Full wwPDB EM Validation Report

May 27, 2024 – 01:56 AM EDT

PDB ID	:	7SOM
EMDB ID	:	EMD-25361
Title	:	Ciliary C2 central pair apparatus isolated from Chlamydomonas reinhardtii
Authors	:	Gui, M.; Wang, X.; Dutcher, S.K.; Brown, A.; Zhang, R.
Deposited on	:	2021-11-01
Resolution	:	3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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.

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	443	5% 97% .
1	AC	443	. 97% .
1	AE	443	. 97% .
1	AG	443	. 97% .
1	AI	443	. 97% .
1	AK	443	. 97% .
1	BA	443	7% 98% .
1	BC	443	. 96% .
1	BE	443	6% 98% .
1	BG	443	. 96% .
1	BI	443	7% 98% .
1	BK	443	. 96% .
1	CA	443	. 96% .
1	CC	443	. 96% .
1	CE	443	. 96% .
1	CG	443	. 96% .
1	CI	443	. 96% .

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Mol	Chain	Length	Quality of chain
1	CK	443	96%
1	DC	443	96%
1	DE	443	96%
1	DG	443	96%
1	DI	443	96%
1	DK	443	5% 96%
1	EA	443	9% 96%
1	EC	443	6% 96%
1	EE	443	96%
1	EG	443	5% 96%
1	EI	443	5% 96%
1	EK	443	6% 96%
1	FA	443	5% 96%
1	FC	443	6% 96%
1	FE	443	96%
1	FG	443	96%
1	FI	443	96%
1	FK	443	5% 96%
1	GC	443	6% 96%
1	GE	443	5% 96%
1	GG	443	5% 96%
1	GI	443	5% 96%
1	GK	443	6% 96%
1	GM	443	7% 96%
1	HC	443	18% 96%

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Mol	Chain	Length	Quality of chain
1	HE	443	18% 96%
1	HG	443	13% 96%
1	HI	443	14% 96%
1	HK	443	16% 96%
1	HM	443	16% 96%
1	IC	443	11% 96%
1	IE	443	11% 96%
1	IG	443	10% 96%
1	II	443	10% 96%
1	IK	443	10% 96%
1	IM	443	10% 96%
1	JC	443	6% 96%
1	JE	443	96%
1	JG	443	96%
1	JI	443	96%
1	JK	443	96%
1	JM	443	5% 96%
1	KC	443	96%
1	KE	443	5% 96%
1	KG	443	96%
1	KI	443	96%
1	KK	443	5% 96%
1	LC	443	96%
1	LE	443	96%
1	LG	443	96%

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Mol	Chain	Length	Quality of chain
1	LI	443	96%
1	LK	443	6% 96%
1	MC	443	6% 97%
1	ME	443	96%
1	MG	443	97%
1	MI	443	96%
1	MK	443	6% 97%
2	AB	451	5% 96%
2	AD	451	7% 96%
2	AF	451	96%
2	AH	451	95% 5%
2	AJ	451	5% 96%
2	AL	451	6% 95% 5%
2	BB	451	7% 97%
2	BD	451	5% 95% 5%
2	BF	451	6% 97%
2	BH	451	95% 5%
2	BJ	451	8% 97%
2	BL	451	7% 95% 5%
2	CB	451	95% 5%
2	CD	451	95% 5%
2	CF	451	95% 5%
2	CH	451	95% 5%
2	CJ	451	95% 5%
2	DB	451	95% 5%

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Mol	Chain	Length	Quality of chain
2	DD	451	95% 5%
2	DF	451	95% 5%
2	DH	451	95% 5%
2	DJ	451	5% 95% 5%
2	DL	451	5% 95% 5%
2	EB	451	6% 97%
2	ED	451	8% 95% 5%
2	EF	451	5% 97%
2	EH	451	95% 5%
2	EJ	451	5% 97%
2	EL	451	7% 95% 5%
2	FB	451	6% 95% 5%
2	FD	451	5% 95% 5%
2	FF	451	95% 5%
2	FH	451	5% 95% 5%
2	FJ	451	95% 5%
2	FL	451	5% 95% 5%
2	GD	451	7% 95% 5%
2	GF	451	95% 5%
2	GH	451	6% 95% 5%
2	GJ	451	5% 95% 5%
2	GL	451	6% 95% 5%
2	HD	451	16% 95% 5%
2	HF	451	11% 95% 5%
2	HH	451	14% 95% 5%

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Mol	Chain	Length	Quality of chain
2	HJ	451	11% 95% 5%
2	HL	451	16% 95% 5%
2	ID	451	10% 95% 5%
2	IF	451	8% 95% 5%
2	IH	451	10% 95% 5%
2	IJ	451	7% 95% 5%
2	IL	451	11% 95% 5%
2	JB	451	5% 95% 5%
2	JD	451	6% 95% 5%
2	JF	451	5% 95% 5%
2	JH	451	5% 95% 5%
2	JJ	451	95% 5%
2	JL	451	5% 95% 5%
2	KB	451	5% 95% 5%
2	KD	451	7% 95% 5%
2	KF	451	95% 5%
2	KH	451	5% 95% 5%
2	KJ	451	6% 95% 5%
2	KL	451	6% 95% 5%
2	LB	451	95% 5%
2	LD	451	5% 95% 5%
2	LF	451	95% 5%
2	LH	451	6% 95% 5%
2	LJ	451	5% 95% 5%
2	LL	451	6% 95% 5%

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Mol	Chain	Length	Quality of chain
2	MB	451	7% 95% 5%
2	MD	451	8% 97%
2	MF	451	5% 95% 5%
2	MH	451	6% 98%
2	MJ	451	5% 95% 5%
2	ML	451	7% 98%
3	a	618	8% 53% 47%
3	b	618	14% 100%
3	c	618	13% 99%
3	d	618	6% 48% 52%
4	e	201	15% 93% 7%
4	f	201	13% 93% 7%
4	g	201	6% 72% 28%
5	h	758	17% 77% 23%
5	i	758	12% 77% 23%
5	j	758	16% 77% 23%
6	k	528	17% 73% 27%
6	l	528	16% 73% 27%
6	s	528	12% 54% 46%
7	m	421	15% 83% 16%
7	n	421	12% 83% 16%
7	o	421	17% 83% 16%
8	p	89	19% 99%
8	q	89	13% 99%
8	r	89	16% 99%

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Mol	Chain	Length	Quality of chain
9	A	190	23% 98%
9	B	190	17% 98%
9	C	190	28% 98%
10	P	606	50% 71% 29%
10	Q	606	36% 71% 29%
10	R	606	50% 71% 29%
10	S	606	32% 71% 29%
10	Z	606	15% 85%
10	aa	606	34% 48% 52%
10	cc	606	15% 85%
11	T	93	28% 68% 32%
11	U	93	23% 62% 38%
11	V	93	37% 72% 28%
11	W	93	25% 68% 32%
12	D	2257	20% 67% 33%
12	E	2257	20% 67% 33%
12	bb	2257	8% 92%
13	F	1074	27% 91% 9%
13	G	1074	31% 92% 8%
13	H	1074	27% 91% 9%
13	I	1074	31% 92% 8%
14	J	976	15% 68% 32%
14	K	976	14% 68% 32%
15	L	222	32% 48% 52%
15	M	222	42% 48% 52%

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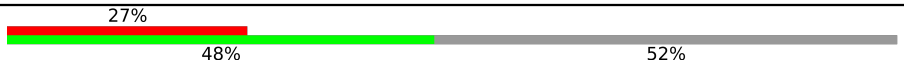
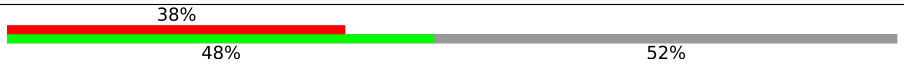
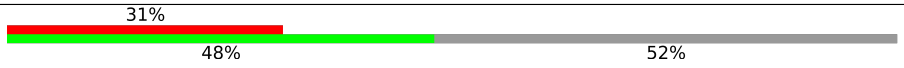
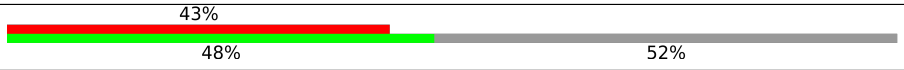
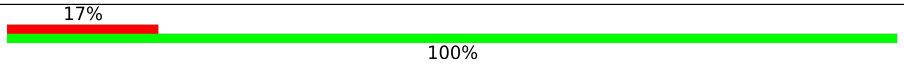
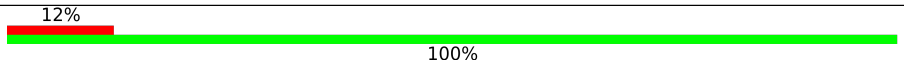
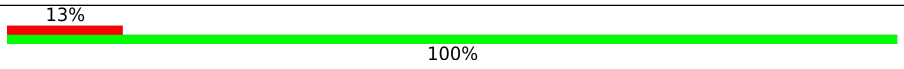
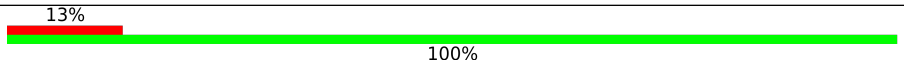
Mol	Chain	Length	Quality of chain
15	N	222	
15	O	222	
15	X	222	
15	Y	222	
16	A1	48	
17	A2	77	
17	A4	77	
18	A3	47	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 618760 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	AC	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
1	AE	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	AG	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	AI	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	AK	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	BA	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
1	BC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	BE	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
1	BG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	BI	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
1	BK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	DE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	DG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	DI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	DK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EA	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FA	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	GK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	II	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JI	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	JK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JM	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	KC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	KE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	KG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	KI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	KK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	MC	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	ME	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	MG	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	MI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	MK	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	CA	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	432	Total	C	N	O	S	0	0
			3355	2124	570	639	22		
2	AD	432	Total	C	N	O	S	0	0
			3355	2123	570	640	22		
2	AF	432	Total	C	N	O	S	0	0
			3355	2124	570	639	22		
2	AH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AJ	432	Total	C	N	O	S	0	0
			3355	2124	570	639	22		
2	AL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	BB	438	Total	C	N	O	S	0	0
			3393	2146	577	648	22		
2	BD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	BF	438	Total	C	N	O	S	0	0
			3393	2146	577	648	22		
2	BH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	BJ	438	Total	C	N	O	S	0	0
			3393	2146	577	648	22		
2	BL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	CB	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	CD	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	CF	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	CH	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	CJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	DB	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	DD	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	DF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	DH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	DJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	DL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	EB	438	Total	C	N	O	S	0	0
			3393	2146	577	648	22		
2	ED	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	EF	439	Total	C	N	O	S	0	0
			3399	2149	578	650	22		
2	EH	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	EJ	438	Total	C	N	O	S	0	0
			3393	2146	577	648	22		
2	EL	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	FB	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	HD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	HF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	HH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	HJ	428	Total	C	N	O	S	0	0
			3326	2108	566	630	22		
2	HL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	ID	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	IF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	IH	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	IJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	IL	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	JB	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	JD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	JF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	JH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	JJ	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	JL	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	KB	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	KD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	KF	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	KH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	KJ	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	KL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	LB	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	LD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	LF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	LH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	LJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	LL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	MB	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	MD	439	Total	C	N	O	S	0	0
			3399	2149	578	650	22		
2	MF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	MH	440	Total	C	N	O	S	0	0
			3404	2152	579	651	22		
2	MJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	ML	440	Total	C	N	O	S	0	0
			3404	2152	579	651	22		

- Molecule 3 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	325	Total	C	N	O	S	0	0
			2380	1491	422	453	14		
3	b	617	Total	C	N	O	S	0	0
			4537	2823	824	857	33		
3	c	617	Total	C	N	O	S	0	0
			4537	2823	824	857	33		
3	d	295	Total	C	N	O	S	0	0
			2180	1345	407	409	19		

- Molecule 4 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	186	Total	C	N	O	S	0	0
			1464	886	289	286	3		
4	f	186	Total	C	N	O	S	0	0
			1464	886	289	286	3		
4	g	145	Total	C	N	O	S	0	0
			1136	690	220	223	3		

- Molecule 5 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	585	Total	C	N	O	S	0	0
			4525	2788	856	866	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	i	585	Total	C	N	O	S	0	0
			4525	2788	856	866	15		
5	j	585	Total	C	N	O	S	0	0
			4525	2788	856	866	15		

- Molecule 6 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	388	Total	C	N	O	S	0	0
			3017	1857	582	572	6		
6	l	388	Total	C	N	O	S	0	0
			3017	1857	582	572	6		
6	s	285	Total	C	N	O	S	0	0
			2208	1369	420	415	4		

- Molecule 7 is a protein called FAP65.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	m	352	Total	C	N	O	S	0	0
			2737	1685	532	512	8		
7	n	352	Total	C	N	O	S	0	0
			2737	1685	532	512	8		
7	o	352	Total	C	N	O	S	0	0
			2737	1685	532	512	8		

- Molecule 8 is a protein called FAP70.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	88	Total	C	N	O	S	0	0
			698	432	135	129	2		
8	q	88	Total	C	N	O	S	0	0
			698	432	135	129	2		
8	r	88	Total	C	N	O	S	0	0
			698	432	135	129	2		

- Molecule 9 is a protein called FAP147.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	186	Total	C	N	O	S	0	0
			1530	982	266	275	7		
9	B	186	Total	C	N	O	S	0	0
			1530	982	266	275	7		

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Mol	Chain	Residues	Atoms	AltConf	Trace
9	C	186	Total C N O S 1530 982 266 275 7	0	0

- Molecule 10 is a protein called FAP178.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	P	433	Total C N O S 2493 1507 495 486 5	0	0
10	Q	432	Total C N O S 2488 1504 494 485 5	0	0
10	R	433	Total C N O S 2493 1507 495 486 5	0	0
10	S	432	Total C N O S 2488 1504 494 485 5	0	0
10	aa	292	Total C N O 1435 850 292 293	0	0
10	cc	89	Total C N O S 758 475 147 131 5	0	0
10	Z	92	Total C N O S 775 486 150 134 5	0	0

- Molecule 11 is a protein called Flagellar WD repeat-containing protein Pf20.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	T	63	Total C N O 312 186 63 63	0	0
11	U	58	Total C N O 287 171 58 58	0	0
11	V	67	Total C N O 332 198 67 67	0	0
11	W	63	Total C N O 312 186 63 63	0	0

- Molecule 12 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	bb	175	Total C N O S 1065 650 211 202 2	0	0
12	D	1516	Total C N O 7474 4442 1516 1516	0	0
12	E	1516	Total C N O 7474 4442 1516 1516	0	0

- Molecule 13 is a protein called FAP196.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	F	982	Total 4832	C 2868	N 982	O 982	0	0
13	G	993	Total 4884	C 2898	N 993	O 993	0	0
13	H	982	Total 4832	C 2868	N 982	O 982	0	0
13	I	993	Total 4884	C 2898	N 993	O 993	0	0

- Molecule 14 is a protein called FAP213.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	666	Total 3874	C 2350	N 768	O 752	S 4	0	0
14	K	666	Total 3874	C 2350	N 768	O 752	S 4	0	0

- Molecule 15 is a protein called FAP225.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	107	Total 841	C 534	N 154	O 149	S 4	0	0
15	Y	107	Total 841	C 534	N 154	O 149	S 4	0	0
15	L	107	Total 841	C 534	N 154	O 149	S 4	0	0
15	M	107	Total 841	C 534	N 154	O 149	S 4	0	0
15	N	107	Total 841	C 534	N 154	O 149	S 4	0	0
15	X	107	Total 841	C 534	N 154	O 149	S 4	0	0

- Molecule 16 is a protein called FAP239.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	A1	48	Total 240	C 144	N 48	O 48	0	0

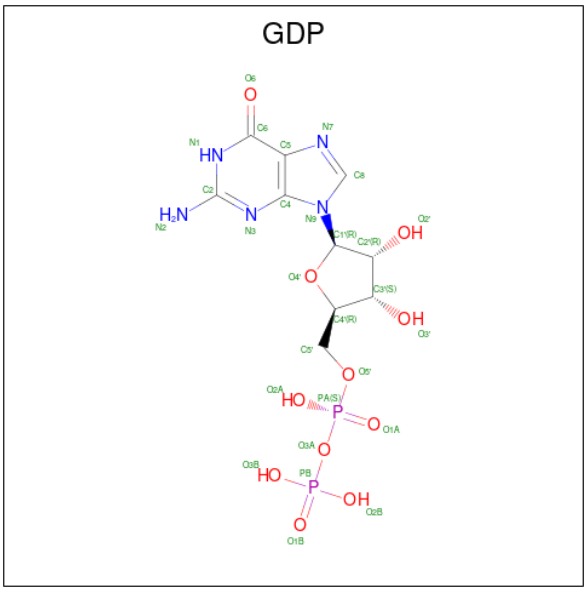
- Molecule 17 is a protein called FAP388.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	A2	77	Total 385	C 231	N 77	O 77	0	0
17	A4	77	Total 385	C 231	N 77	O 77	0	0

- Molecule 18 is a protein called FAP424.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	A3	47	Total 235	C 141	N 47	O 47	0	0

- Molecule 19 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
19	AA	1	Total 28	C 10	N 5	O 11	P 2	0
19	AC	1	Total 28	C 10	N 5	O 11	P 2	0
19	AE	1	Total 28	C 10	N 5	O 11	P 2	0
19	AG	1	Total 28	C 10	N 5	O 11	P 2	0
19	AI	1	Total 28	C 10	N 5	O 11	P 2	0
19	AK	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
19	BA	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	BC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	BE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	BG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	BI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	BK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	CC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	CE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	CG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	CI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	CK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	DE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	DG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	DI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	DK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	EA	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	EC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	EE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	EG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	EI	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
19	EK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	FA	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	FC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	FE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	FG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	FI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	FK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	GC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	GE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	GG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	GI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	GK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	GM	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	HC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	HE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	HG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	HI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	HK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	HM	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	IC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	IE	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
19	IG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	II	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	IK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	IM	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	JC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	JE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	JG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	JI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	JK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	JM	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	KC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	KE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	KG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	KI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	KK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	LC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	LE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	LG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	LI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	LK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	MC	1	Total	C	N	O	P	0
			28	10	5	11	2	

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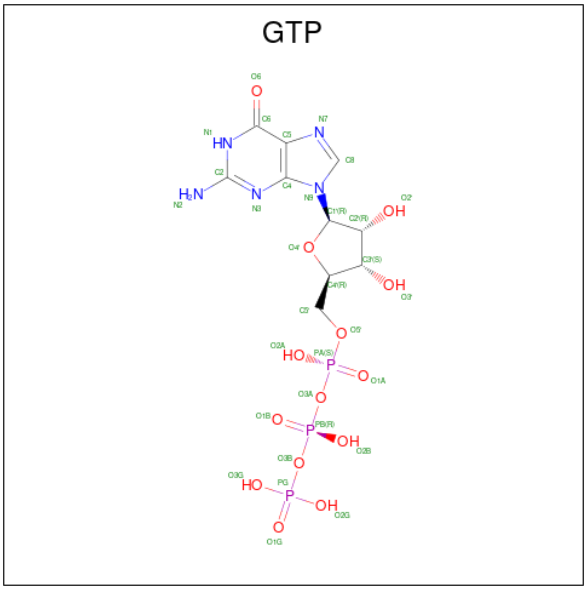
Mol	Chain	Residues	Atoms					AltConf
19	ME	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	MG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	MI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	MK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	CA	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 20 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
20	AB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AL	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
20	BB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	BD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	BF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	BH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	BJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	BL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	CB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	CD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	CF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	CJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	DB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	DD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	DF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	DH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	DJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	DL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	EB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	ED	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	EF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	EH	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
20	EJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	EL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	FB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	FD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	FF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	FH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	FJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	FL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	GD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	GF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	GH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	GJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	GL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	HD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	HF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	HI	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	HJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	HL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	ID	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	IF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	IH	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
20	IJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	IL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	JB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	JD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	JF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	JH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	JJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	JL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	KB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	KD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	KF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	KH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	KJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	KL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	LB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	LD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	LF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	LH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	LJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	LL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	MB	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
20	MD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	MF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	MH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	MJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	ML	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	AB	1	Total	Mg	0
			1	1	
21	AD	1	Total	Mg	0
			1	1	
21	AF	1	Total	Mg	0
			1	1	
21	AH	1	Total	Mg	0
			1	1	
21	AJ	1	Total	Mg	0
			1	1	
21	AL	1	Total	Mg	0
			1	1	
21	BB	1	Total	Mg	0
			1	1	
21	BD	1	Total	Mg	0
			1	1	
21	BF	1	Total	Mg	0
			1	1	
21	BH	1	Total	Mg	0
			1	1	
21	BJ	1	Total	Mg	0
			1	1	
21	BL	1	Total	Mg	0
			1	1	
21	CB	1	Total	Mg	0
			1	1	
21	CD	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
21	CF	1	Total Mg 1 1	0
21	CH	1	Total Mg 1 1	0
21	CJ	1	Total Mg 1 1	0
21	DB	1	Total Mg 1 1	0
21	DD	1	Total Mg 1 1	0
21	DF	1	Total Mg 1 1	0
21	DH	1	Total Mg 1 1	0
21	DJ	1	Total Mg 1 1	0
21	DL	1	Total Mg 1 1	0
21	EB	1	Total Mg 1 1	0
21	EE	1	Total Mg 1 1	0
21	EF	1	Total Mg 1 1	0
21	EH	1	Total Mg 1 1	0
21	EJ	1	Total Mg 1 1	0
21	EL	1	Total Mg 1 1	0
21	FB	1	Total Mg 1 1	0
21	FD	1	Total Mg 1 1	0
21	FF	1	Total Mg 1 1	0
21	FH	1	Total Mg 1 1	0
21	FJ	1	Total Mg 1 1	0
21	FL	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
21	GD	1	Total Mg 1 1	0
21	GF	1	Total Mg 1 1	0
21	GH	1	Total Mg 1 1	0
21	GJ	1	Total Mg 1 1	0
21	GL	1	Total Mg 1 1	0
21	HD	1	Total Mg 1 1	0
21	HF	1	Total Mg 1 1	0
21	HH	1	Total Mg 1 1	0
21	HJ	1	Total Mg 1 1	0
21	HL	1	Total Mg 1 1	0
21	ID	1	Total Mg 1 1	0
21	IF	1	Total Mg 1 1	0
21	IH	1	Total Mg 1 1	0
21	IJ	1	Total Mg 1 1	0
21	IL	1	Total Mg 1 1	0
21	JB	1	Total Mg 1 1	0
21	JD	1	Total Mg 1 1	0
21	JF	1	Total Mg 1 1	0
21	JH	1	Total Mg 1 1	0
21	JJ	1	Total Mg 1 1	0
21	JL	1	Total Mg 1 1	0

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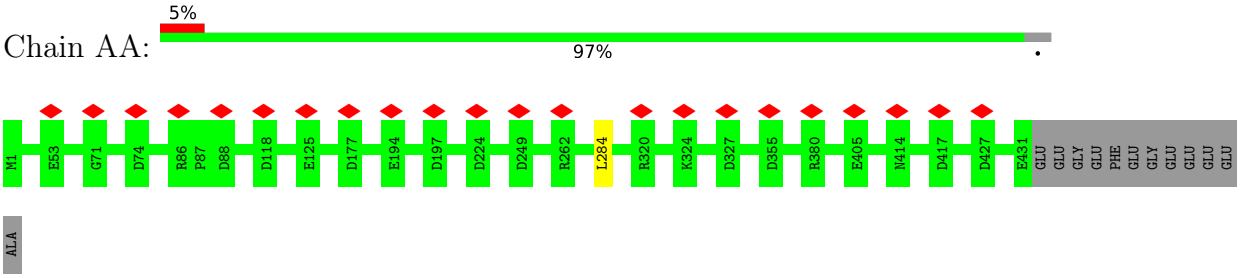
Mol	Chain	Residues	Atoms	AltConf
21	KB	1	Total Mg 1 1	0
21	KD	1	Total Mg 1 1	0
21	KF	1	Total Mg 1 1	0
21	KI	1	Total Mg 1 1	0
21	KJ	1	Total Mg 1 1	0
21	KL	1	Total Mg 1 1	0
21	LB	1	Total Mg 1 1	0
21	LD	1	Total Mg 1 1	0
21	LF	1	Total Mg 1 1	0
21	LH	1	Total Mg 1 1	0
21	LJ	1	Total Mg 1 1	0
21	LL	1	Total Mg 1 1	0
21	MB	1	Total Mg 1 1	0
21	MD	1	Total Mg 1 1	0
21	MF	1	Total Mg 1 1	0
21	MH	1	Total Mg 1 1	0
21	MJ	1	Total Mg 1 1	0
21	ML	1	Total Mg 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

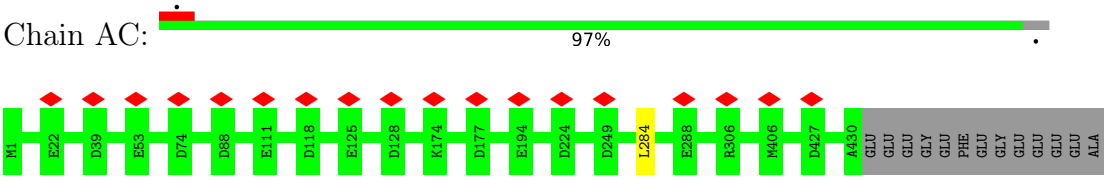
• Molecule 1: Tubulin beta

Chain AA:



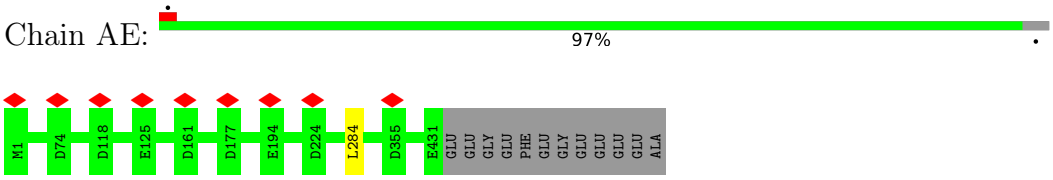
• Molecule 1: Tubulin beta

Chain AC:



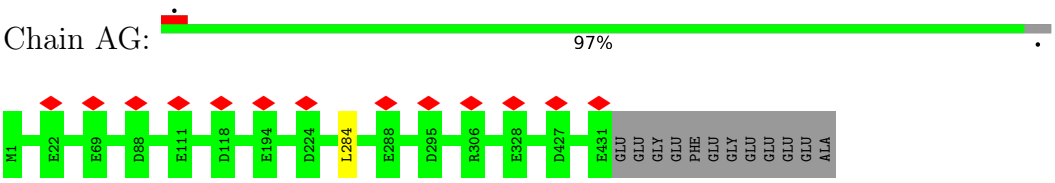
• Molecule 1: Tubulin beta

Chain AE:



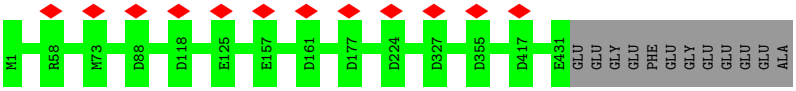
• Molecule 1: Tubulin beta

Chain AG:



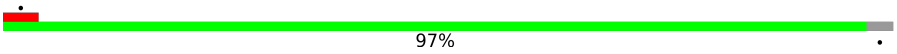
• Molecule 1: Tubulin beta

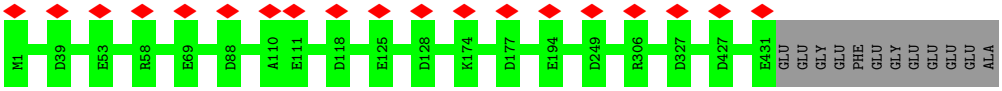
Chain AI:



