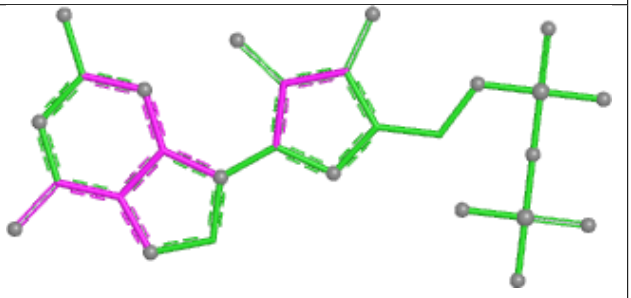


Rings

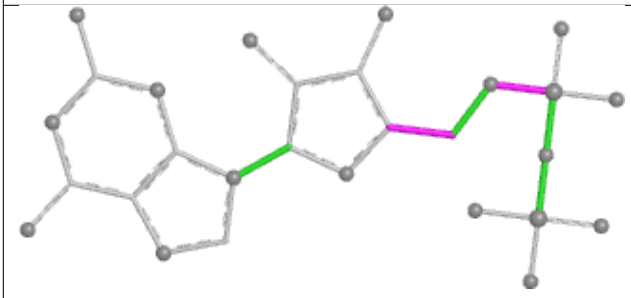
Ligand GDP SB 501



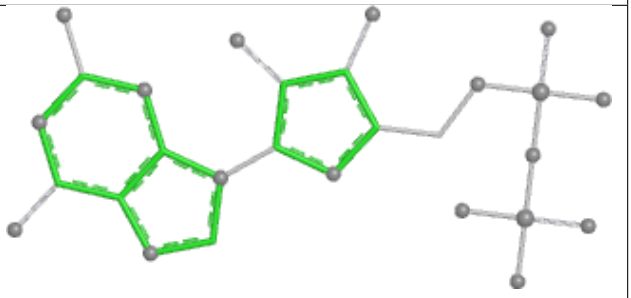
Bond lengths



Bond angles

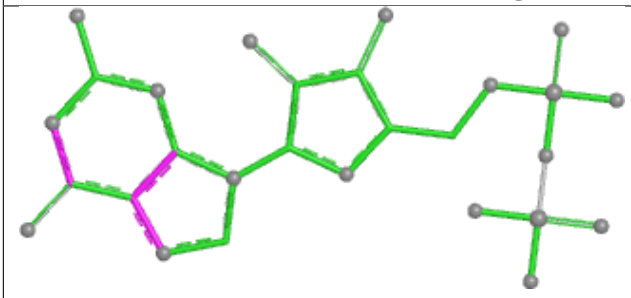


Torsions

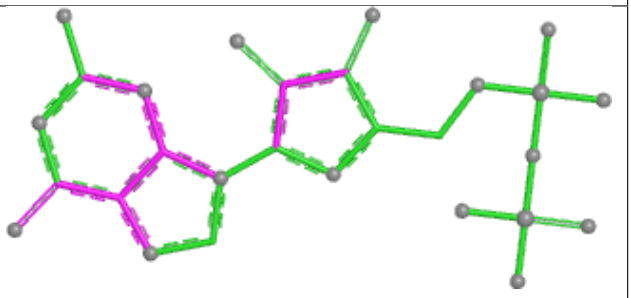


Rings

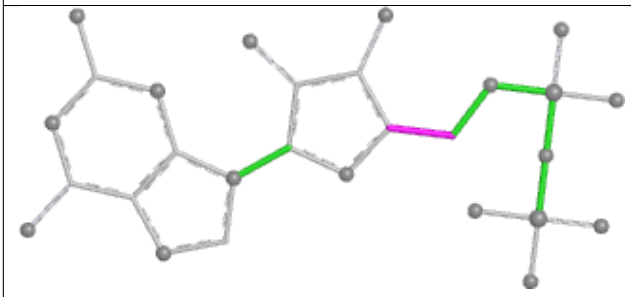
Ligand GDP OL 500



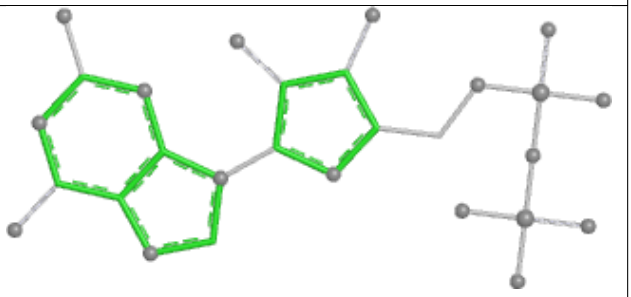
Bond lengths



Bond angles

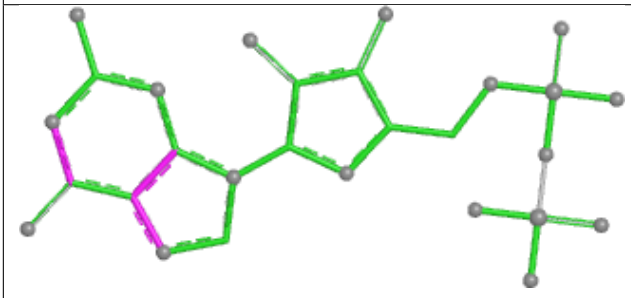


Torsions

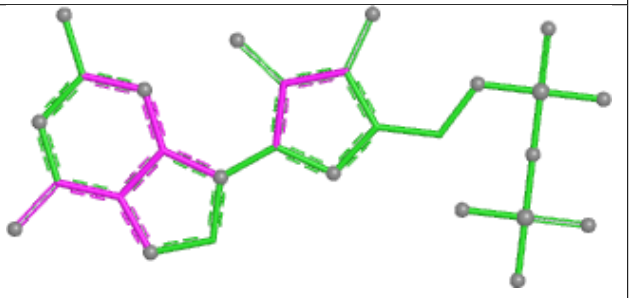


Rings

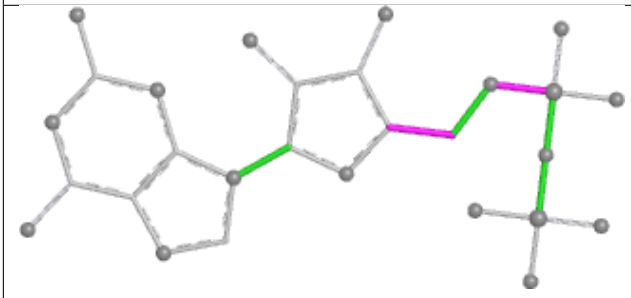
Ligand GDP IT 501



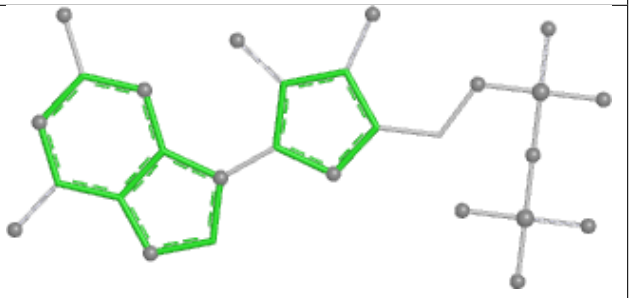
Bond lengths



Bond angles

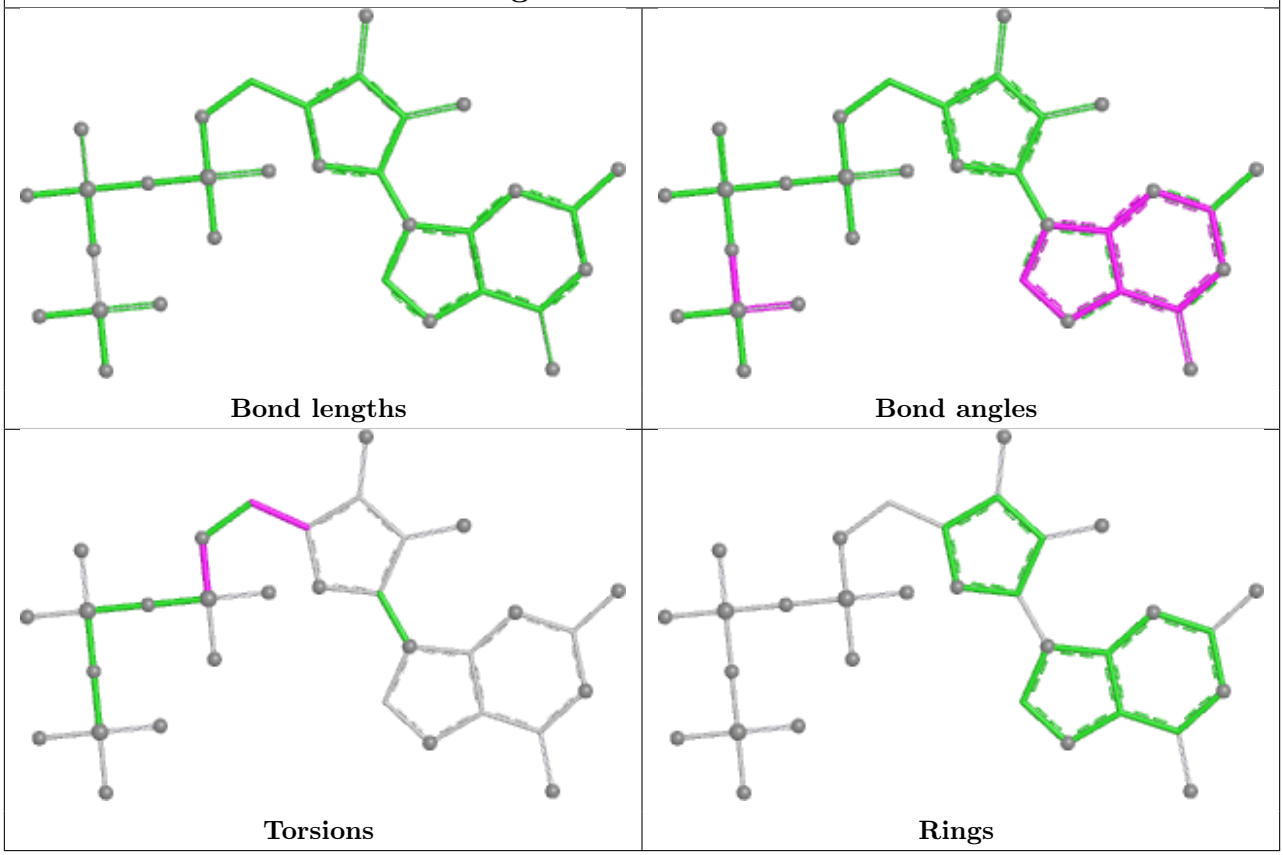


Torsions

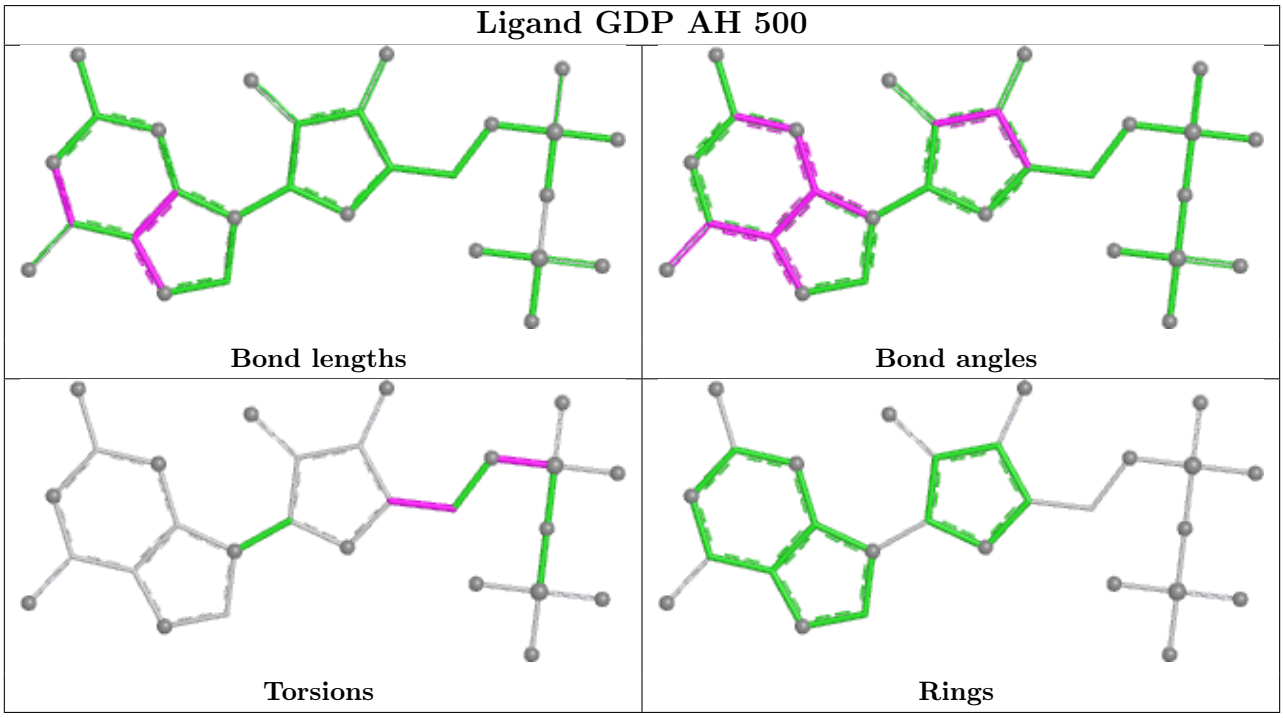


Rings

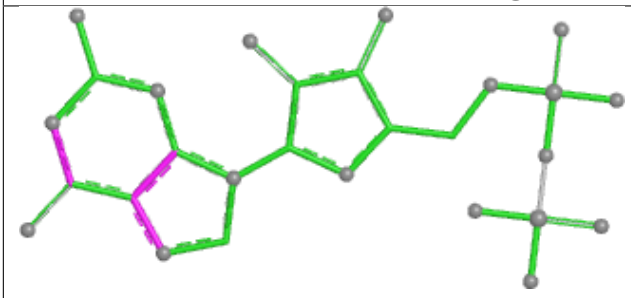
Ligand GTP ED 501



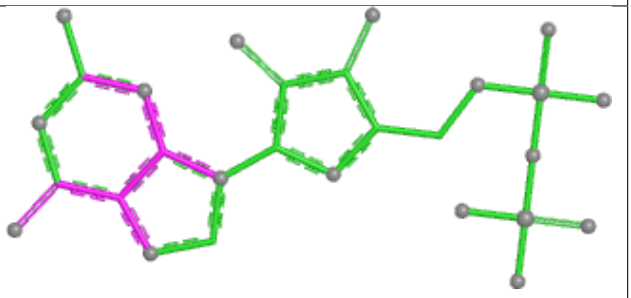
Ligand GDP AH 500



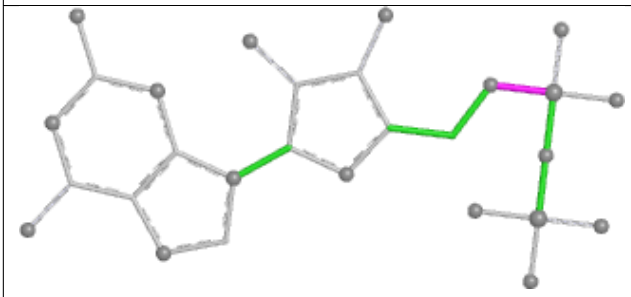
Ligand GDP UX 500



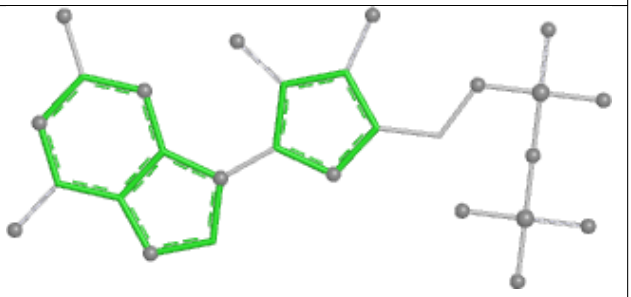
Bond lengths



Bond angles

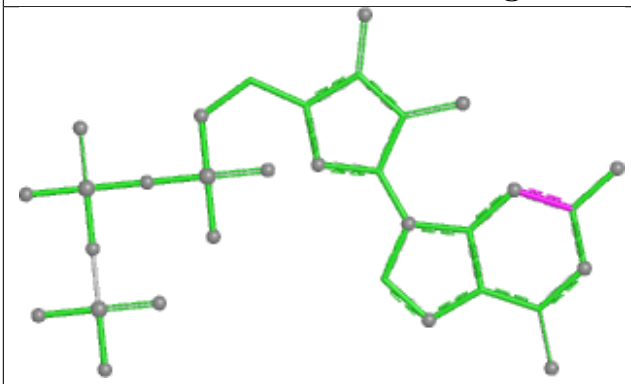


Torsions

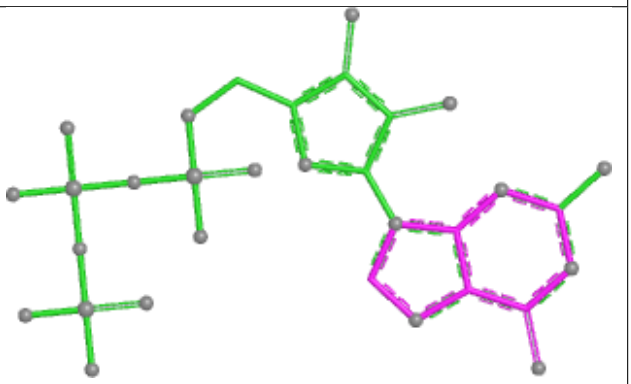


Rings

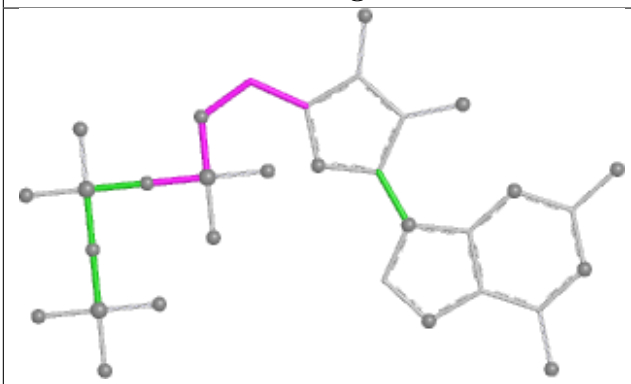
Ligand GTP WK 501



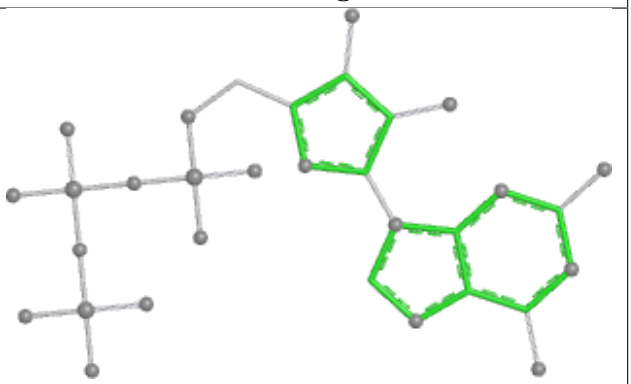
Bond lengths



Bond angles

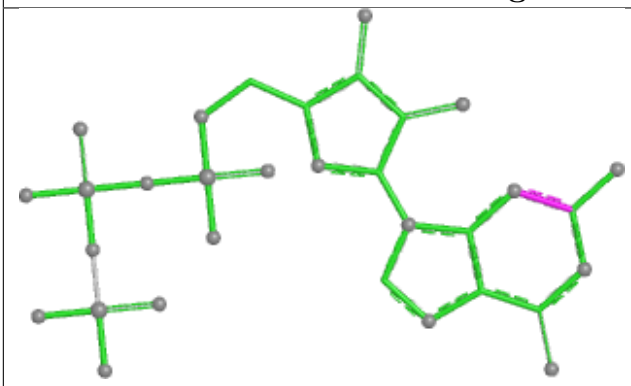


Torsions

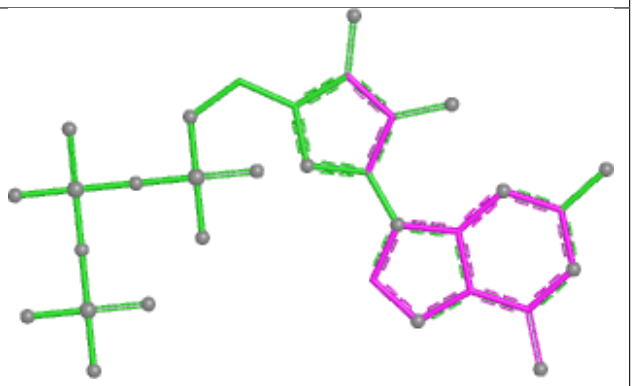


Rings

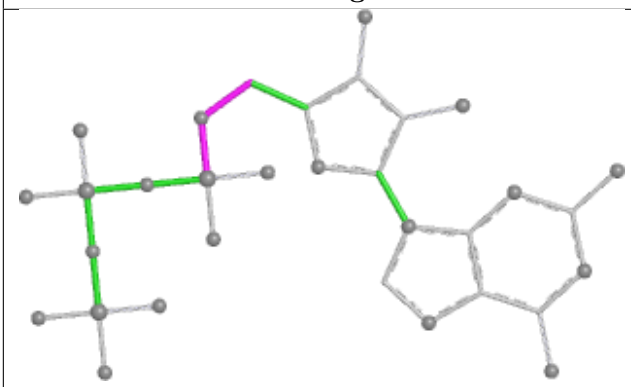
Ligand GTP SM 501



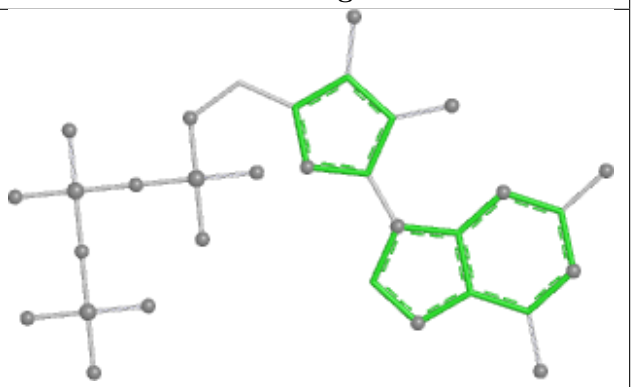
Bond lengths



Bond angles

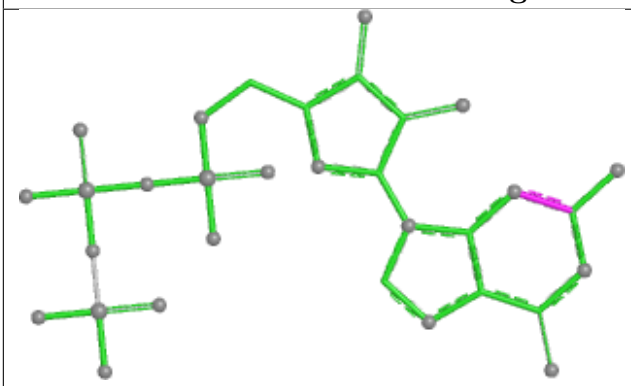


Torsions

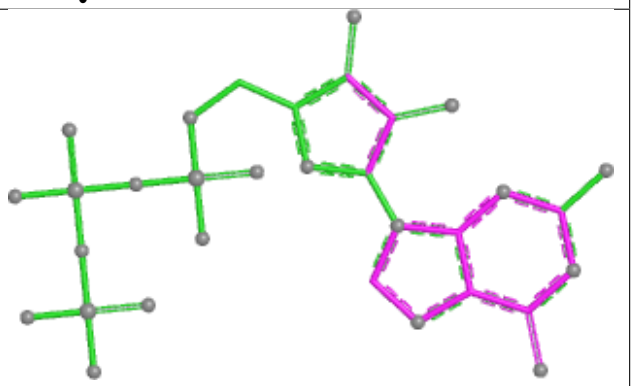


Rings

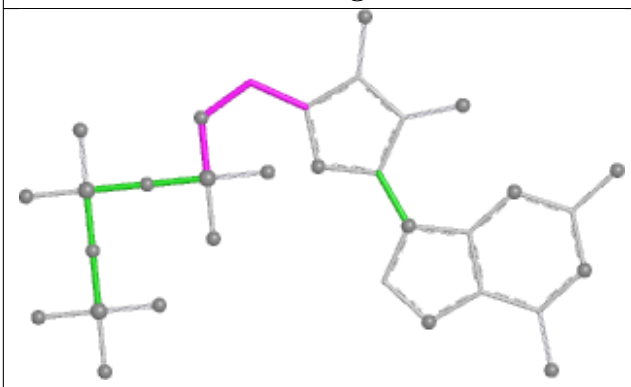
Ligand GTP TQ 501



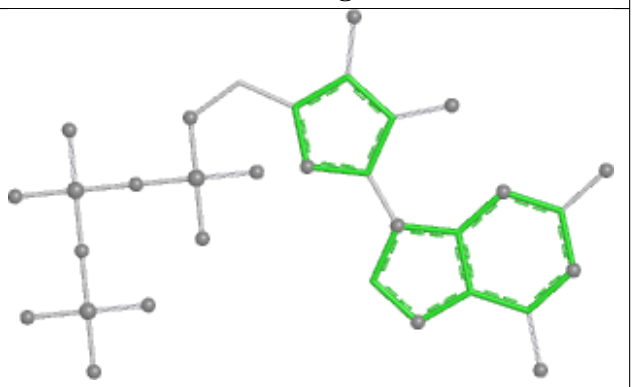
Bond lengths



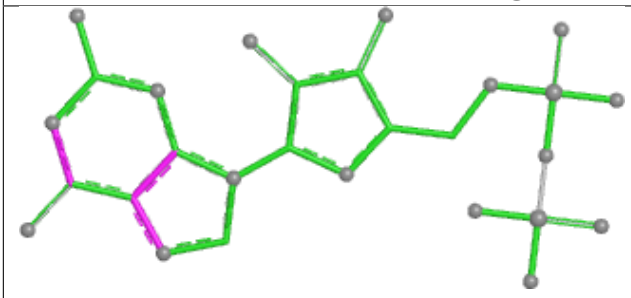
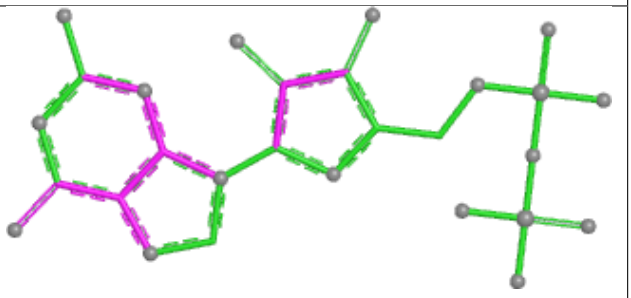
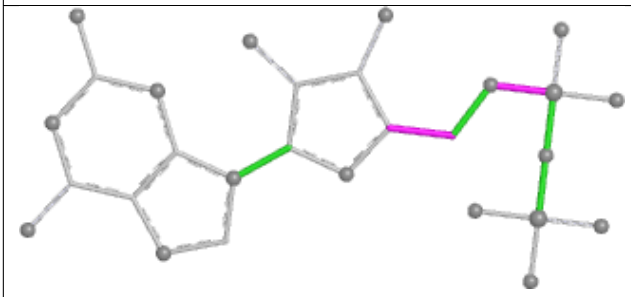
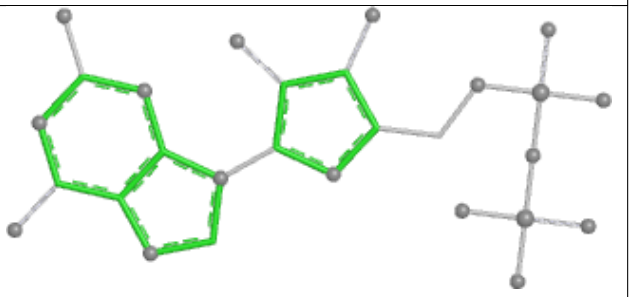
Bond angles

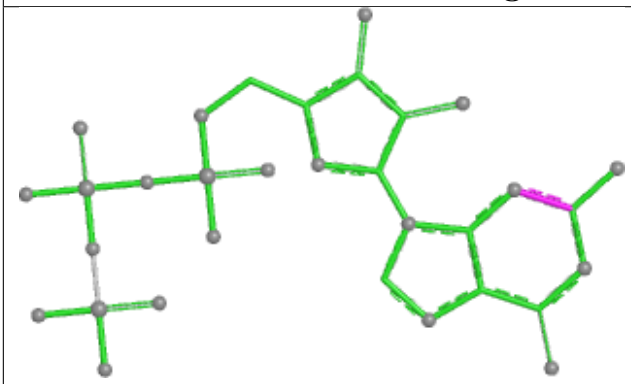
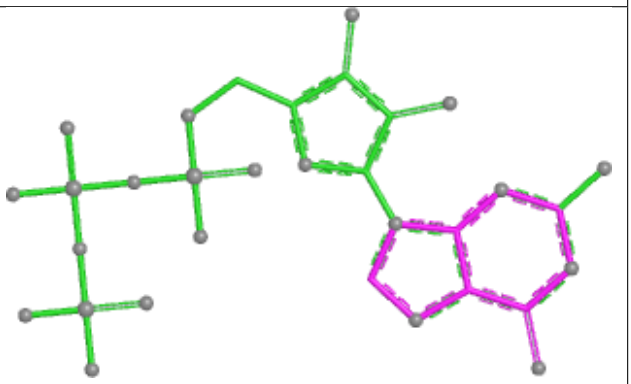
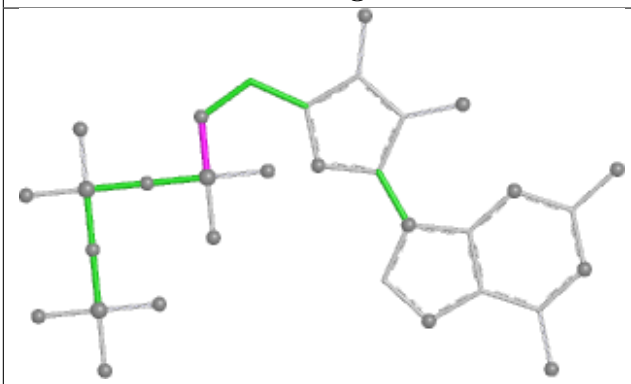
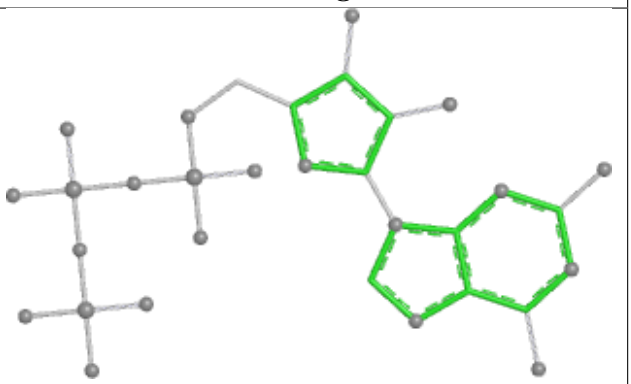


Torsions

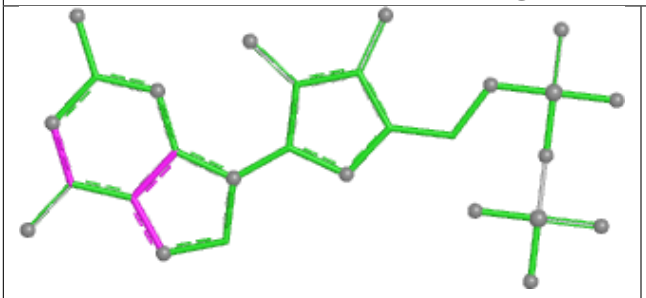


Rings

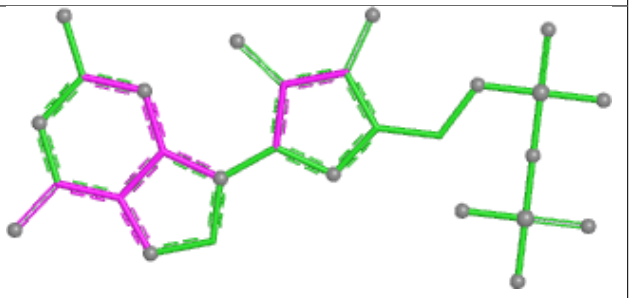
Ligand GDP NT 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP WU 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

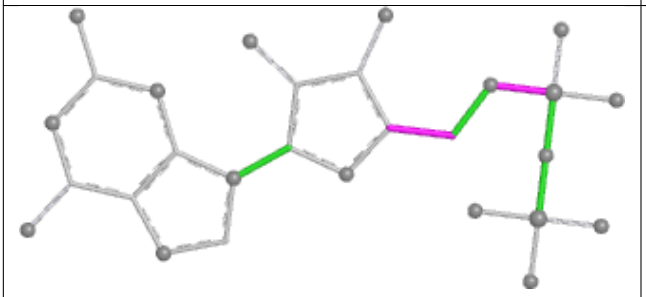
Ligand GDP PJ 500



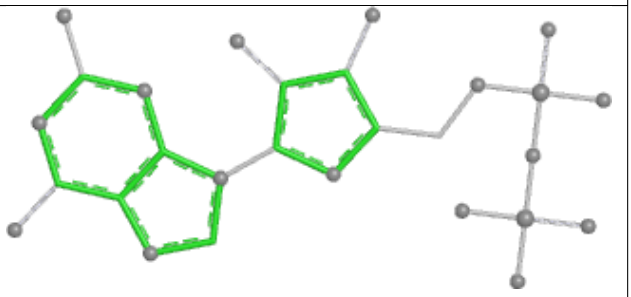
Bond lengths



Bond angles

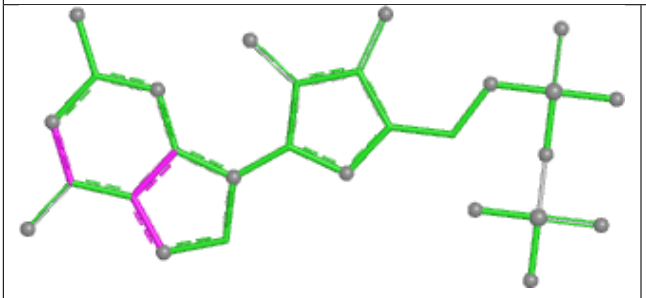


Torsions

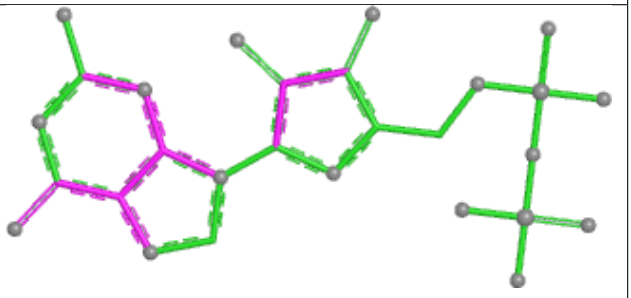


Rings

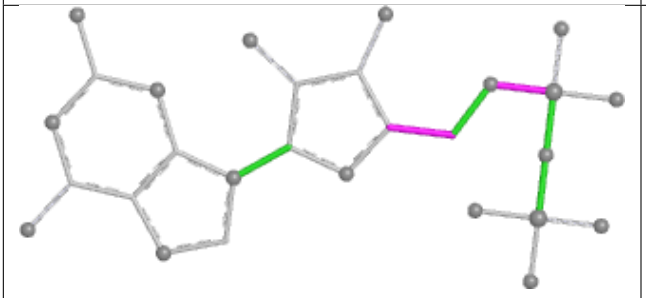
Ligand GDP OH 500



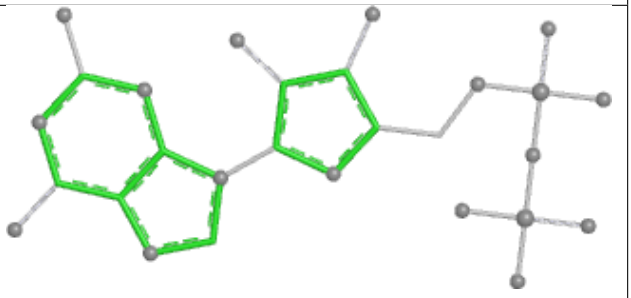
Bond lengths



Bond angles

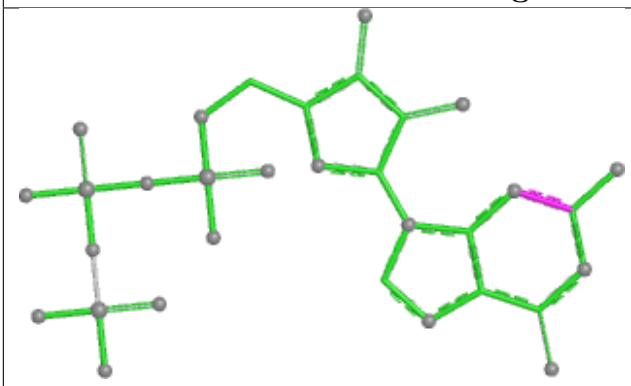


Torsions

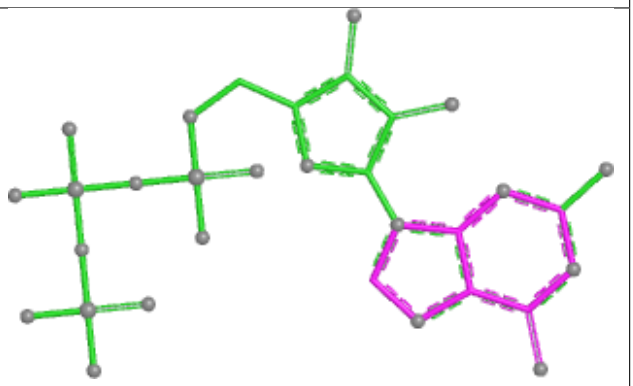


Rings

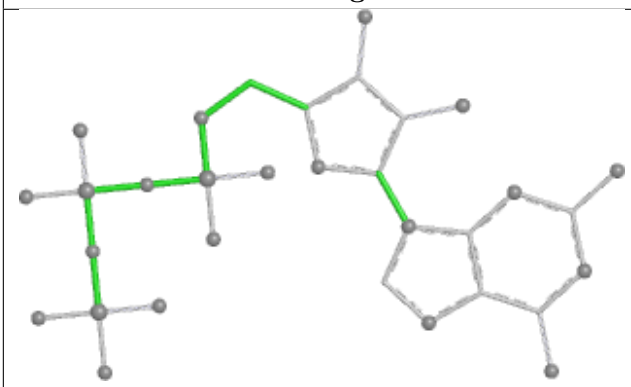
Ligand GTP SK 501



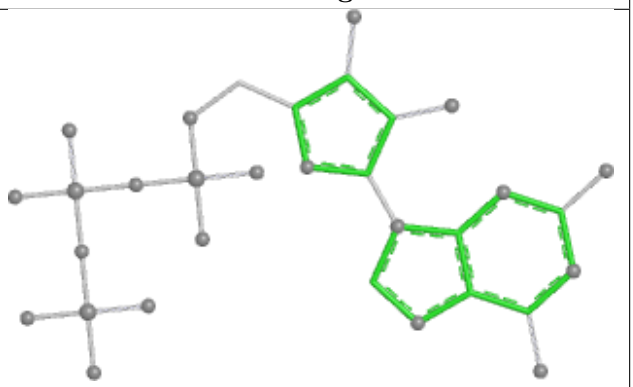
Bond lengths



Bond angles

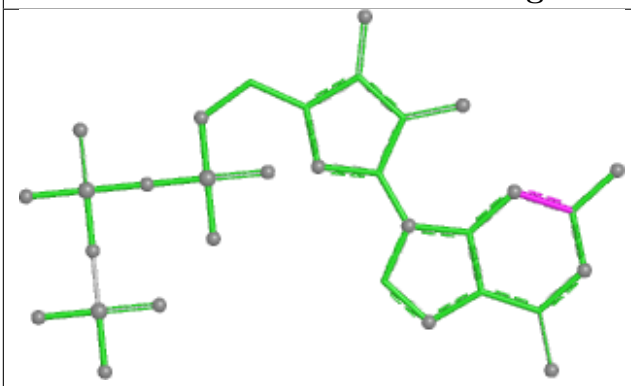


Torsions

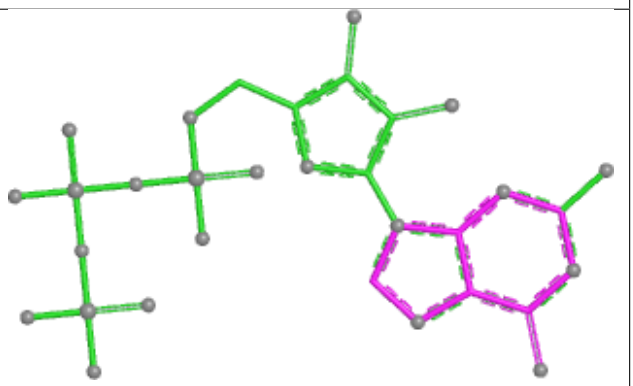


Rings

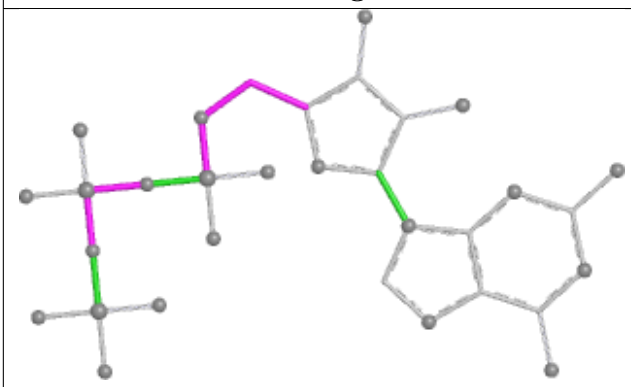
Ligand GTP J 501



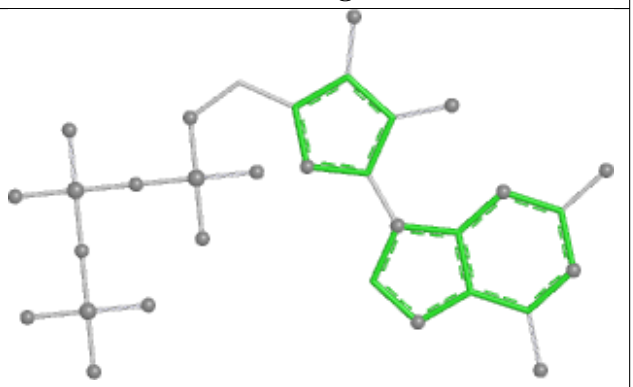
Bond lengths



Bond angles

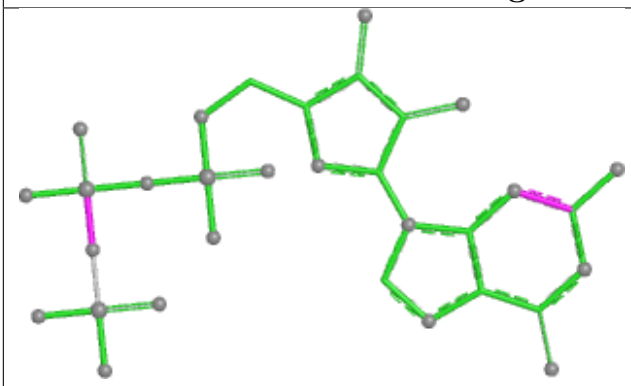


Torsions

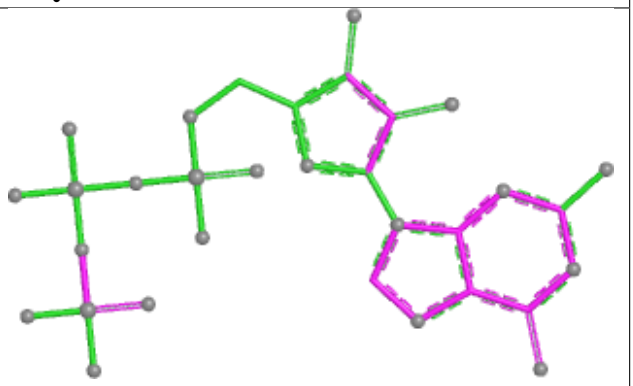


Rings

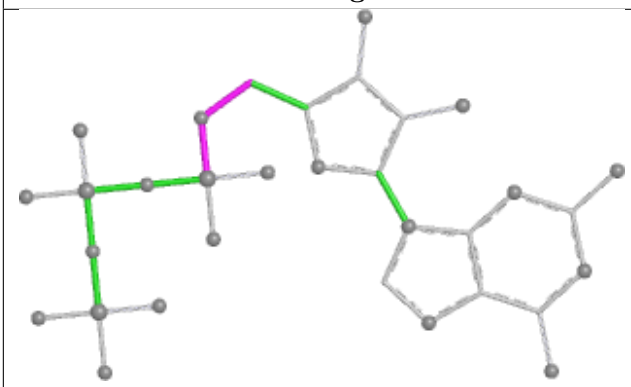
Ligand GTP QU 501



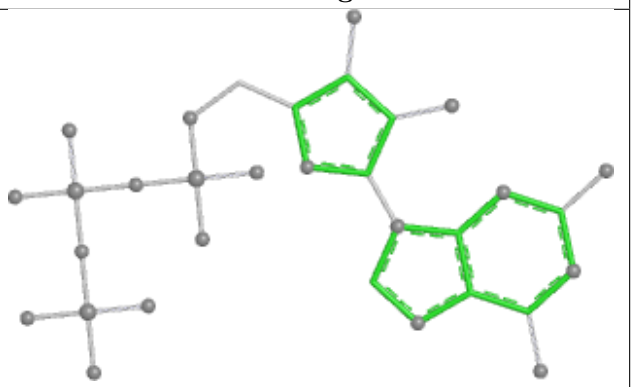
Bond lengths



Bond angles

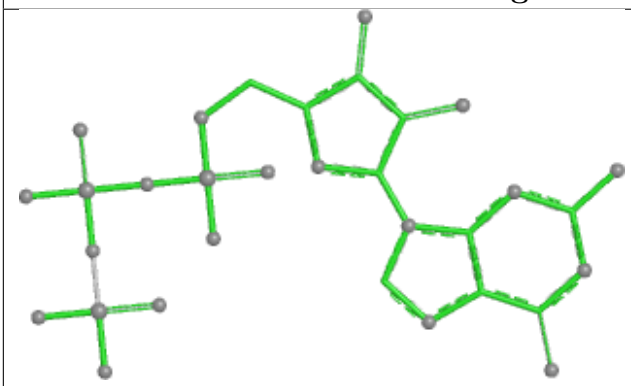


Torsions

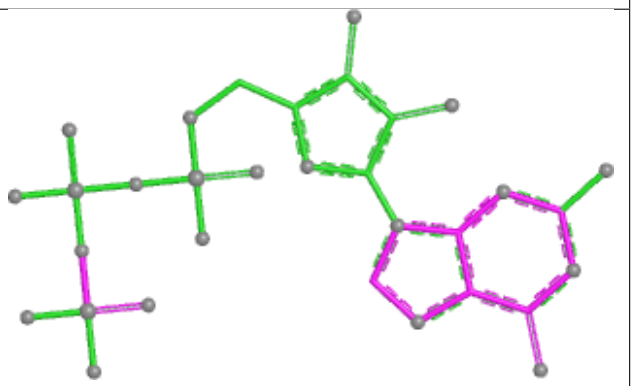


Rings

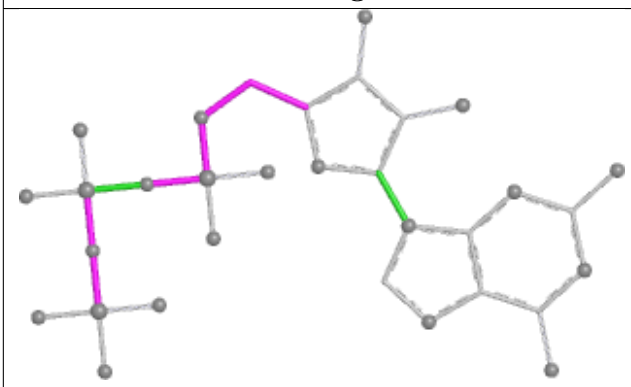
Ligand GTP DL 501



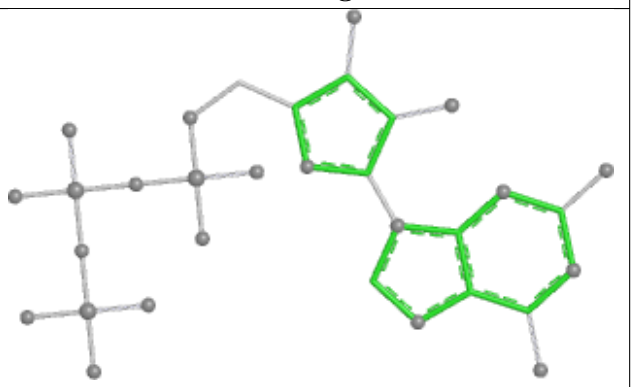
Bond lengths



Bond angles

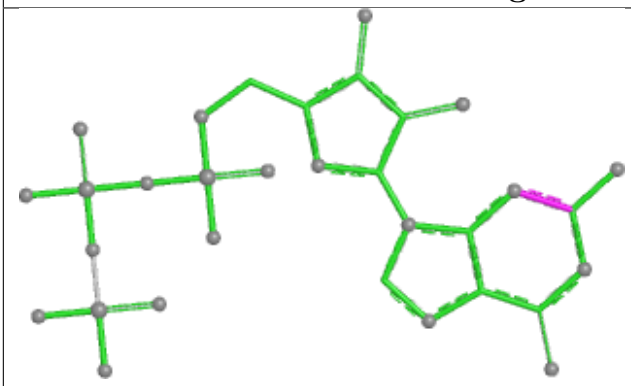


Torsions

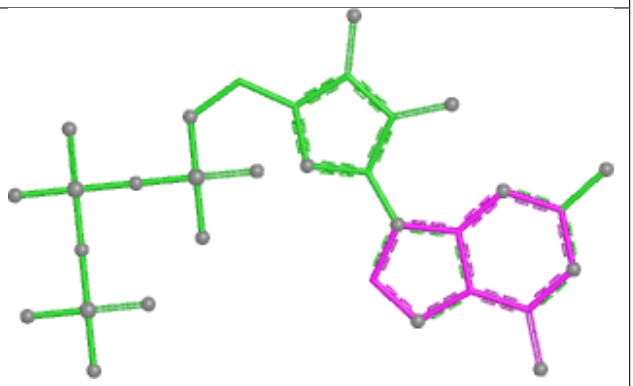


Rings

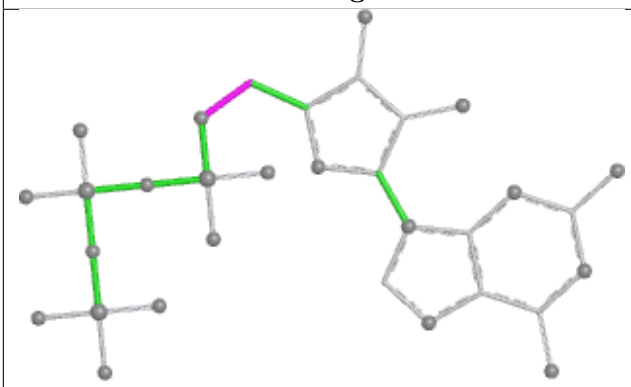
Ligand GTP RR 501



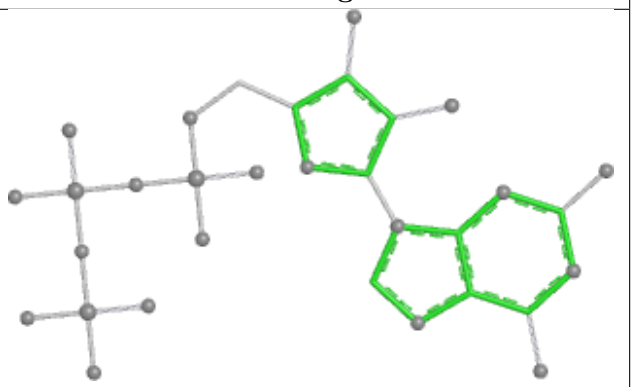
Bond lengths



Bond angles

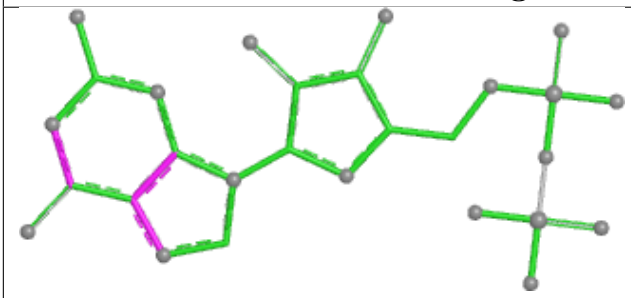


Torsions

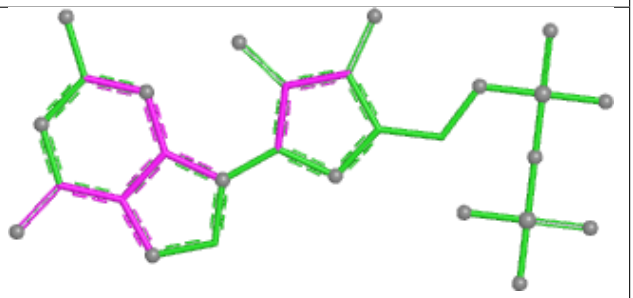


Rings

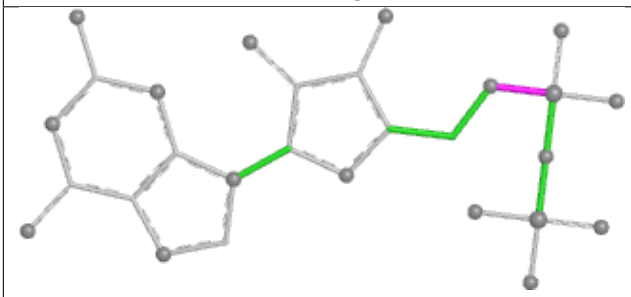
Ligand GDP AZ 500



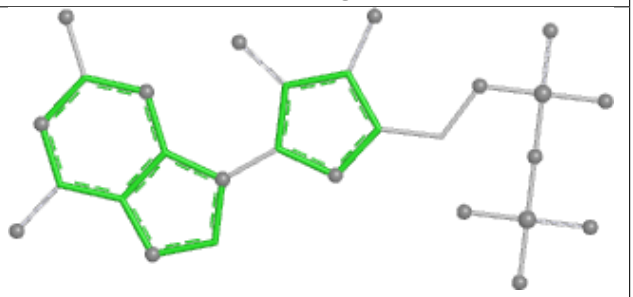
Bond lengths



Bond angles

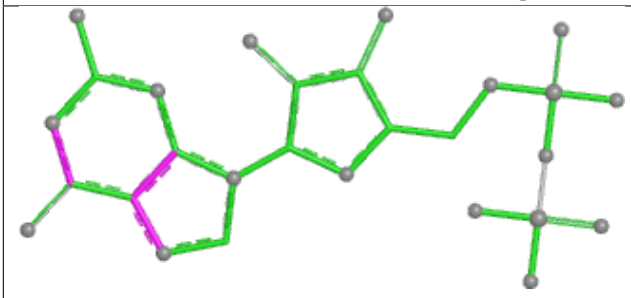


Torsions

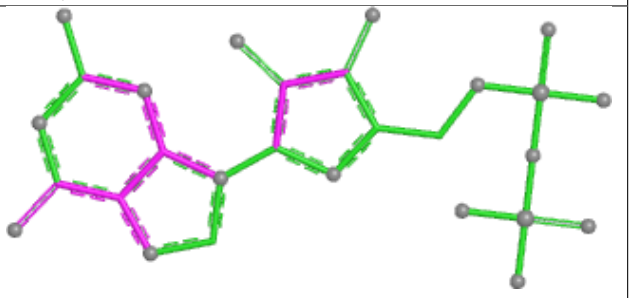


Rings

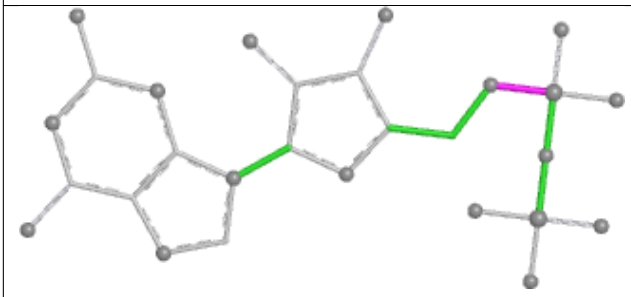
Ligand GDP QI 500



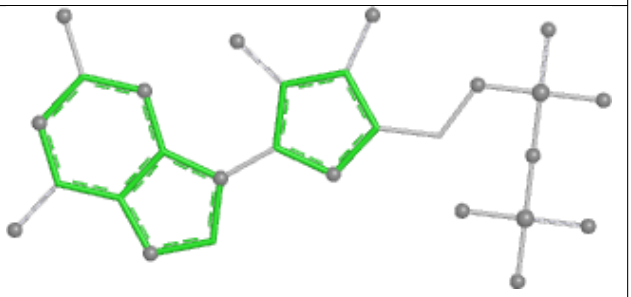
Bond lengths



Bond angles

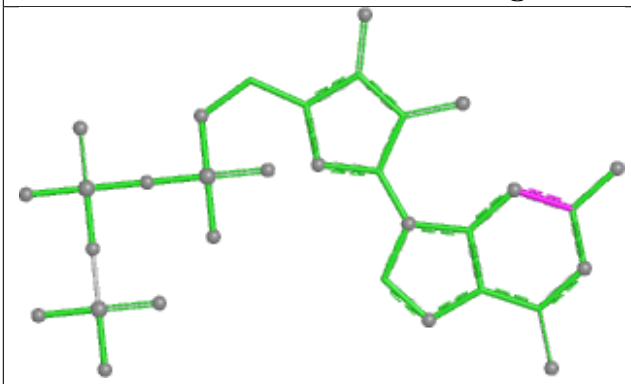


Torsions

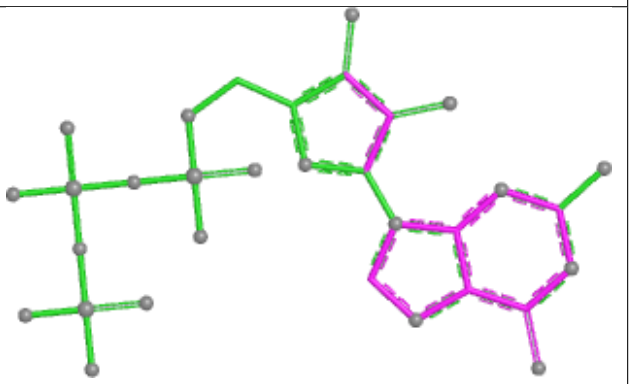


Rings

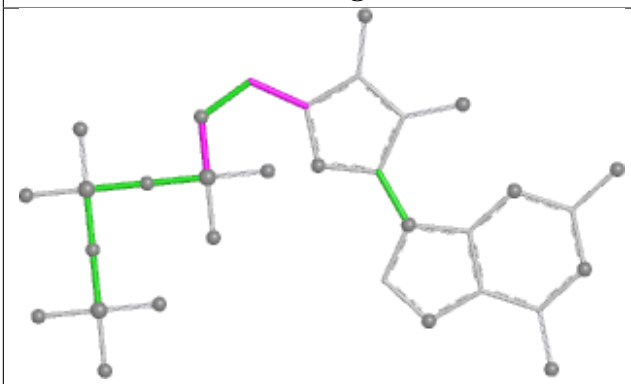
Ligand GTP VY 501



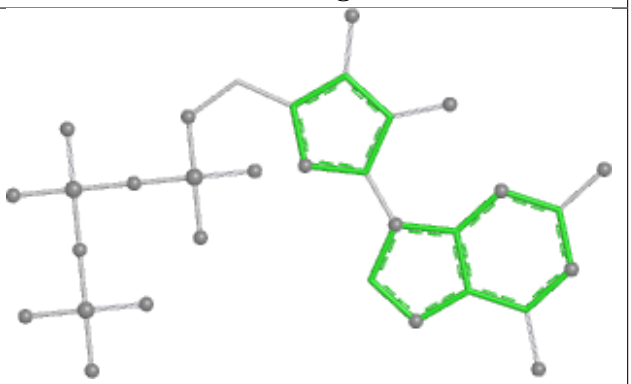
Bond lengths



Bond angles

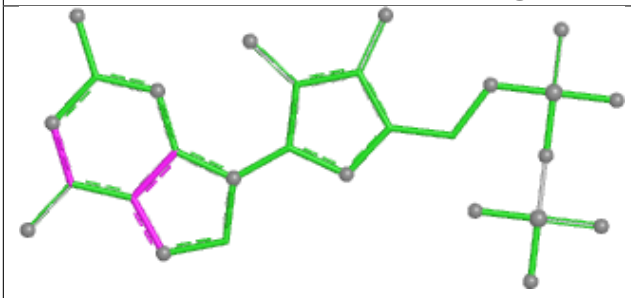


Torsions

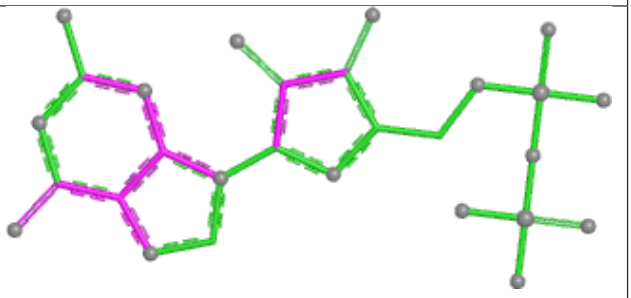


Rings

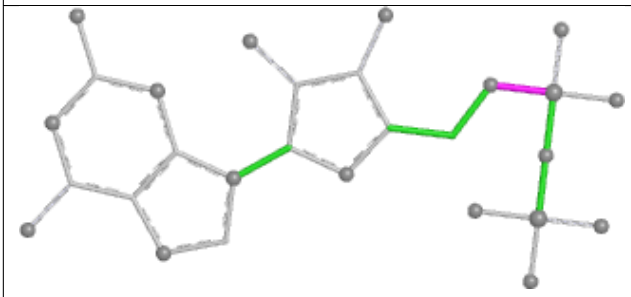
Ligand GDP HJ 500



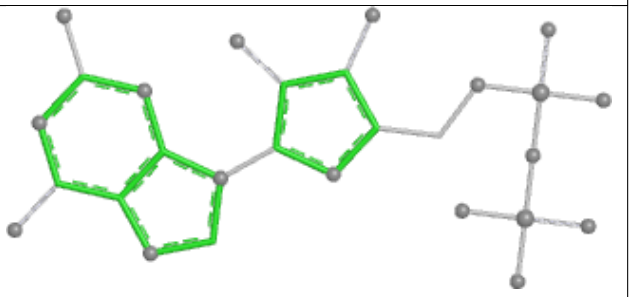
Bond lengths



Bond angles

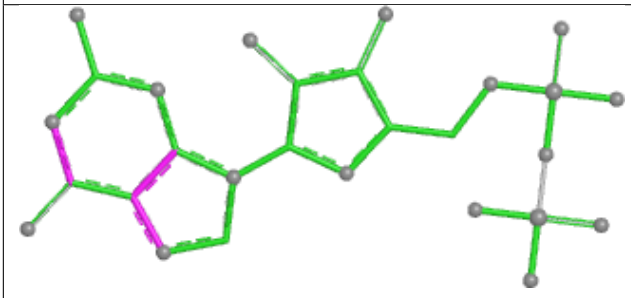


Torsions

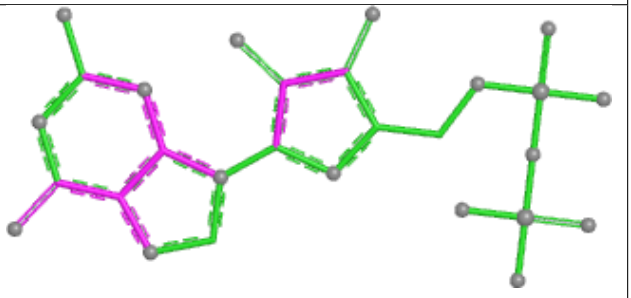


Rings

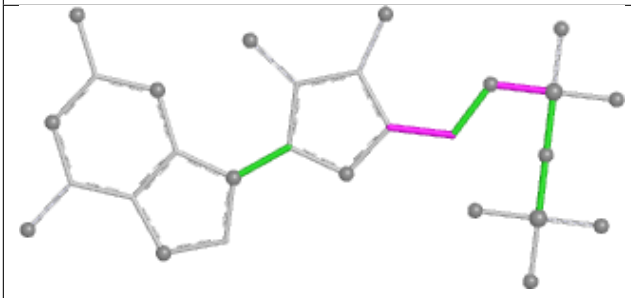
Ligand GDP OV 500



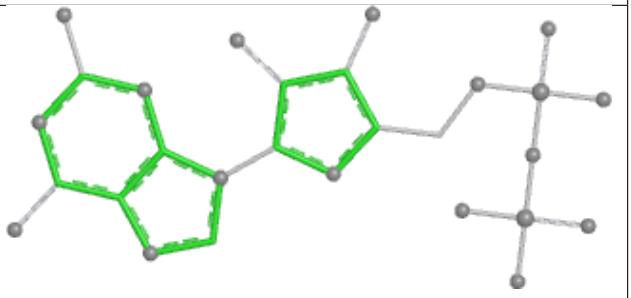
Bond lengths



Bond angles

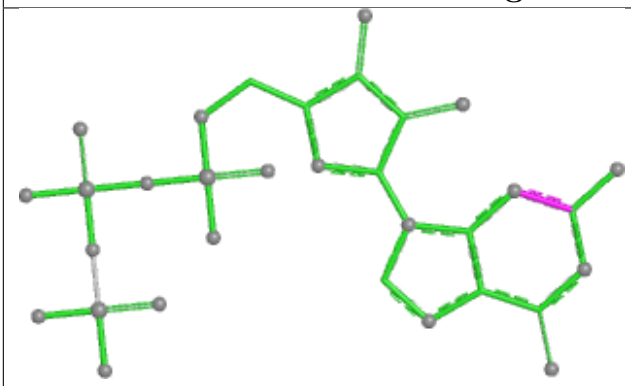


Torsions

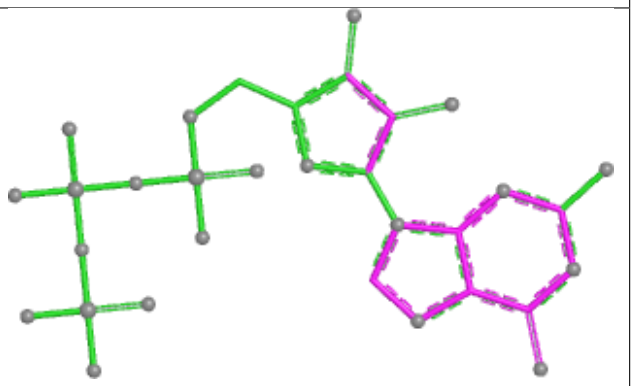


Rings

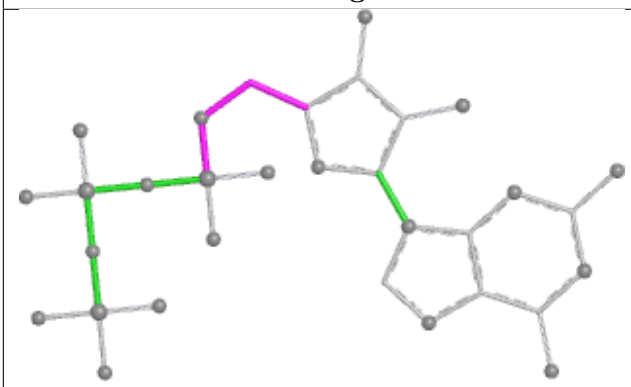
Ligand GTP MO 501



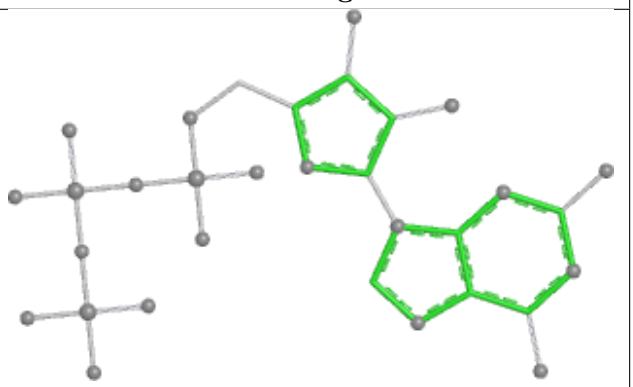
Bond lengths



Bond angles

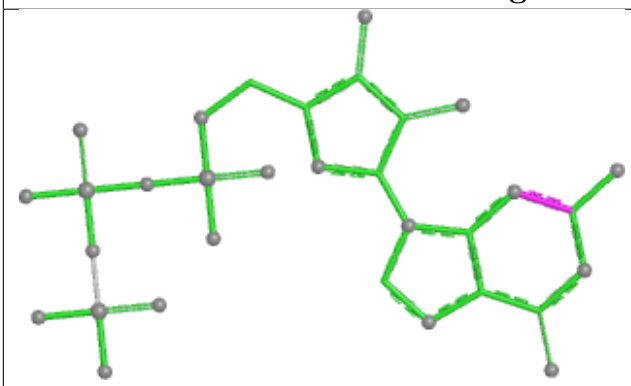


Torsions

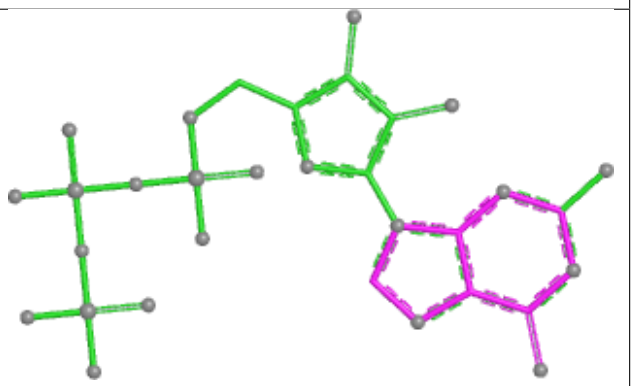


Rings

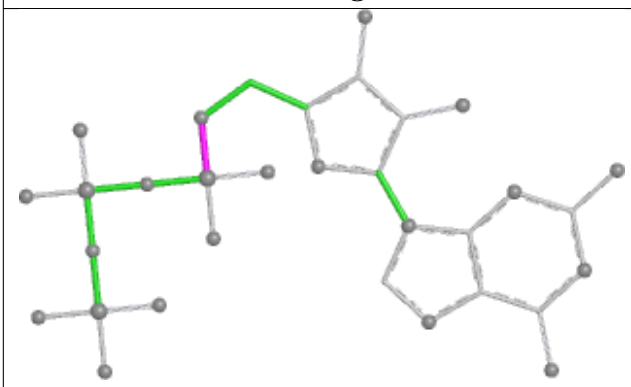
Ligand GTP KP 502



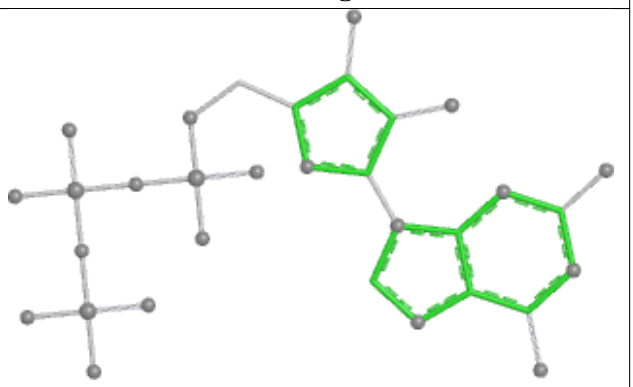
Bond lengths



Bond angles

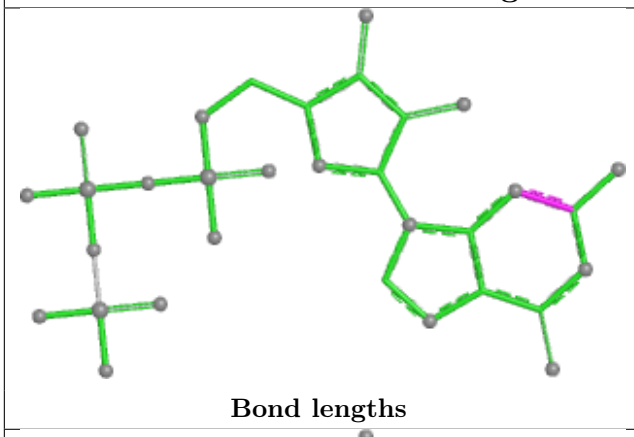


Torsions

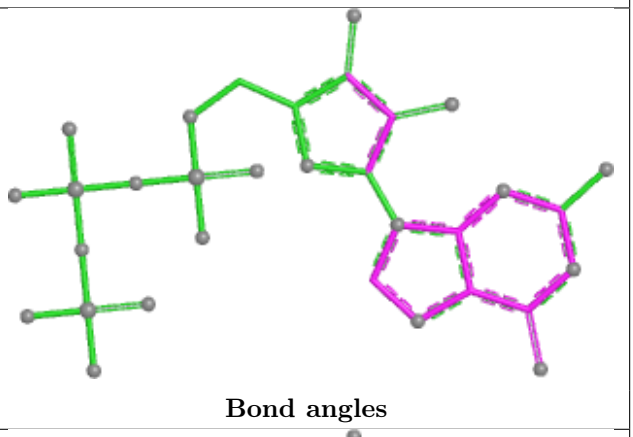


Rings

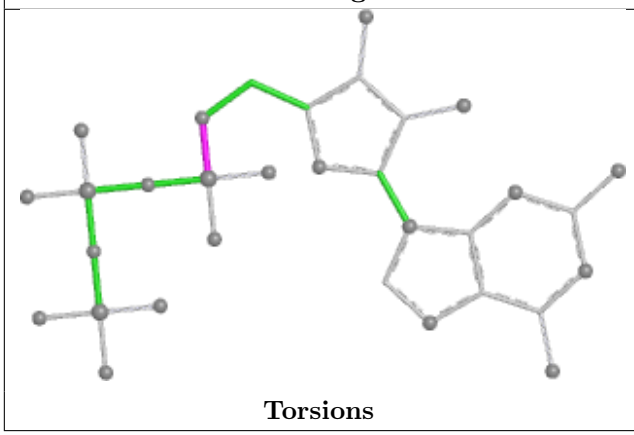
Ligand GTP WM 501



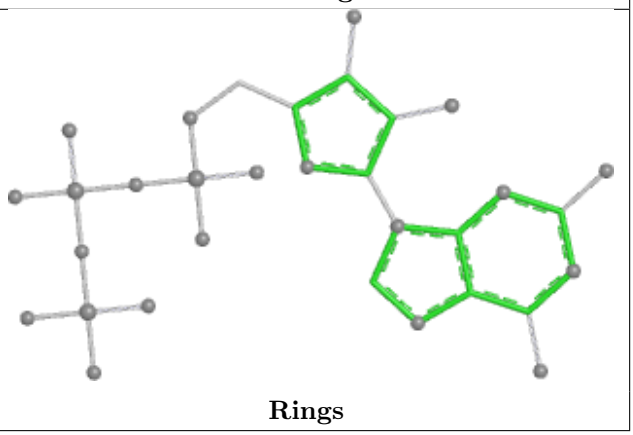
Bond lengths



Bond angles

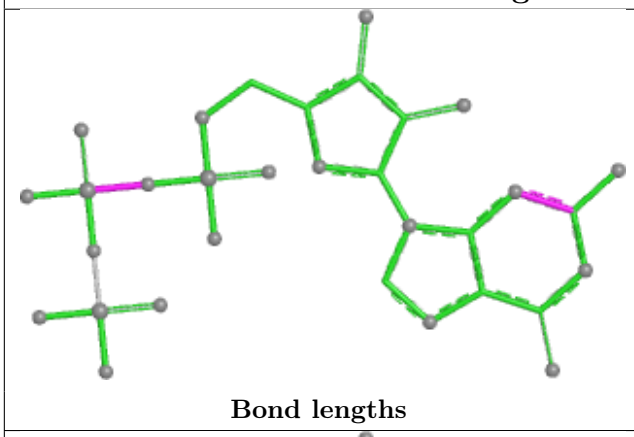


Torsions

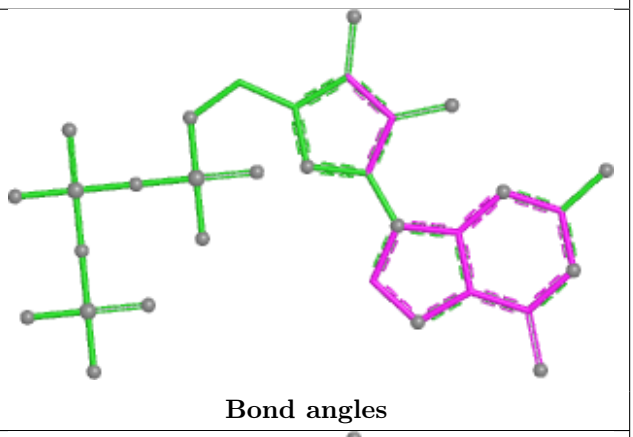


Rings

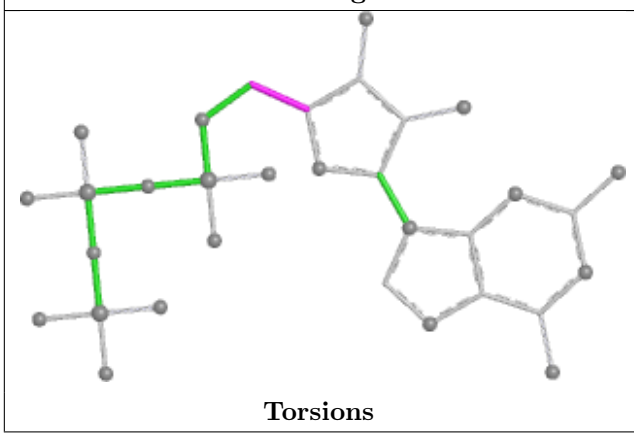
Ligand GTP KL 501



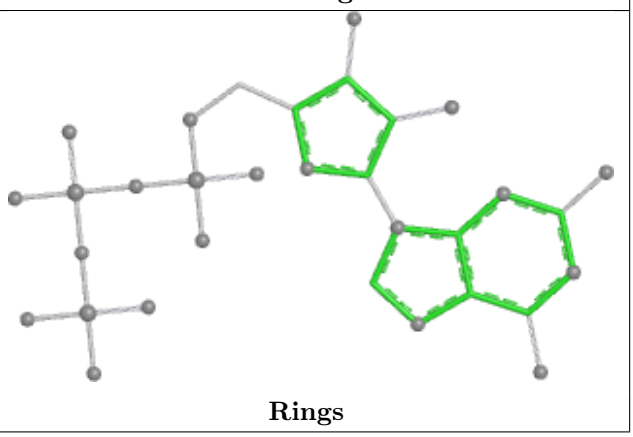
Bond lengths



Bond angles

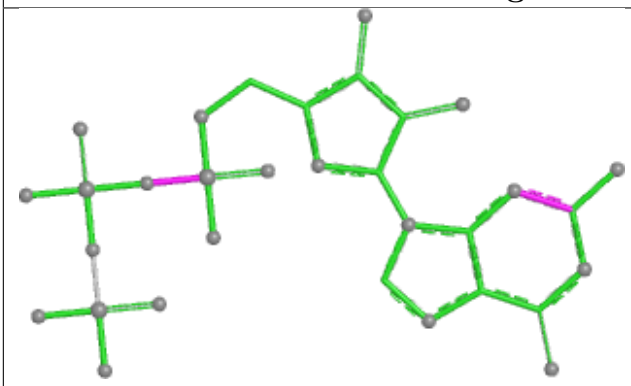


Torsions

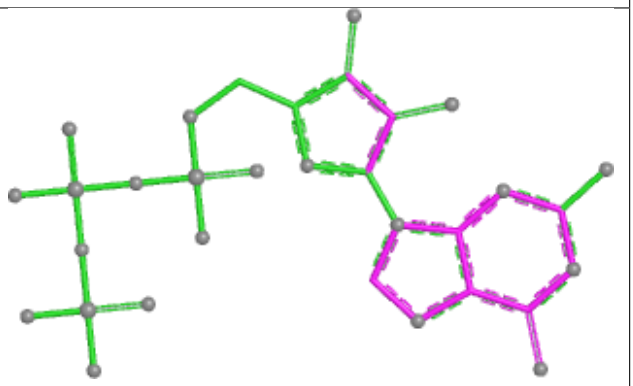


Rings

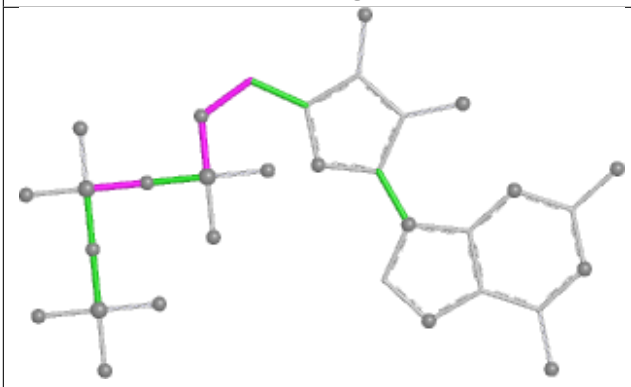
Ligand GTP ME 501



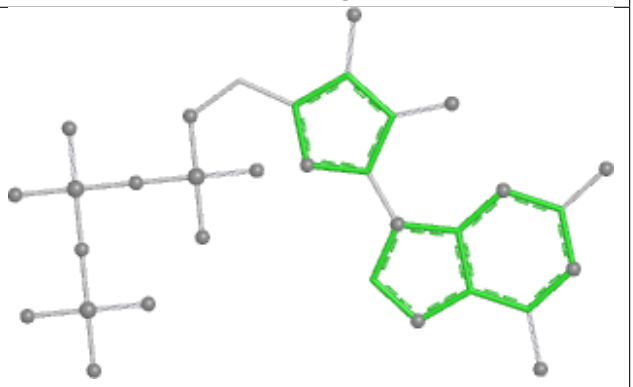
Bond lengths



Bond angles

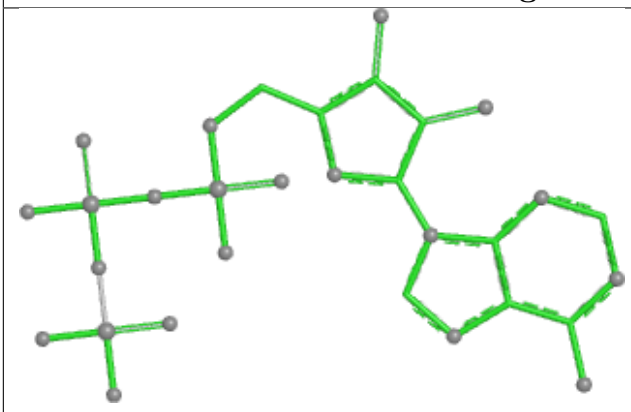


Torsions

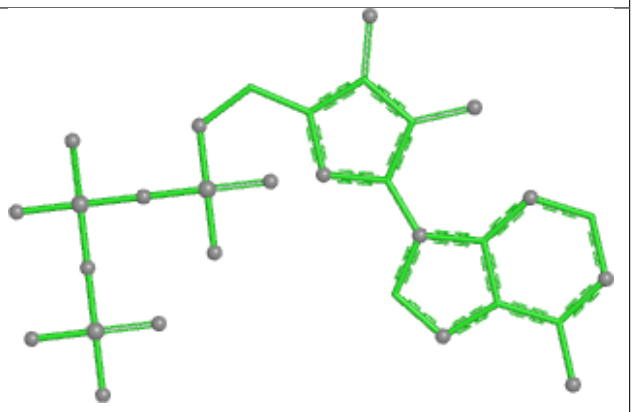


Rings

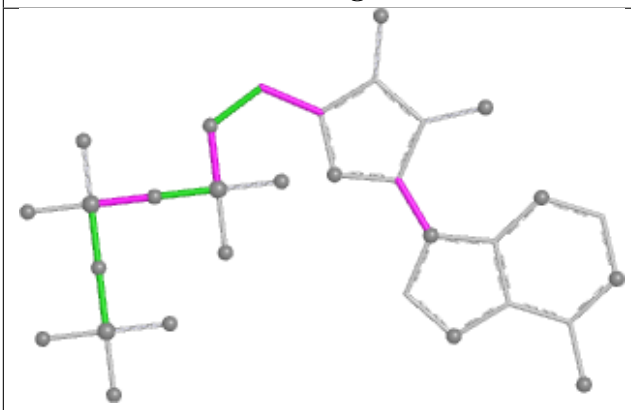
Ligand ATP 2x 501



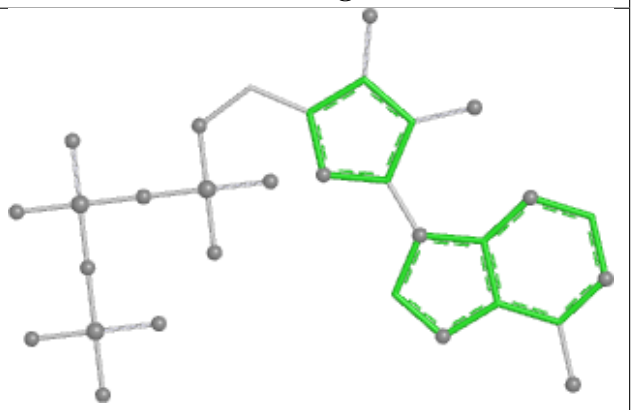
Bond lengths



Bond angles

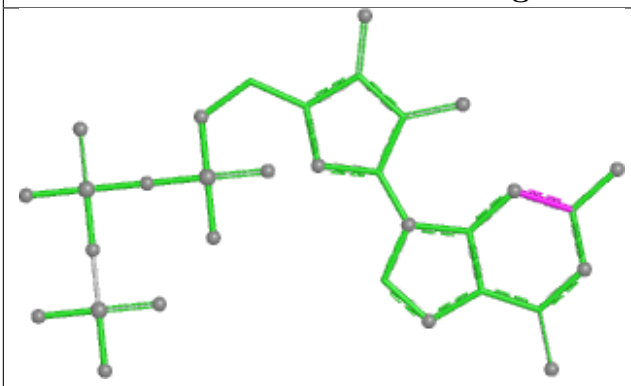


Torsions

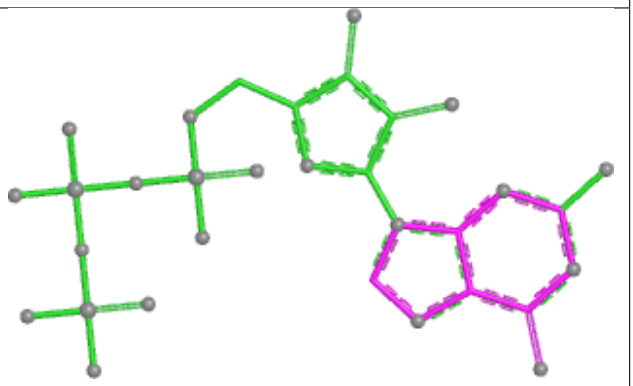


Rings

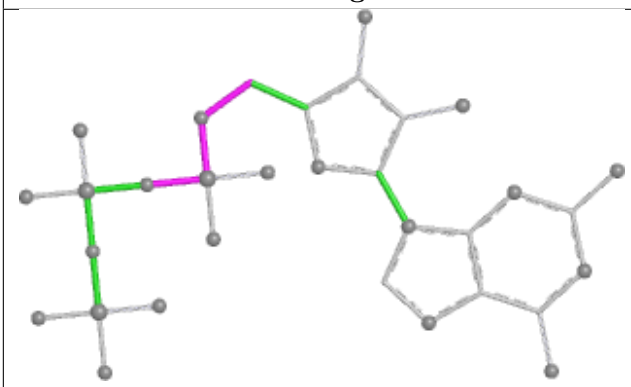
Ligand GTP IM 501



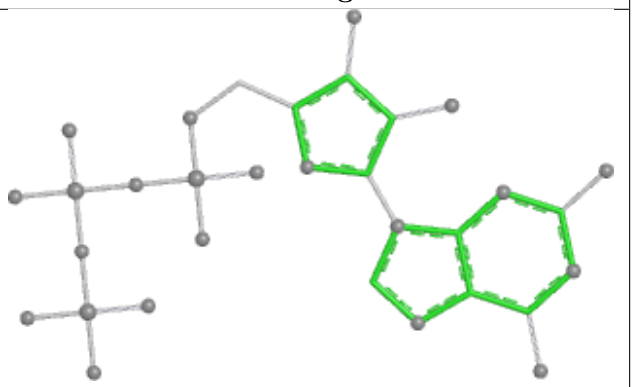
Bond lengths



Bond angles

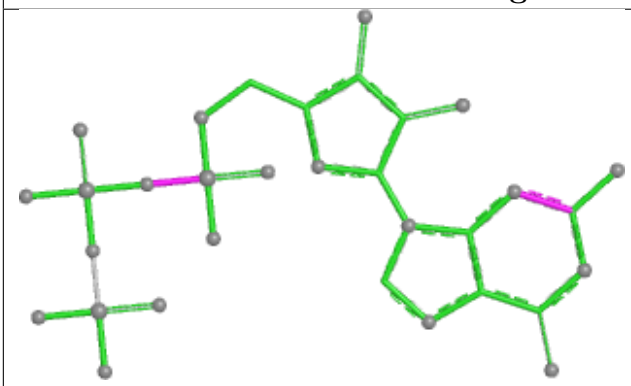


Torsions

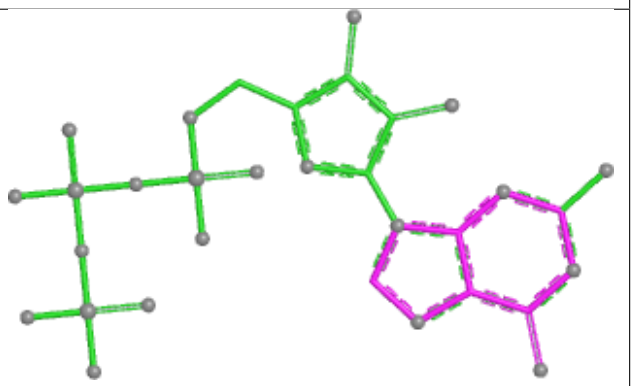


Rings

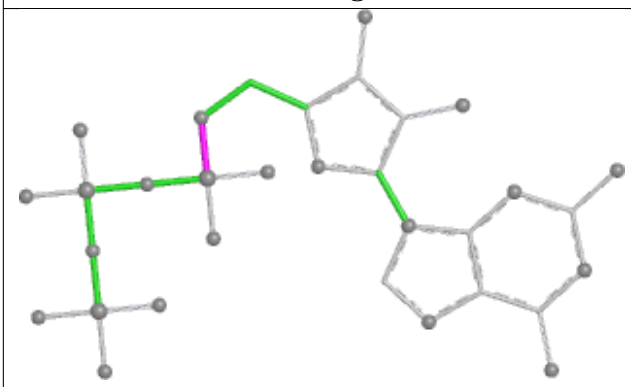
Ligand GTP RB 501



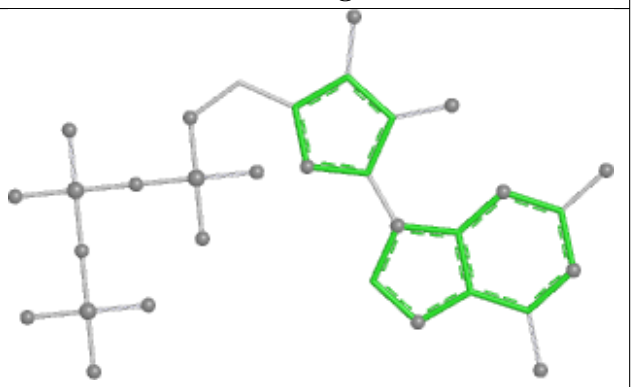
Bond lengths



Bond angles

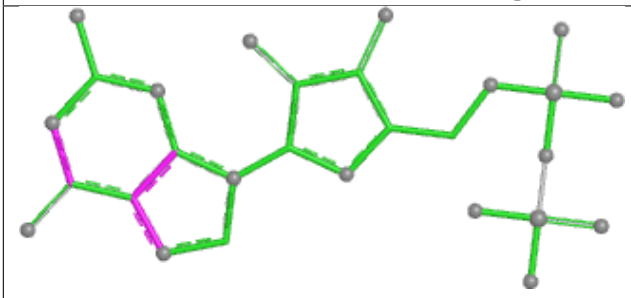


Torsions

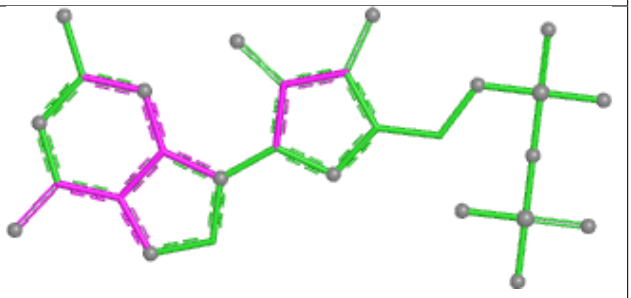


Rings

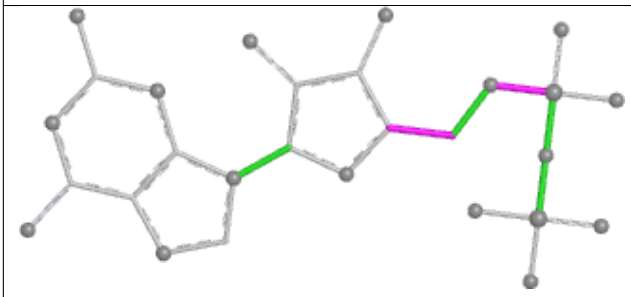
Ligand GDP EN 500



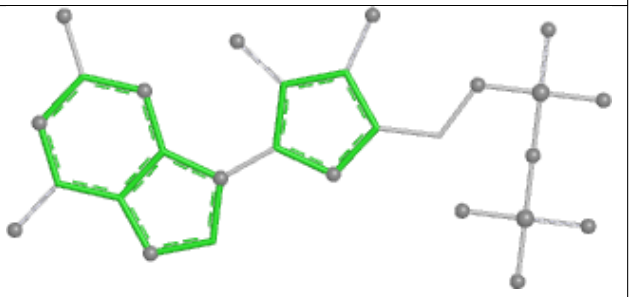
Bond lengths



Bond angles

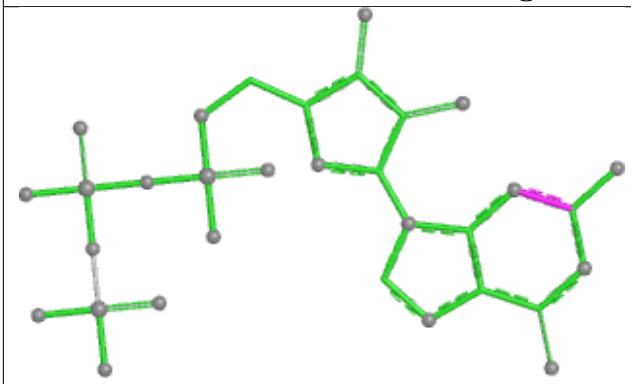


Torsions

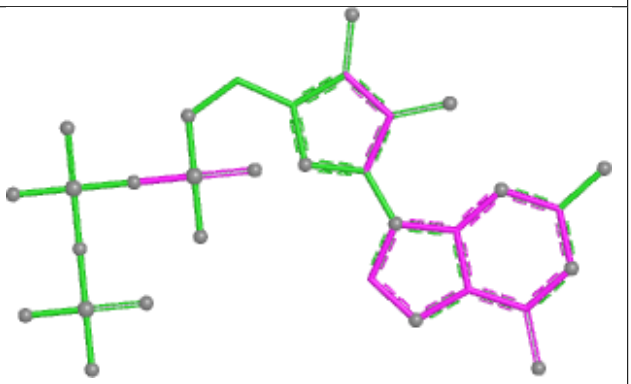


Rings

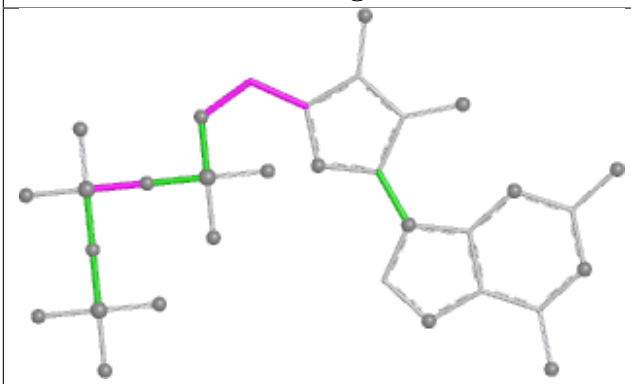
Ligand GTP FI 501



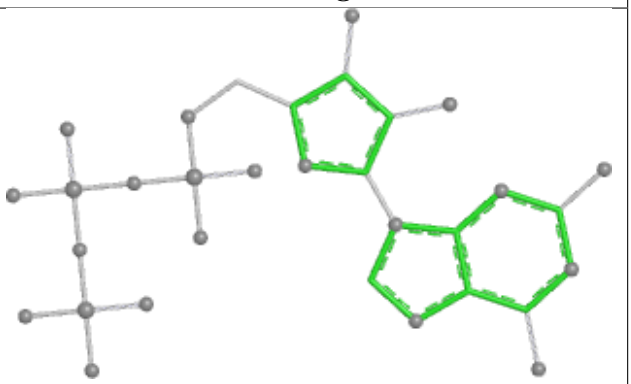
Bond lengths



Bond angles

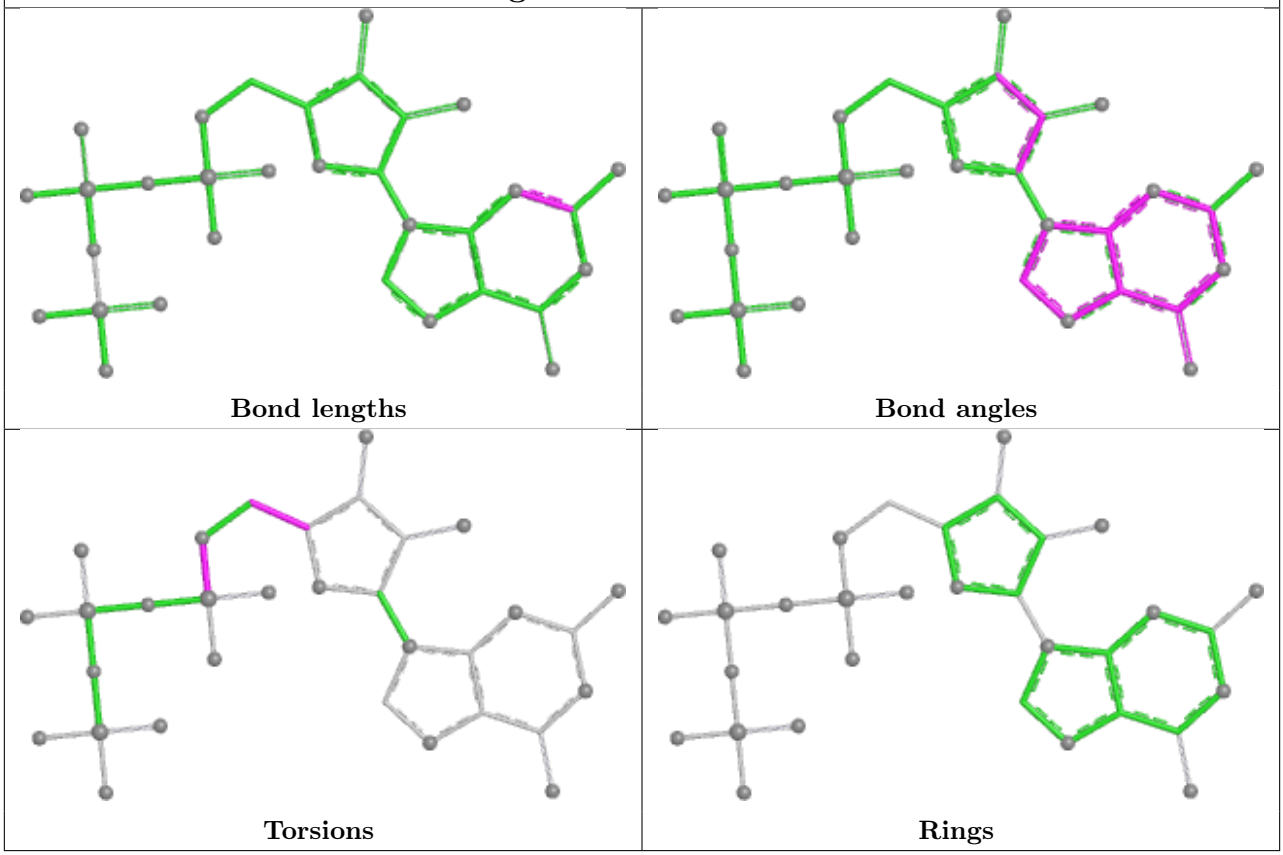


Torsions

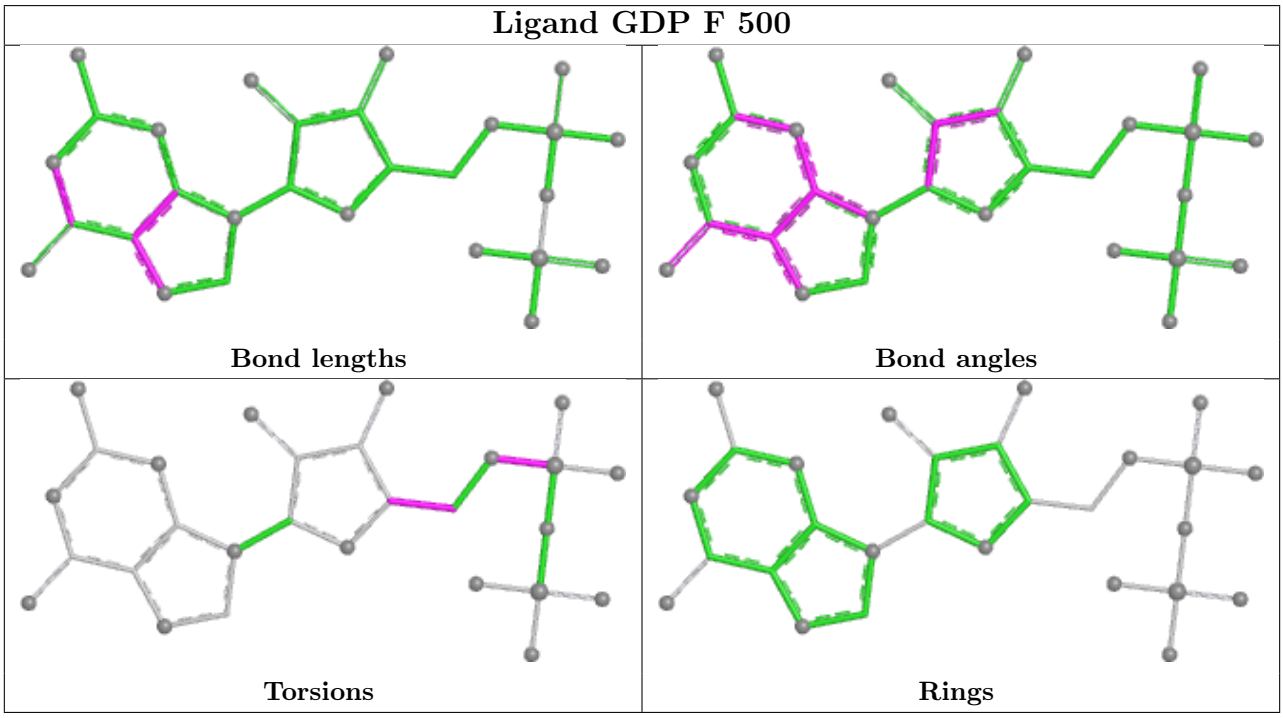


Rings

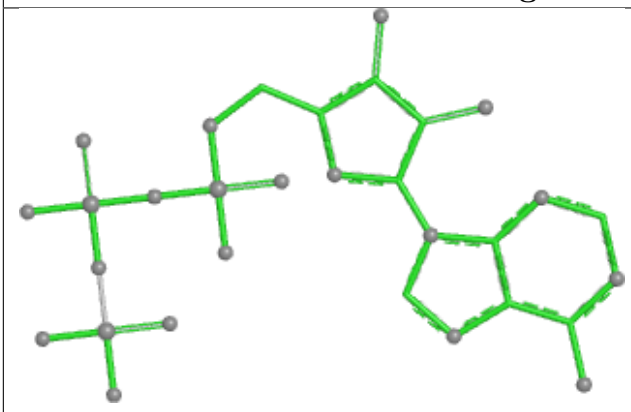
Ligand GTP UG 501



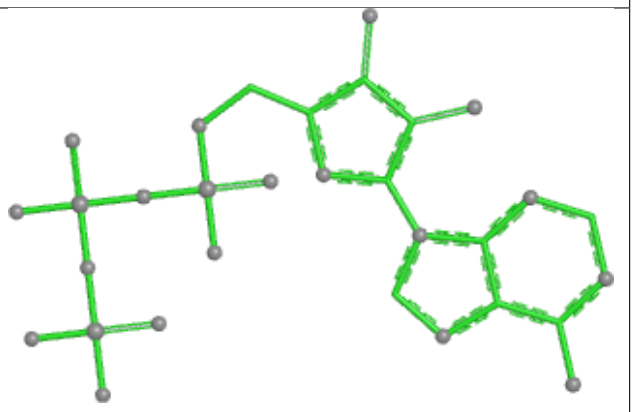
Ligand GDP F 500



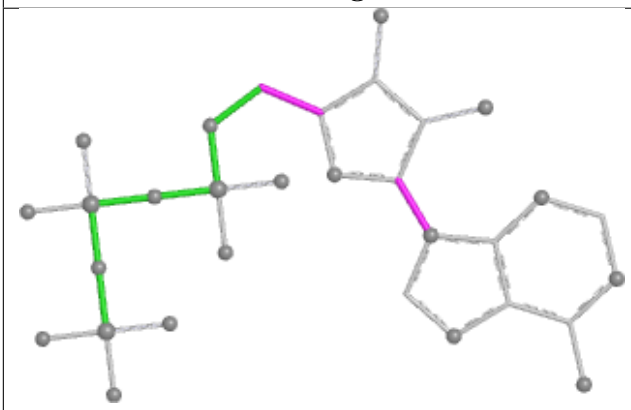
Ligand ATP 2v 501



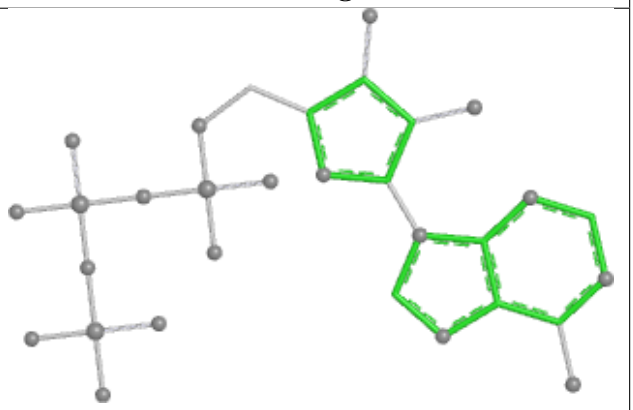
Bond lengths



Bond angles

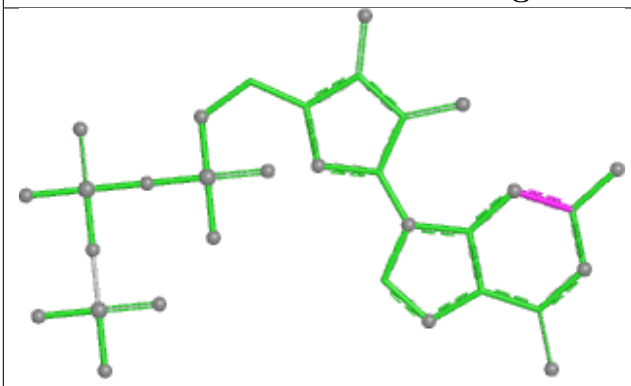


Torsions

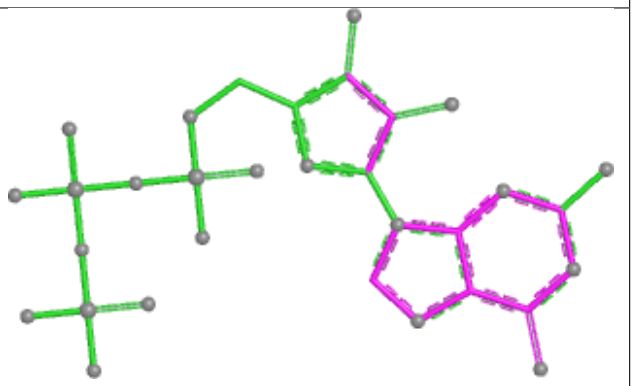


Rings

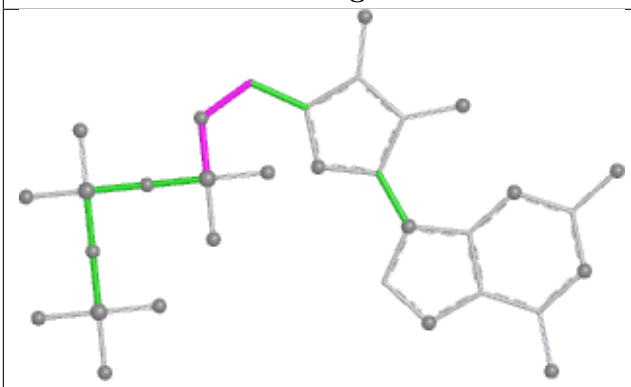
Ligand GTP OS 501



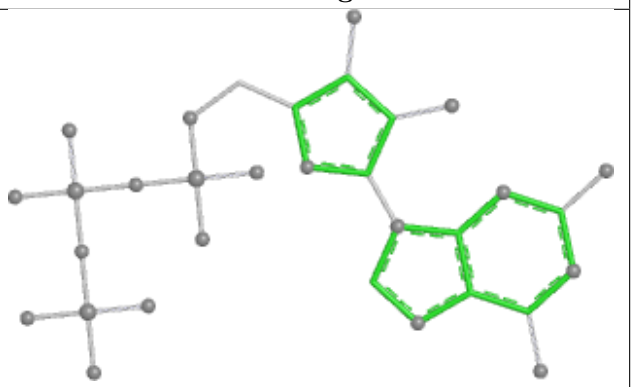
Bond lengths



Bond angles

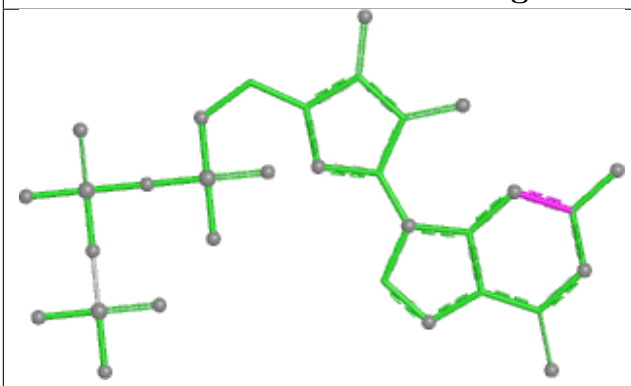


Torsions

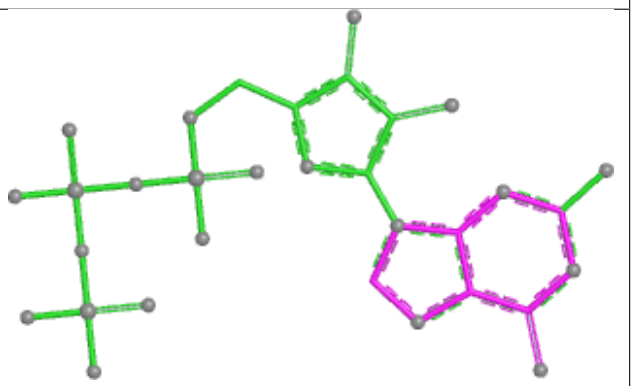


Rings

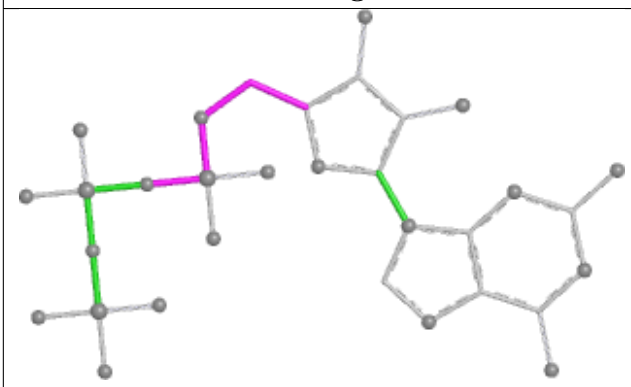
Ligand GTP LD 502



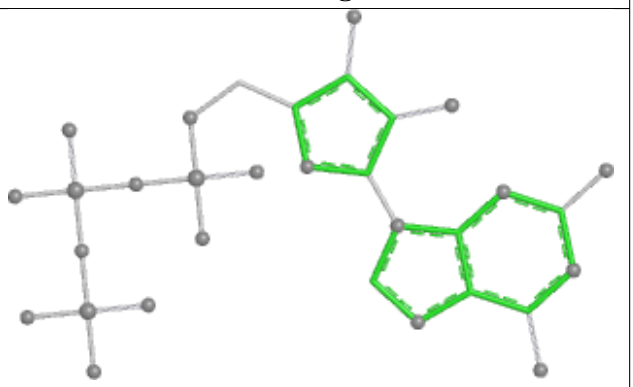
Bond lengths



Bond angles

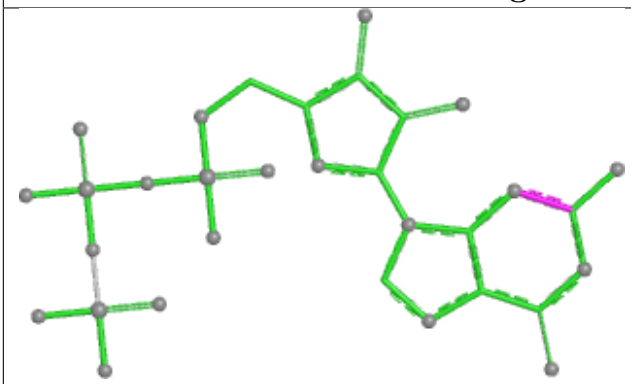


Torsions

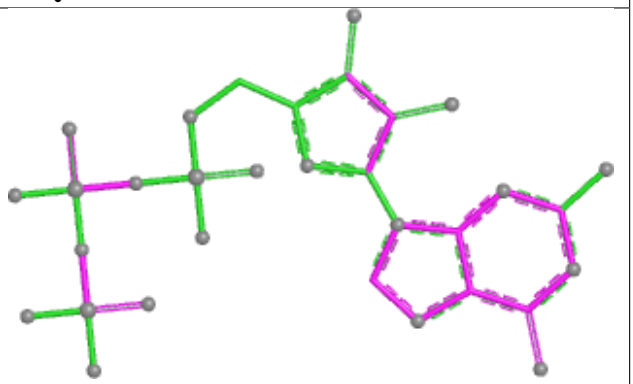


Rings

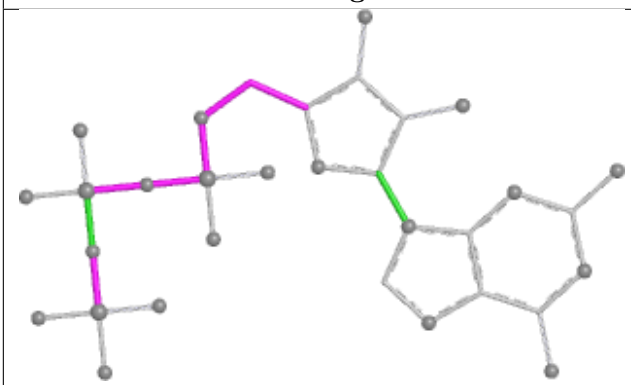
Ligand GTP QT 501



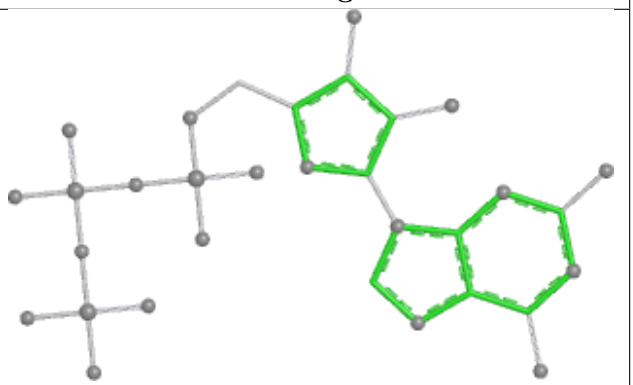
Bond lengths



Bond angles

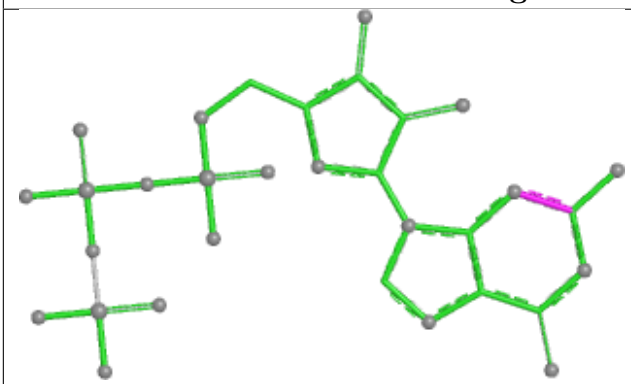


Torsions

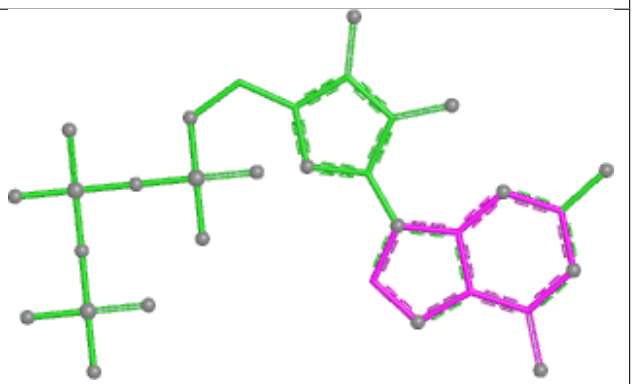


Rings

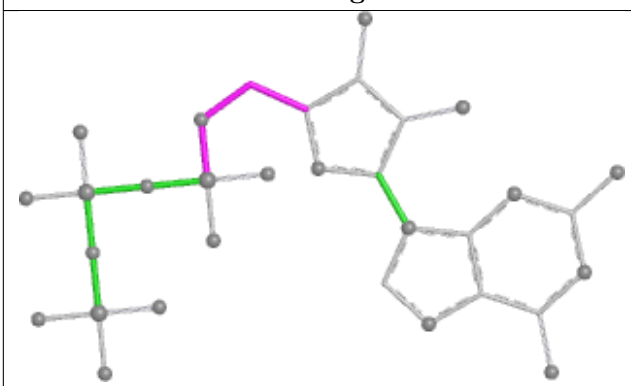
Ligand GTP TO 501



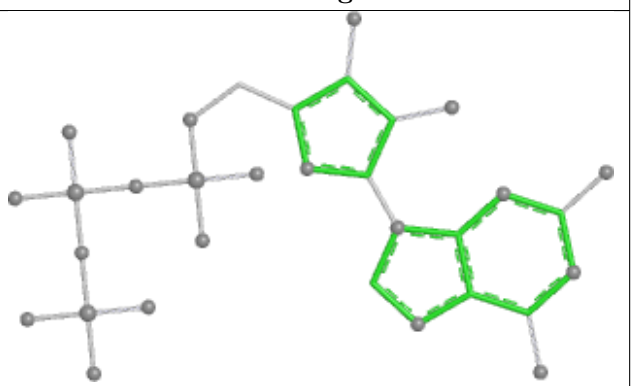
Bond lengths



Bond angles

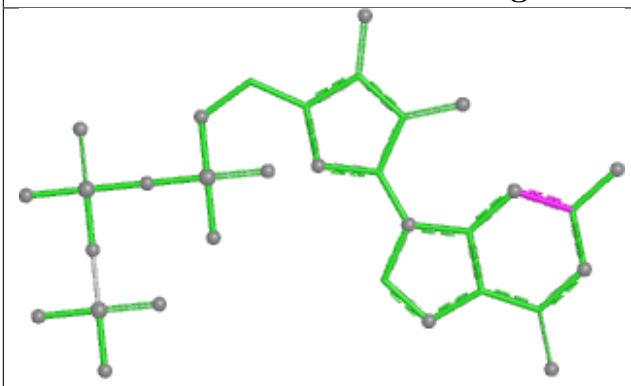


Torsions

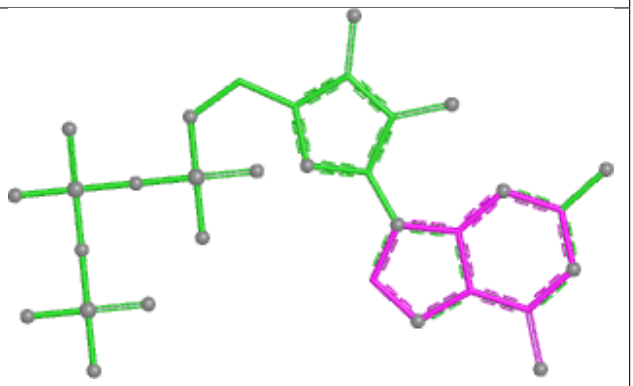


Rings

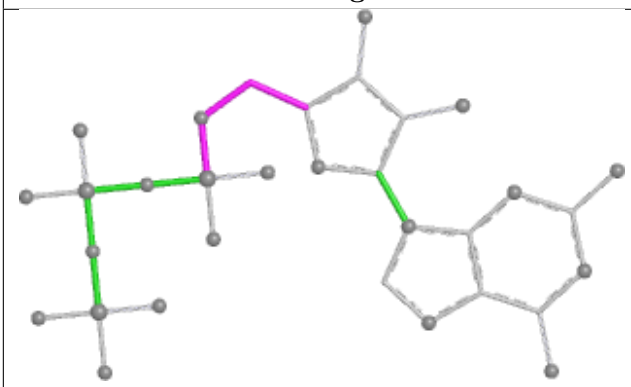
Ligand GTP TC 501



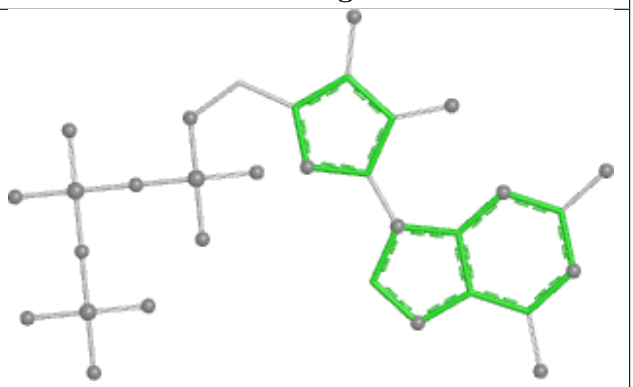
Bond lengths



Bond angles

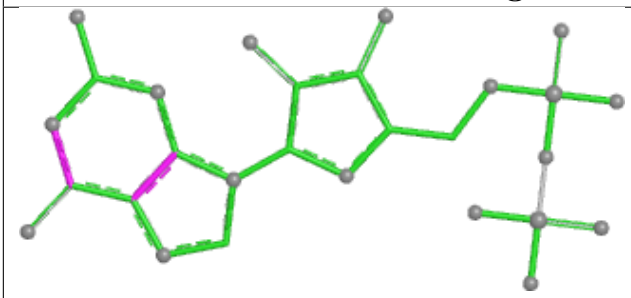


Torsions

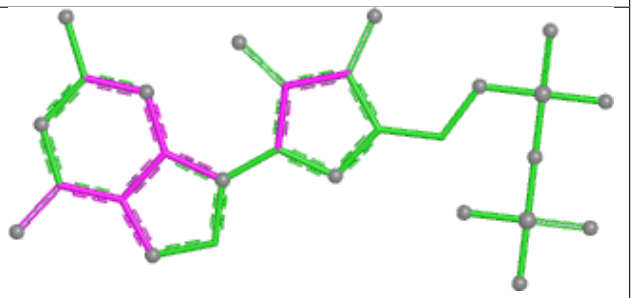


Rings

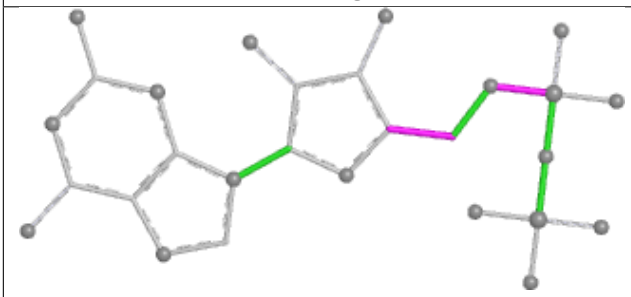
Ligand GDP HN 501



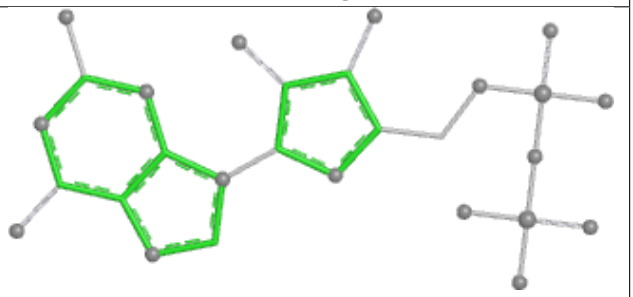
Bond lengths



Bond angles

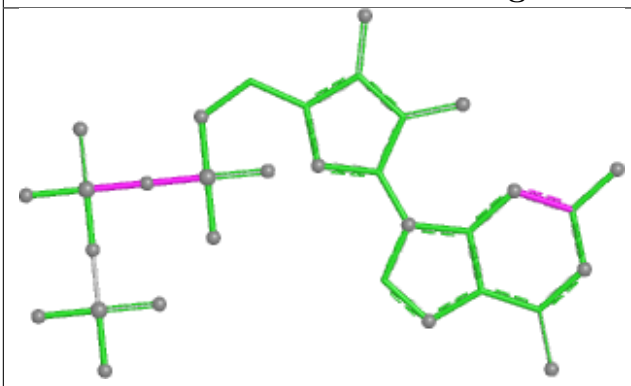


Torsions

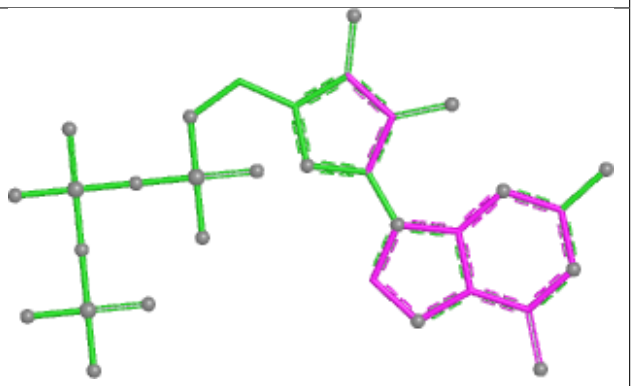


Rings

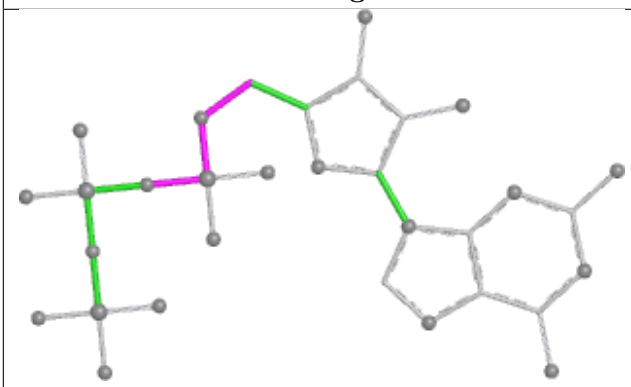
Ligand GTP NR 501



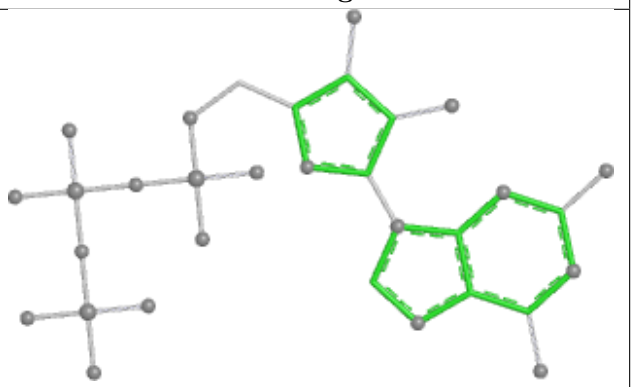
Bond lengths



Bond angles

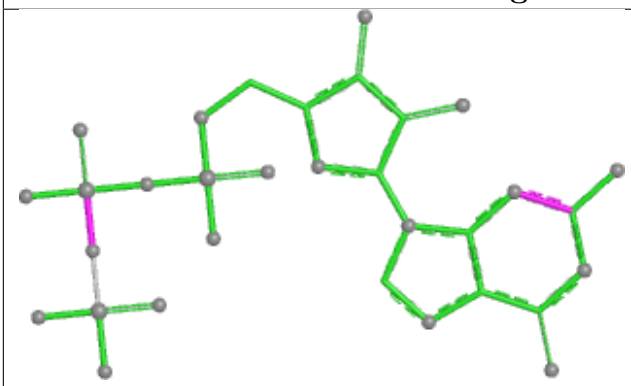


Torsions

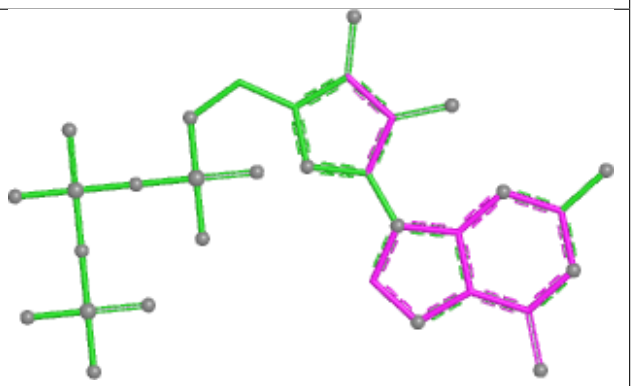


Rings

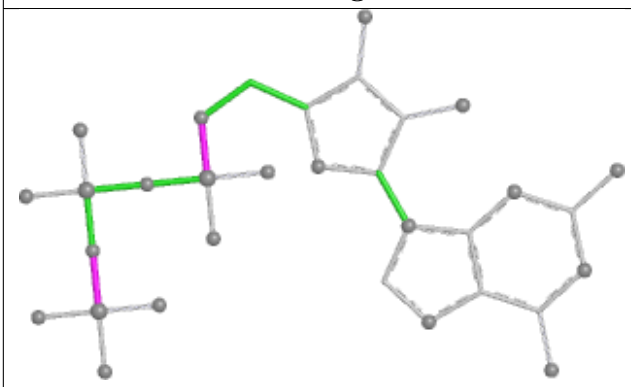
Ligand GTP KF 501



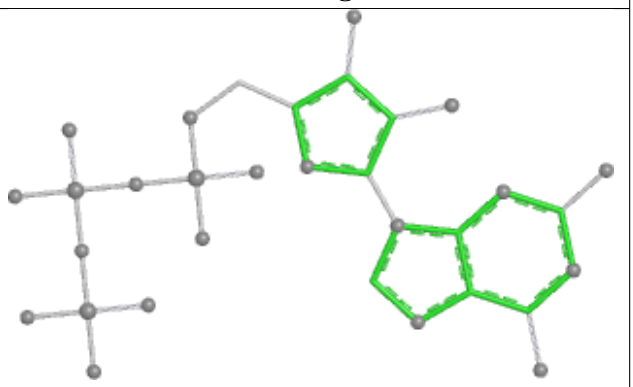
Bond lengths



Bond angles

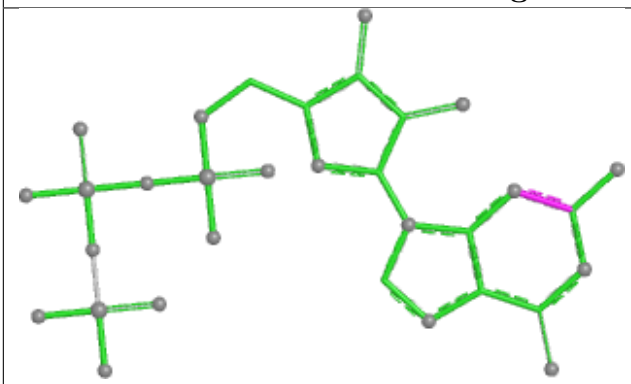


Torsions

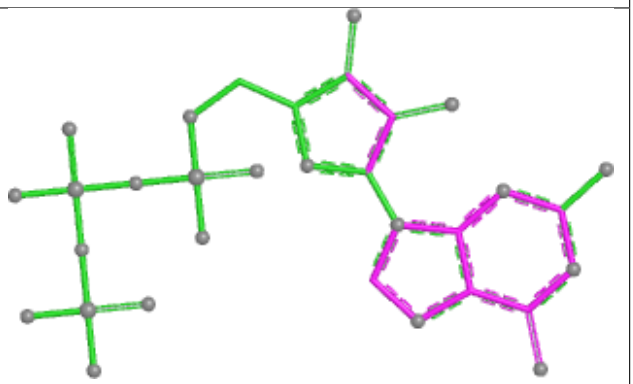


Rings

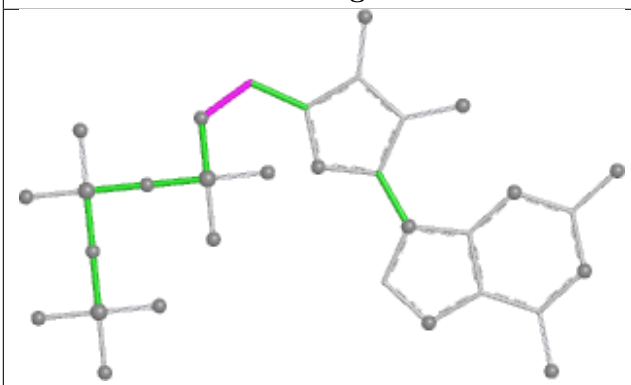
Ligand GTP VE 501



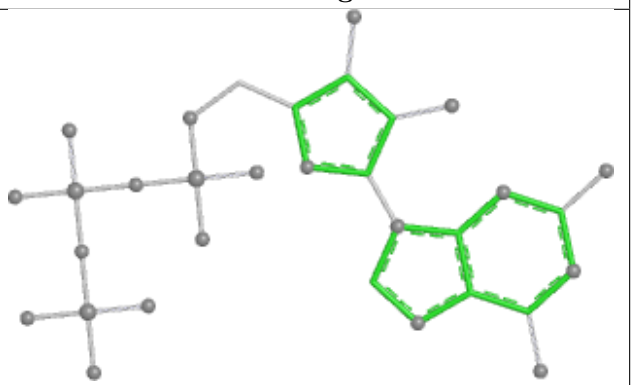
Bond lengths



Bond angles

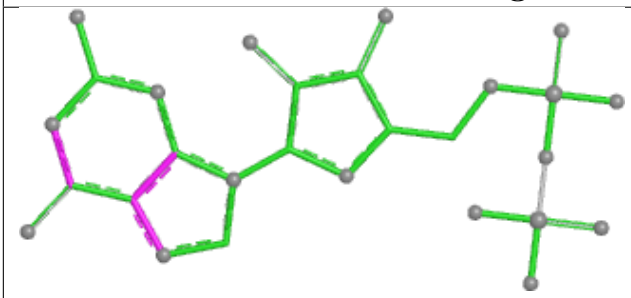


Torsions

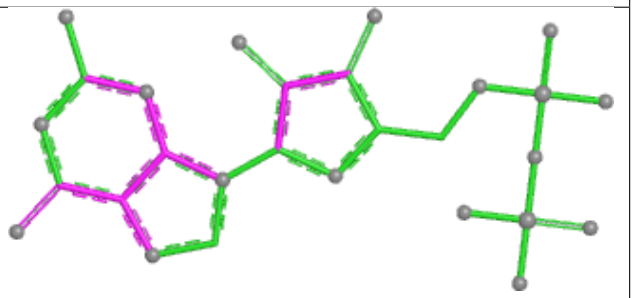


Rings

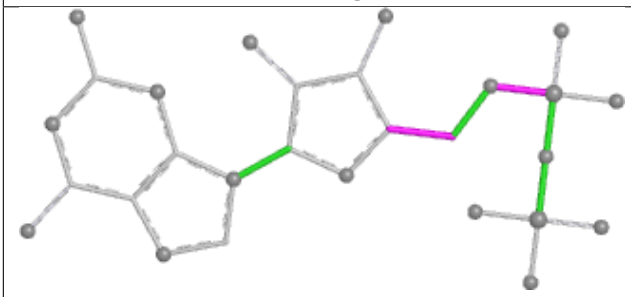
Ligand GDP NF 500



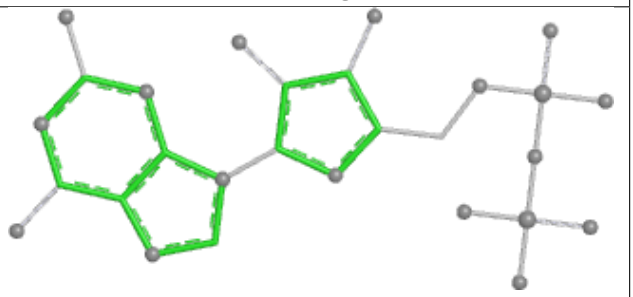
Bond lengths



Bond angles

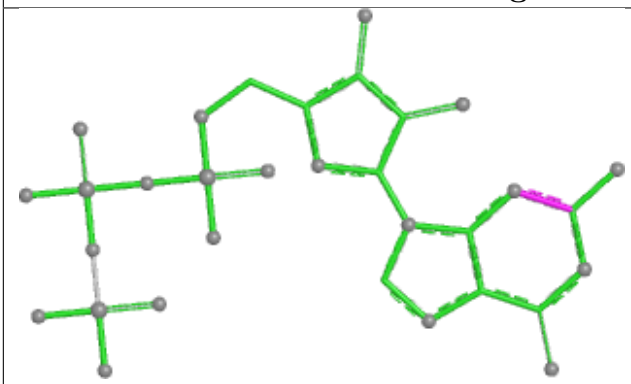


Torsions

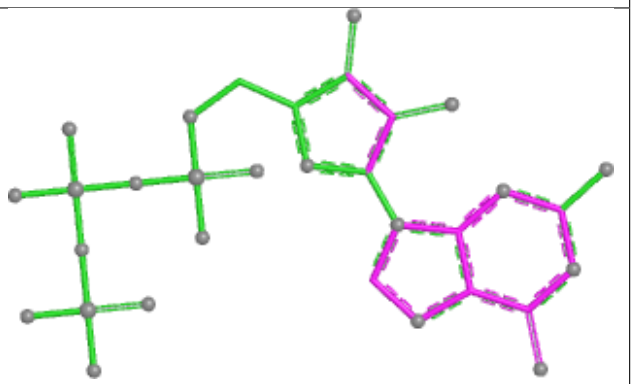


Rings

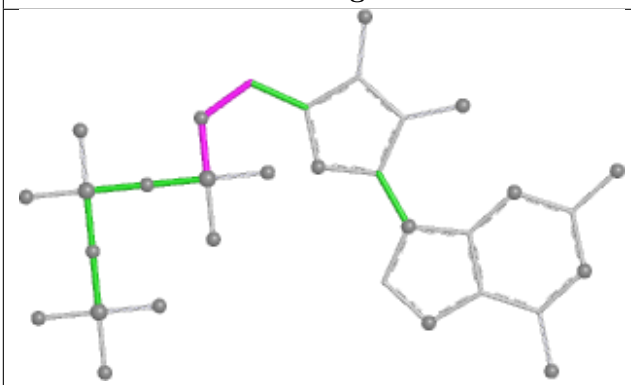
Ligand GTP VT 501



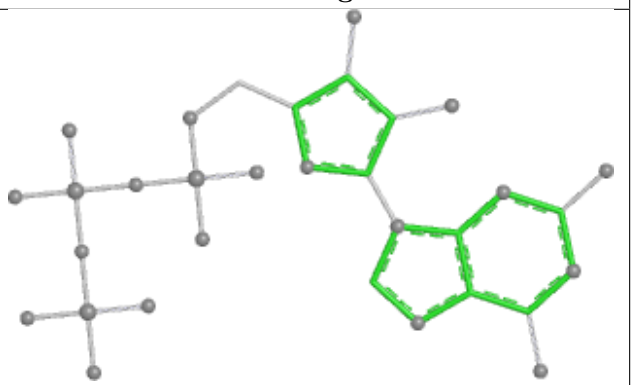
Bond lengths



Bond angles

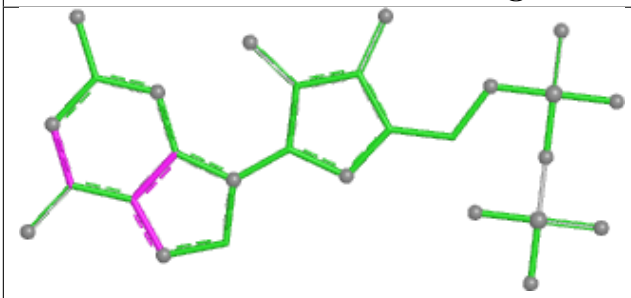


Torsions

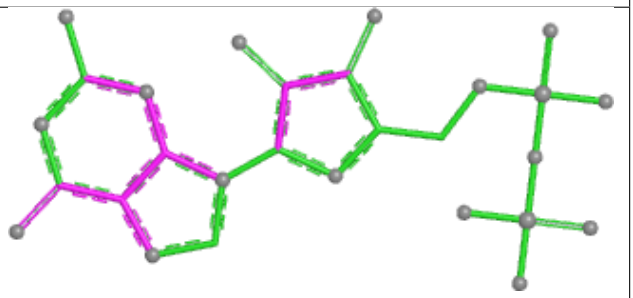


Rings

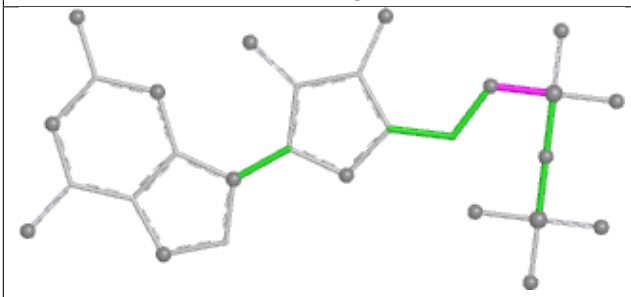
Ligand GDP UR 500



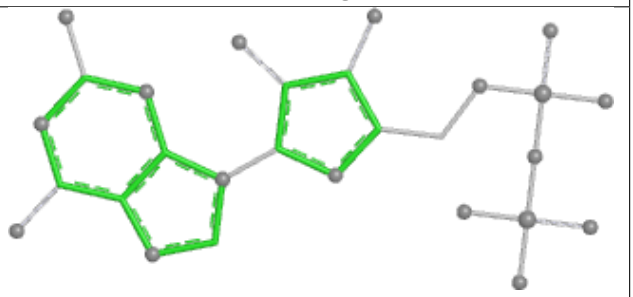
Bond lengths



Bond angles

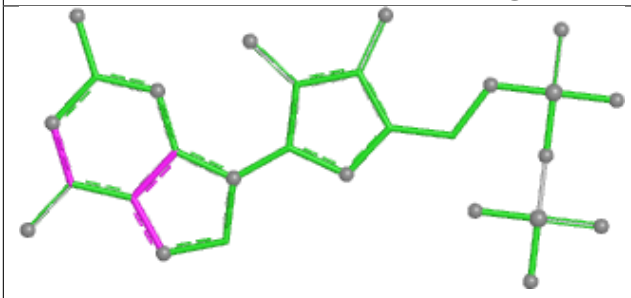


Torsions

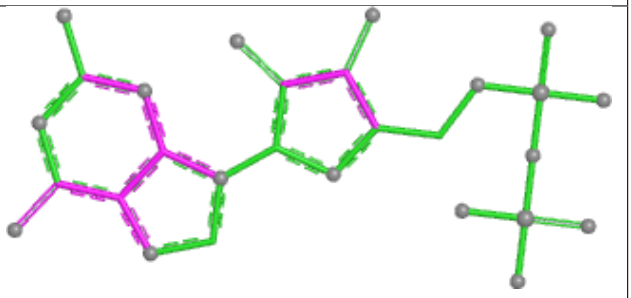


Rings

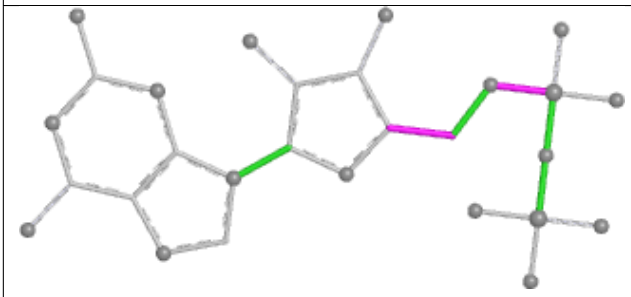
Ligand GDP MF 500



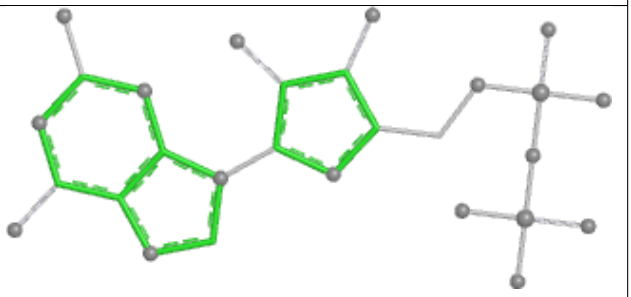
Bond lengths



Bond angles

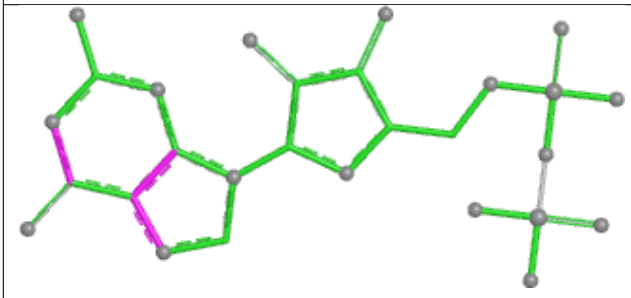


Torsions

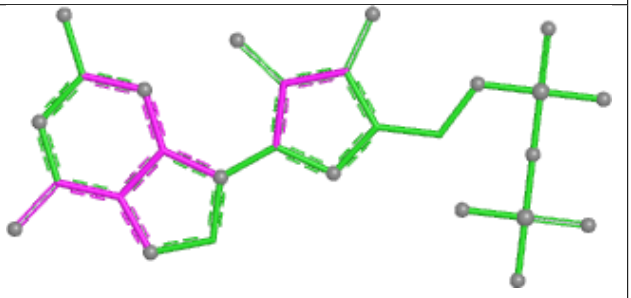


Rings

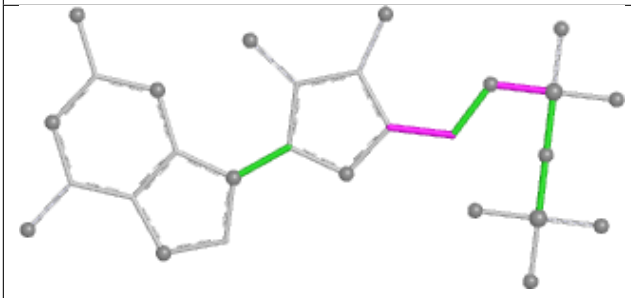
Ligand GDP KU 500



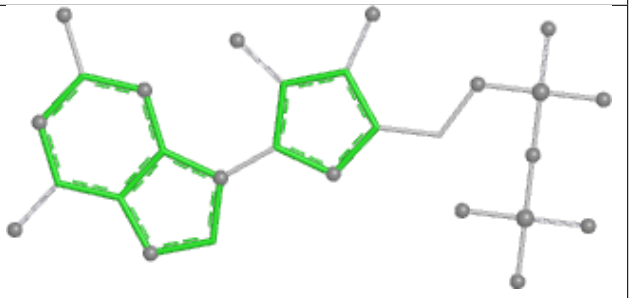
Bond lengths



Bond angles

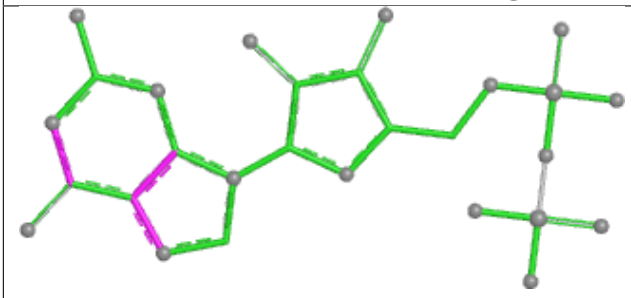


Torsions

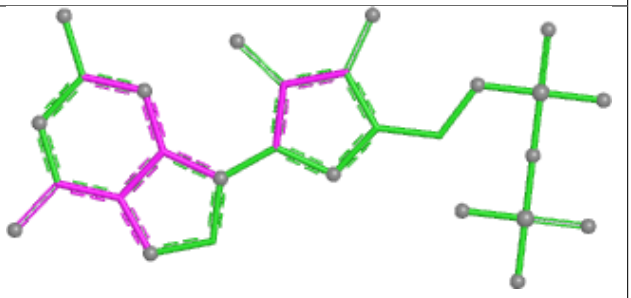


Rings

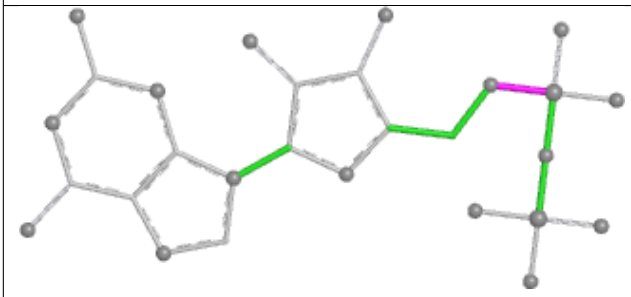
Ligand GDP MP 500



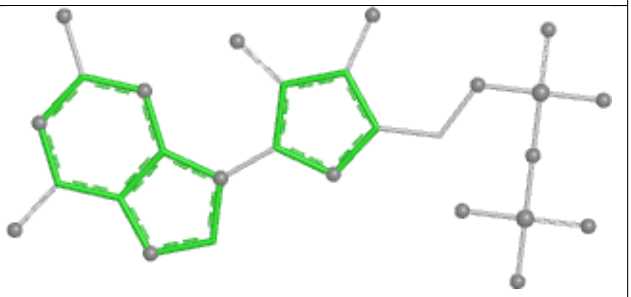
Bond lengths



Bond angles

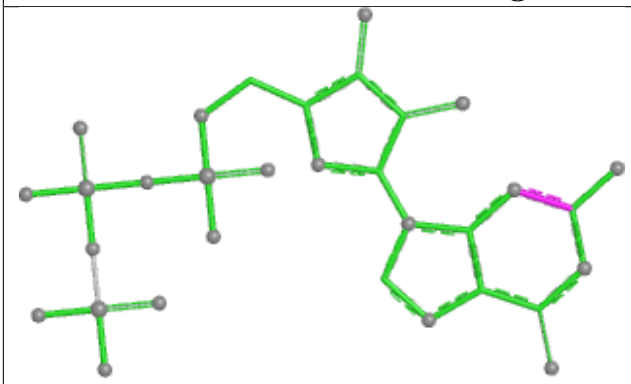


Torsions

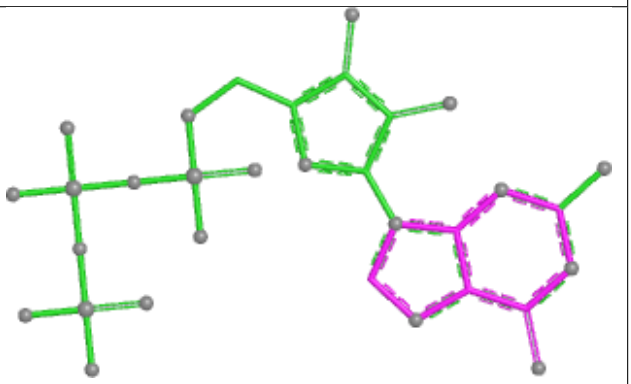


Rings

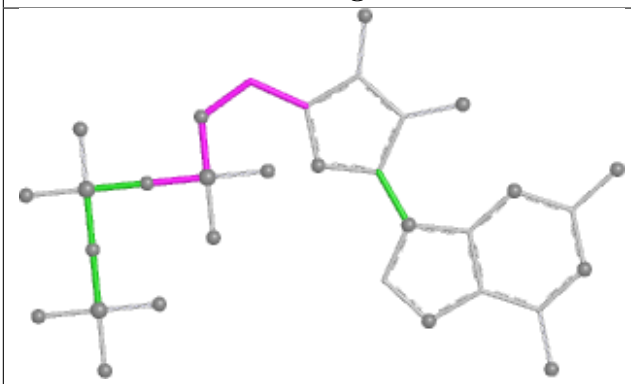
Ligand GTP TK 501



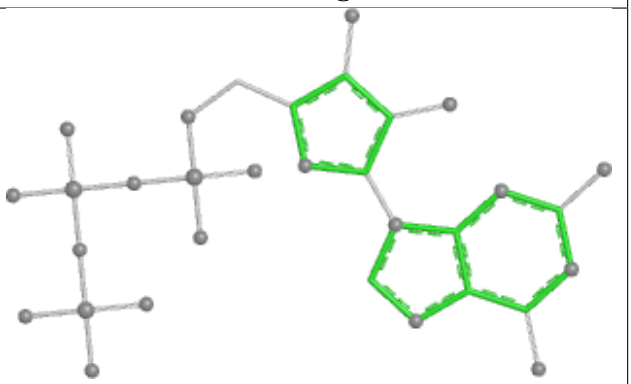
Bond lengths



Bond angles

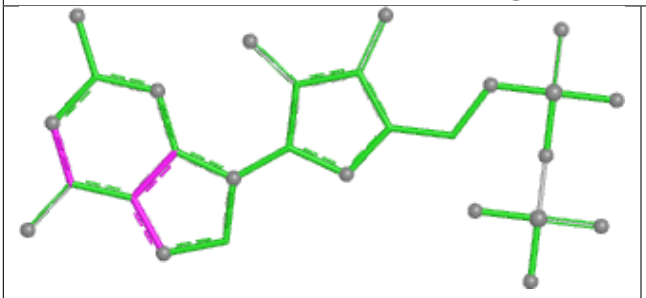


Torsions

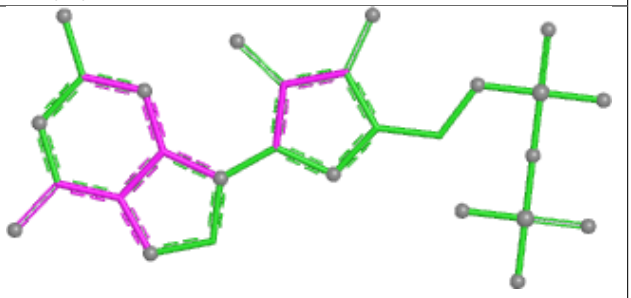


Rings

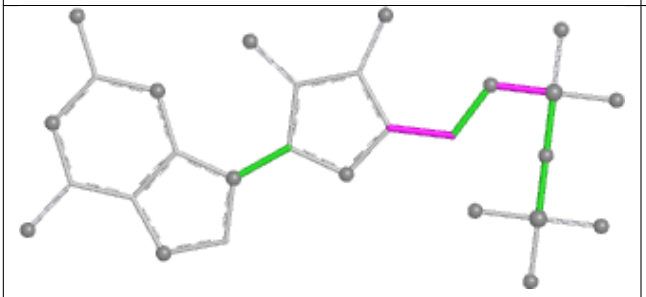
Ligand GDP QQ 500



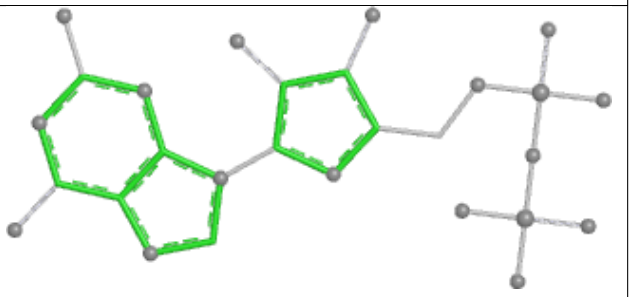
Bond lengths



Bond angles

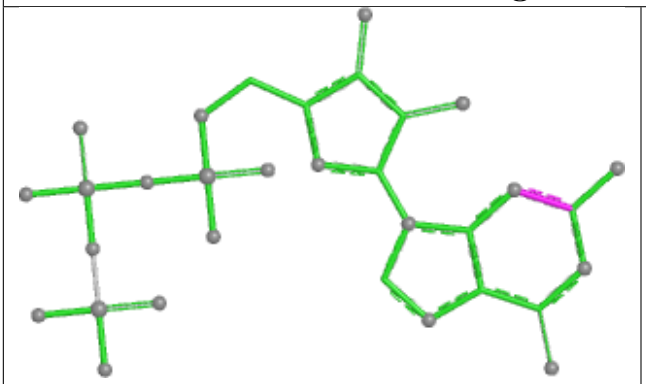


Torsions

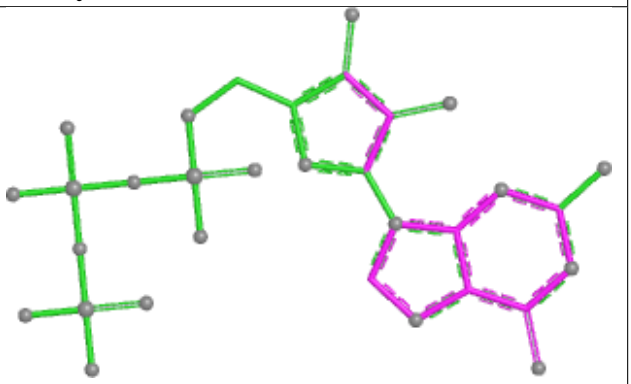


Rings

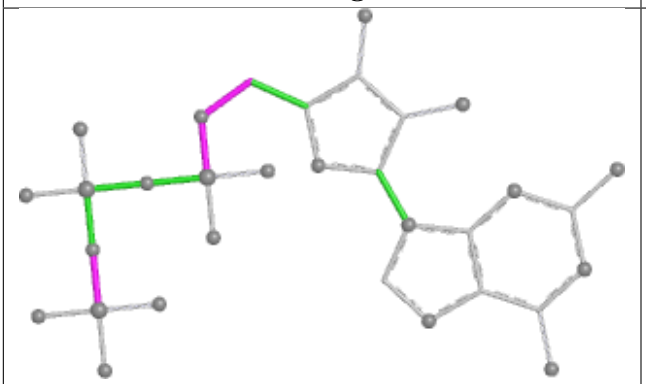
Ligand GTP FQ 501



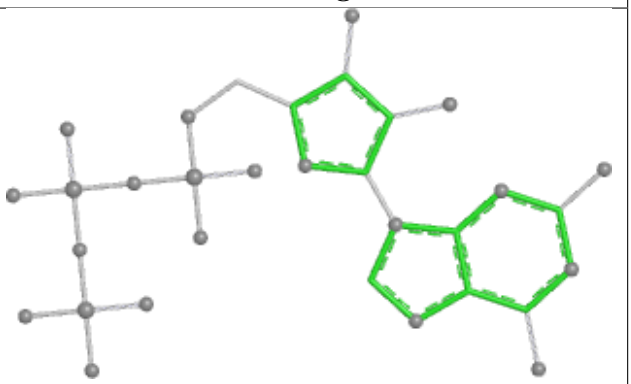
Bond lengths



Bond angles

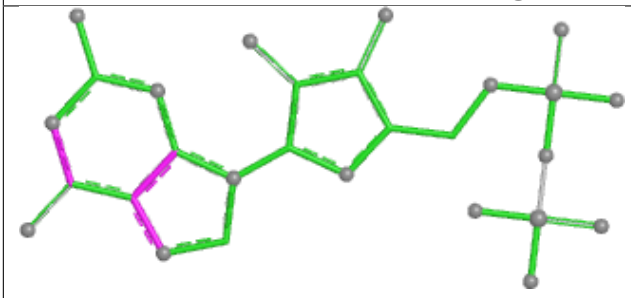


Torsions

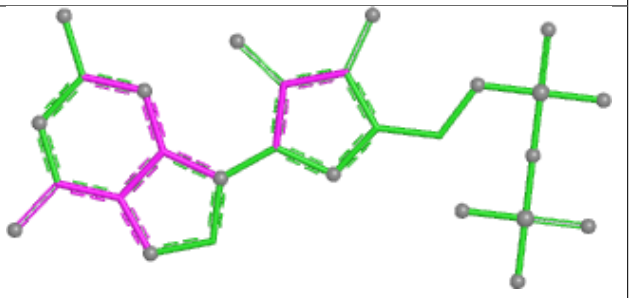


Rings

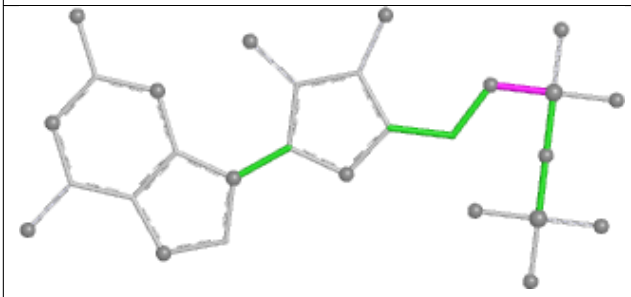
Ligand GDP NL 500



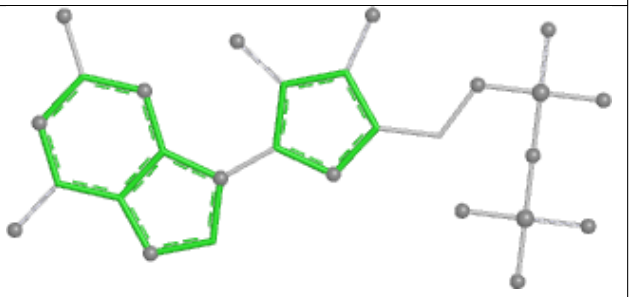
Bond lengths



Bond angles

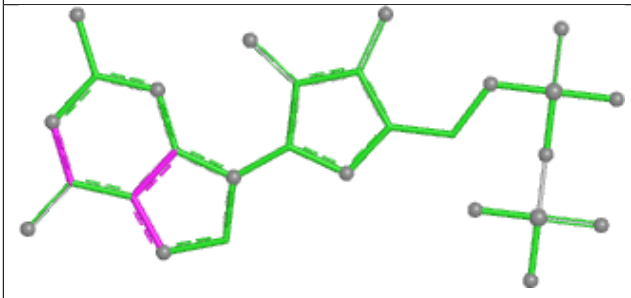


Torsions

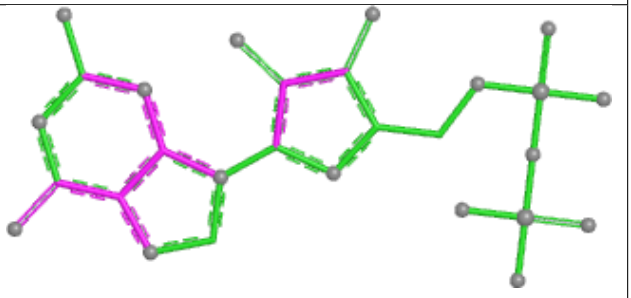


Rings

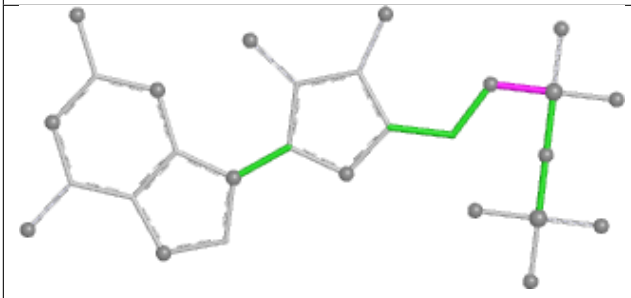
Ligand GDP WT 500



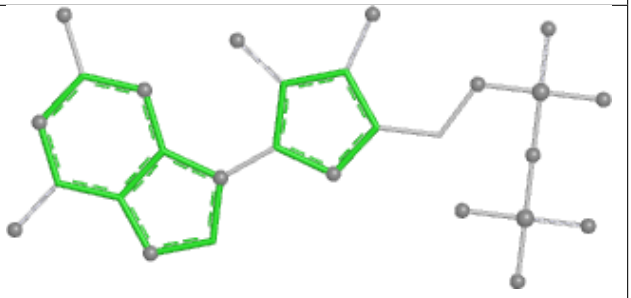
Bond lengths



Bond angles

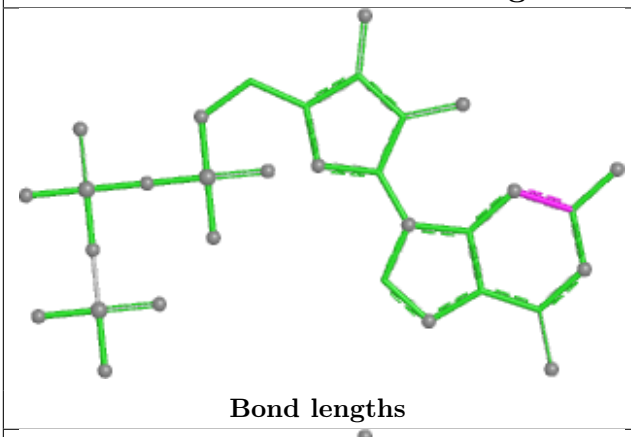


Torsions

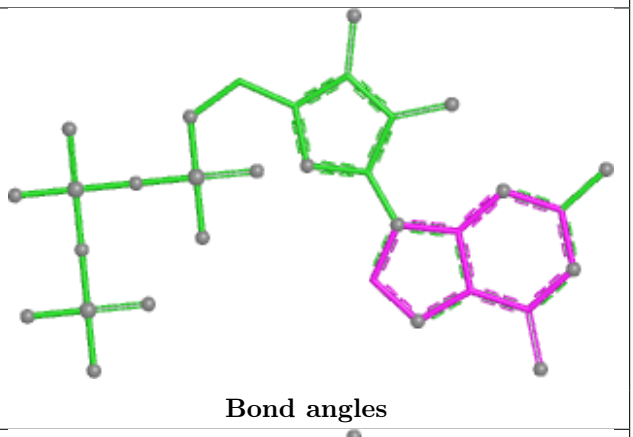


Rings

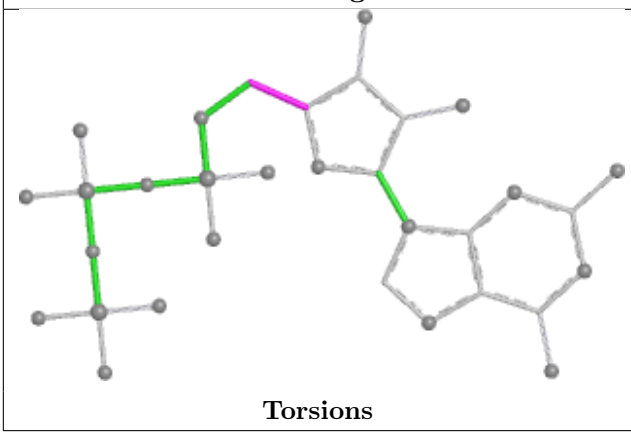
Ligand GTP RH 501



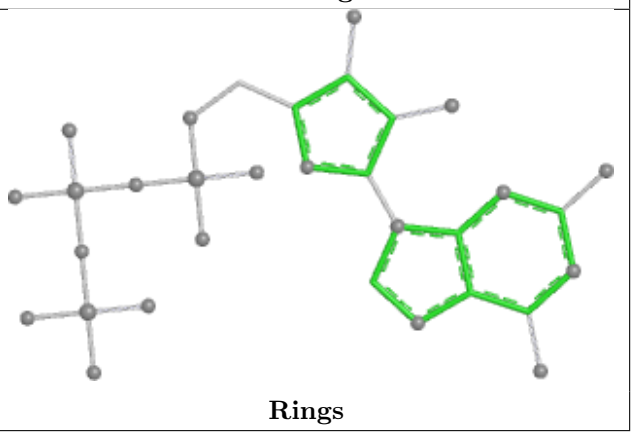
Bond lengths



Bond angles

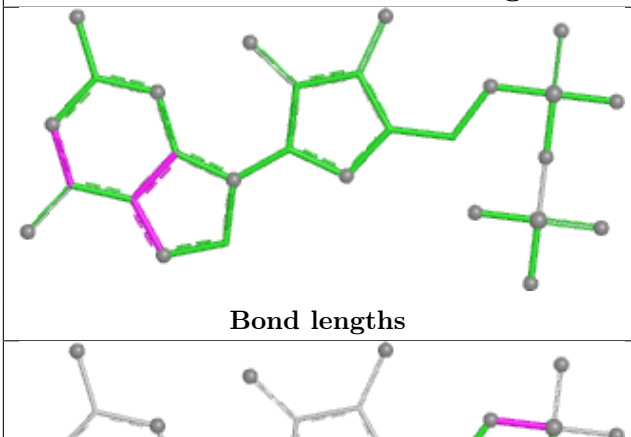


Torsions

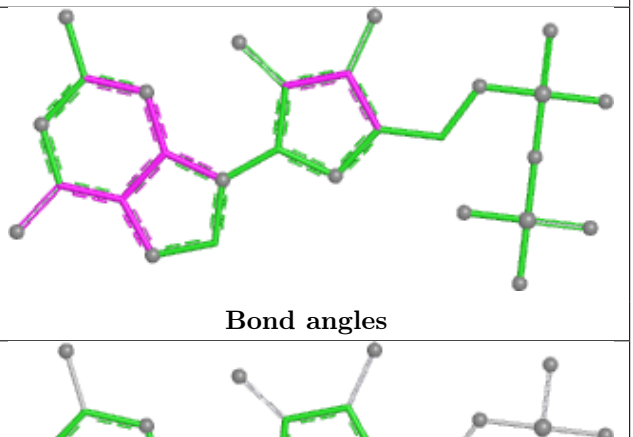


Rings

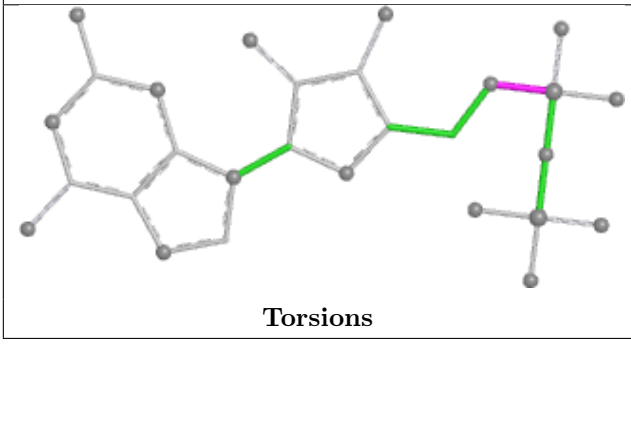
Ligand GDP RM 500



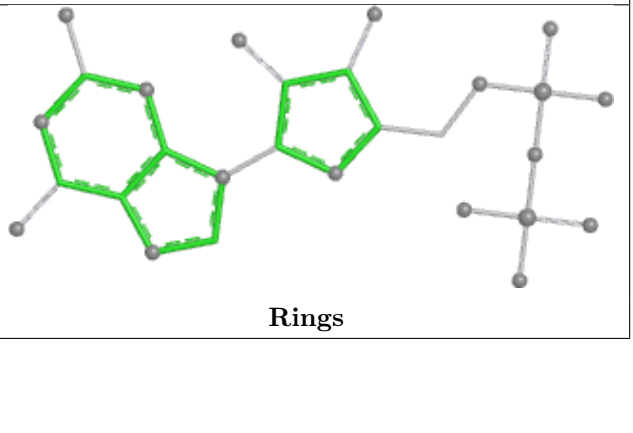
Bond lengths



Bond angles

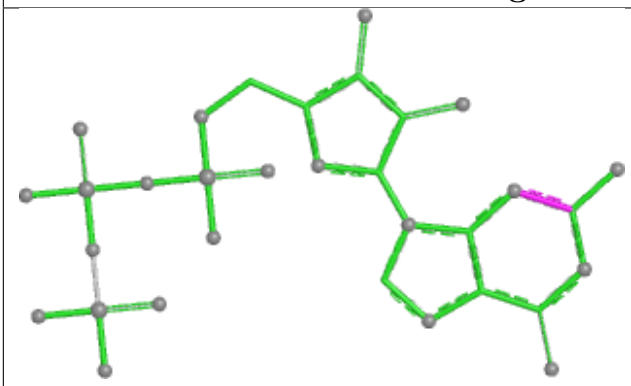


Torsions

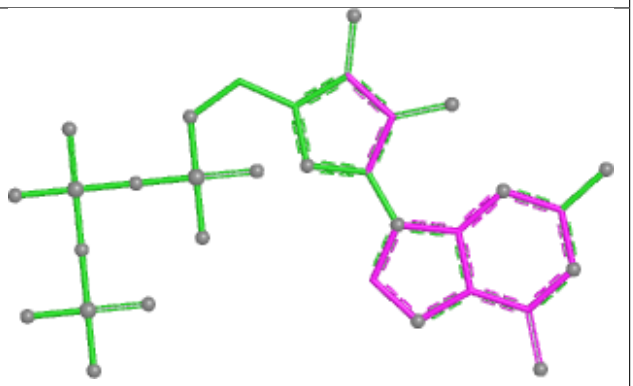


Rings

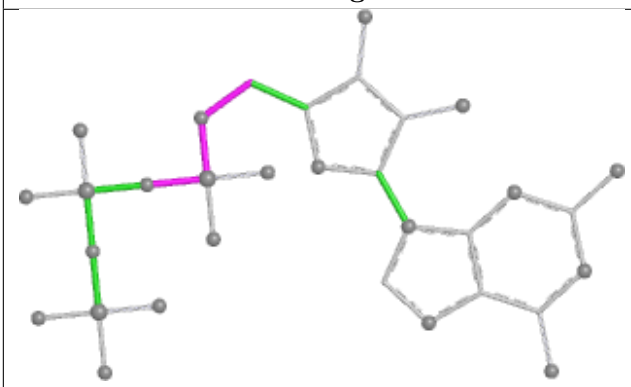
Ligand GTP KB 502



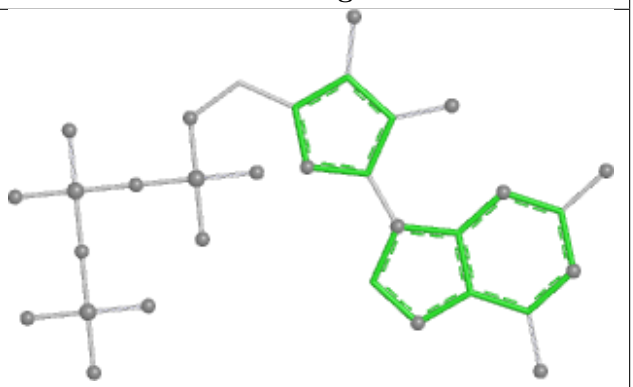
Bond lengths



Bond angles

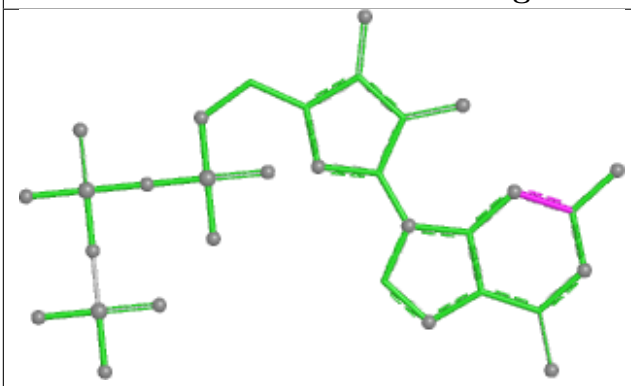


Torsions

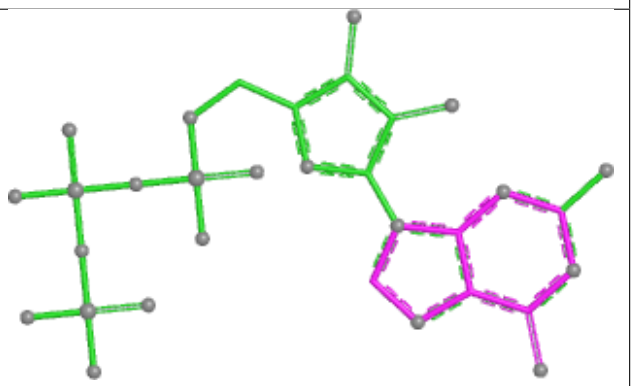


Rings

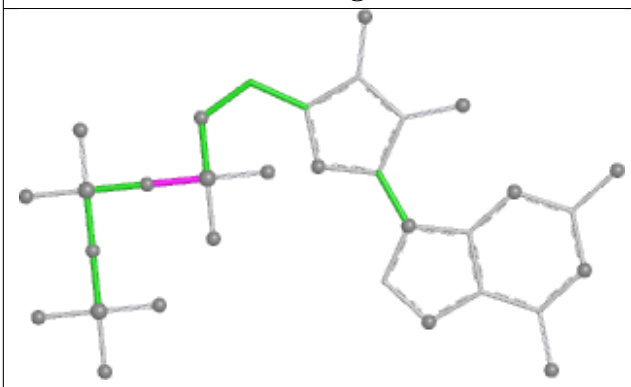
Ligand GTP BS 501



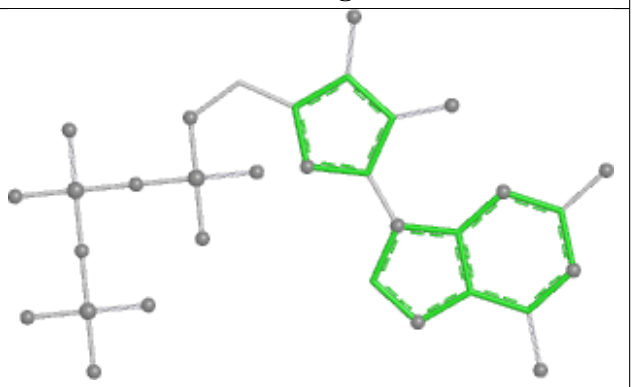
Bond lengths



Bond angles

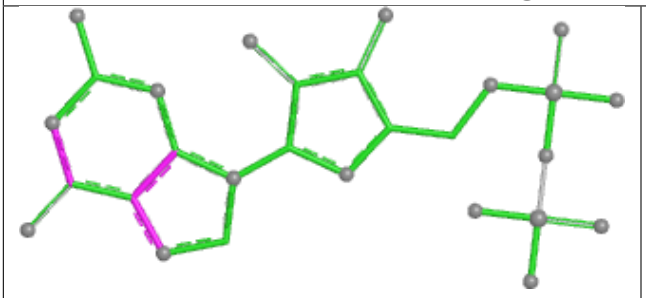


Torsions

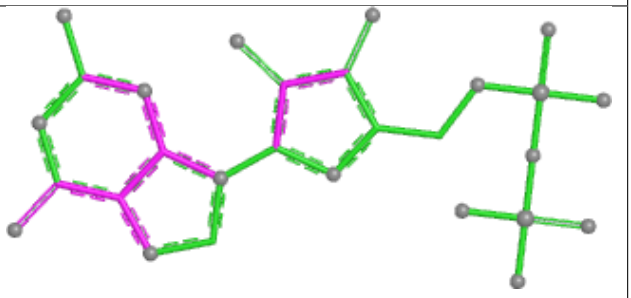


Rings

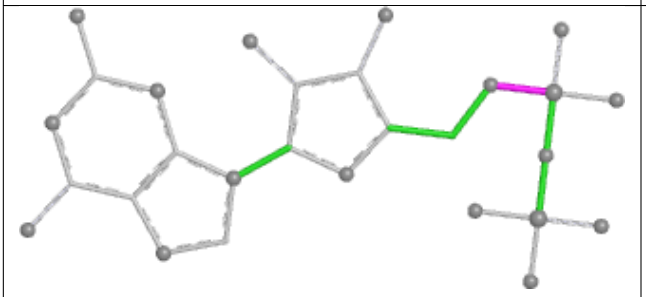
Ligand GDP IJ 500



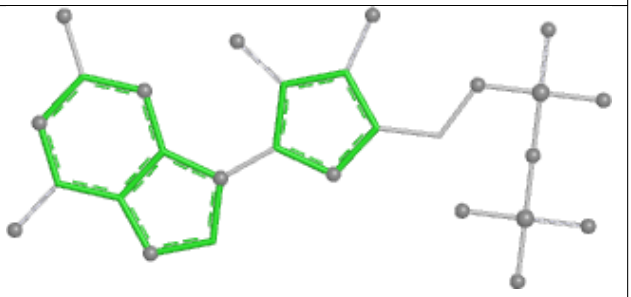
Bond lengths



Bond angles

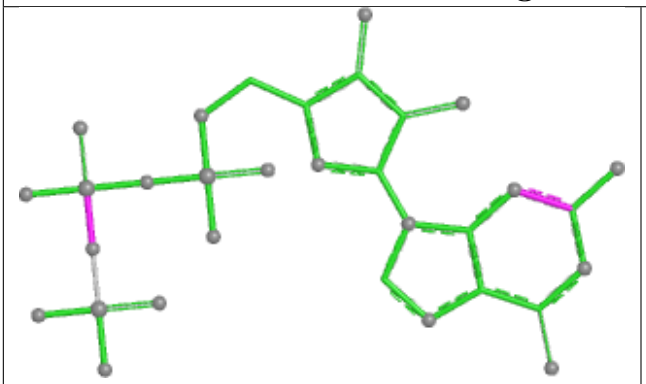


Torsions

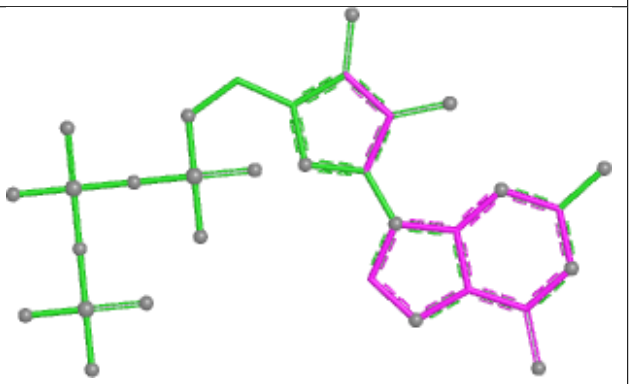


Rings

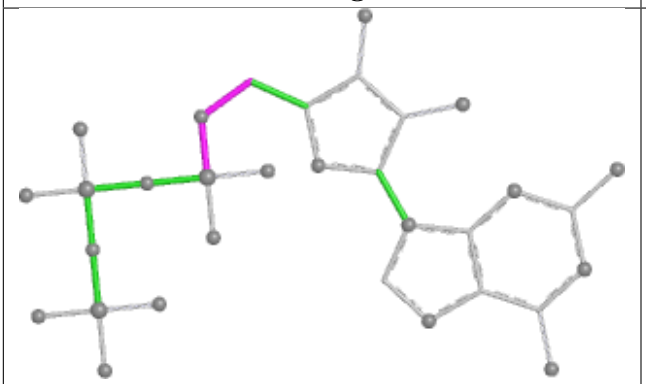
Ligand GTP IC 501



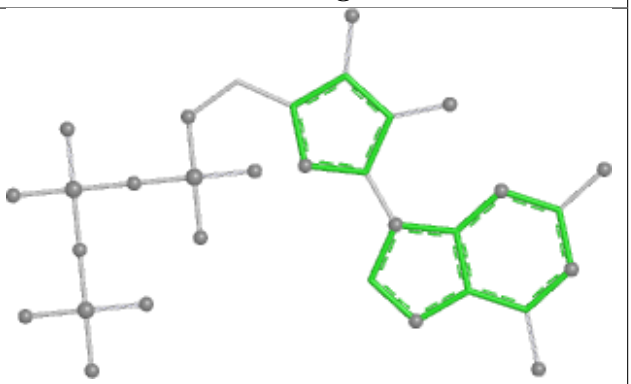
Bond lengths



Bond angles

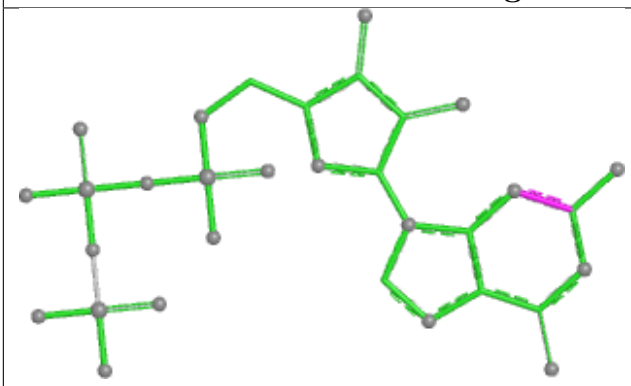


Torsions

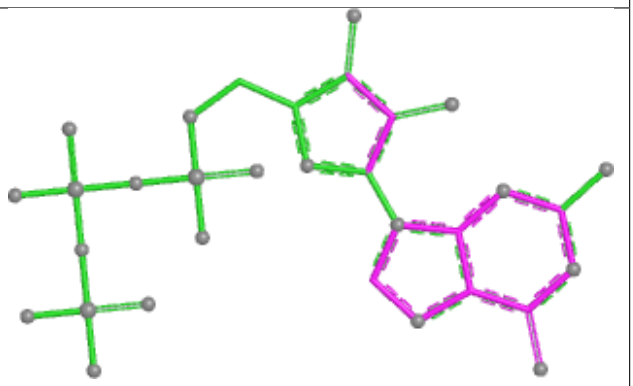


Rings

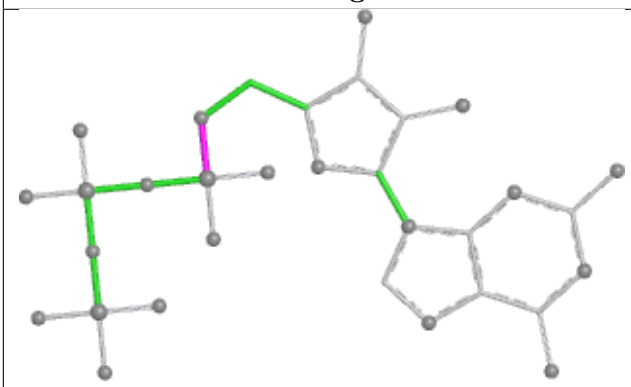
Ligand GTP WO 501



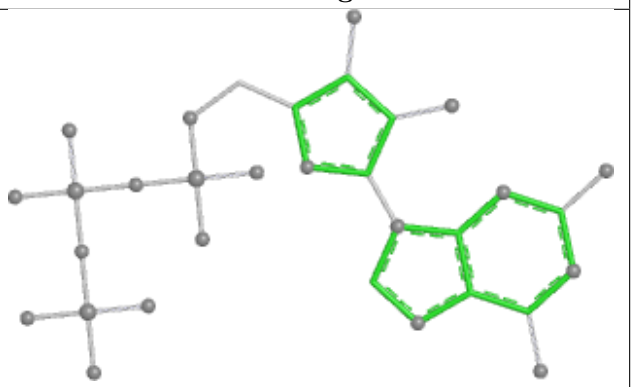
Bond lengths



Bond angles

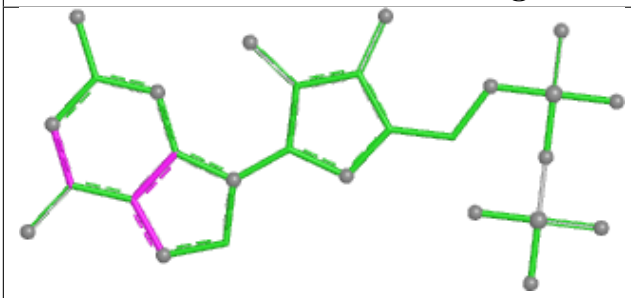


Torsions

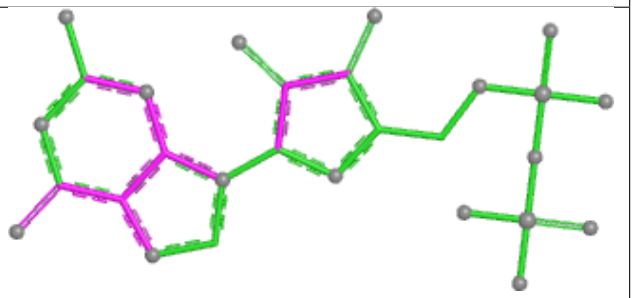


Rings

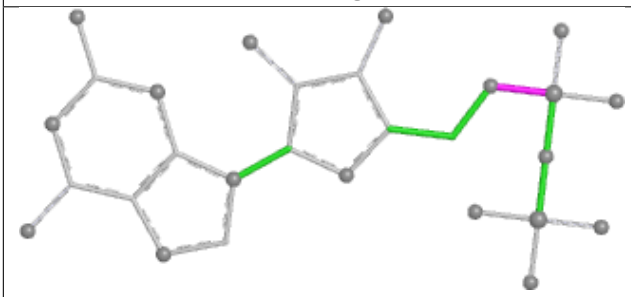
Ligand GDP EP 500



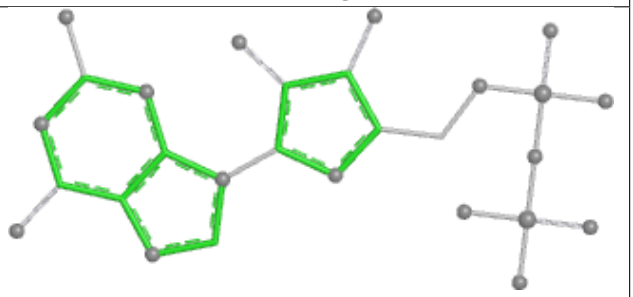
Bond lengths



Bond angles

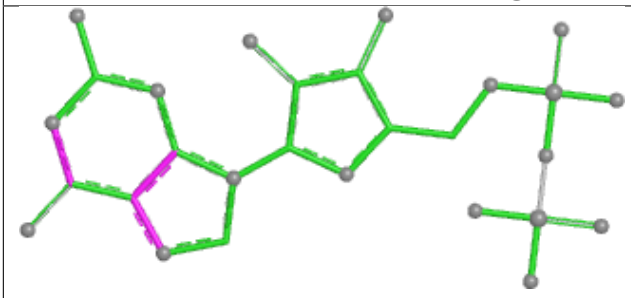


Torsions

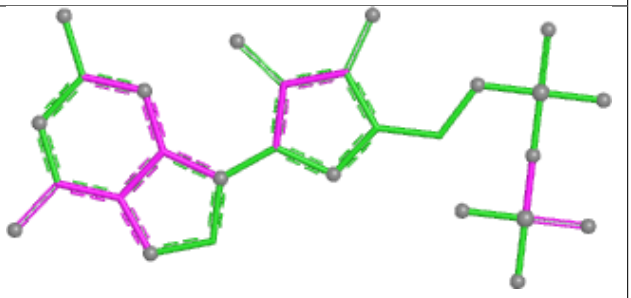


Rings

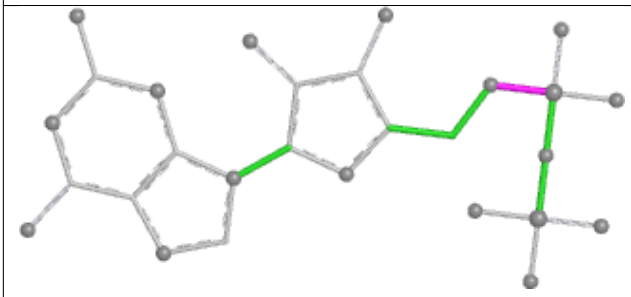
Ligand GDP BD 500



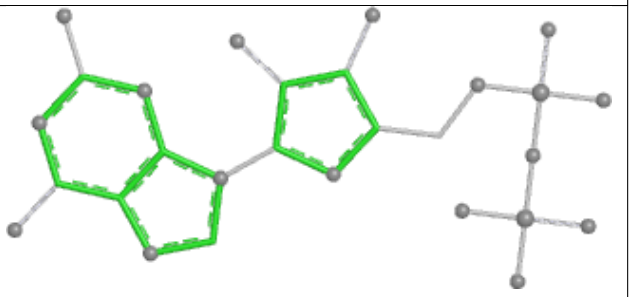
Bond lengths



Bond angles

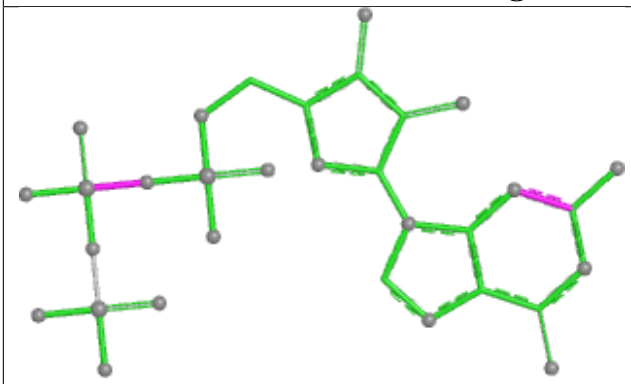


Torsions

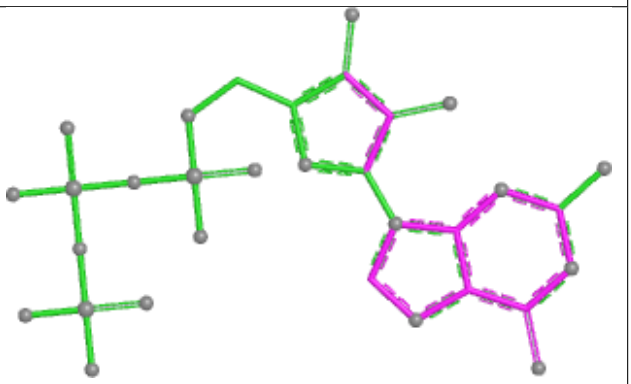


Rings

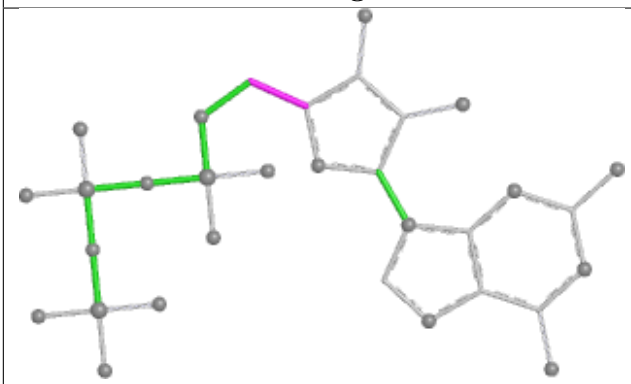
Ligand GTP KX 501



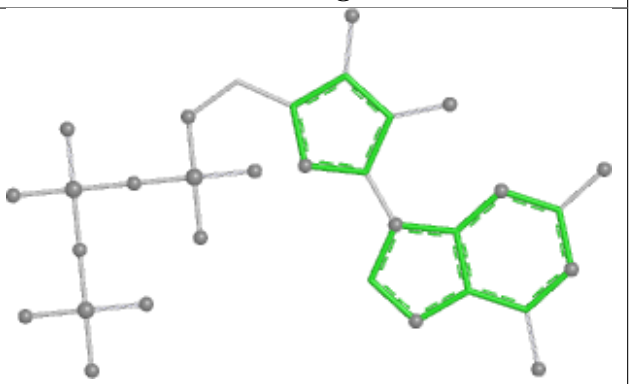
Bond lengths



Bond angles

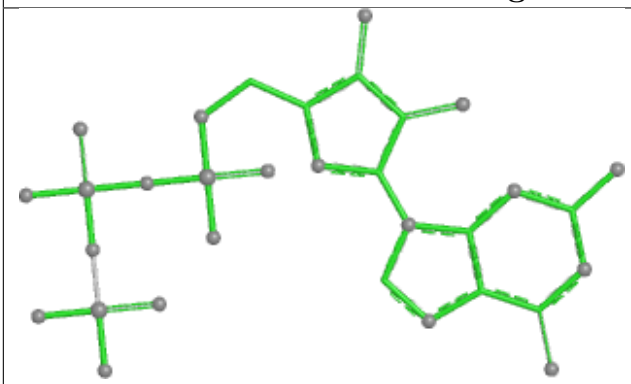


Torsions

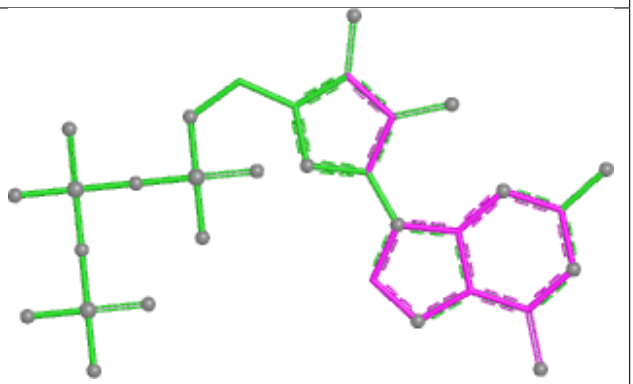


Rings

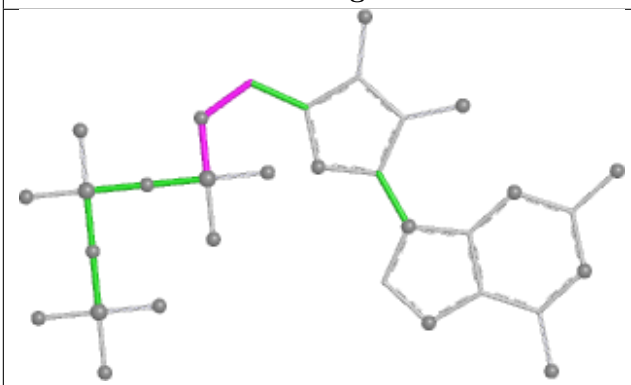
Ligand GTP GO 501



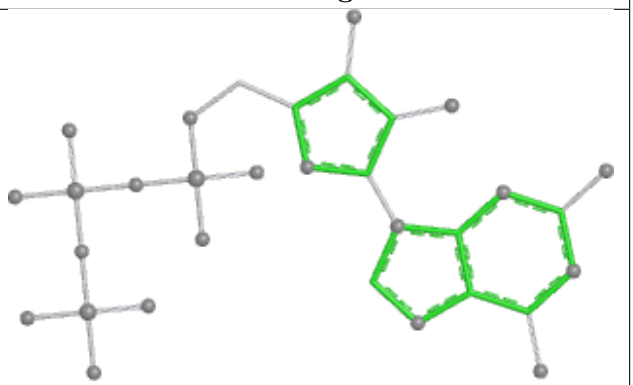
Bond lengths



Bond angles

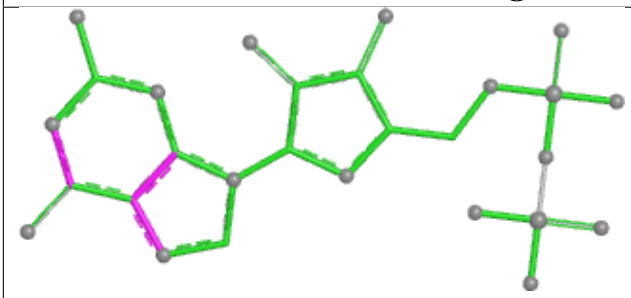


Torsions

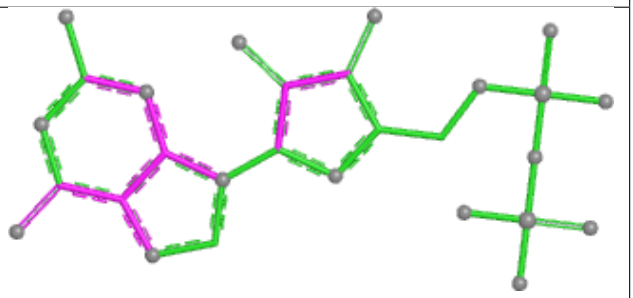


Rings

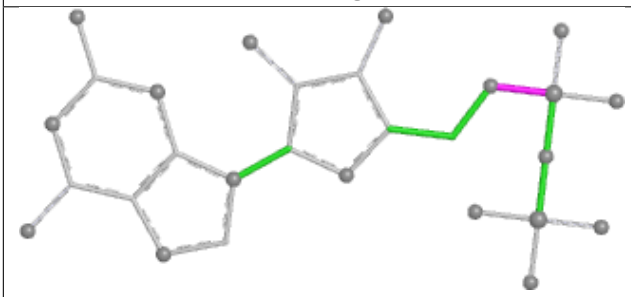
Ligand GDP VB 500



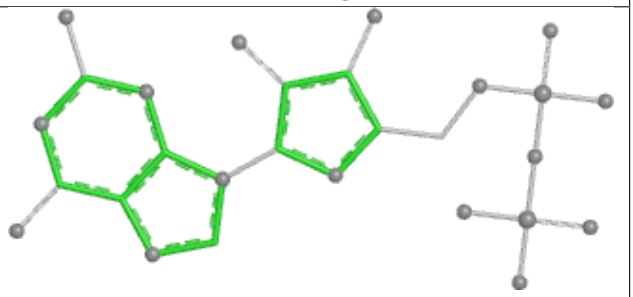
Bond lengths



Bond angles

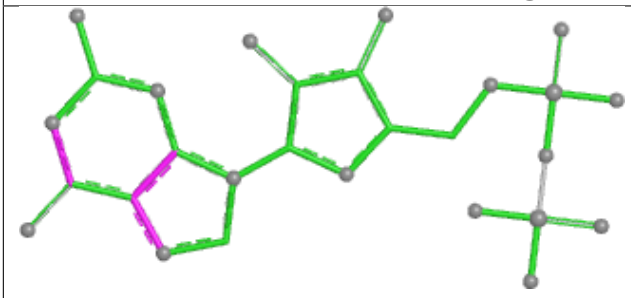


Torsions

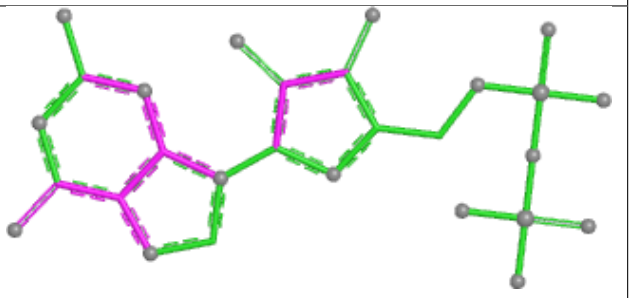


Rings

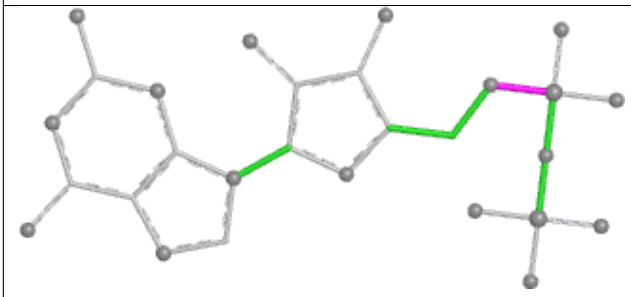
Ligand GDP V 500



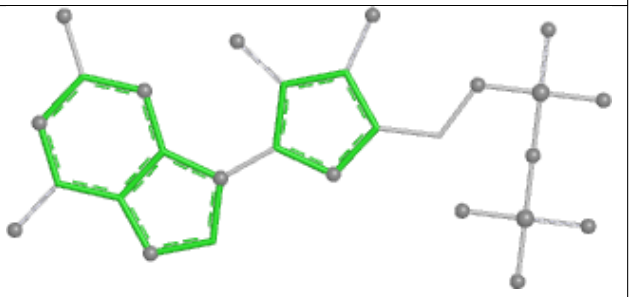
Bond lengths



Bond angles

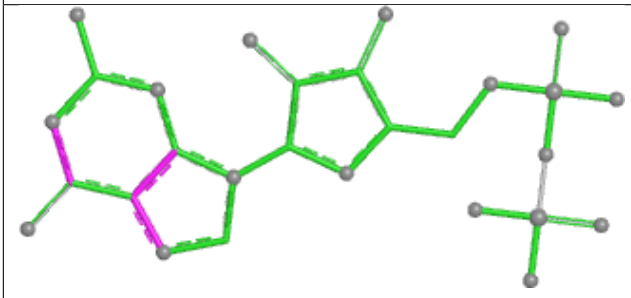


Torsions

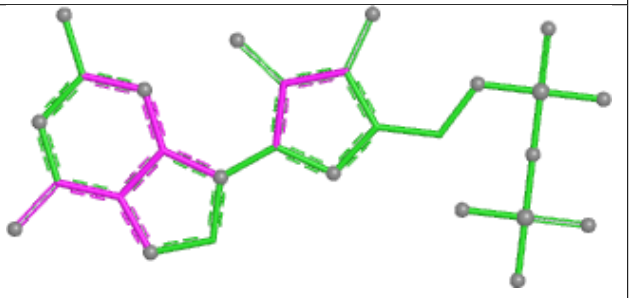


Rings

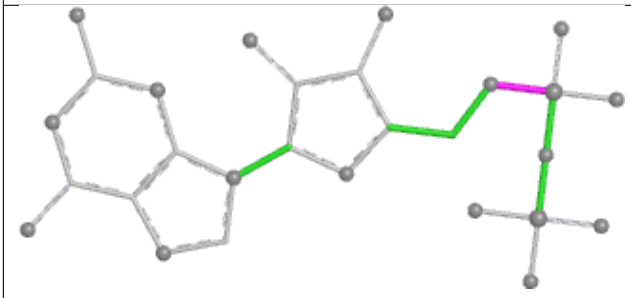
Ligand GDP WP 500



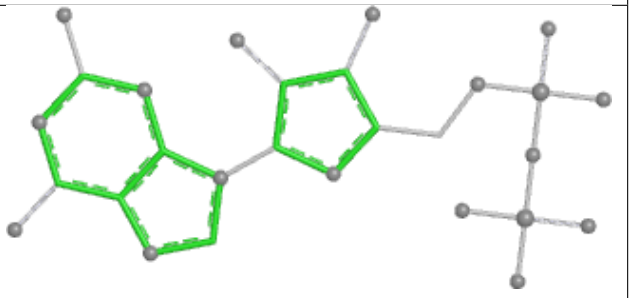
Bond lengths



Bond angles

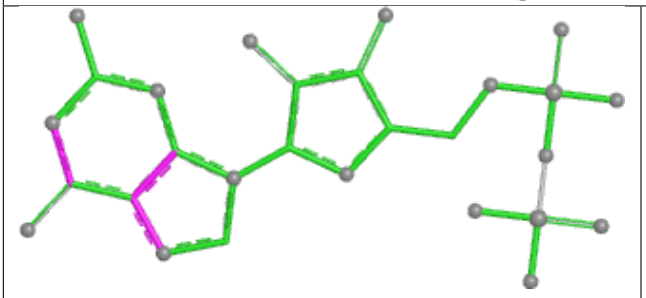


Torsions

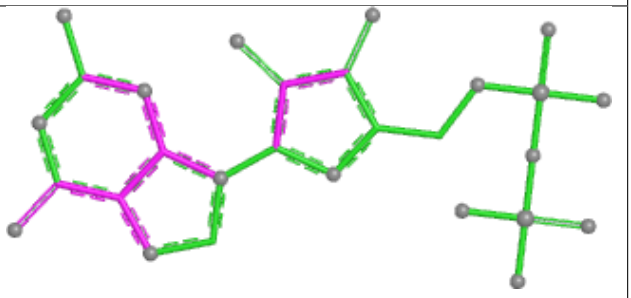


Rings

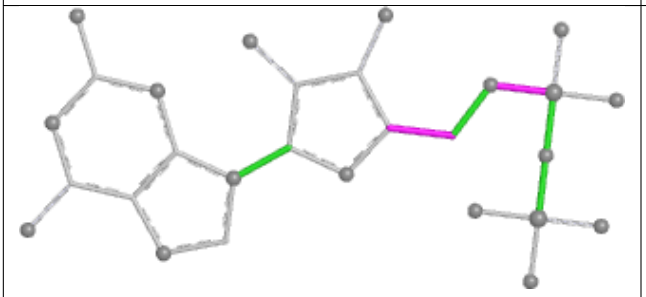
Ligand GDP FJ 501



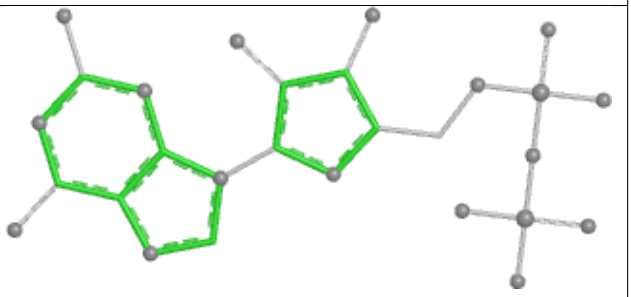
Bond lengths



Bond angles

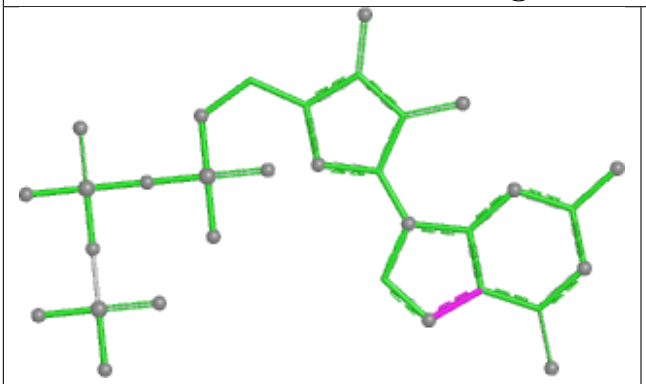


Torsions

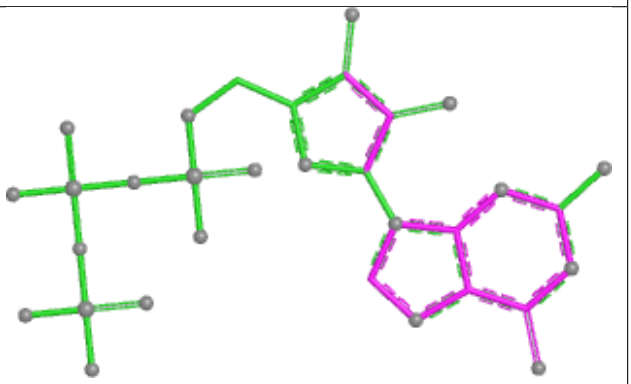


Rings

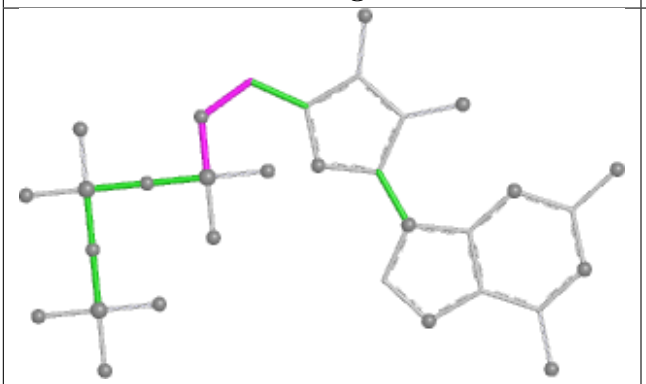
Ligand GTP AP 501



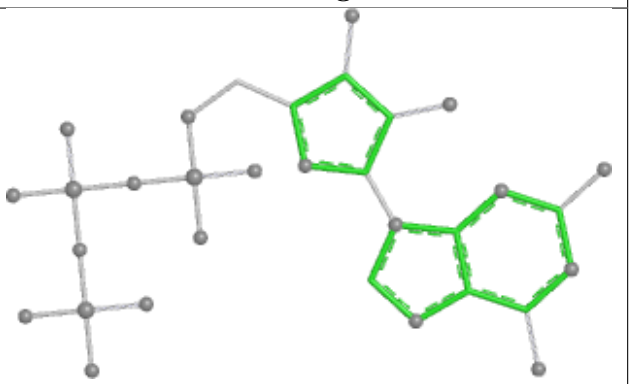
Bond lengths



Bond angles

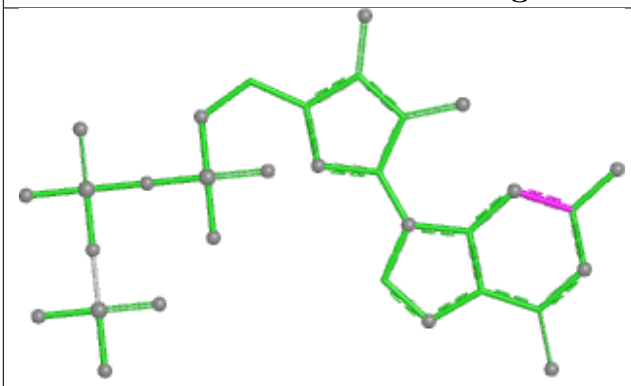


Torsions

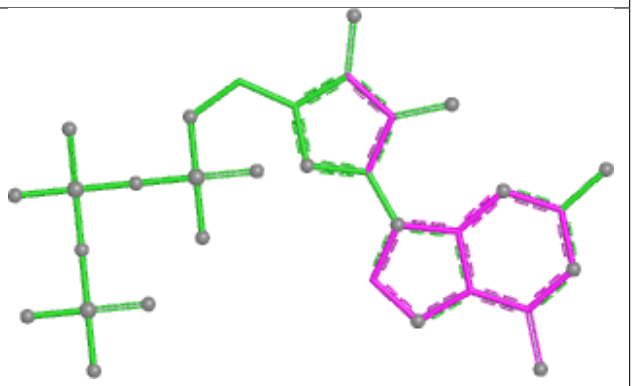


Rings

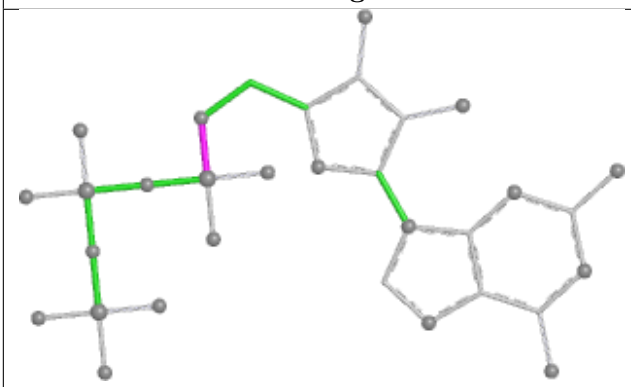
Ligand GTP LN 502



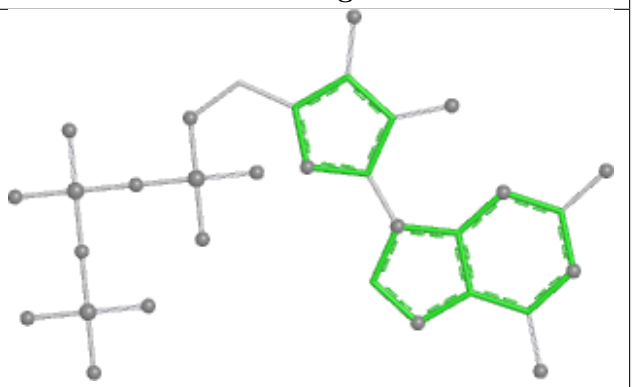
Bond lengths



Bond angles

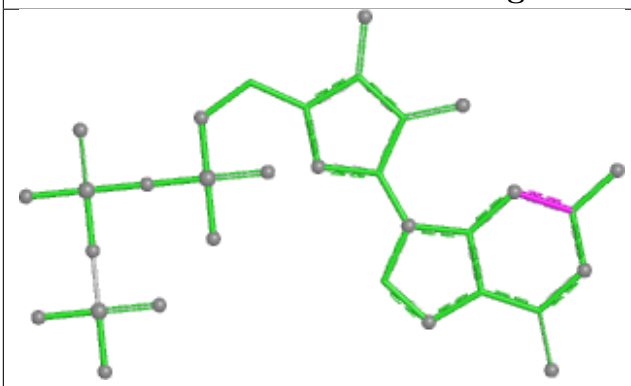


Torsions

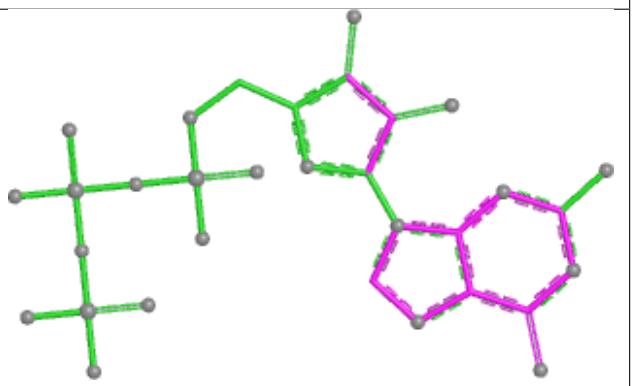


Rings

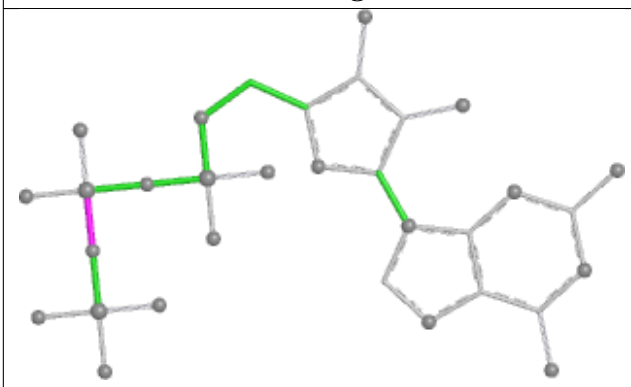
Ligand GTP WS 501



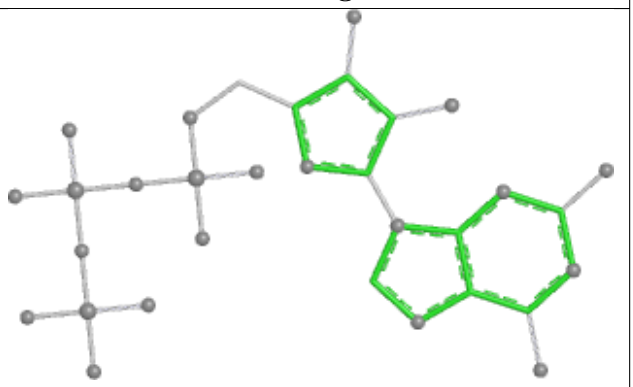
Bond lengths



Bond angles

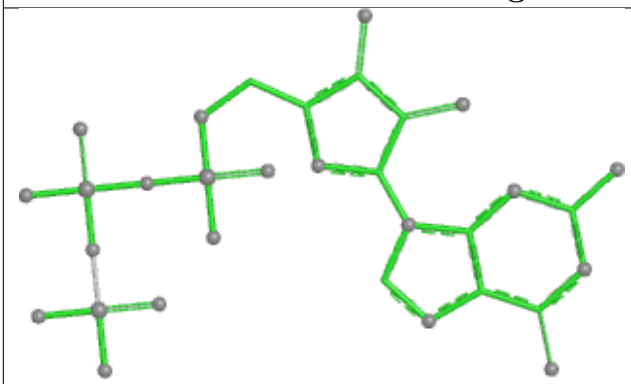


Torsions

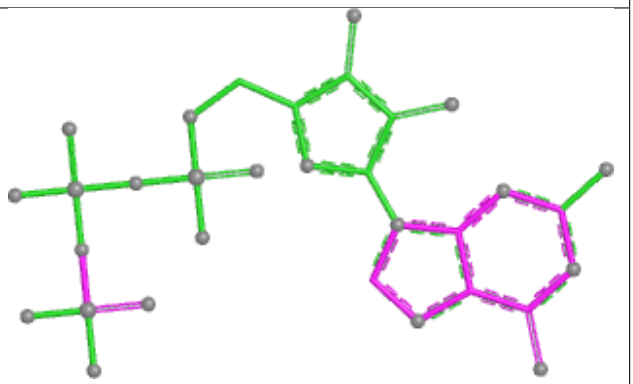


Rings

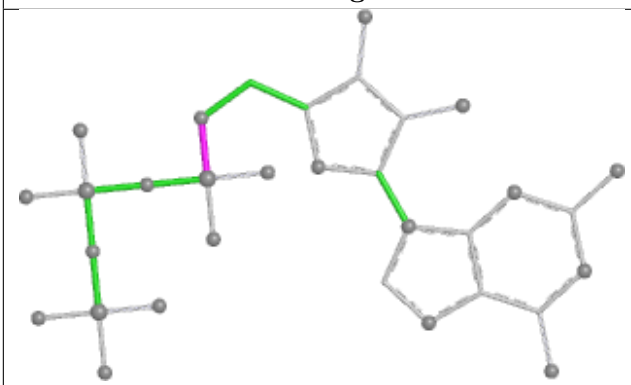
Ligand GTP GK 501



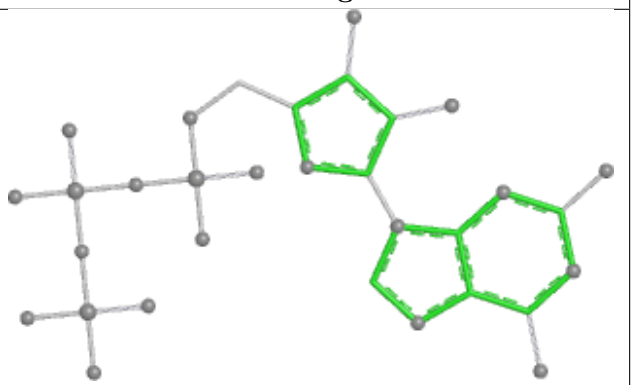
Bond lengths



Bond angles

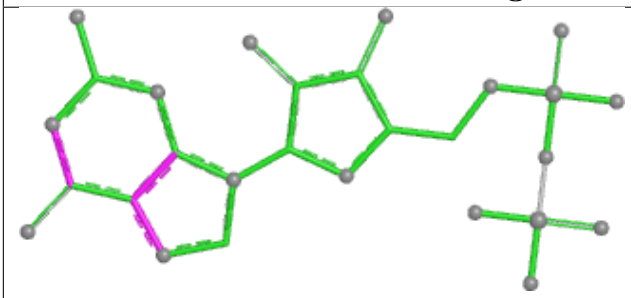


Torsions

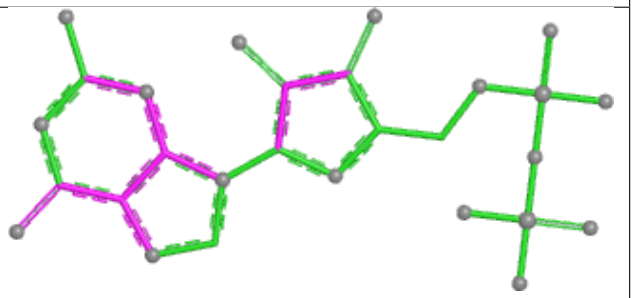


Rings

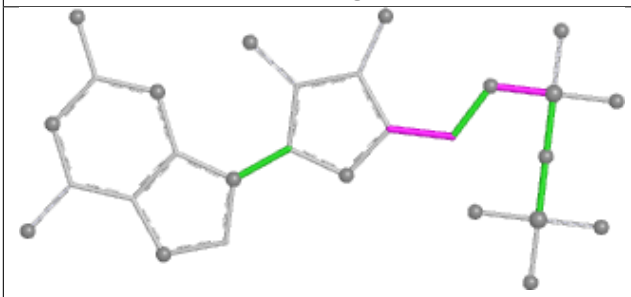
Ligand GDP NR 500



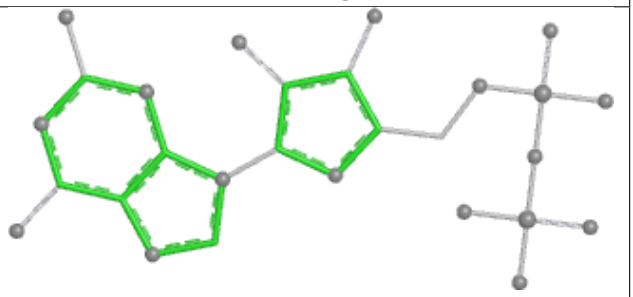
Bond lengths



Bond angles

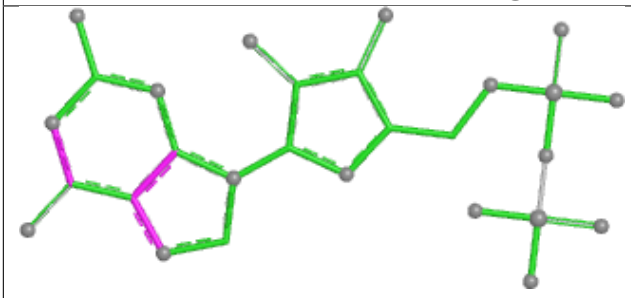


Torsions

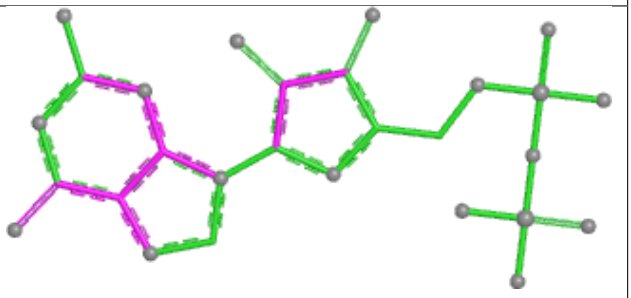


Rings

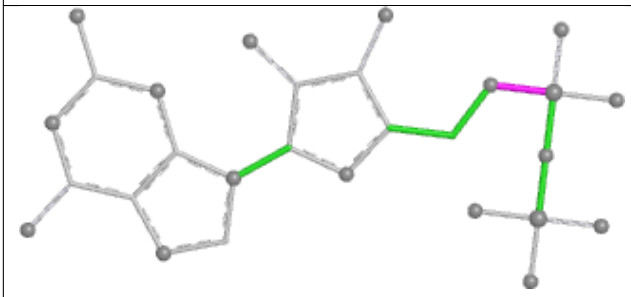
Ligand GDP ML 500



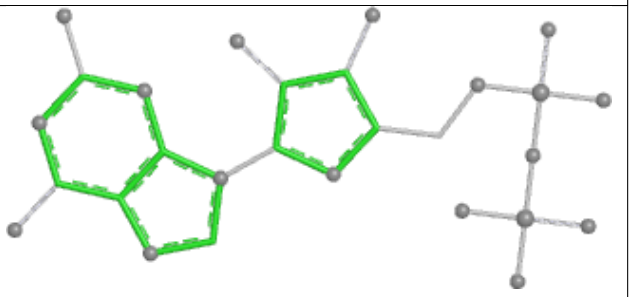
Bond lengths



Bond angles

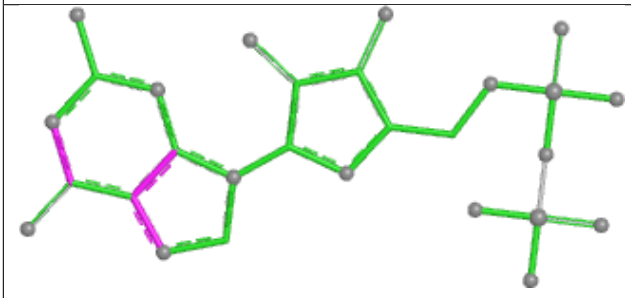


Torsions

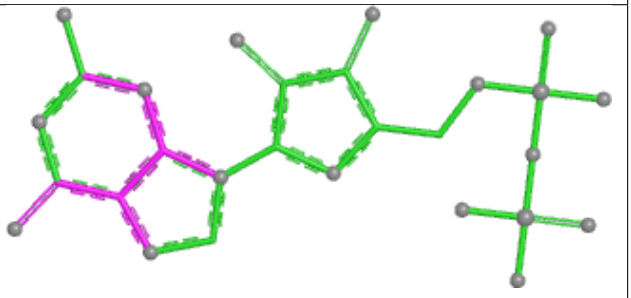


Rings

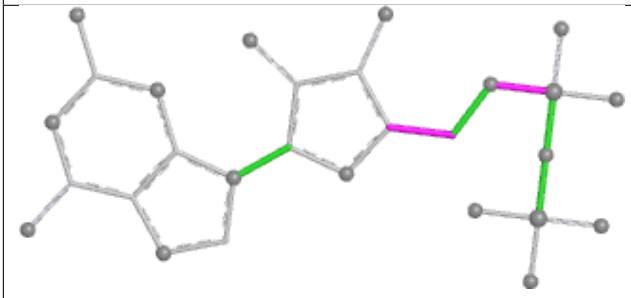
Ligand GDP LG 501



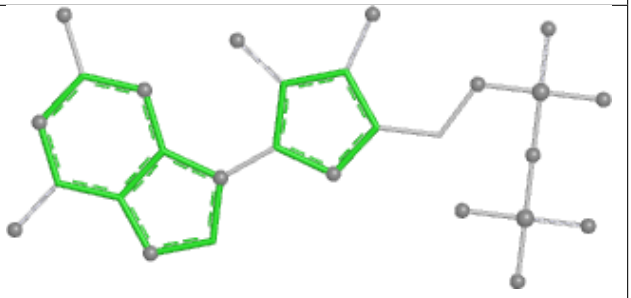
Bond lengths



Bond angles

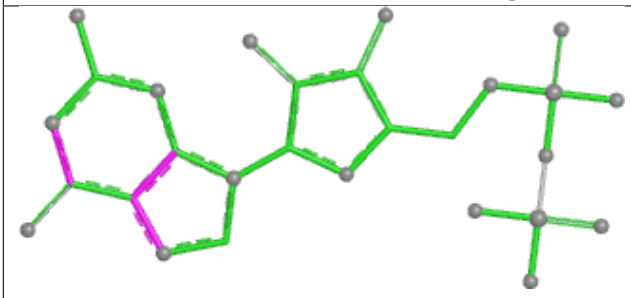


Torsions

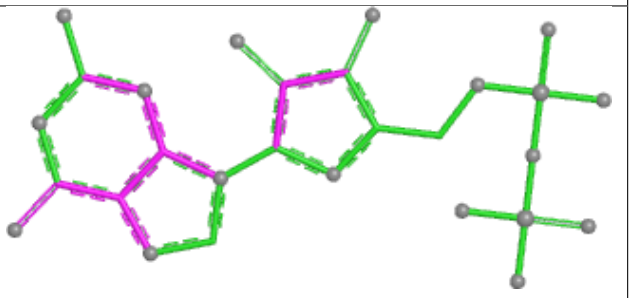


Rings

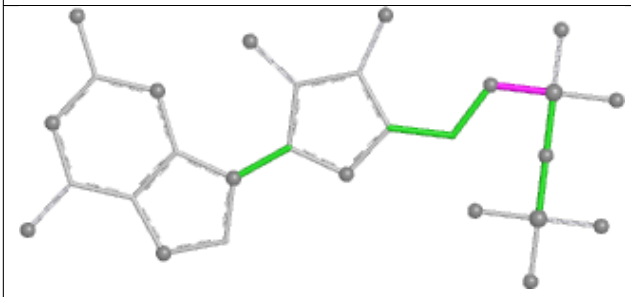
Ligand GDP MH 500



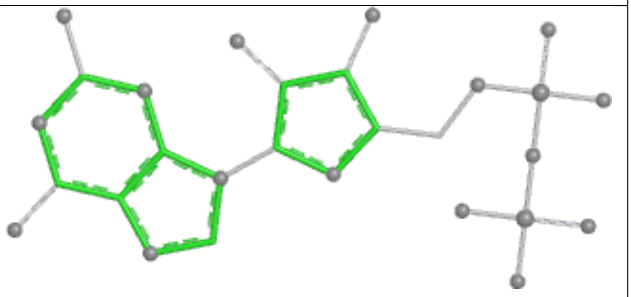
Bond lengths



Bond angles

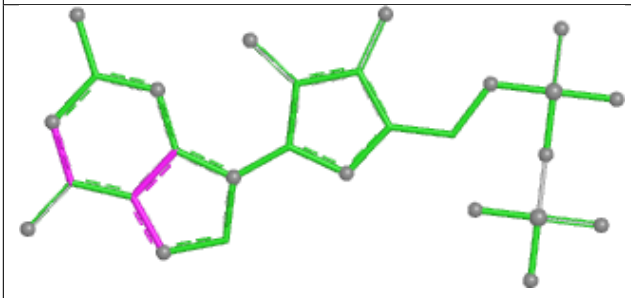


Torsions

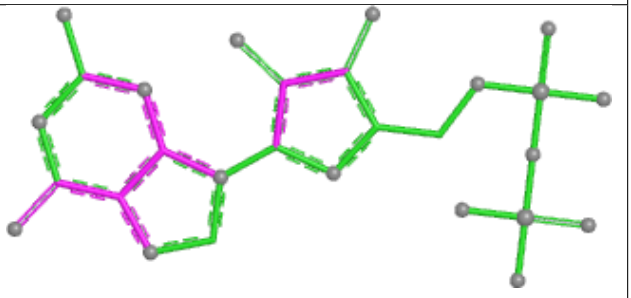


Rings

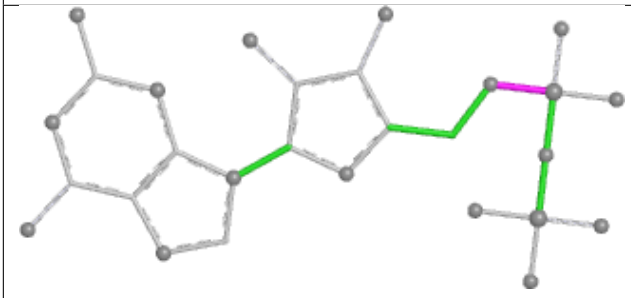
Ligand GDP DW 501



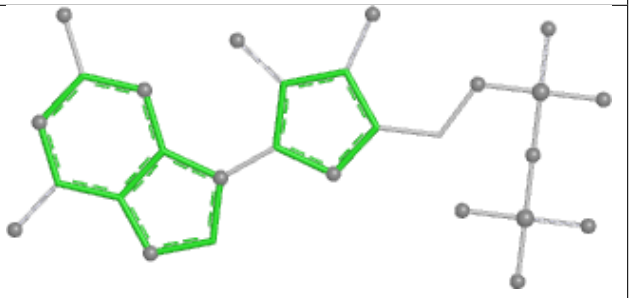
Bond lengths



Bond angles

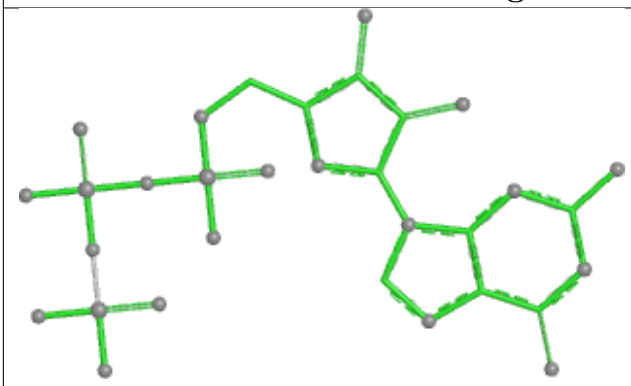


Torsions

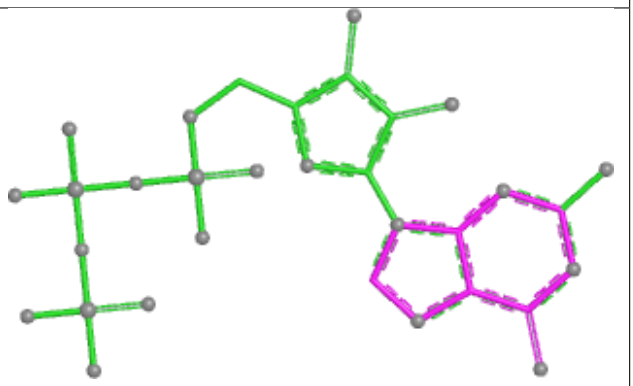


Rings

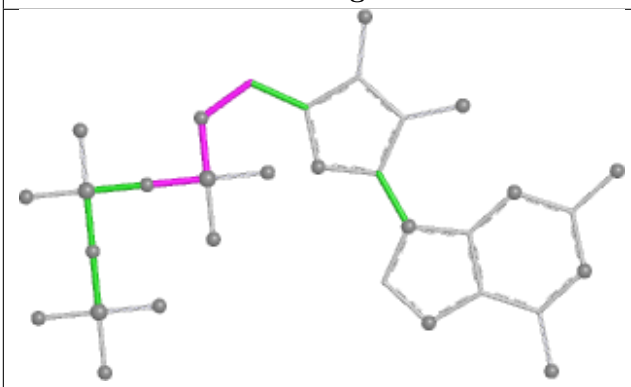
Ligand GTP EM 501



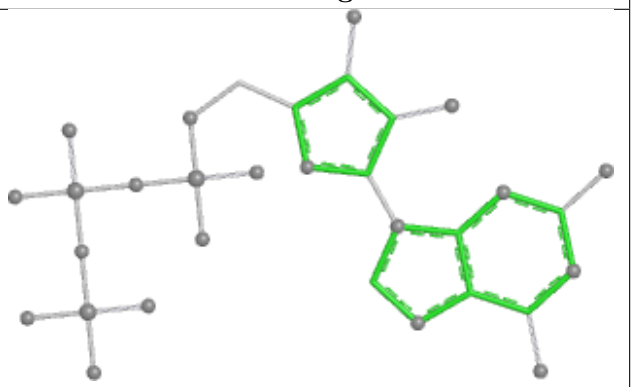
Bond lengths



Bond angles

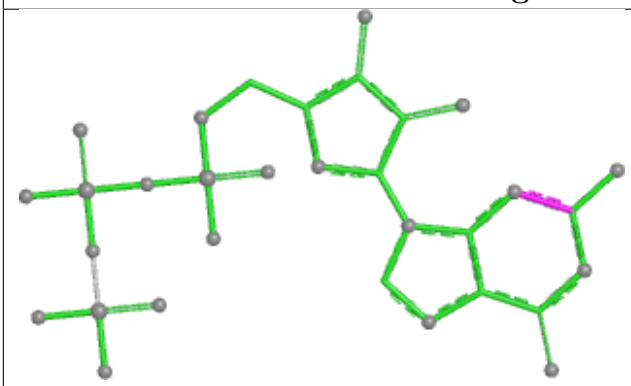


Torsions

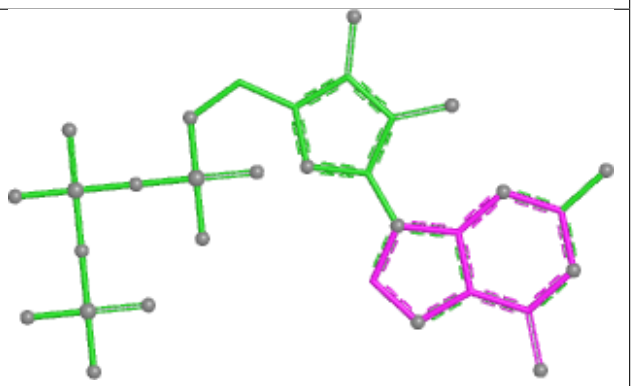


Rings

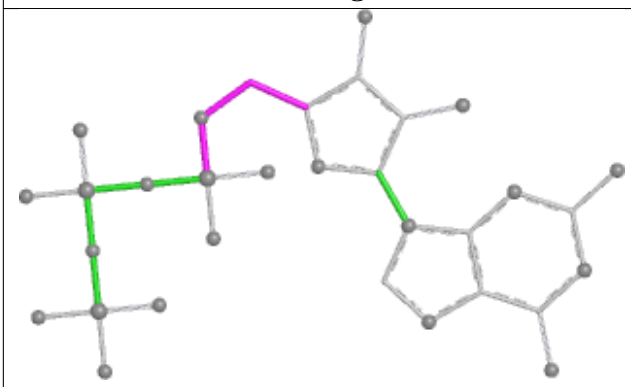
Ligand GTP GS 501



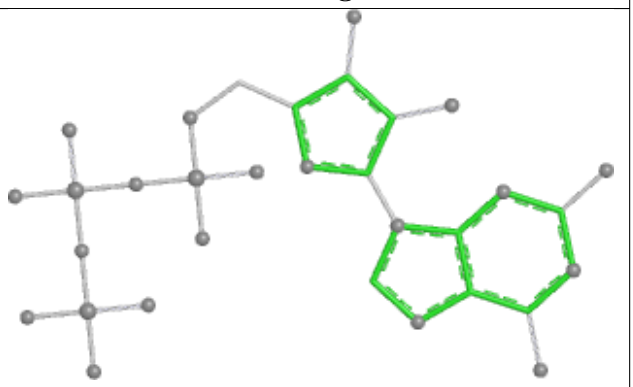
Bond lengths



Bond angles

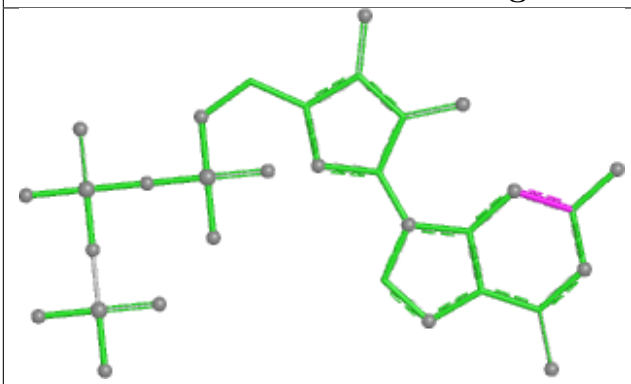


Torsions

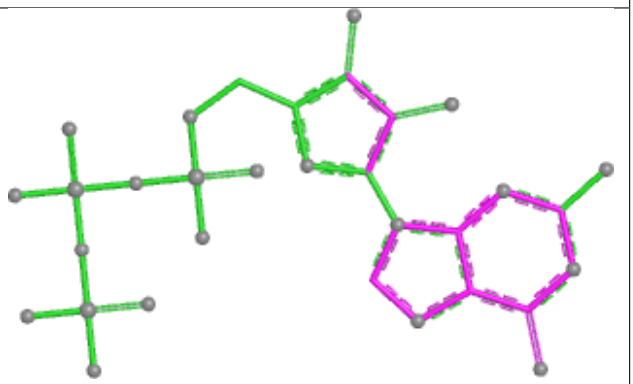


Rings

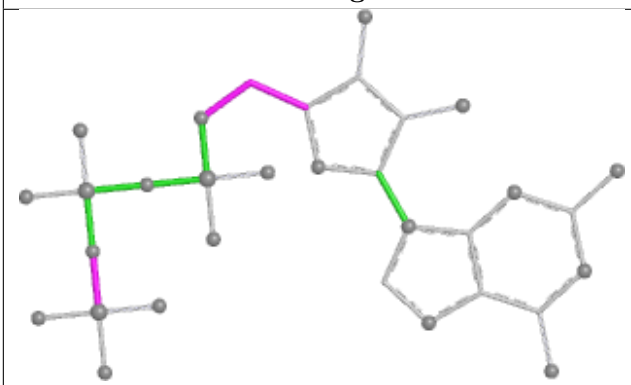
Ligand GTP KT 501



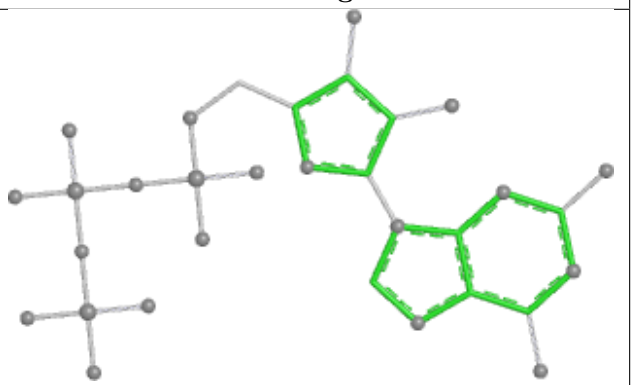
Bond lengths



Bond angles

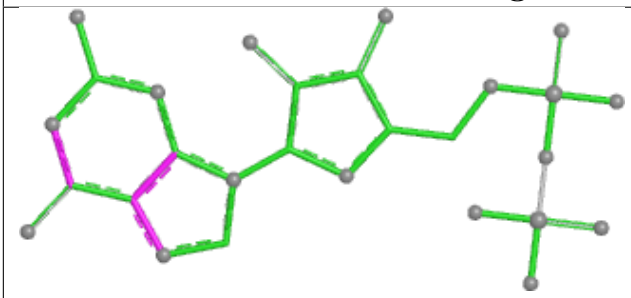


Torsions

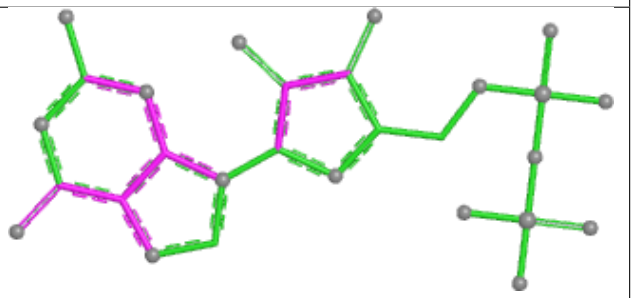


Rings

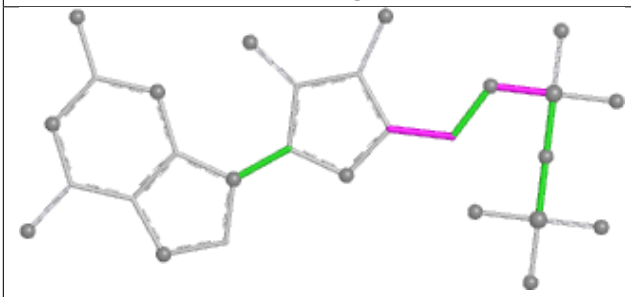
Ligand GDP OP 501



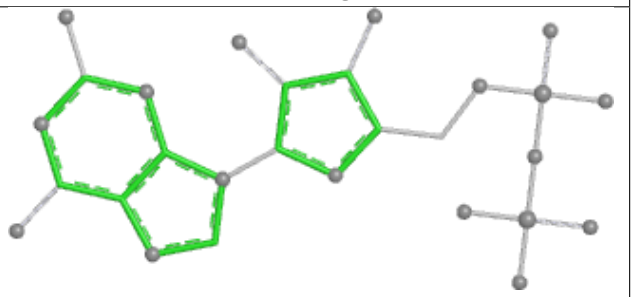
Bond lengths



Bond angles

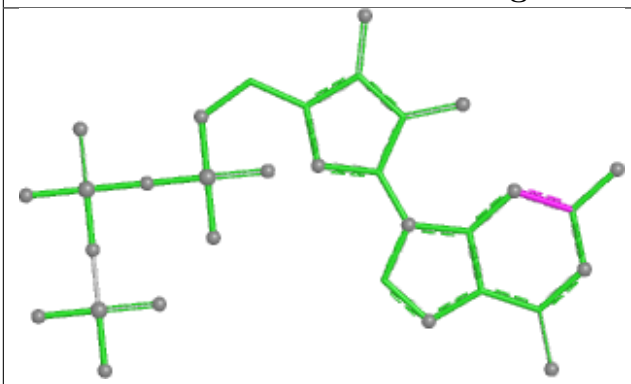


Torsions

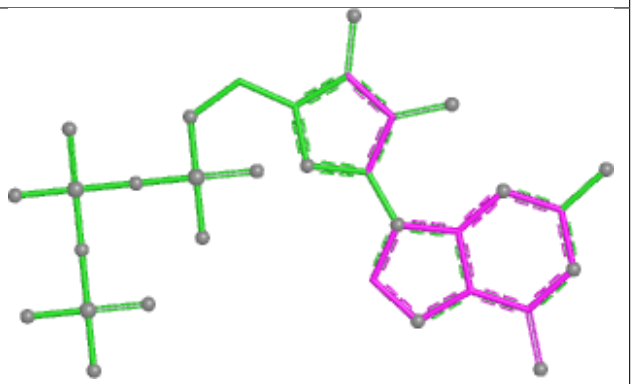


Rings

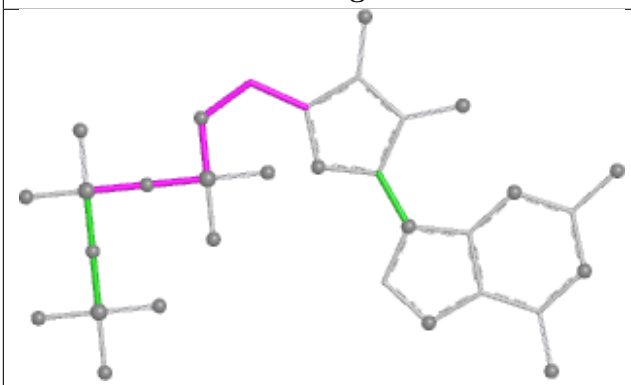
Ligand GTP UE 501



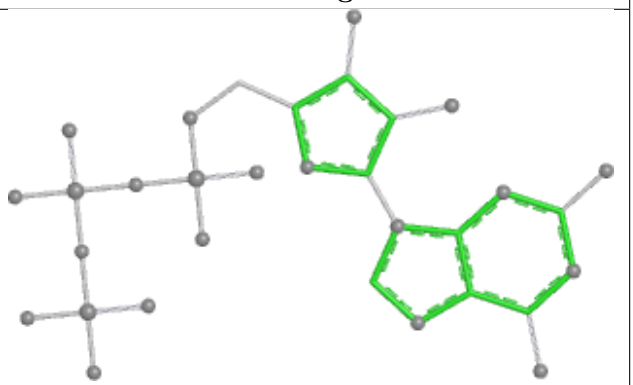
Bond lengths



Bond angles

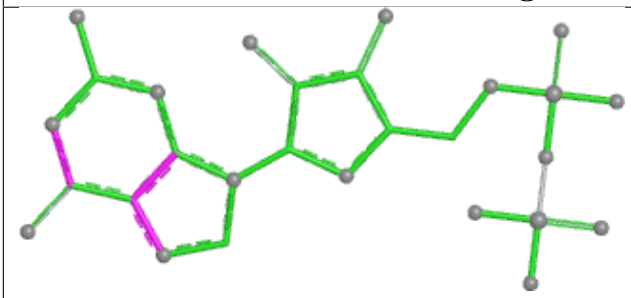


Torsions

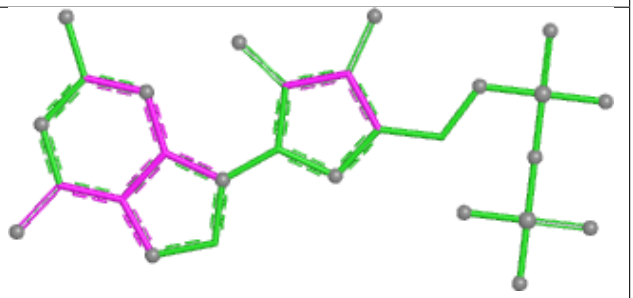


Rings

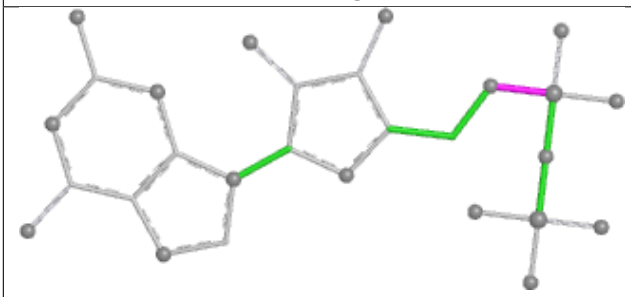
Ligand GDP JI 500



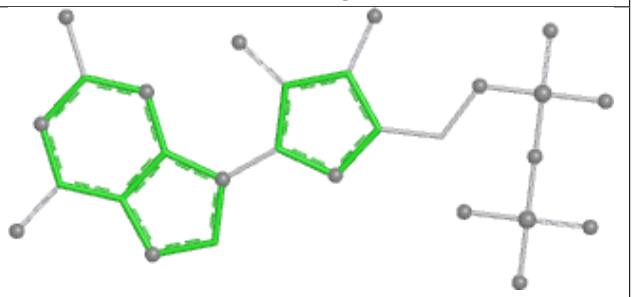
Bond lengths



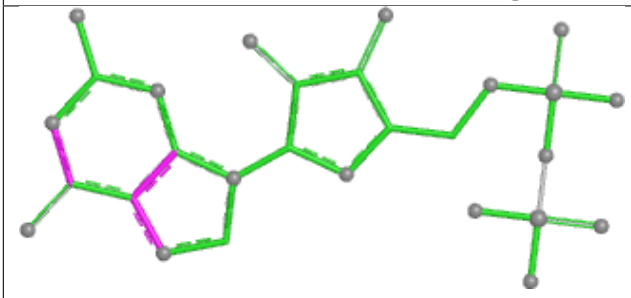
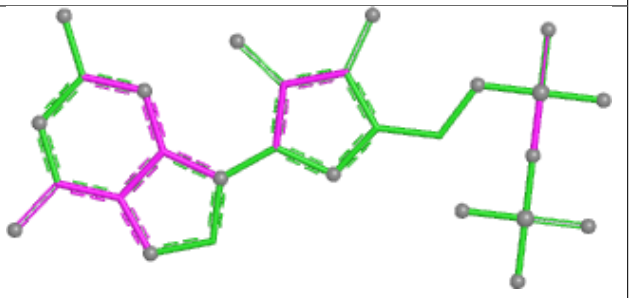
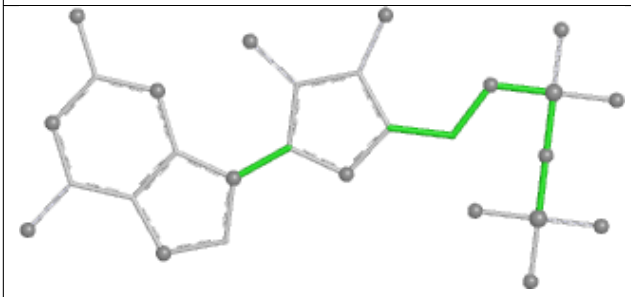
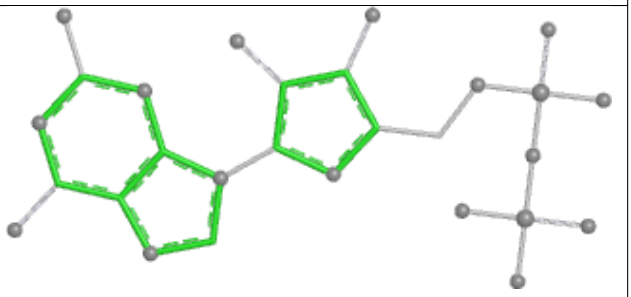
Bond angles

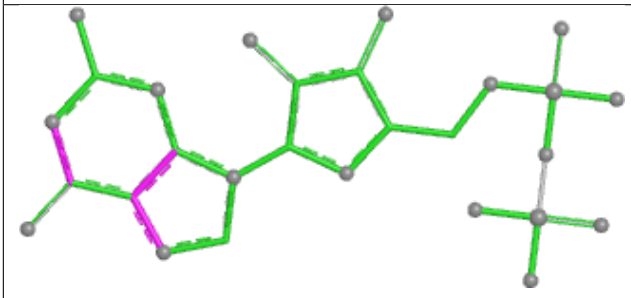
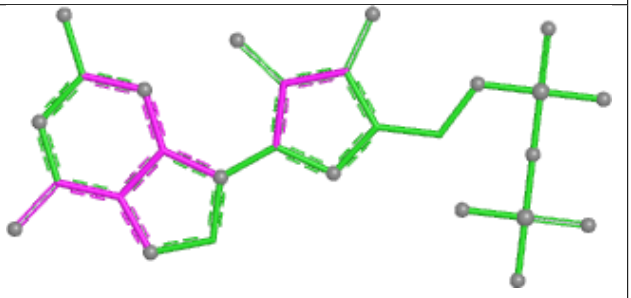
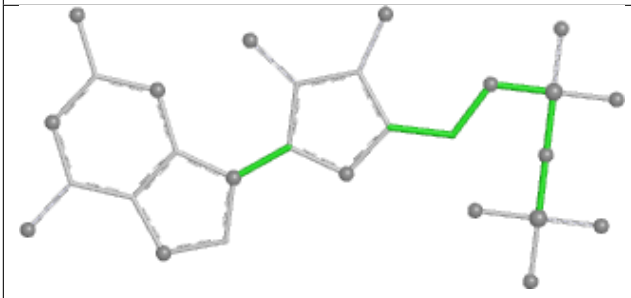
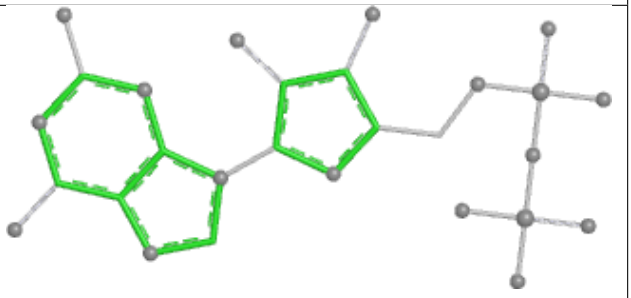


Torsions

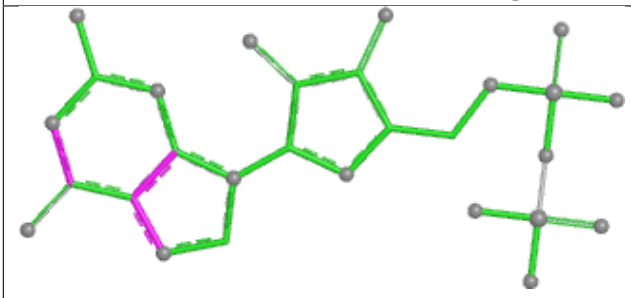


Rings

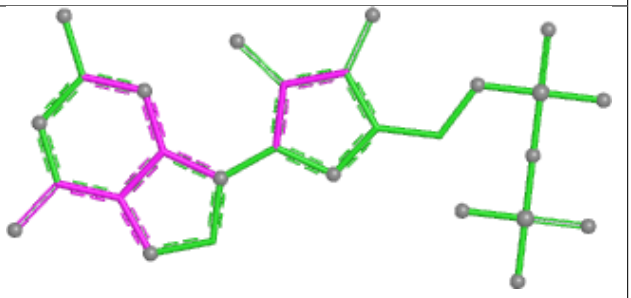
Ligand GDP ND 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP RU 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

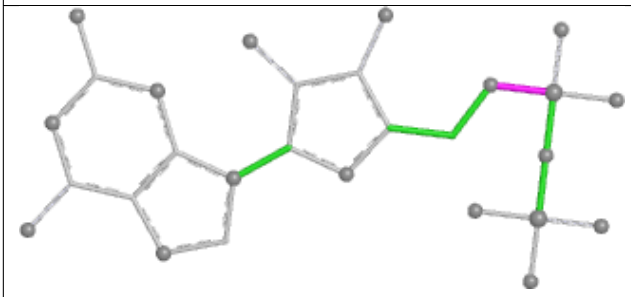
Ligand GDP HX 501



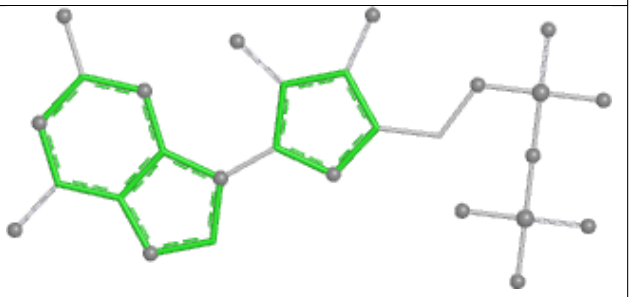
Bond lengths



Bond angles

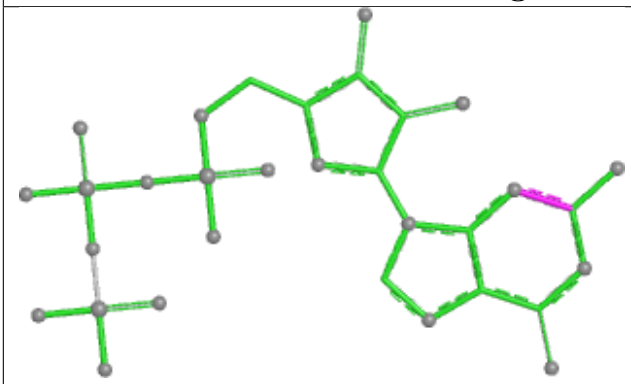


Torsions

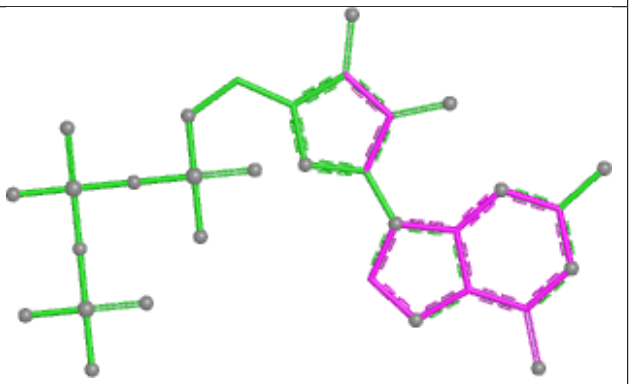


Rings

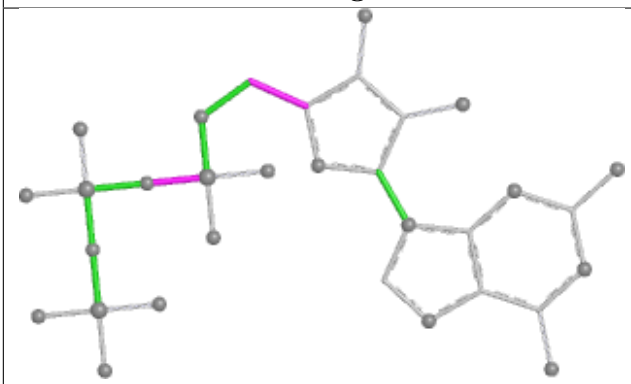
Ligand GTP DT 501



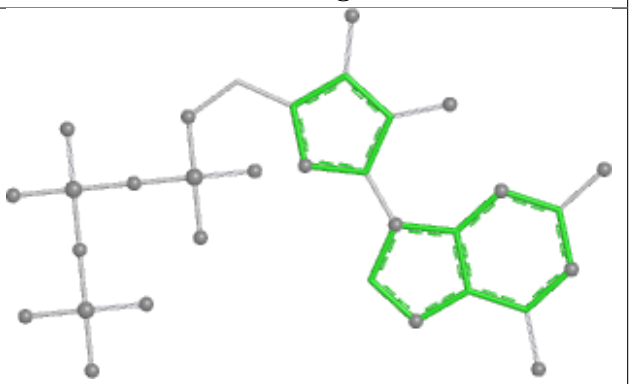
Bond lengths



Bond angles

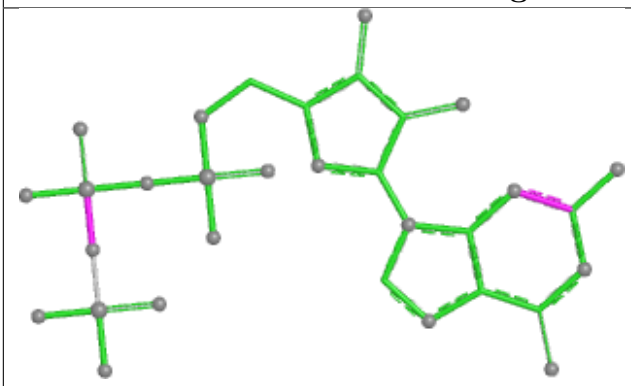


Torsions

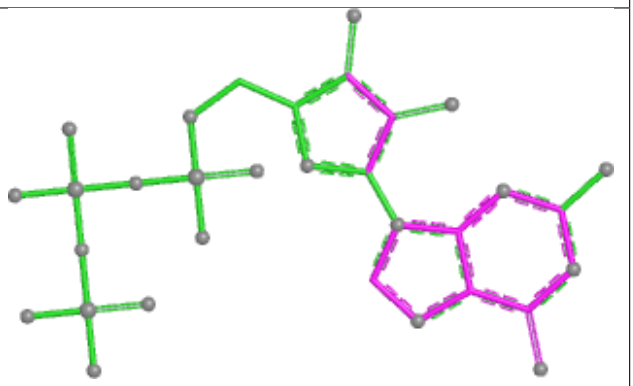


Rings

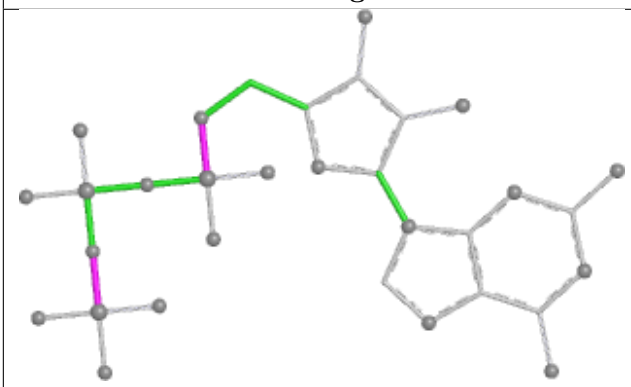
Ligand GTP NE 501



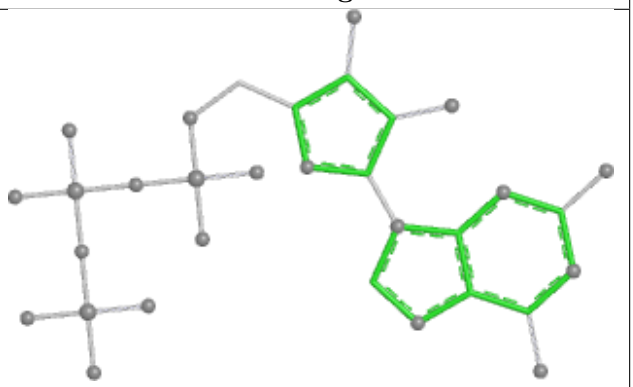
Bond lengths



Bond angles

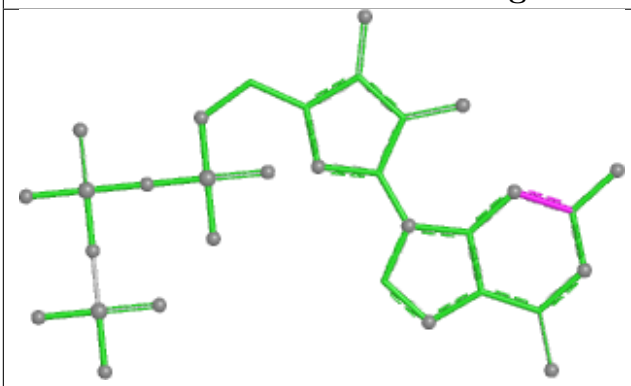


Torsions

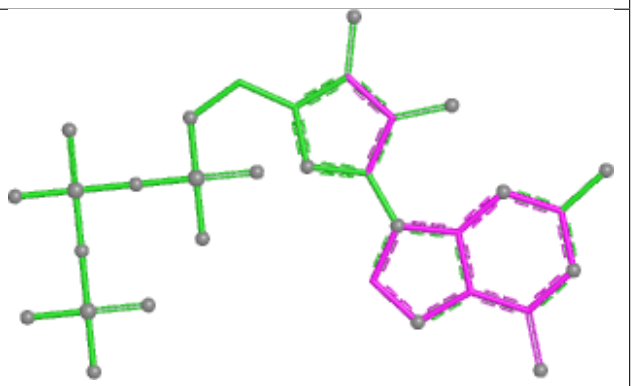


Rings

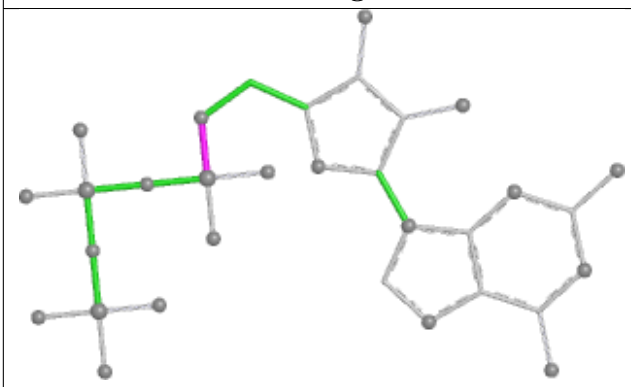
Ligand GTP UC 501



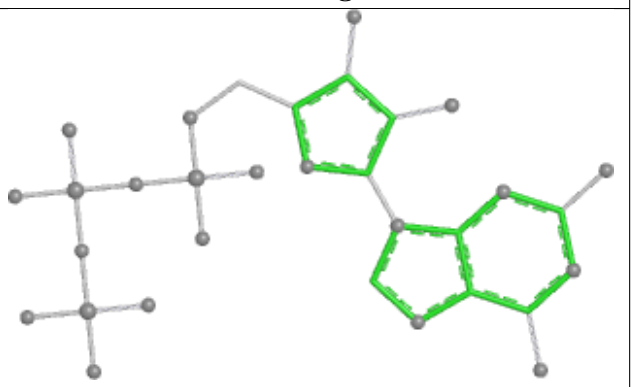
Bond lengths



Bond angles

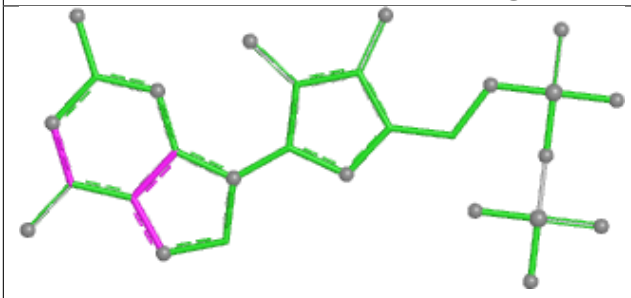


Torsions

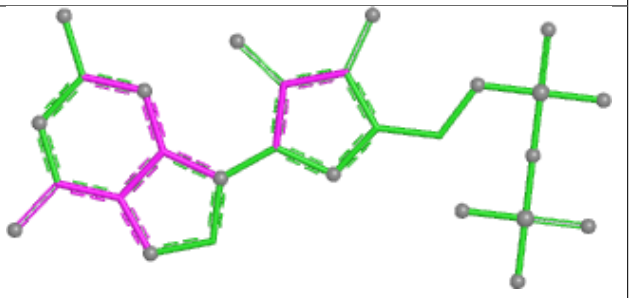


Rings

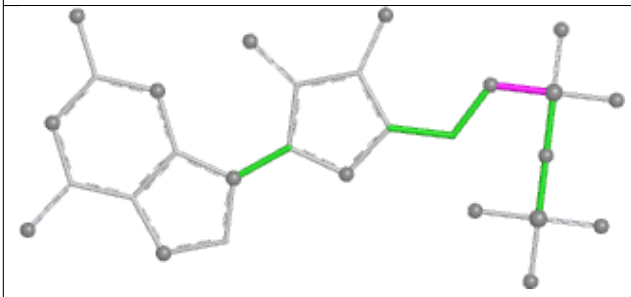
Ligand GDP MT 500



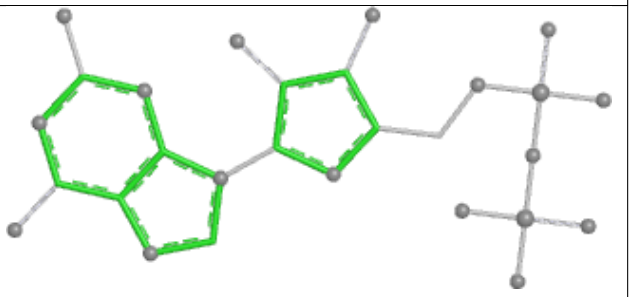
Bond lengths



Bond angles

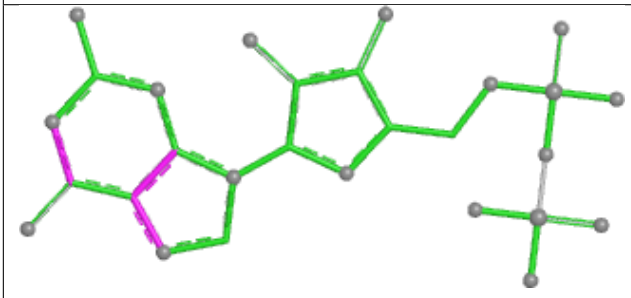


Torsions

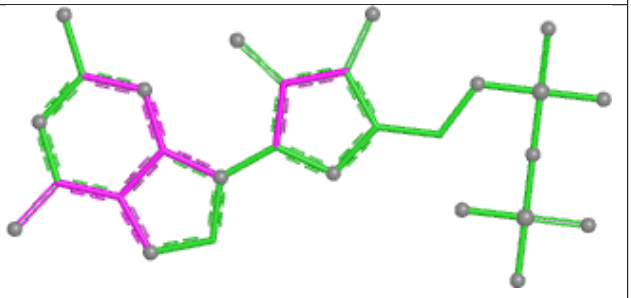


Rings

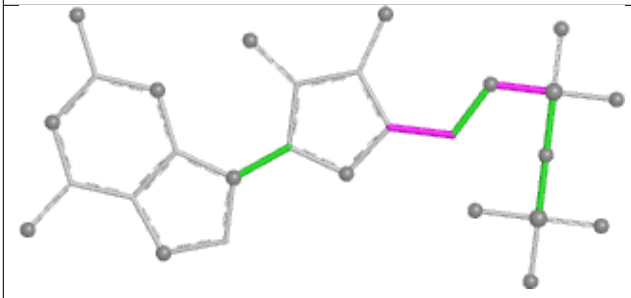
Ligand GDP PP 500



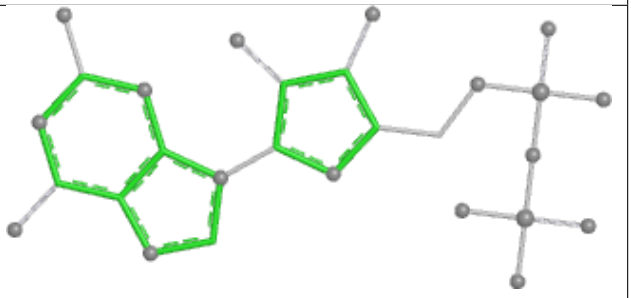
Bond lengths



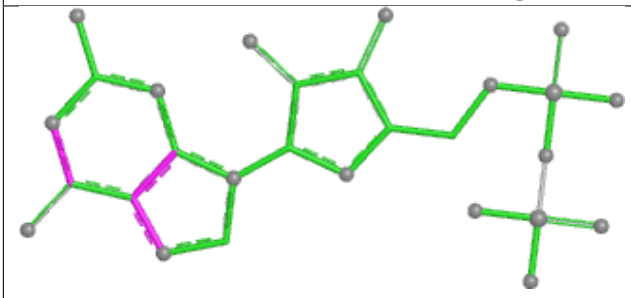
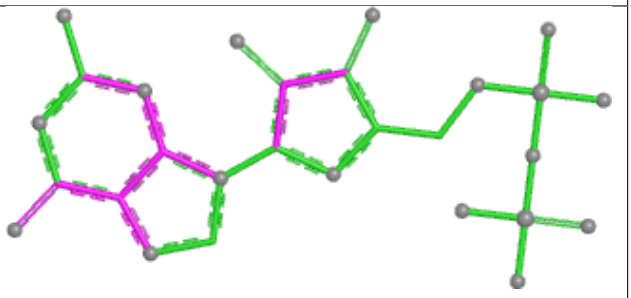
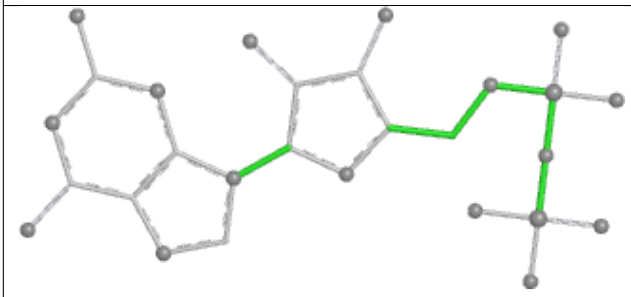
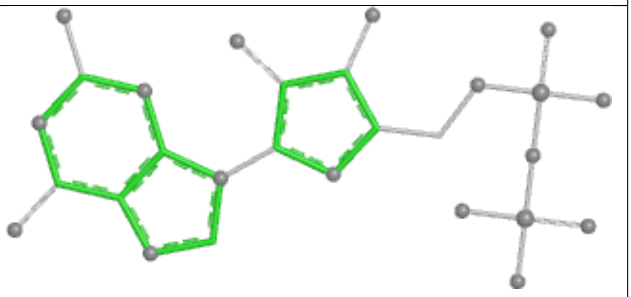
Bond angles

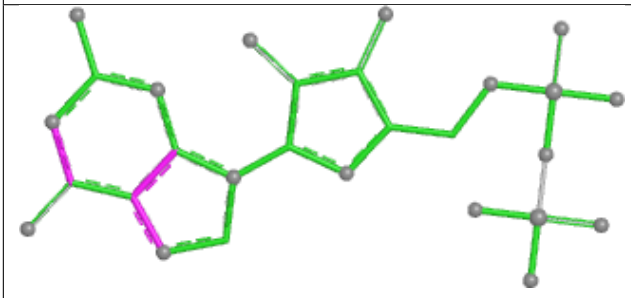
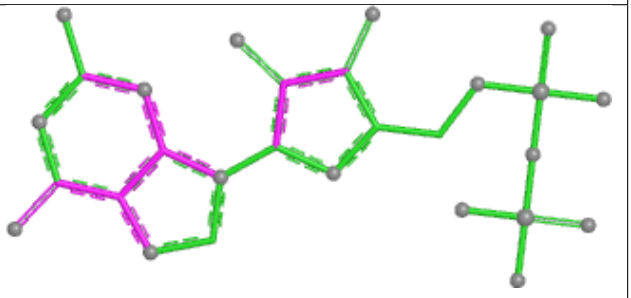
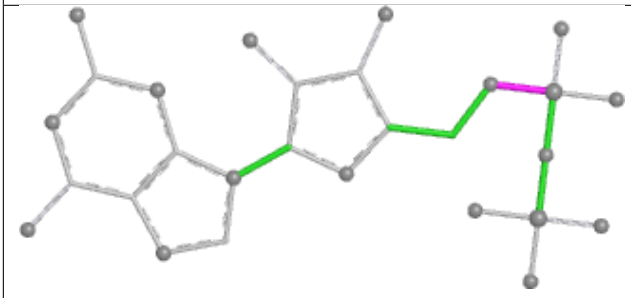
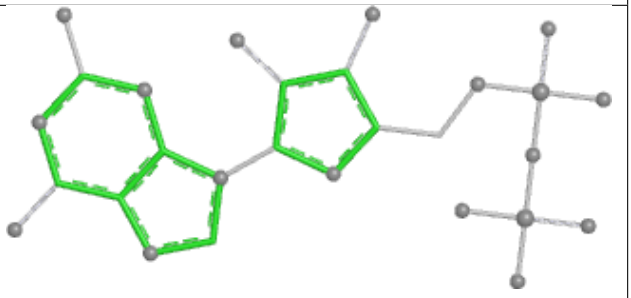


Torsions

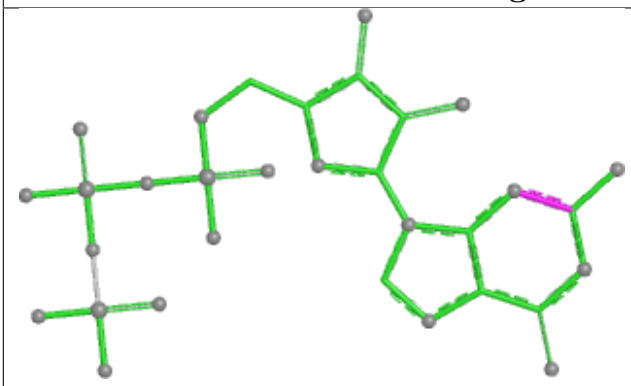


Rings

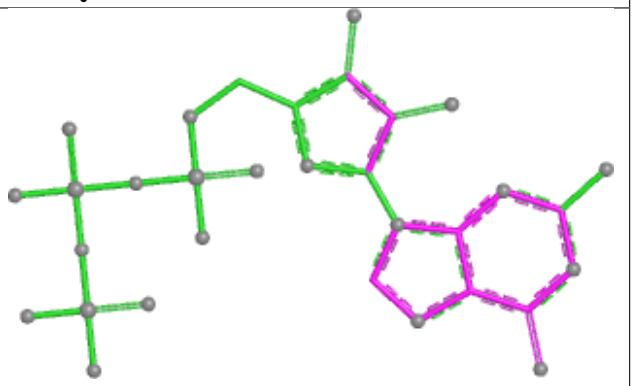
Ligand GDP TL 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP UD 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

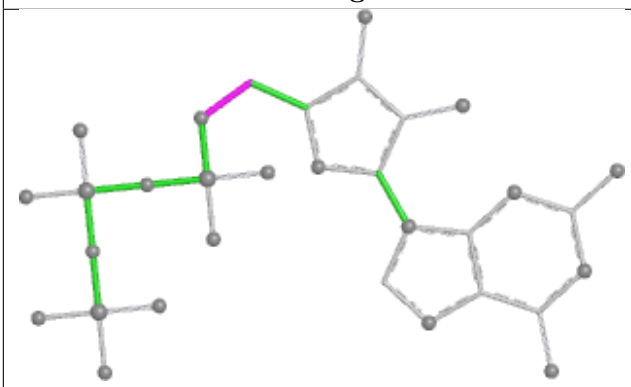
Ligand GTP VQ 501



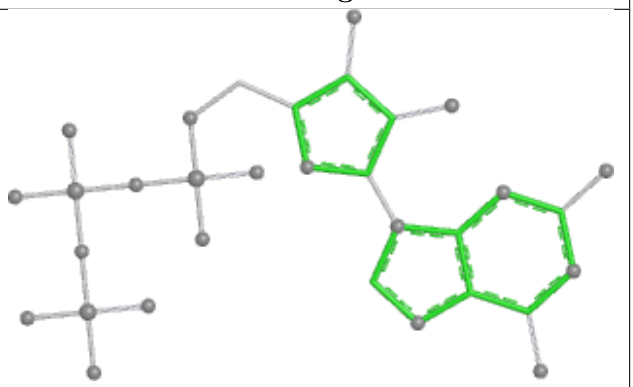
Bond lengths



Bond angles

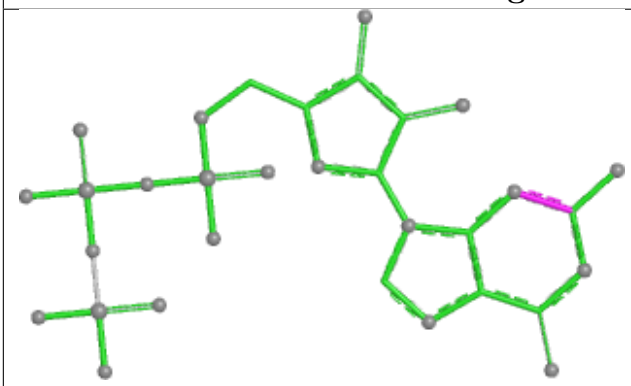


Torsions

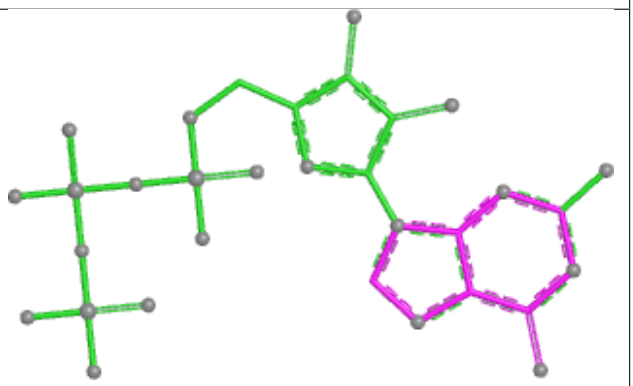


Rings

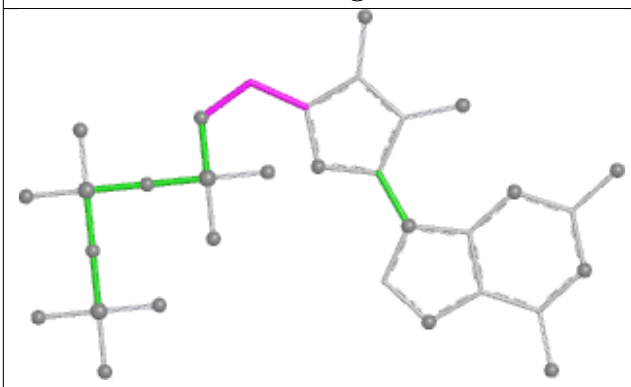
Ligand GTP KN 502



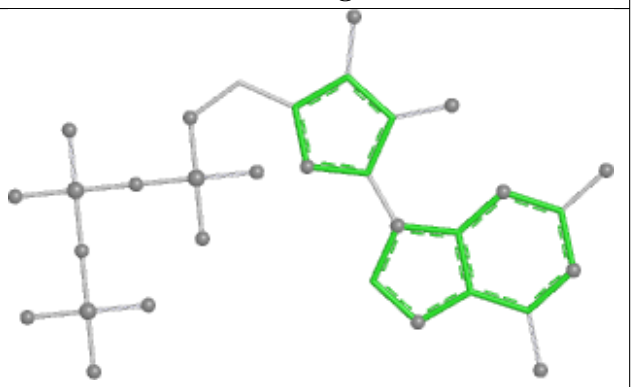
Bond lengths



Bond angles

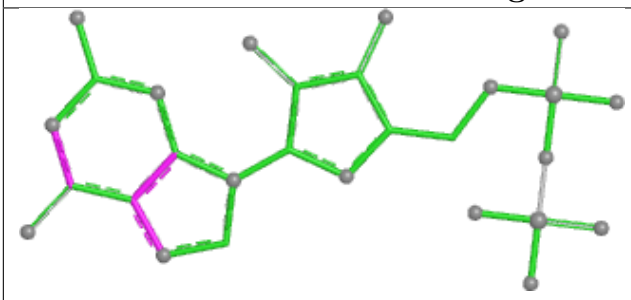


Torsions

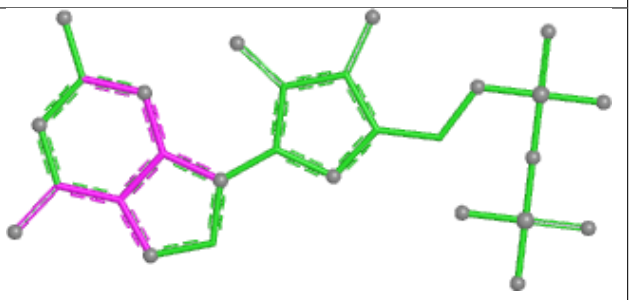


Rings

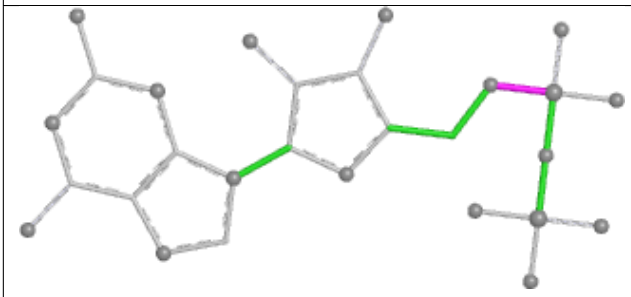
Ligand GDP PH 500



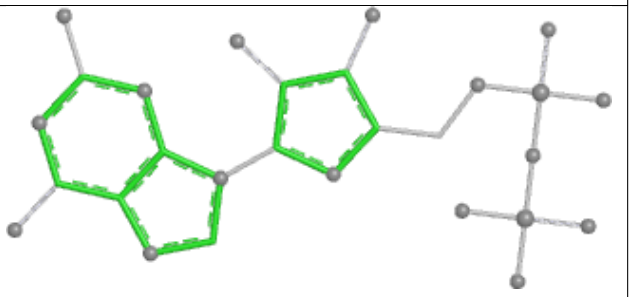
Bond lengths



Bond angles

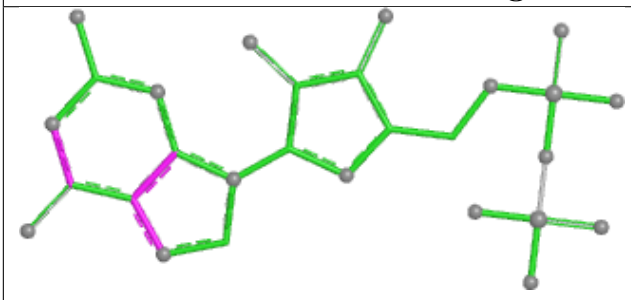


Torsions

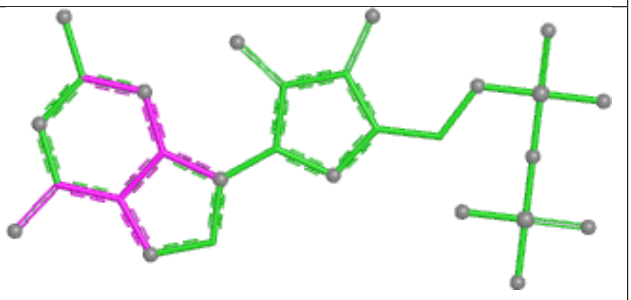


Rings

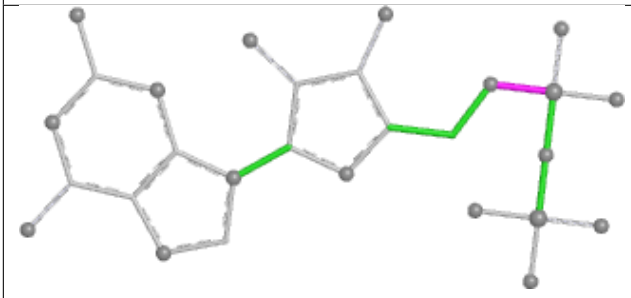
Ligand GDP AR 500



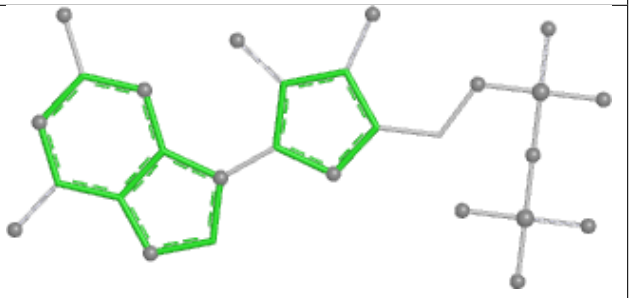
Bond lengths



Bond angles

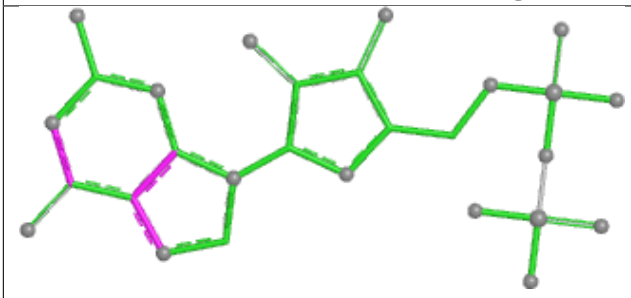


Torsions

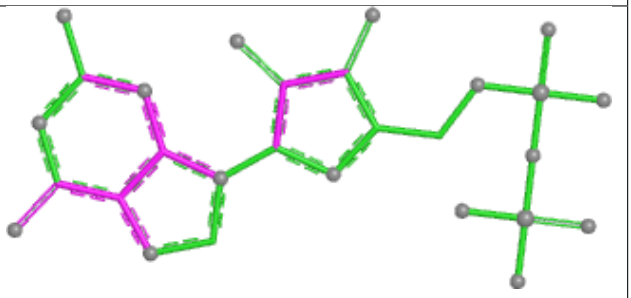


Rings

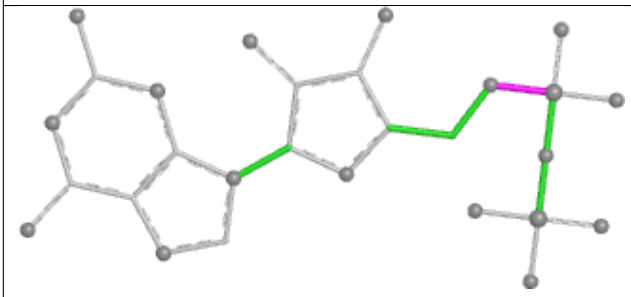
Ligand GDP FV 501



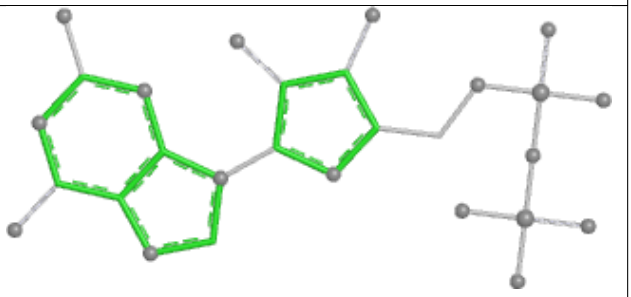
Bond lengths



Bond angles

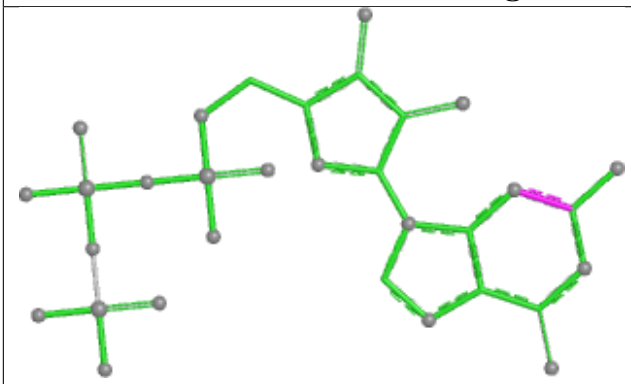


Torsions

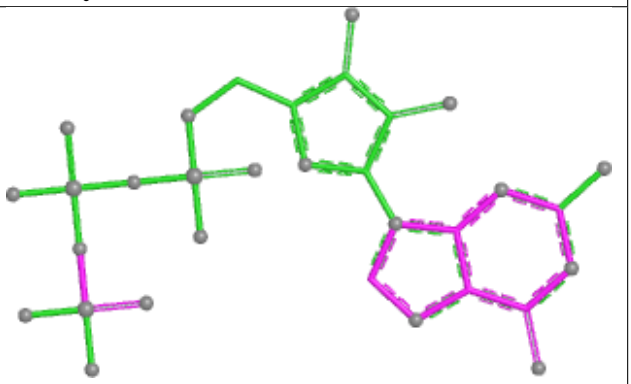


Rings

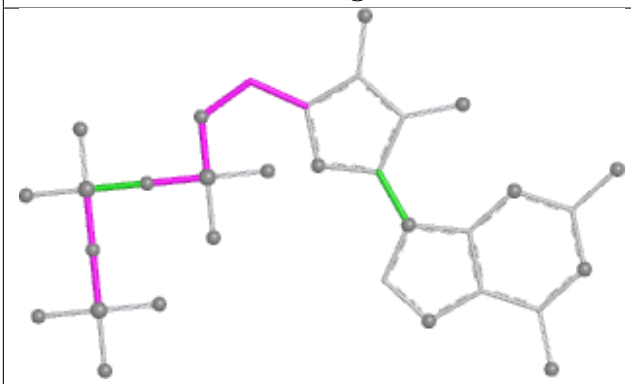
Ligand GTP WQ 501



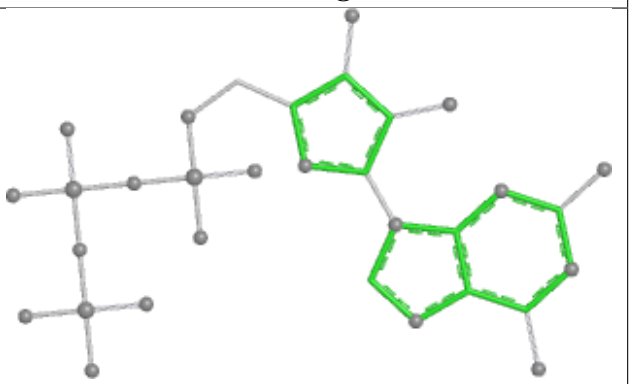
Bond lengths



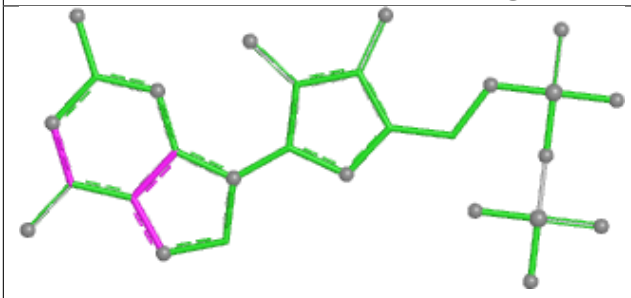
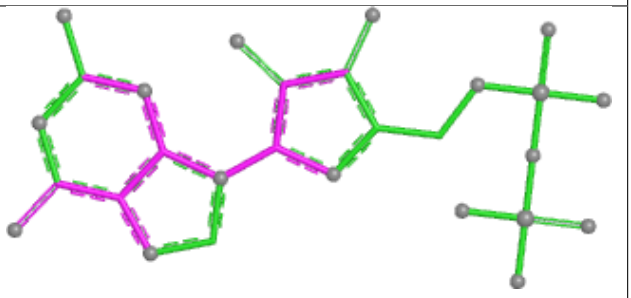
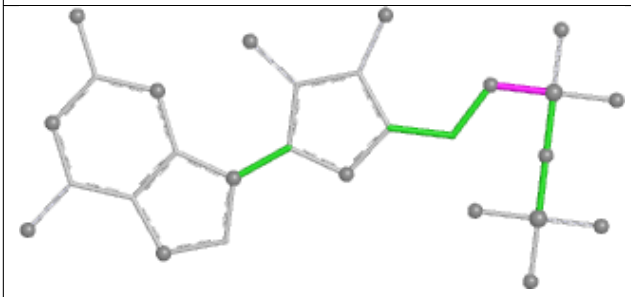
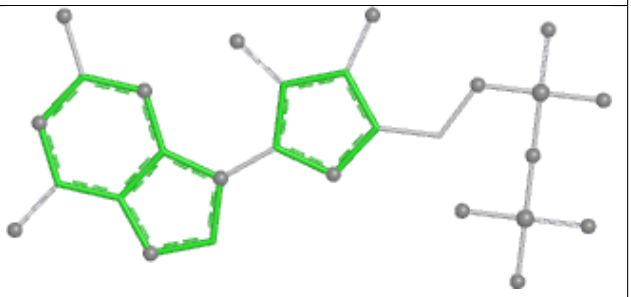
Bond angles

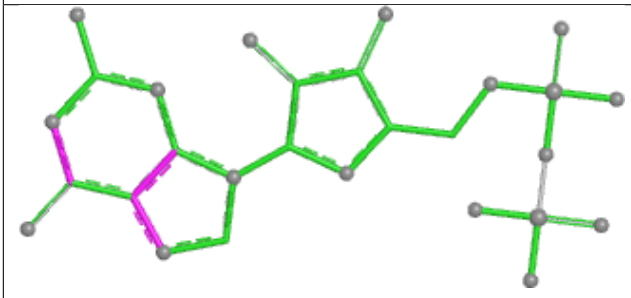
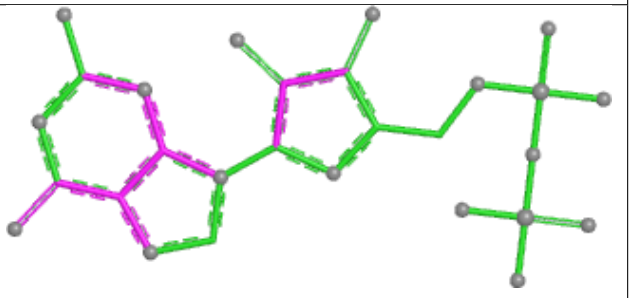
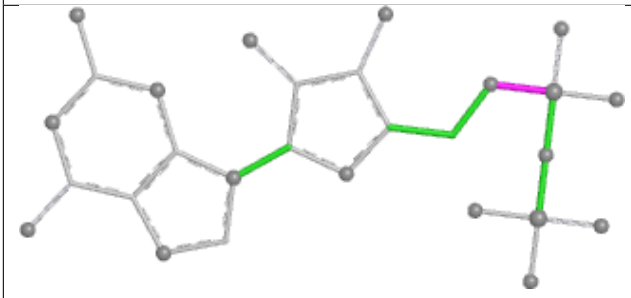
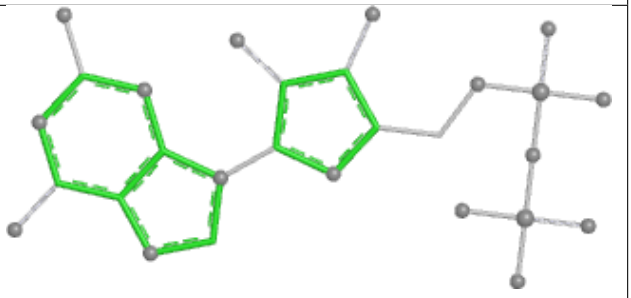


Torsions

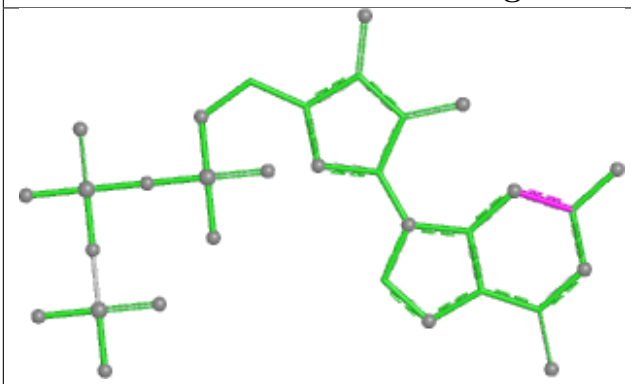


Rings

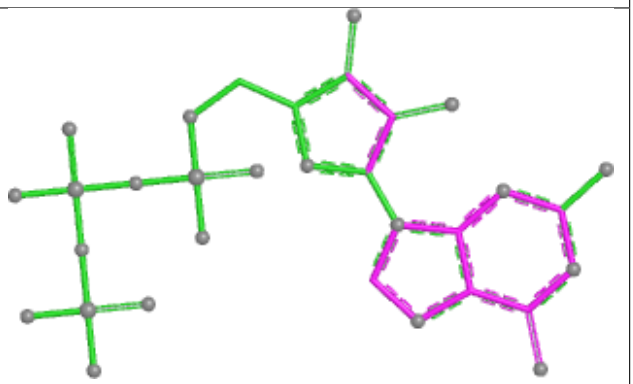
Ligand GDP CM 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP W 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

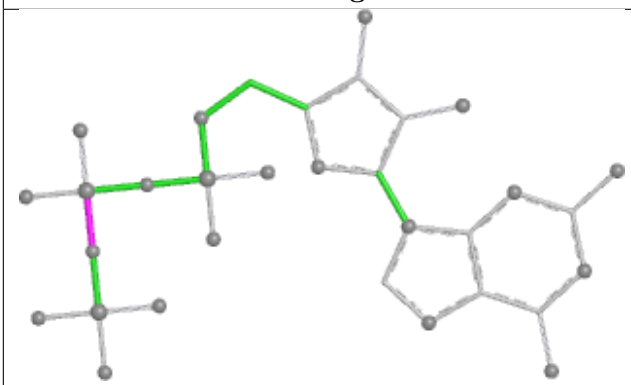
Ligand GTP WG 501



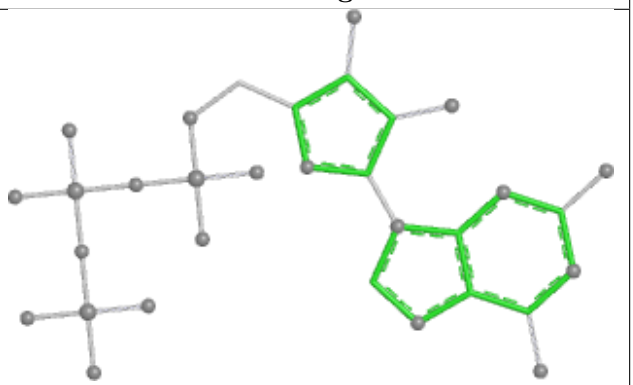
Bond lengths



Bond angles

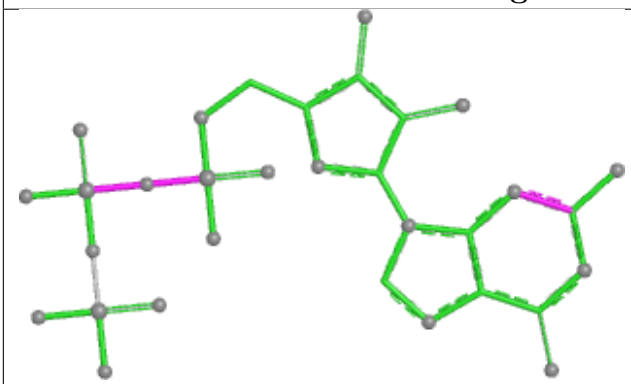


Torsions

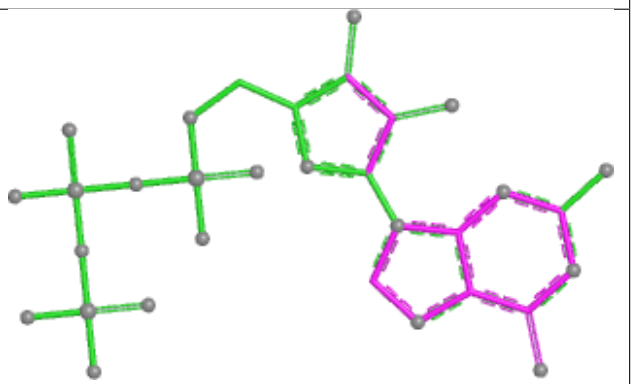


Rings

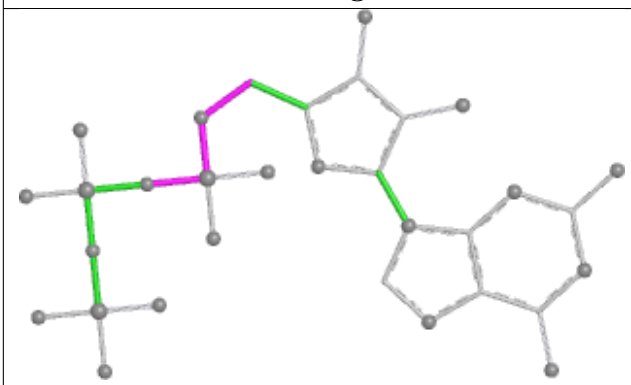
Ligand GTP NF 501



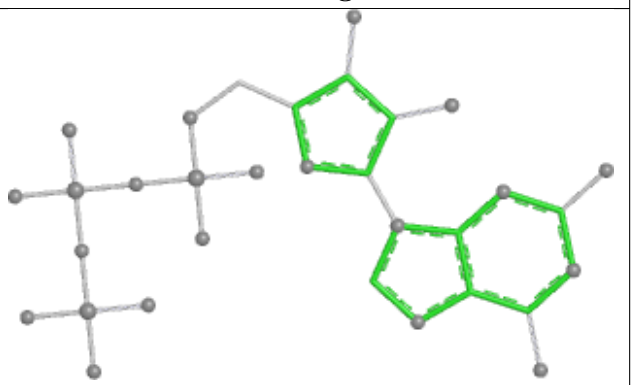
Bond lengths



Bond angles

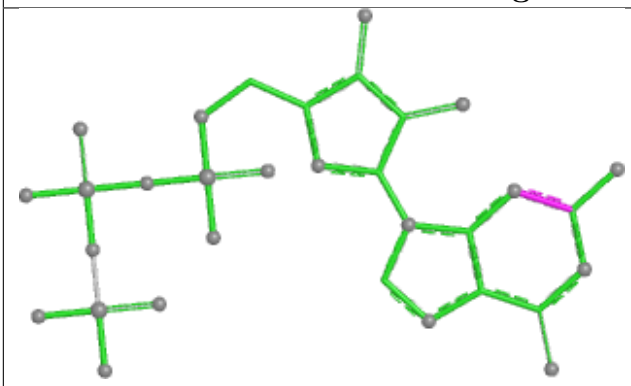


Torsions

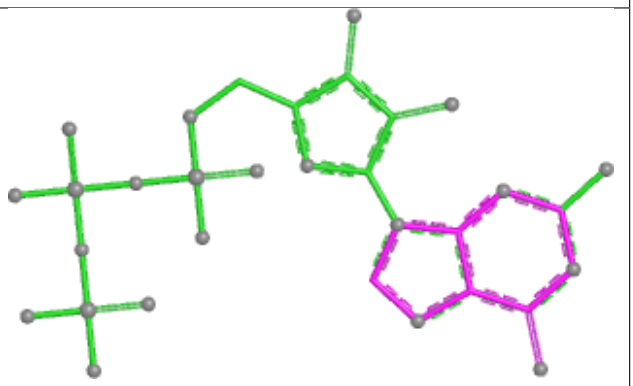


Rings

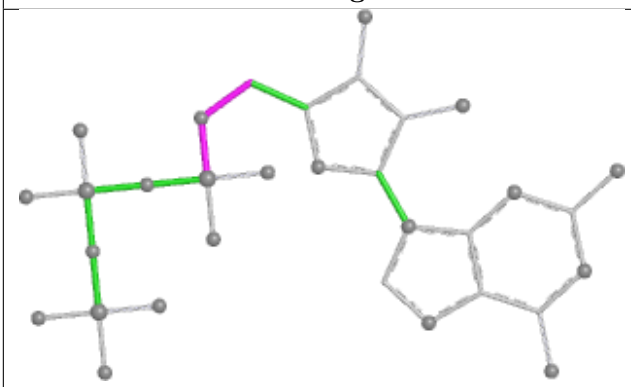
Ligand GTP KJ 501



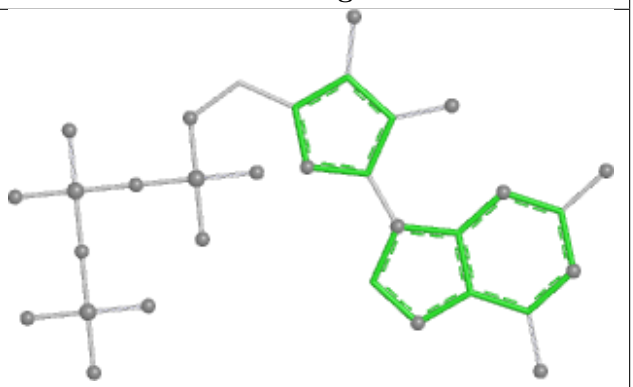
Bond lengths



Bond angles

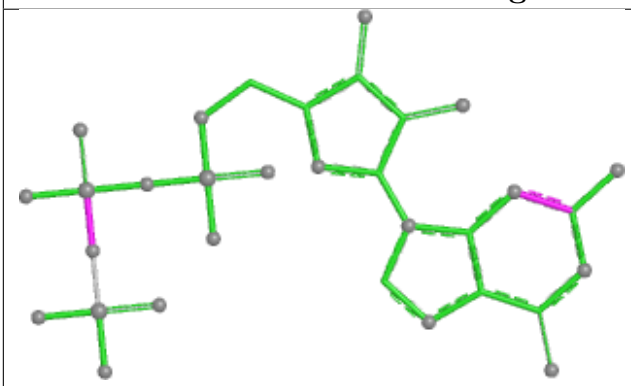


Torsions

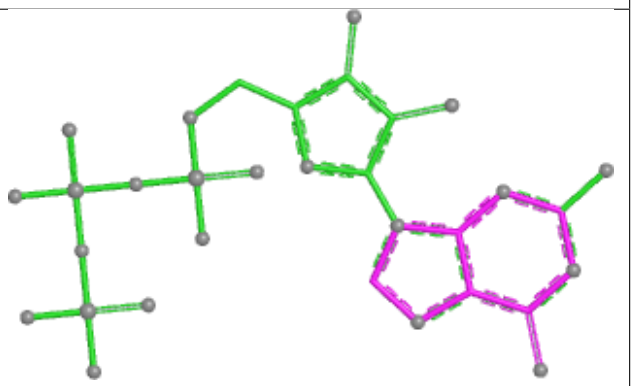


Rings

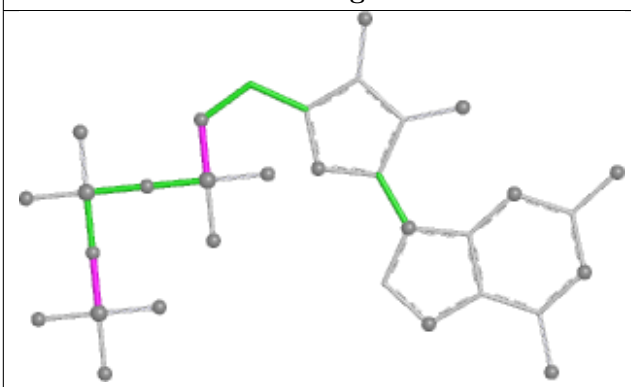
Ligand GTP VO 501



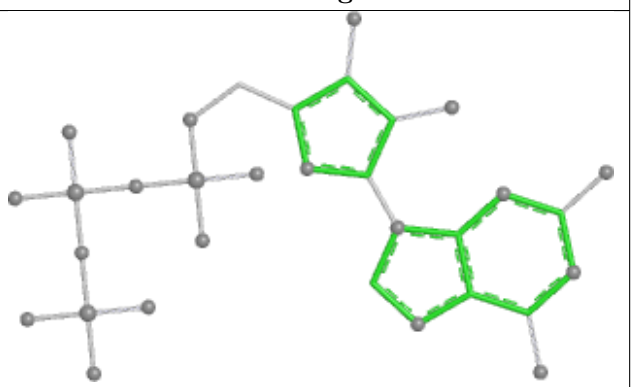
Bond lengths



Bond angles

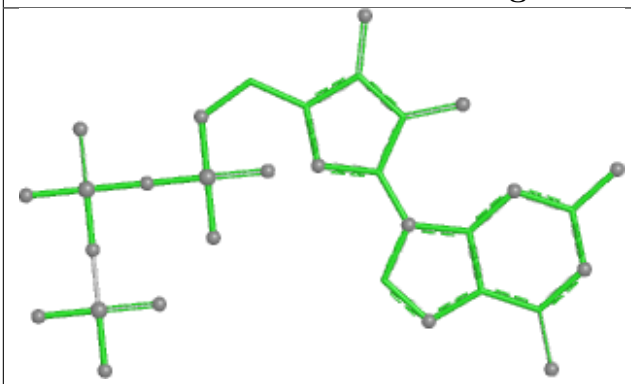


Torsions

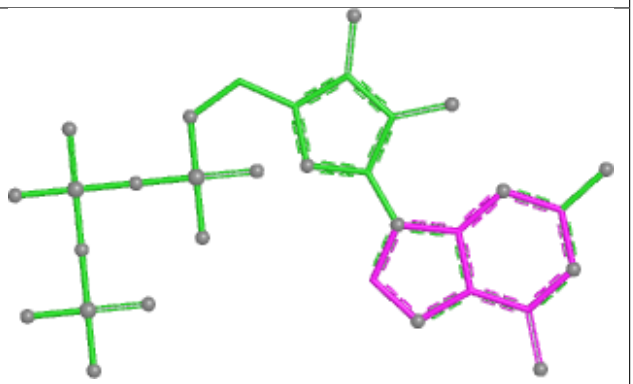


Rings

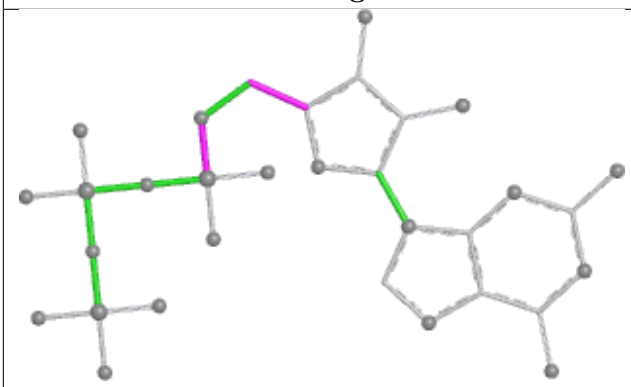
Ligand GTP BY 501



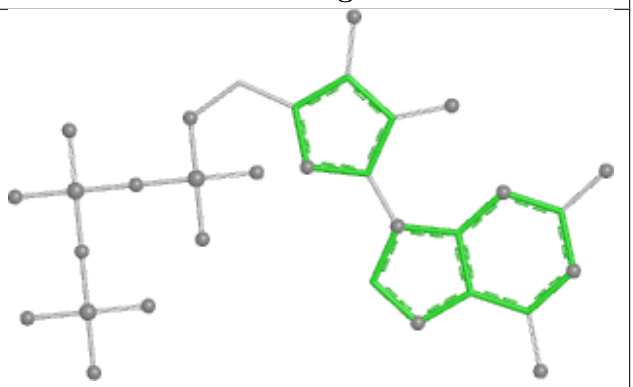
Bond lengths



Bond angles

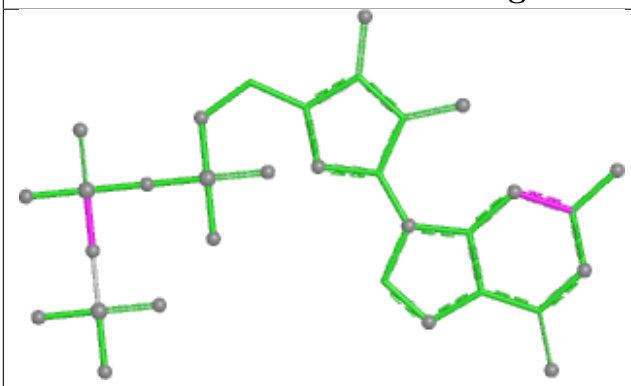


Torsions

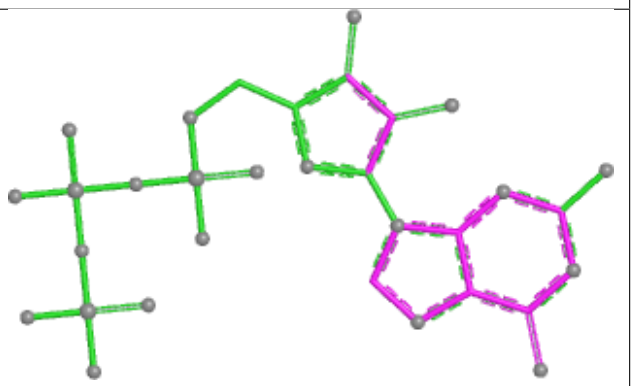


Rings

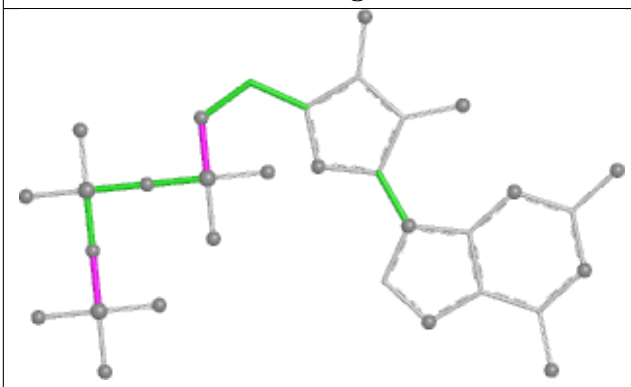
Ligand GTP KR 501



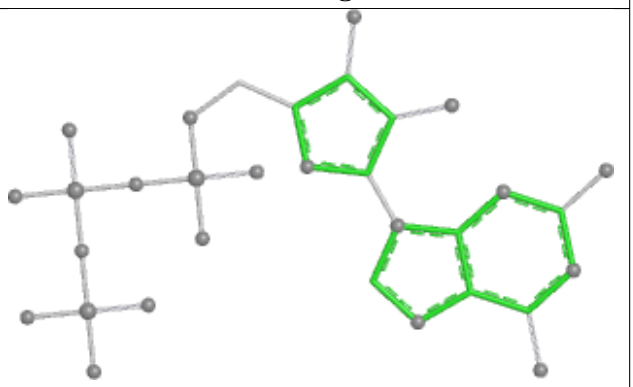
Bond lengths



Bond angles

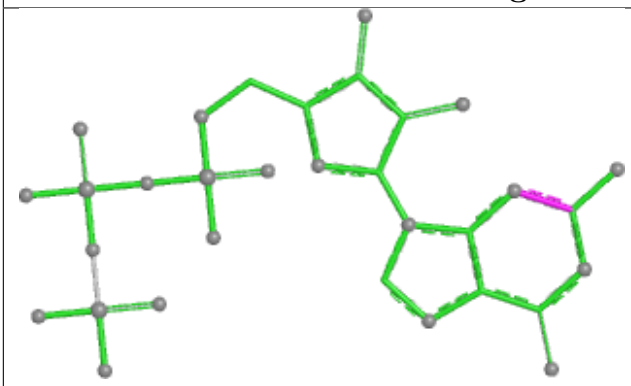


Torsions

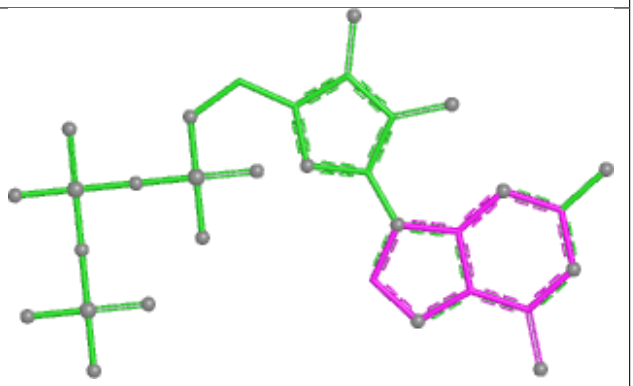


Rings

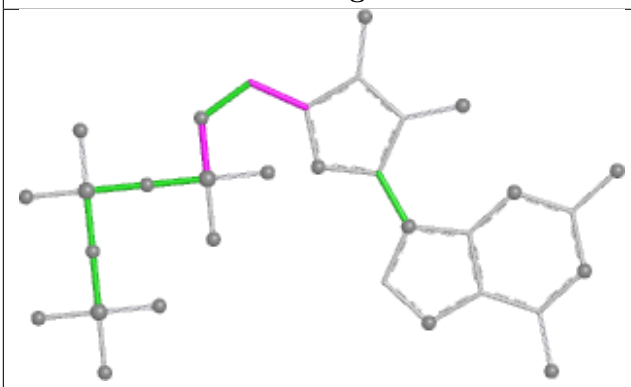
Ligand GTP PU 501



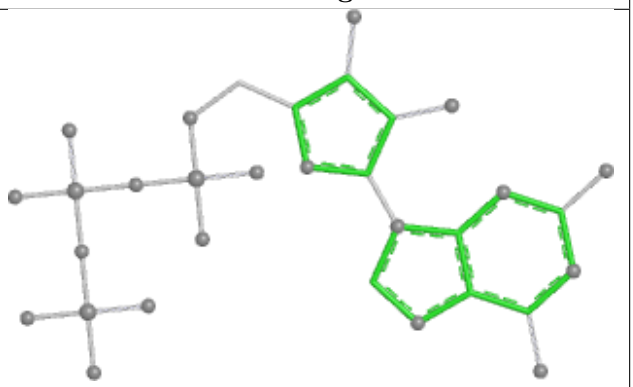
Bond lengths



Bond angles

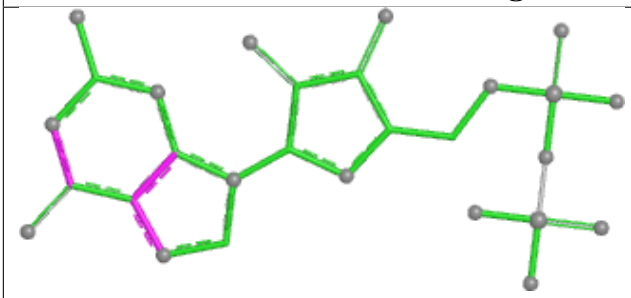


Torsions

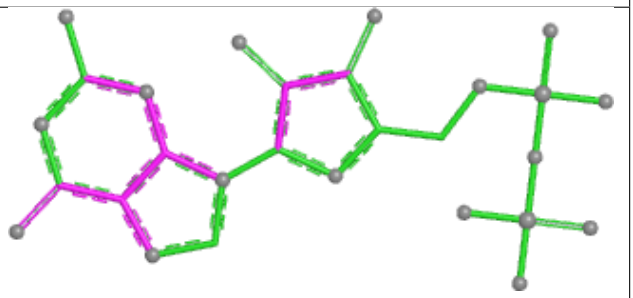


Rings

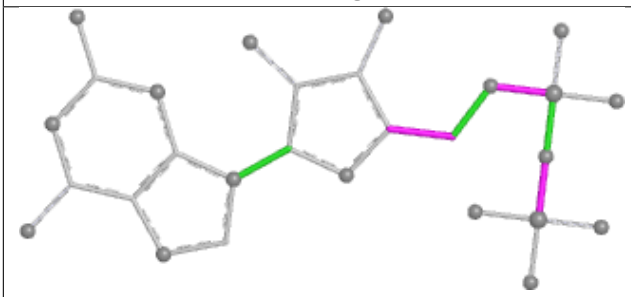
Ligand GDP CK 501



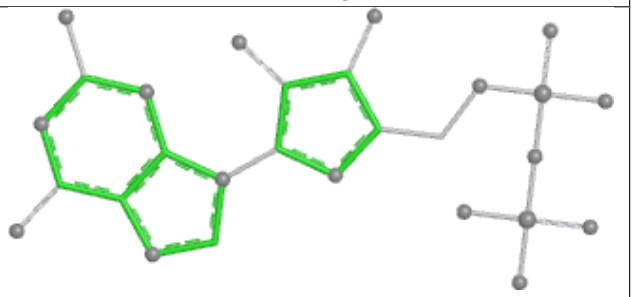
Bond lengths



Bond angles

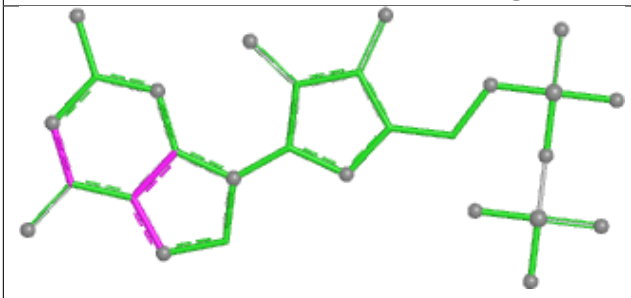


Torsions

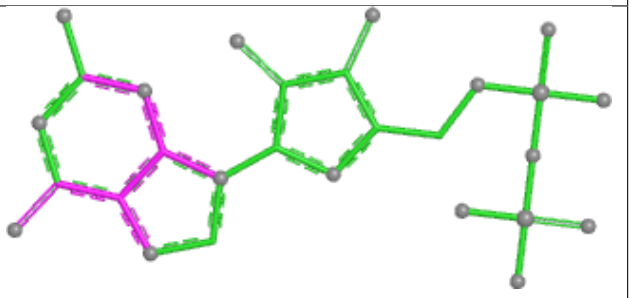


Rings

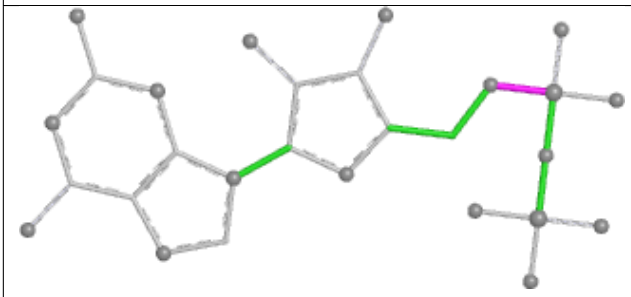
Ligand GDP DY 500



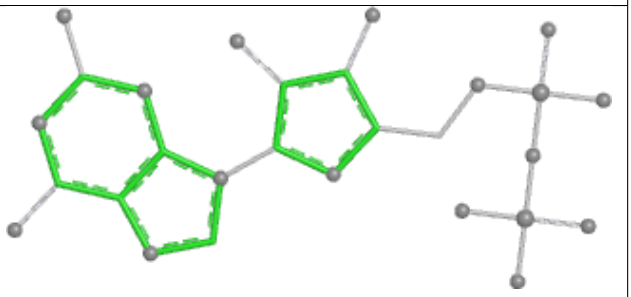
Bond lengths



Bond angles

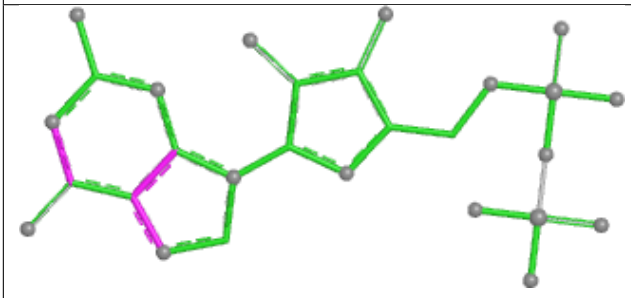


Torsions

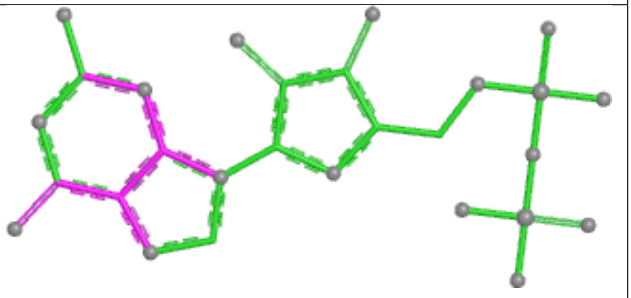


Rings

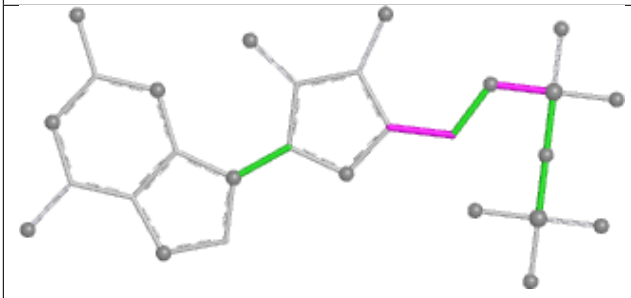
Ligand GDP EB 500



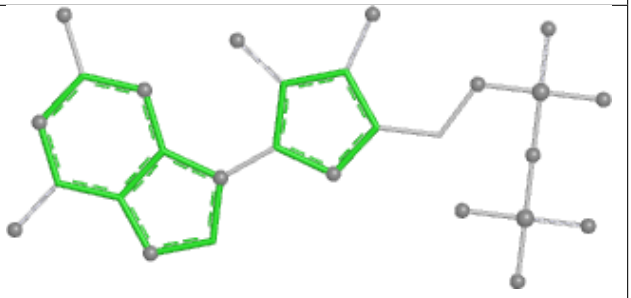
Bond lengths



Bond angles

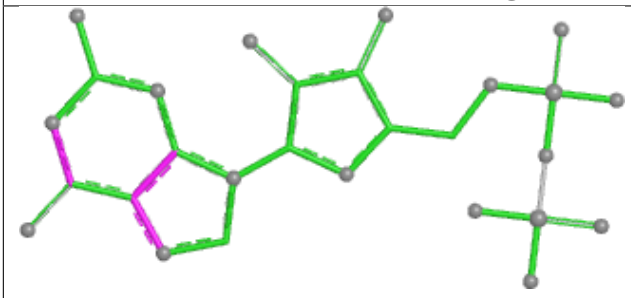


Torsions

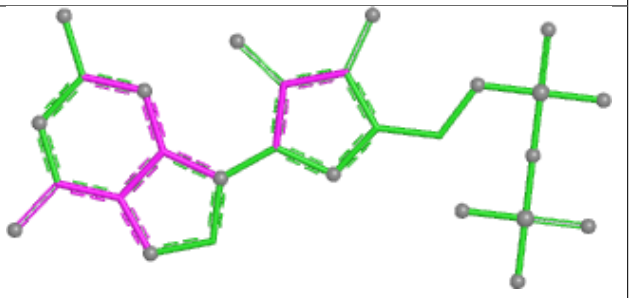


Rings

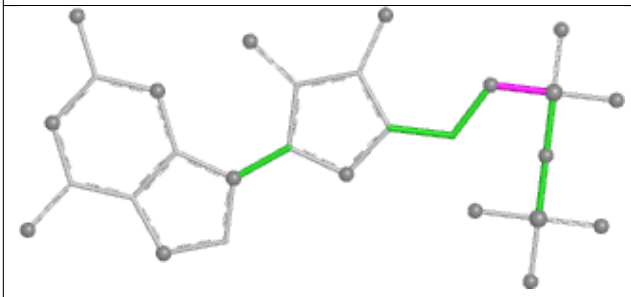
Ligand GDP WB 500



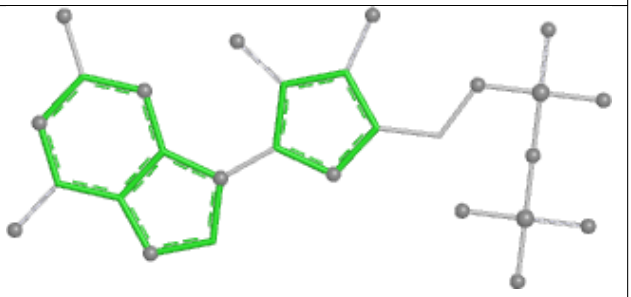
Bond lengths



Bond angles

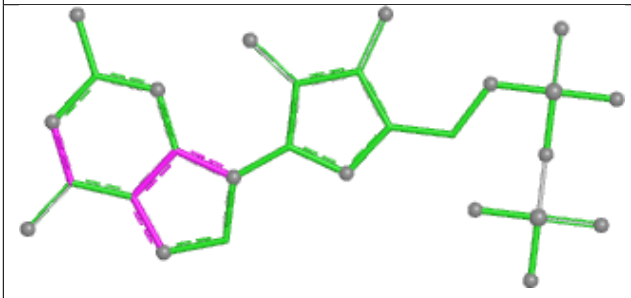


Torsions

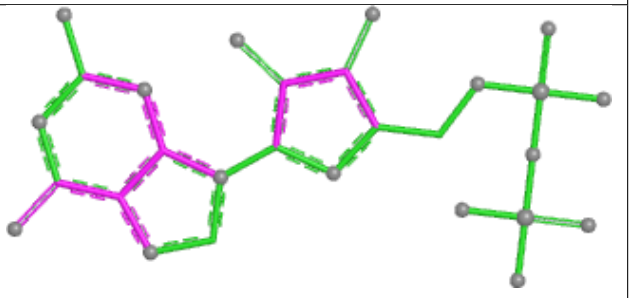


Rings

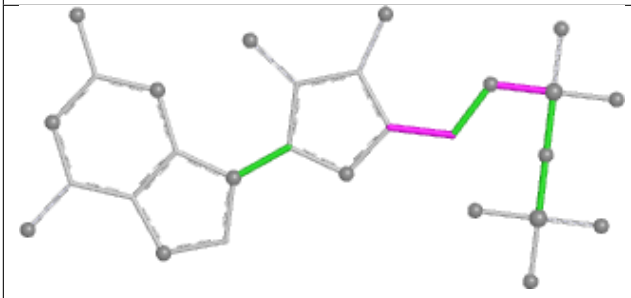
Ligand GDP AL 500



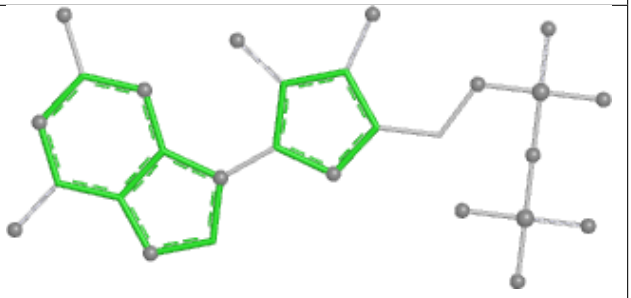
Bond lengths



Bond angles

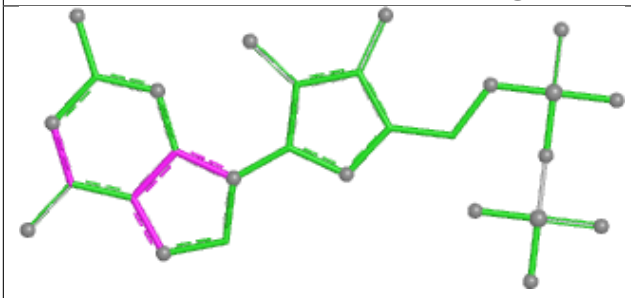


Torsions

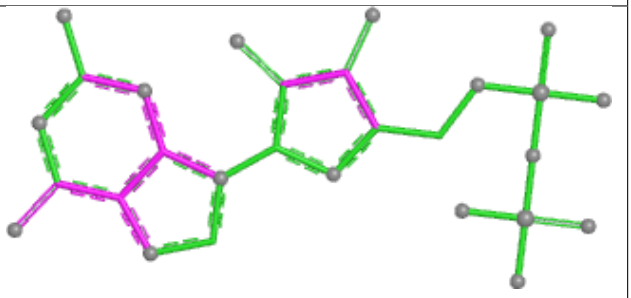


Rings

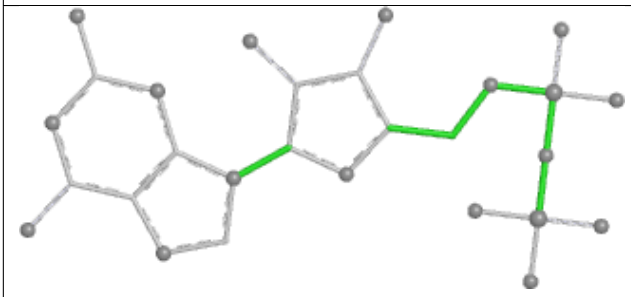
Ligand GDP FH 500



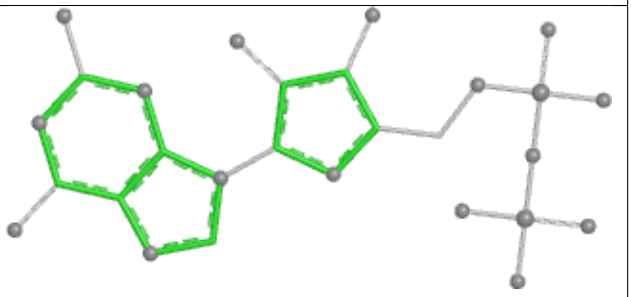
Bond lengths



Bond angles

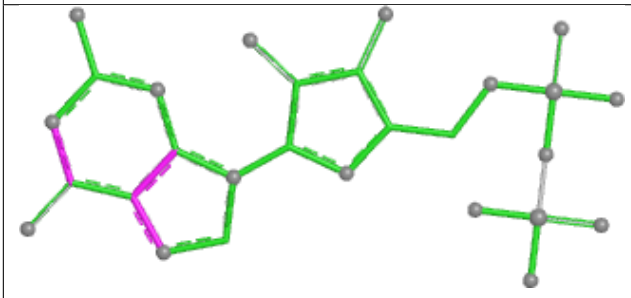


Torsions

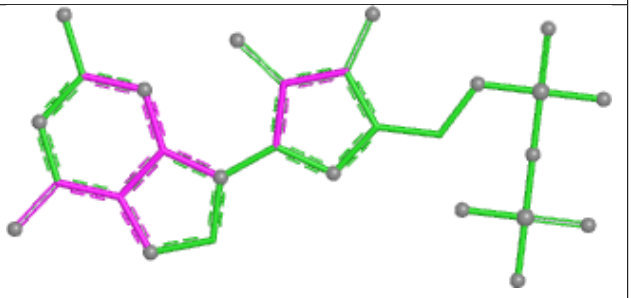


Rings

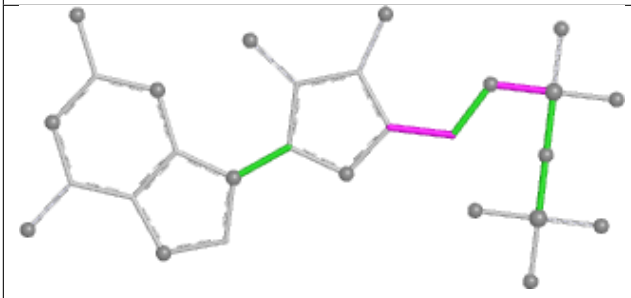
Ligand GDP NN 500



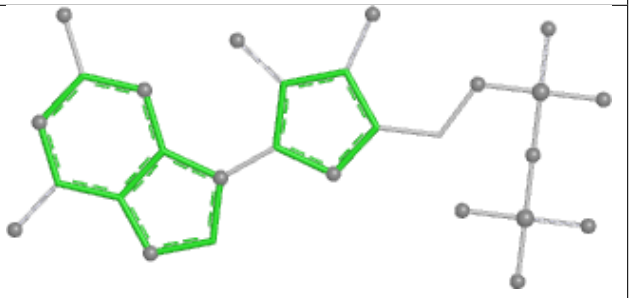
Bond lengths



Bond angles

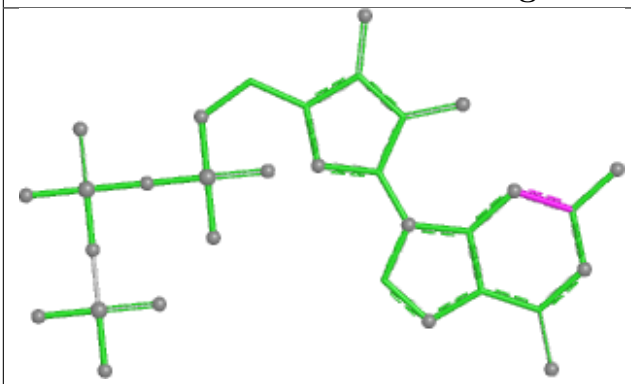


Torsions

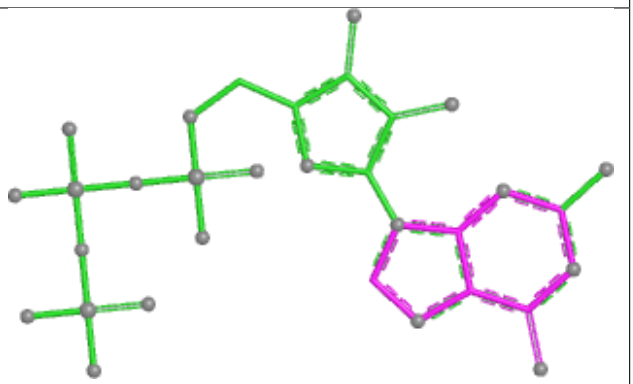


Rings

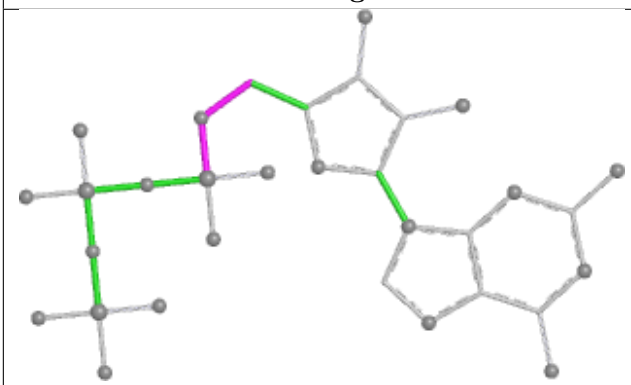
Ligand GTP SI 501



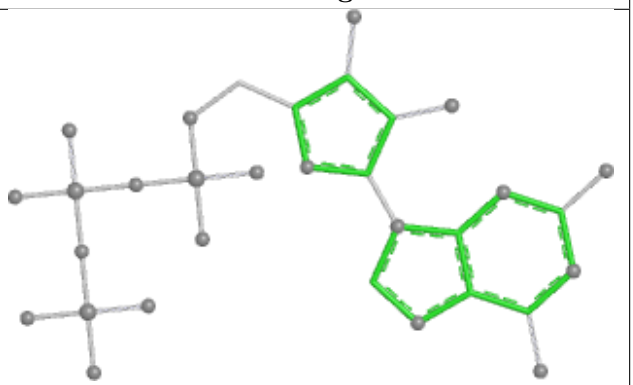
Bond lengths



Bond angles

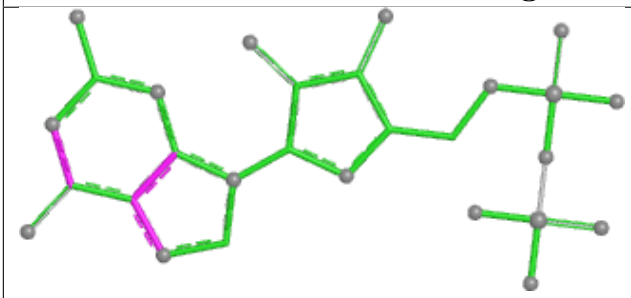


Torsions

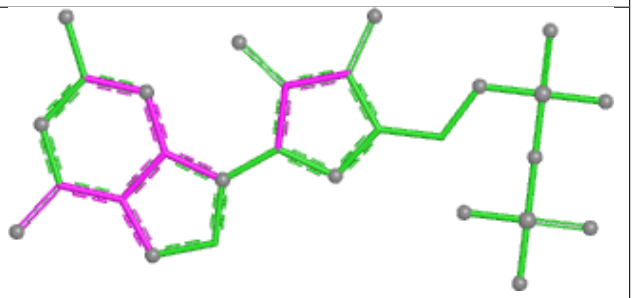


Rings

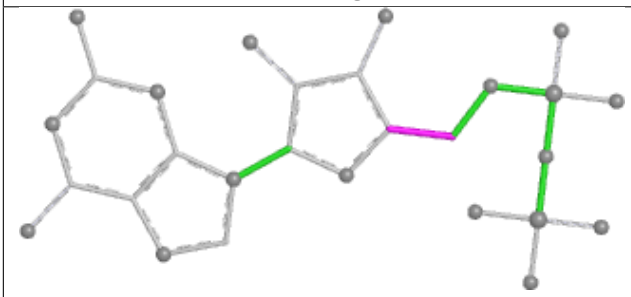
Ligand GDP G 500



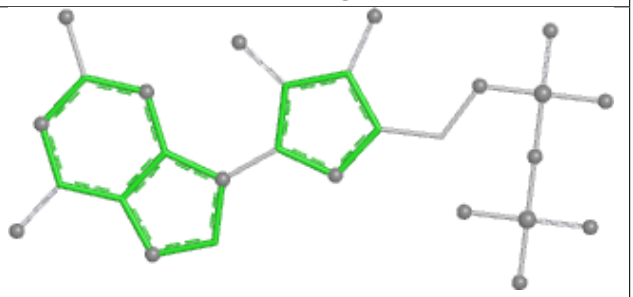
Bond lengths



Bond angles

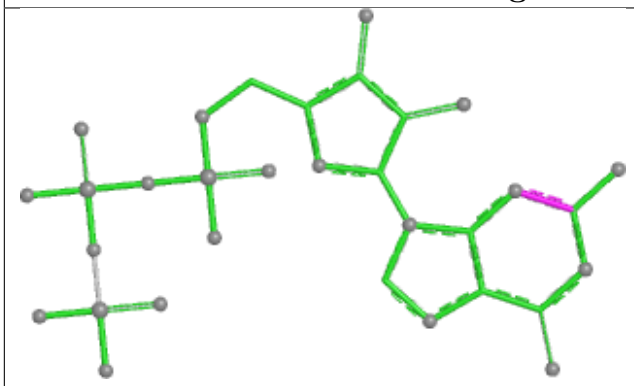


Torsions

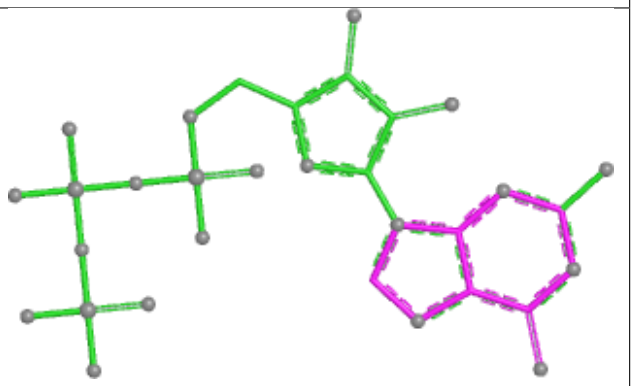


Rings

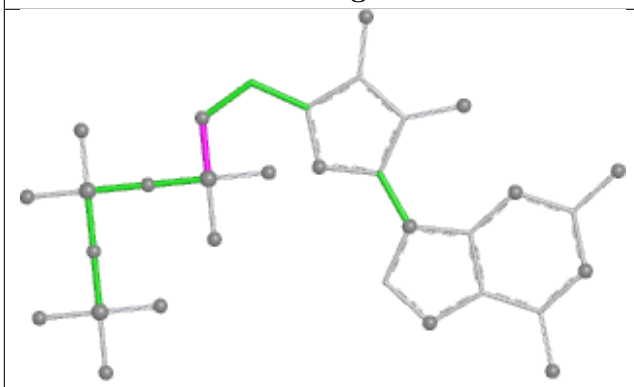
Ligand GTP KD 502



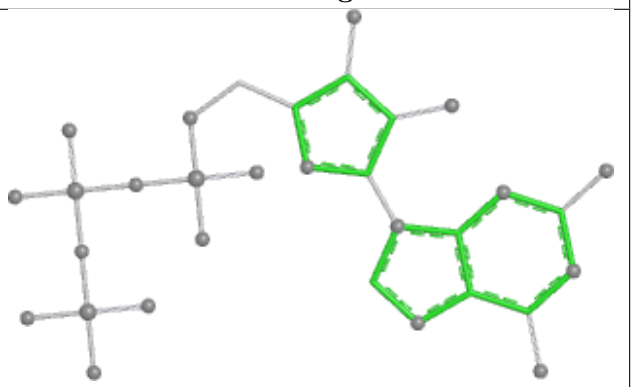
Bond lengths



Bond angles

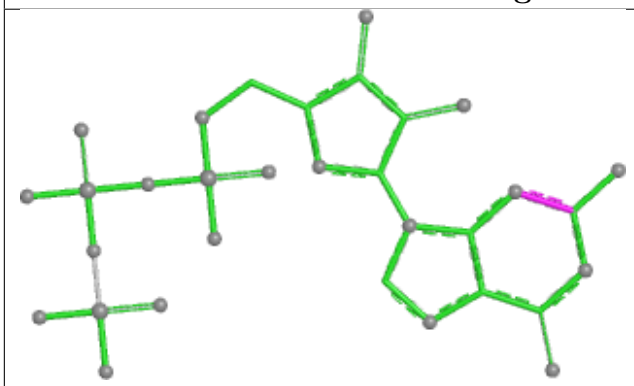


Torsions

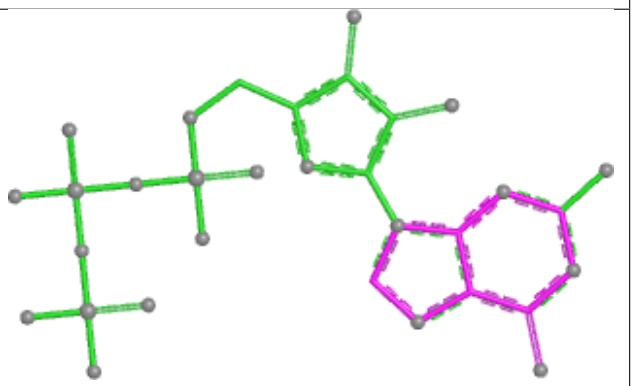


Rings

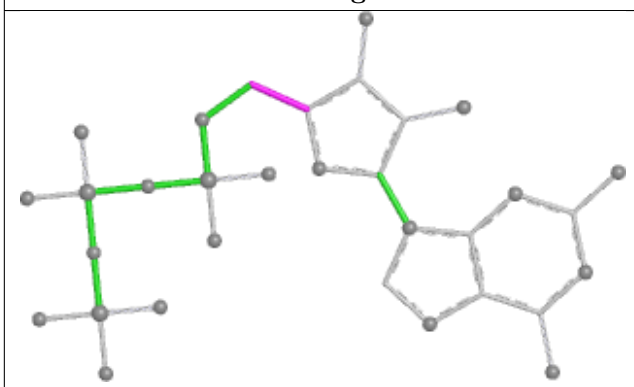
Ligand GTP RJ 501



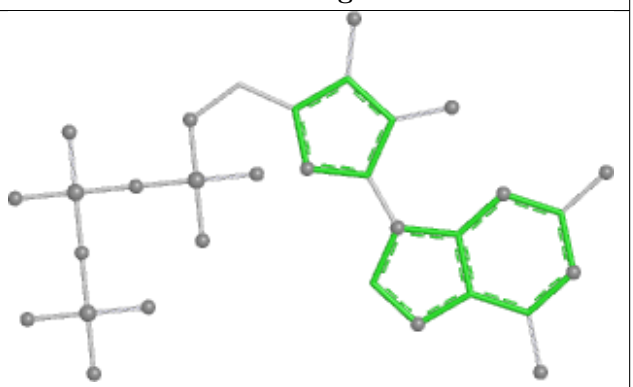
Bond lengths



Bond angles

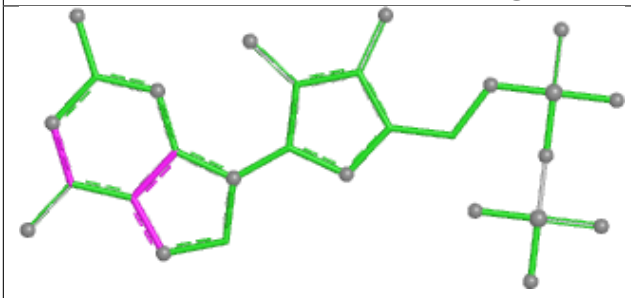


Torsions

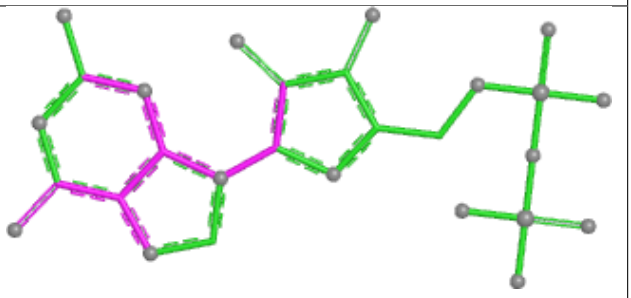


Rings

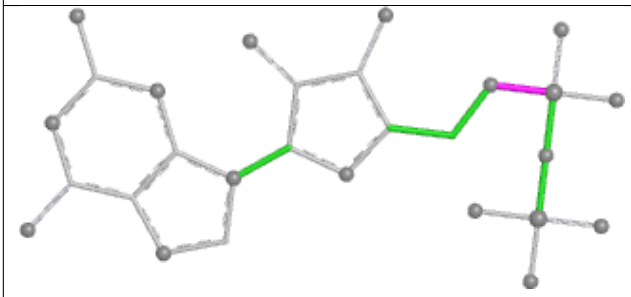
Ligand GDP CA 500



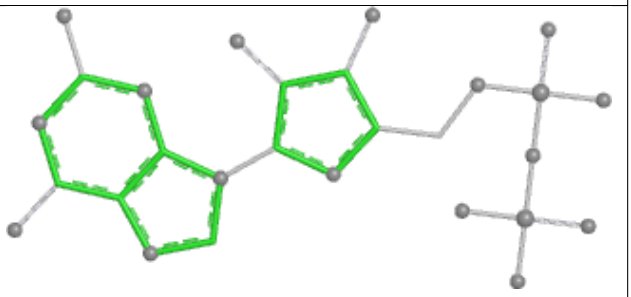
Bond lengths



Bond angles

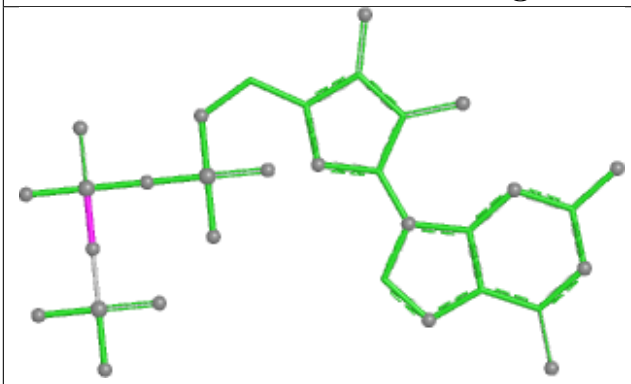


Torsions

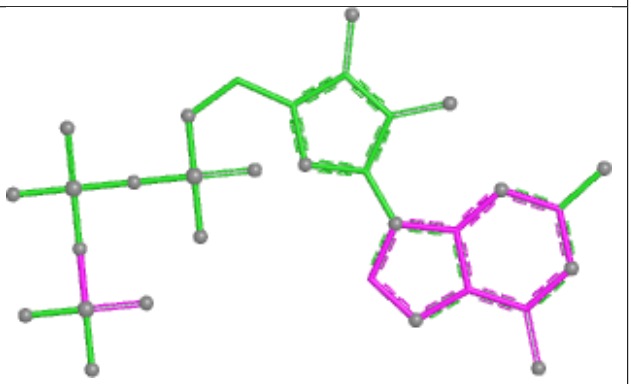


Rings

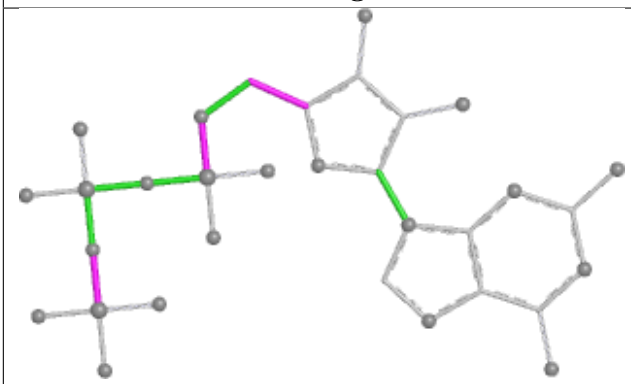
Ligand GTP EP 501



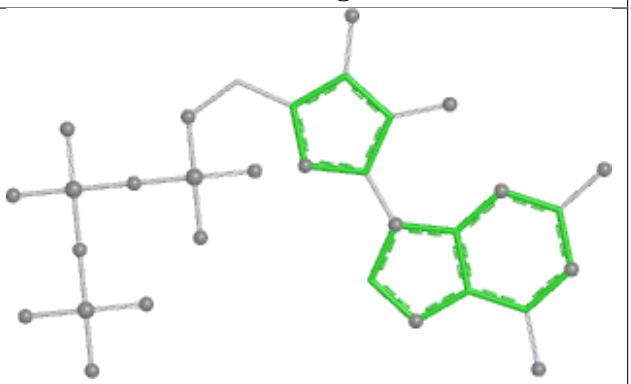
Bond lengths



Bond angles

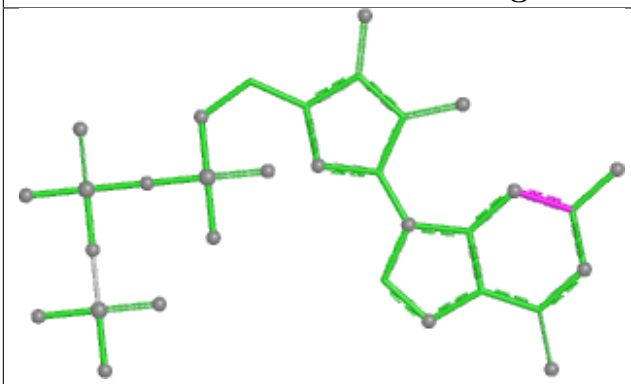


Torsions

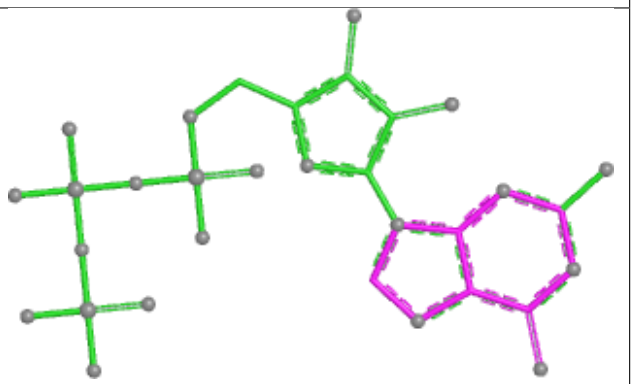


Rings

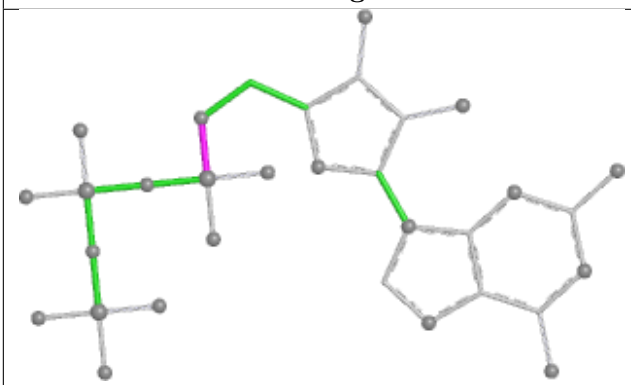
Ligand GTP PC 501



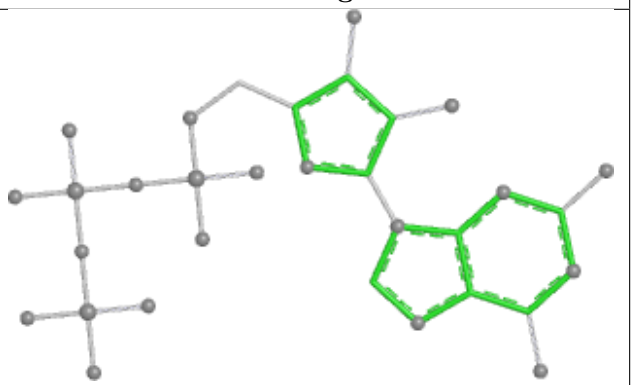
Bond lengths



Bond angles

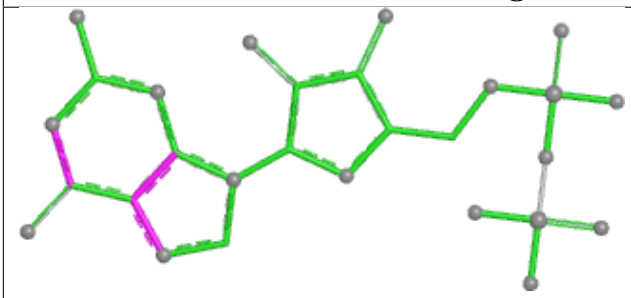


Torsions

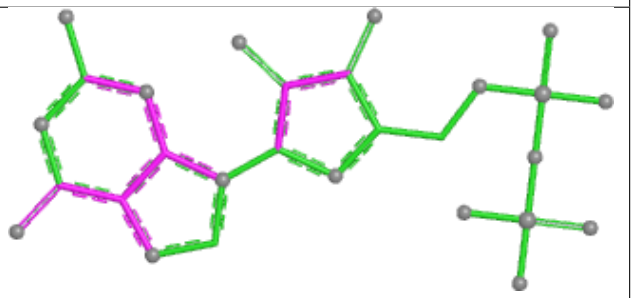


Rings

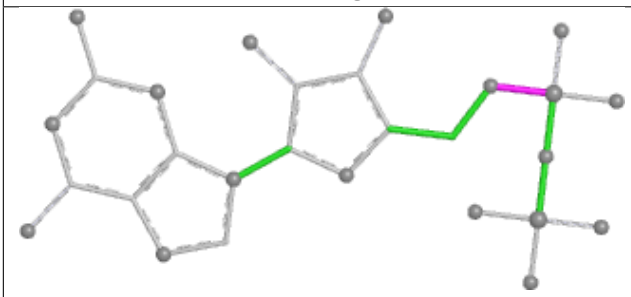
Ligand GDP UT 500



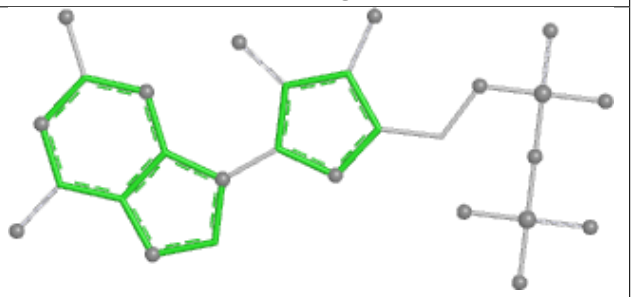
Bond lengths



Bond angles

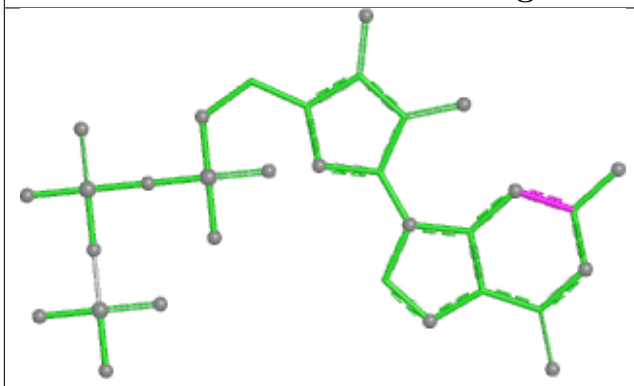


Torsions

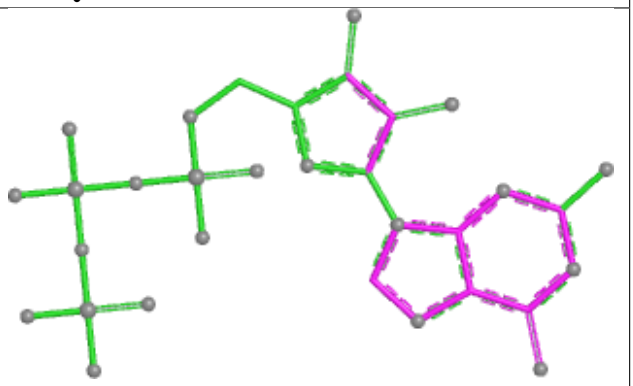


Rings

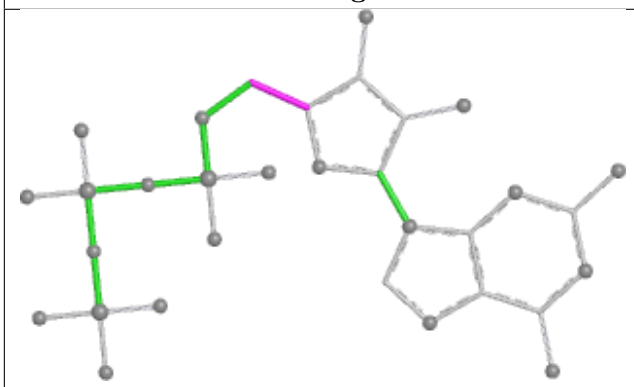
Ligand GTP IQ 501



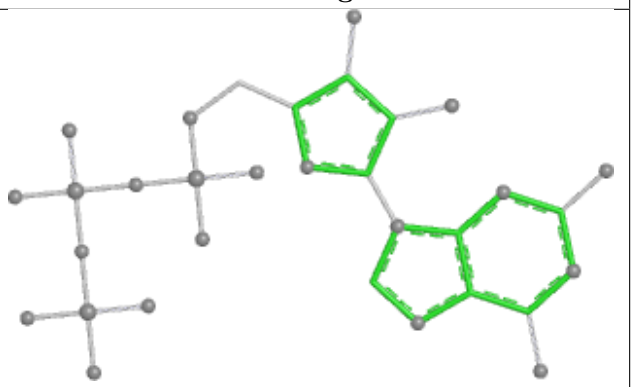
Bond lengths



Bond angles

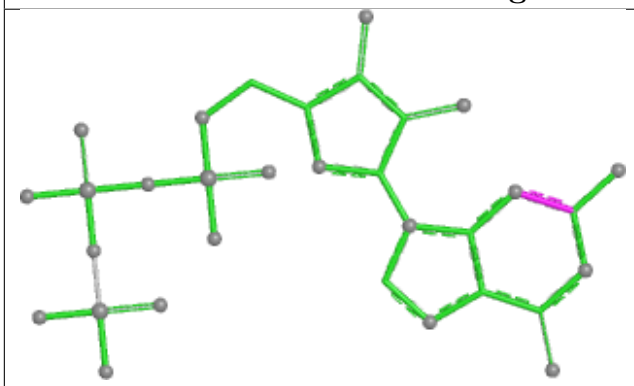


Torsions

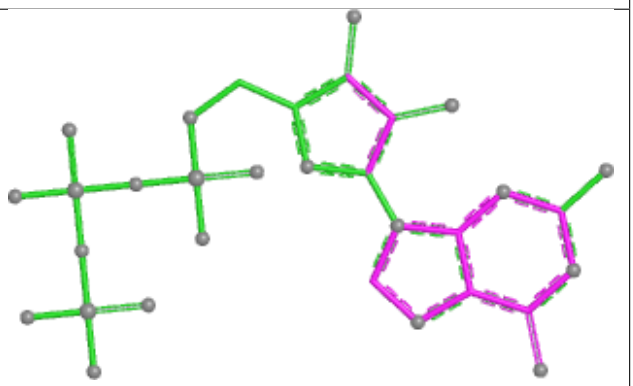


Rings

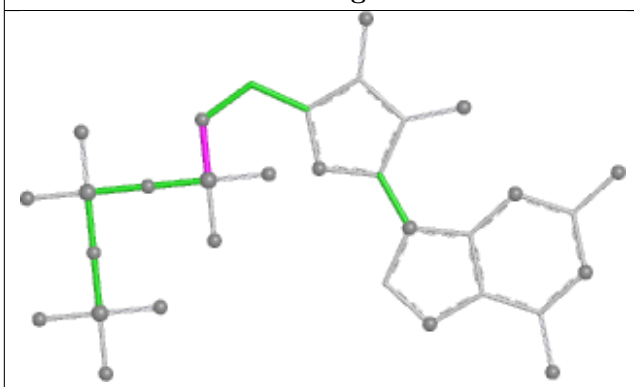
Ligand GTP UU 501



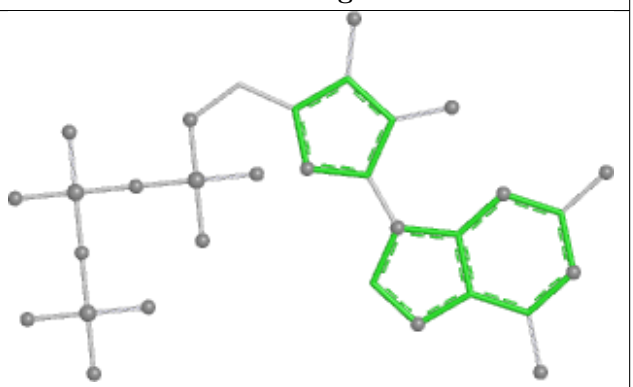
Bond lengths



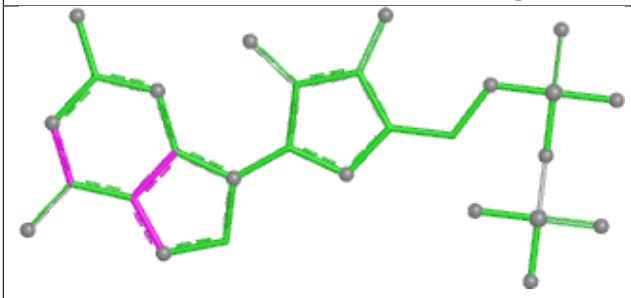
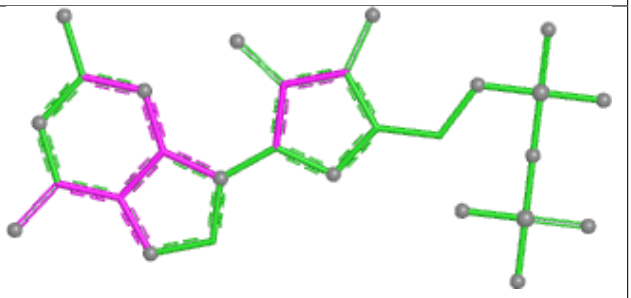
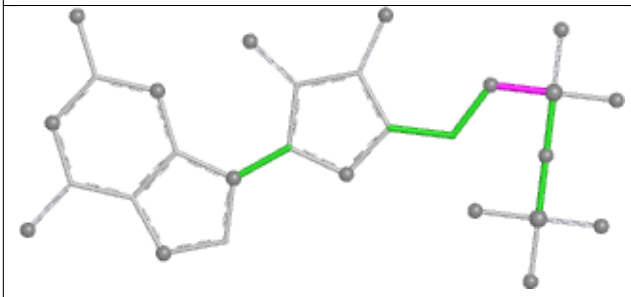
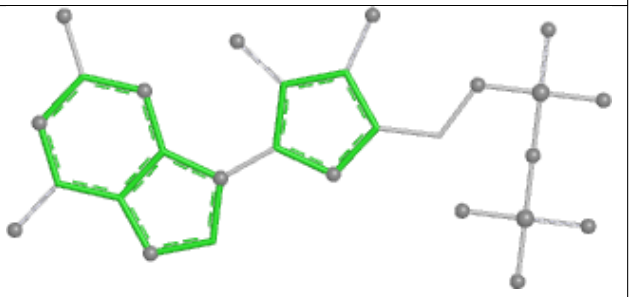
Bond angles

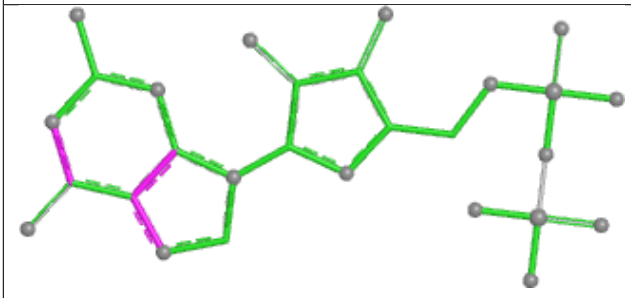
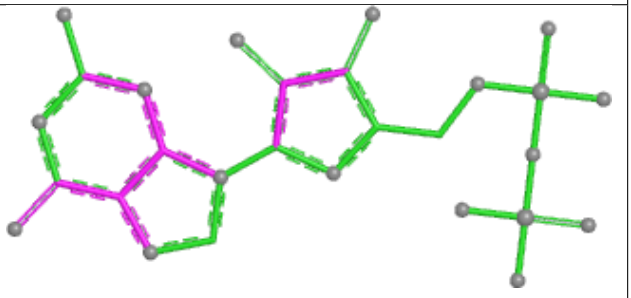
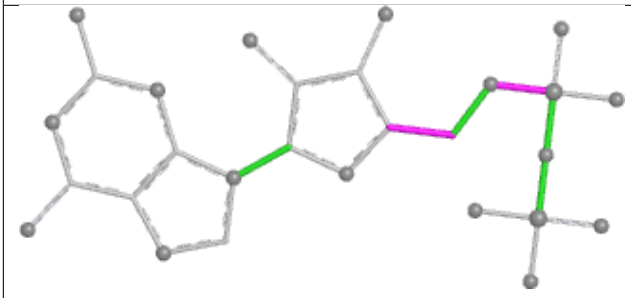
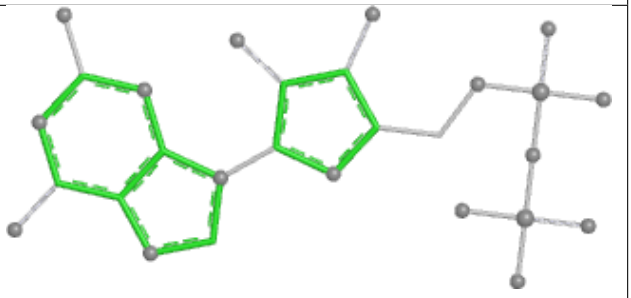


Torsions

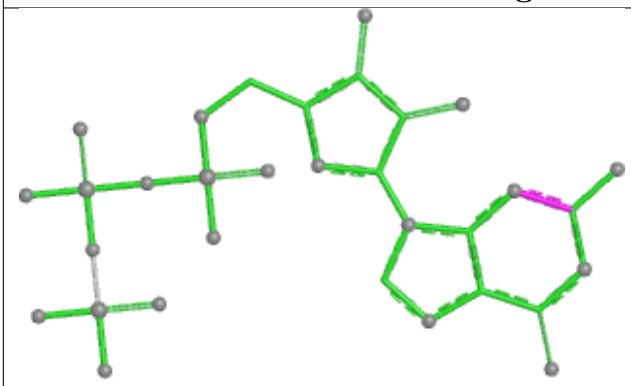


Rings

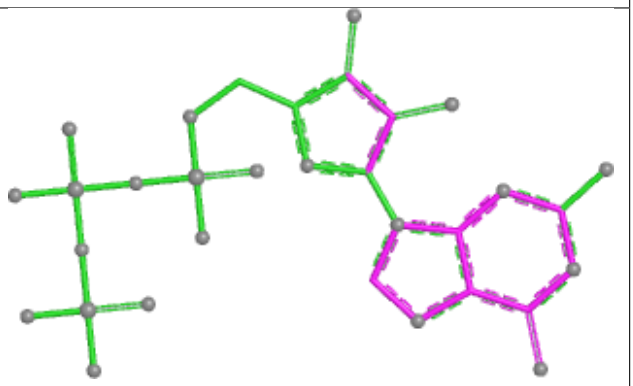
Ligand GDP UL 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP LU 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

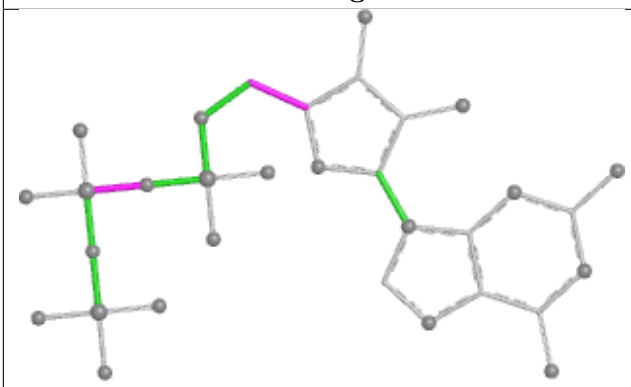
Ligand GTP AI 501



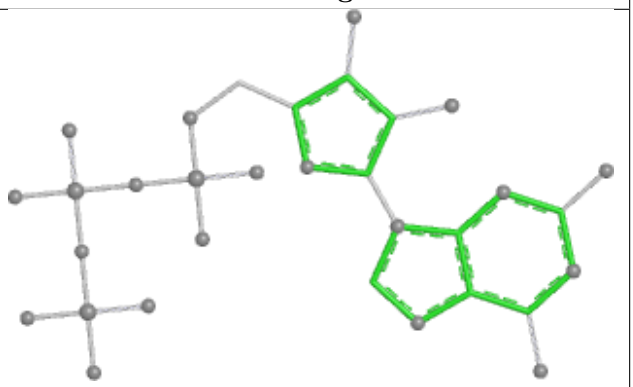
Bond lengths



Bond angles

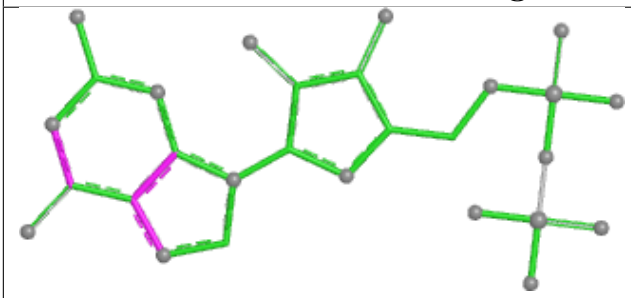


Torsions

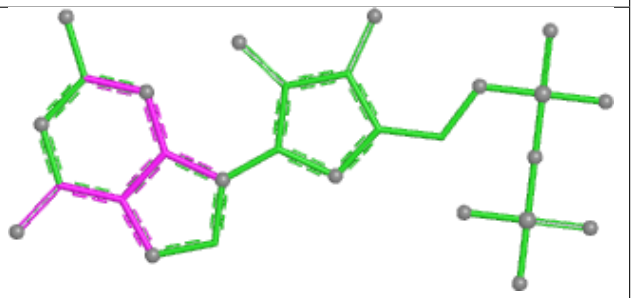


Rings

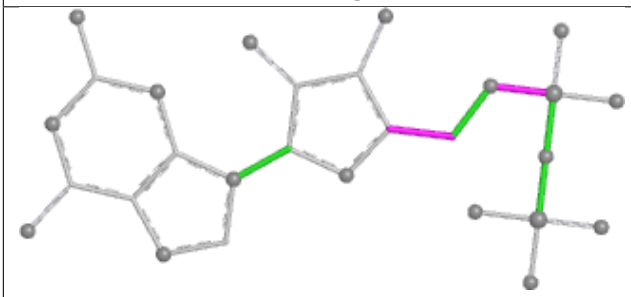
Ligand GDP PR 501



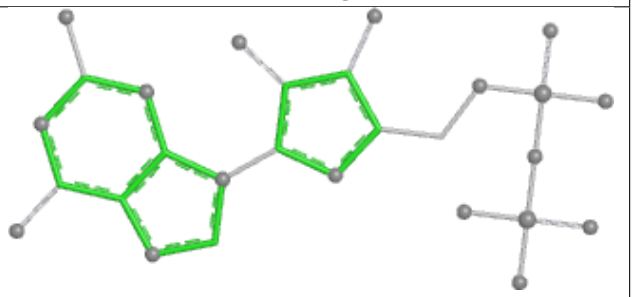
Bond lengths



Bond angles

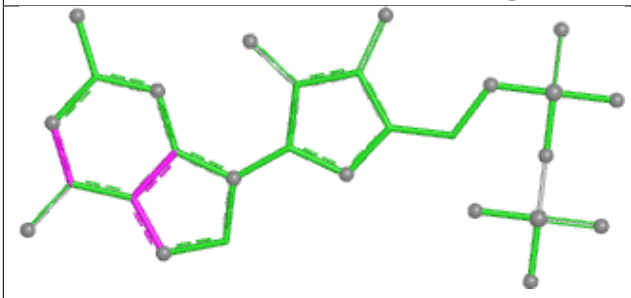


Torsions

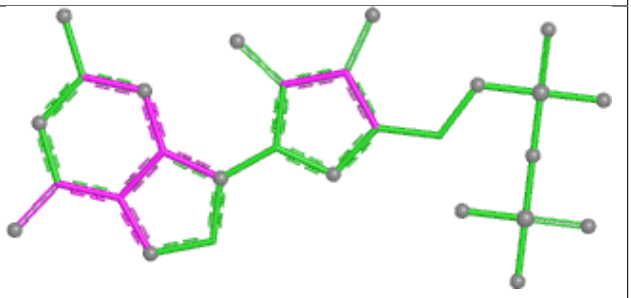


Rings

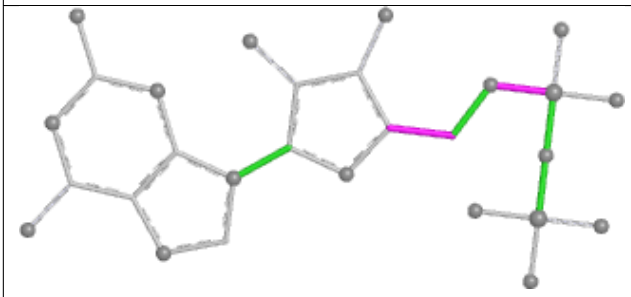
Ligand GDP MN 500



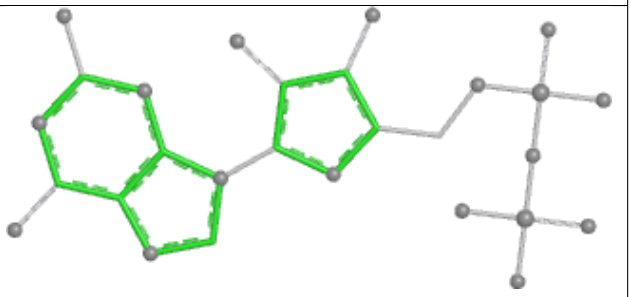
Bond lengths



Bond angles

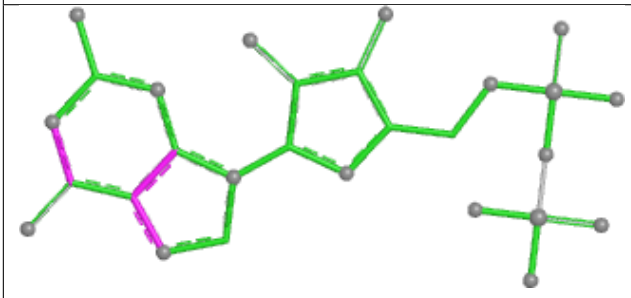


Torsions

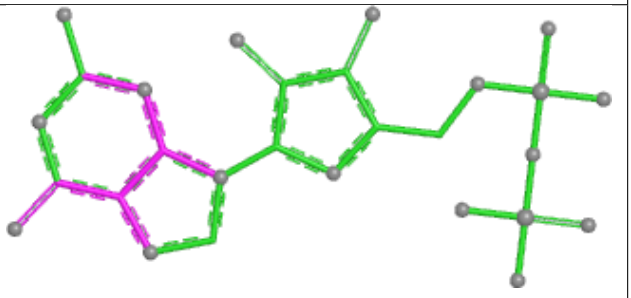


Rings

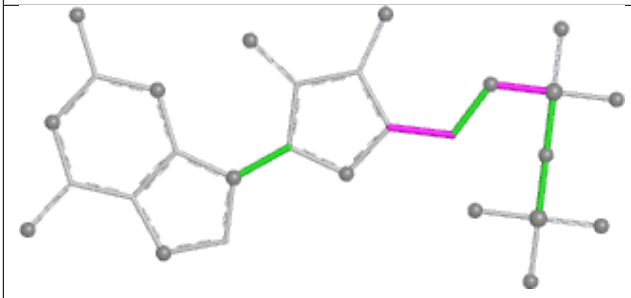
Ligand GDP BX 500



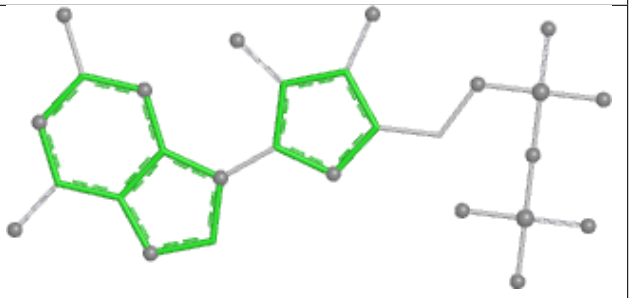
Bond lengths



Bond angles

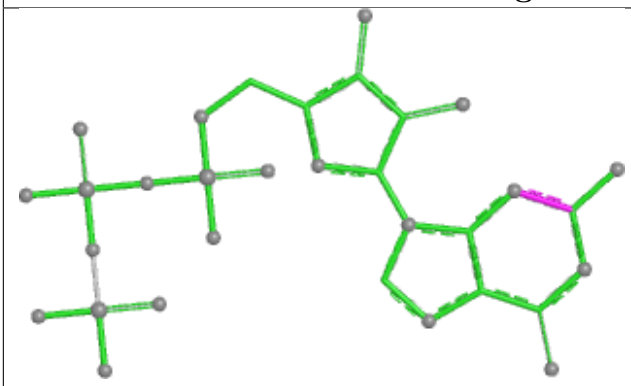


Torsions

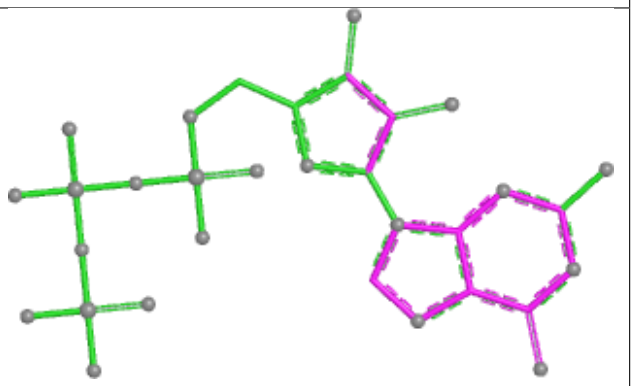


Rings

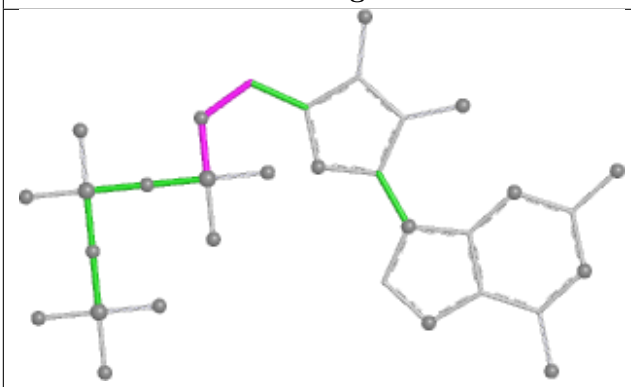
Ligand GTP JF 501



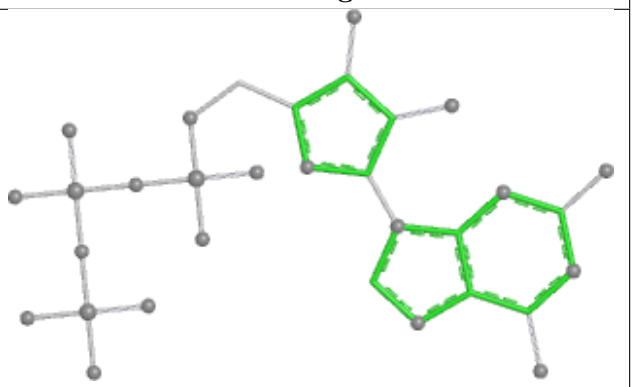
Bond lengths



Bond angles

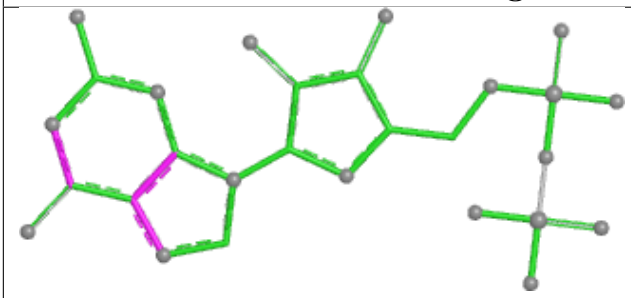


Torsions

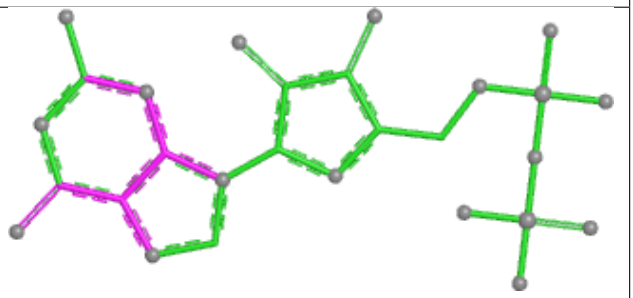


Rings

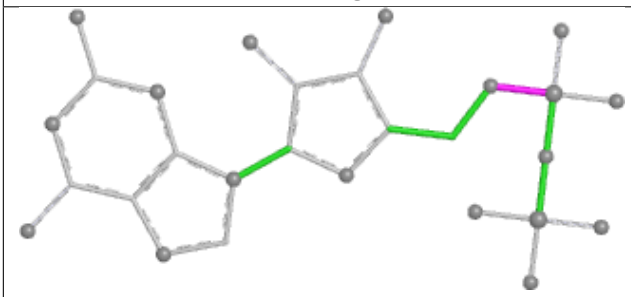
Ligand GDP DG 500



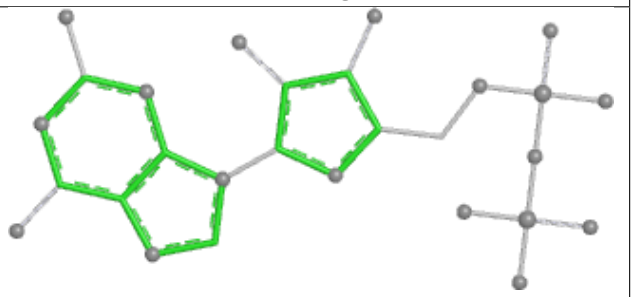
Bond lengths



Bond angles

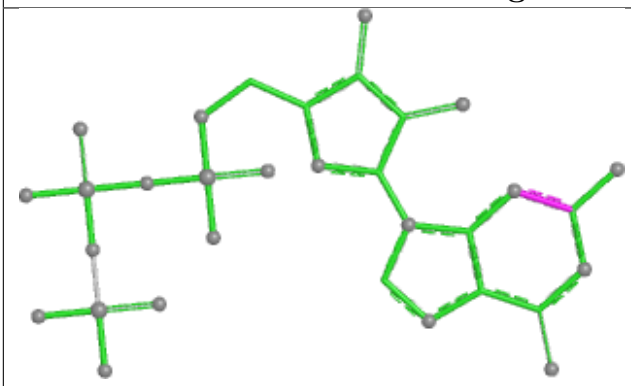


Torsions

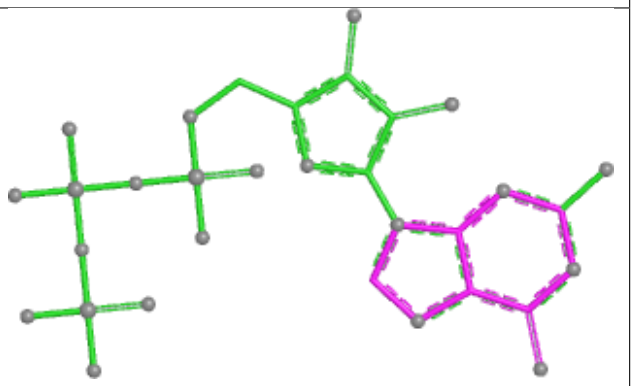


Rings

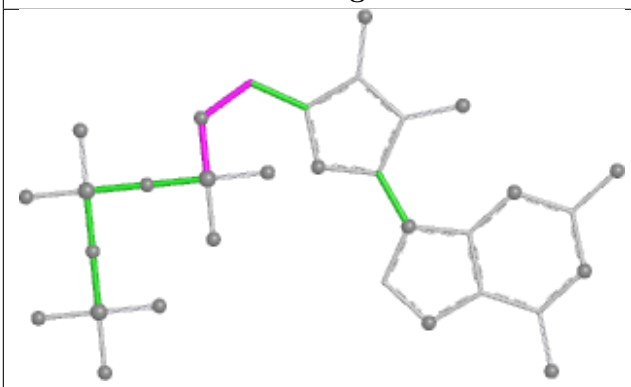
Ligand GTP KV 501



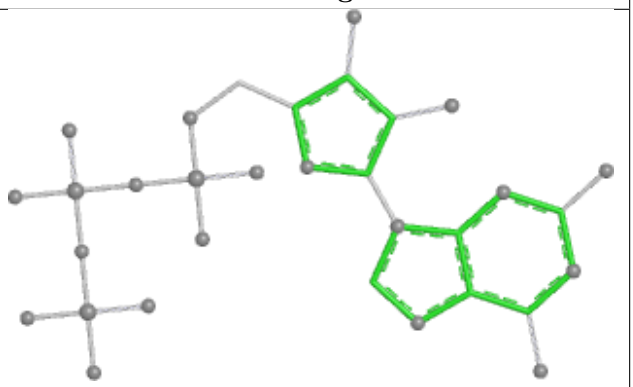
Bond lengths



Bond angles

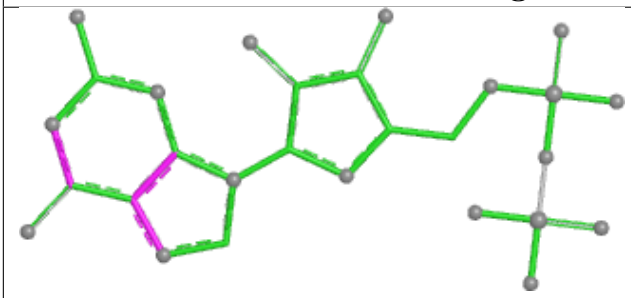


Torsions

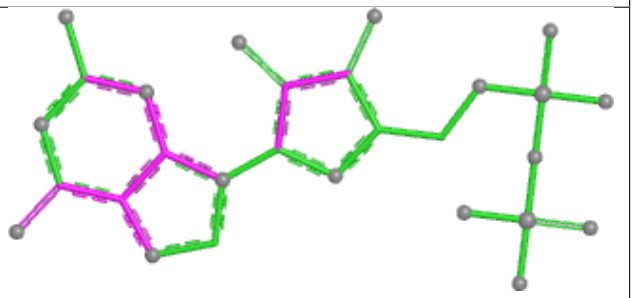


Rings

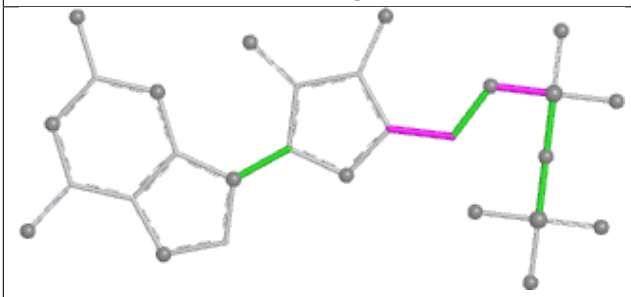
Ligand GDP GL 500



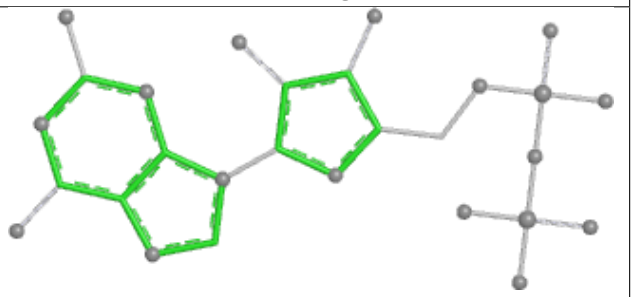
Bond lengths



Bond angles

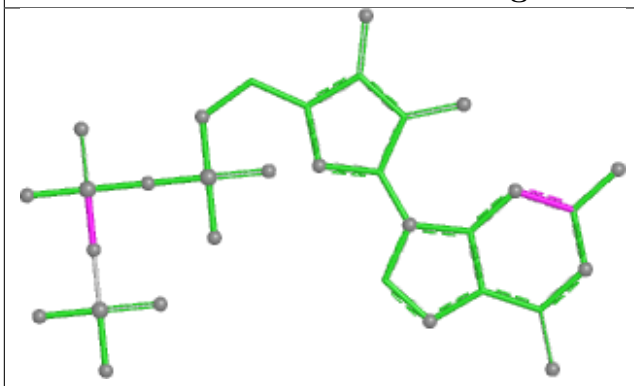


Torsions

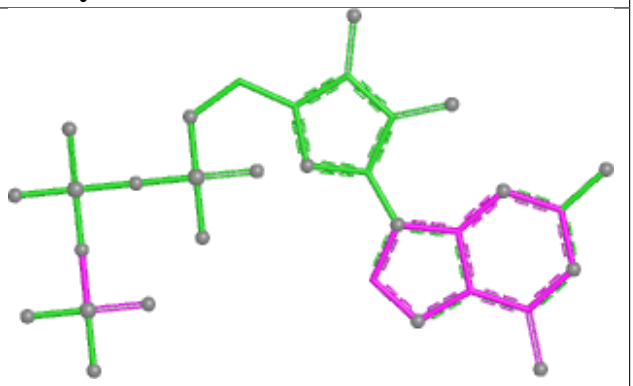


Rings

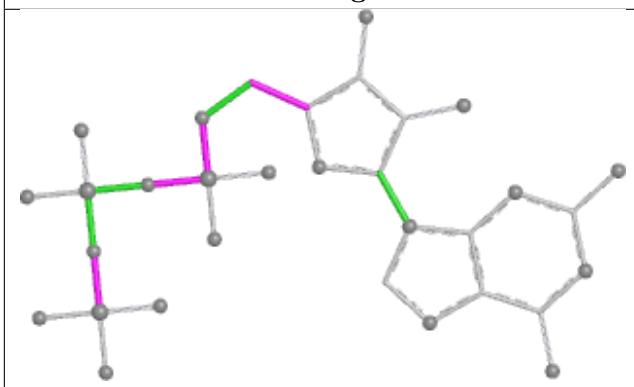
Ligand GTP CQ 501



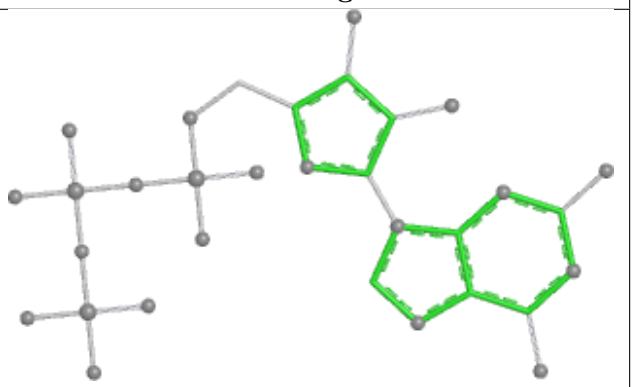
Bond lengths



Bond angles

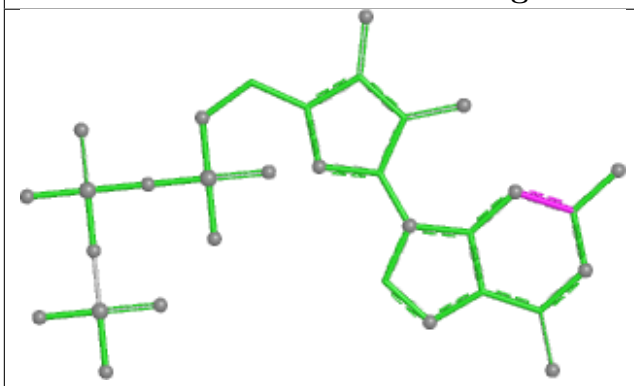


Torsions

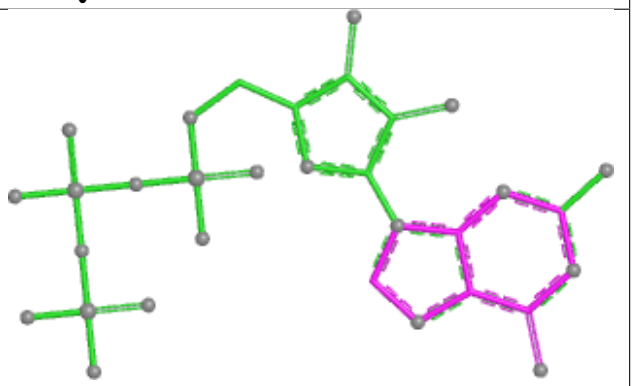


Rings

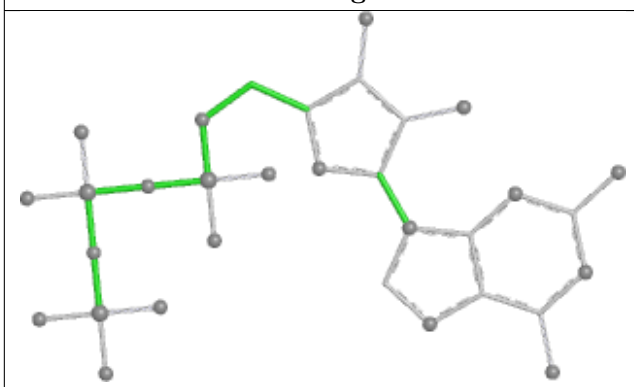
Ligand GTP PQ 501



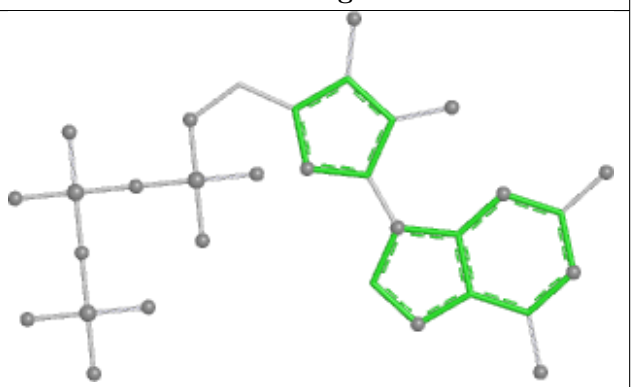
Bond lengths



Bond angles

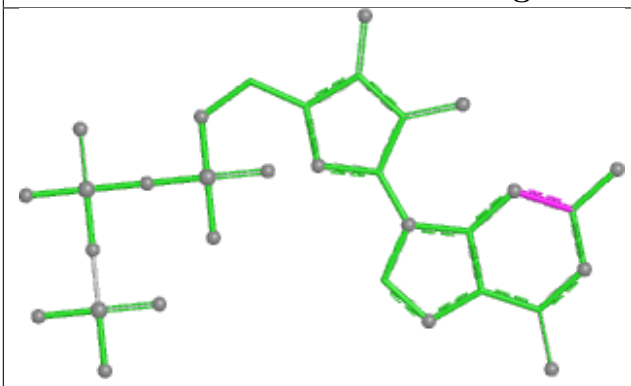


Torsions

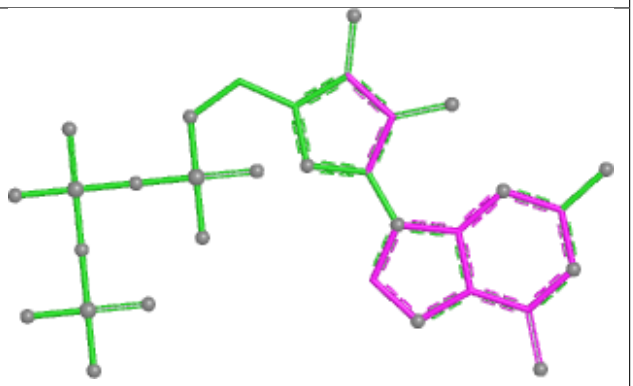


Rings

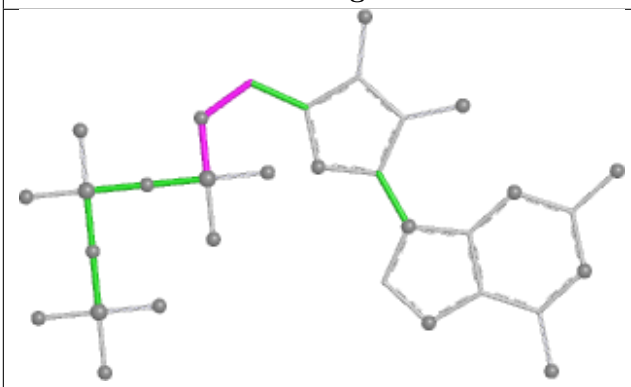
Ligand GTP JR 501



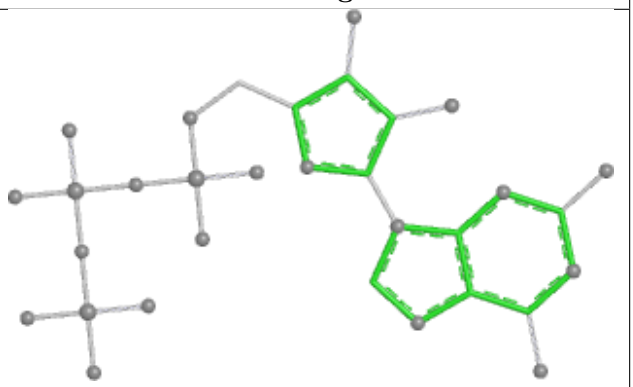
Bond lengths



Bond angles

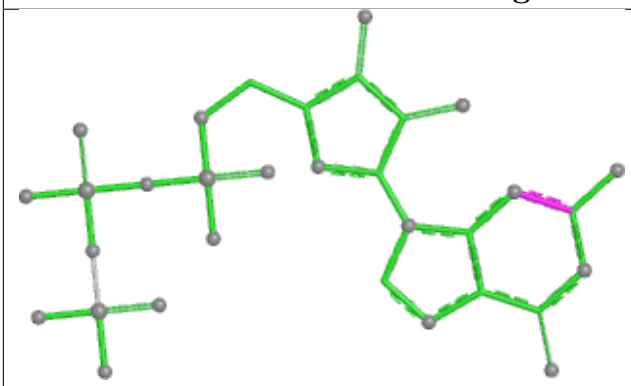


Torsions

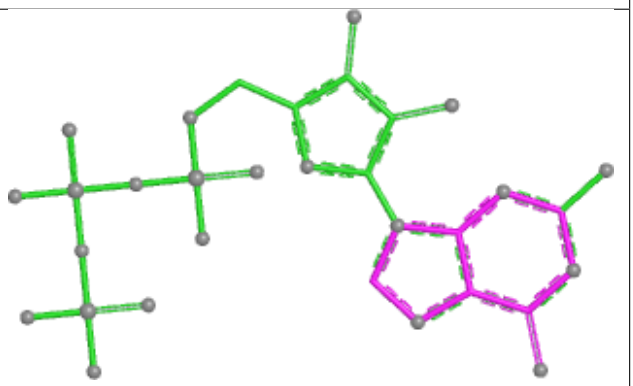


Rings

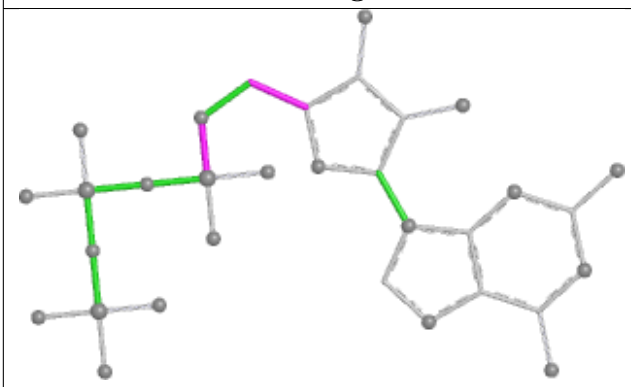
Ligand GTP JD 501



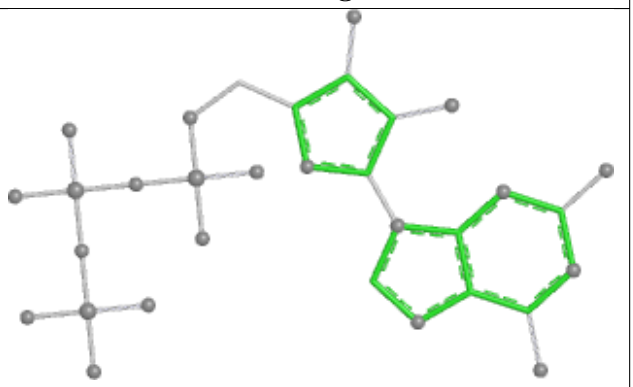
Bond lengths



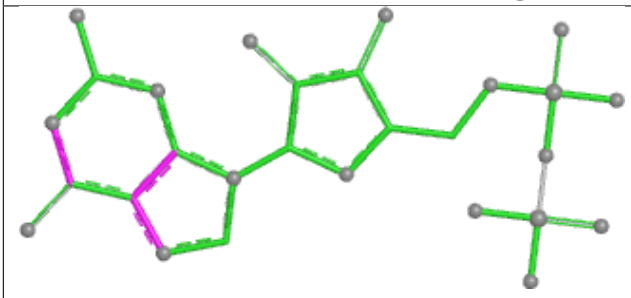
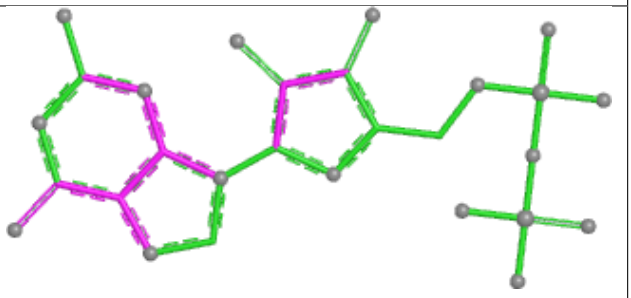
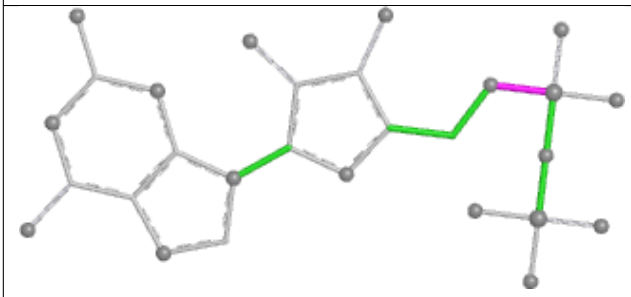
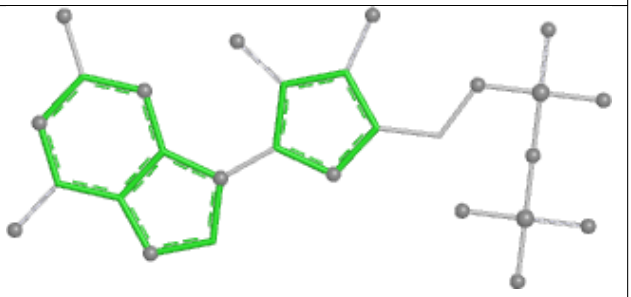
Bond angles

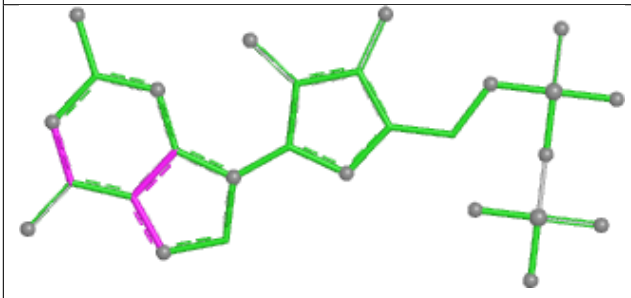
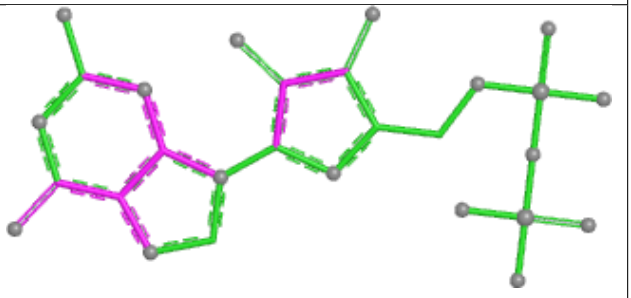
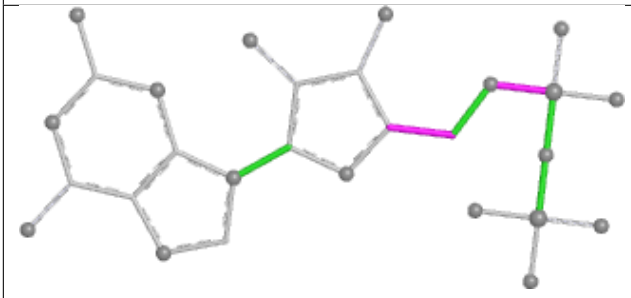
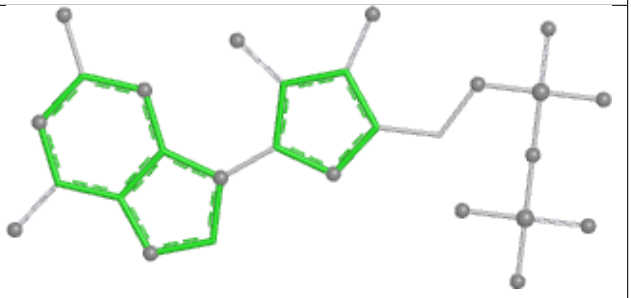


Torsions

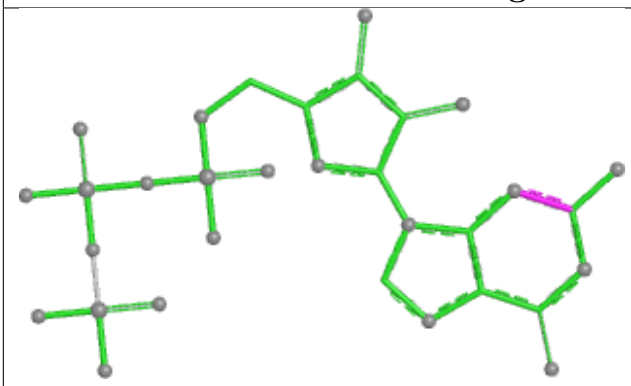


Rings

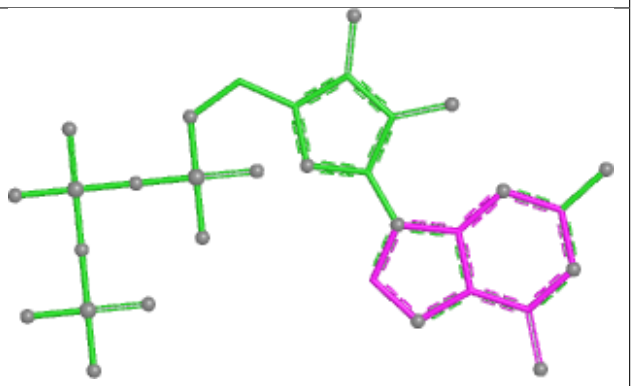
Ligand GDP EF 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP P 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

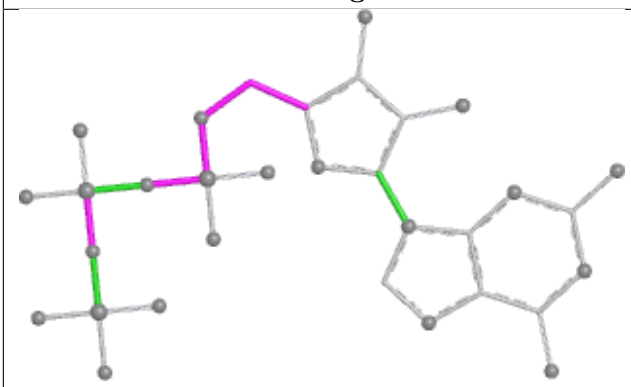
Ligand GTP AA 501



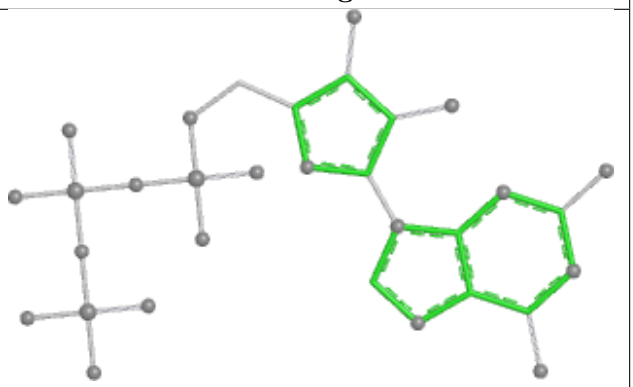
Bond lengths



Bond angles

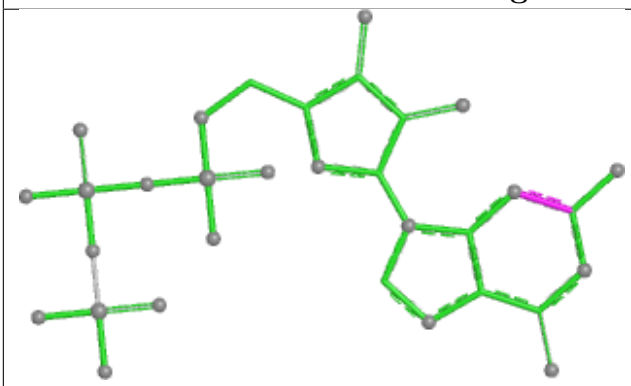


Torsions

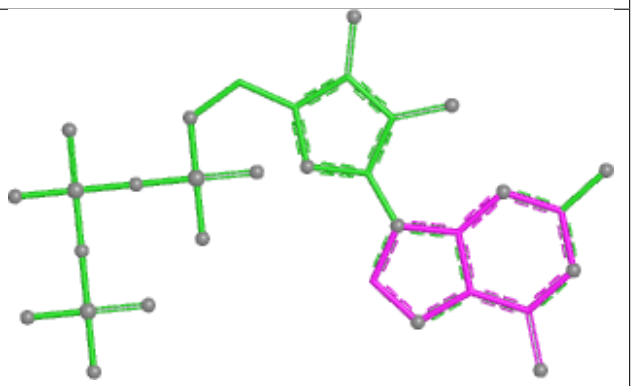


Rings

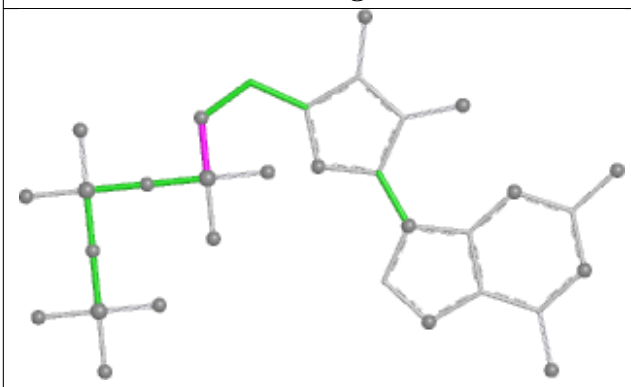
Ligand GTP EA 501



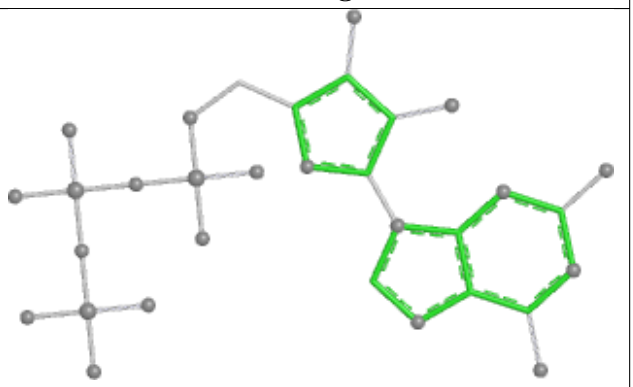
Bond lengths



Bond angles

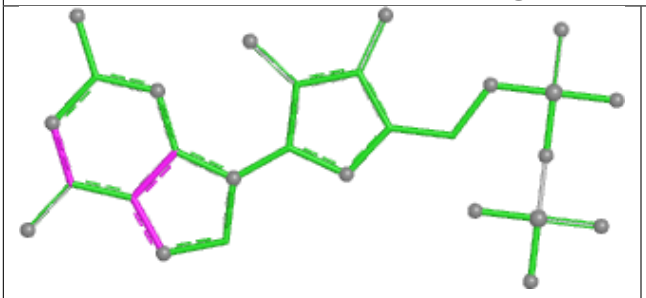


Torsions

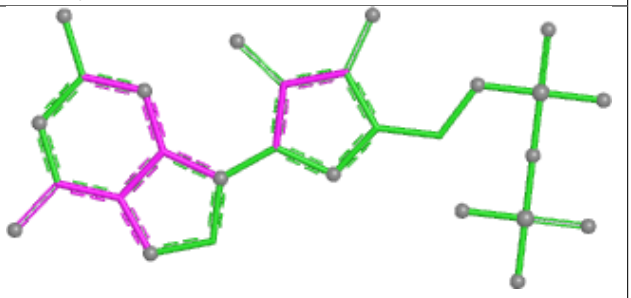


Rings

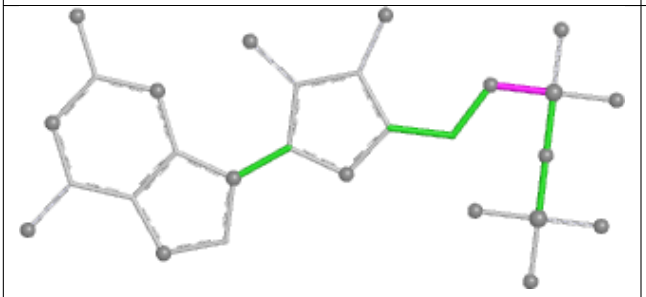
Ligand GDP LQ 500



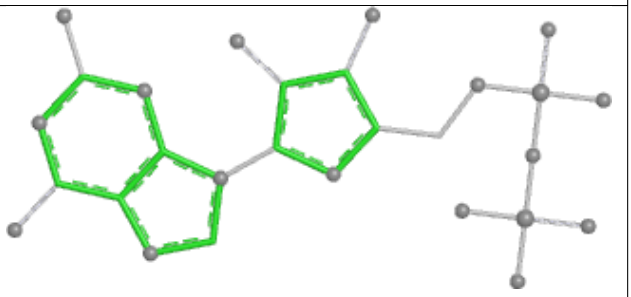
Bond lengths



Bond angles

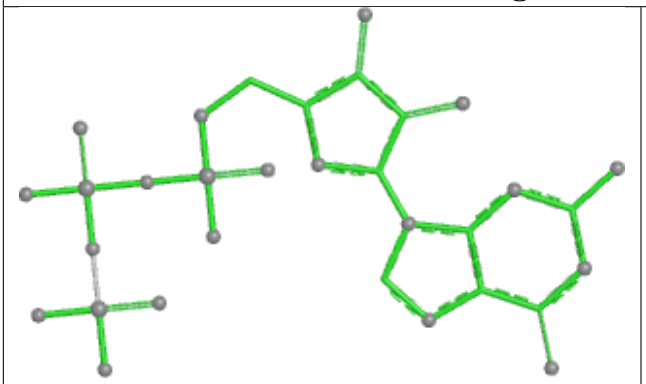


Torsions

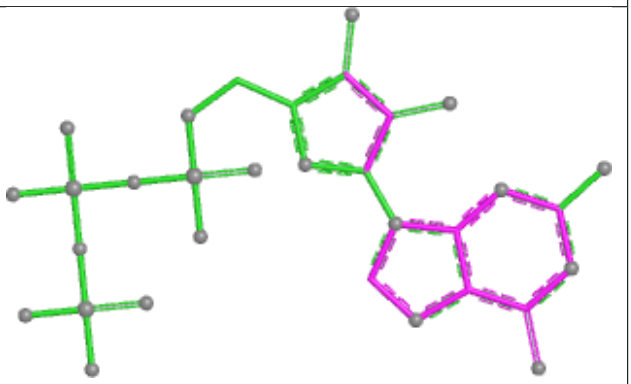


Rings

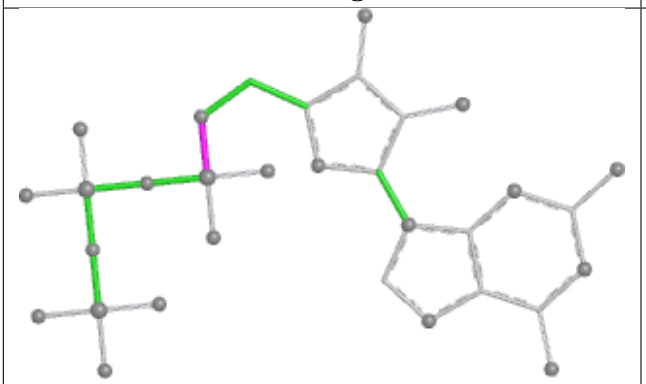
Ligand GTP EC 501



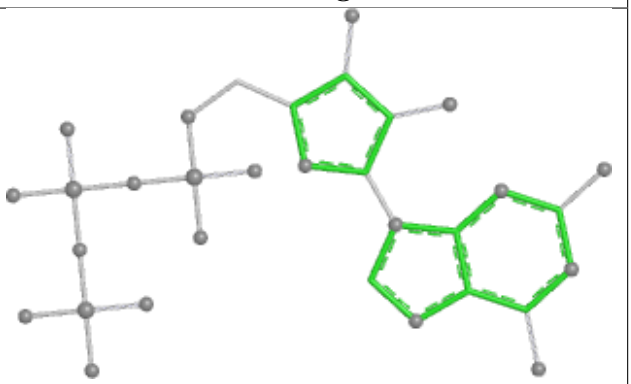
Bond lengths



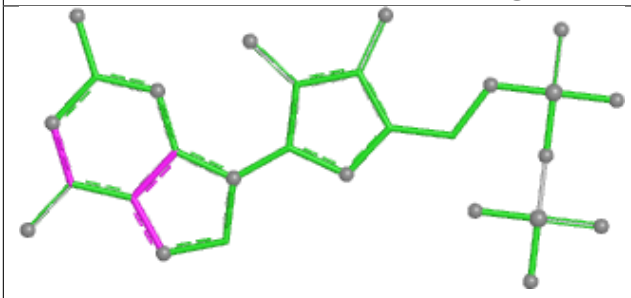
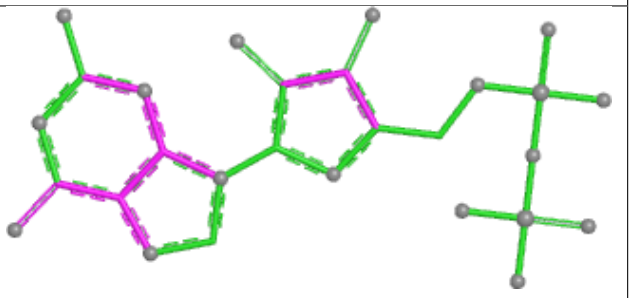
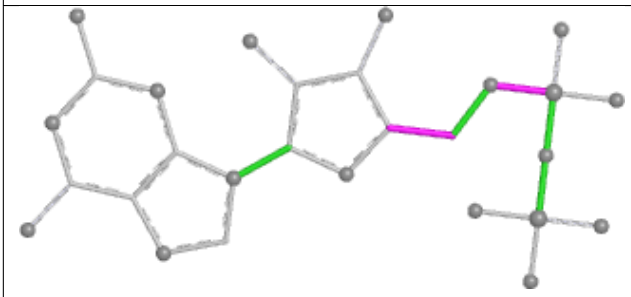
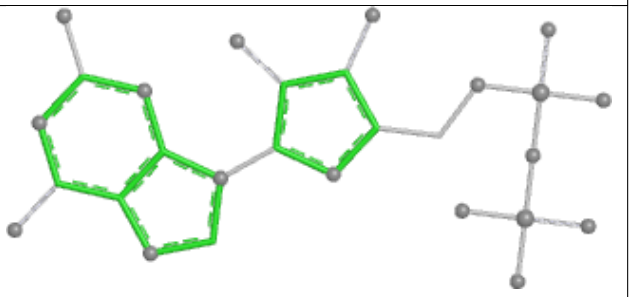
Bond angles

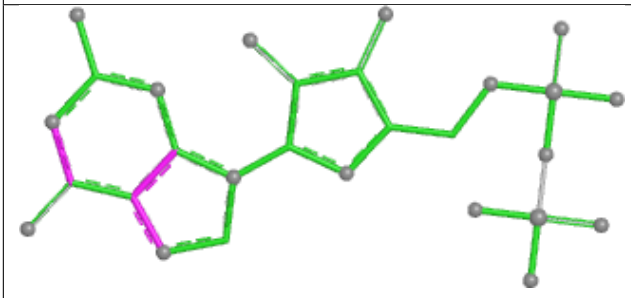
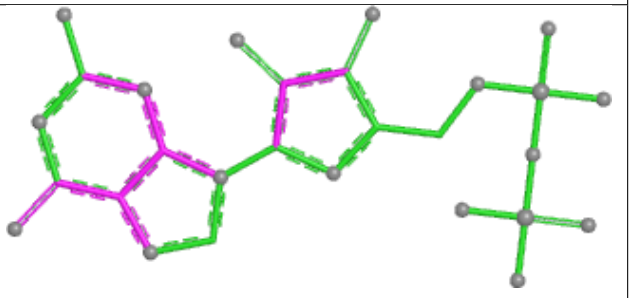
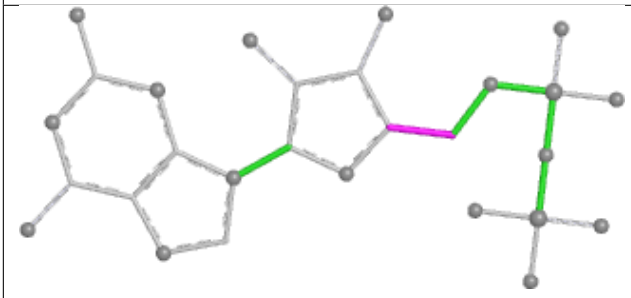
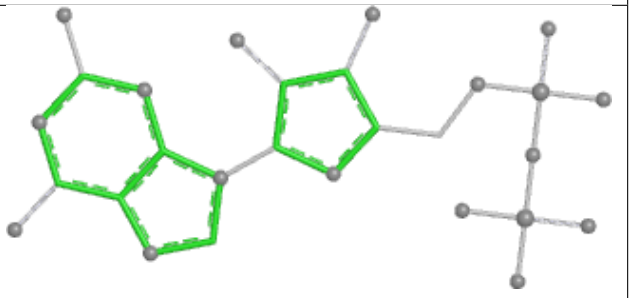


Torsions

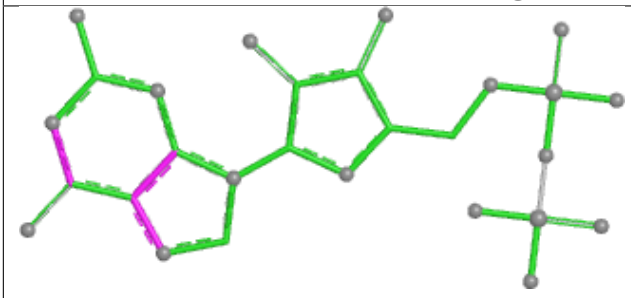


Rings

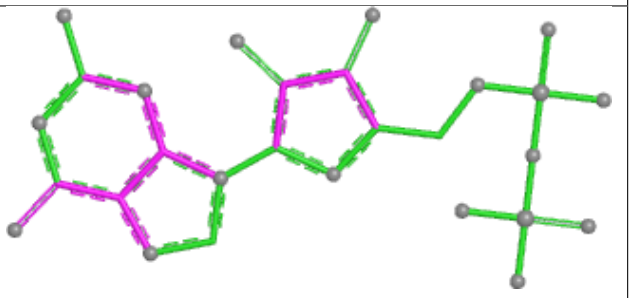
Ligand GDP OT 500	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP OX 500	
	
Bond lengths	Bond angles
	
Torsions	Rings

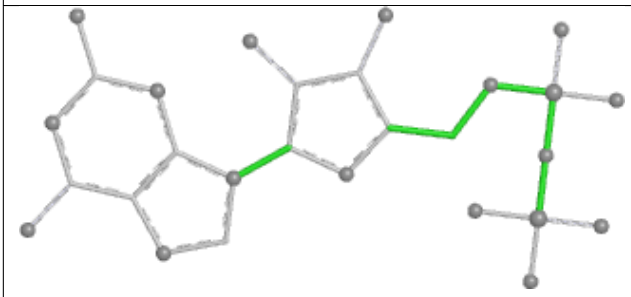
Ligand GDP RE 500



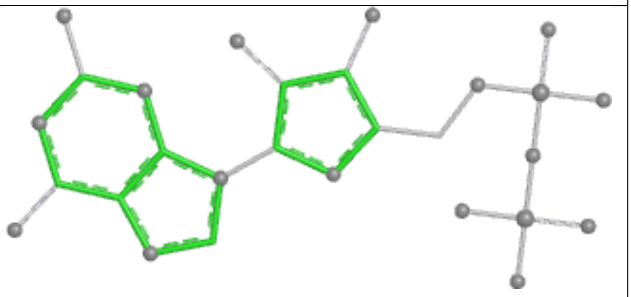
Bond lengths



Bond angles

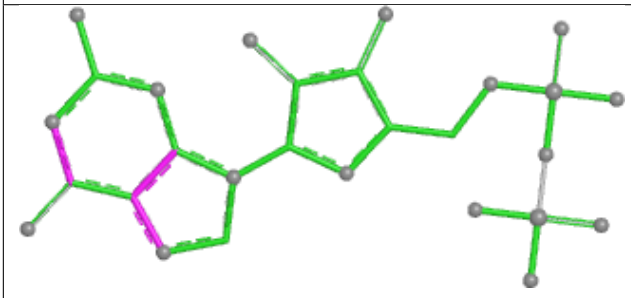


Torsions

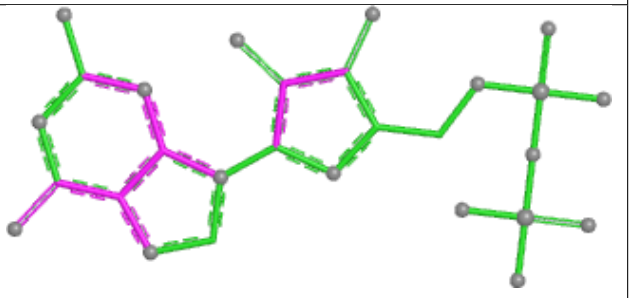


Rings

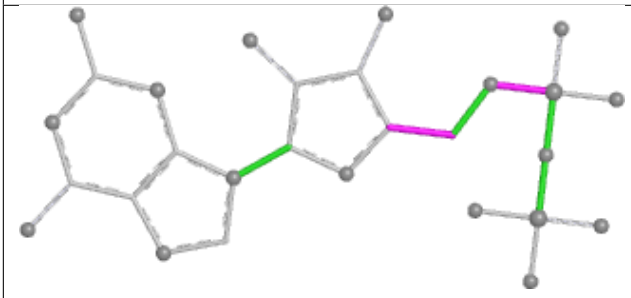
Ligand GDP QE 500



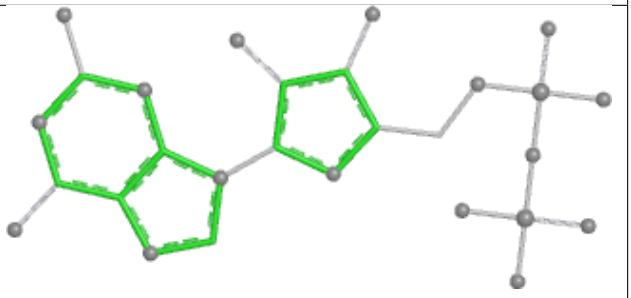
Bond lengths



Bond angles

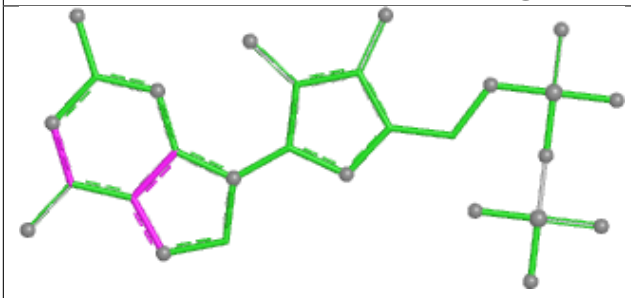


Torsions

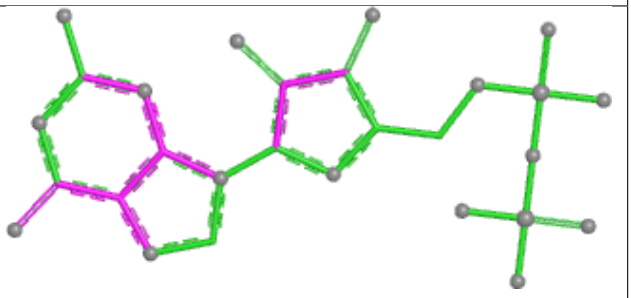


Rings

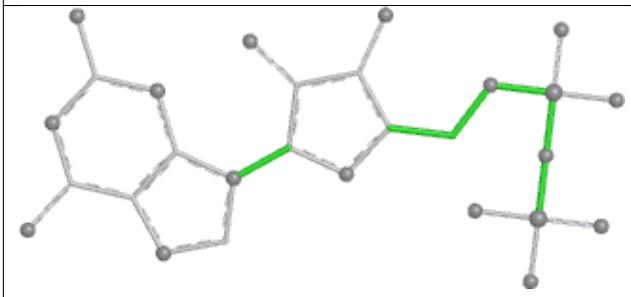
Ligand GDP IL 501



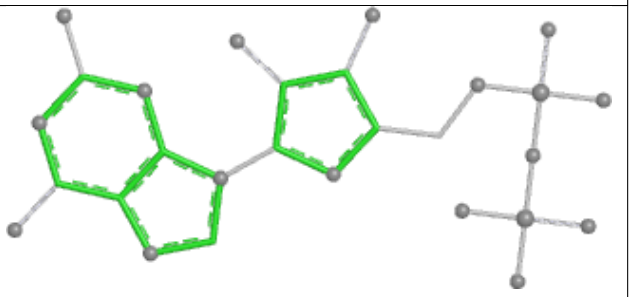
Bond lengths



Bond angles

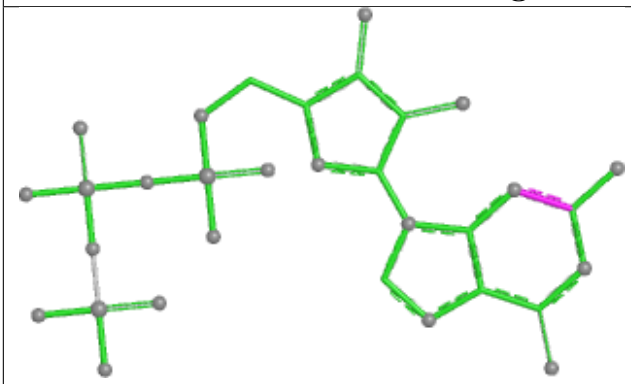


Torsions

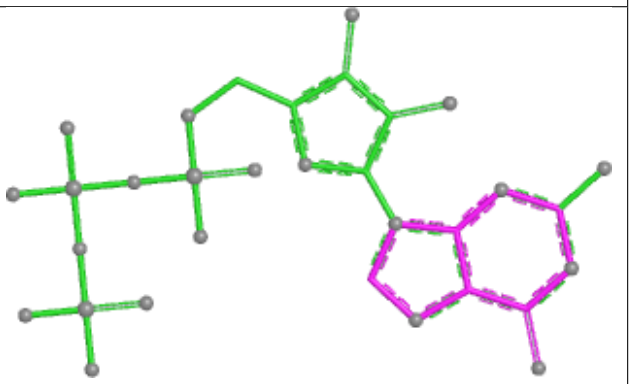


Rings

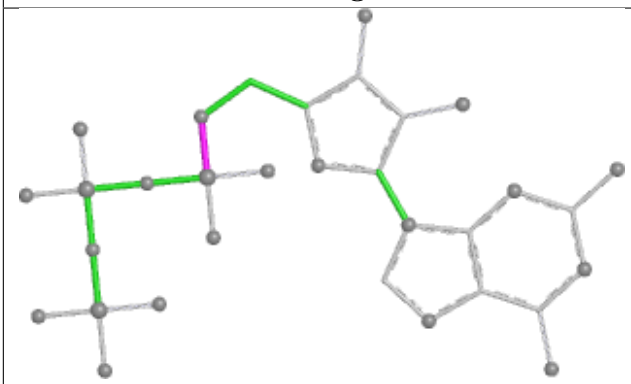
Ligand GTP PY 501



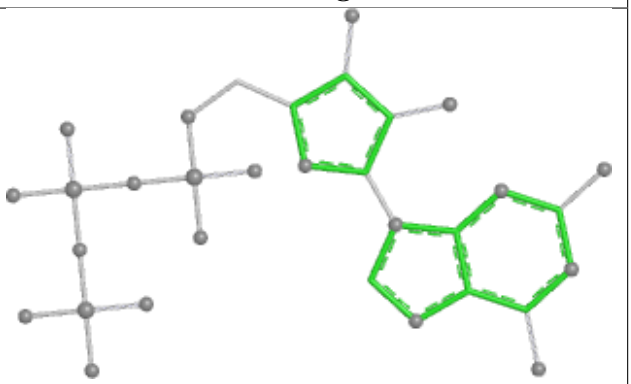
Bond lengths



Bond angles

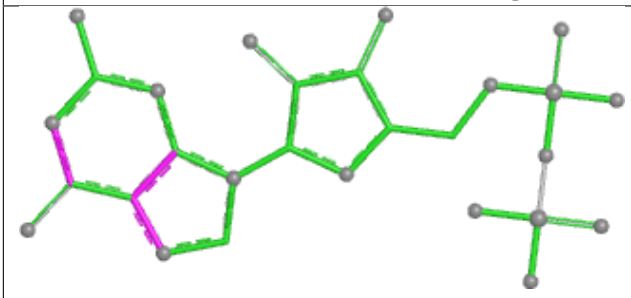


Torsions

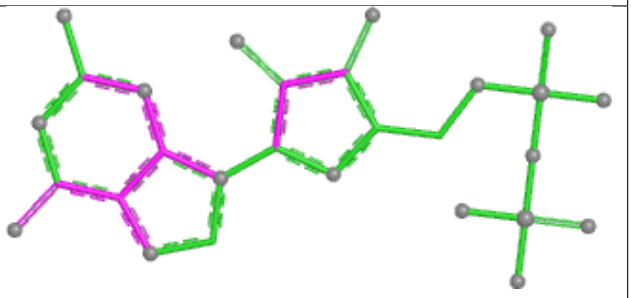


Rings

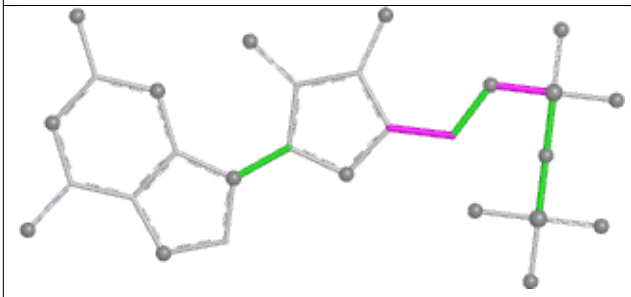
Ligand GDP GX 500



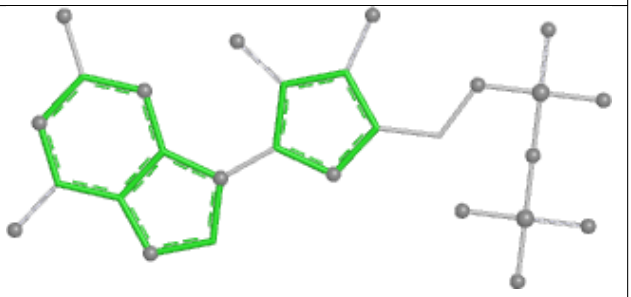
Bond lengths



Bond angles

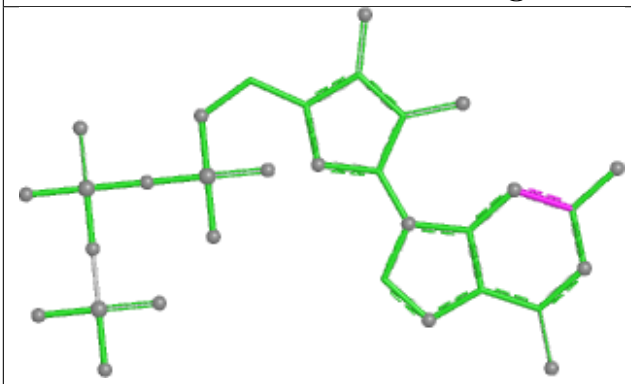


Torsions

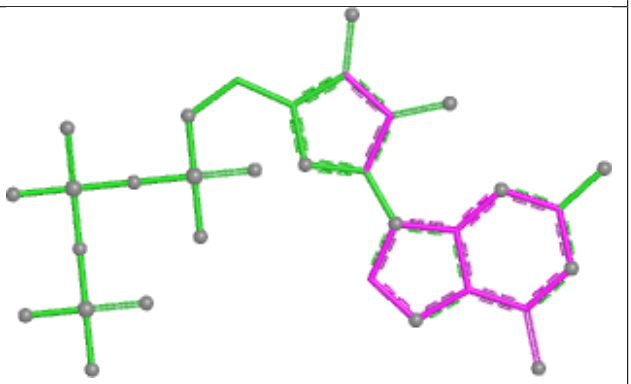


Rings

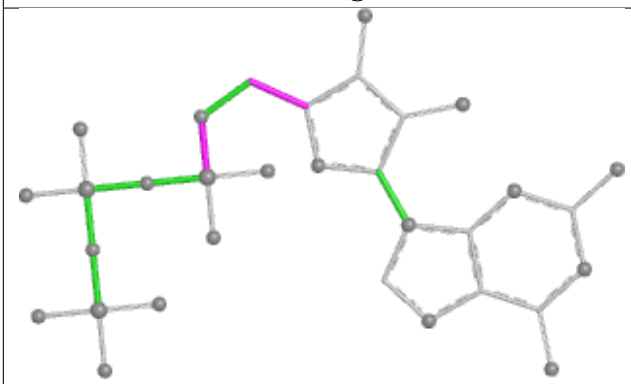
Ligand GTP GU 501



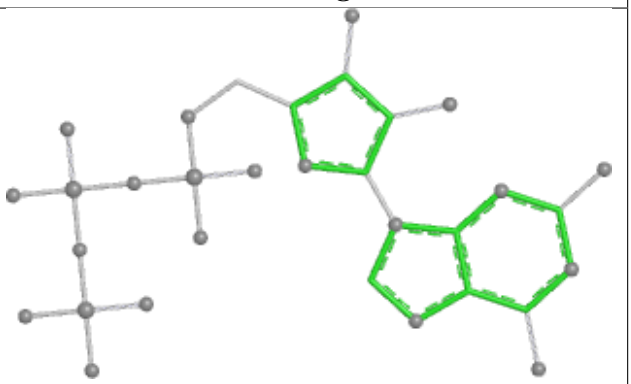
Bond lengths



Bond angles

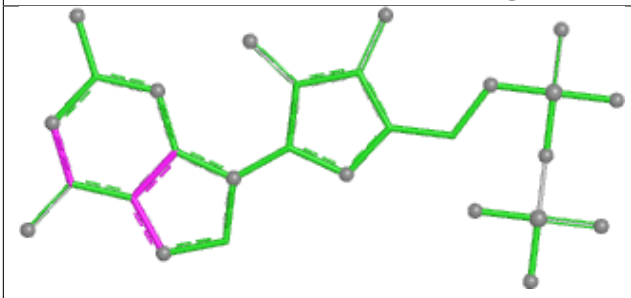


Torsions

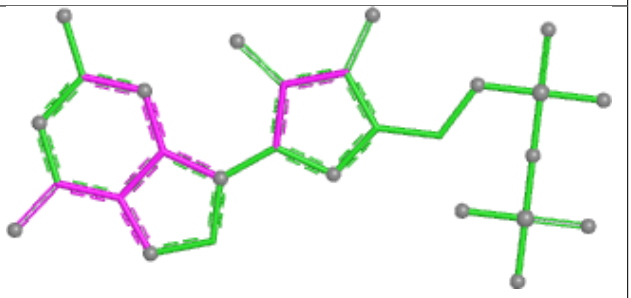


Rings

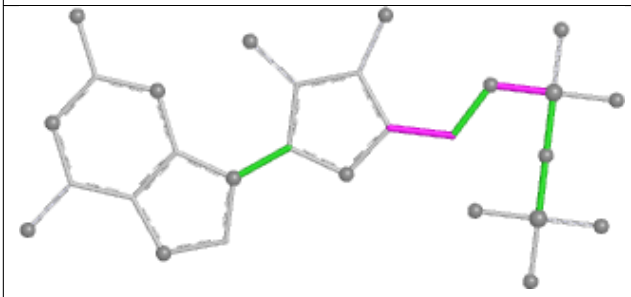
Ligand GDP KM 500



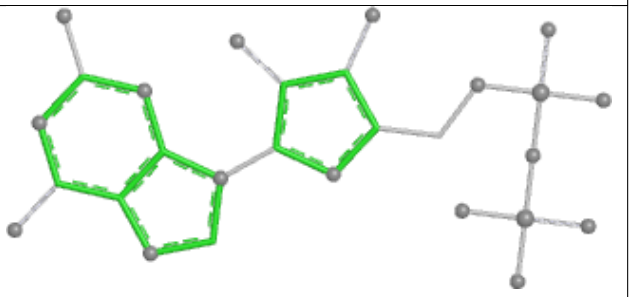
Bond lengths



Bond angles

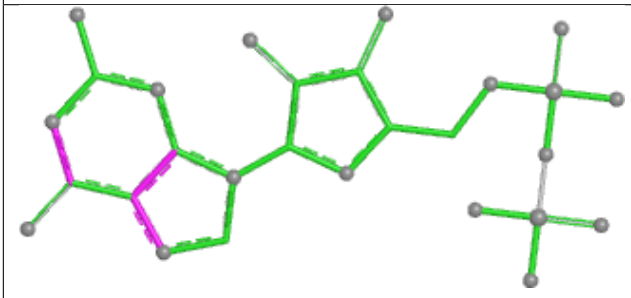


Torsions

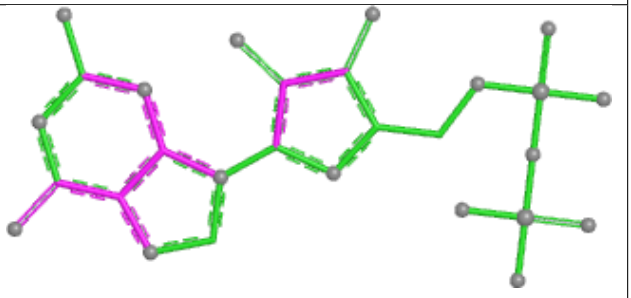


Rings

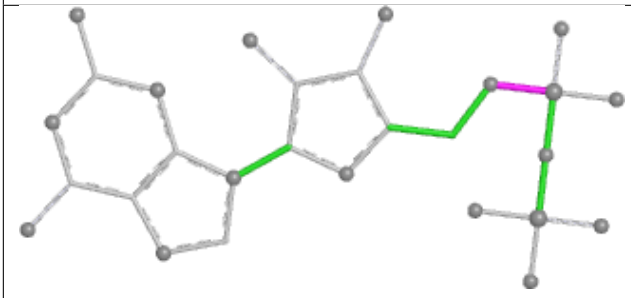
Ligand GDP JA 500



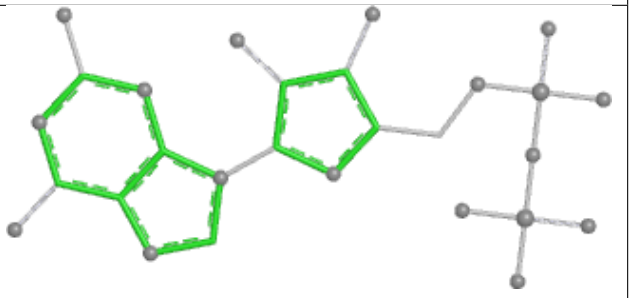
Bond lengths



Bond angles

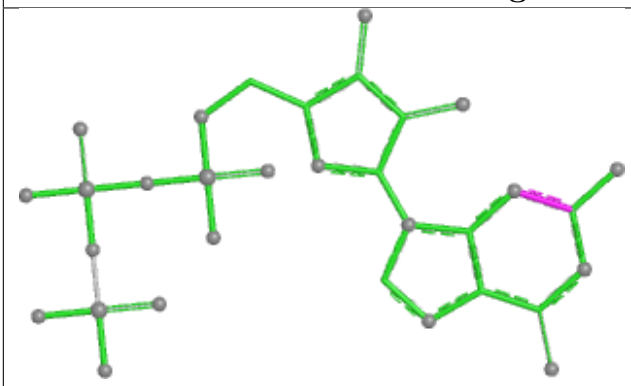


Torsions

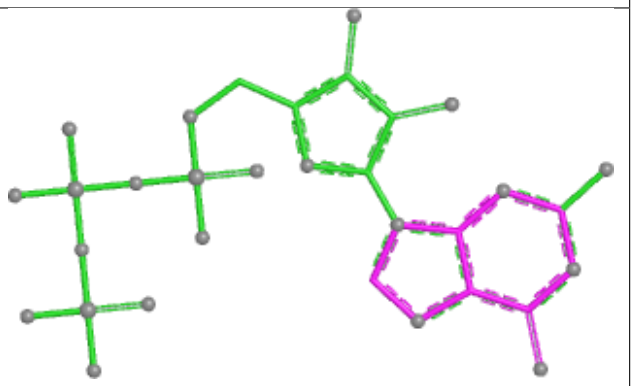


Rings

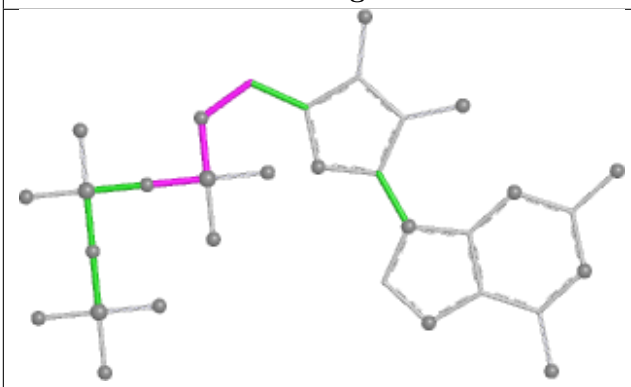
Ligand GTP OA 501



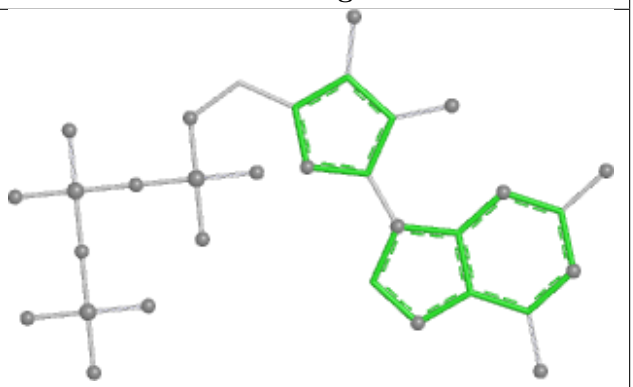
Bond lengths



Bond angles

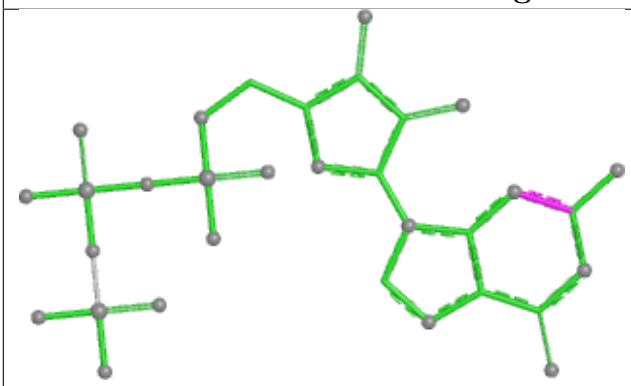


Torsions

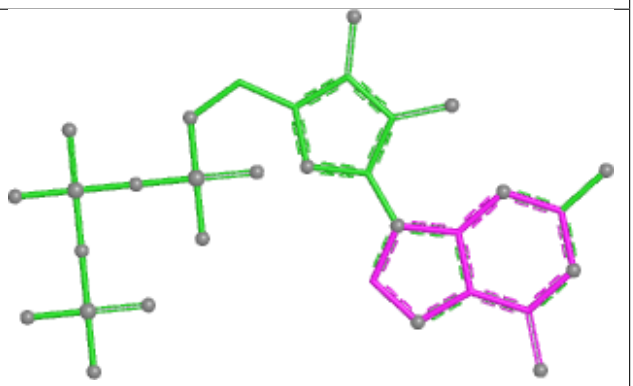


Rings

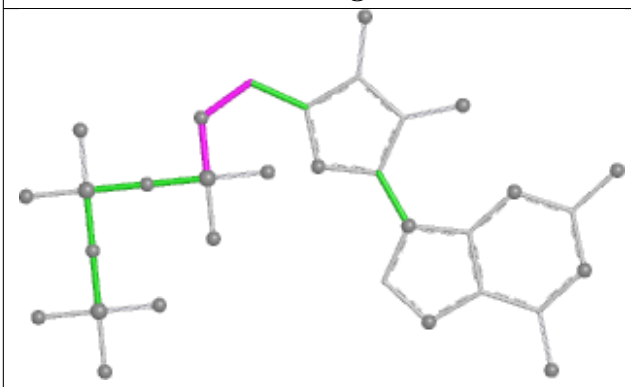
Ligand GTP JB 501



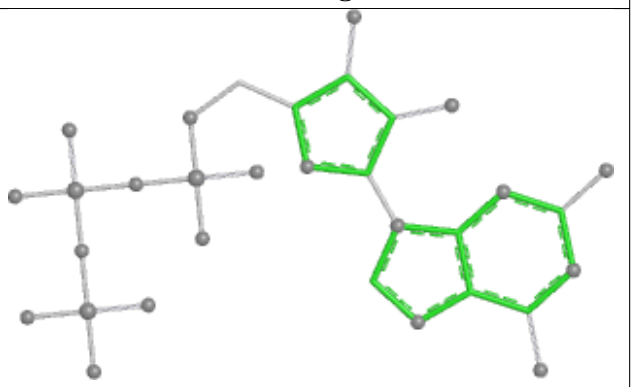
Bond lengths



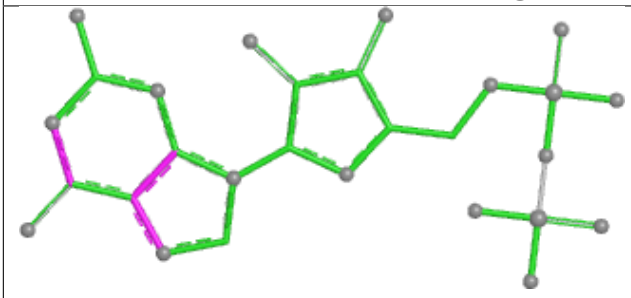
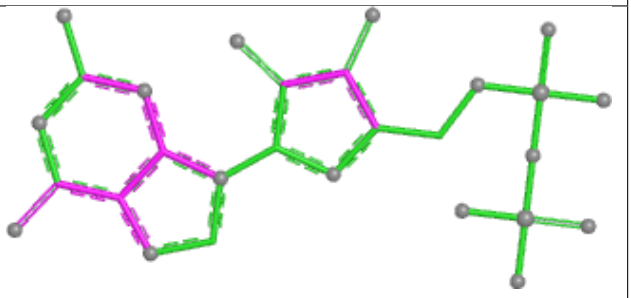
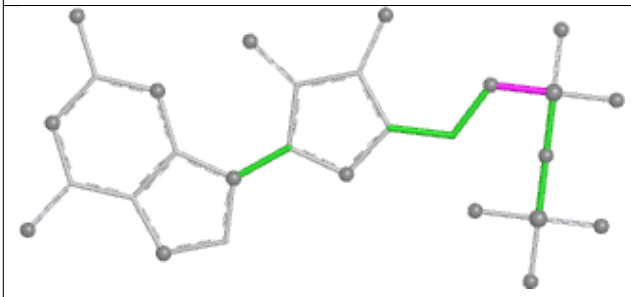
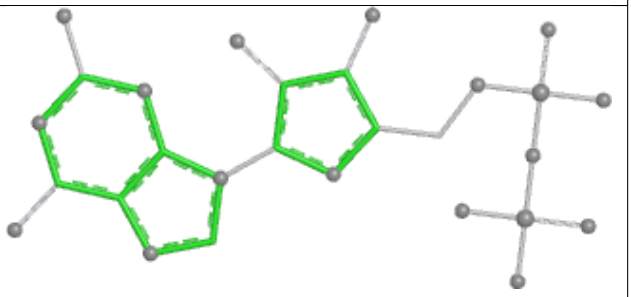
Bond angles

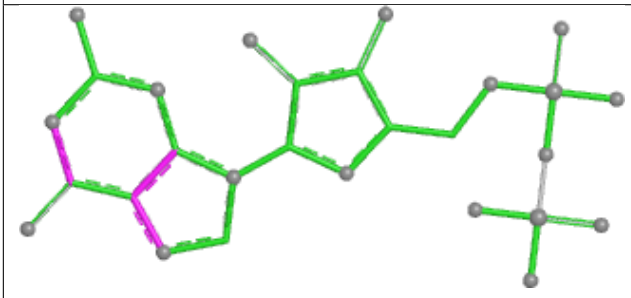
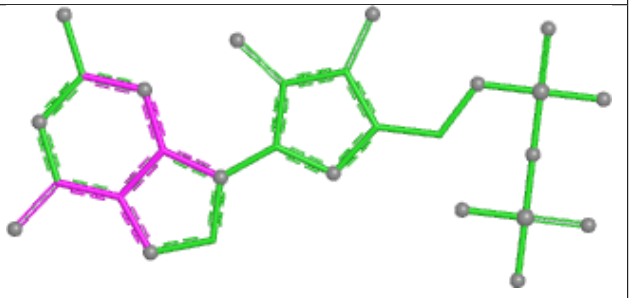
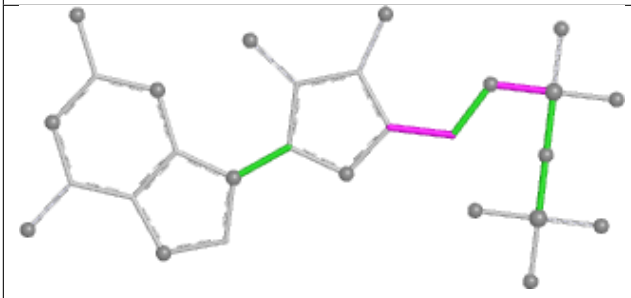
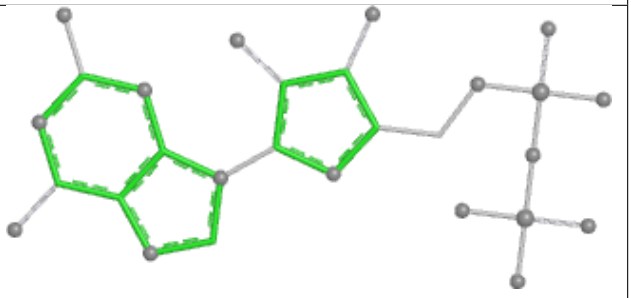


Torsions

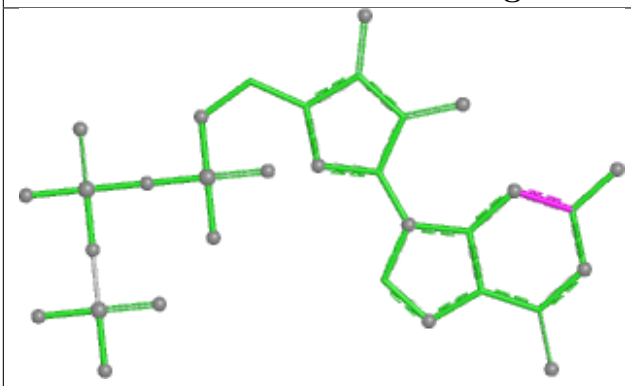


Rings

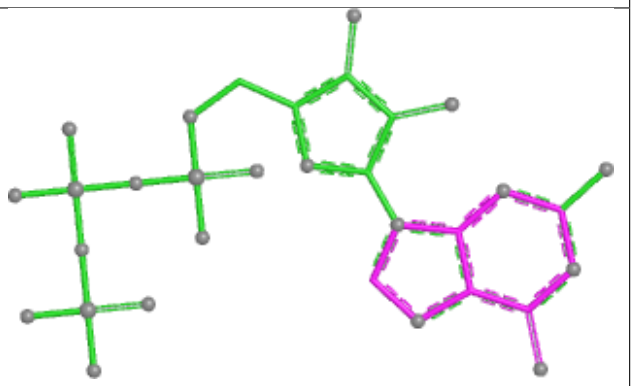
Ligand GDP JU 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP GV 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

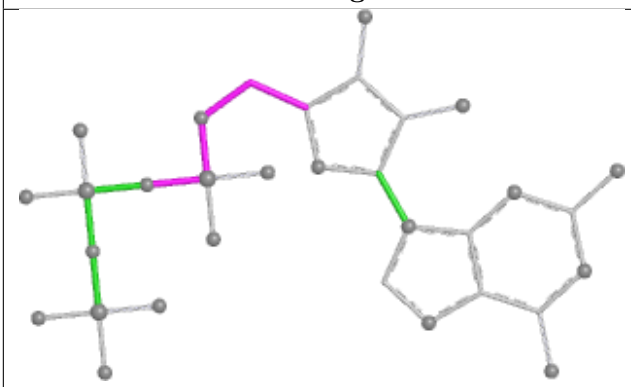
Ligand GTP VW 501



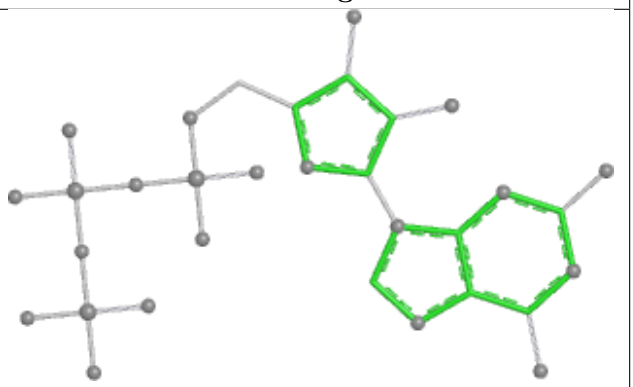
Bond lengths



Bond angles

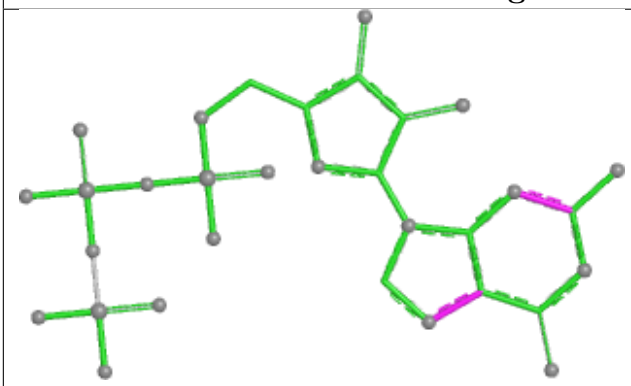


Torsions

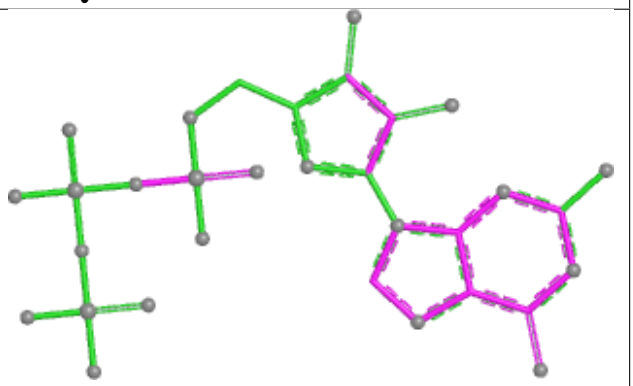


Rings

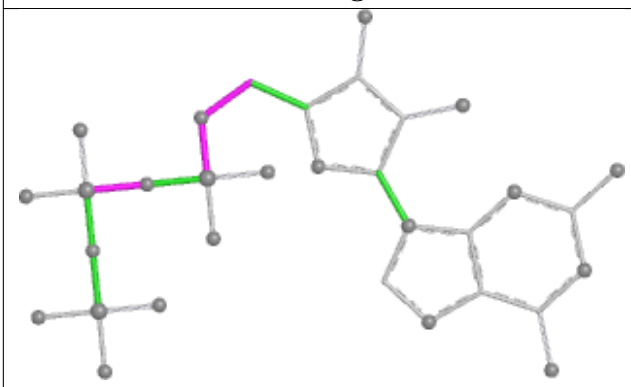
Ligand GTP GQ 501



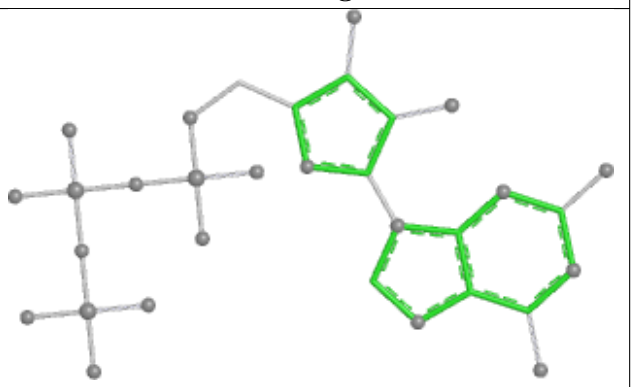
Bond lengths



Bond angles

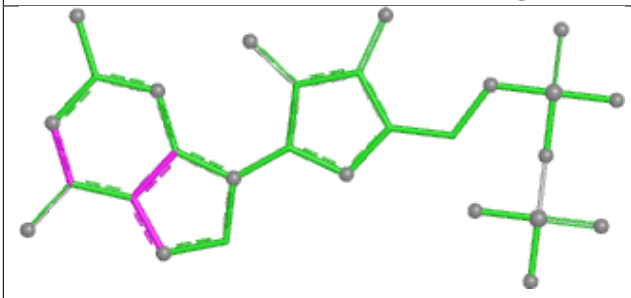


Torsions

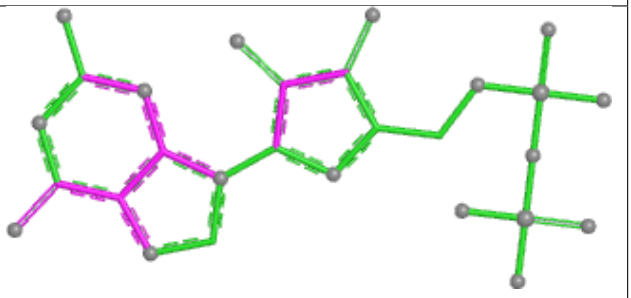


Rings

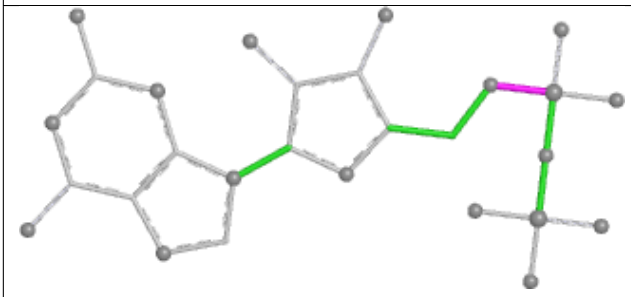
Ligand GDP SF 500



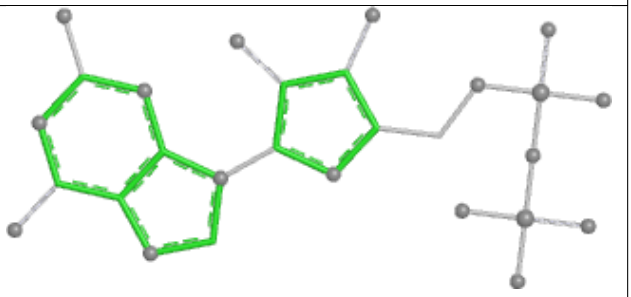
Bond lengths



Bond angles

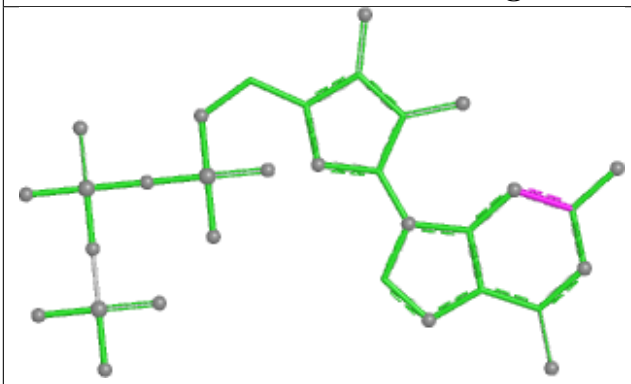


Torsions

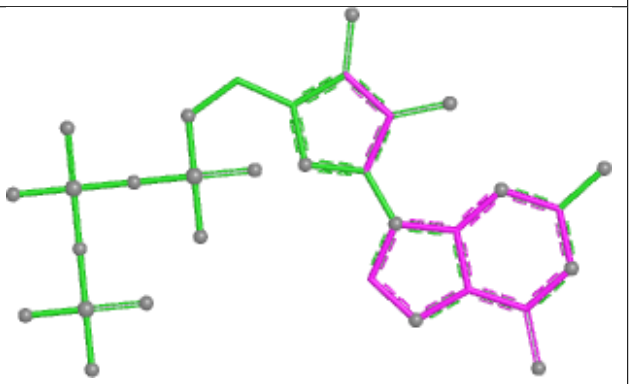


Rings

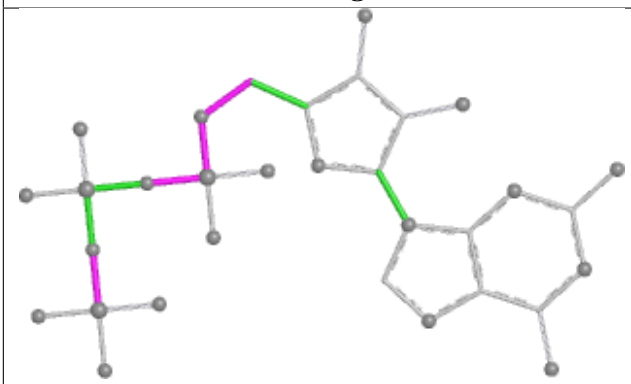
Ligand GTP UM 501



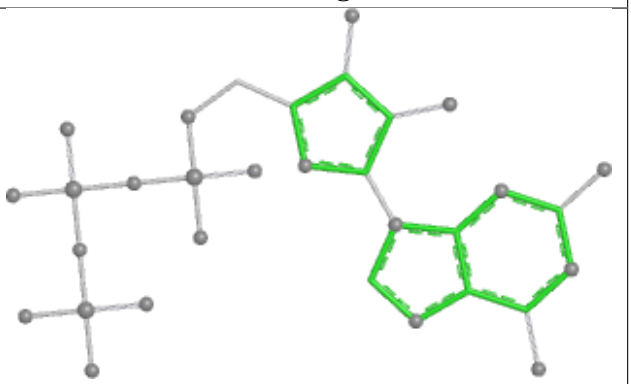
Bond lengths



Bond angles

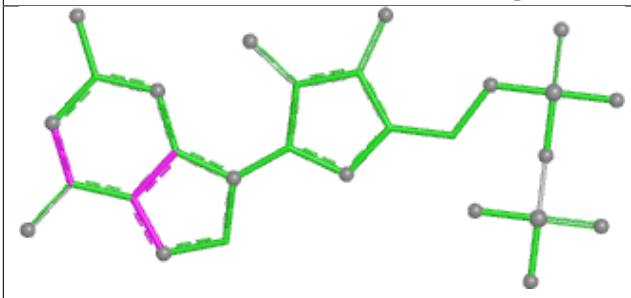


Torsions

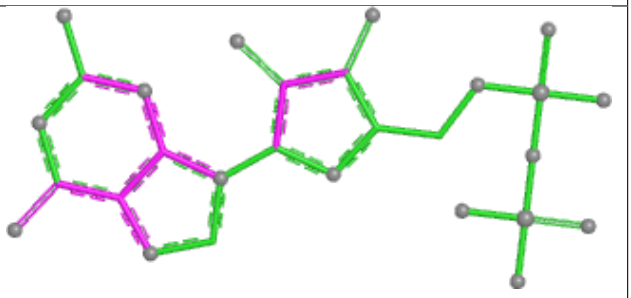


Rings

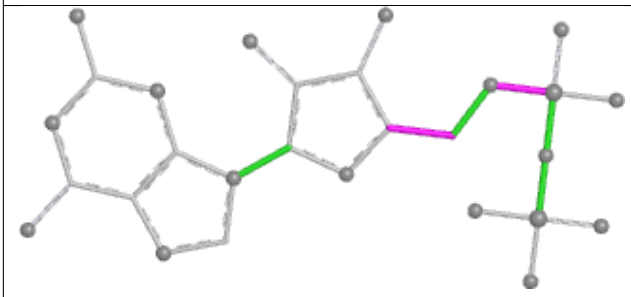
Ligand GDP PV 500



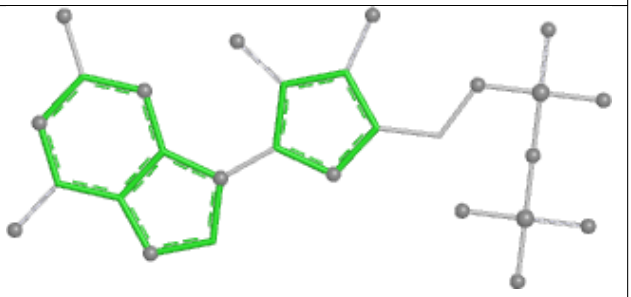
Bond lengths



Bond angles

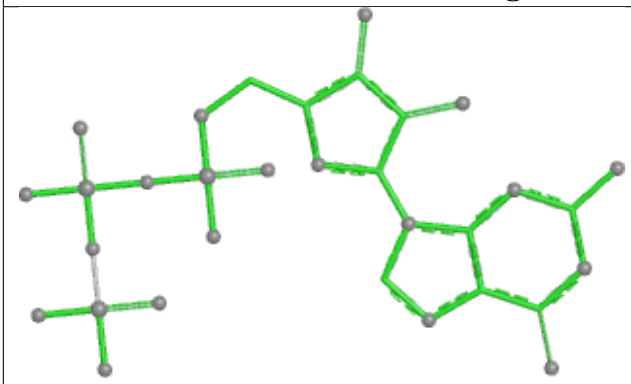


Torsions

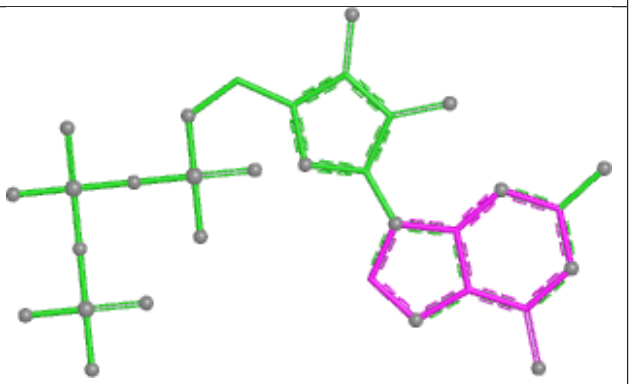


Rings

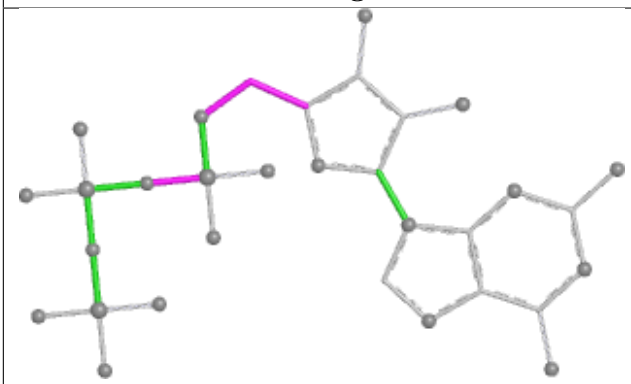
Ligand GTP CW 501



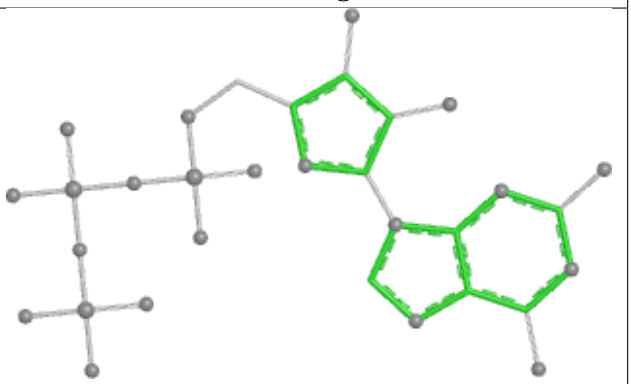
Bond lengths



Bond angles

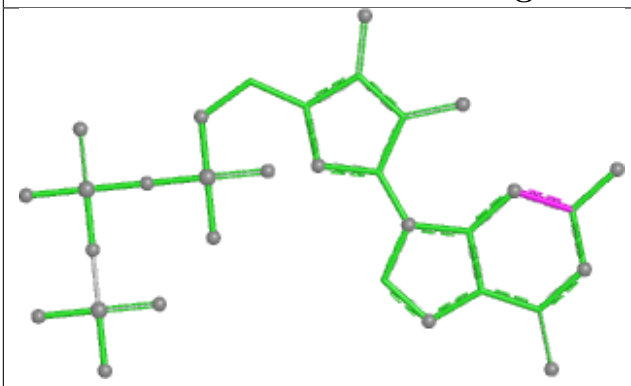


Torsions

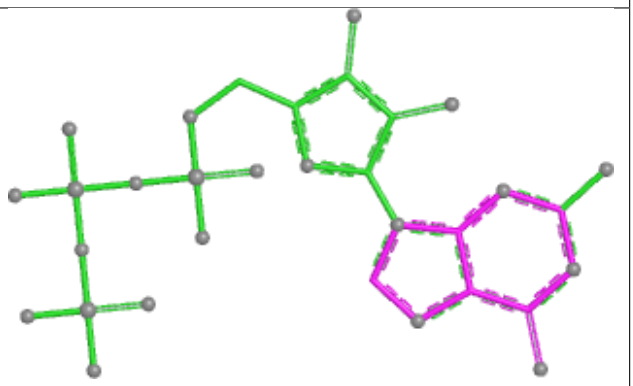


Rings

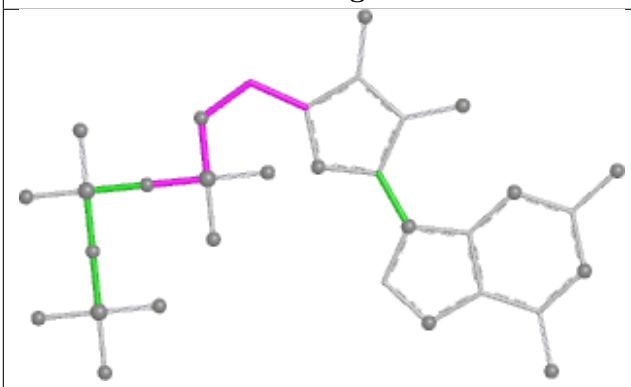
Ligand GTP IA 501



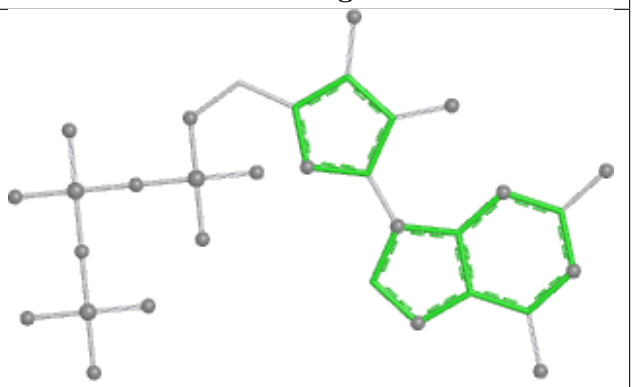
Bond lengths



Bond angles

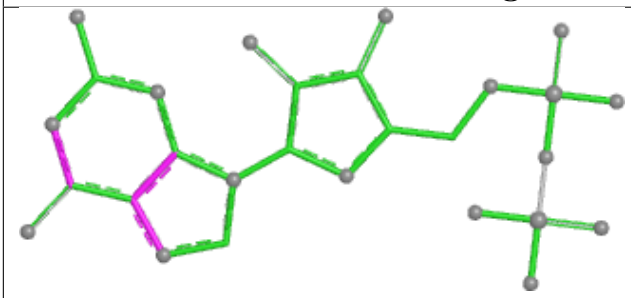


Torsions

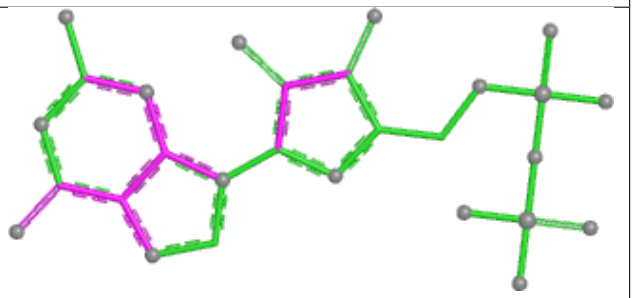


Rings

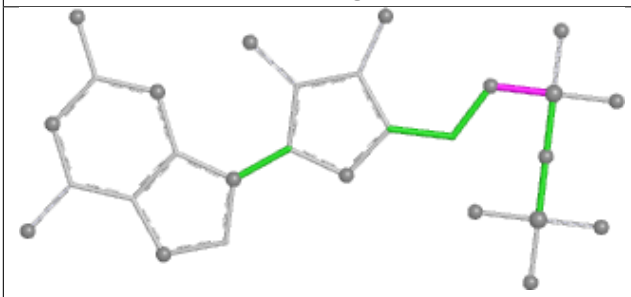
Ligand GDP WH 500



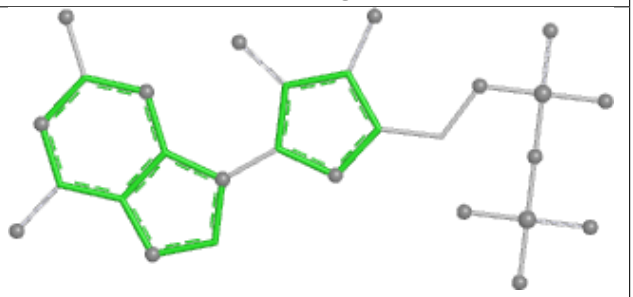
Bond lengths



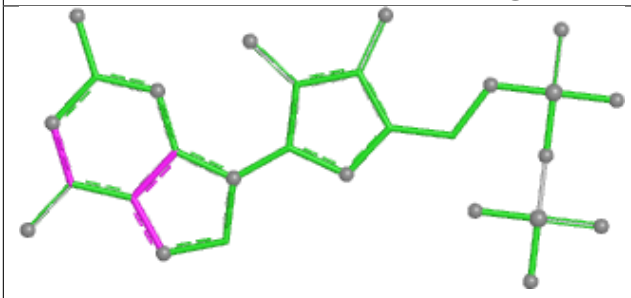
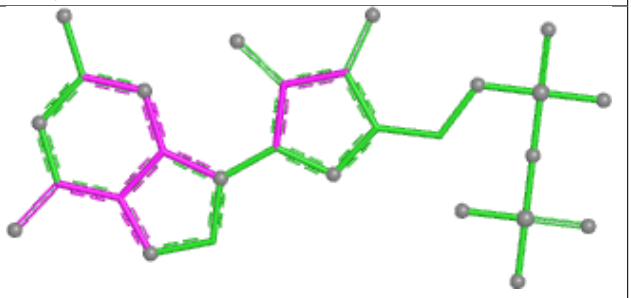
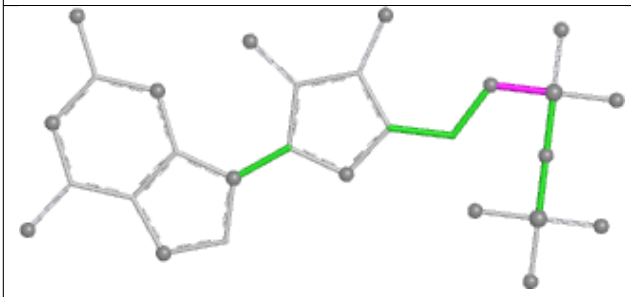
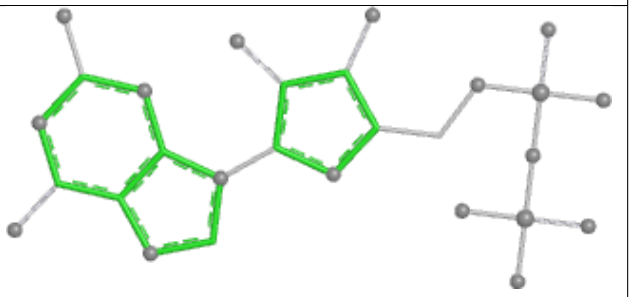
Bond angles

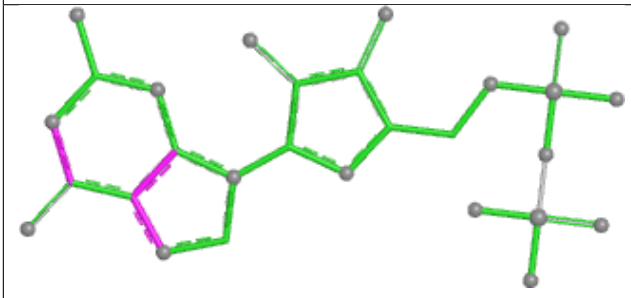
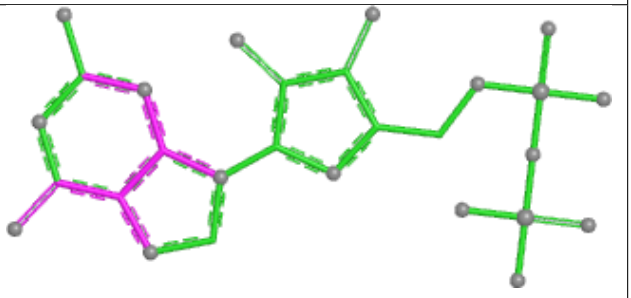
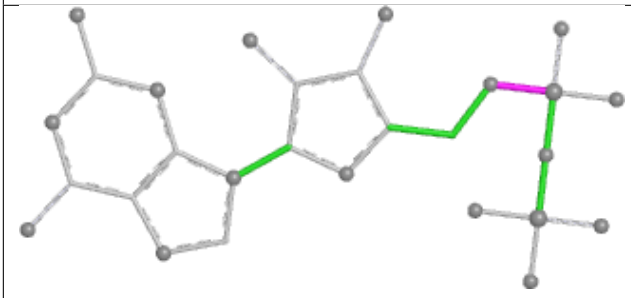
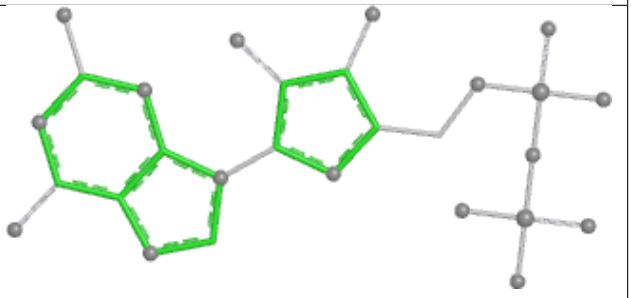


Torsions

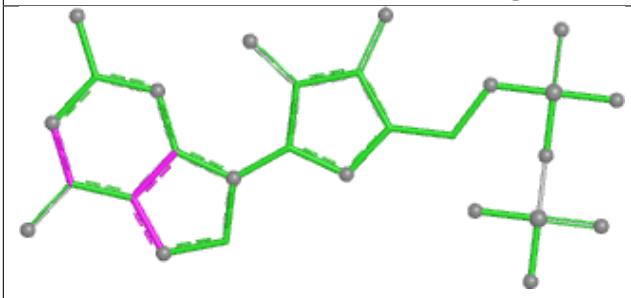


Rings

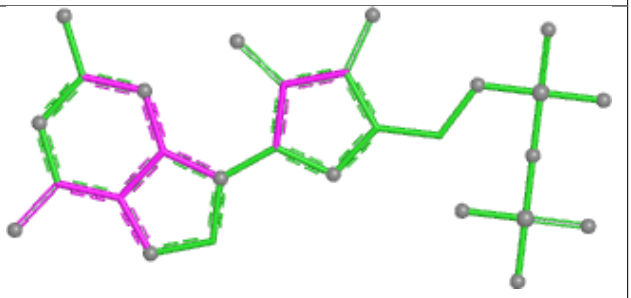
Ligand GDP QG 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP IP 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

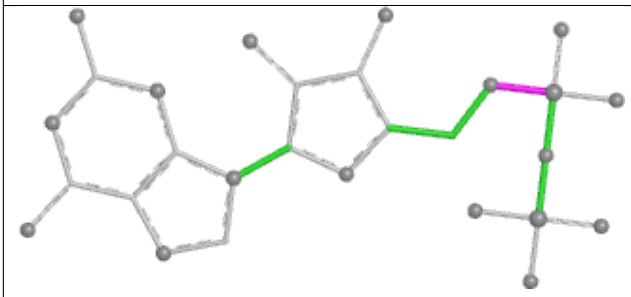
Ligand GDP UV 500



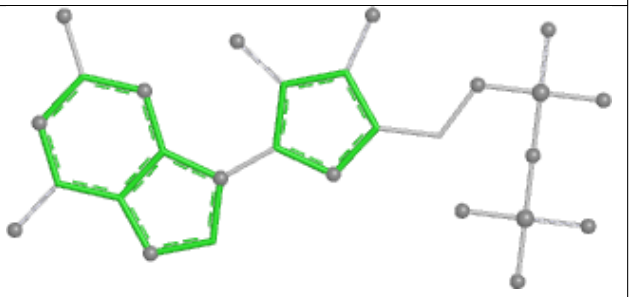
Bond lengths



Bond angles

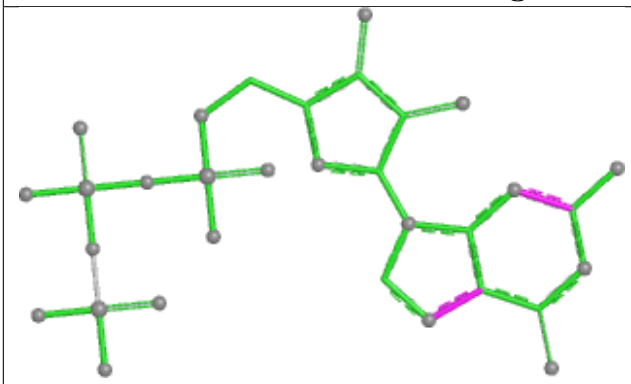


Torsions

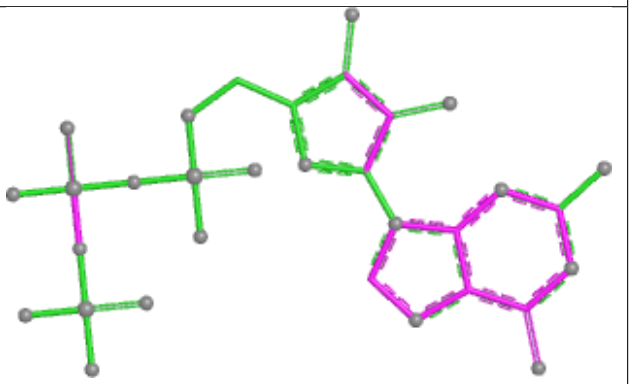


Rings

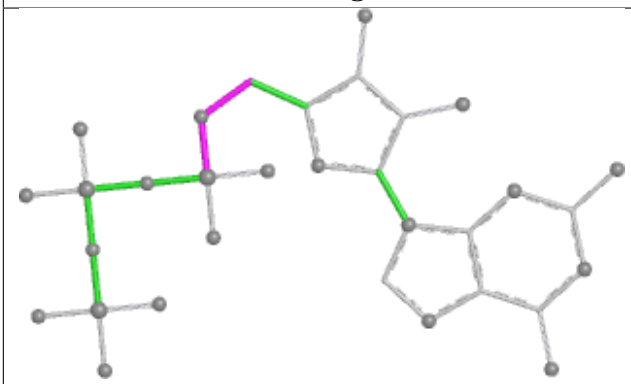
Ligand GTP BU 501



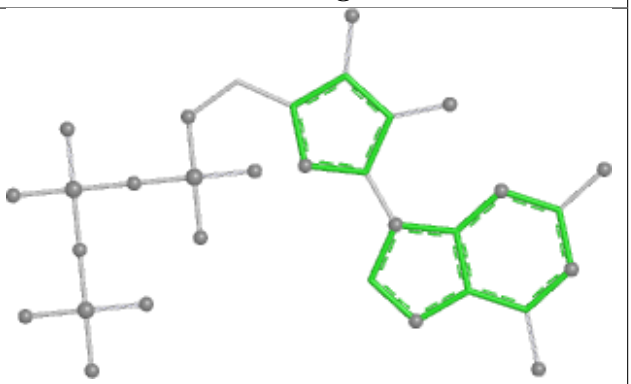
Bond lengths



Bond angles

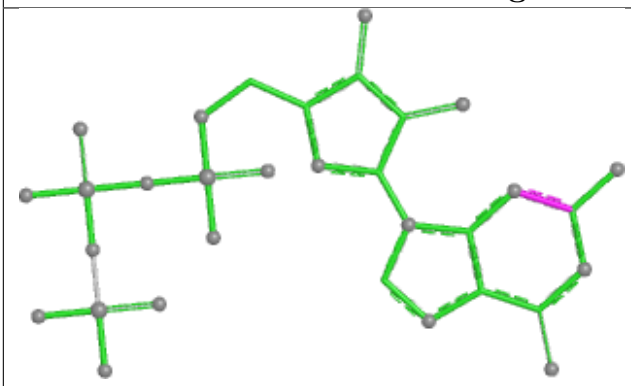


Torsions

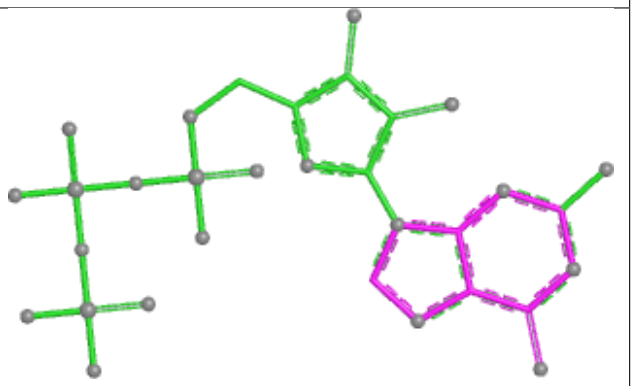


Rings

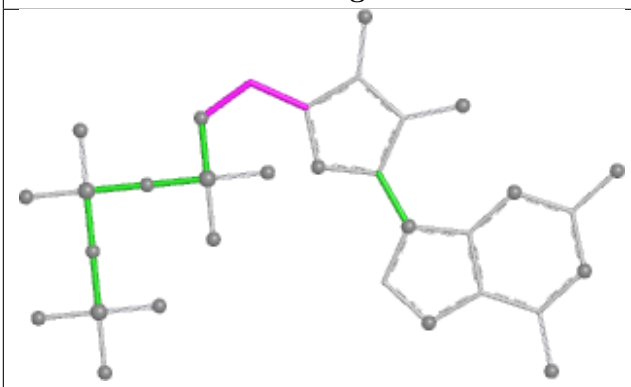
Ligand GTP CK 503



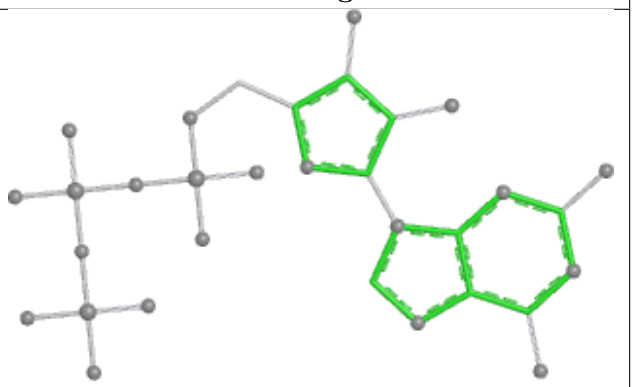
Bond lengths



Bond angles

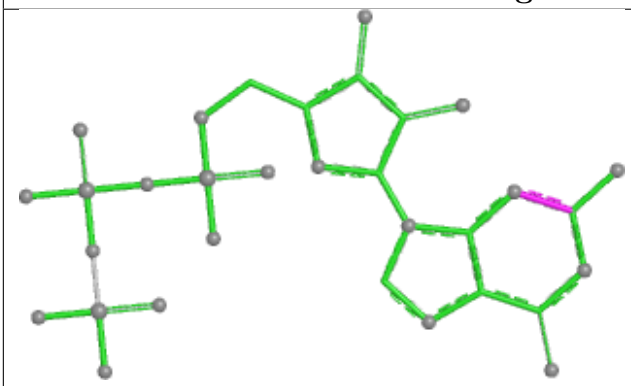


Torsions

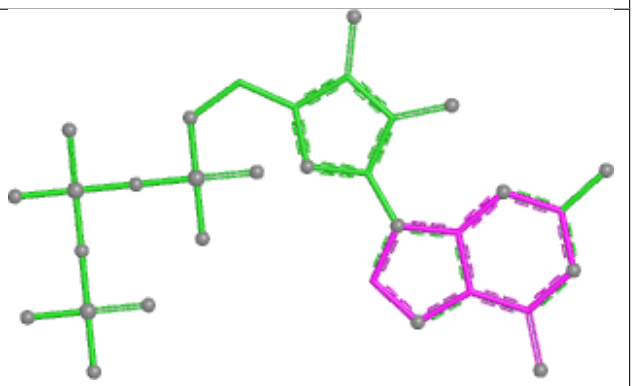


Rings

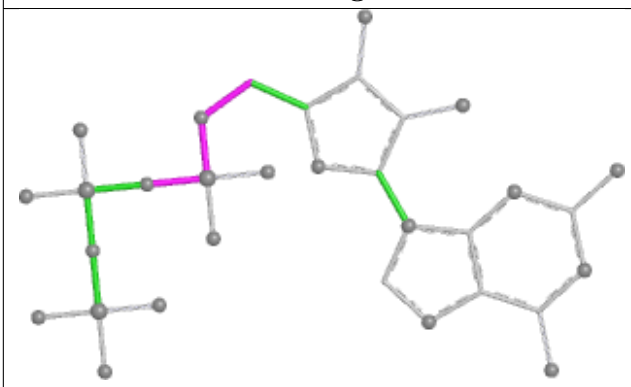
Ligand GTP IY 501



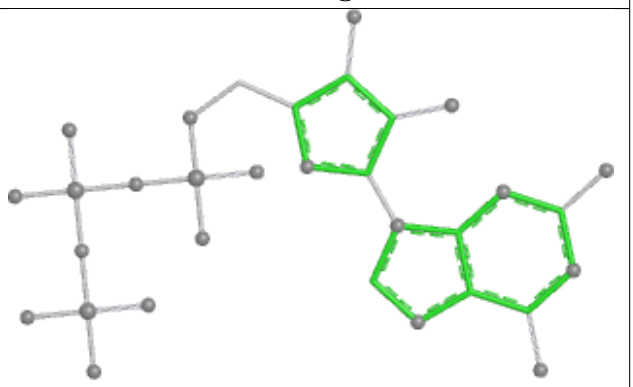
Bond lengths



Bond angles

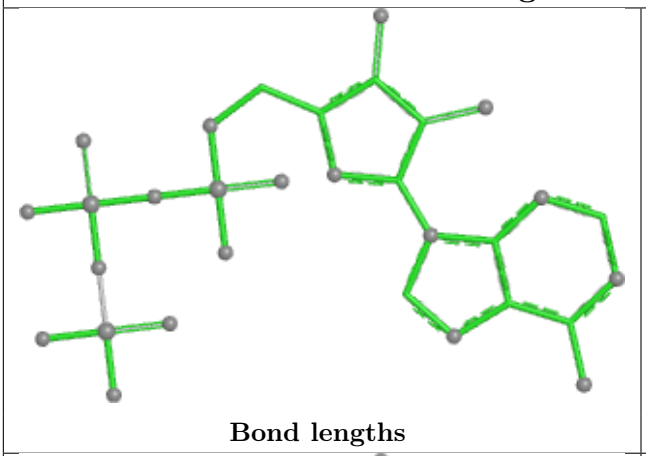


Torsions

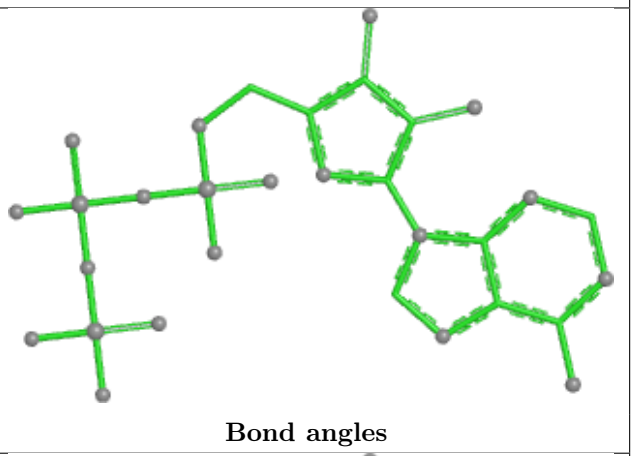


Rings

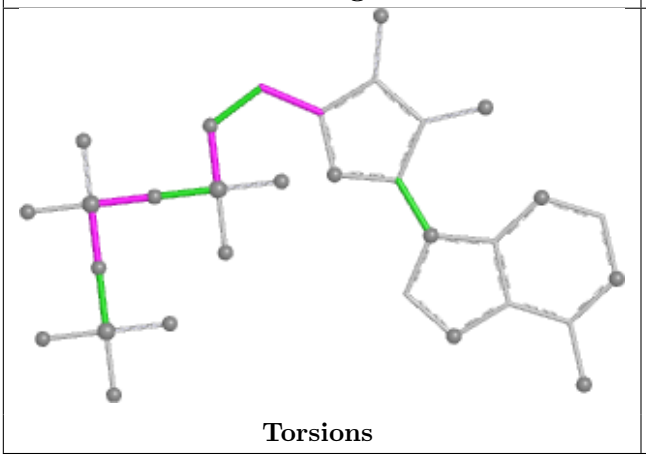
Ligand ATP 6u 700



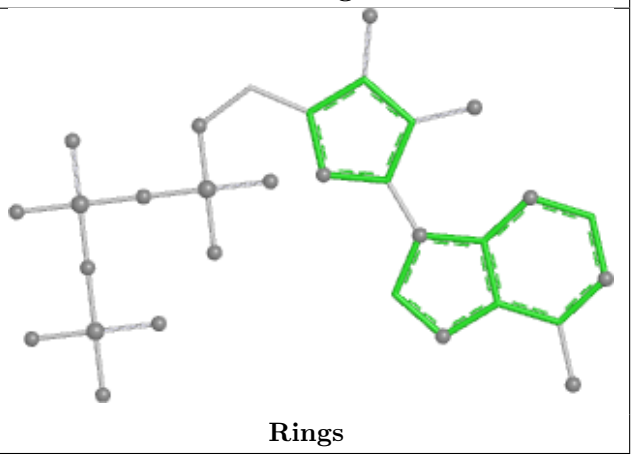
Bond lengths



Bond angles

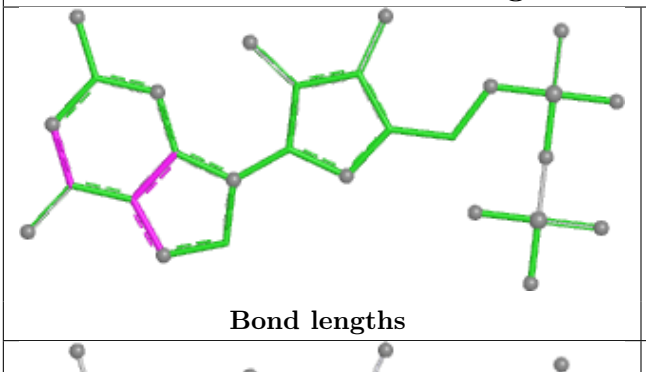


Torsions

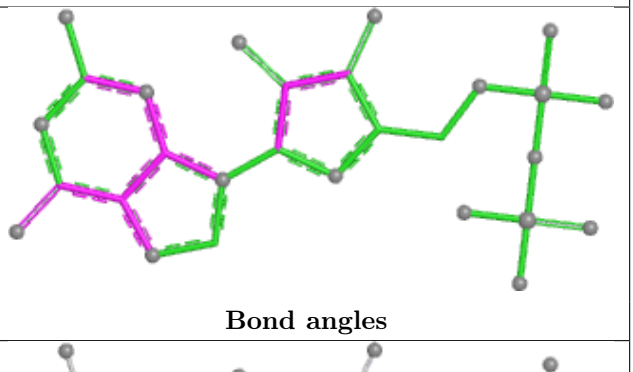


Rings

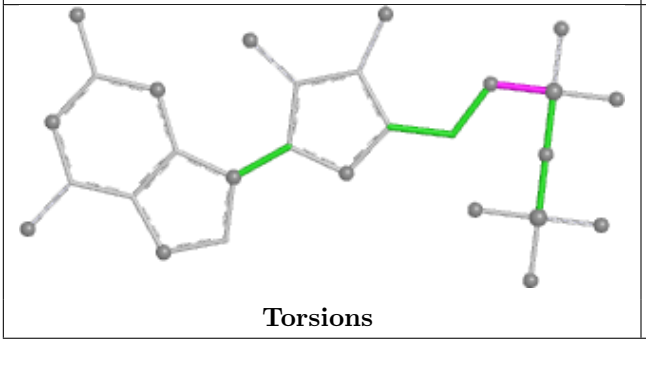
Ligand GDP VD 500



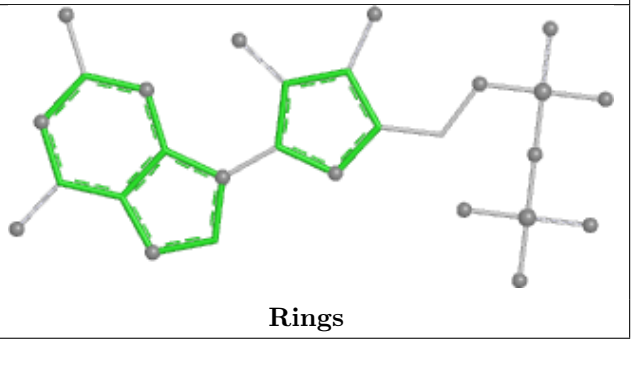
Bond lengths



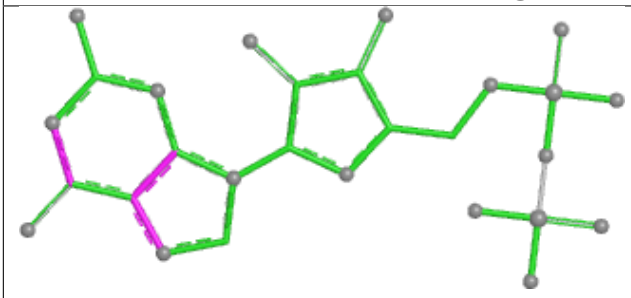
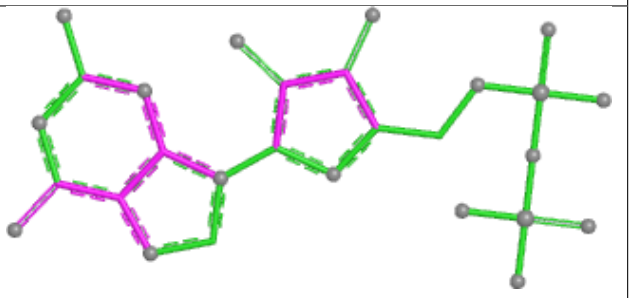
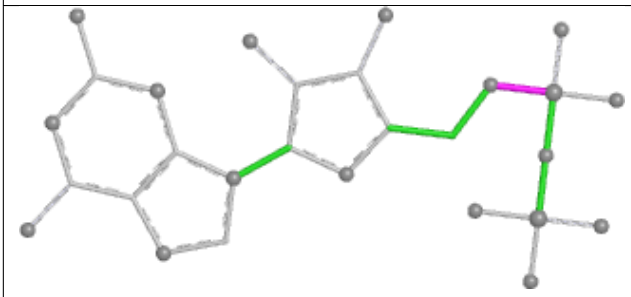
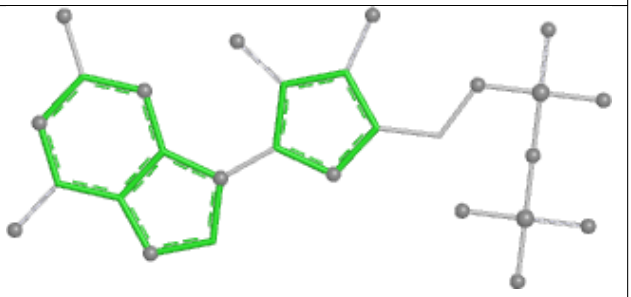
Bond angles

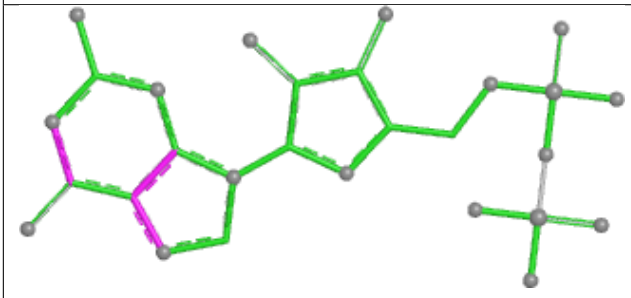
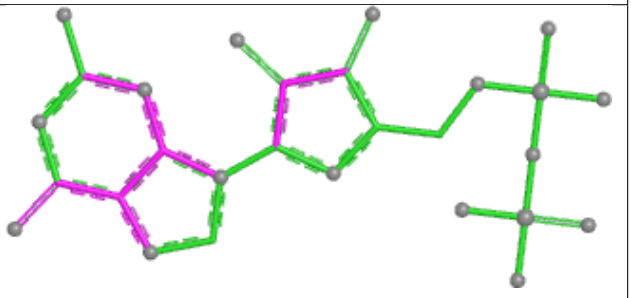
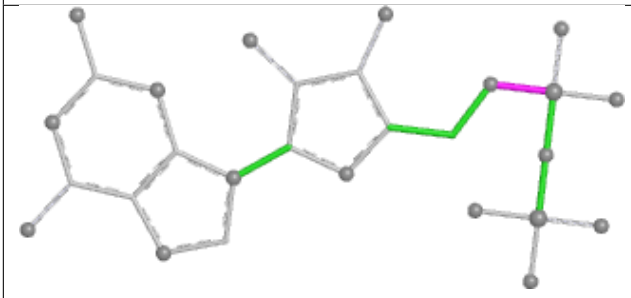
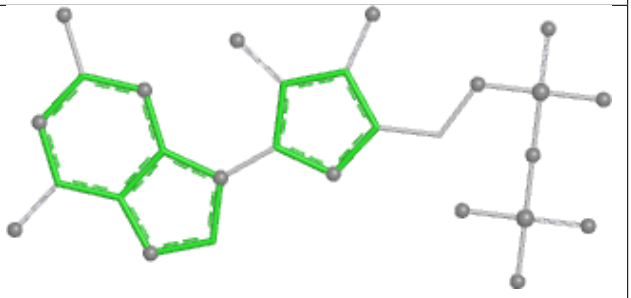


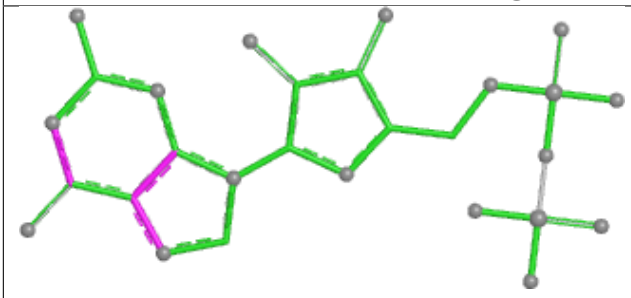
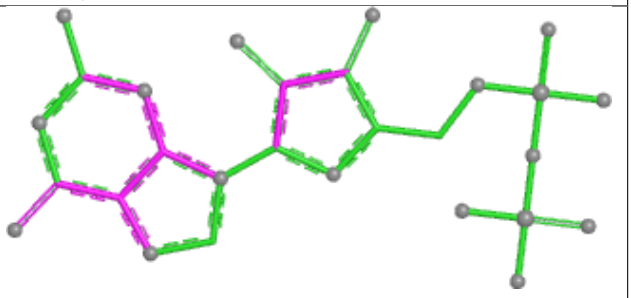
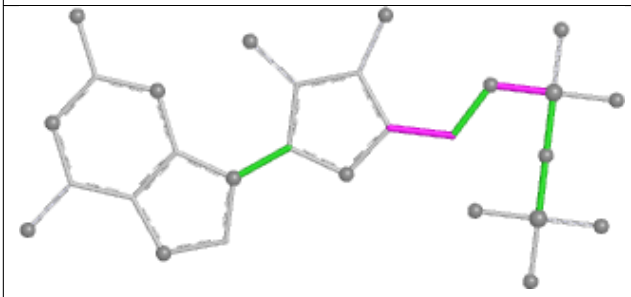
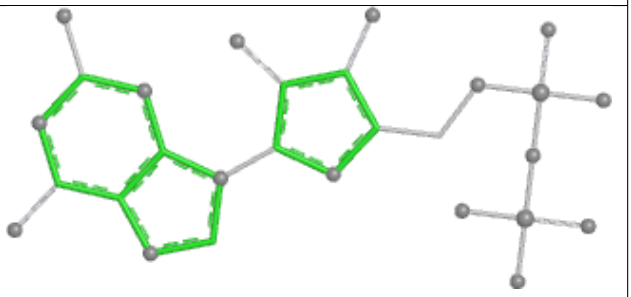
Torsions

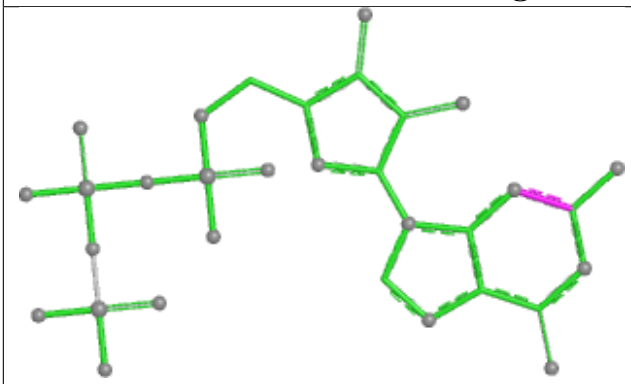
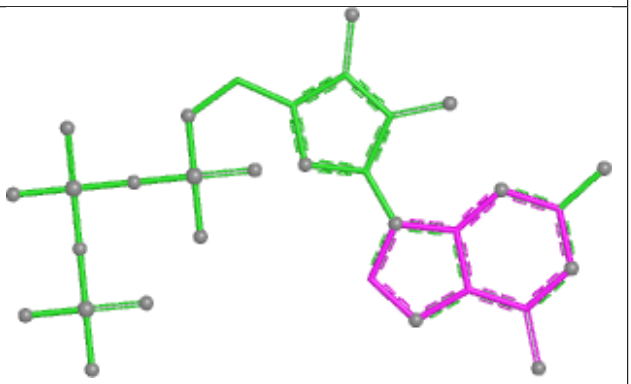
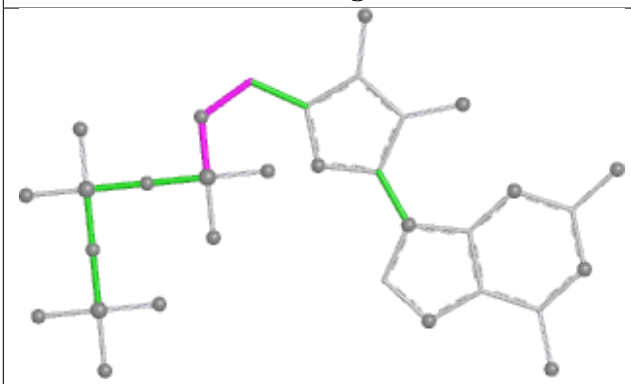
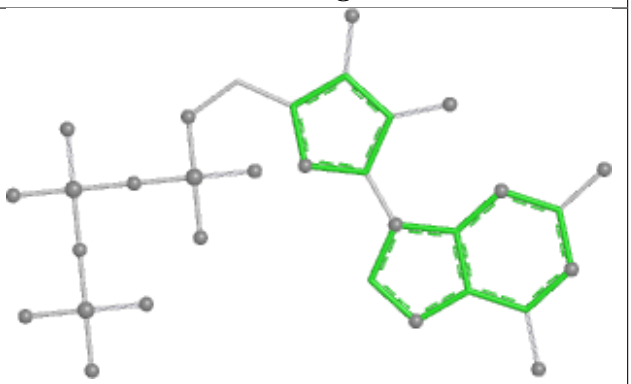


Rings

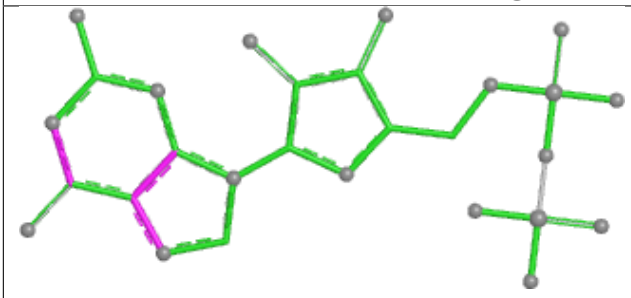
Ligand GDP VJ 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP WV 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

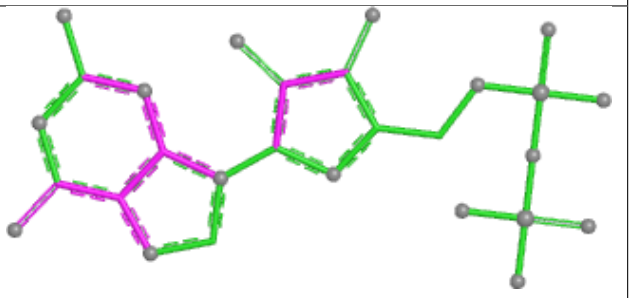
Ligand GDP CQ 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP LR 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

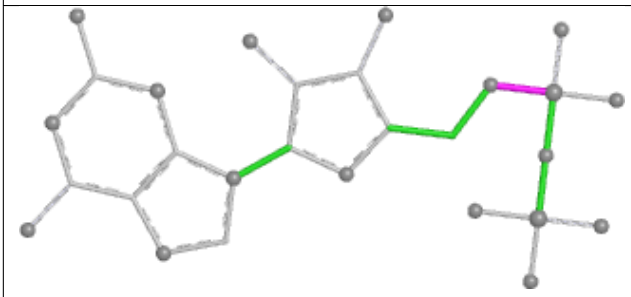
Ligand GDP UP 500



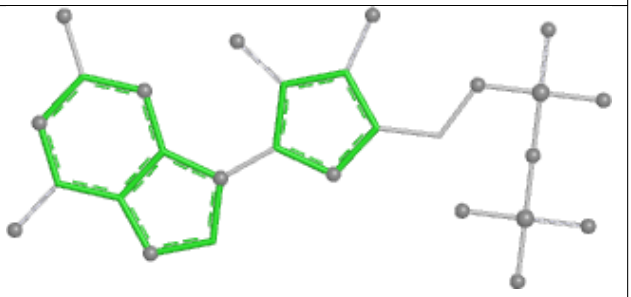
Bond lengths



Bond angles

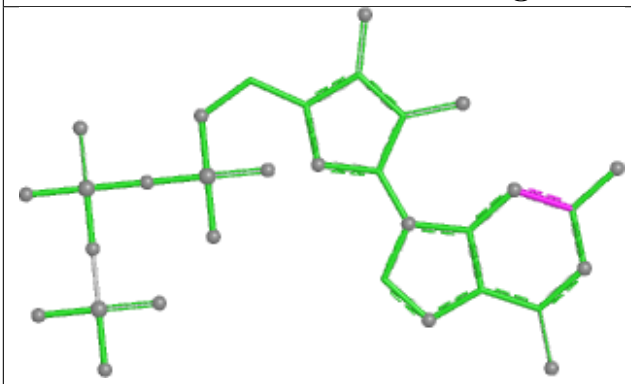


Torsions

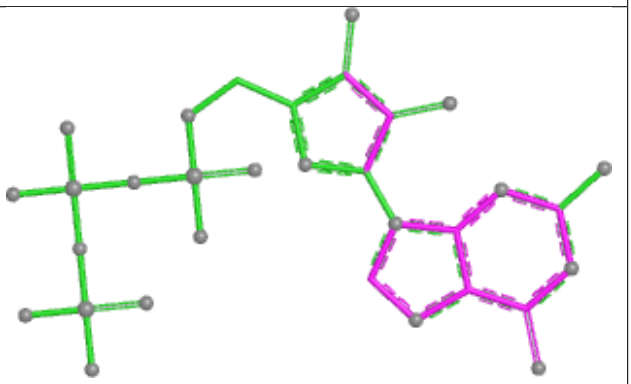


Rings

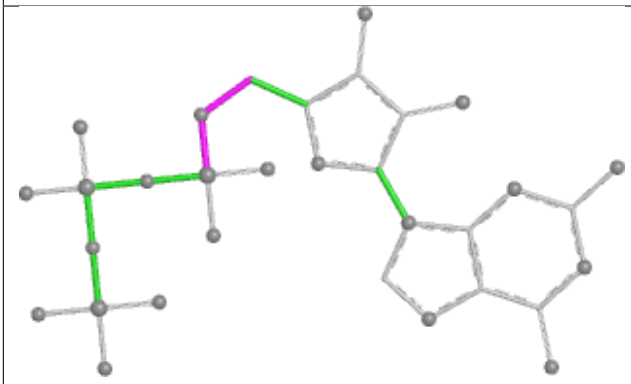
Ligand GTP JN 501



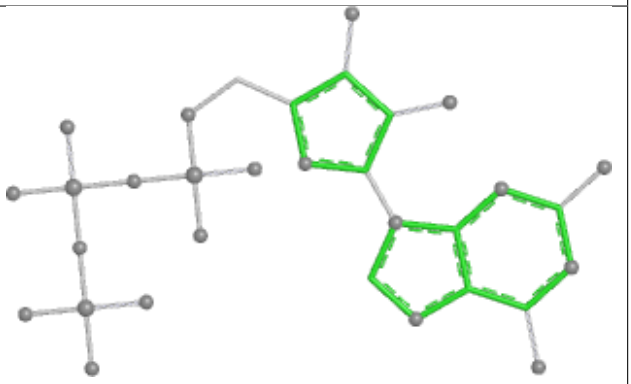
Bond lengths



Bond angles

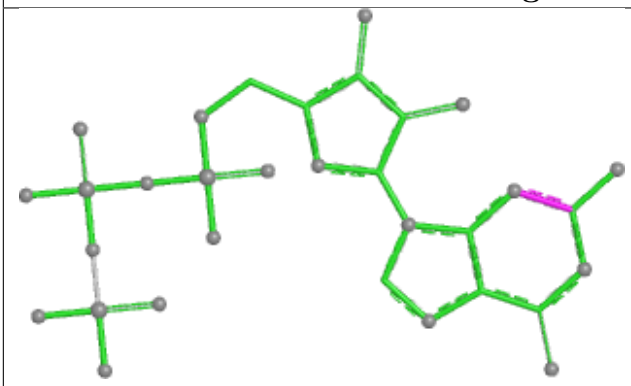


Torsions

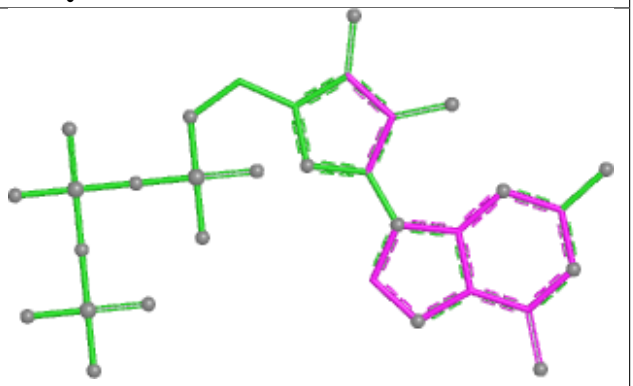


Rings

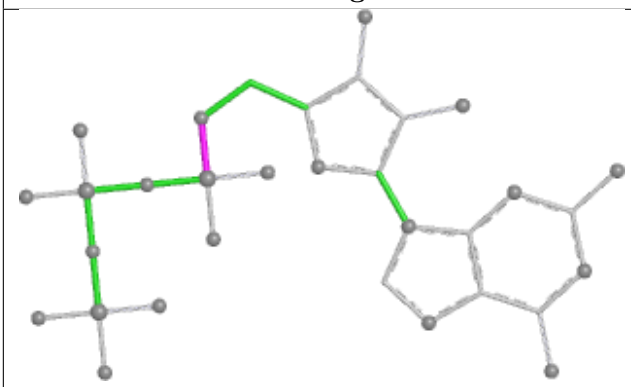
Ligand GTP Q 501



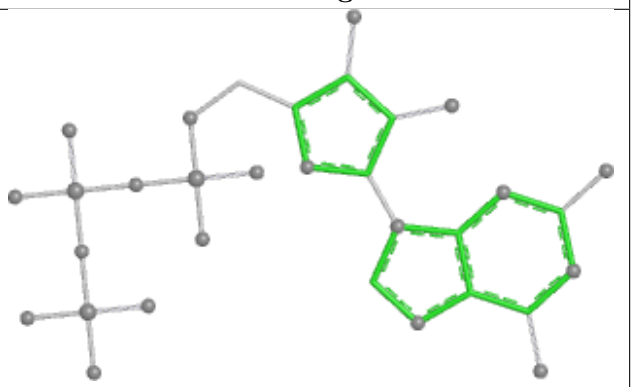
Bond lengths



Bond angles

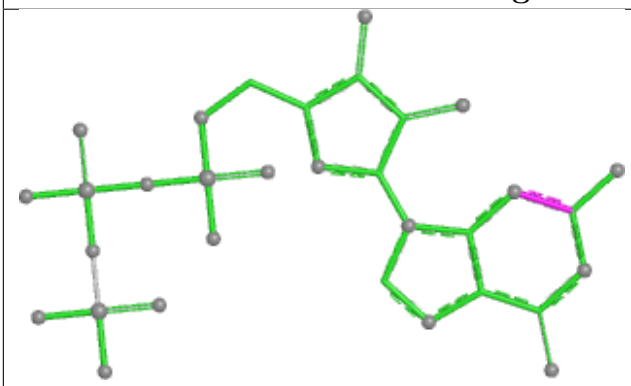


Torsions

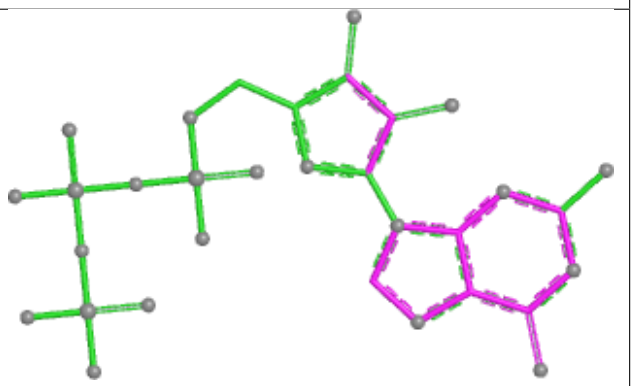


Rings

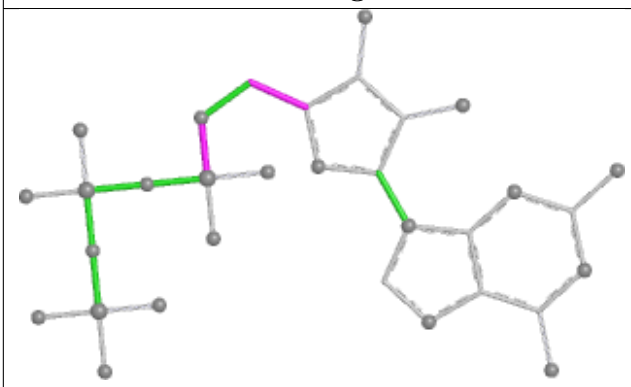
Ligand GTP JH 501



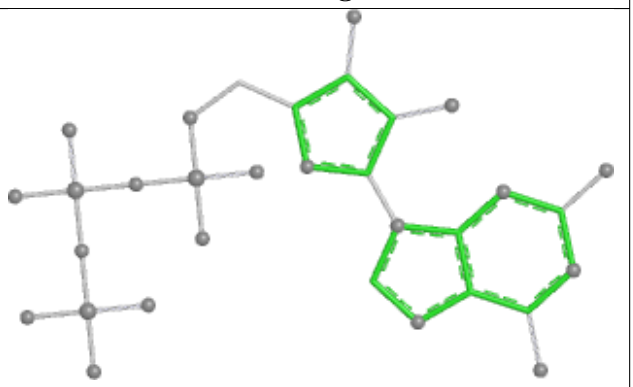
Bond lengths



Bond angles

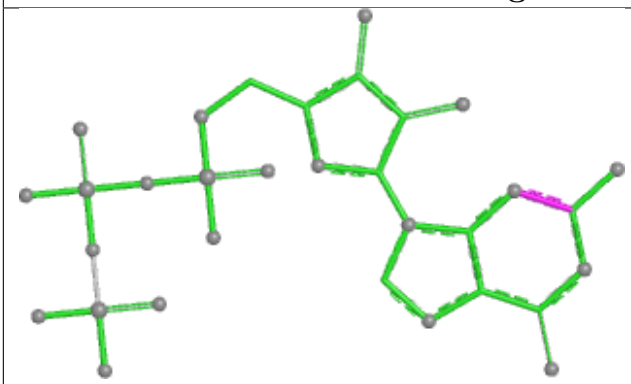


Torsions

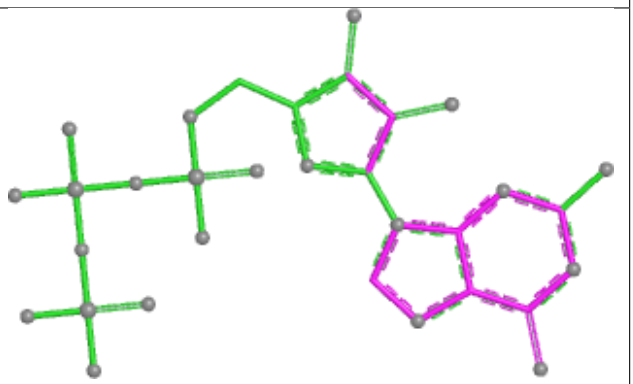


Rings

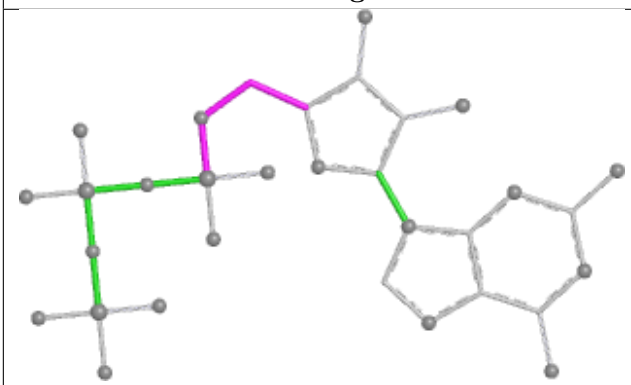
Ligand GTP OU 501



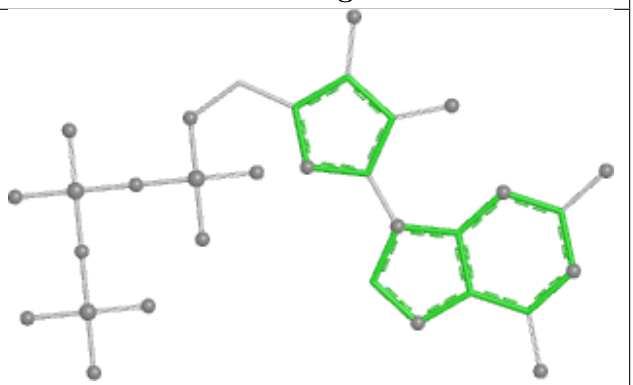
Bond lengths



Bond angles

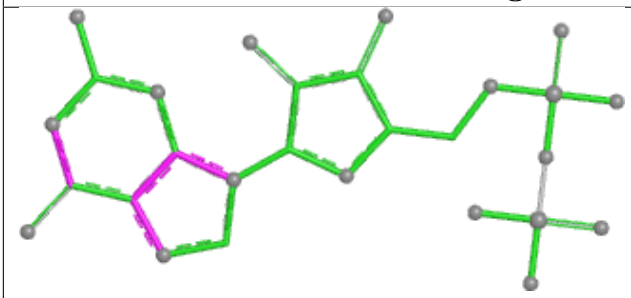


Torsions

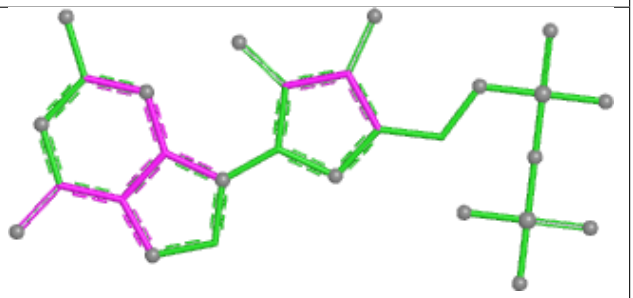


Rings

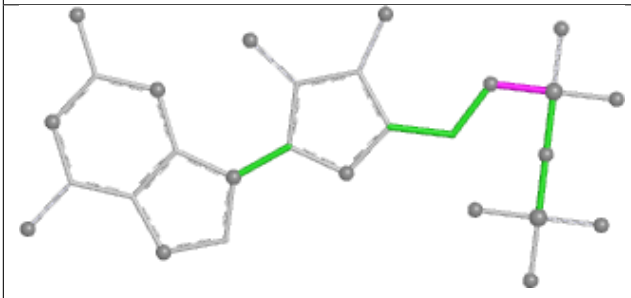
Ligand GDP AN 500



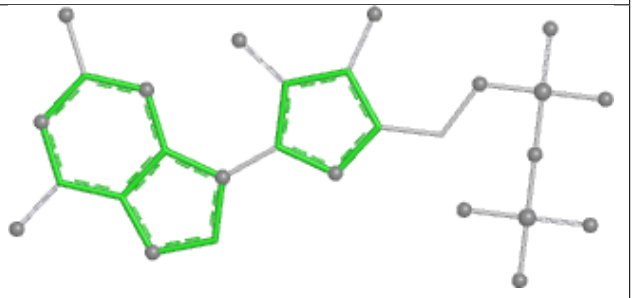
Bond lengths



Bond angles

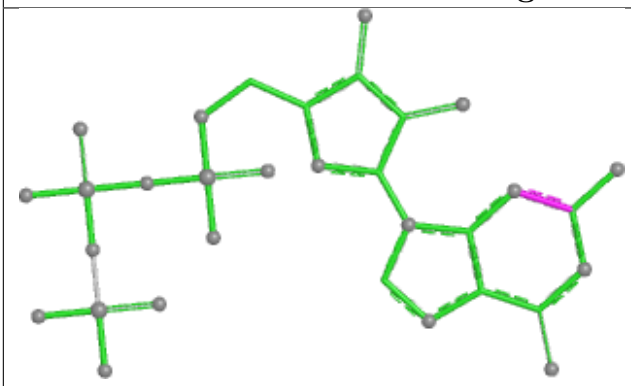


Torsions

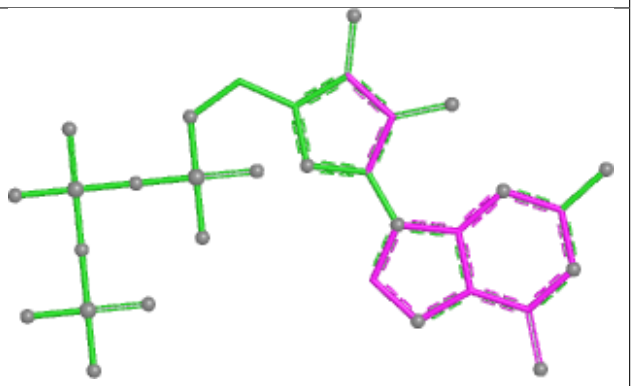


Rings

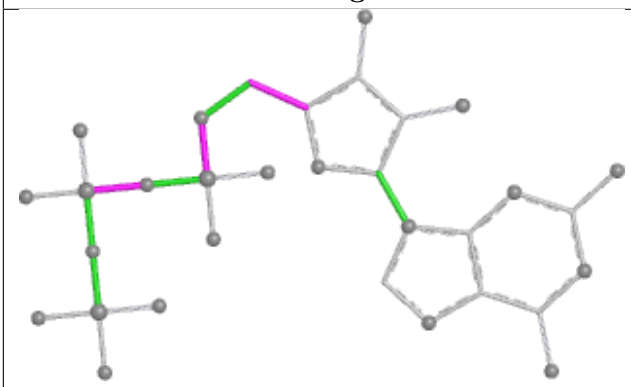
Ligand GTP EI 501



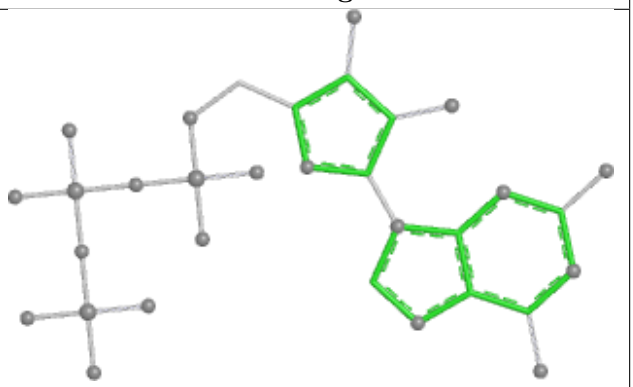
Bond lengths



Bond angles

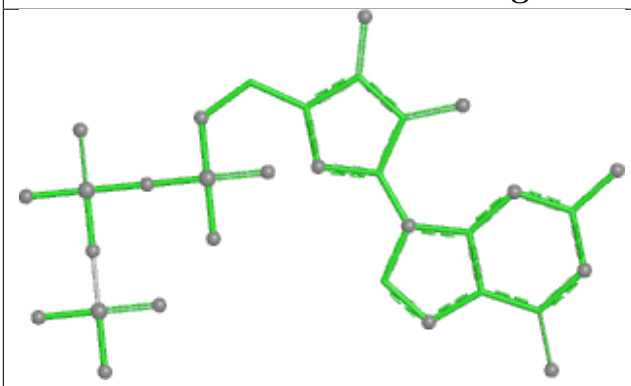


Torsions

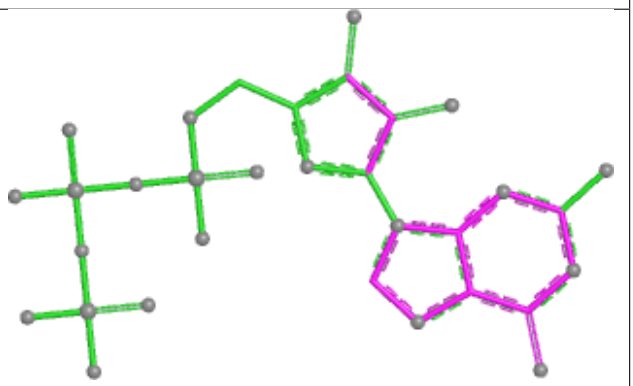


Rings

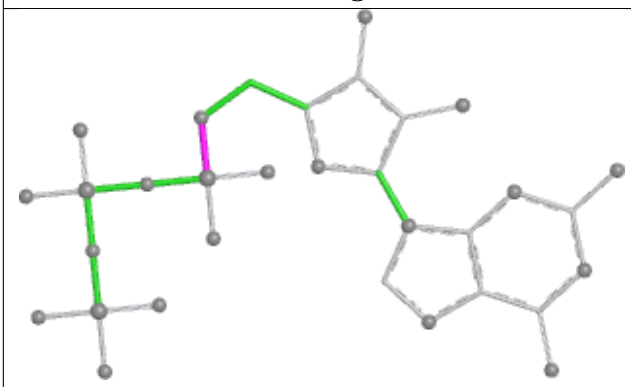
Ligand GTP FO 501



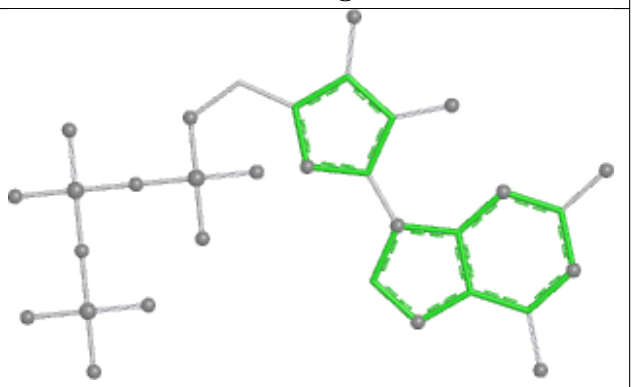
Bond lengths



Bond angles

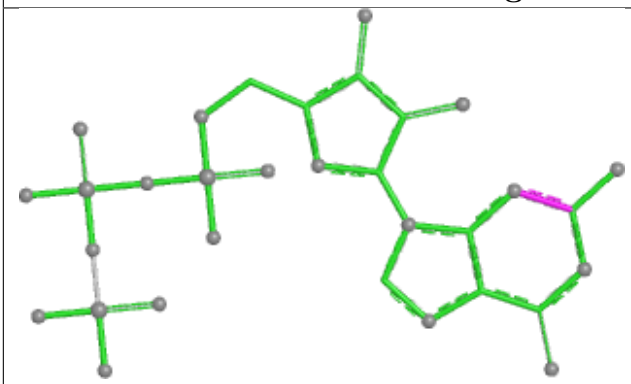


Torsions

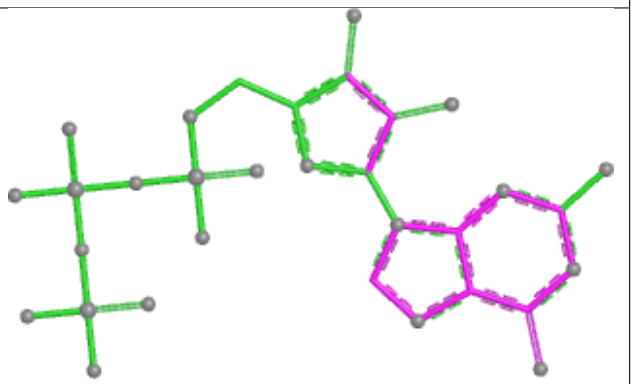


Rings

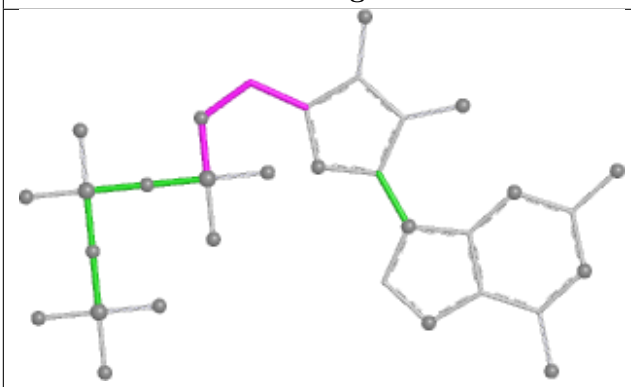
Ligand GTP PW 501



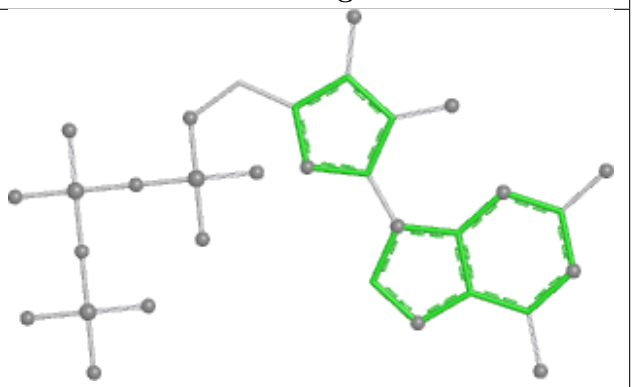
Bond lengths



Bond angles

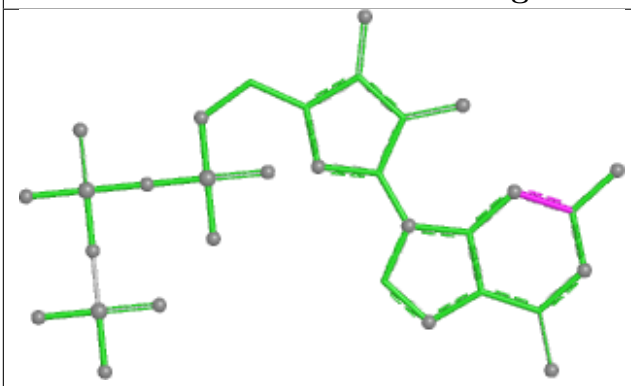


Torsions

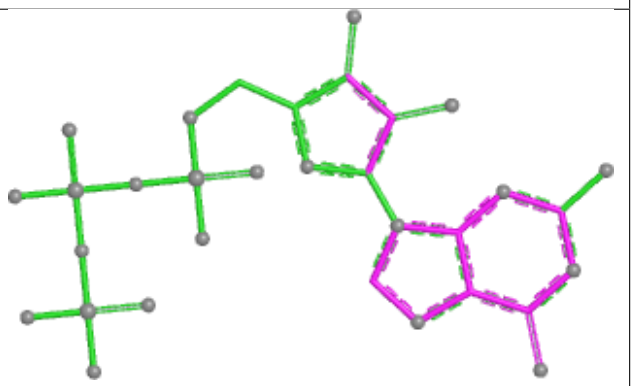


Rings

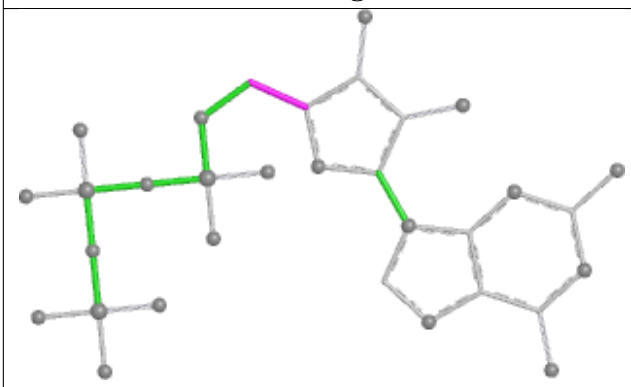
Ligand GTP RT 501



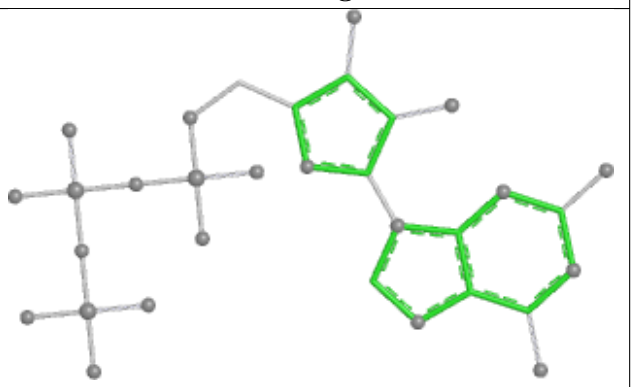
Bond lengths



Bond angles

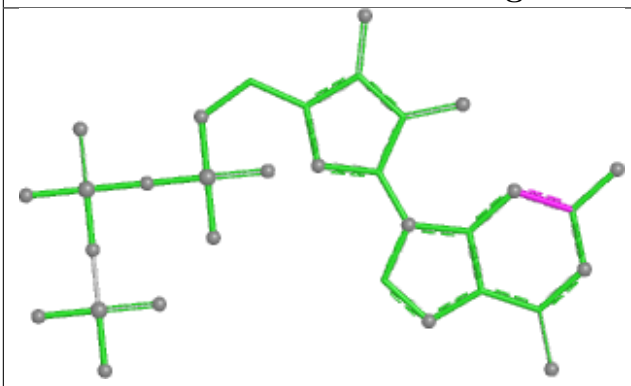


Torsions

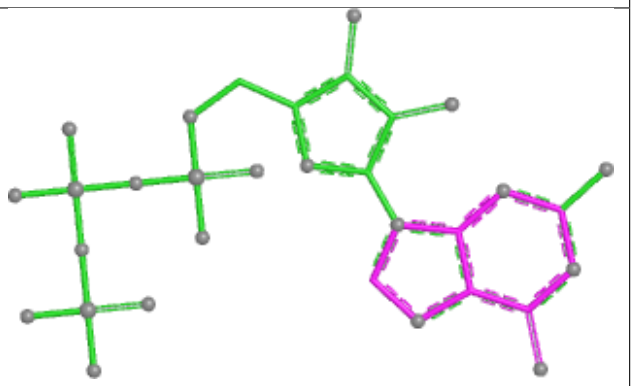


Rings

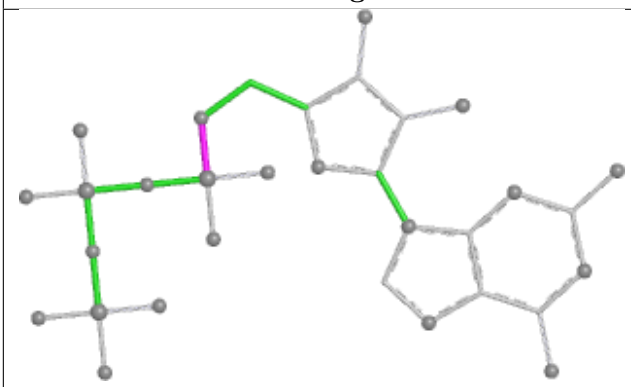
Ligand GTP AW 501



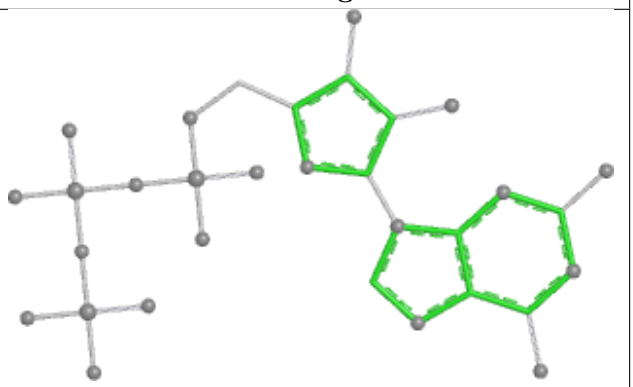
Bond lengths



Bond angles

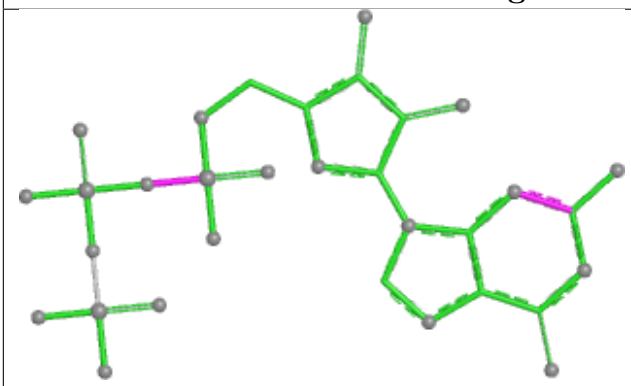


Torsions

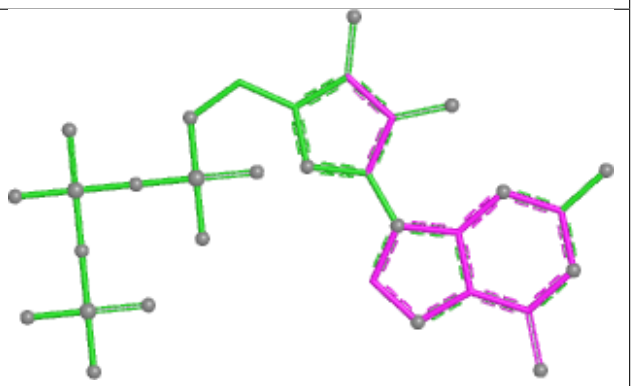


Rings

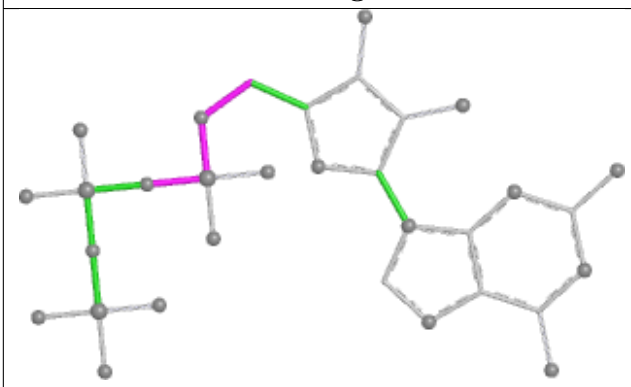
Ligand GTP NY 501



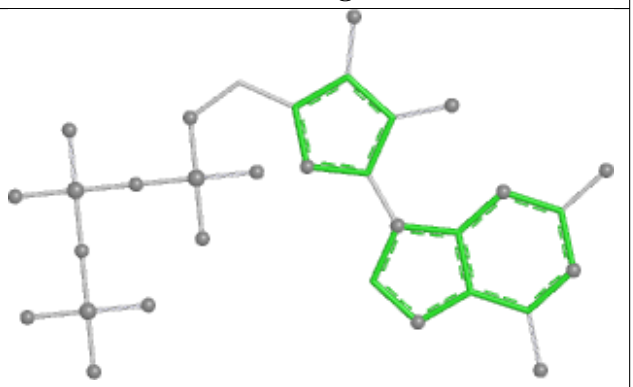
Bond lengths



Bond angles

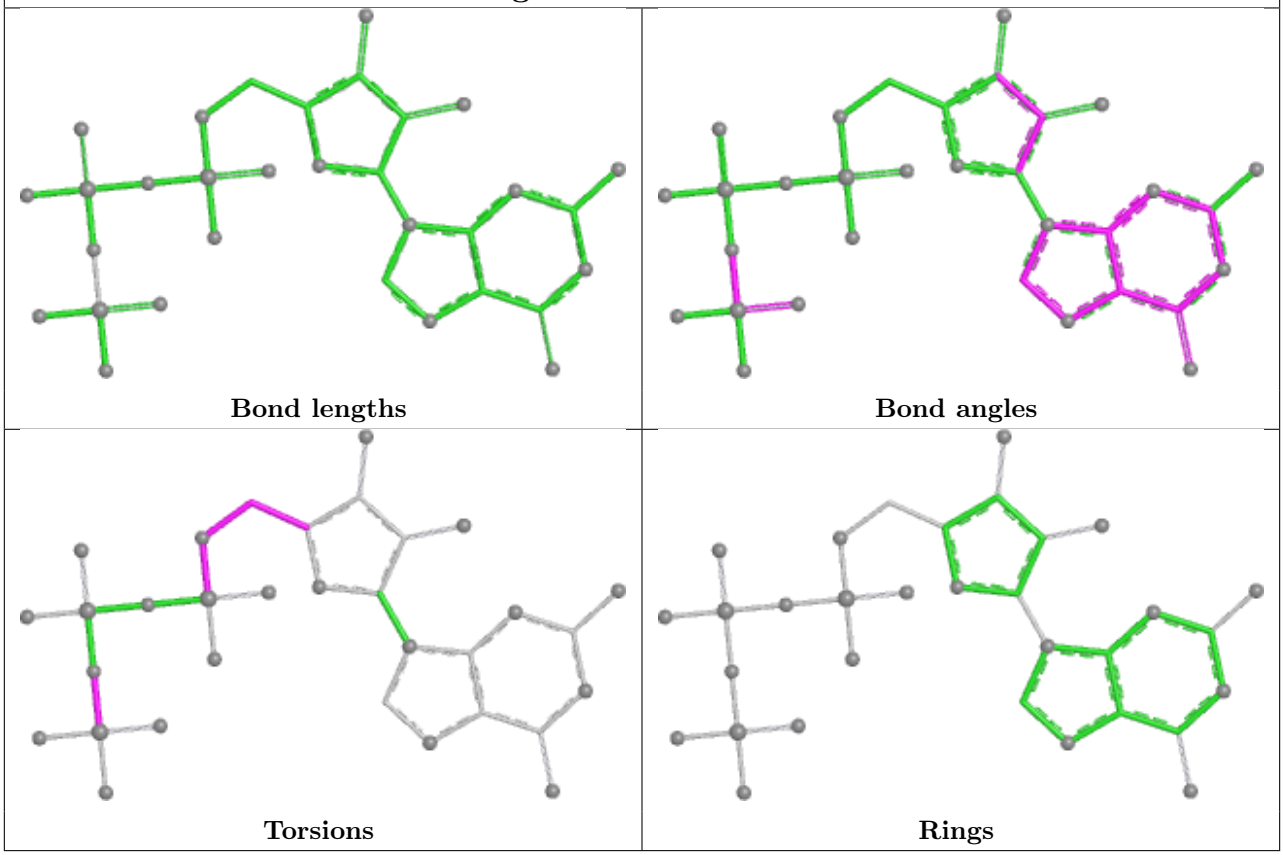


Torsions

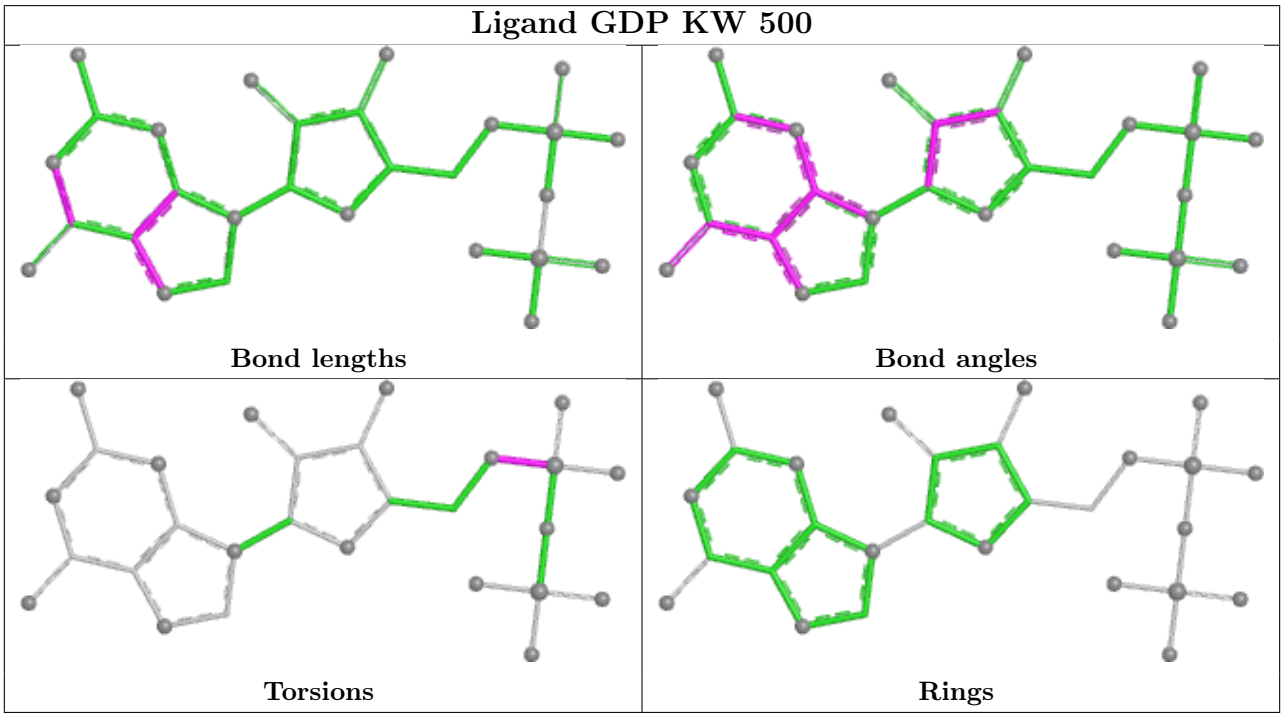


Rings

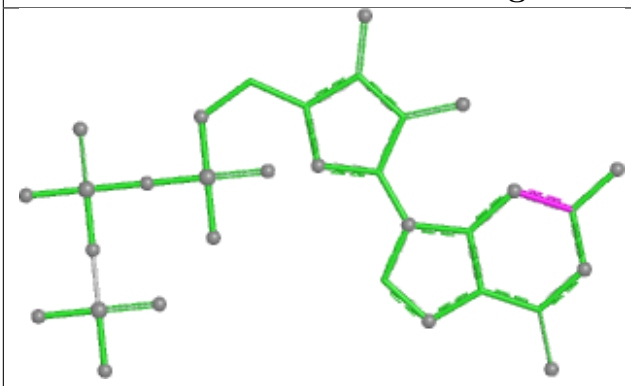
Ligand GTP BE 501



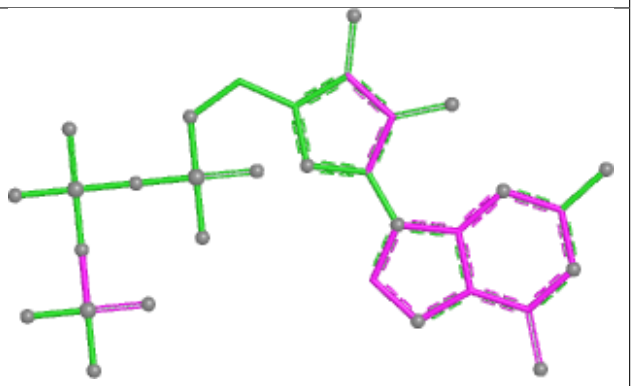
Ligand GDP KW 500



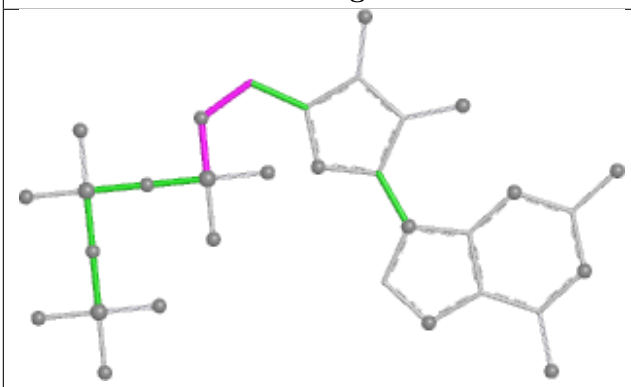
Ligand GTP AD 501



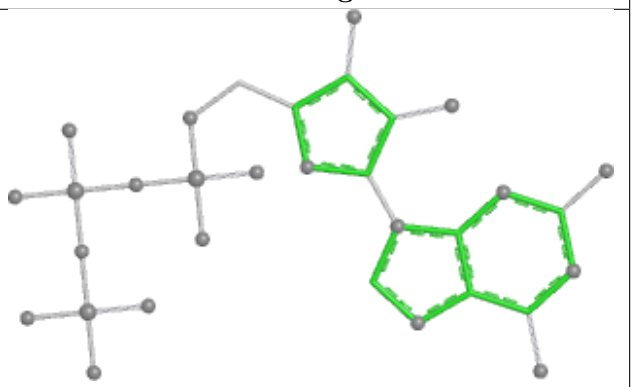
Bond lengths



Bond angles

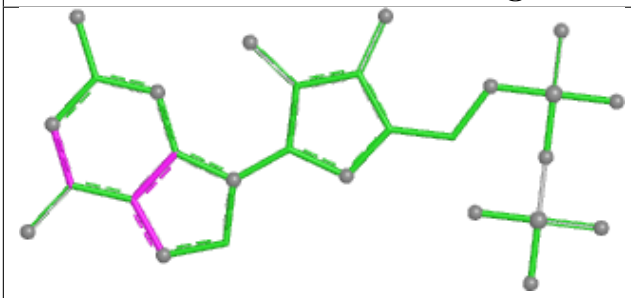


Torsions

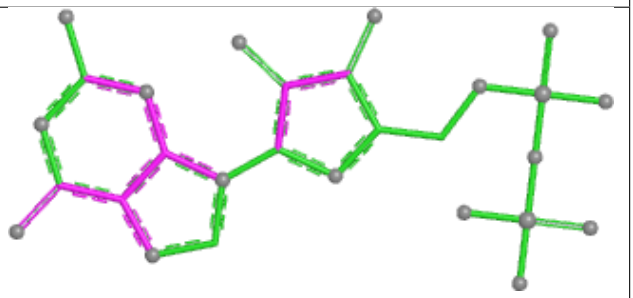


Rings

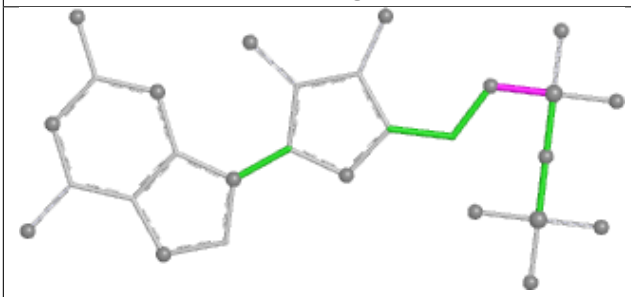
Ligand GDP UH 500



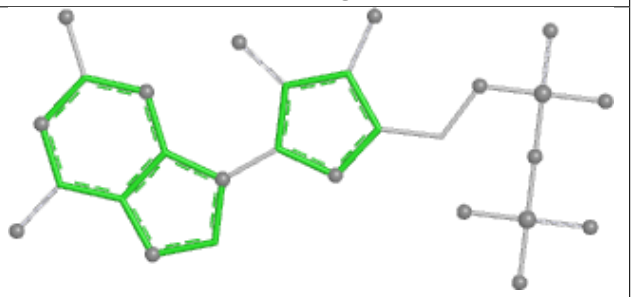
Bond lengths



Bond angles

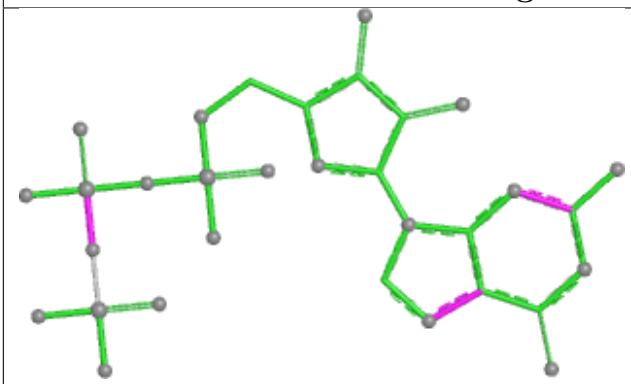


Torsions

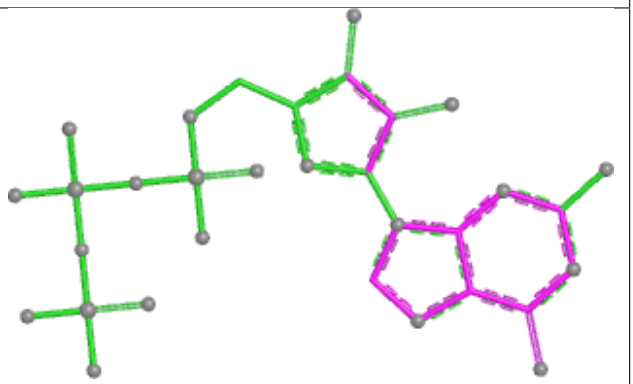


Rings

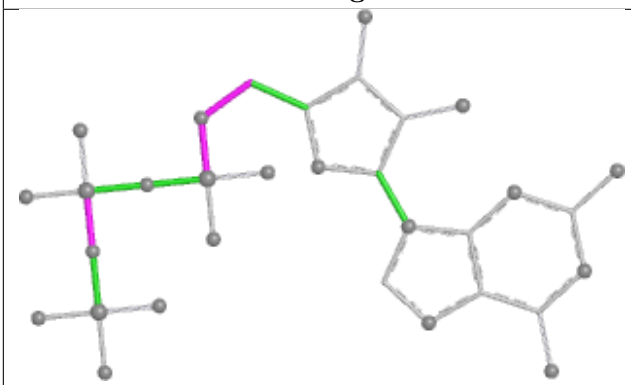
Ligand GTP BI 501



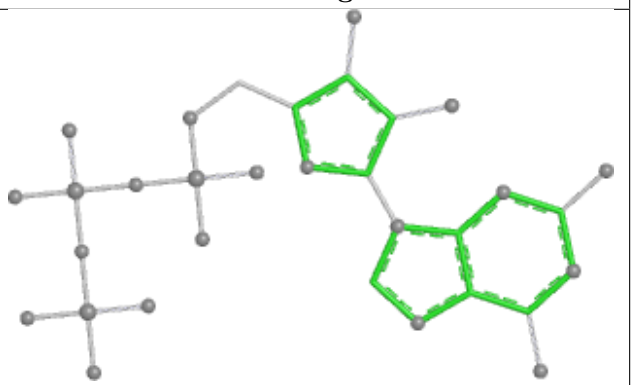
Bond lengths



Bond angles

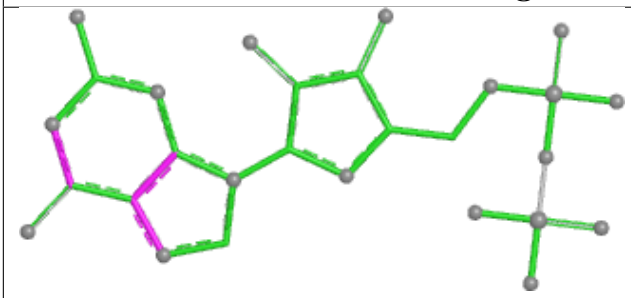


Torsions

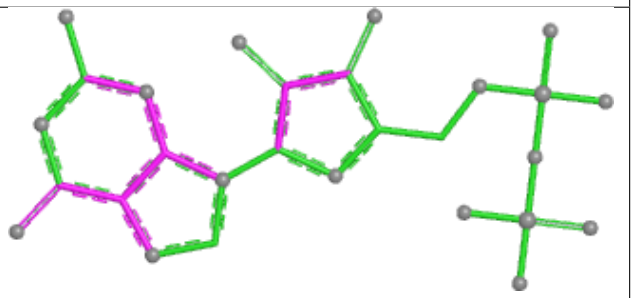


Rings

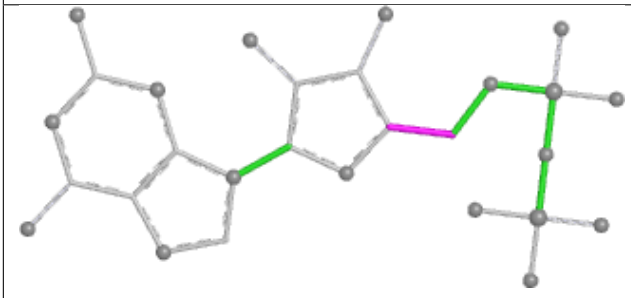
Ligand GDP JS 500



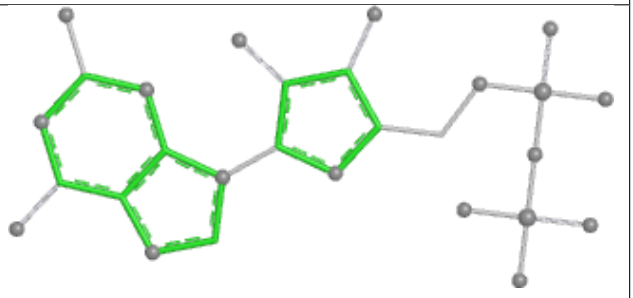
Bond lengths



Bond angles

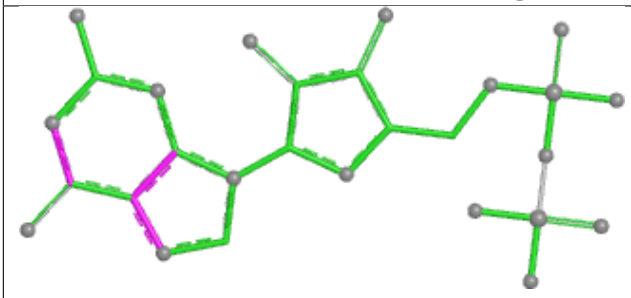


Torsions

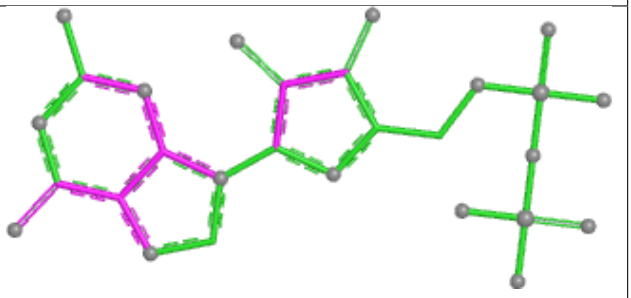


Rings

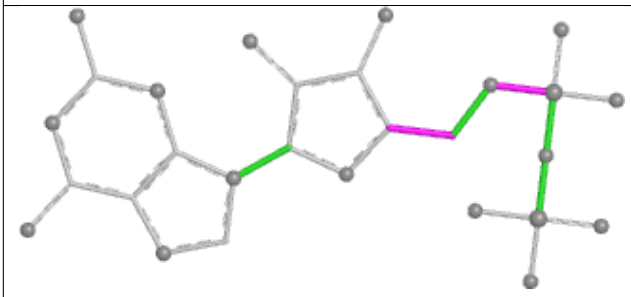
Ligand GDP SV 501



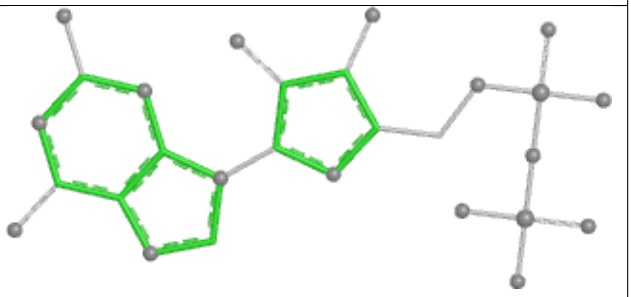
Bond lengths



Bond angles

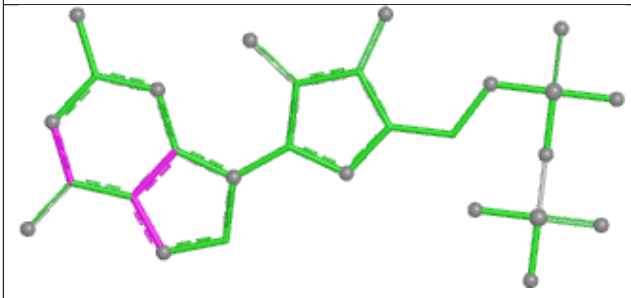


Torsions

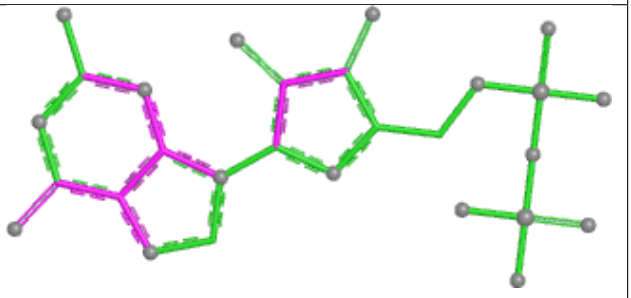


Rings

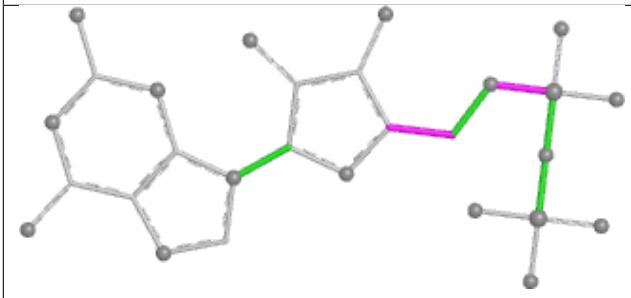
Ligand GDP AB 500



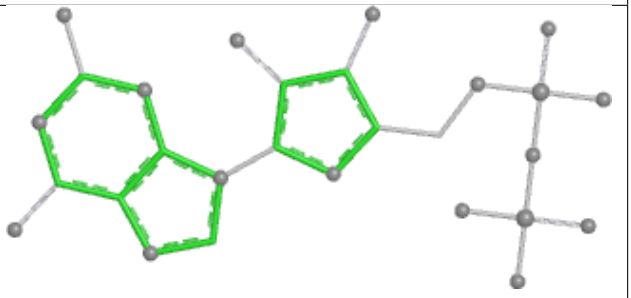
Bond lengths



Bond angles

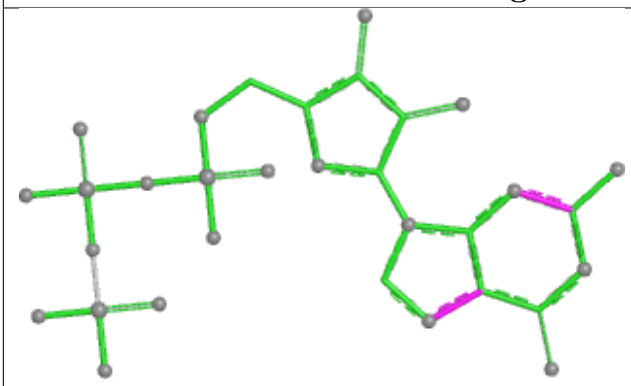


Torsions

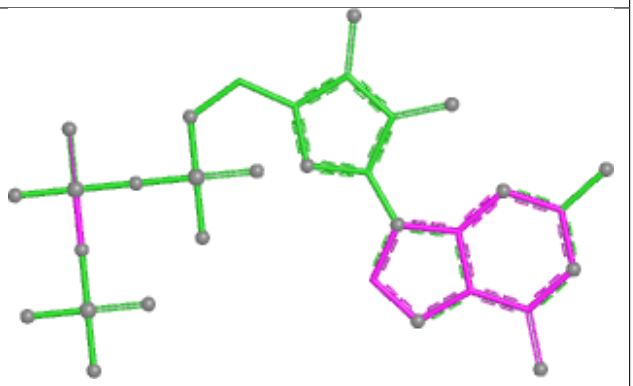


Rings

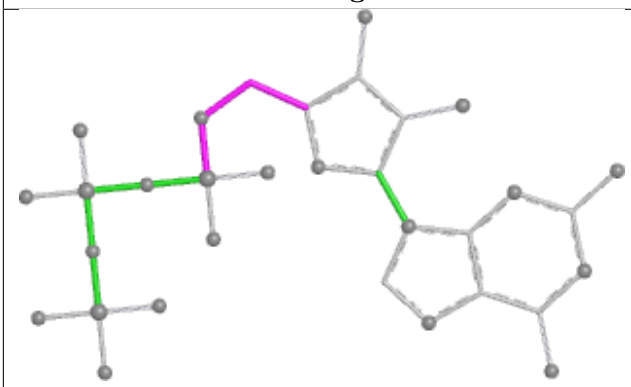
Ligand GTP DE 501



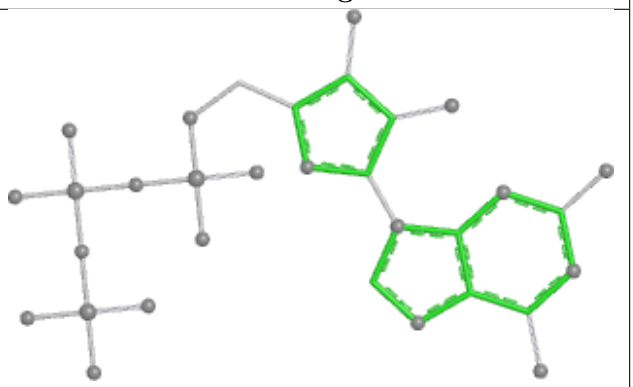
Bond lengths



Bond angles

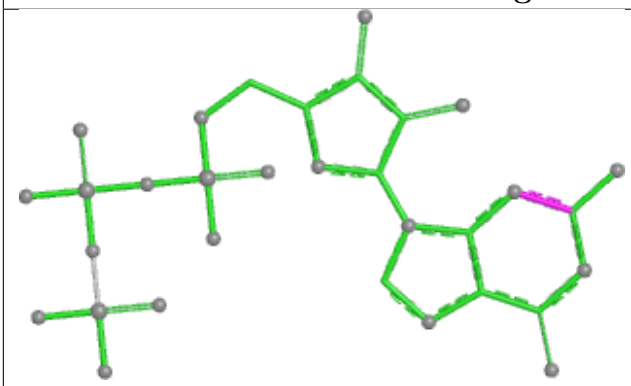


Torsions

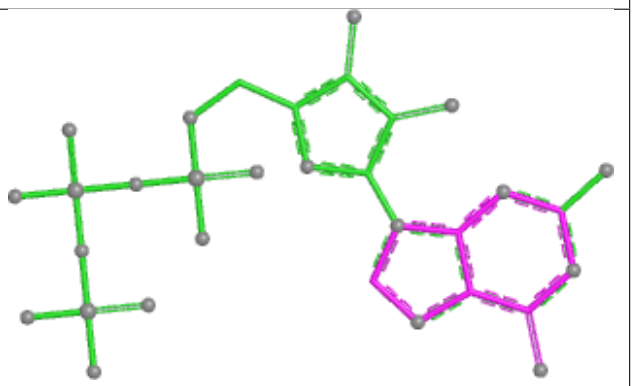


Rings

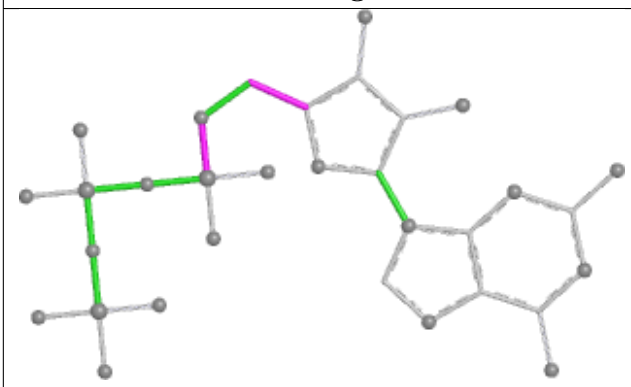
Ligand GTP JP 501



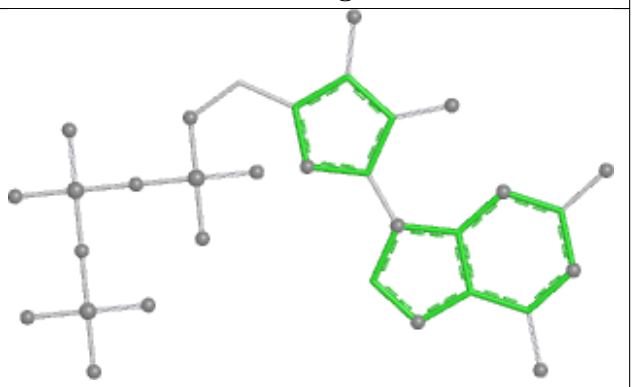
Bond lengths



Bond angles

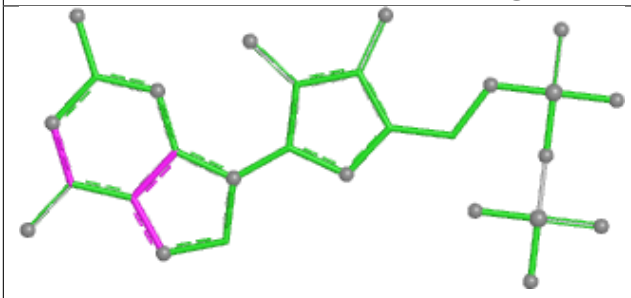


Torsions

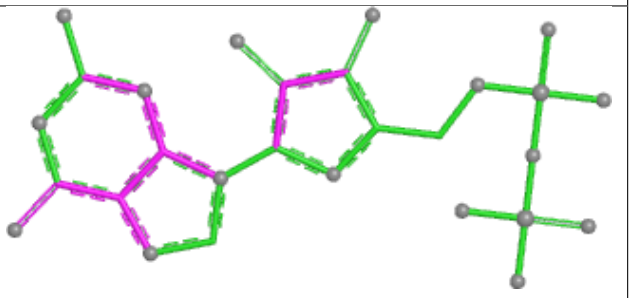


Rings

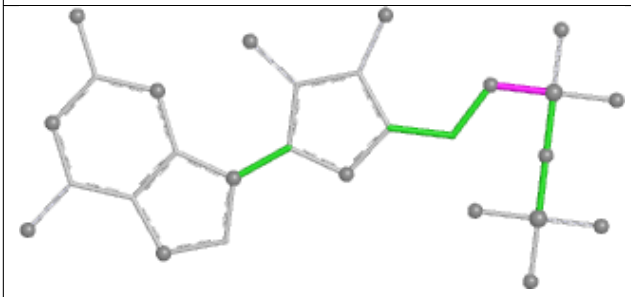
Ligand GDP TH 500



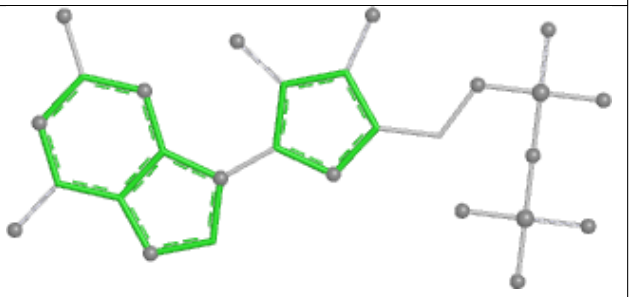
Bond lengths



Bond angles

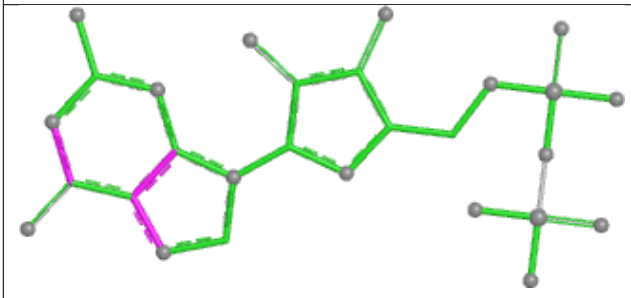


Torsions

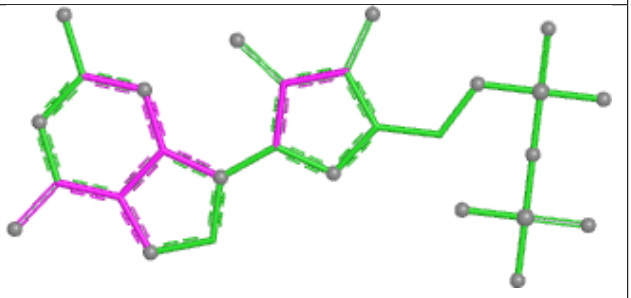


Rings

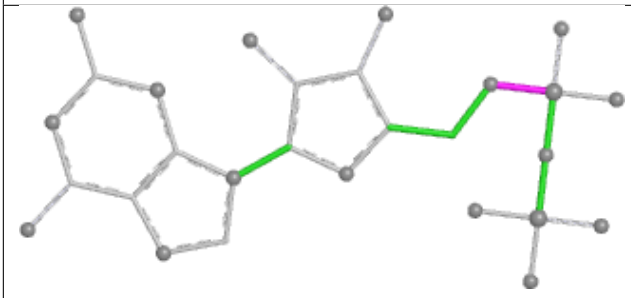
Ligand GDP KE 500



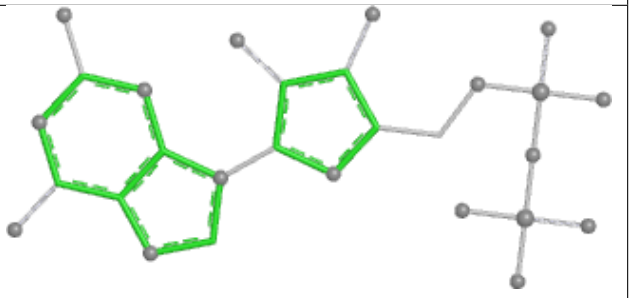
Bond lengths



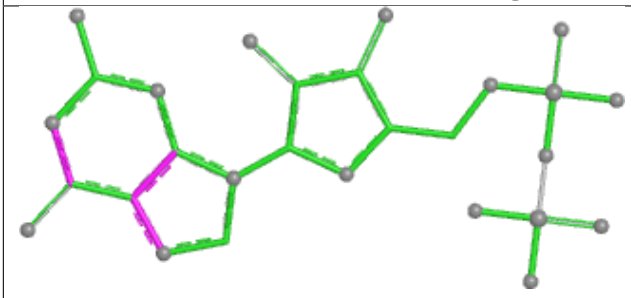
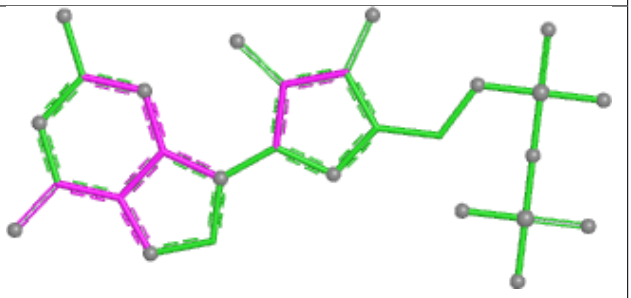
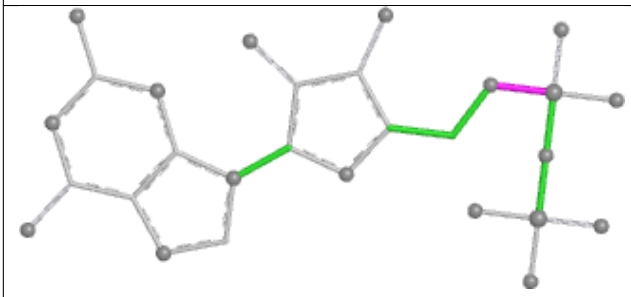
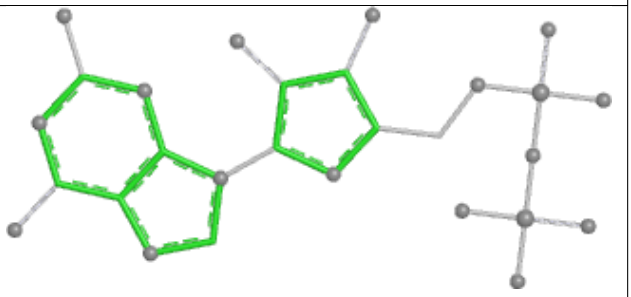
Bond angles

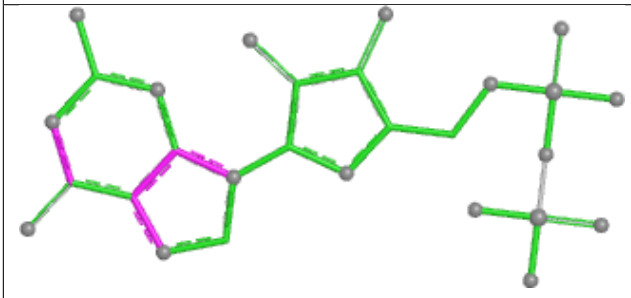
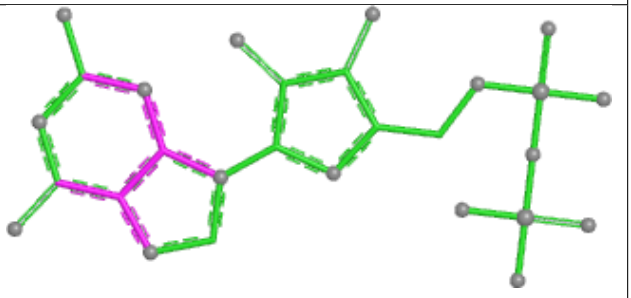
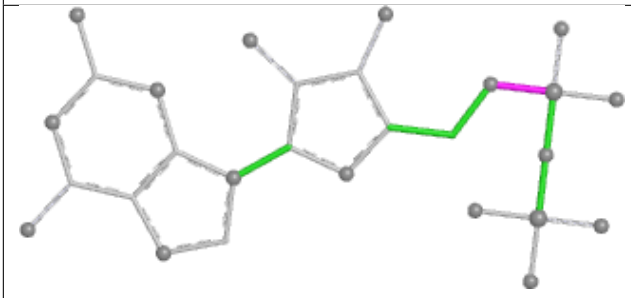
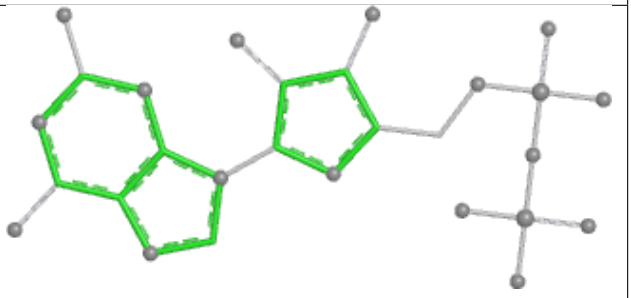


Torsions

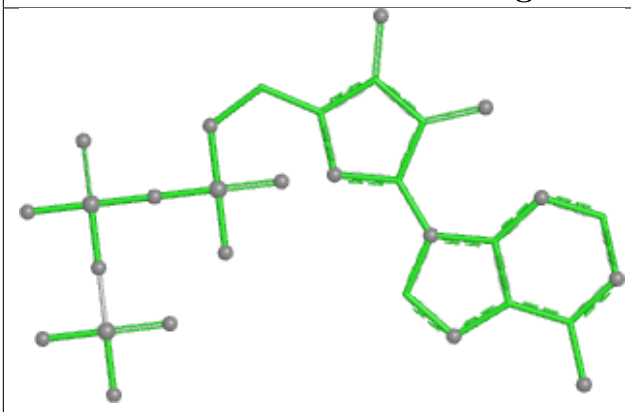


Rings

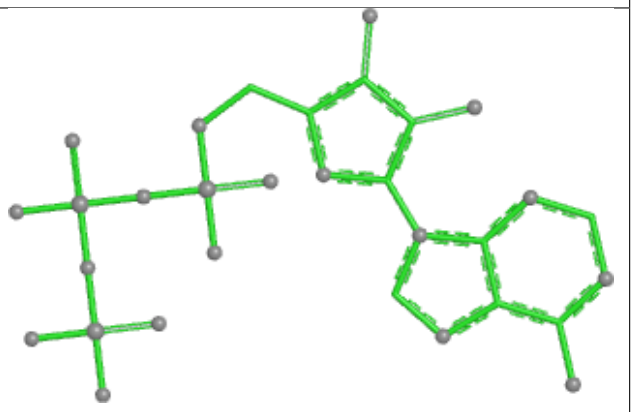
Ligand GDP KG 500	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP DO 500	
	
Bond lengths	Bond angles
	
Torsions	Rings

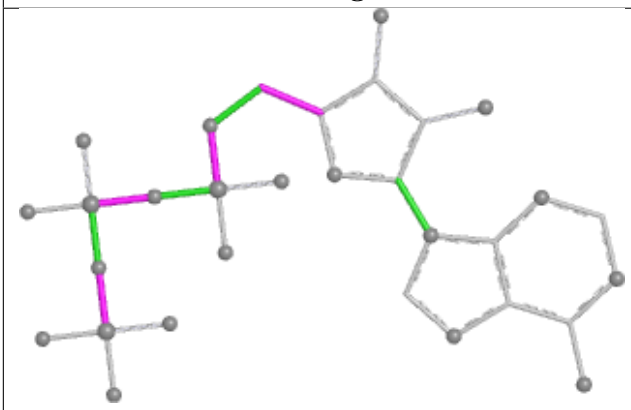
Ligand ATP 9R 500



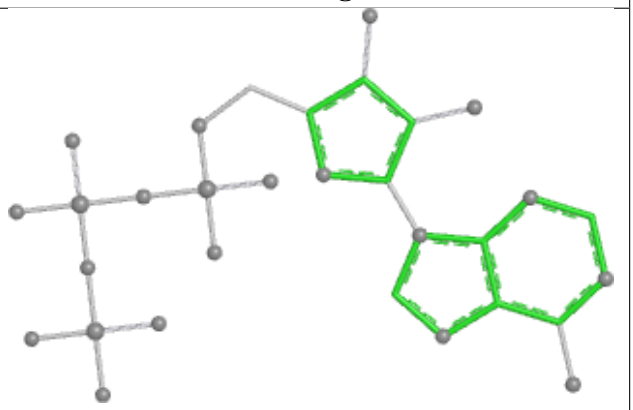
Bond lengths



Bond angles

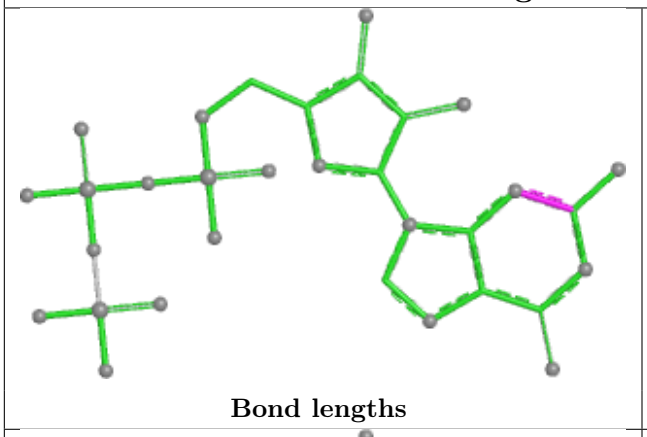


Torsions

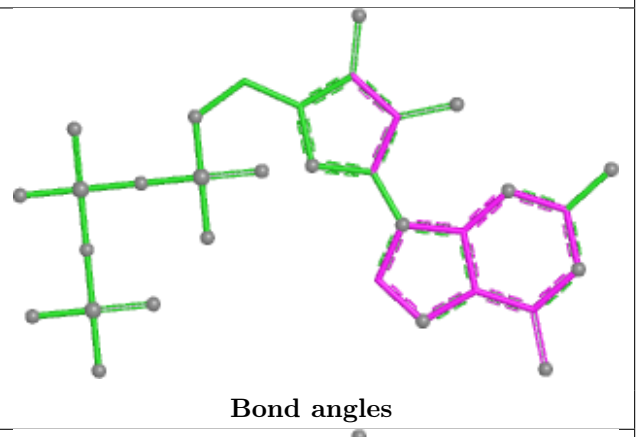


Rings

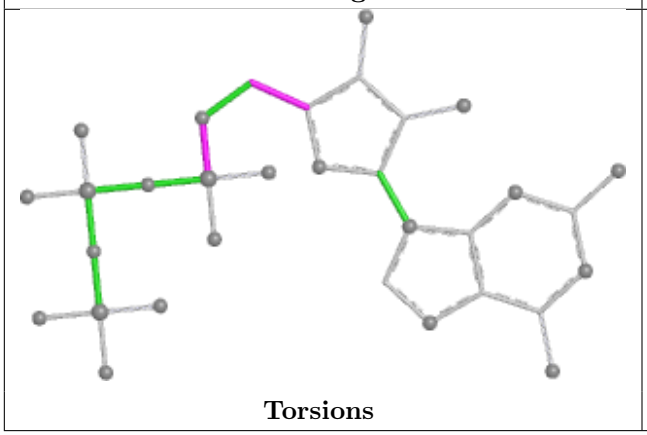
Ligand GTP JT 501



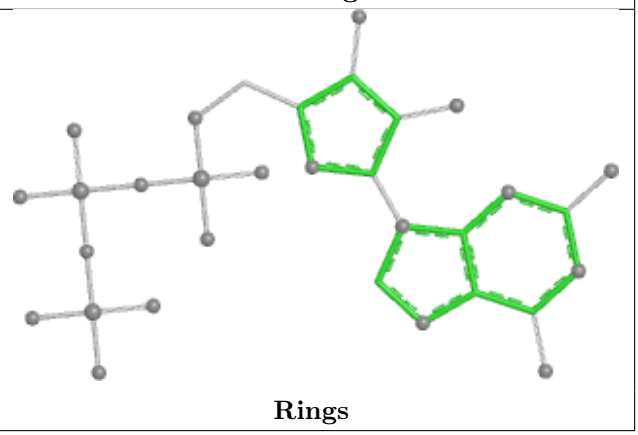
Bond lengths



Bond angles

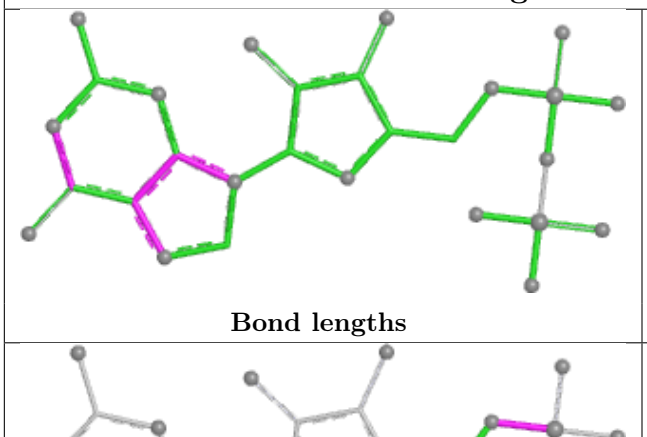


Torsions

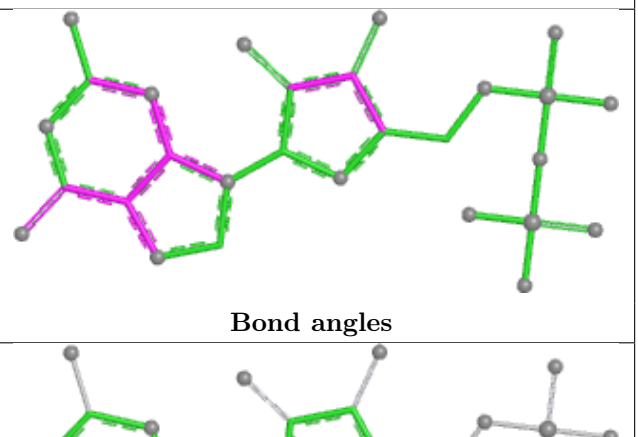


Rings

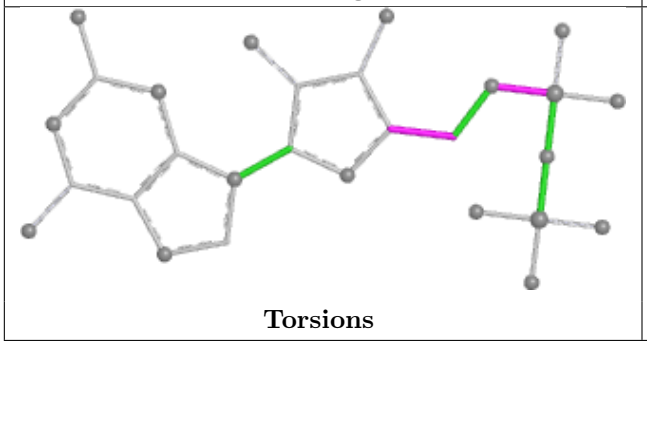
Ligand GDP AV 500



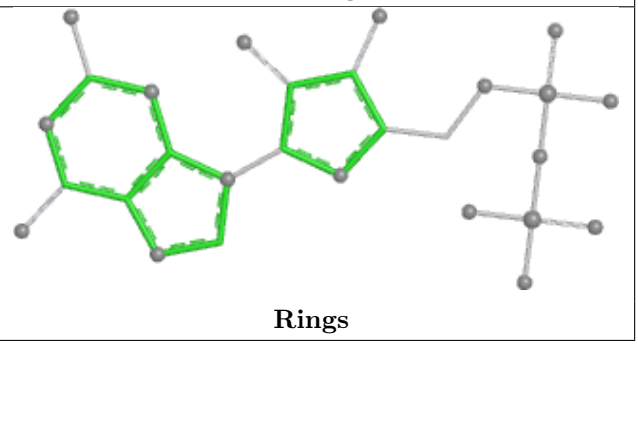
Bond lengths



Bond angles

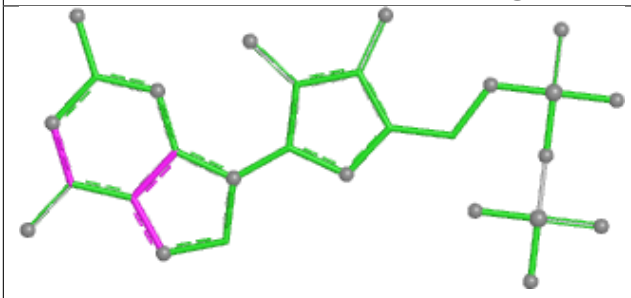


Torsions

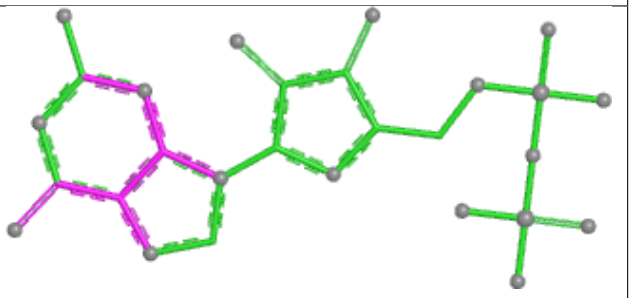


Rings

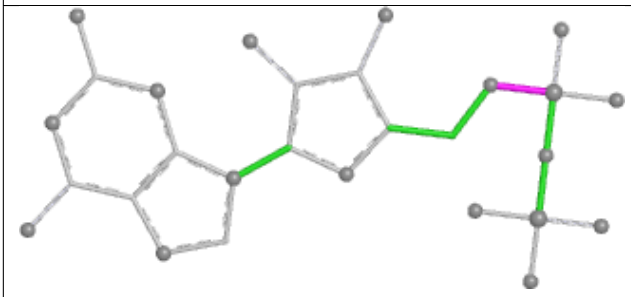
Ligand GDP TR 500



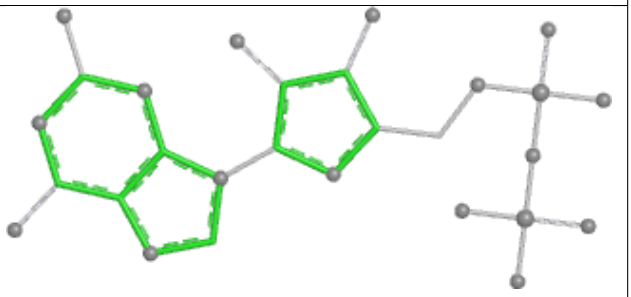
Bond lengths



Bond angles

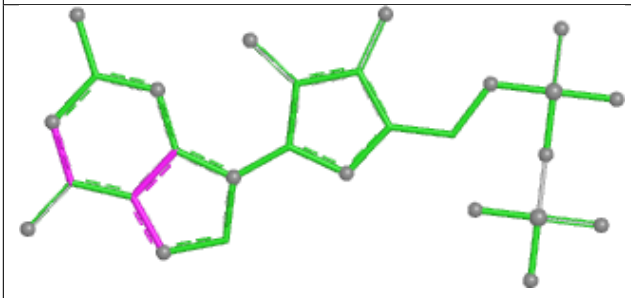


Torsions

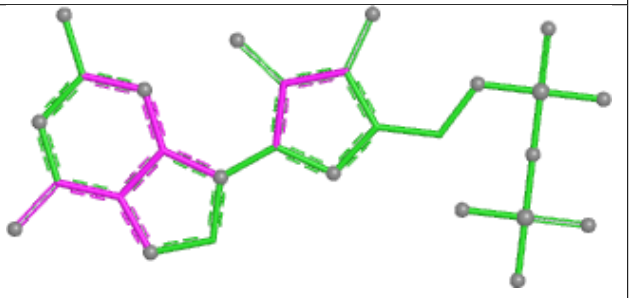


Rings

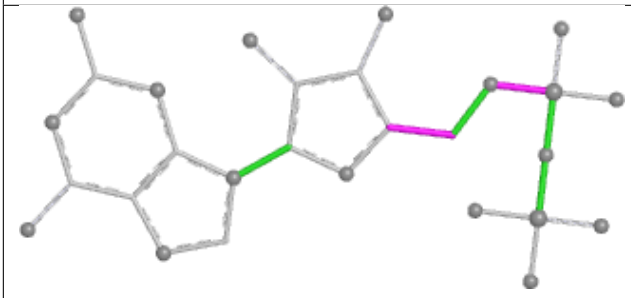
Ligand GDP RW 500



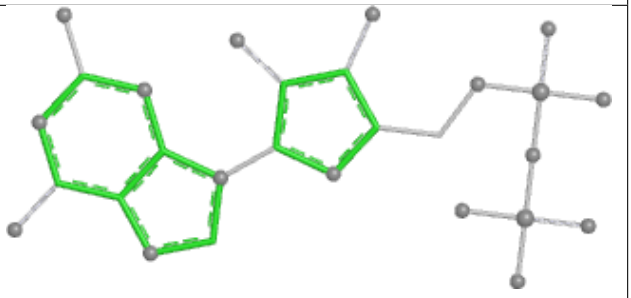
Bond lengths



Bond angles

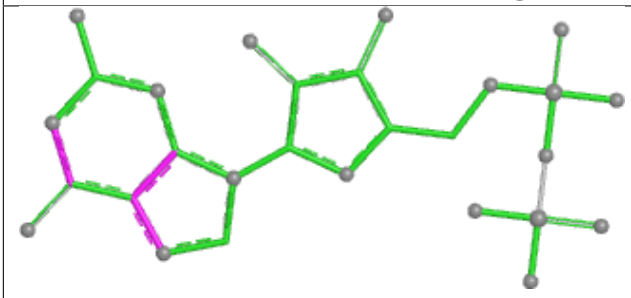


Torsions

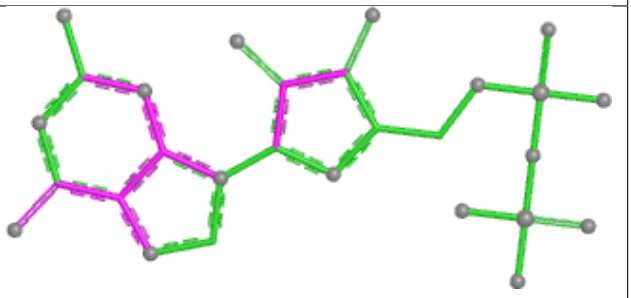


Rings

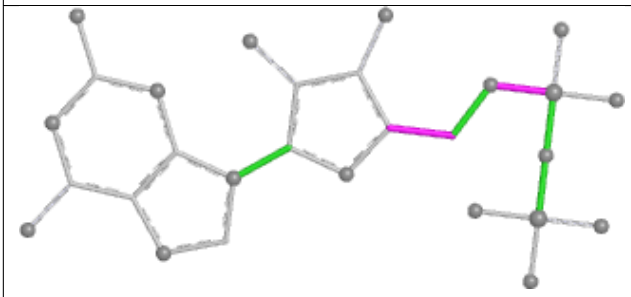
Ligand GDP PF 501



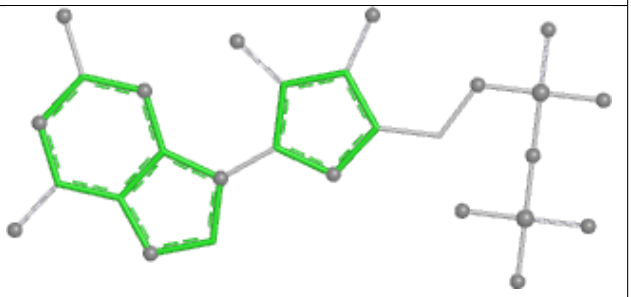
Bond lengths



Bond angles

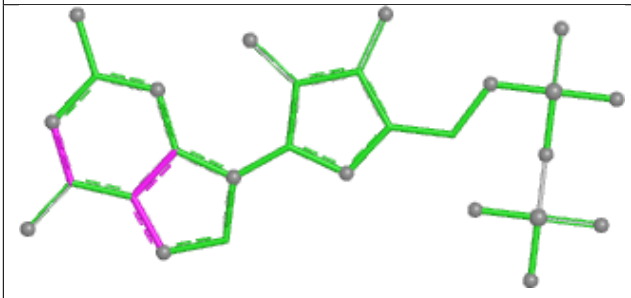


Torsions

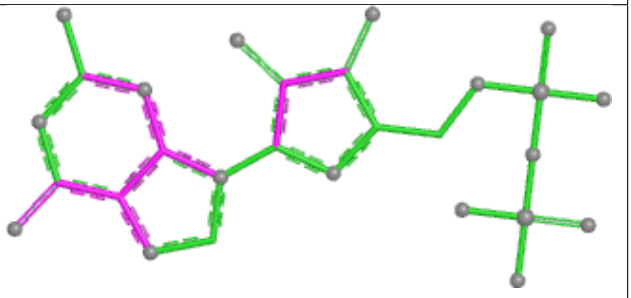


Rings

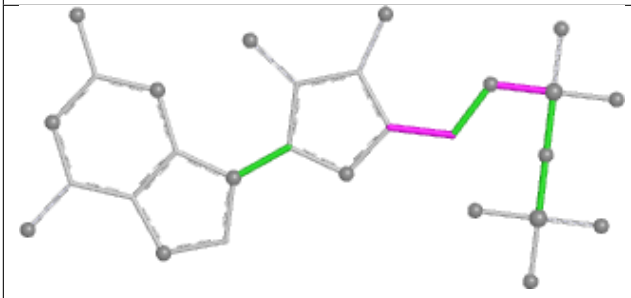
Ligand GDP GF 500



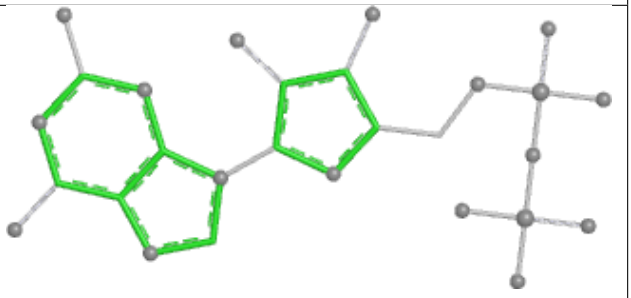
Bond lengths



Bond angles

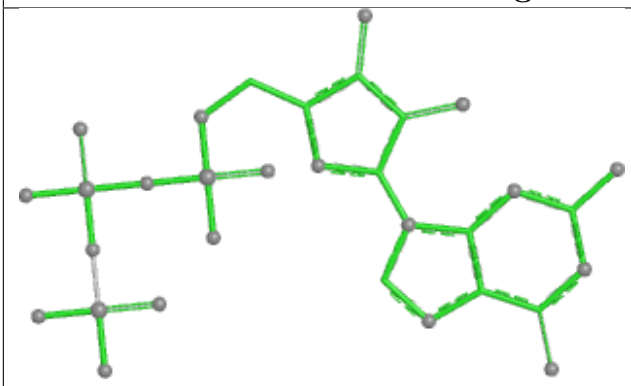


Torsions

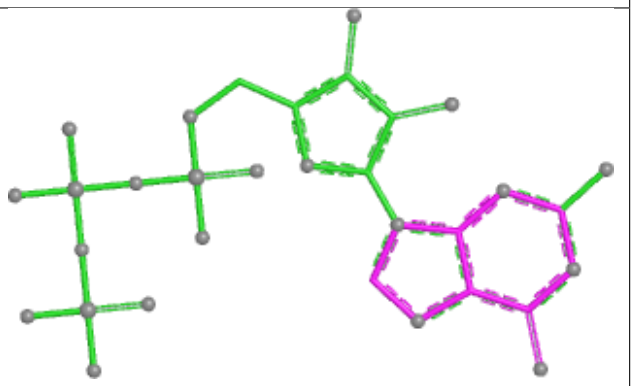


Rings

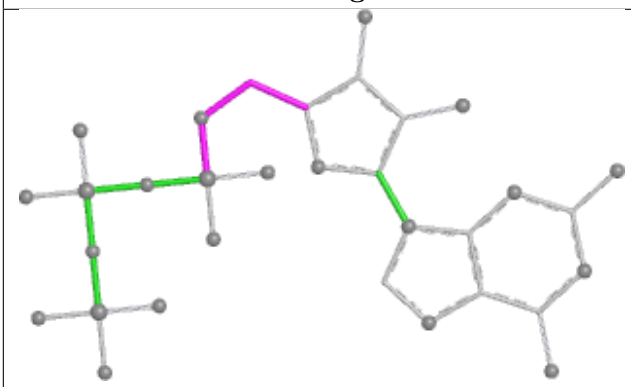
Ligand GTP FS 501



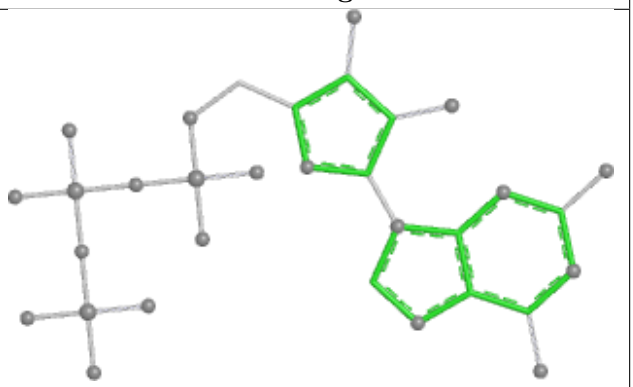
Bond lengths



Bond angles

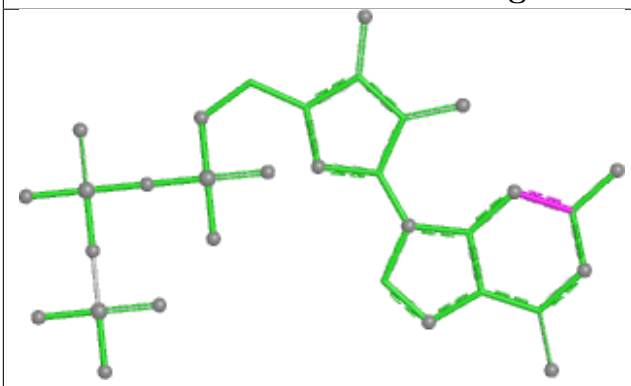


Torsions

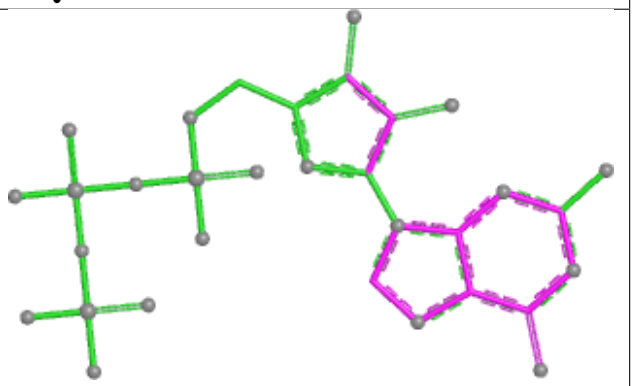


Rings

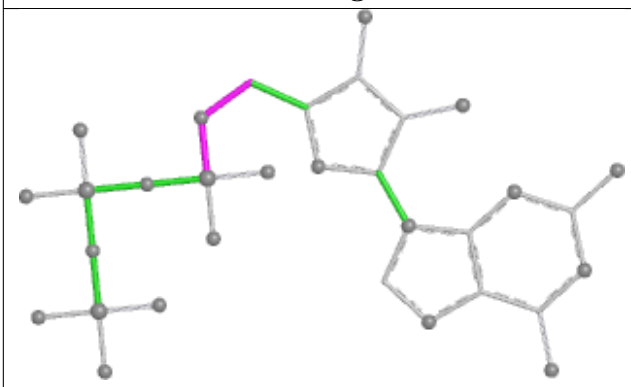
Ligand GTP QR 501



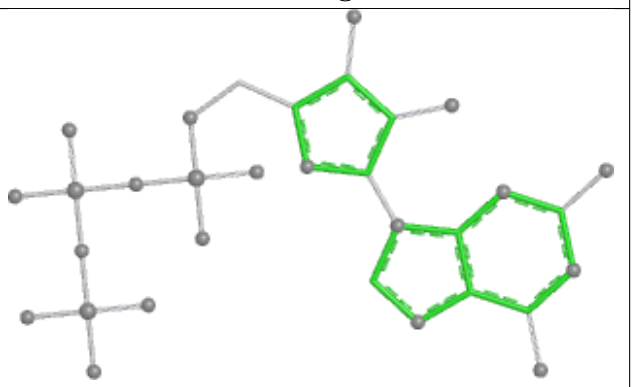
Bond lengths



Bond angles

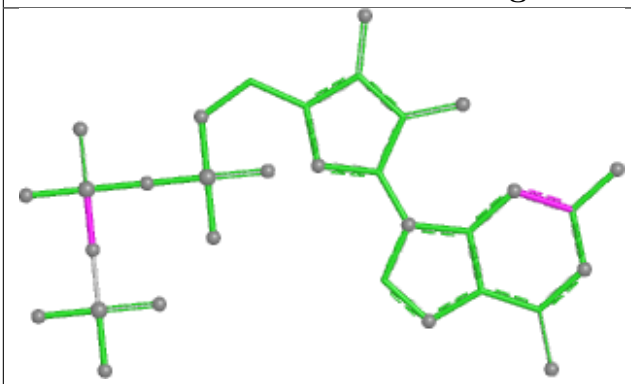


Torsions

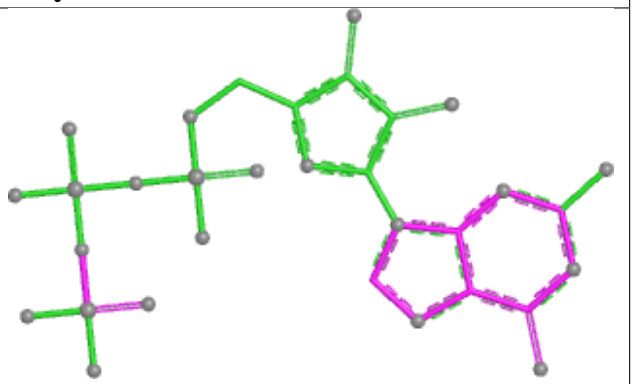


Rings

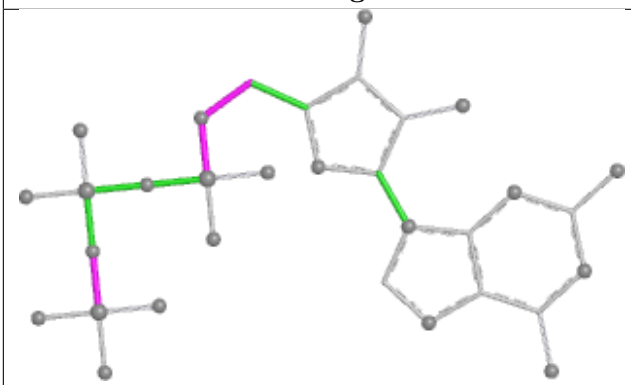
Ligand GTP QC 501



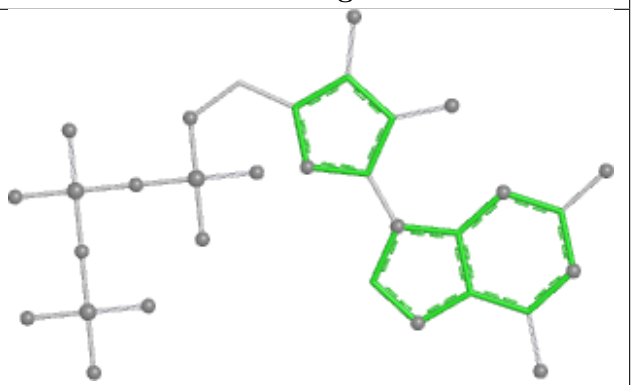
Bond lengths



Bond angles

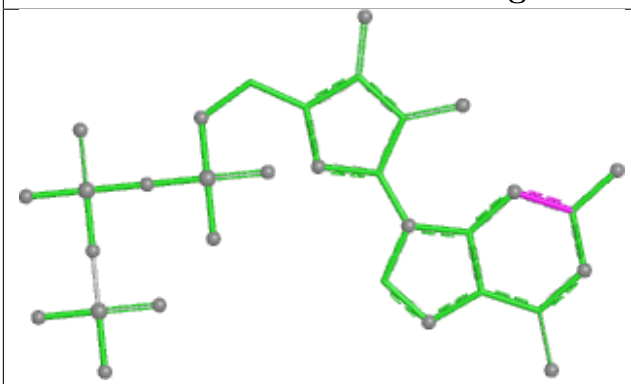


Torsions

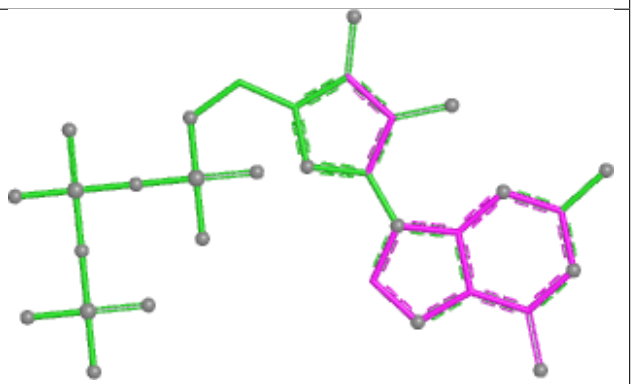


Rings

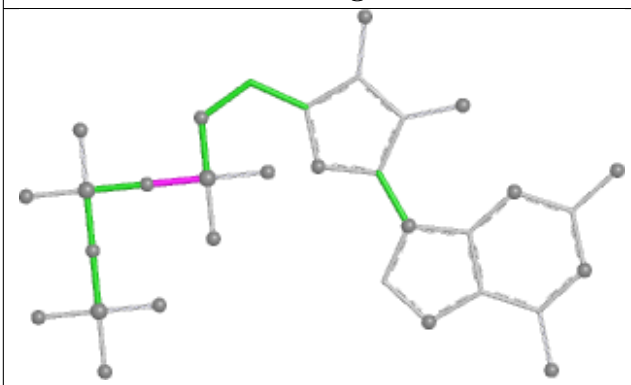
Ligand GTP BG 501



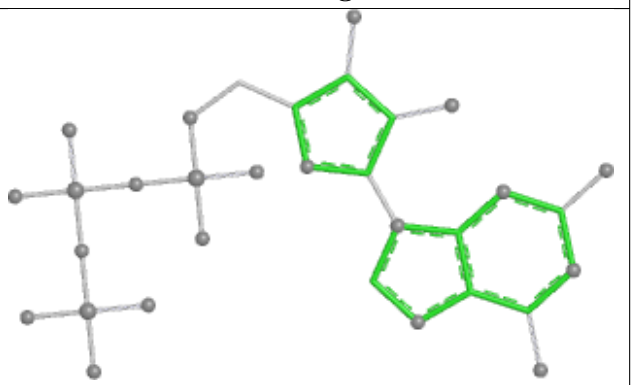
Bond lengths



Bond angles

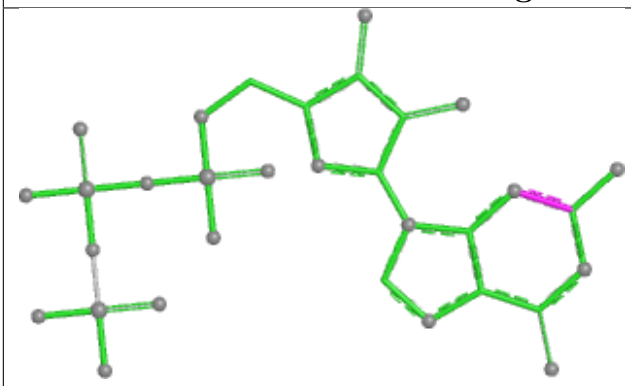


Torsions

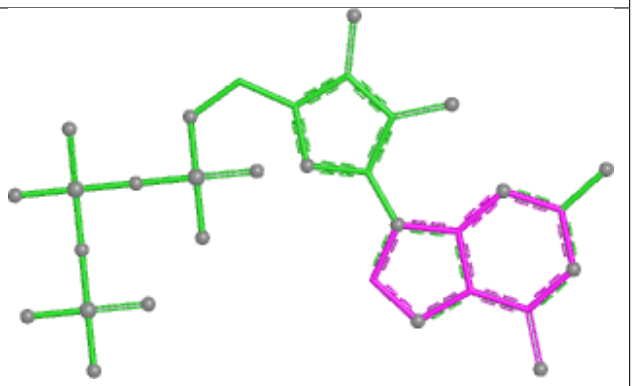


Rings

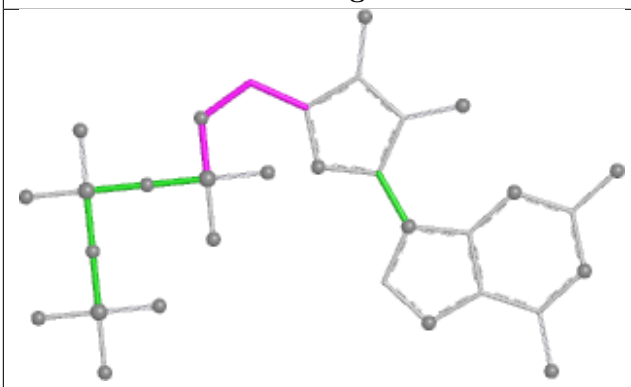
Ligand GTP FJ 503



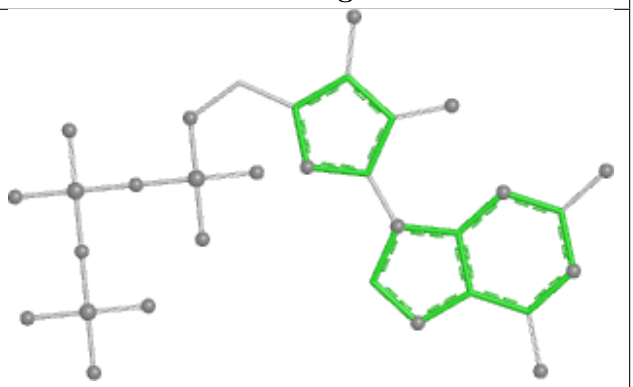
Bond lengths



Bond angles

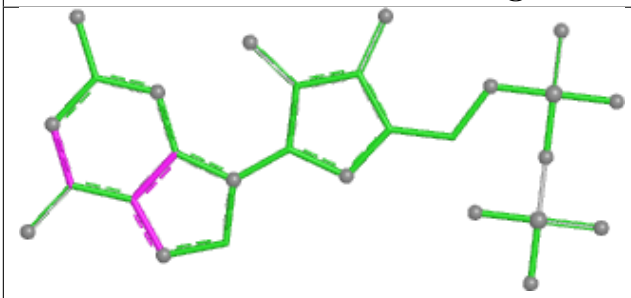


Torsions

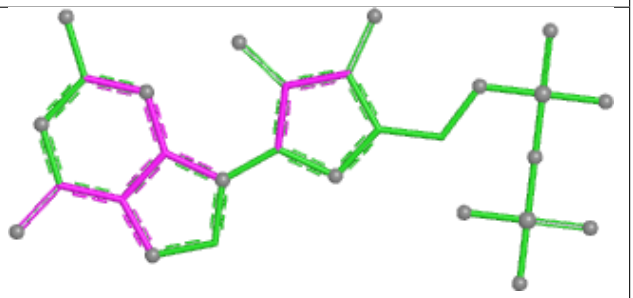


Rings

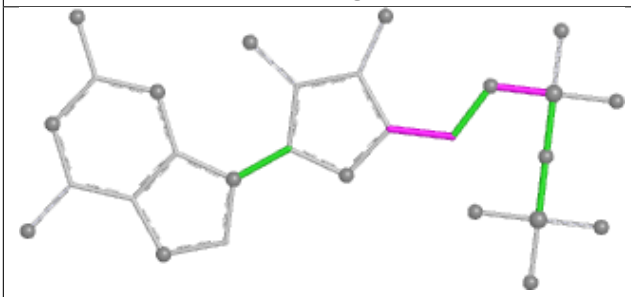
Ligand GDP RK 500



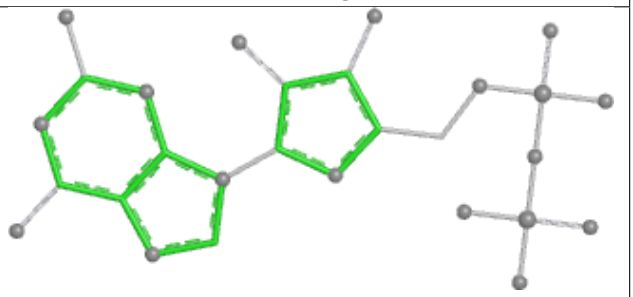
Bond lengths



Bond angles

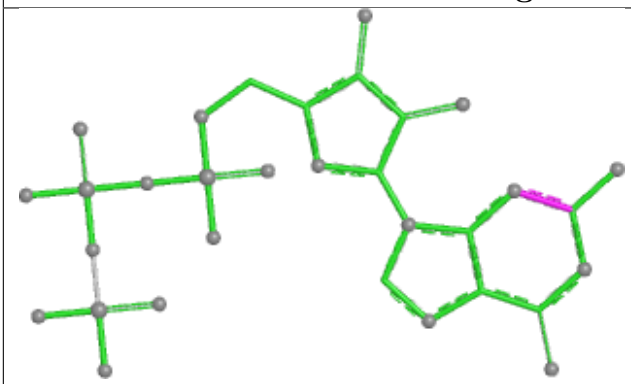


Torsions

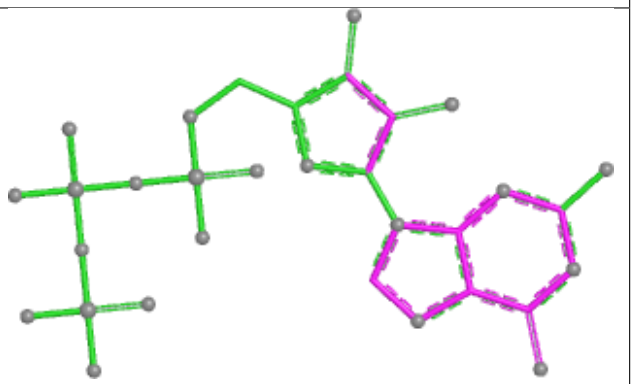


Rings

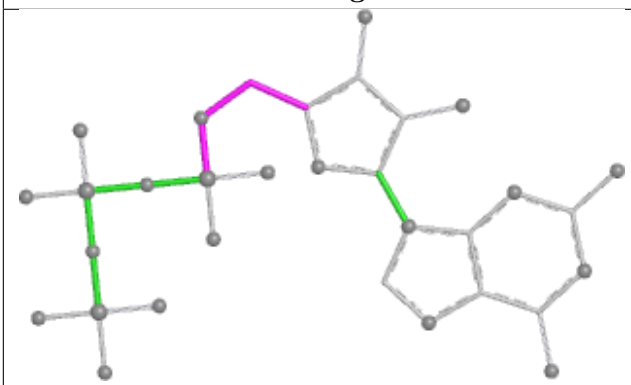
Ligand GTP OI 501



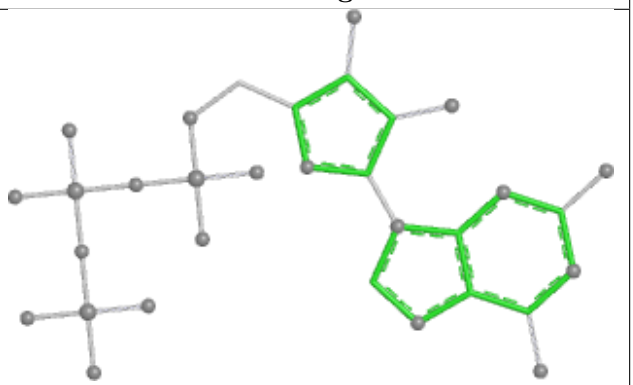
Bond lengths



Bond angles

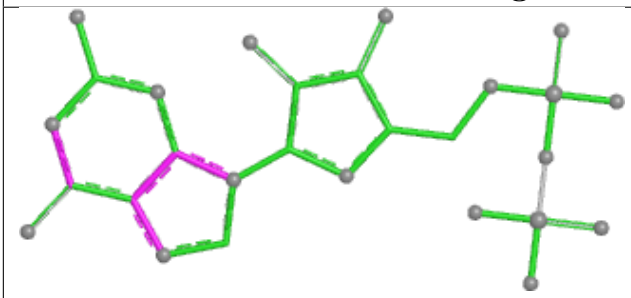


Torsions

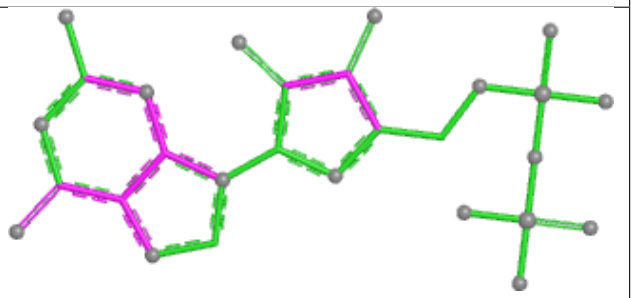


Rings

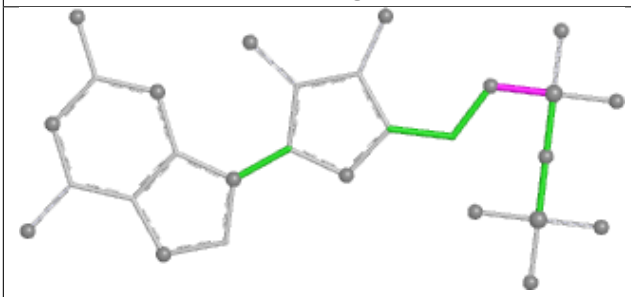
Ligand GDP FT 501



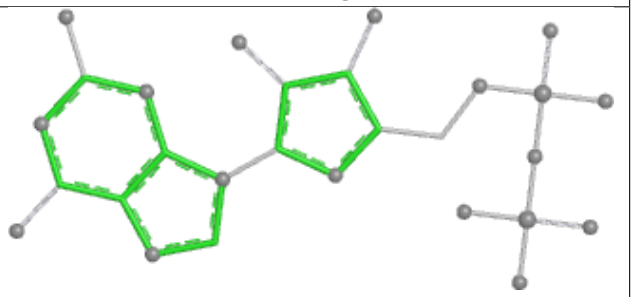
Bond lengths



Bond angles

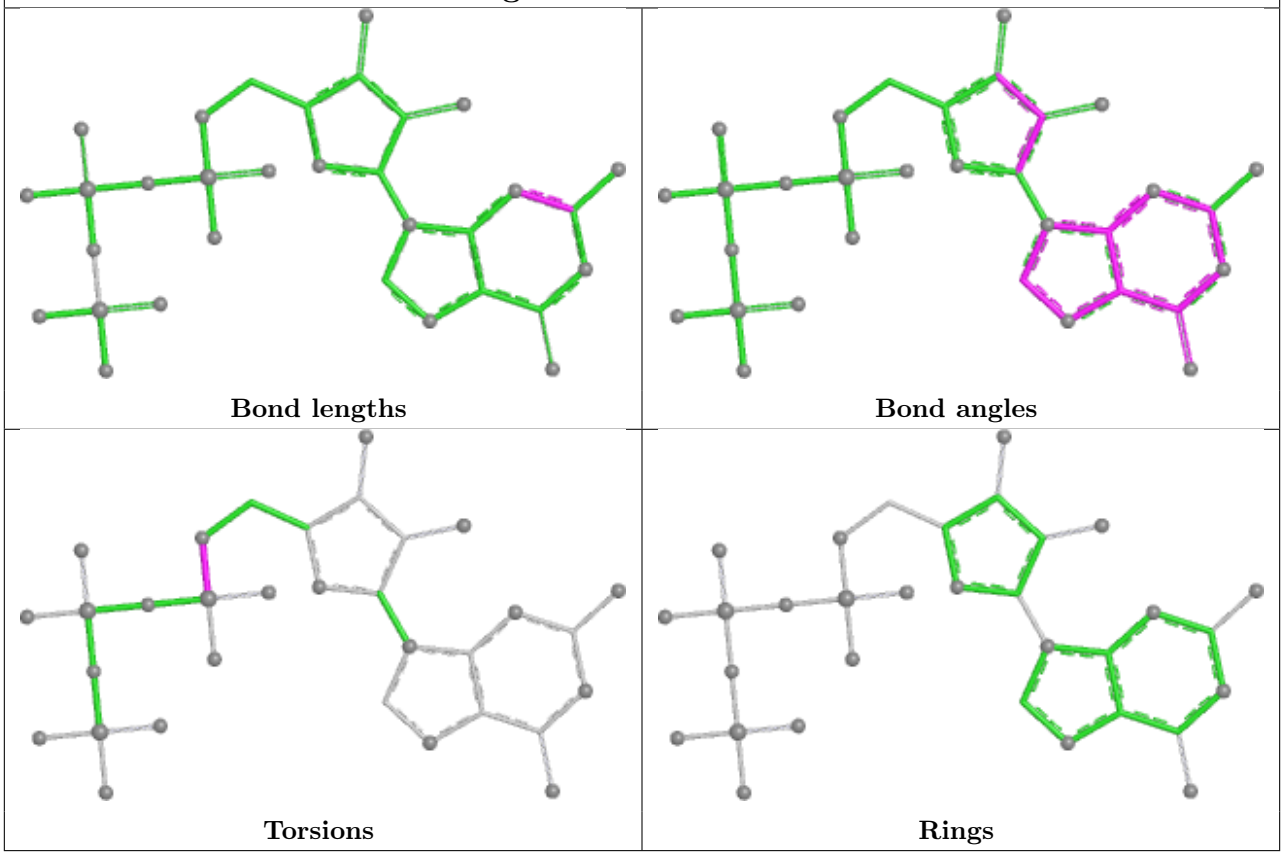


Torsions



Rings

Ligand GTP MM 501



4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
67	5Z	4
67	5Y	4
67	5X	4
67	5a	3
68	5f	2
95	6t	1
68	5c	1
68	5d	1
109	9a	1
68	5e	1
67	5W	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
83	6k	1
16	0i	1
126	9N	1
2	GU	1
2	CB	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5a	233:ASP	C	234:ASP	N	8.58
1	5Z	233:ASP	C	234:ASP	N	8.37
1	5Y	233:ASP	C	234:ASP	N	7.90
1	5X	233:ASP	C	234:ASP	N	7.70
1	5Z	496:PHE	C	497:LEU	N	7.54
1	5a	496:PHE	C	497:LEU	N	7.50
1	5X	496:PHE	C	497:LEU	N	7.34
1	5Y	496:PHE	C	497:LEU	N	6.69
1	6t	1040:LEU	C	1041:GLY	N	6.67
1	5c	1025:LYS	C	1026:SER	N	6.58
1	5d	1025:LYS	C	1026:SER	N	5.60
1	5f	1025:LYS	C	1026:SER	N	5.60
1	9a	525:GLU	C	526:TYR	N	5.23
1	5e	1025:LYS	C	1026:SER	N	4.56
1	5Y	1681:LEU	C	1682:PHE	N	3.24
1	5Z	1681:LEU	C	1682:PHE	N	3.24
1	5W	1681:LEU	C	1682:PHE	N	3.23
1	5Y	735:ARG	C	736:LEU	N	3.23
1	5X	1681:LEU	C	1682:PHE	N	3.19
1	6k	980:ILE	C	981:GLN	N	3.15
1	5X	735:ARG	C	736:LEU	N	3.14
1	5Z	735:ARG	C	736:LEU	N	3.13
1	5a	735:ARG	C	736:LEU	N	3.13
1	5f	776:GLU	C	777:GLU	N	3.08
1	0i	360:ALA	C	361:LYS	N	2.52
1	9N	124:GLU	C	125:MET	N	1.71
1	GU	173:PRO	C	174:SER	N	1.18
1	CB	173:PRO	C	174:SER	N	1.17

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-72629. 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

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

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

6 Map analysis

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

6.1 Map-value distribution

This section was not generated.

6.2 Volume estimate versus contour level

This section was not generated.

6.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

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

8 Map-model fit

This section was not generated.