• Molecule 1: Tubulin beta

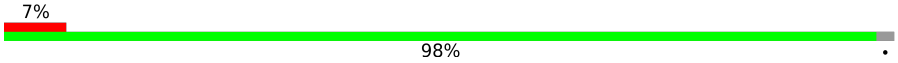
Chain AK:

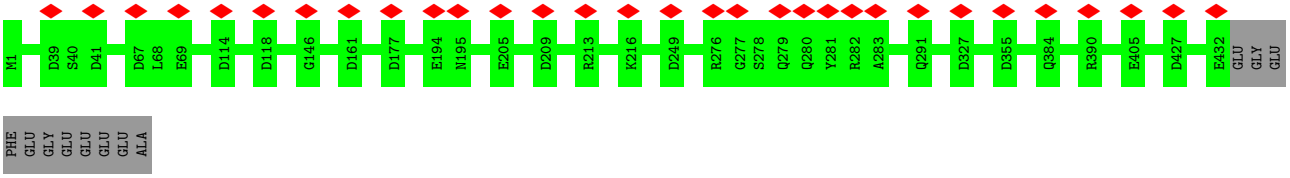




• Molecule 1: Tubulin beta

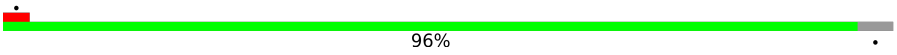
Chain BA:

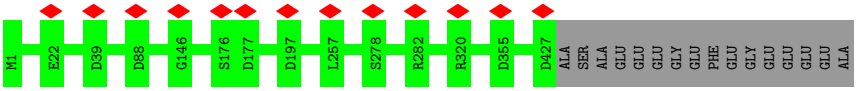




• Molecule 1: Tubulin beta

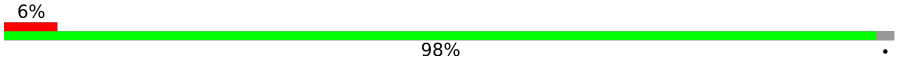
Chain BC:

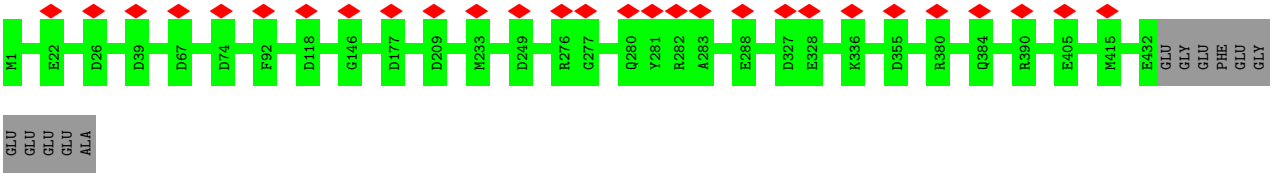




• Molecule 1: Tubulin beta

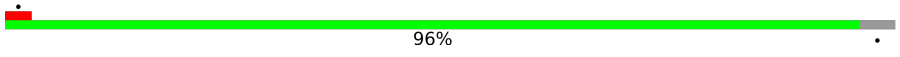
Chain BE:

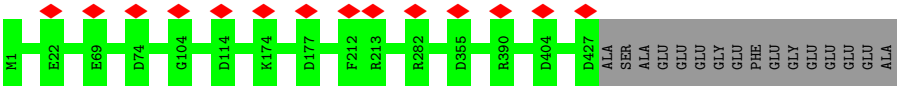




• Molecule 1: Tubulin beta

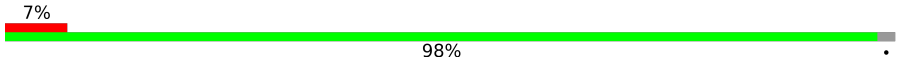
Chain BG:

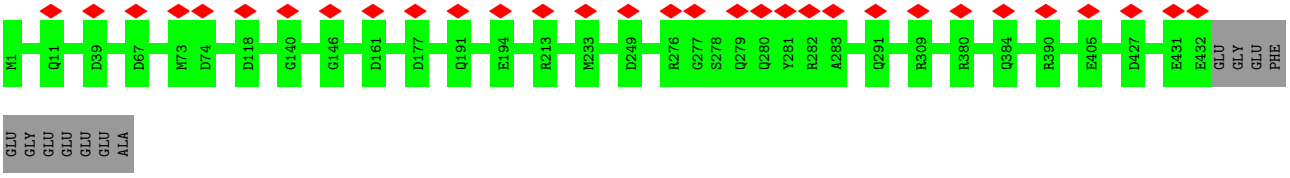




• Molecule 1: Tubulin beta

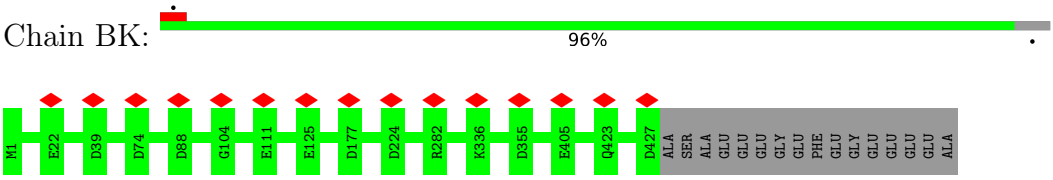
Chain BI:





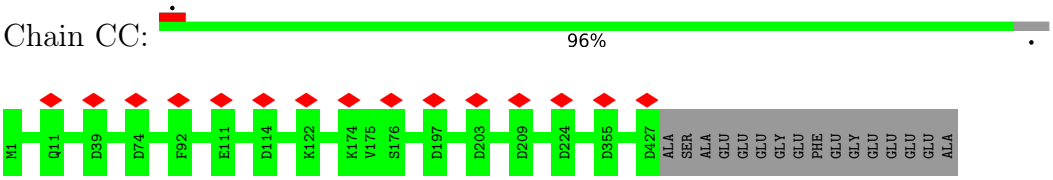
• Molecule 1: Tubulin beta

Chain BK:



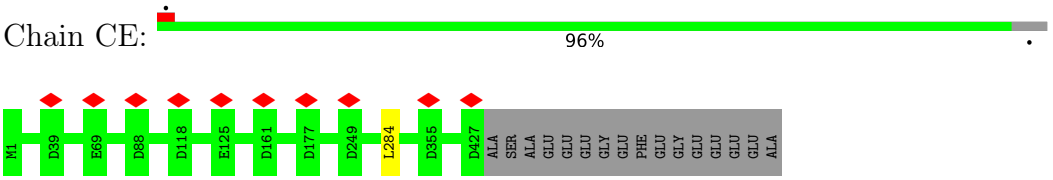
• Molecule 1: Tubulin beta

Chain CC:



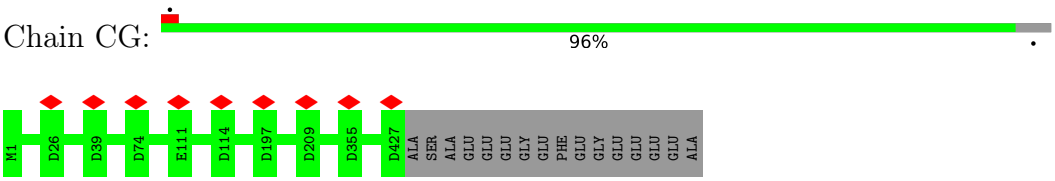
• Molecule 1: Tubulin beta

Chain CE:



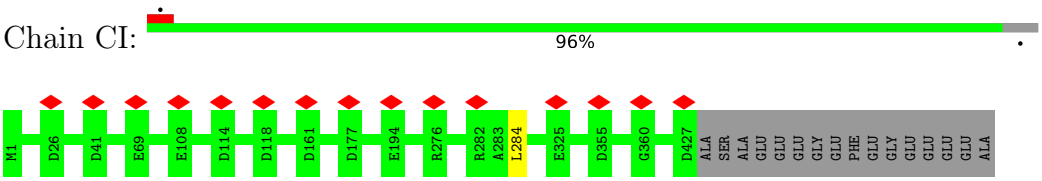
• Molecule 1: Tubulin beta

Chain CG:



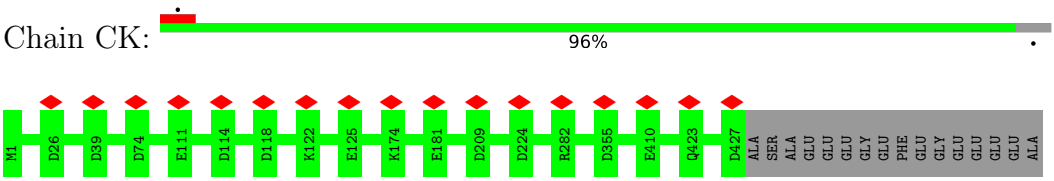
• Molecule 1: Tubulin beta

Chain CI:



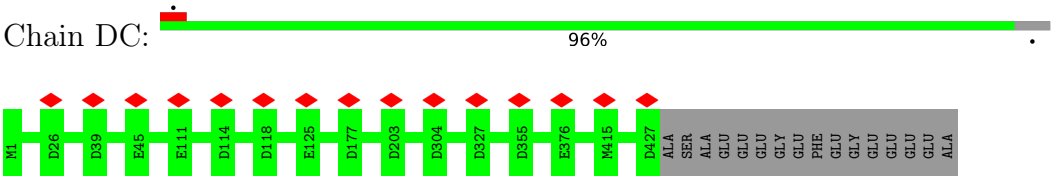
• Molecule 1: Tubulin beta

Chain CK:



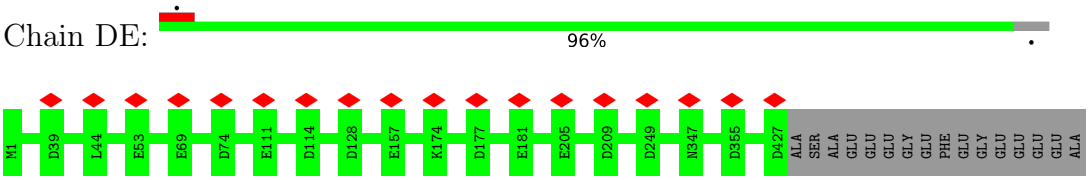
• Molecule 1: Tubulin beta

Chain DC:



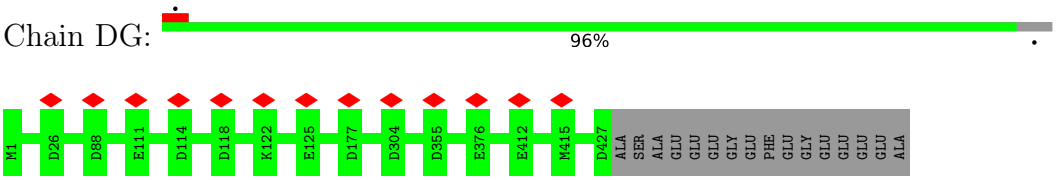
• Molecule 1: Tubulin beta

Chain DE:



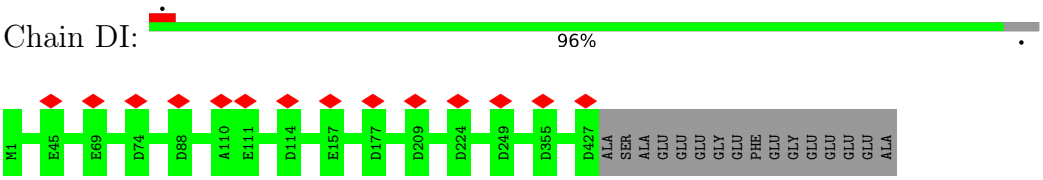
• Molecule 1: Tubulin beta

Chain DG:



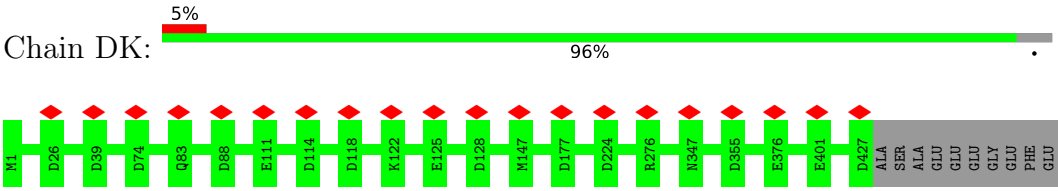
• Molecule 1: Tubulin beta

Chain DI:



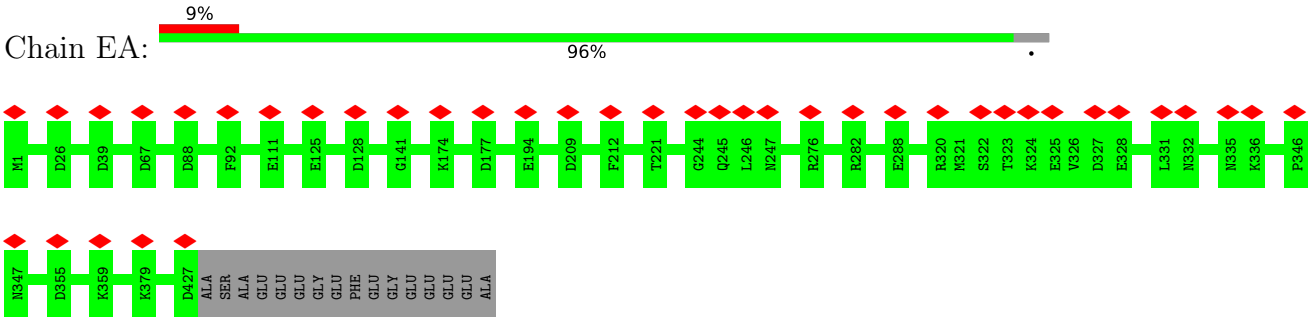
• Molecule 1: Tubulin beta

Chain DK:



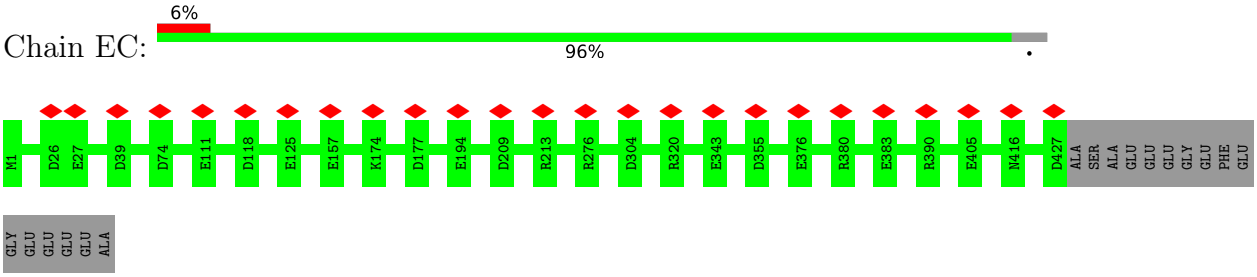
• Molecule 1: Tubulin beta

Chain EA:



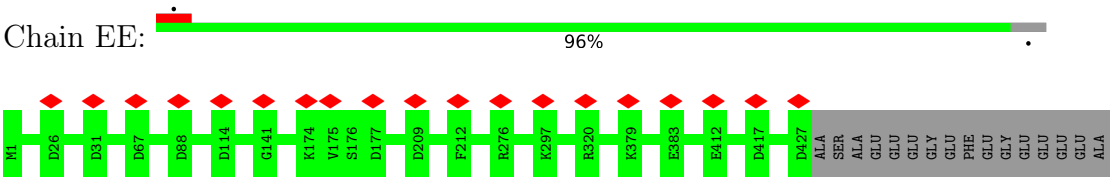
• Molecule 1: Tubulin beta

Chain EC:



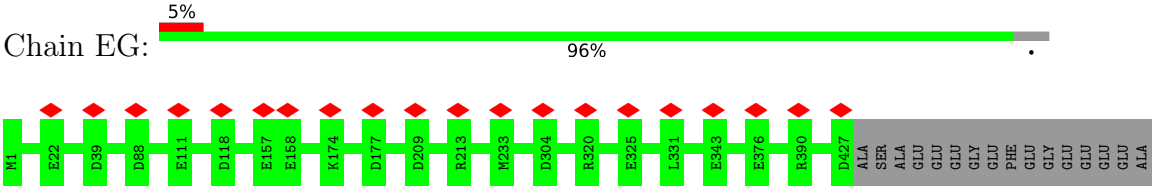
• Molecule 1: Tubulin beta

Chain EE:



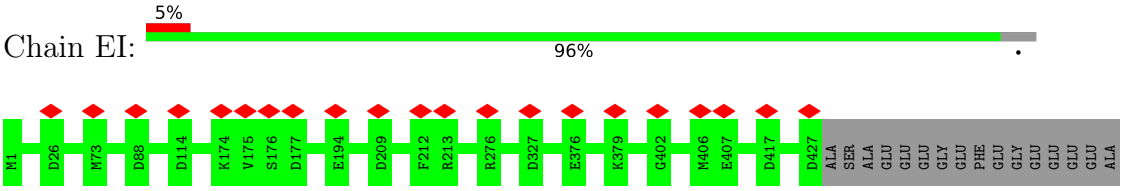
• Molecule 1: Tubulin beta

Chain EG:



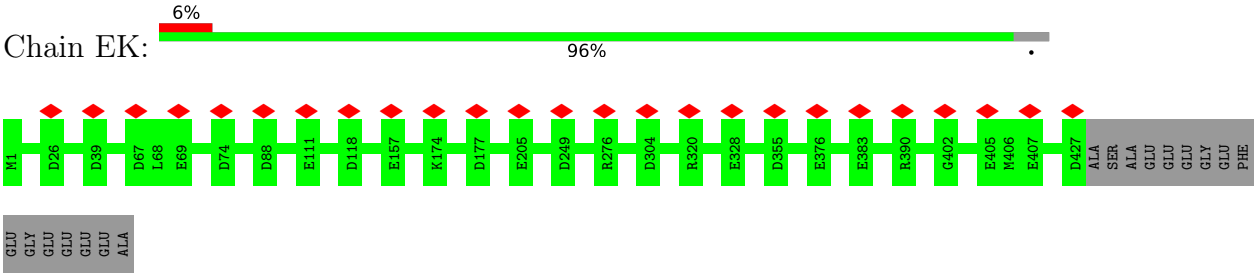
• Molecule 1: Tubulin beta

Chain EI:



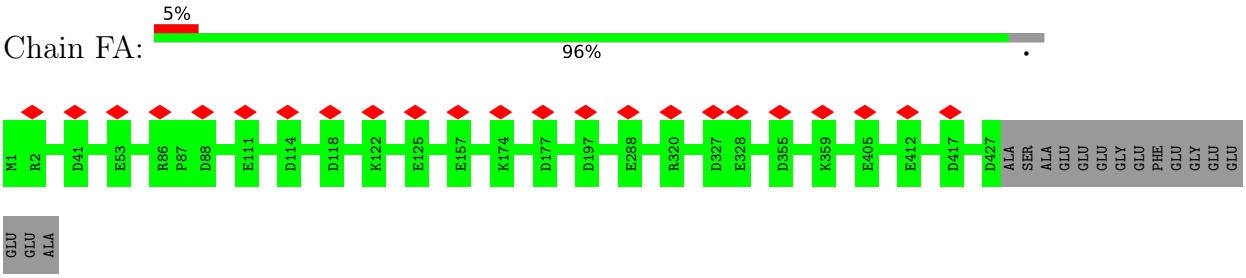
• Molecule 1: Tubulin beta

Chain EK:



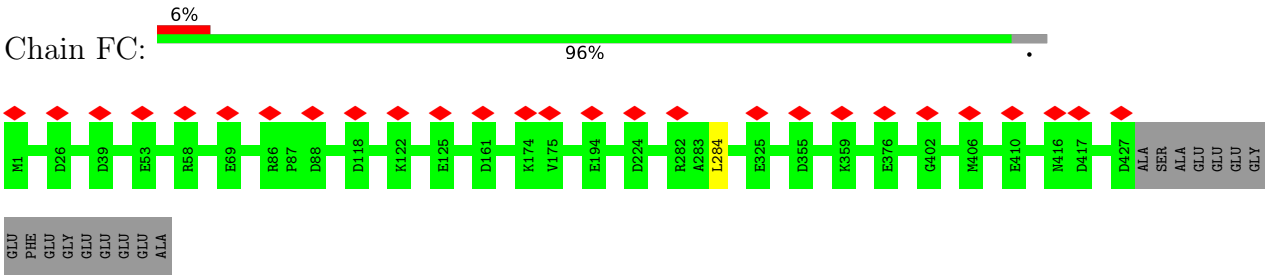
• Molecule 1: Tubulin beta

Chain FA:



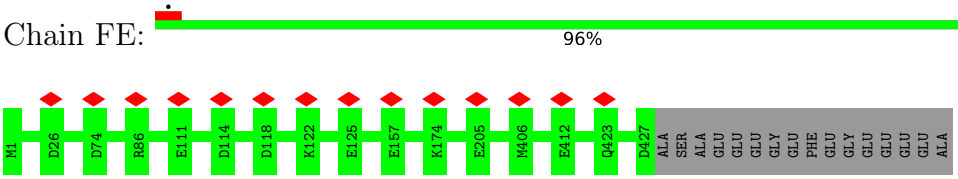
• Molecule 1: Tubulin beta

Chain FC:



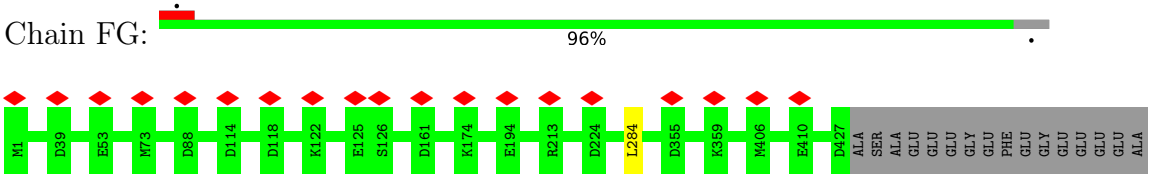
• Molecule 1: Tubulin beta

Chain FE:



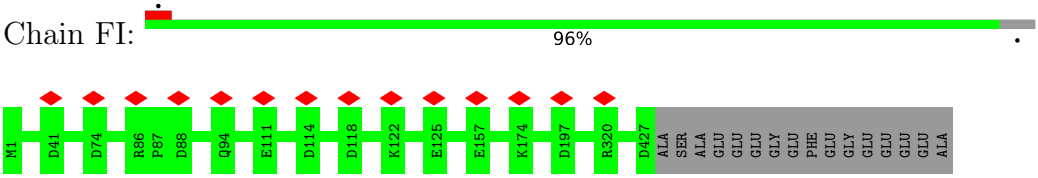
• Molecule 1: Tubulin beta

Chain FG:



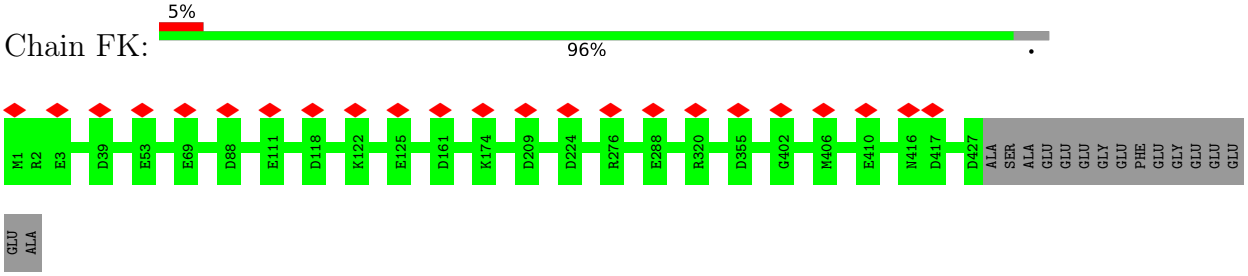
• Molecule 1: Tubulin beta

Chain FI:



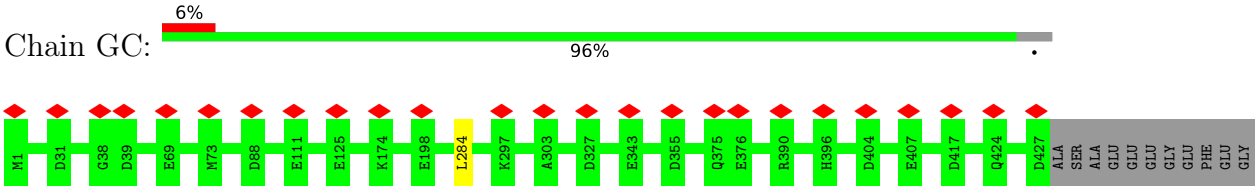
• Molecule 1: Tubulin beta

Chain FK:



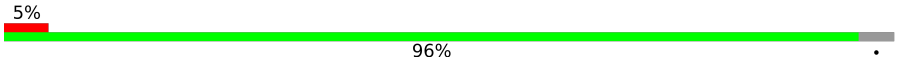
• Molecule 1: Tubulin beta

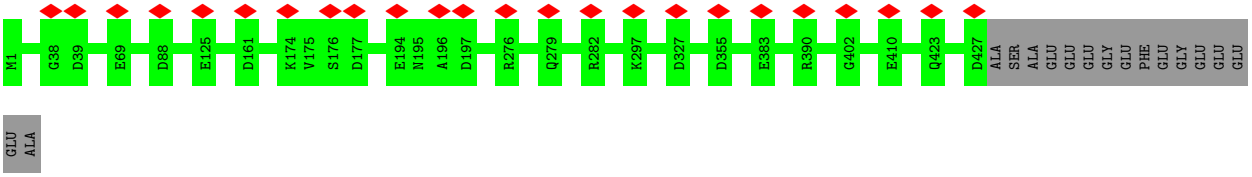
Chain GC:



• Molecule 1: Tubulin beta

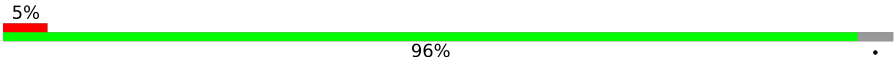
Chain GE:

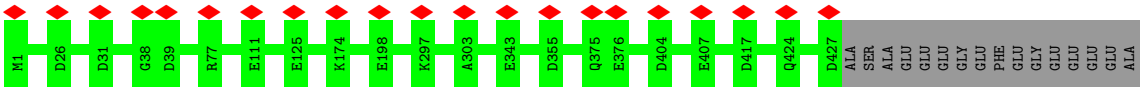




• Molecule 1: Tubulin beta

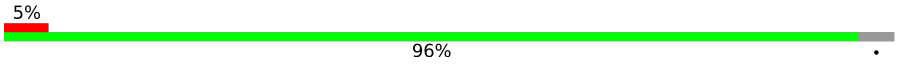
Chain GG:

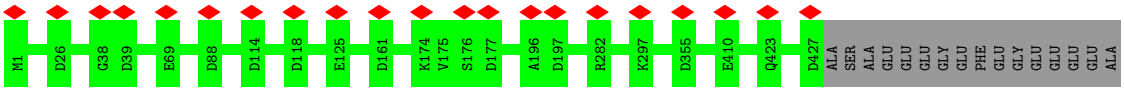




• Molecule 1: Tubulin beta

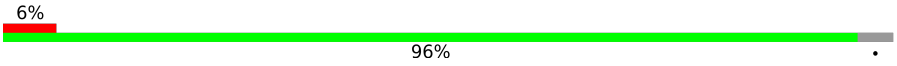
Chain GI:

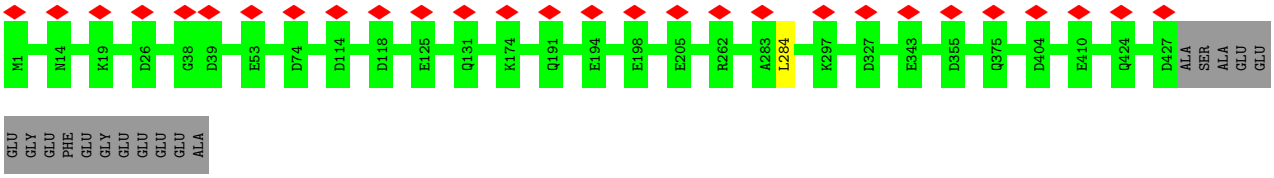




• Molecule 1: Tubulin beta

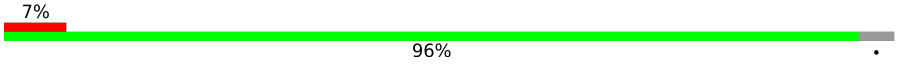
Chain GK:

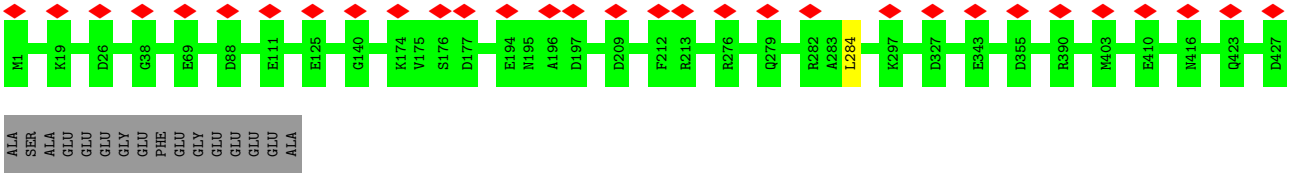




• Molecule 1: Tubulin beta

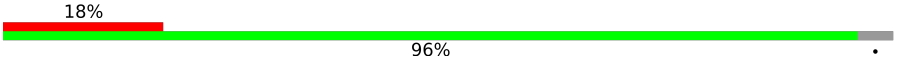
Chain GM:

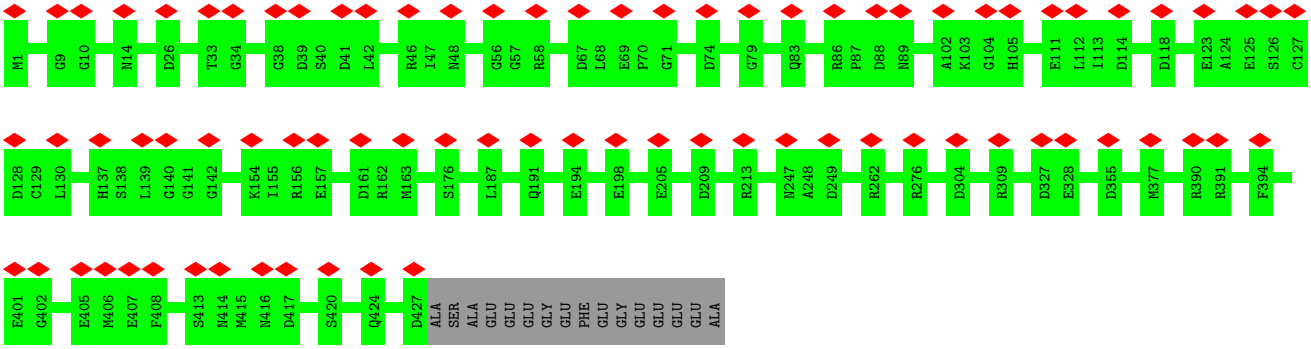




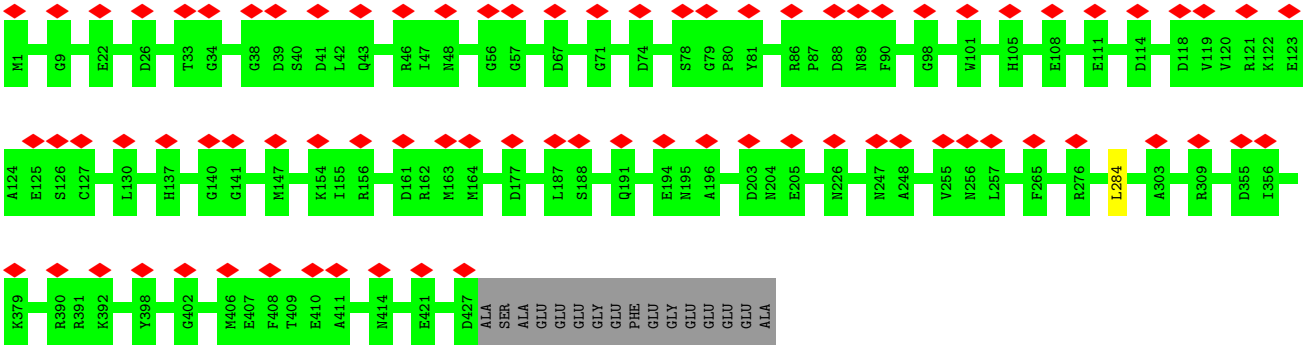
• Molecule 1: Tubulin beta

Chain HC:

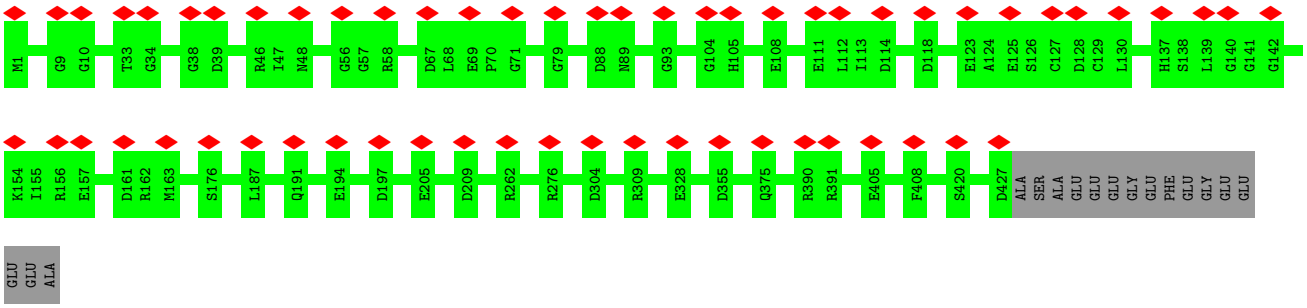




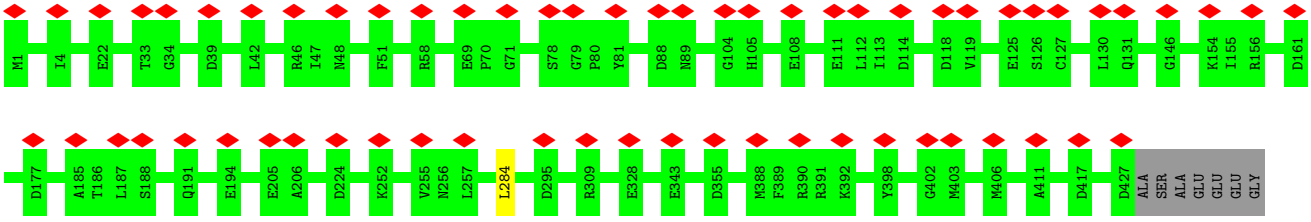
• Molecule 1: Tubulin beta



• Molecule 1: Tubulin beta

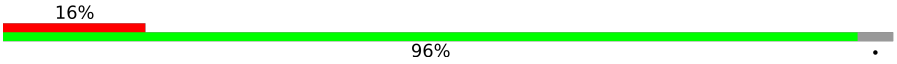


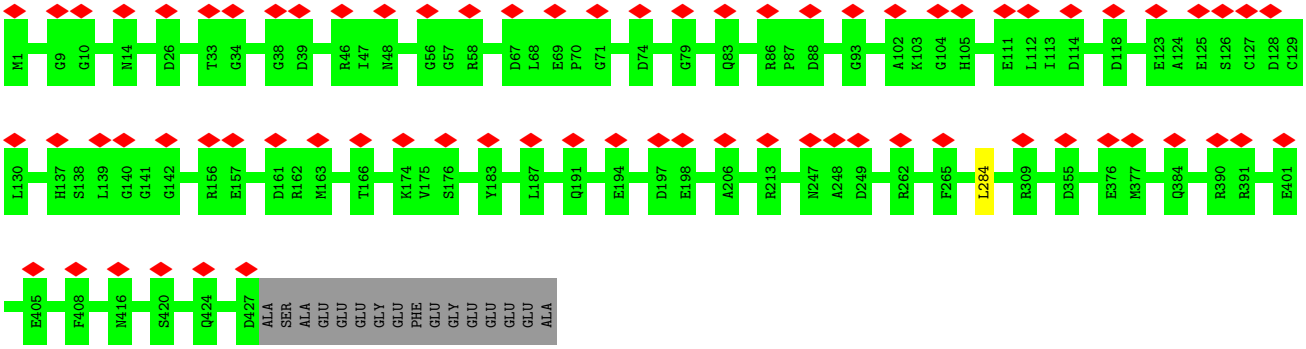
• Molecule 1: Tubulin beta



• Molecule 1: Tubulin beta

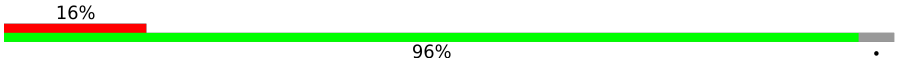
Chain HK:

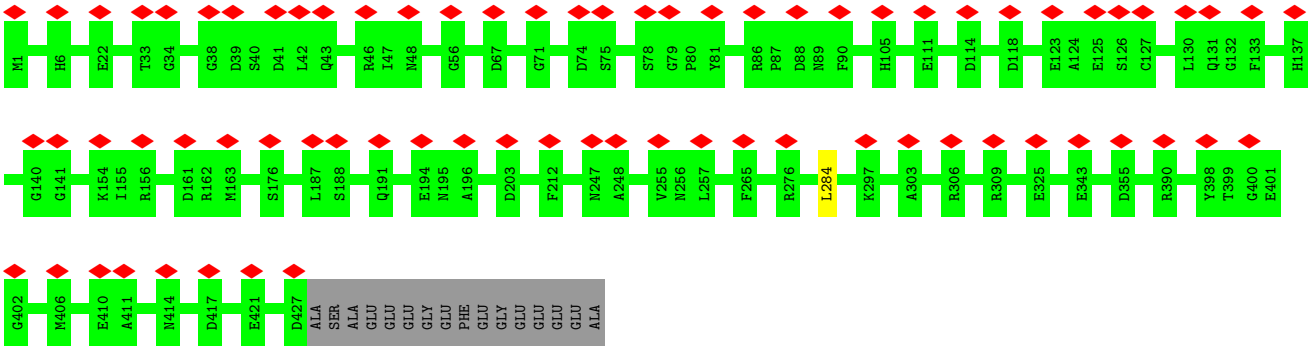




• Molecule 1: Tubulin beta

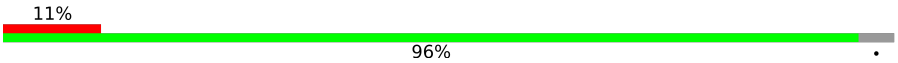
Chain HM:

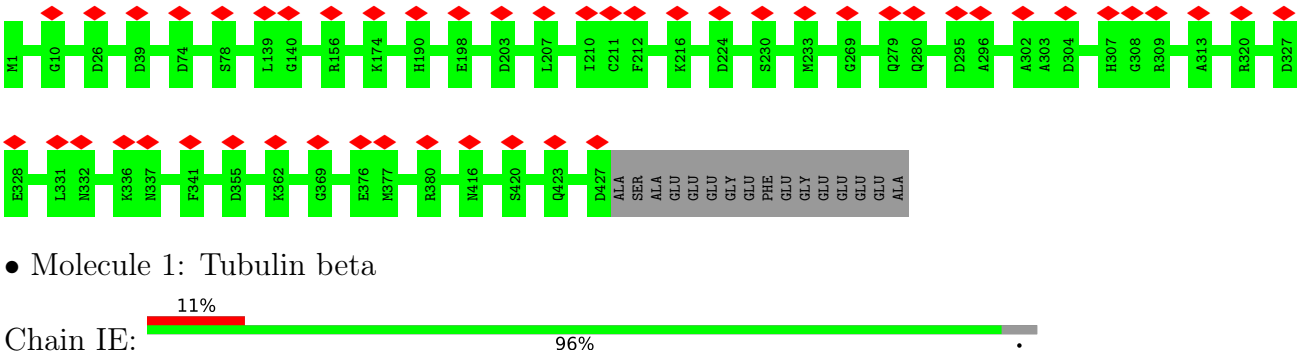




• Molecule 1: Tubulin beta

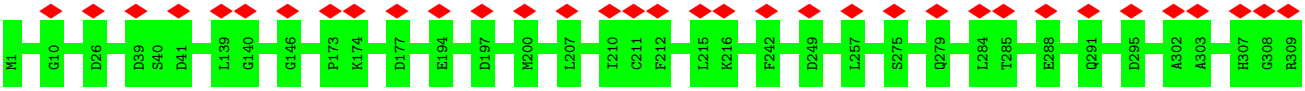
Chain IC:

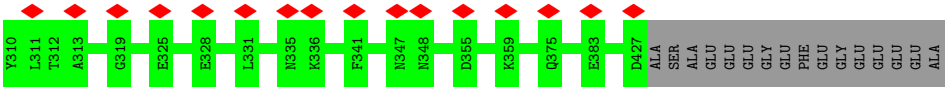




• Molecule 1: Tubulin beta

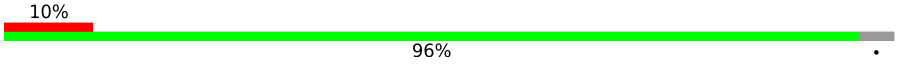
Chain IE:

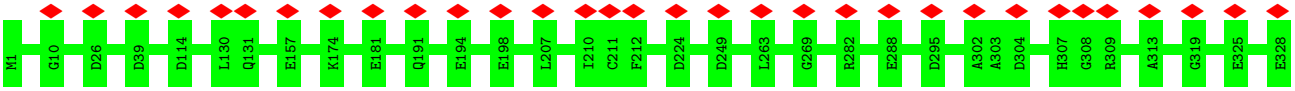


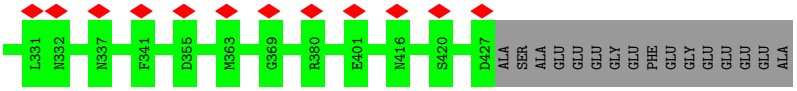


• Molecule 1: Tubulin beta

Chain IG:

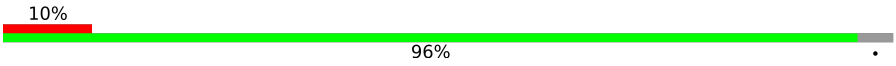


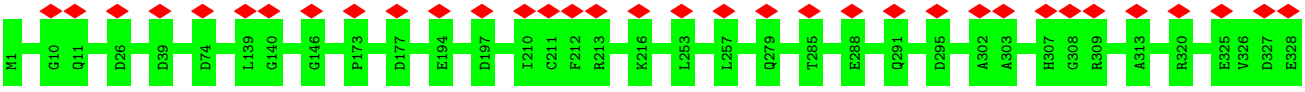


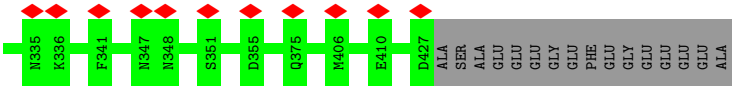


• Molecule 1: Tubulin beta

Chain II:

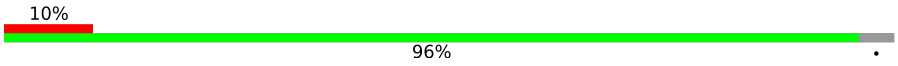


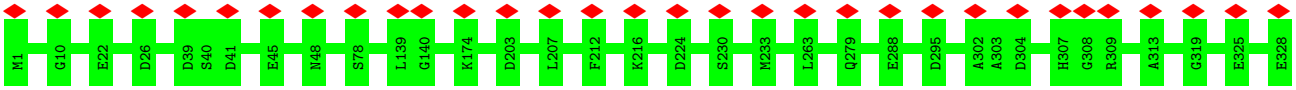


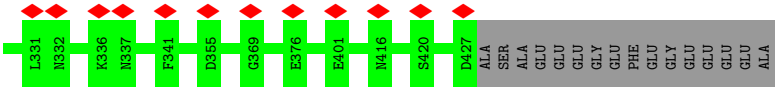


• Molecule 1: Tubulin beta

Chain IK:

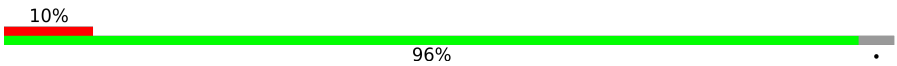


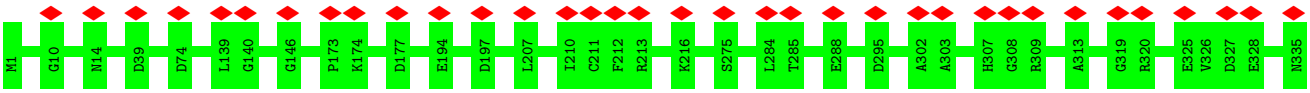


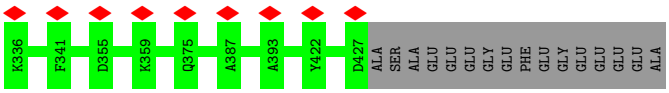


• Molecule 1: Tubulin beta

Chain IM:

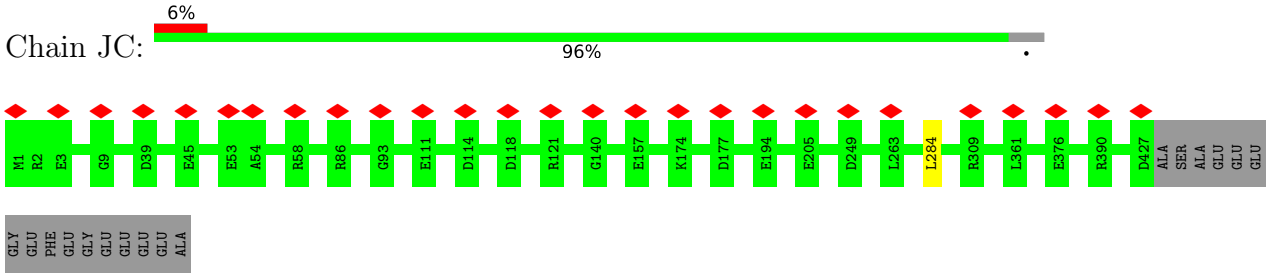






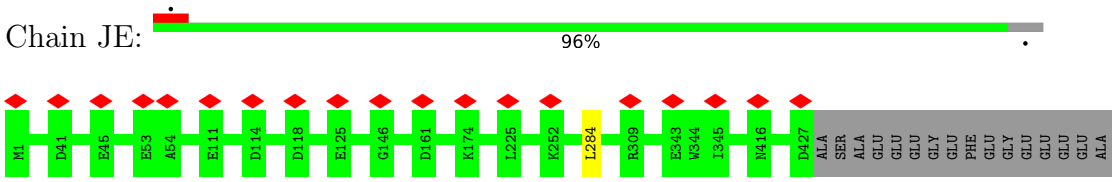
• Molecule 1: Tubulin beta

Chain JC:



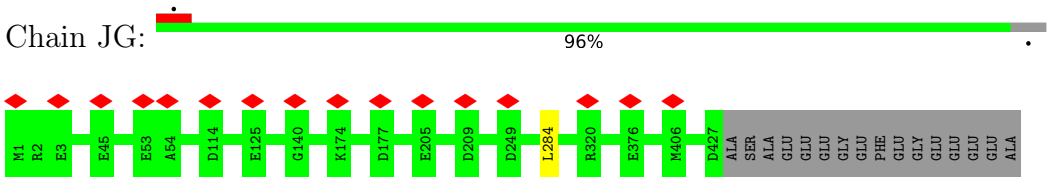
• Molecule 1: Tubulin beta

Chain JE:



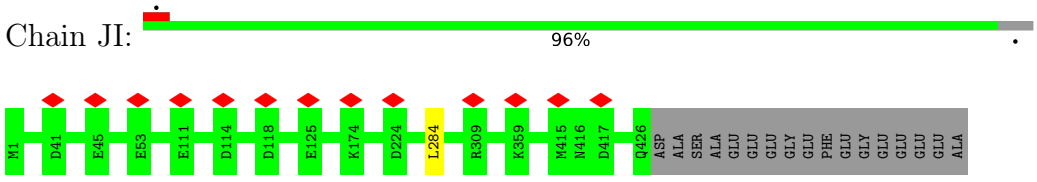
• Molecule 1: Tubulin beta

Chain JG:



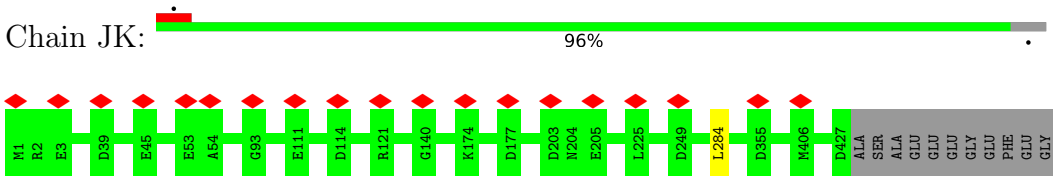
• Molecule 1: Tubulin beta

Chain JI:



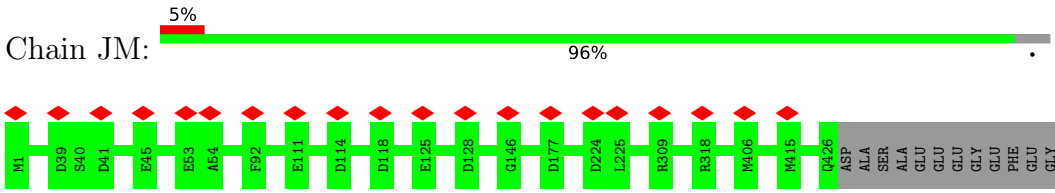
• Molecule 1: Tubulin beta

Chain JK:



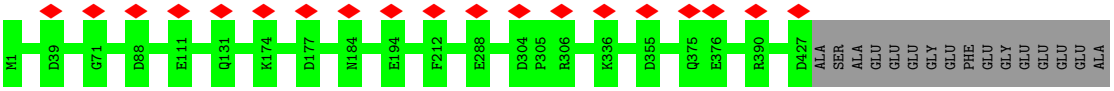
• Molecule 1: Tubulin beta

Chain JM:



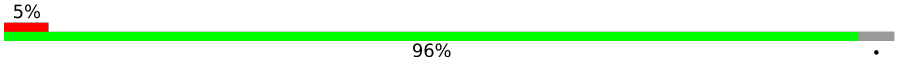
• Molecule 1: Tubulin beta

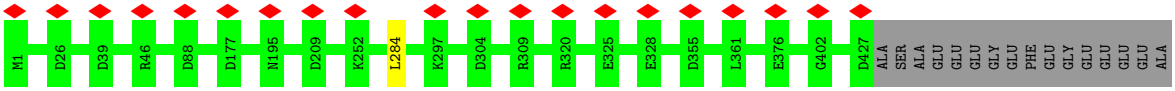
Chain KC:



• Molecule 1: Tubulin beta

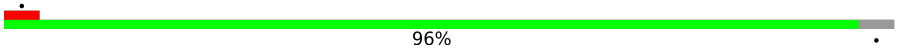
Chain KE:

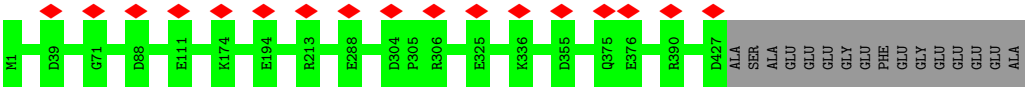




• Molecule 1: Tubulin beta

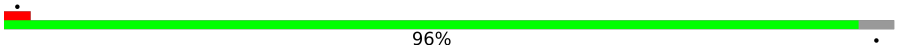
Chain KG:

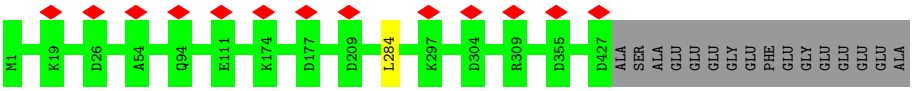




• Molecule 1: Tubulin beta

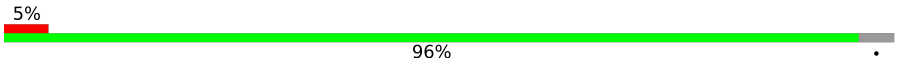
Chain KI:

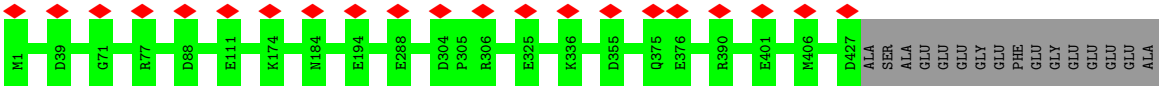




• Molecule 1: Tubulin beta

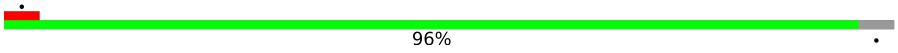
Chain KK:

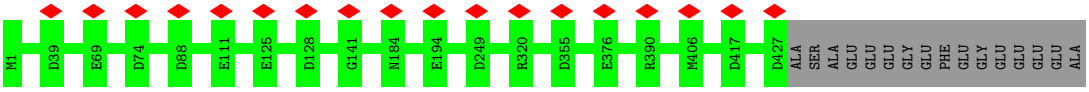




• Molecule 1: Tubulin beta

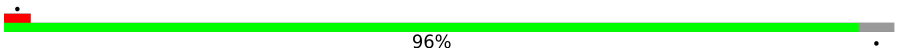
Chain LC:

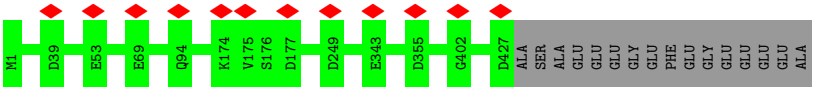




• Molecule 1: Tubulin beta

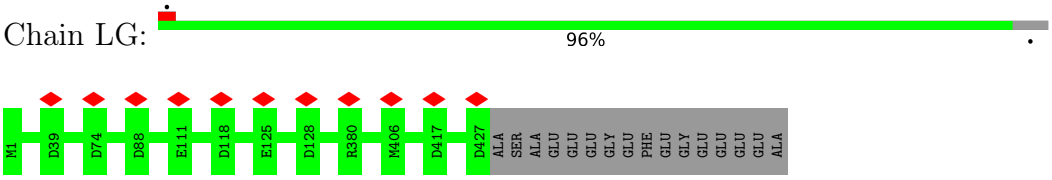
Chain LE:





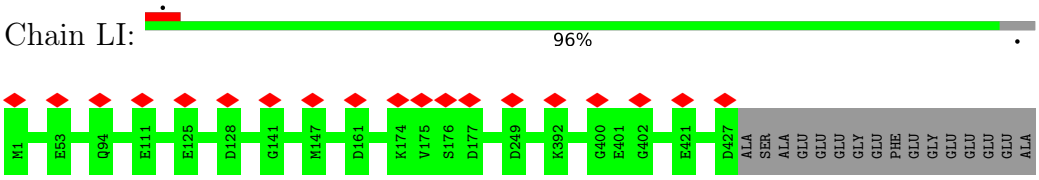
• Molecule 1: Tubulin beta

Chain LG:



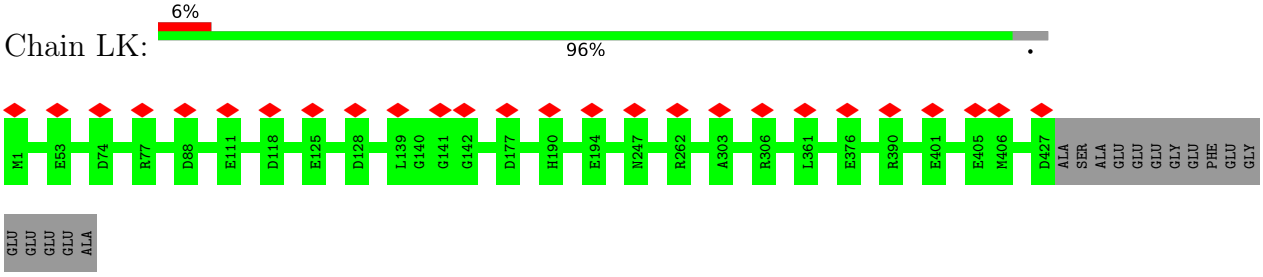
• Molecule 1: Tubulin beta

Chain LI:



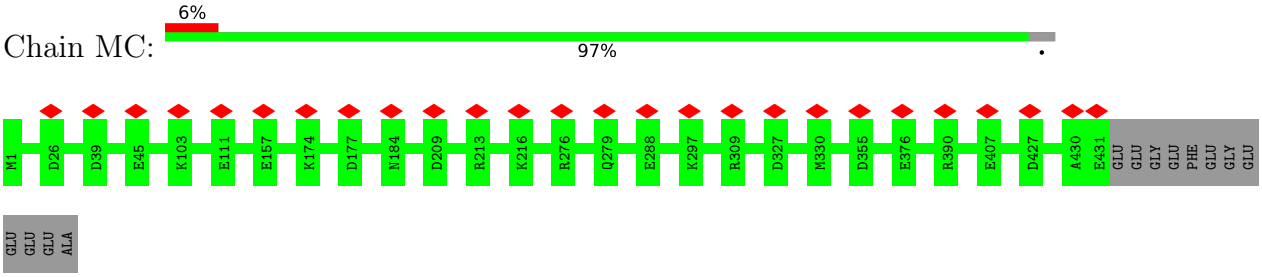
• Molecule 1: Tubulin beta

Chain LK:



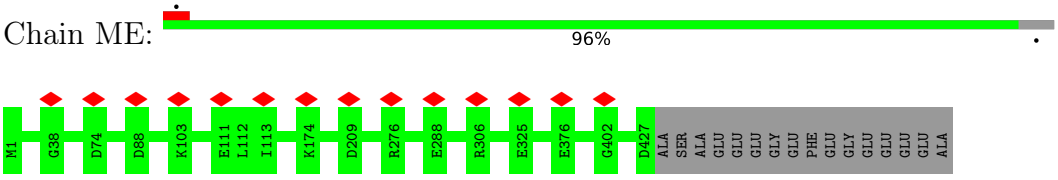
• Molecule 1: Tubulin beta

Chain MC:



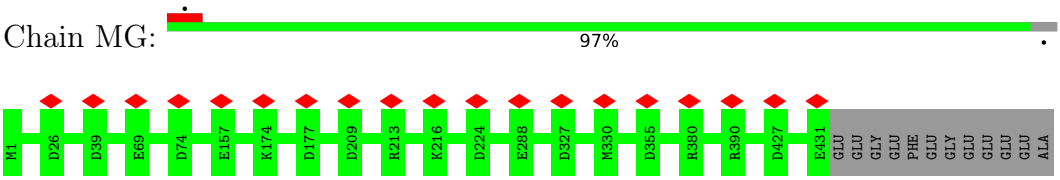
• Molecule 1: Tubulin beta

Chain ME:



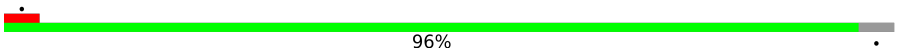
• Molecule 1: Tubulin beta

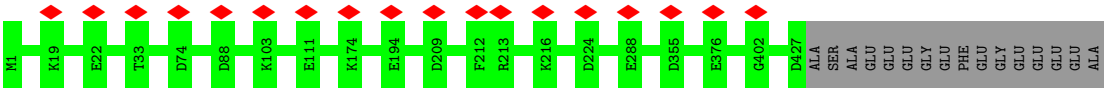
Chain MG:



• Molecule 1: Tubulin beta

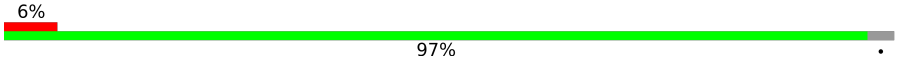
Chain MI:

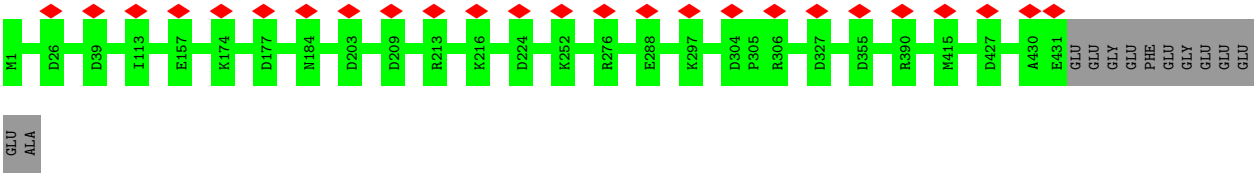




• Molecule 1: Tubulin beta

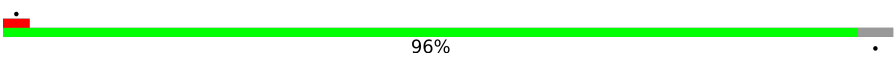
Chain MK:

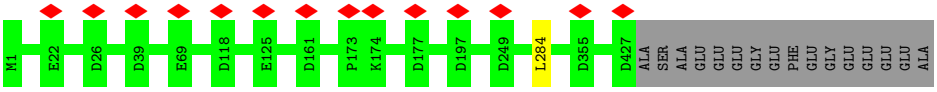




• Molecule 1: Tubulin beta

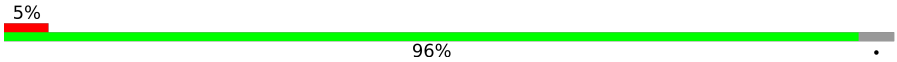
Chain CA:

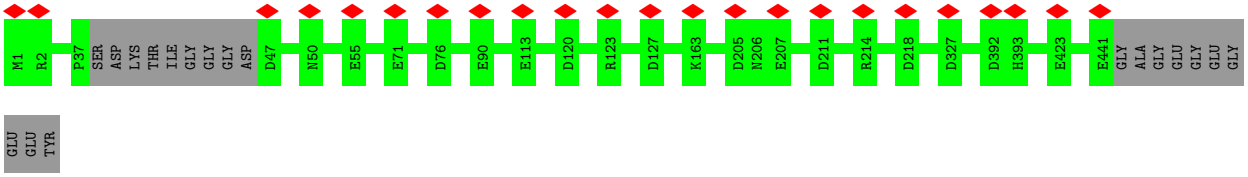




• Molecule 2: Tubulin alpha

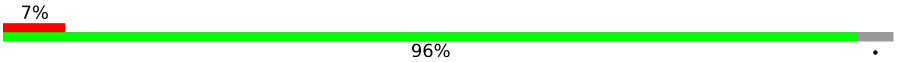
Chain AB:

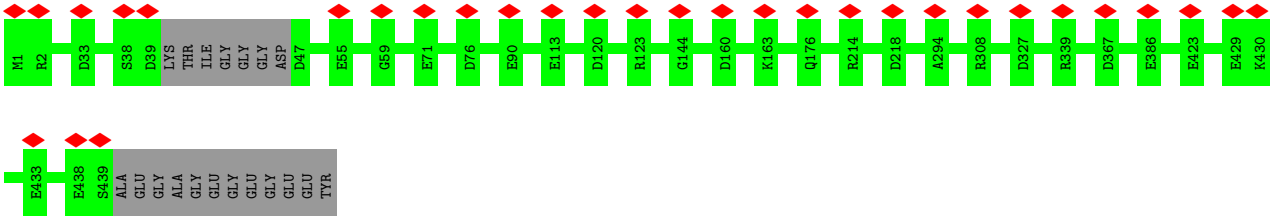




• Molecule 2: Tubulin alpha

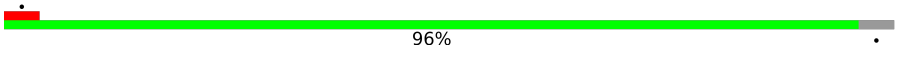
Chain AD:

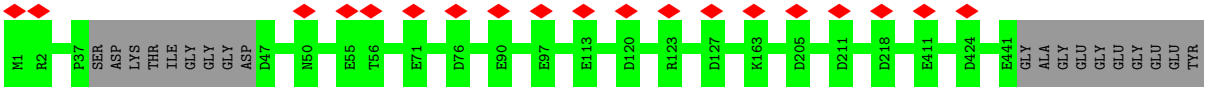




• Molecule 2: Tubulin alpha

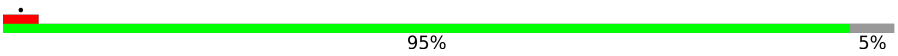
Chain AF:

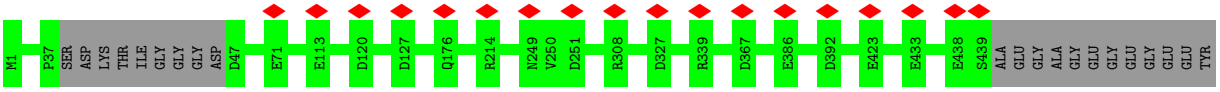




• Molecule 2: Tubulin alpha

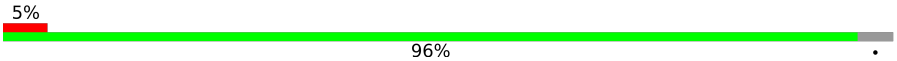
Chain AH:

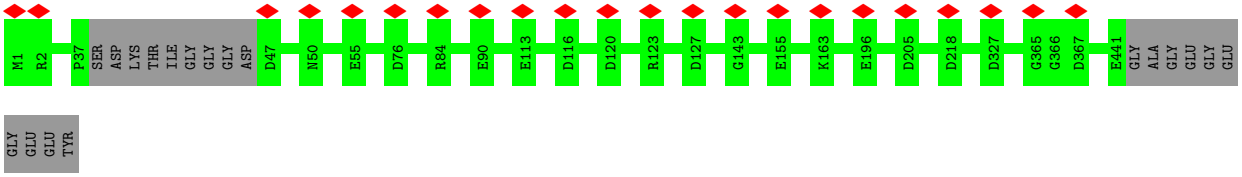




• Molecule 2: Tubulin alpha

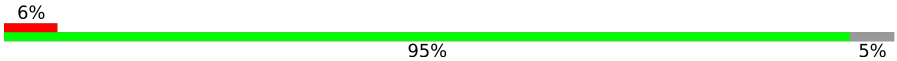
Chain AJ:

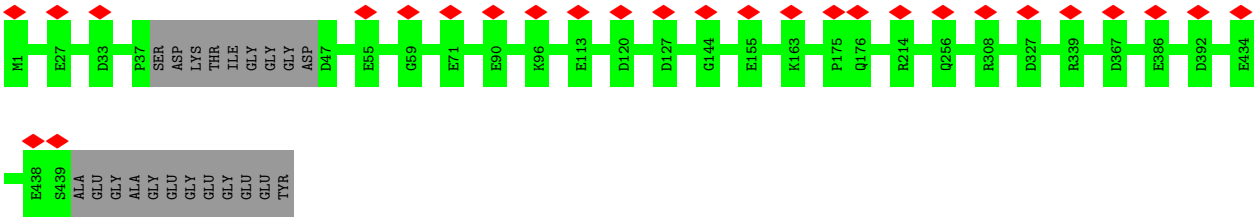




• Molecule 2: Tubulin alpha

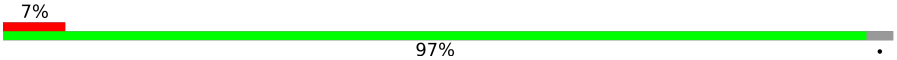
Chain AL:

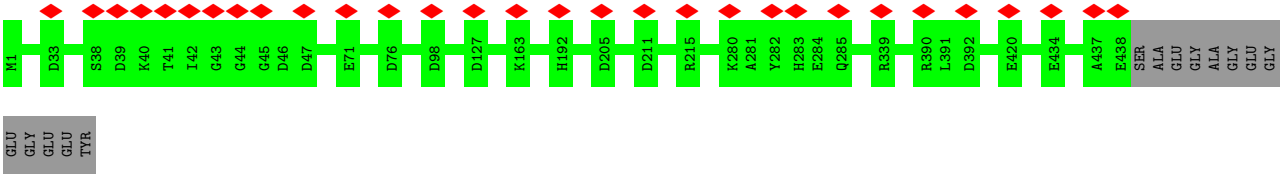




• Molecule 2: Tubulin alpha

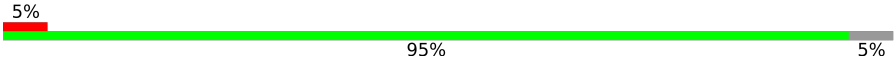
Chain BB:

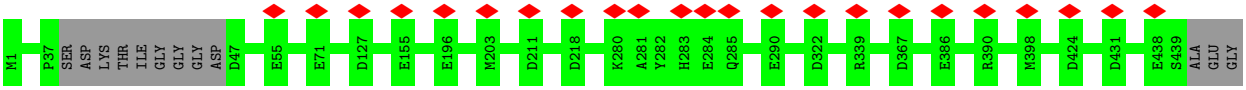


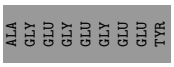


• Molecule 2: Tubulin alpha

Chain BD:

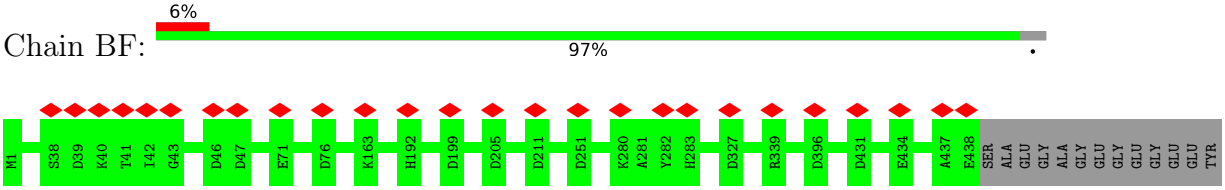






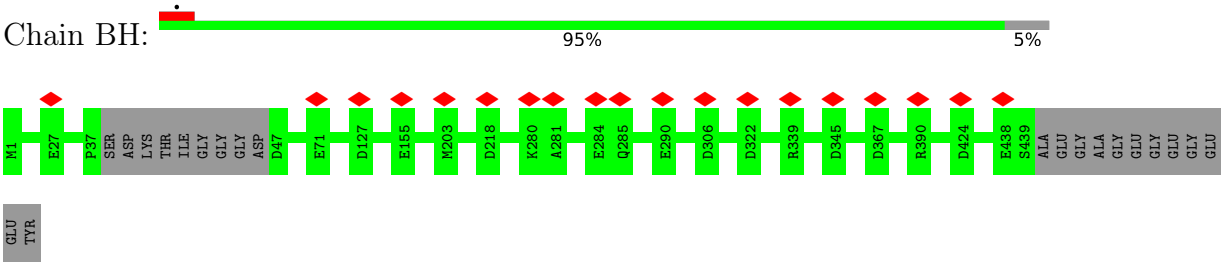
• Molecule 2: Tubulin alpha

Chain BF:



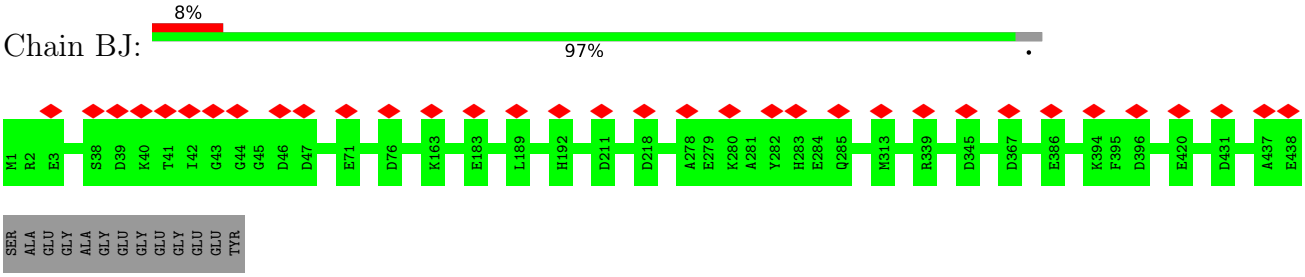
• Molecule 2: Tubulin alpha

Chain BH:



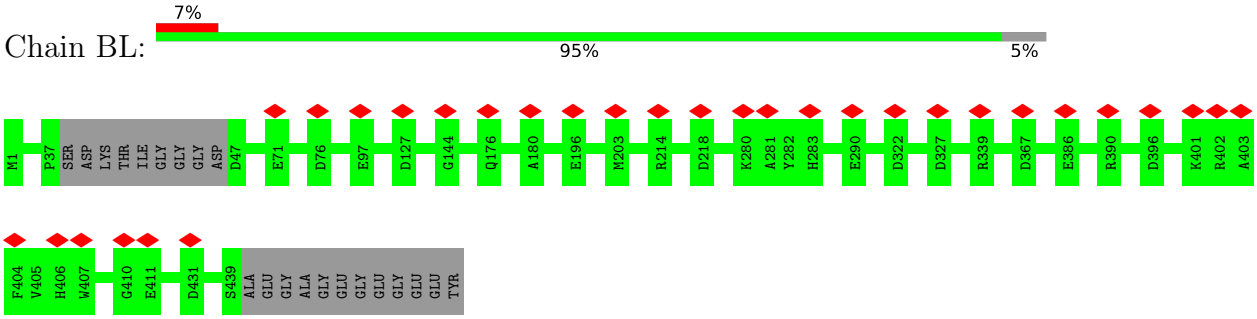
• Molecule 2: Tubulin alpha

Chain BJ:



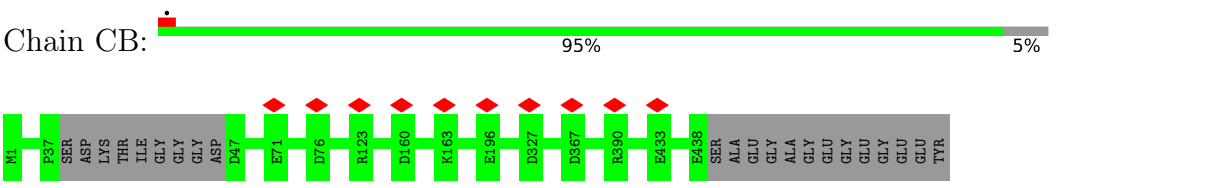
• Molecule 2: Tubulin alpha

Chain BL:



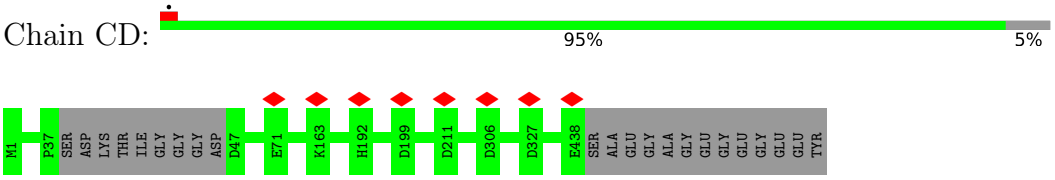
• Molecule 2: Tubulin alpha

Chain CB:



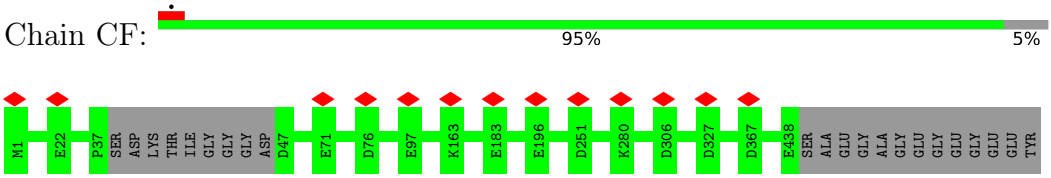
• Molecule 2: Tubulin alpha

Chain CD:



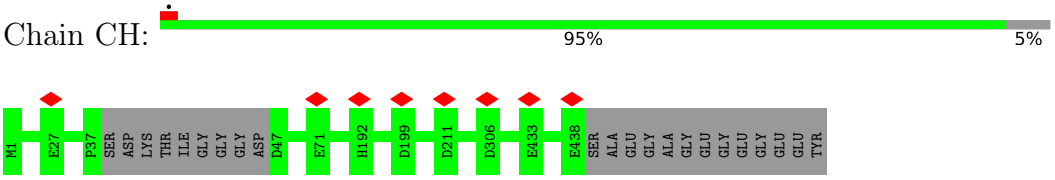
• Molecule 2: Tubulin alpha

Chain CF:



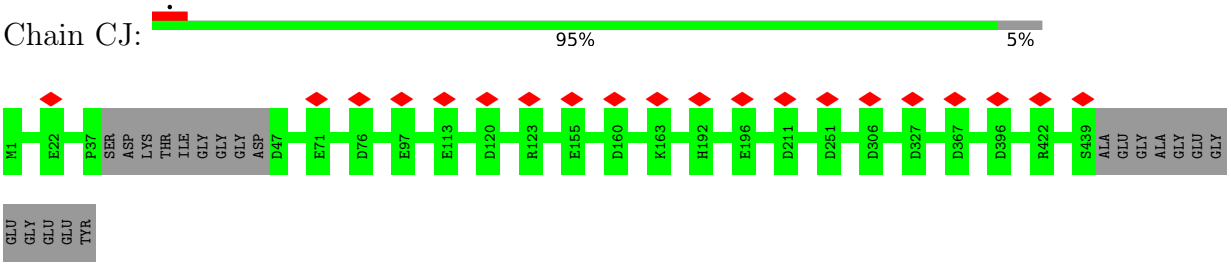
• Molecule 2: Tubulin alpha

Chain CH:



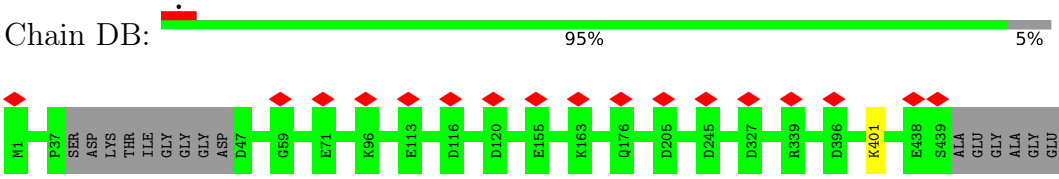
• Molecule 2: Tubulin alpha

Chain CJ:



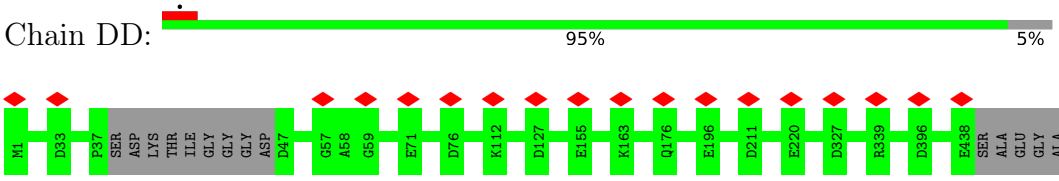
• Molecule 2: Tubulin alpha

Chain DB:



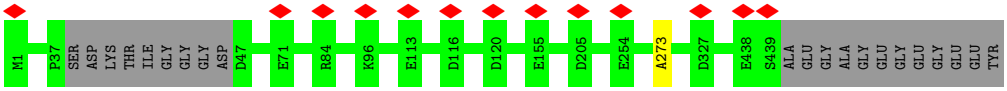
• Molecule 2: Tubulin alpha

Chain DD:



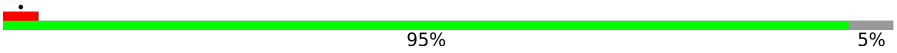
• Molecule 2: Tubulin alpha

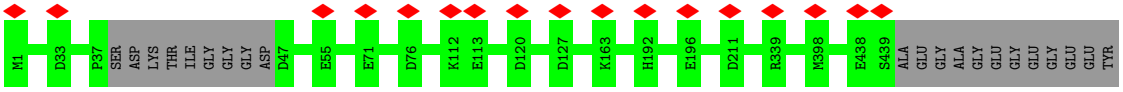
Chain DF:



• Molecule 2: Tubulin alpha

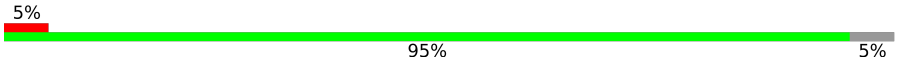
Chain DH:

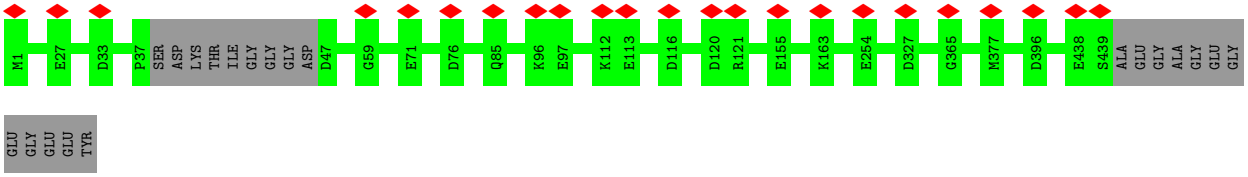




• Molecule 2: Tubulin alpha

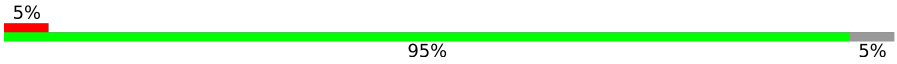
Chain DJ:

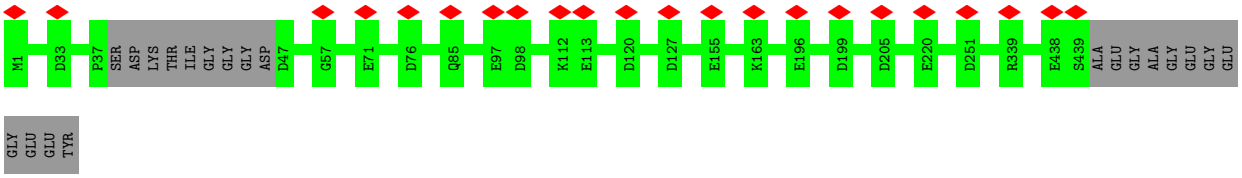




• Molecule 2: Tubulin alpha

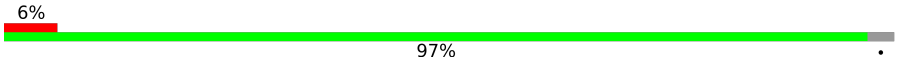
Chain DL:

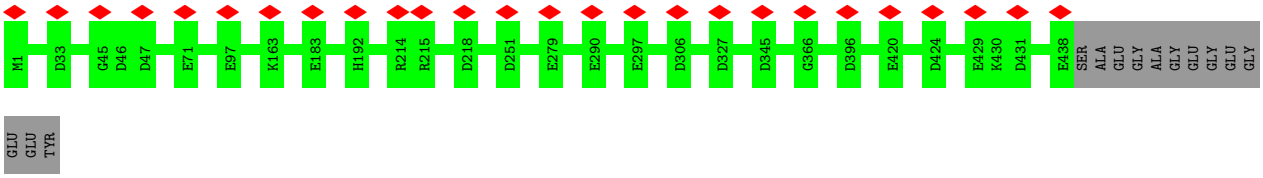




• Molecule 2: Tubulin alpha

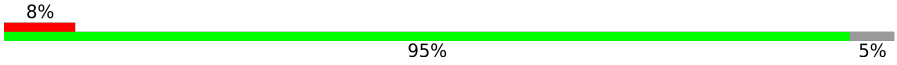
Chain EB:

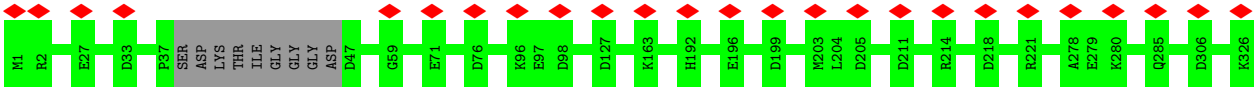


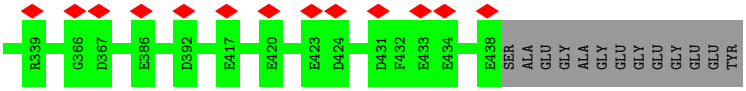


• Molecule 2: Tubulin alpha

Chain ED:

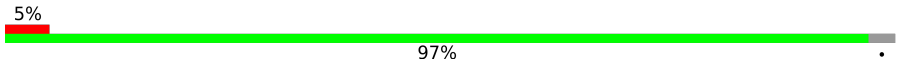


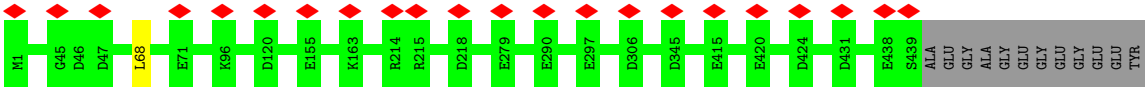




• Molecule 2: Tubulin alpha

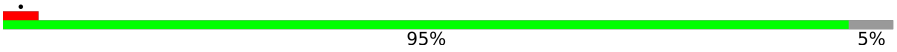
Chain EF:

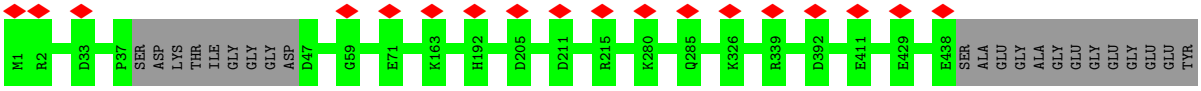




• Molecule 2: Tubulin alpha

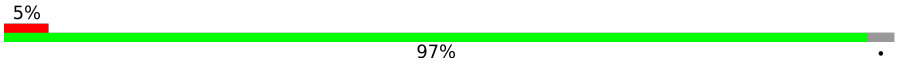
Chain EH:

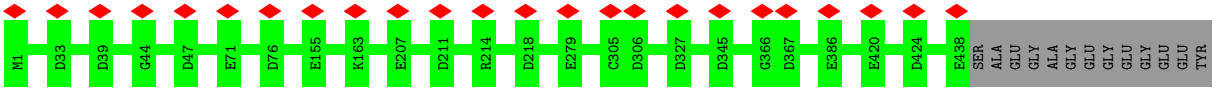




• Molecule 2: Tubulin alpha

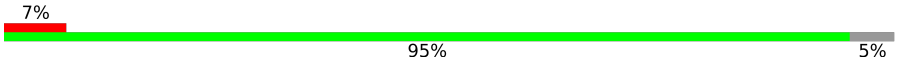
Chain EJ:

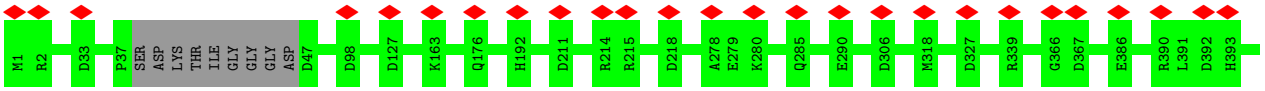


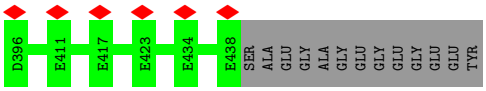


• Molecule 2: Tubulin alpha

Chain EL:

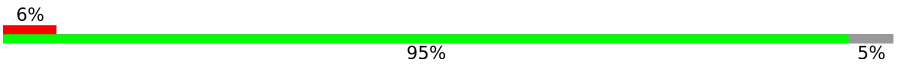


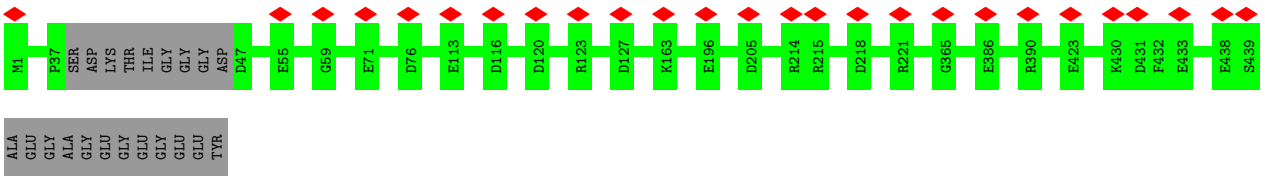




• Molecule 2: Tubulin alpha

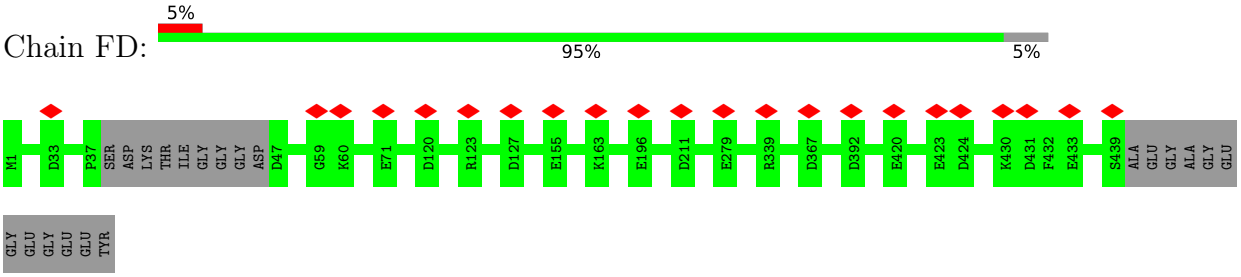
Chain FB:





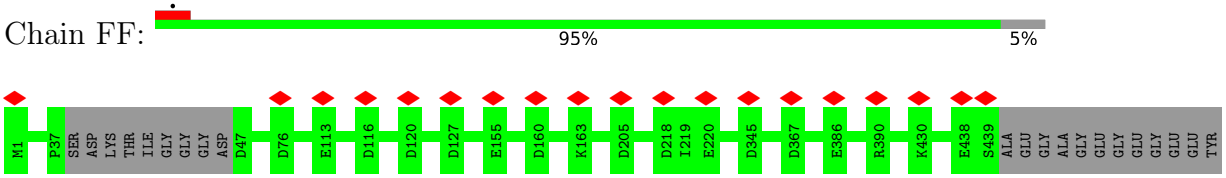
• Molecule 2: Tubulin alpha

Chain FD:



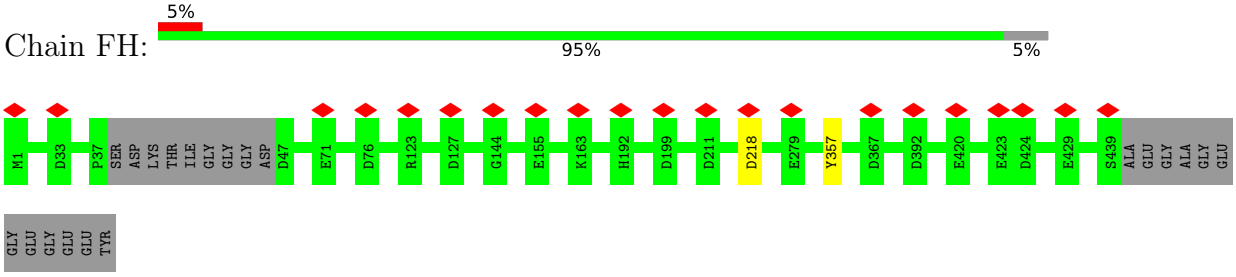
• Molecule 2: Tubulin alpha

Chain FF:



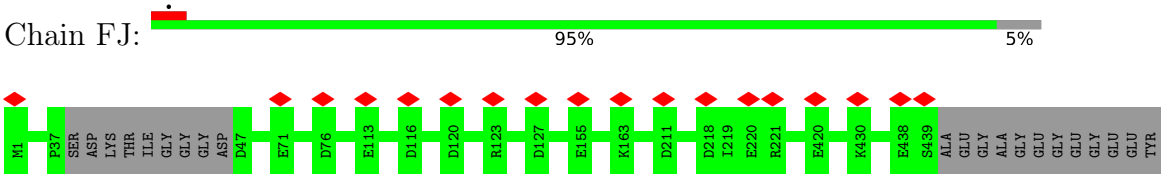
• Molecule 2: Tubulin alpha

Chain FH:



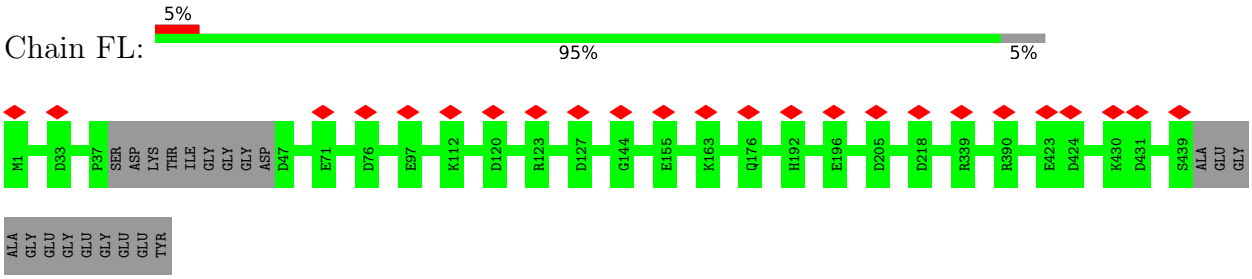
• Molecule 2: Tubulin alpha

Chain FJ:



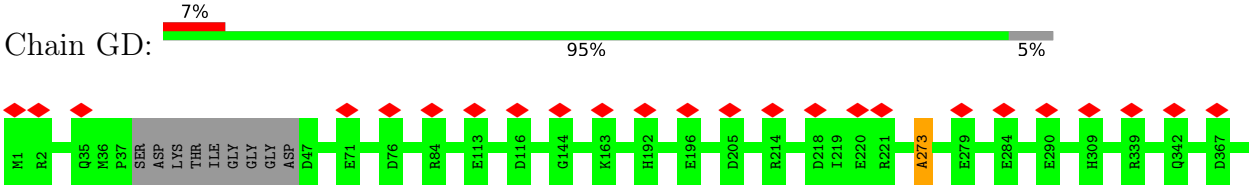
• Molecule 2: Tubulin alpha

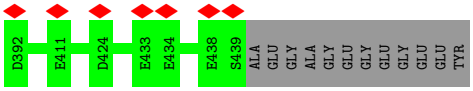
Chain FL:



• Molecule 2: Tubulin alpha

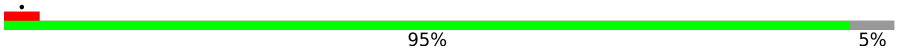
Chain GD:

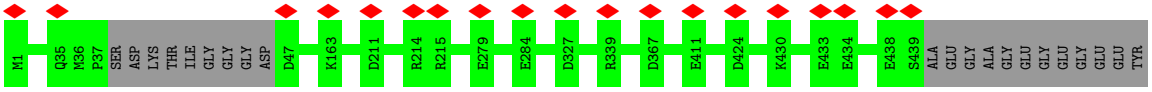




• Molecule 2: Tubulin alpha

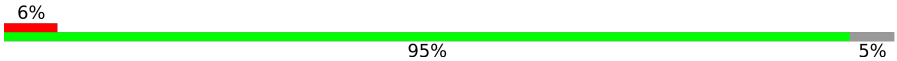
Chain GF:

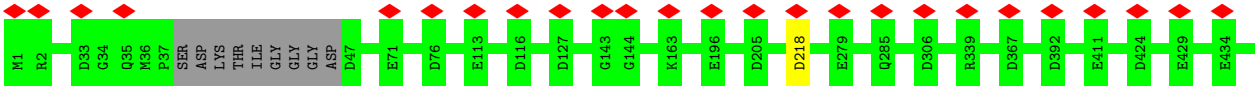


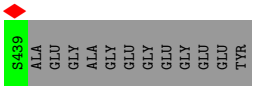


• Molecule 2: Tubulin alpha

Chain GH:

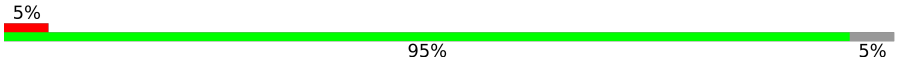


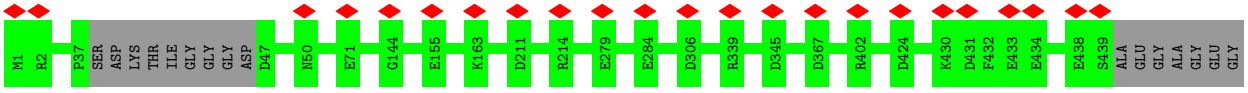




• Molecule 2: Tubulin alpha

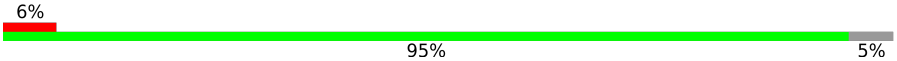
Chain GJ:

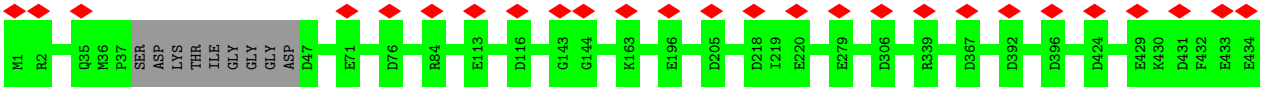


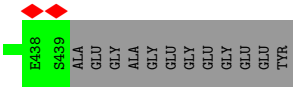


• Molecule 2: Tubulin alpha

Chain GL:

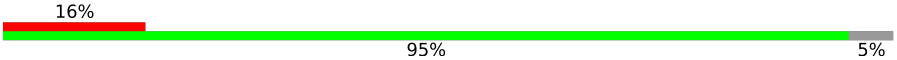


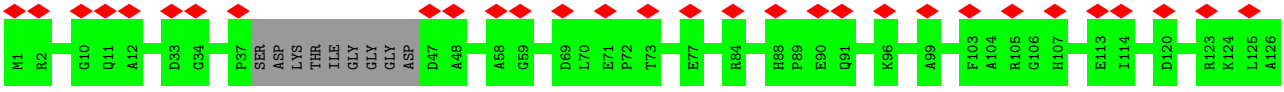


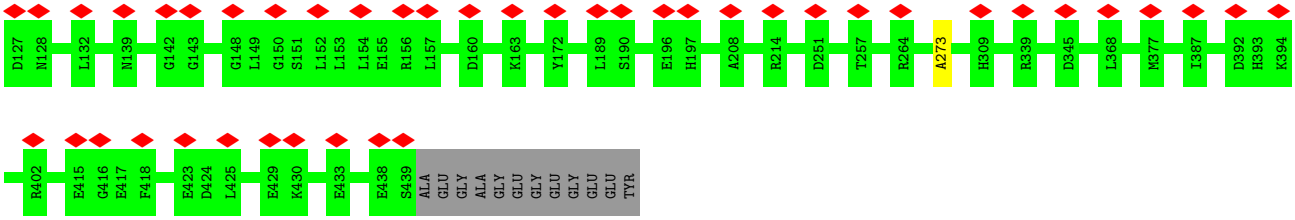


• Molecule 2: Tubulin alpha

Chain HD:

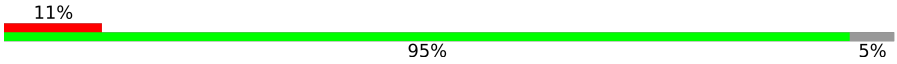


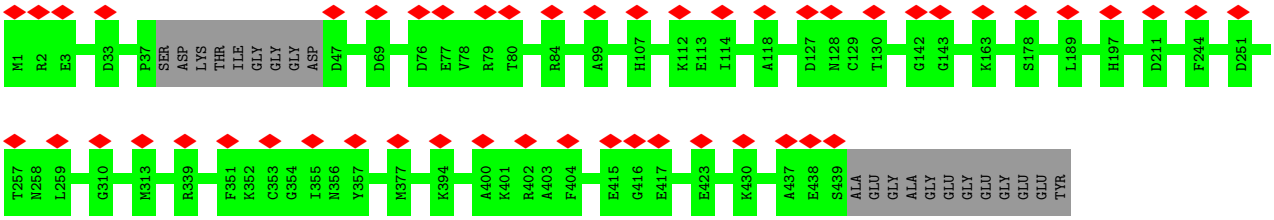




• Molecule 2: Tubulin alpha

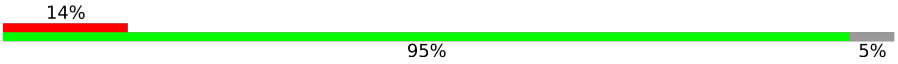
Chain HF:

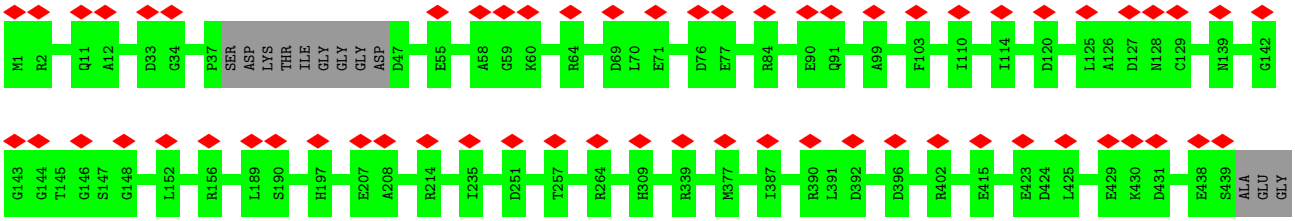




• Molecule 2: Tubulin alpha

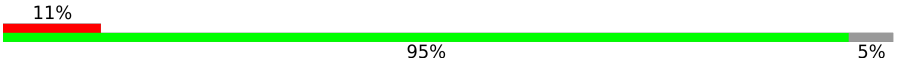
Chain HH:

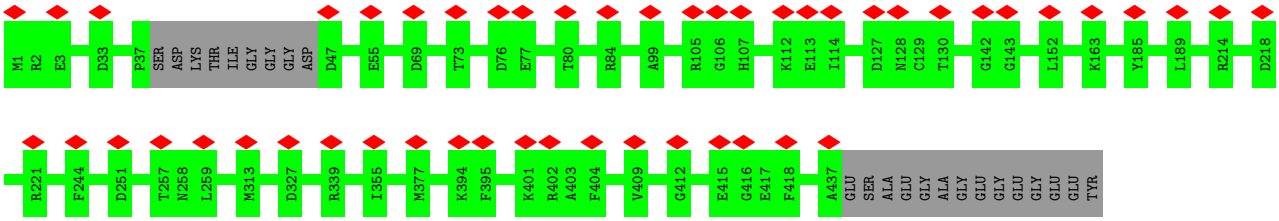




• Molecule 2: Tubulin alpha

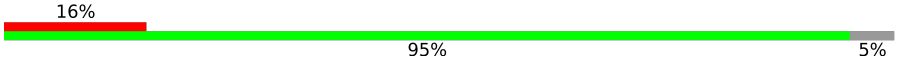
Chain HJ:

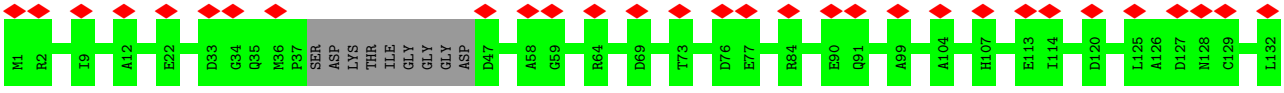


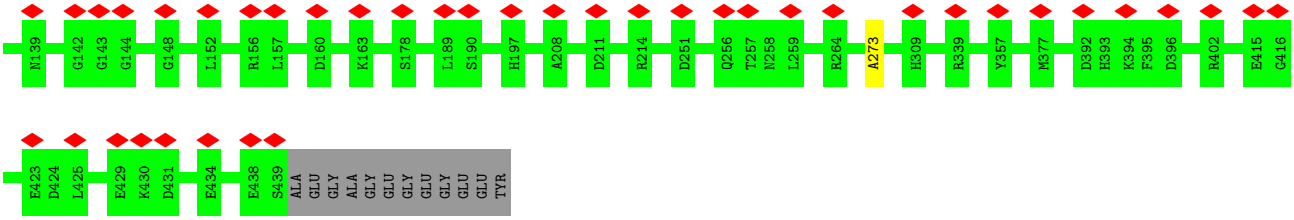


• Molecule 2: Tubulin alpha

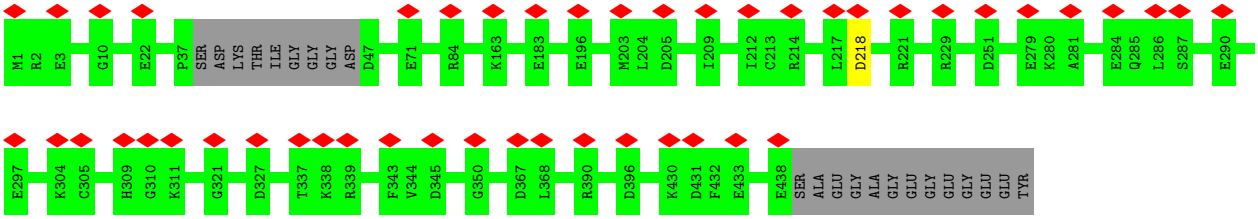
Chain HL:



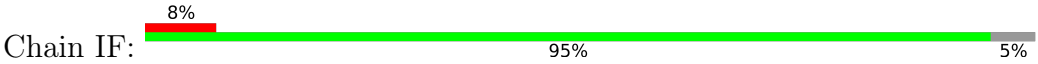


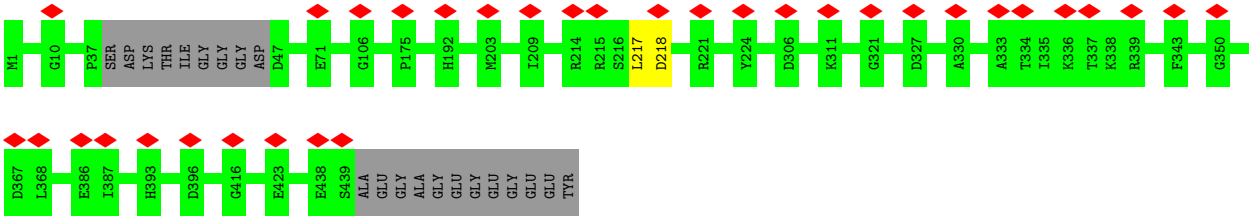


• Molecule 2: Tubulin alpha

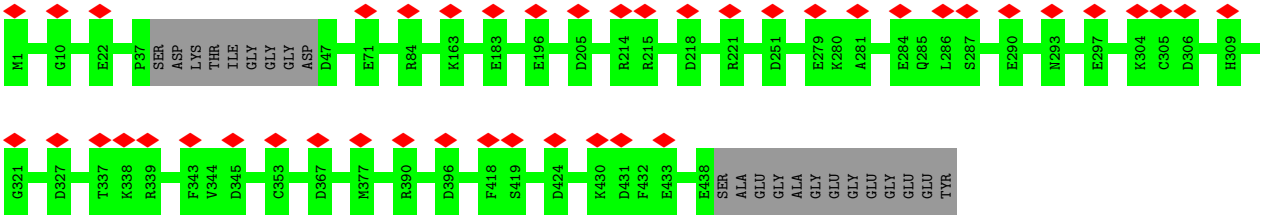


• Molecule 2: Tubulin alpha

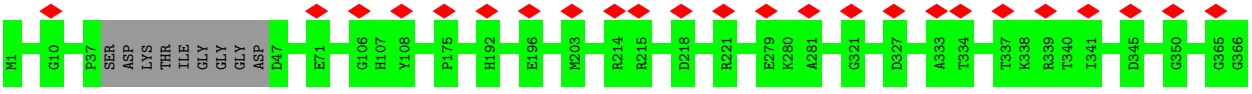


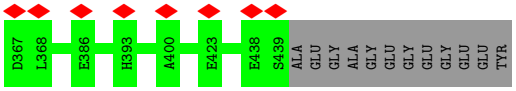


• Molecule 2: Tubulin alpha



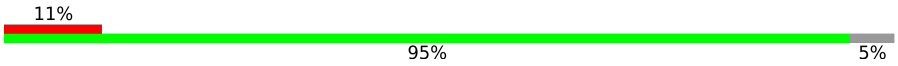
• Molecule 2: Tubulin alpha

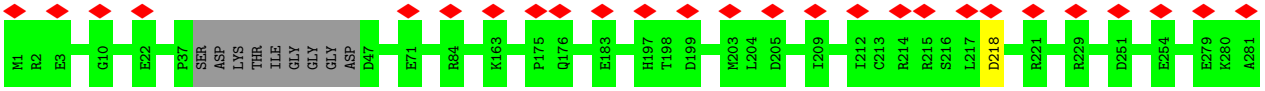


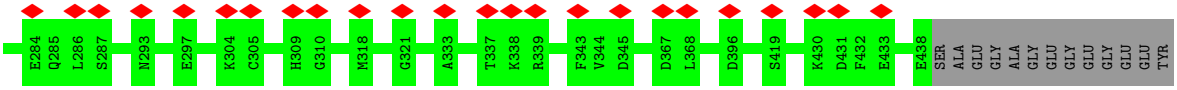


• Molecule 2: Tubulin alpha

Chain IL:

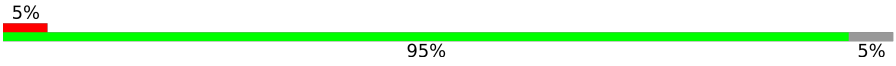


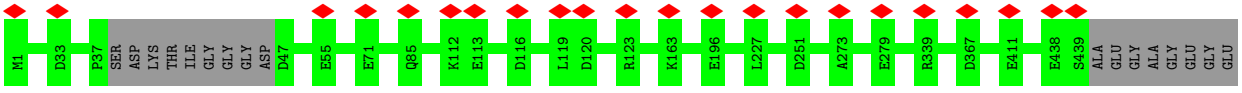




• Molecule 2: Tubulin alpha

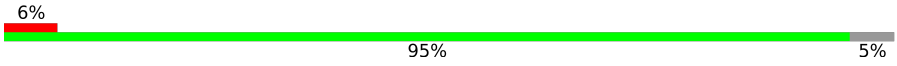
Chain JB:

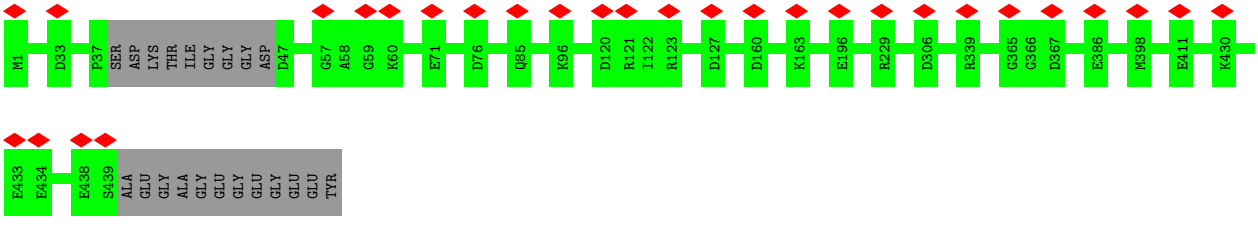




• Molecule 2: Tubulin alpha

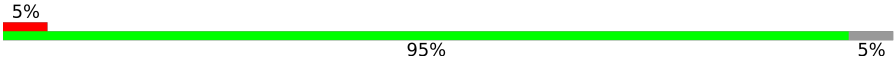
Chain JD:

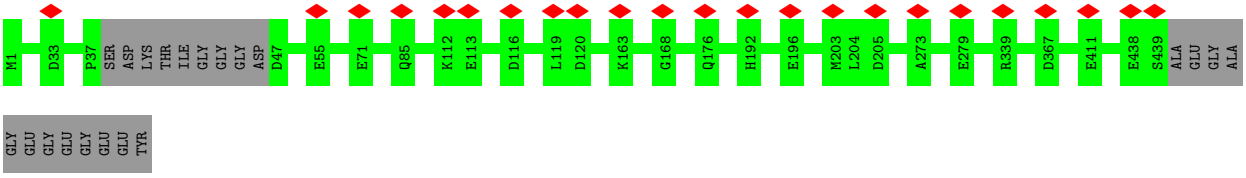




• Molecule 2: Tubulin alpha

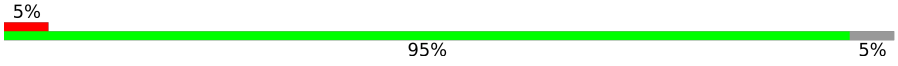
Chain JF:

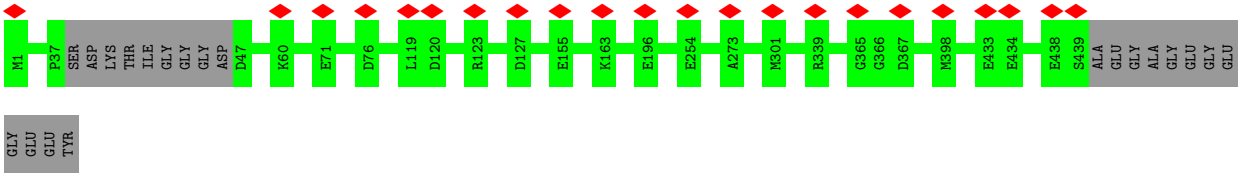




• Molecule 2: Tubulin alpha

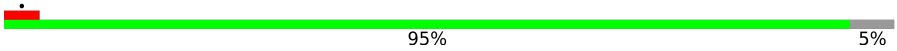
Chain JH:

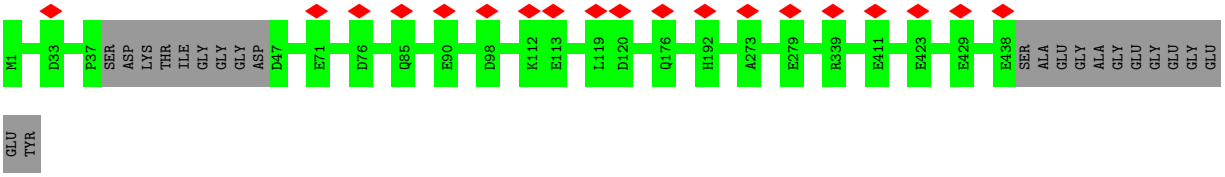




• Molecule 2: Tubulin alpha

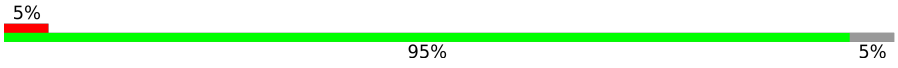
Chain JJ:

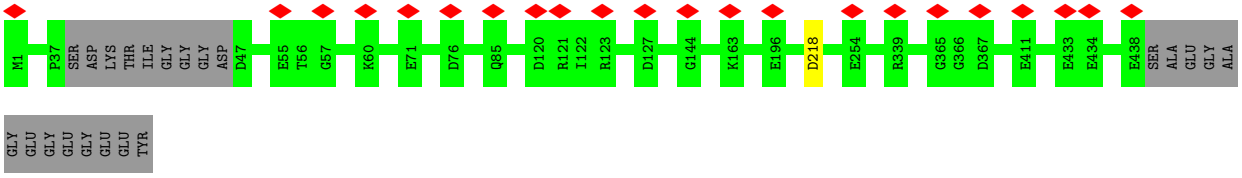




• Molecule 2: Tubulin alpha

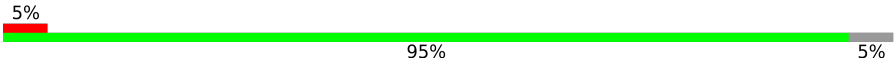
Chain JL:

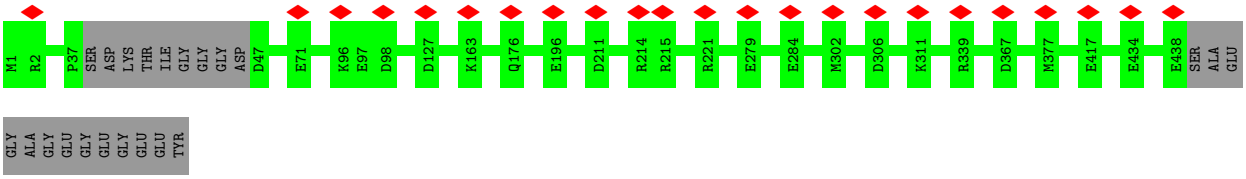




• Molecule 2: Tubulin alpha

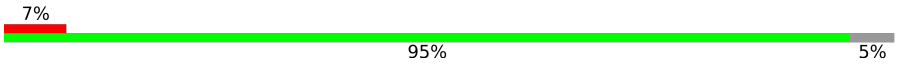
Chain KB:

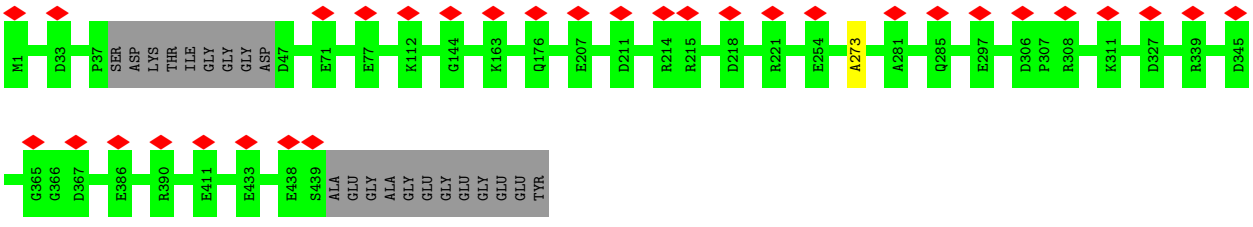




• Molecule 2: Tubulin alpha

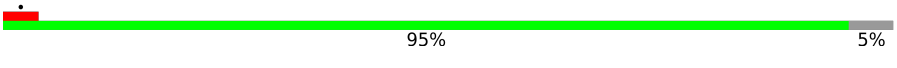
Chain KD:

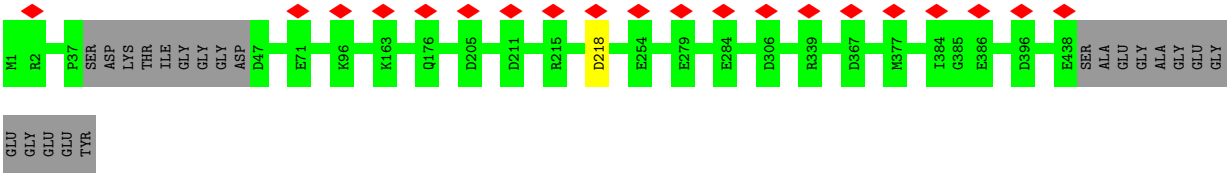




• Molecule 2: Tubulin alpha

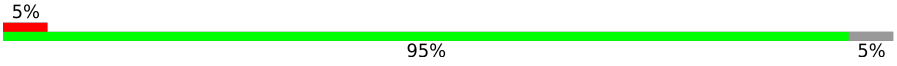
Chain KF:

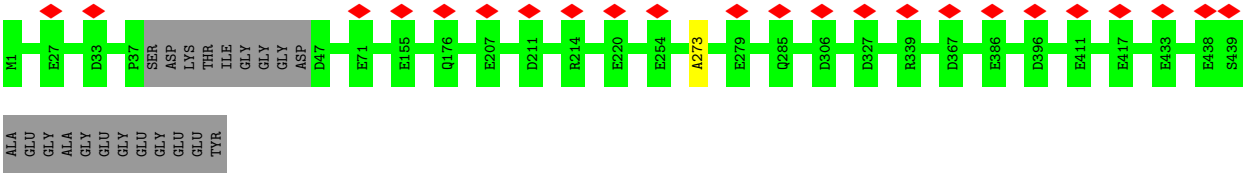




• Molecule 2: Tubulin alpha

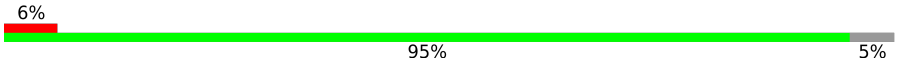
Chain KH:

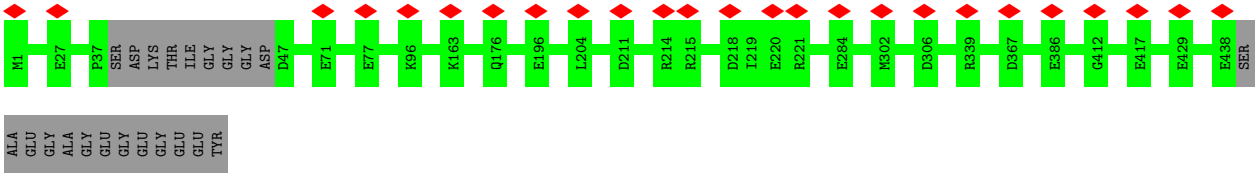




• Molecule 2: Tubulin alpha

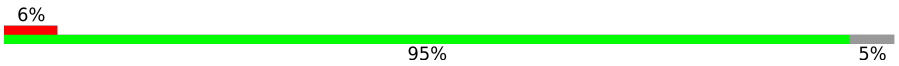
Chain KJ:

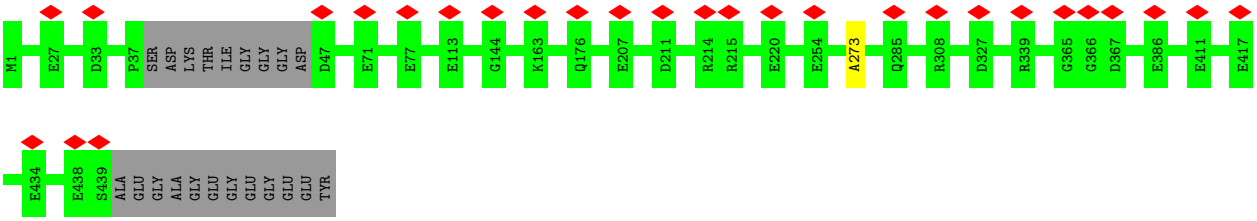




• Molecule 2: Tubulin alpha

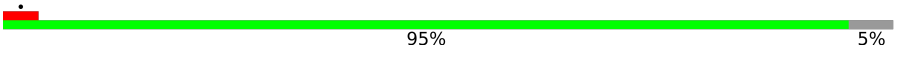
Chain KL:

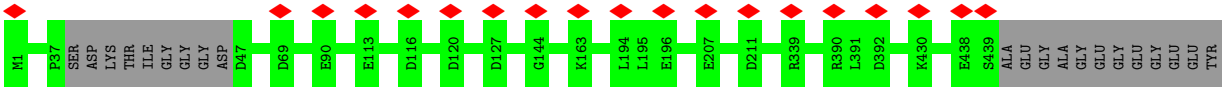




• Molecule 2: Tubulin alpha

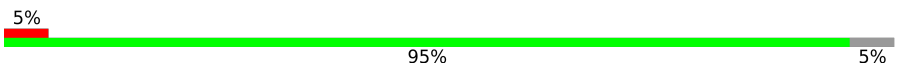
Chain LB:

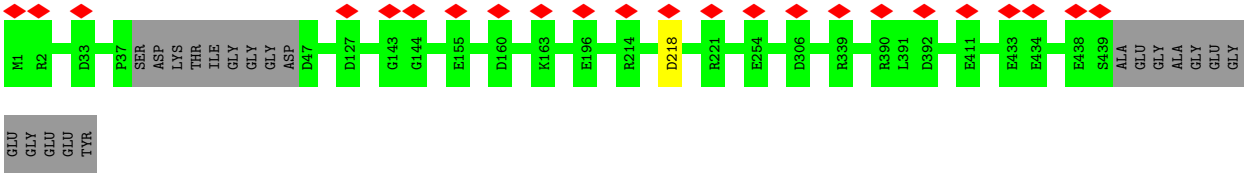




• Molecule 2: Tubulin alpha

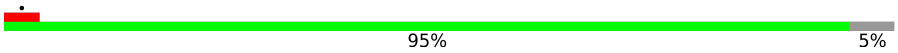
Chain LD:

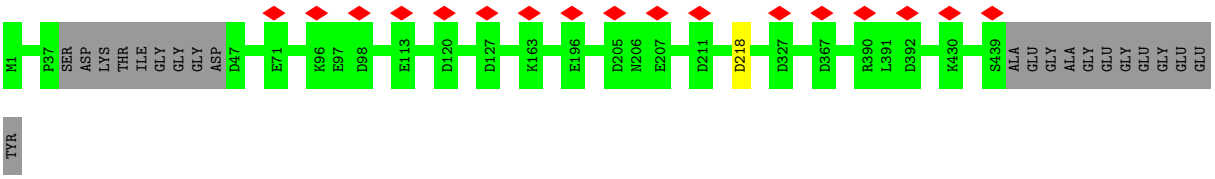




• Molecule 2: Tubulin alpha

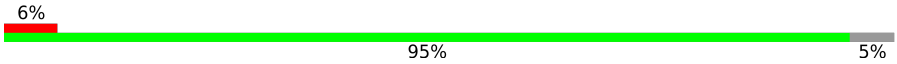
Chain LF:

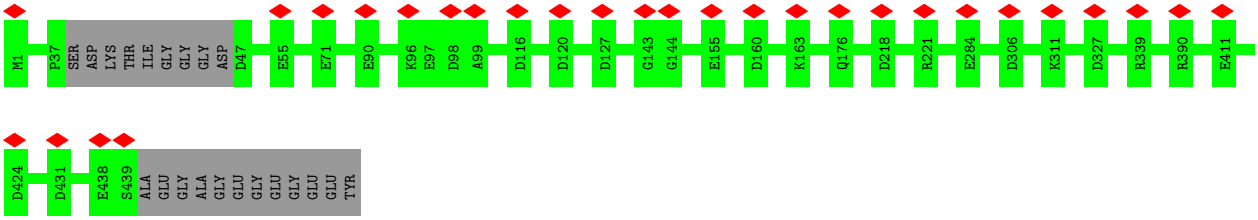




• Molecule 2: Tubulin alpha

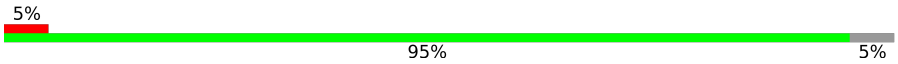
Chain LH:





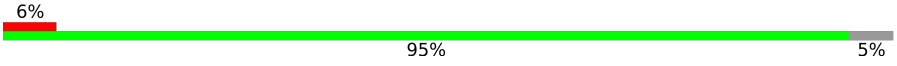
• Molecule 2: Tubulin alpha

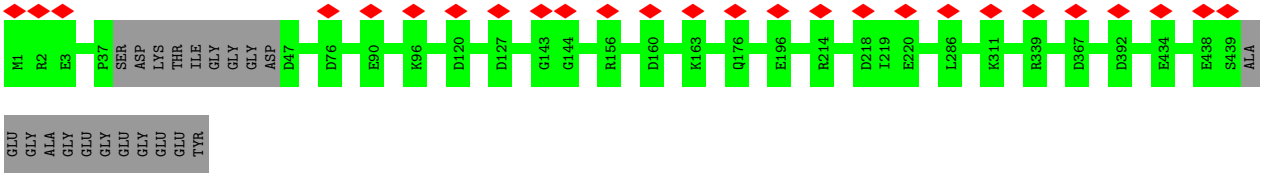
Chain LJ:



• Molecule 2: Tubulin alpha

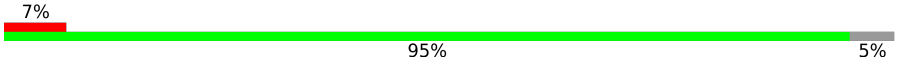
Chain LL:

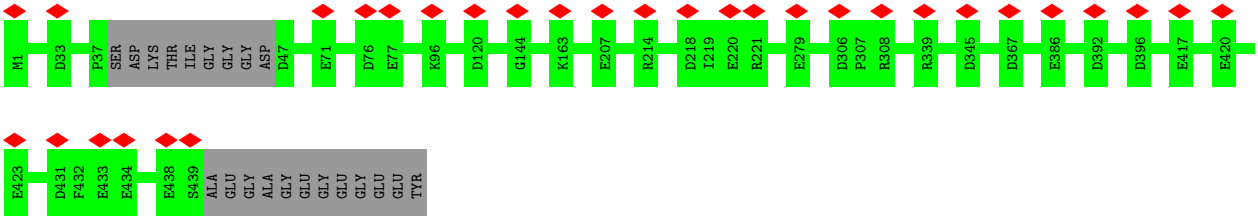




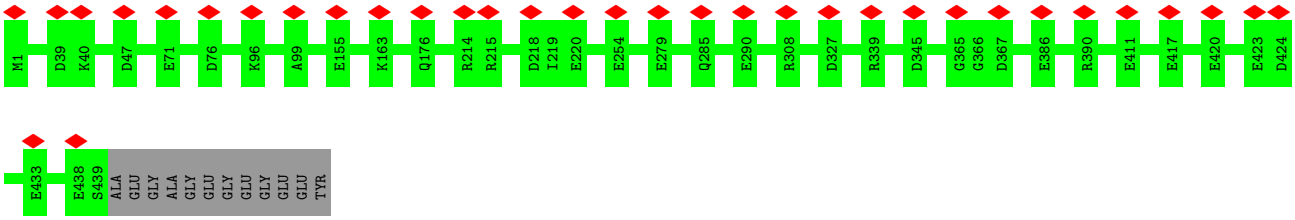
• Molecule 2: Tubulin alpha

Chain MB:

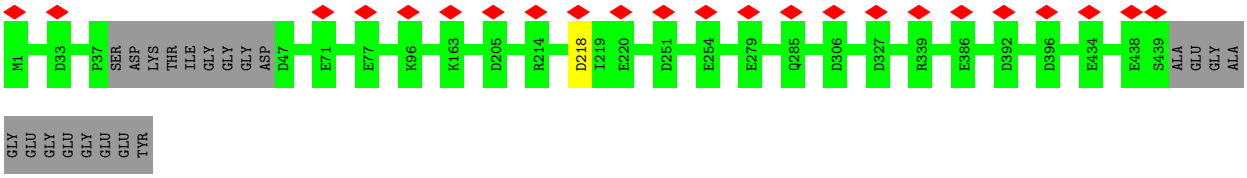




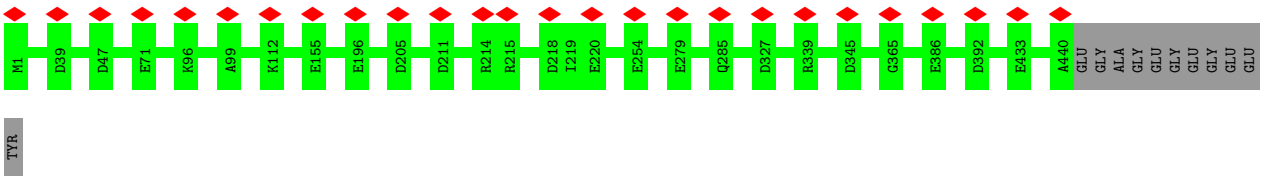
• Molecule 2: Tubulin alpha



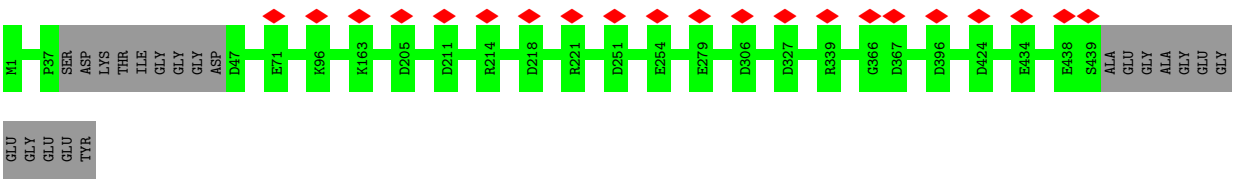
• Molecule 2: Tubulin alpha



• Molecule 2: Tubulin alpha

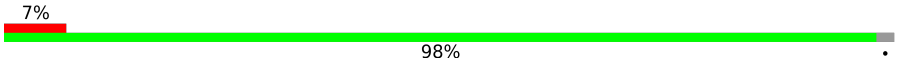


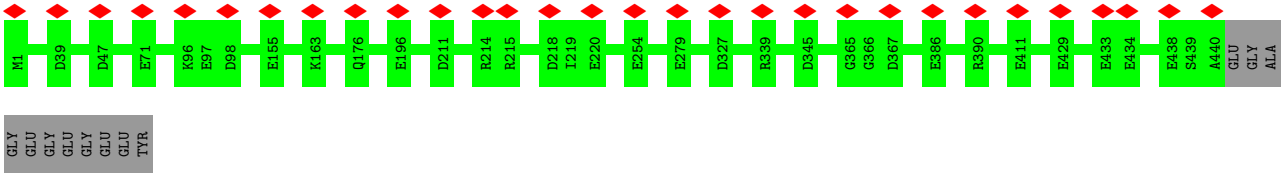
• Molecule 2: Tubulin alpha



• Molecule 2: Tubulin alpha

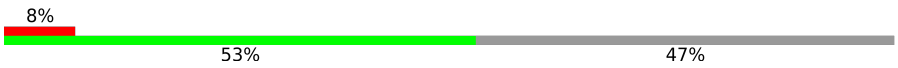
Chain ML:

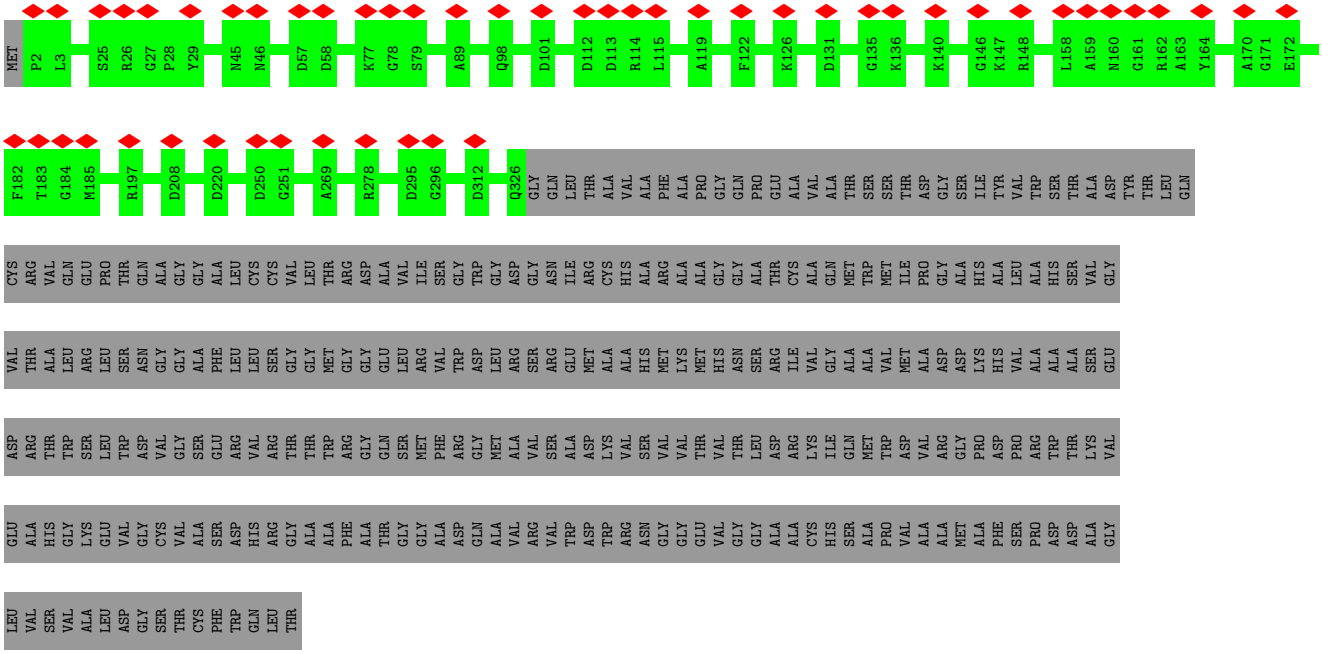




• Molecule 3: Cilia- and flagella-associated protein 20

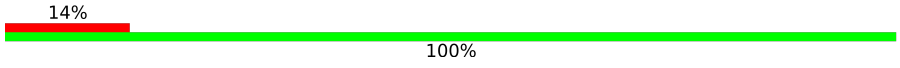
Chain a:

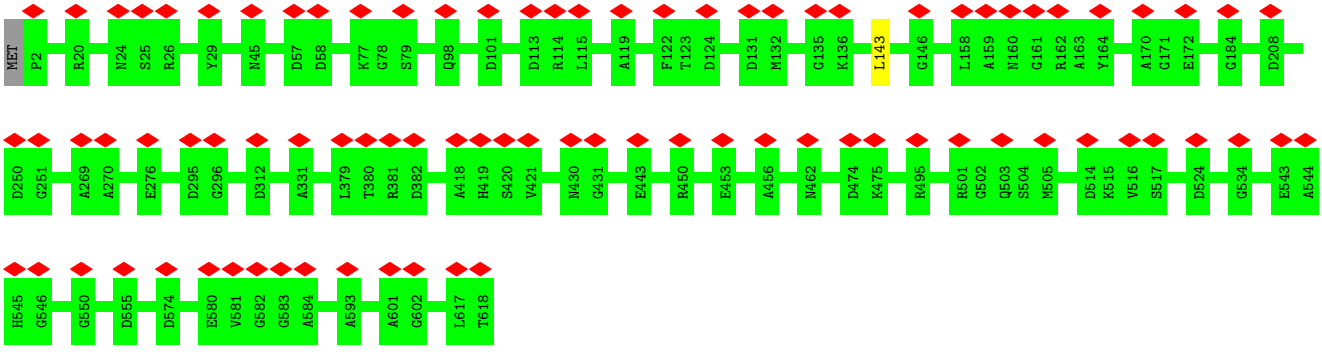




• Molecule 3: Cilia- and flagella-associated protein 20

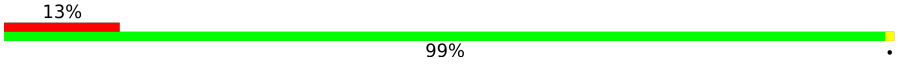
Chain b:

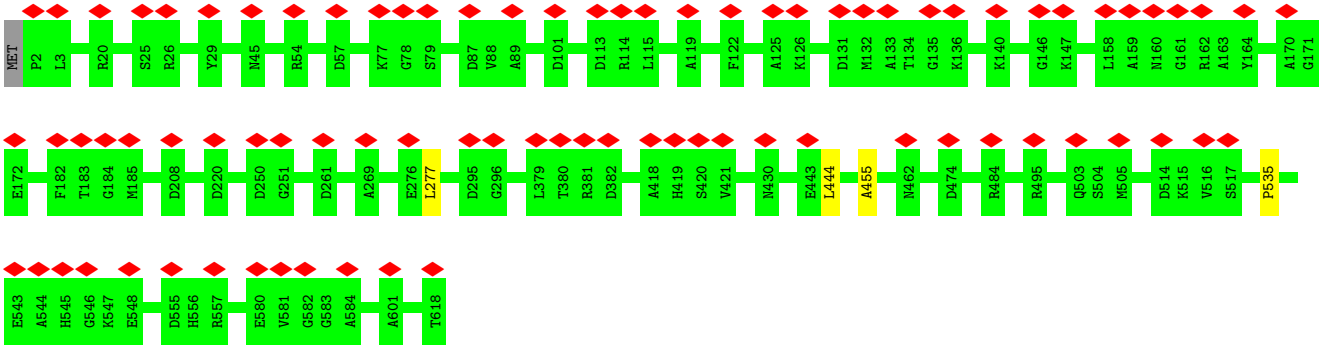




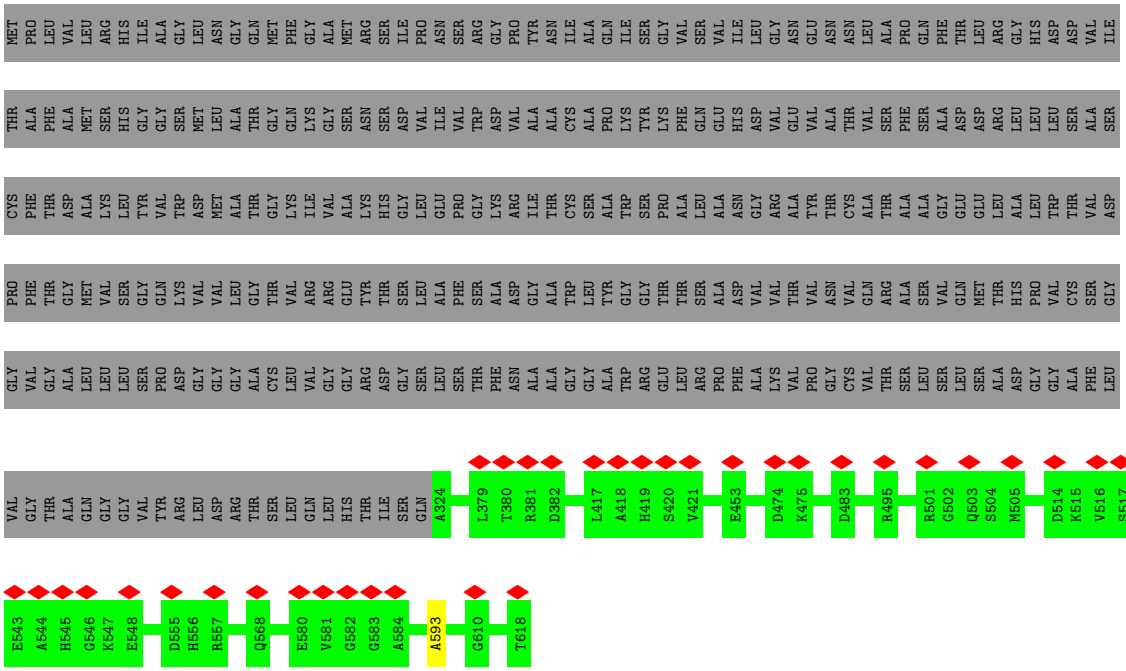
• Molecule 3: Cilia- and flagella-associated protein 20

Chain c:

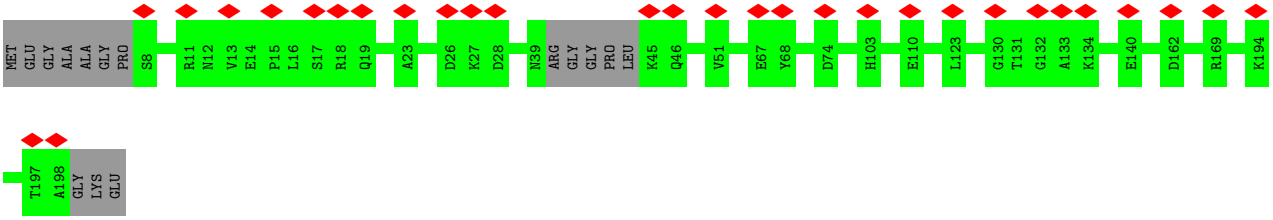




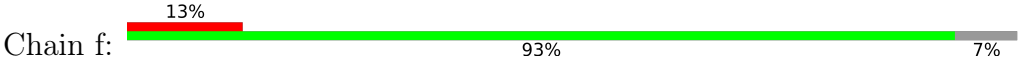
• Molecule 3: Cilia- and flagella-associated protein 20

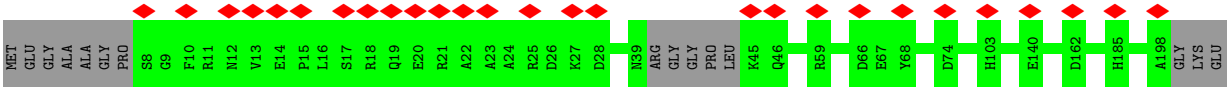


• Molecule 4: Unknown protein



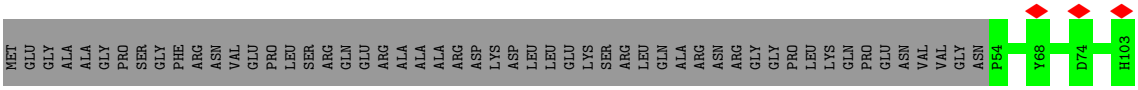
• Molecule 4: Unknown protein

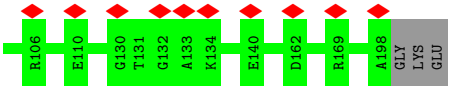




• Molecule 4: Unknown protein

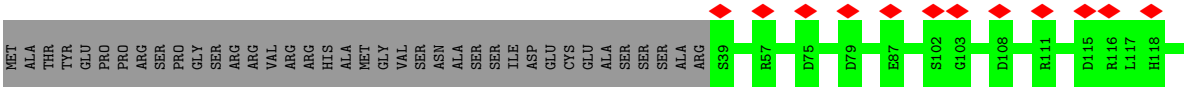
Chain g:

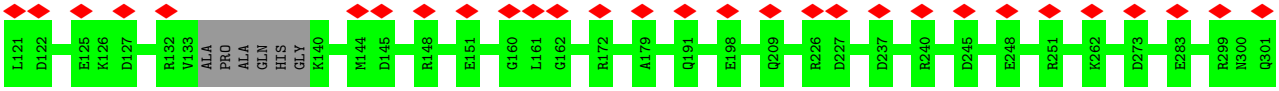


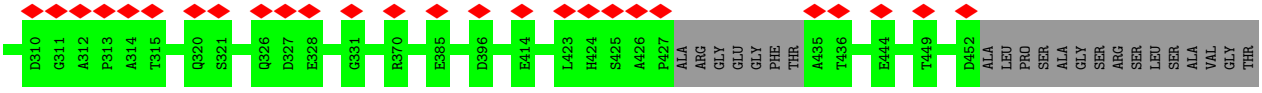


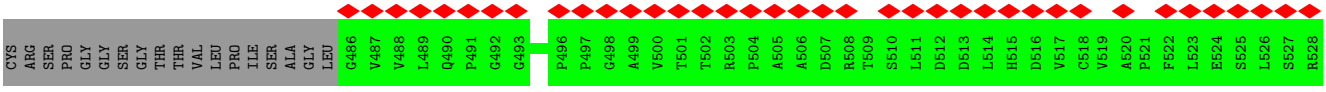
• Molecule 5: Unknown protein

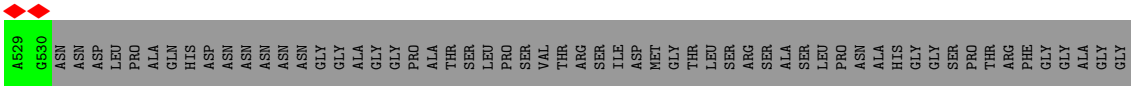
Chain h:

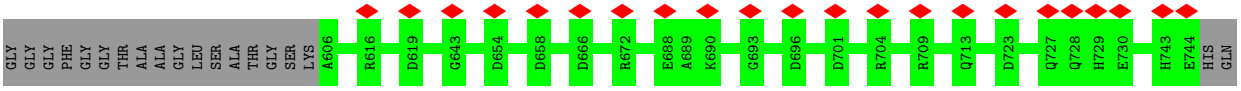






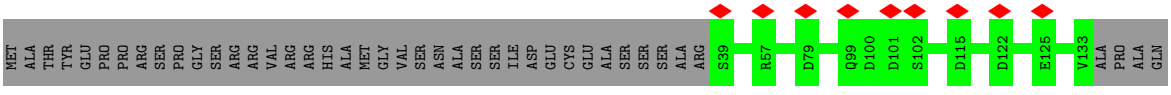


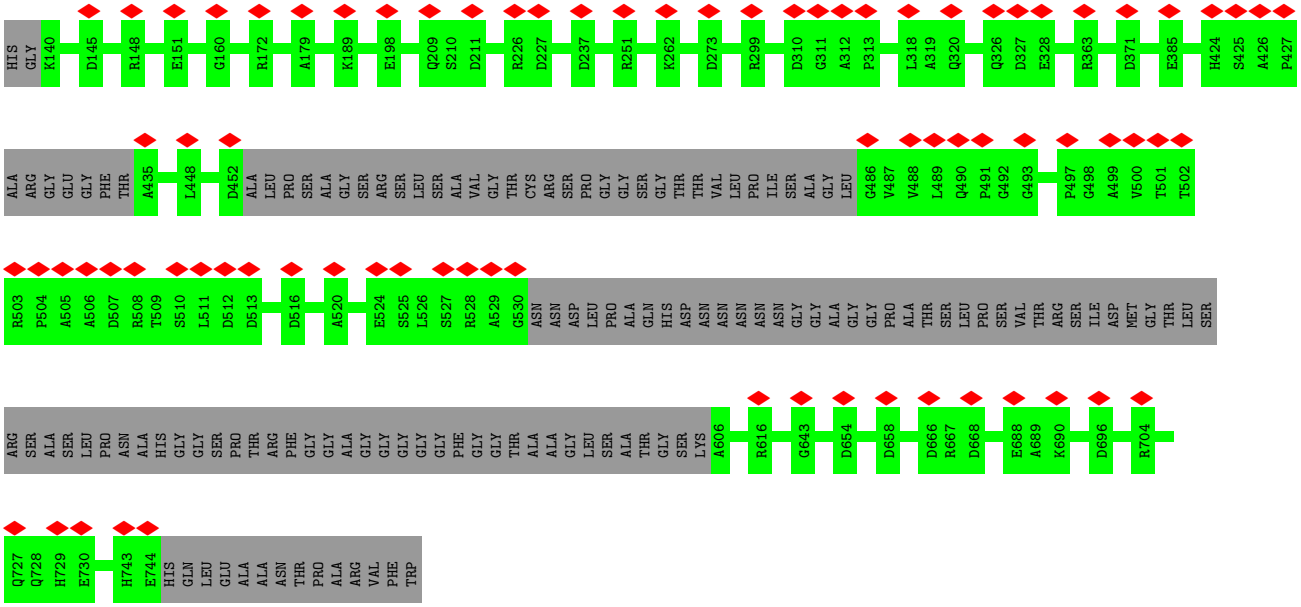




• Molecule 5: Unknown protein

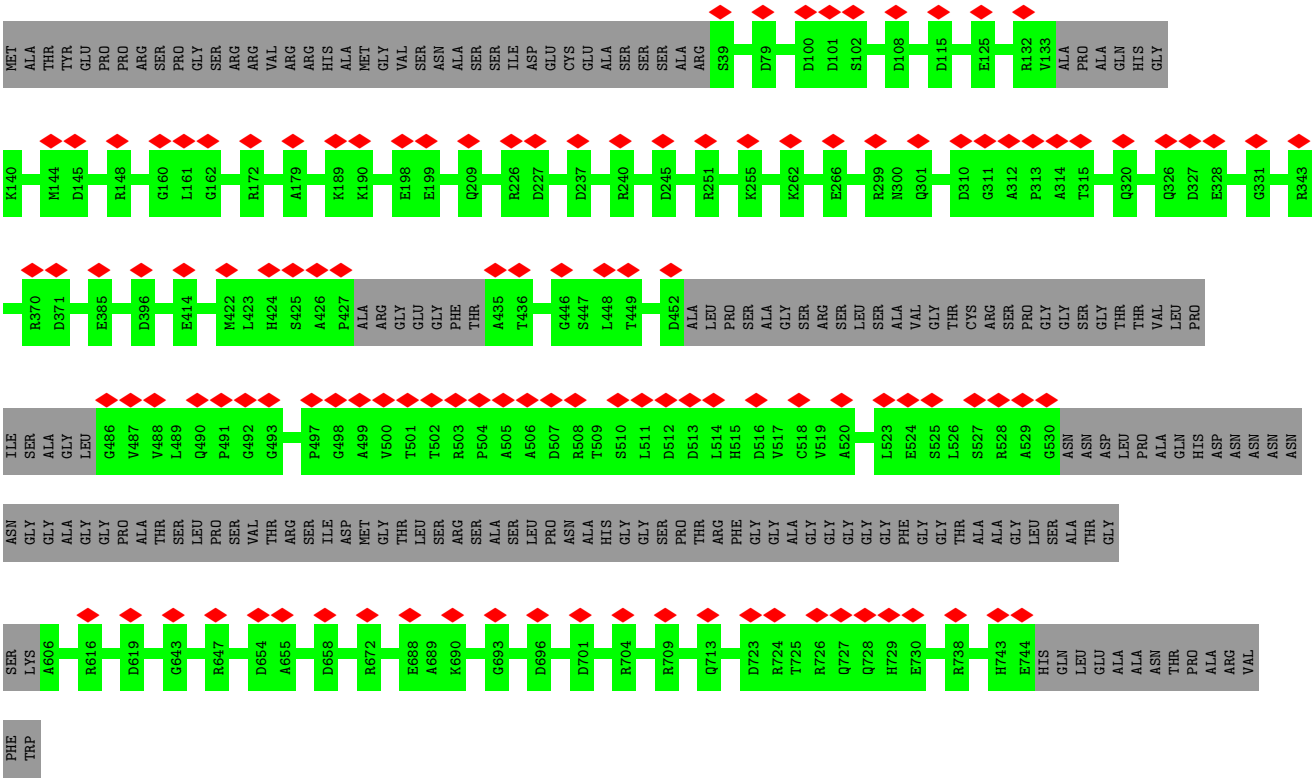
Chain i:





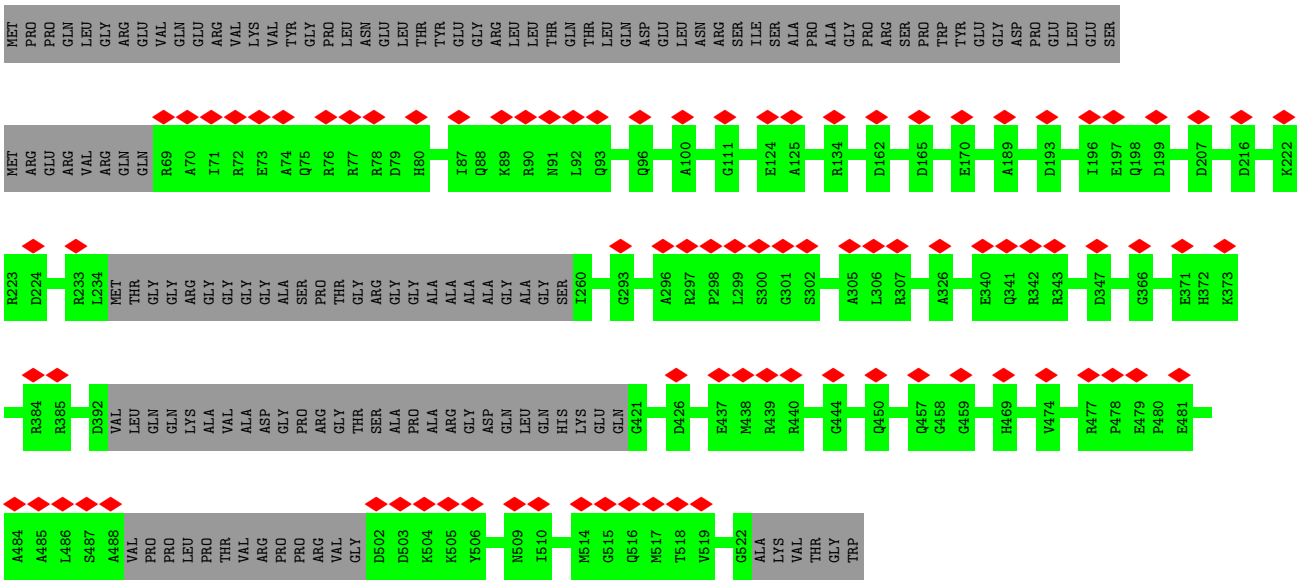
• Molecule 5: Unknown protein

Chain j:



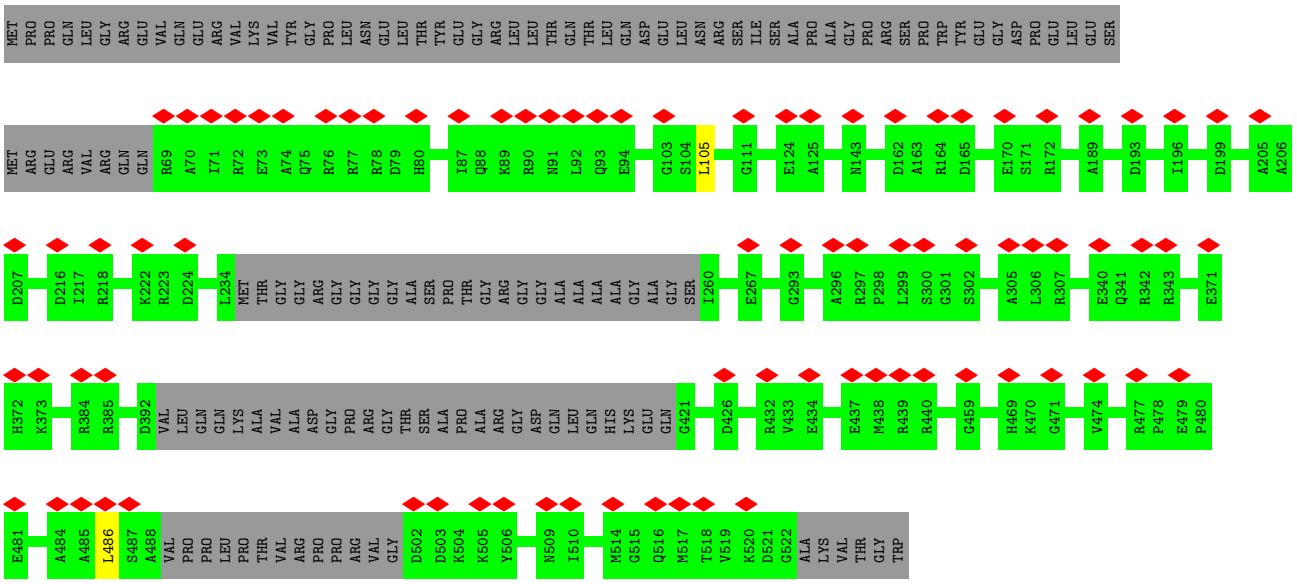
• Molecule 6: Unknown protein

Chain k:



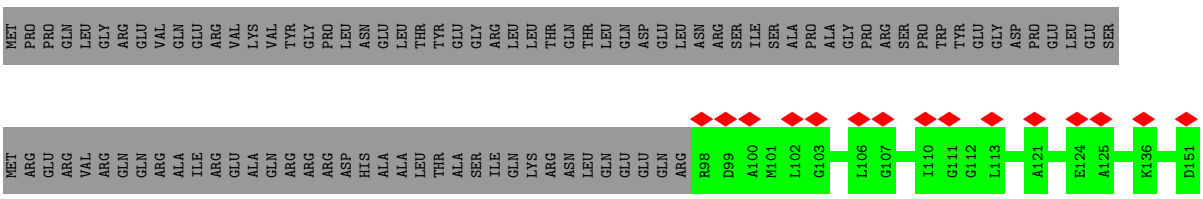
• Molecule 6: Unknown protein

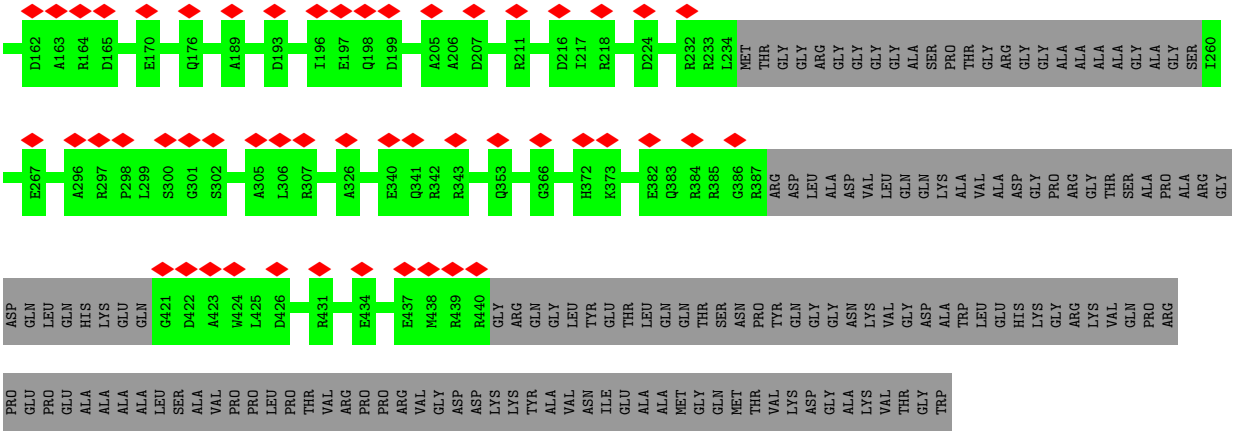
Chain l:



• Molecule 6: Unknown protein

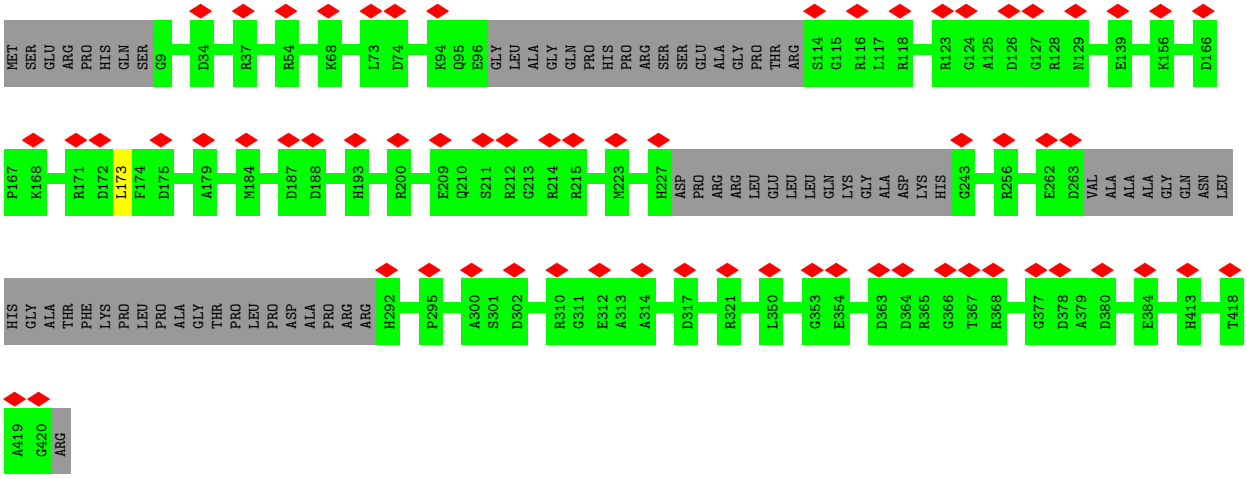
Chain s:





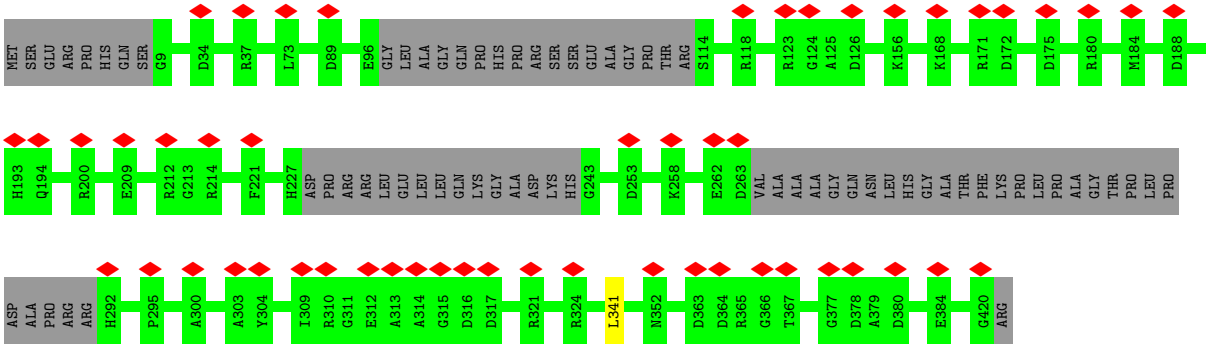
• Molecule 7: FAP65

Chain m:



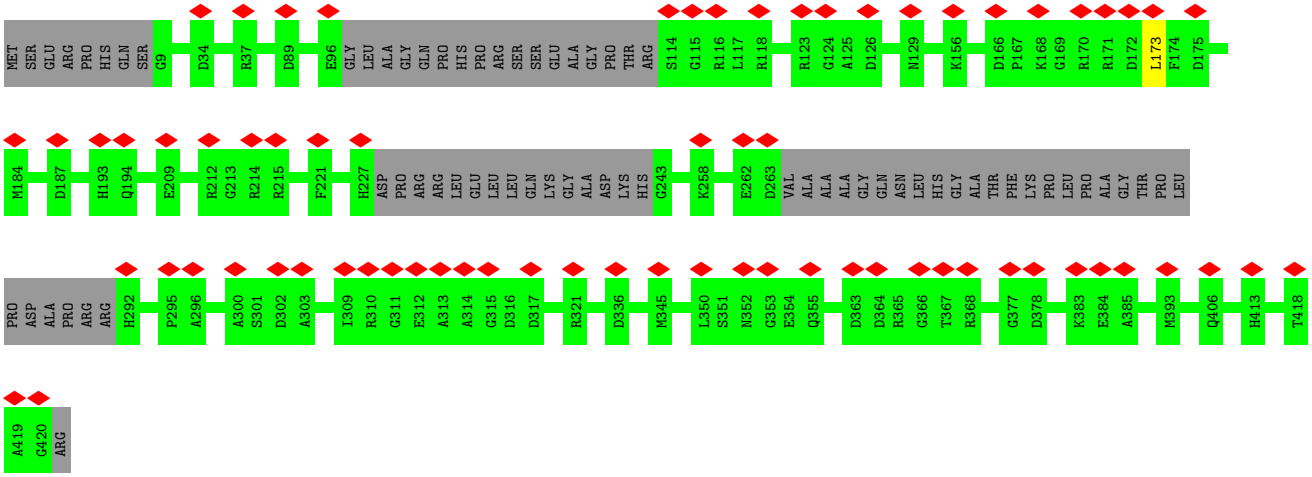
• Molecule 7: FAP65

Chain n:

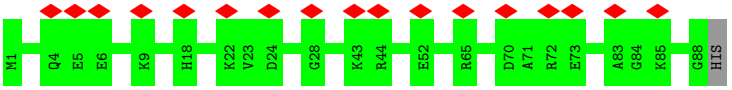


• Molecule 7: FAP65

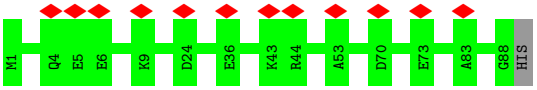
Chain o:



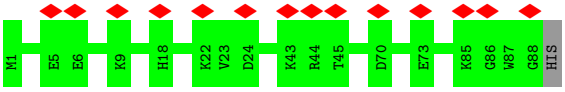
- Molecule 8: FAP70



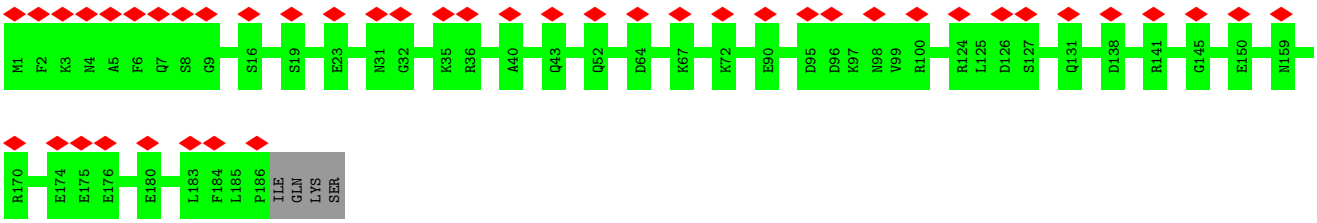
- Molecule 8: FAP70



- Molecule 8: FAP70

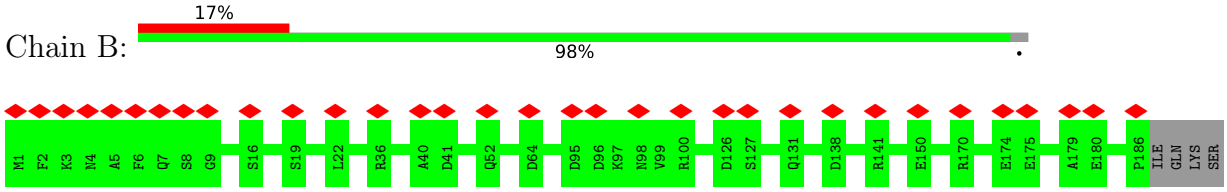


- Molecule 9: FAP147



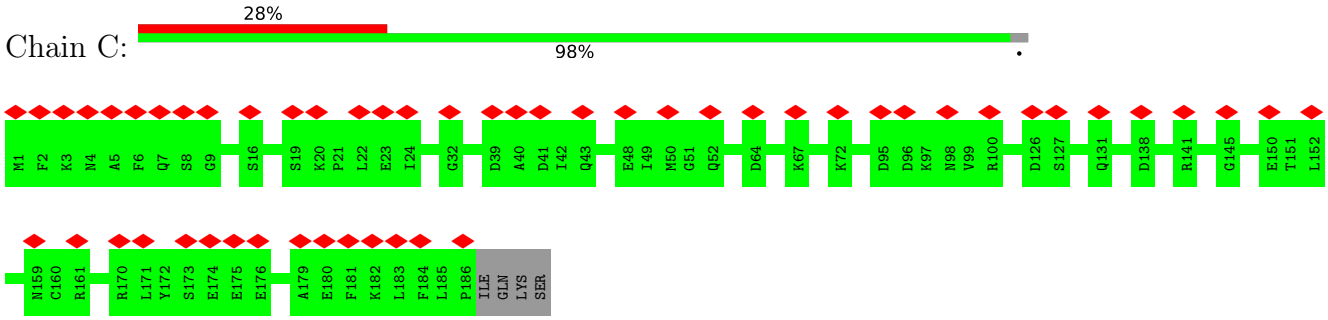
- Molecule 9: FAP147

Chain B:



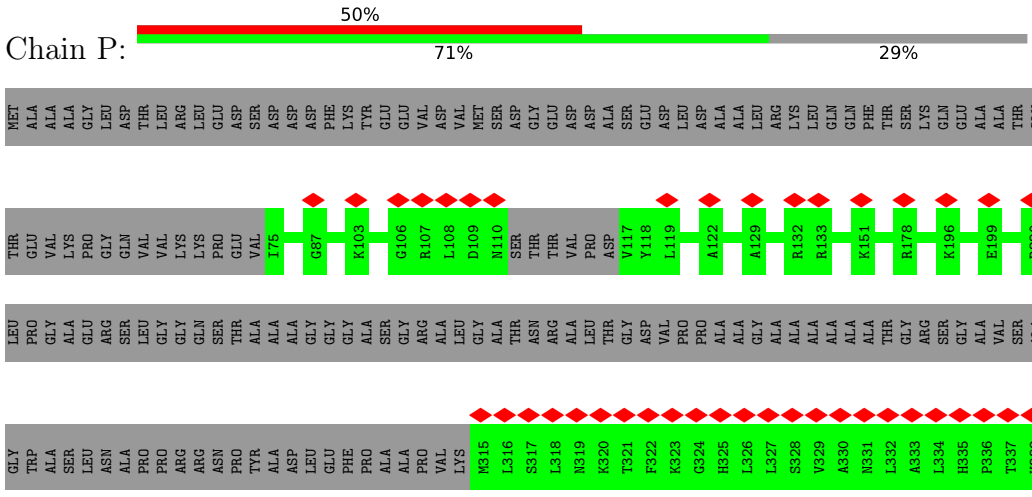
• Molecule 9: FAP147

Chain C:



• Molecule 10: FAP178

Chain P:



• Molecule 10: FAP178

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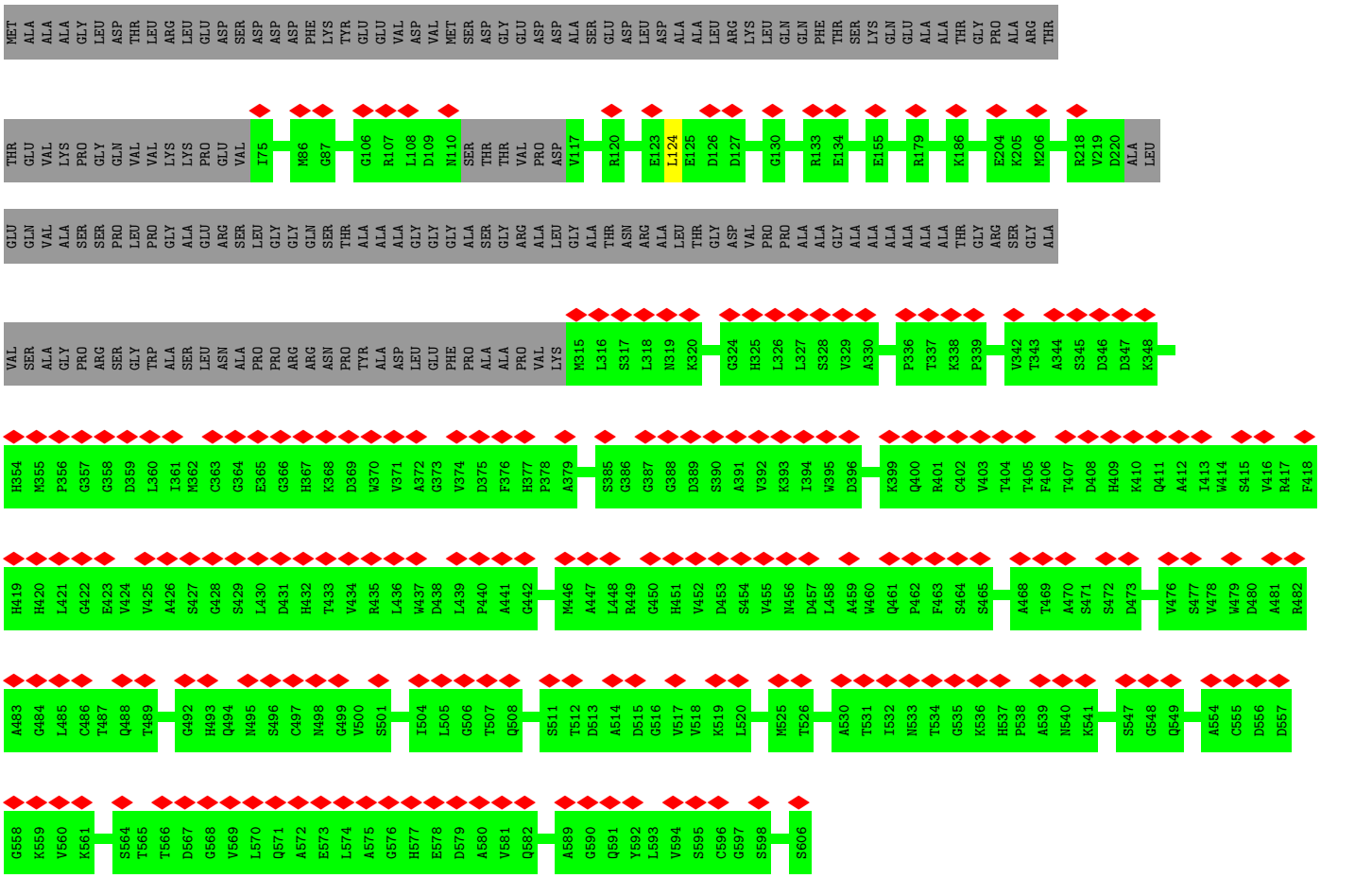

• Molecule 10: FAP178

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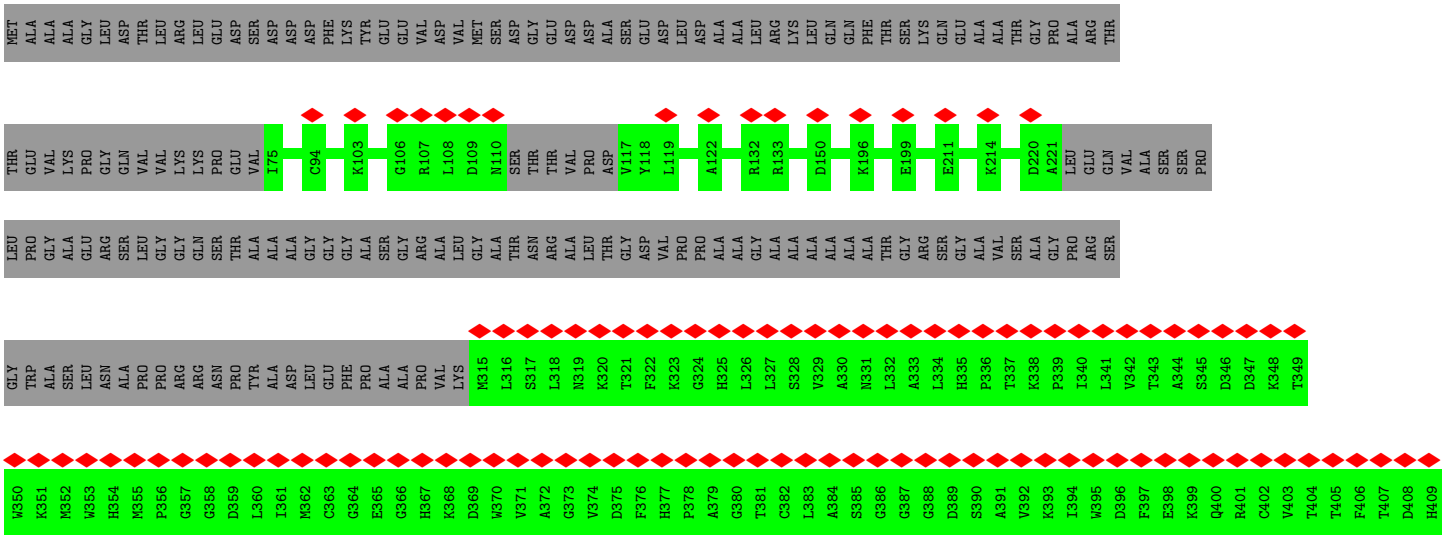

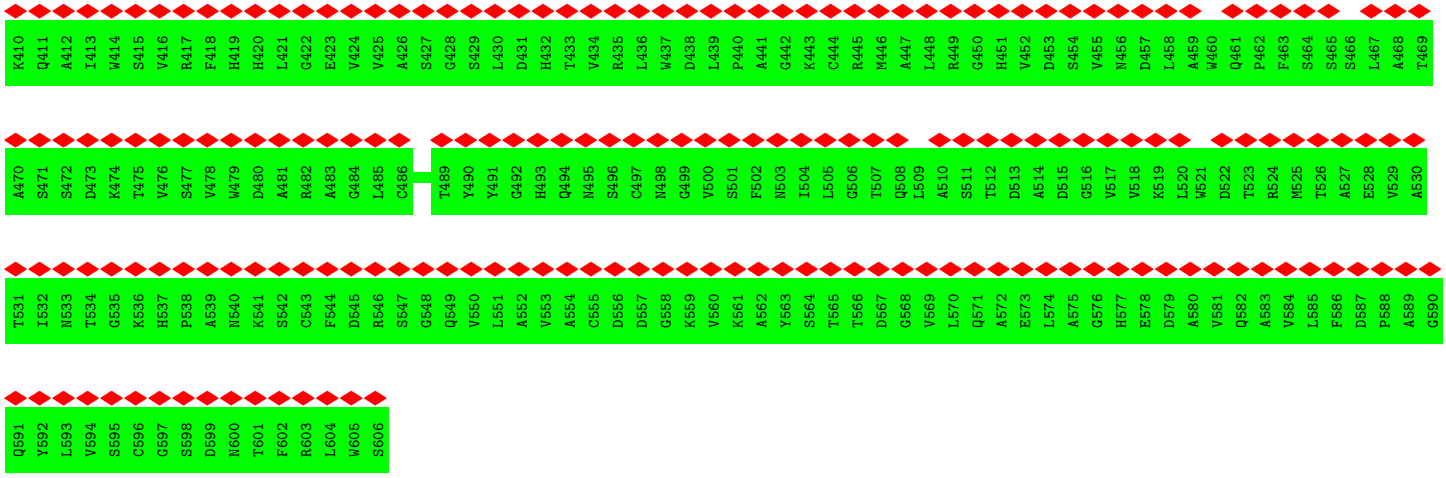

• Molecule 10: FAP178

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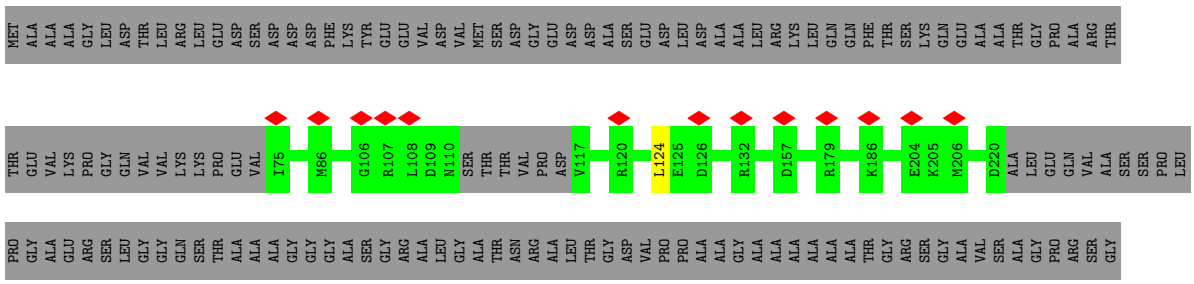
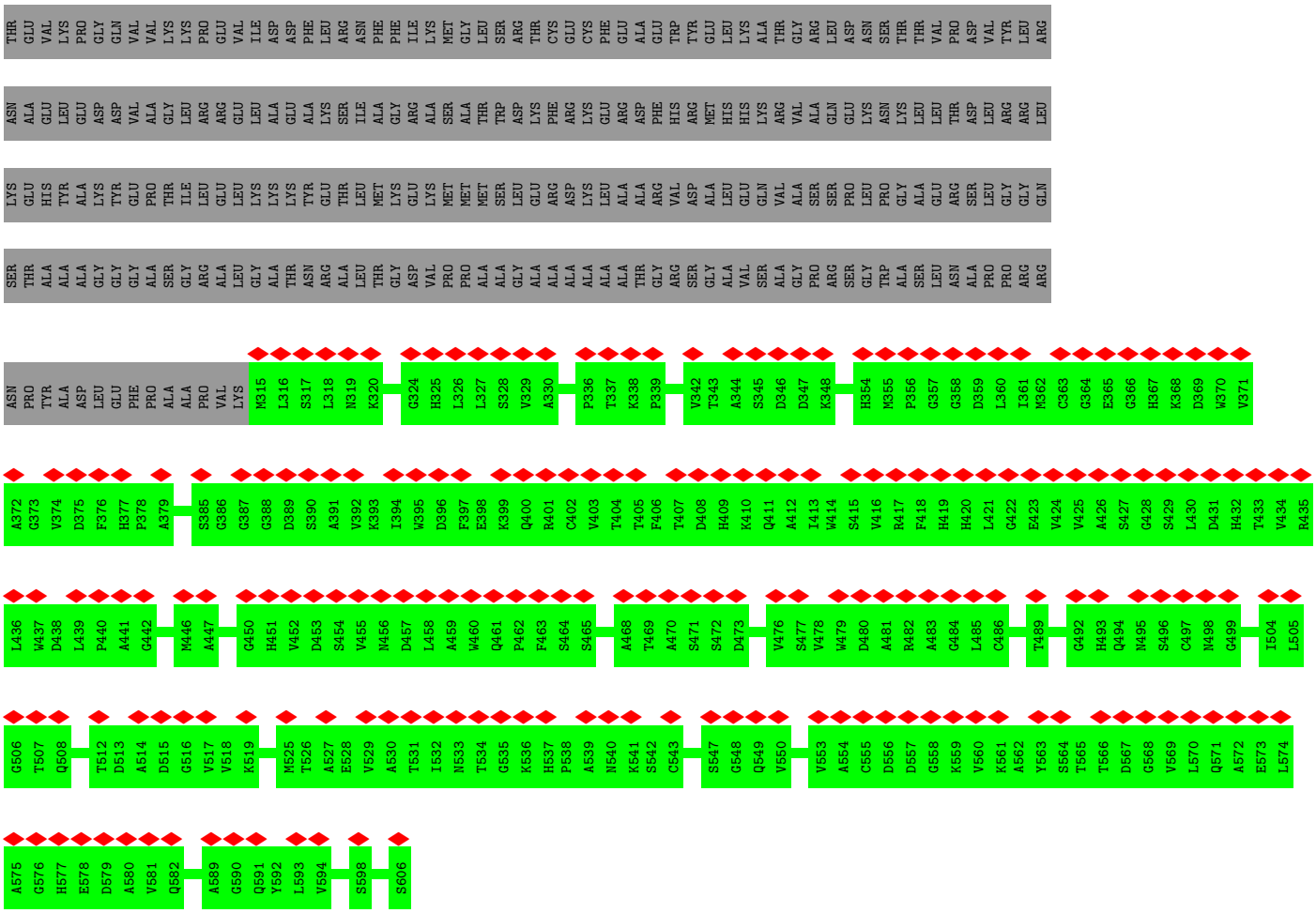


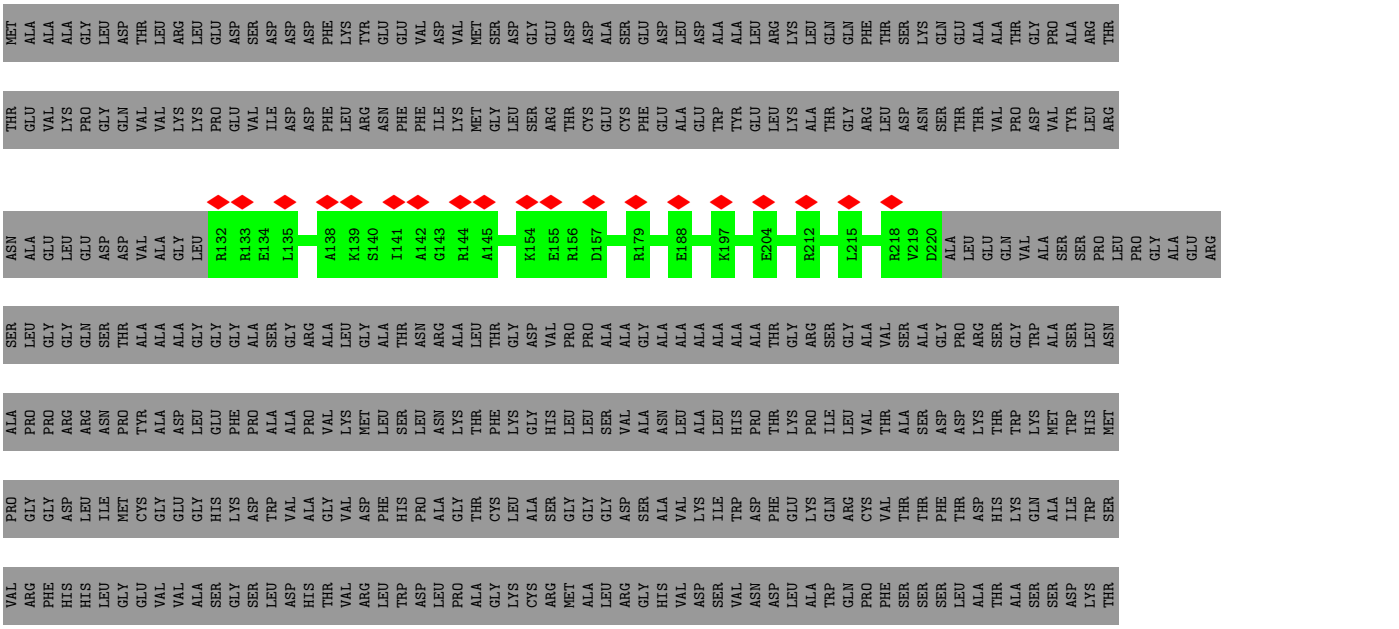
• Molecule 10: FAP178

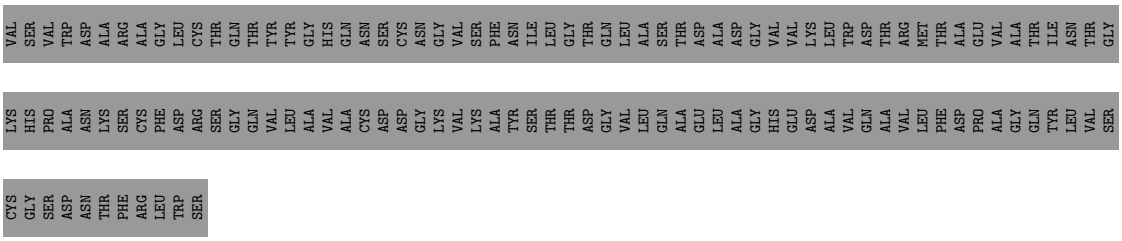
Chain aa:



• Molecule 10: FAP178

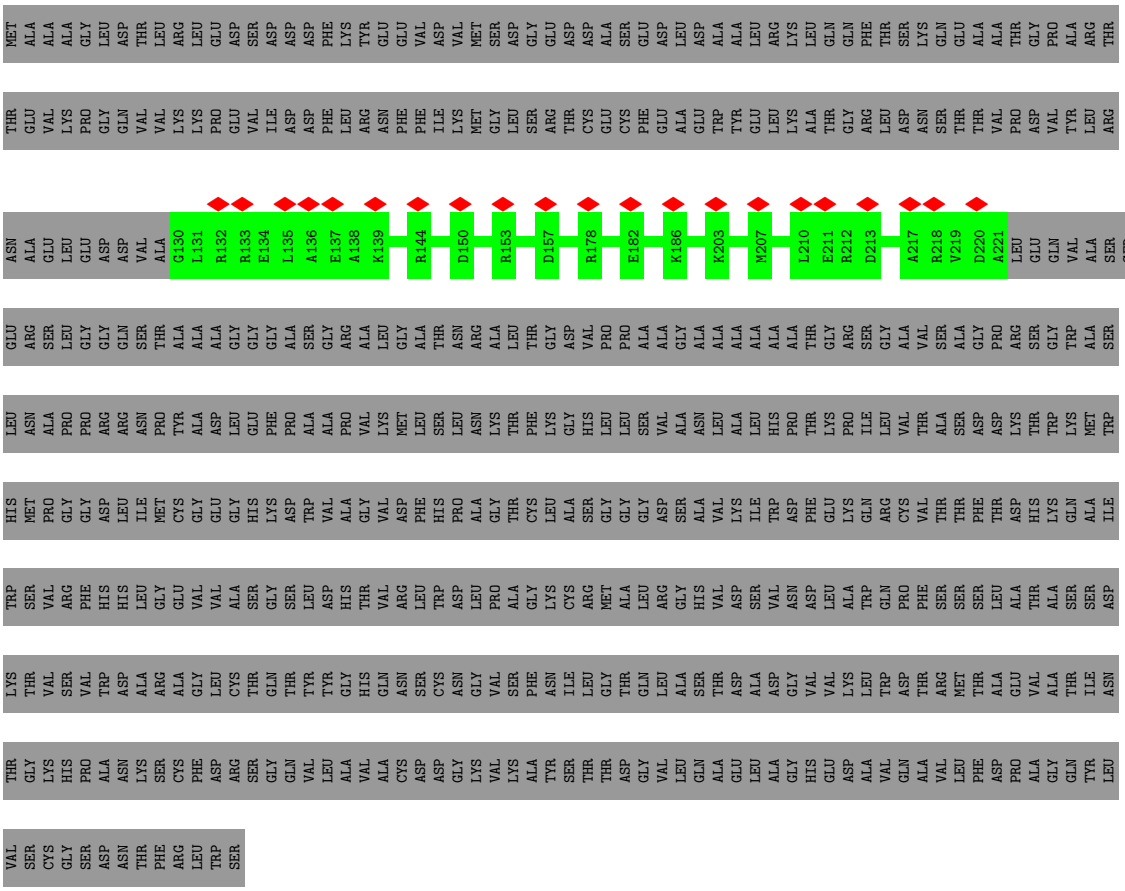
Chain cc:





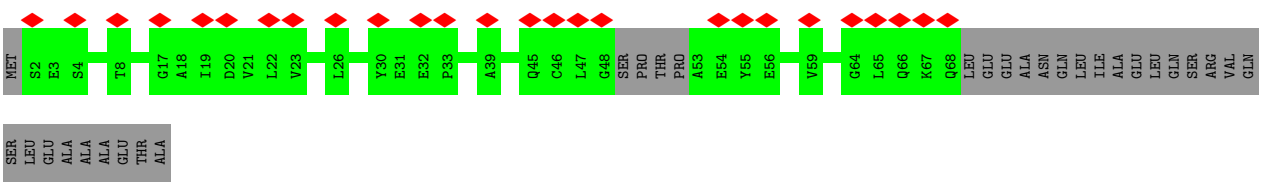
• Molecule 10: FAP178

Chain Z:



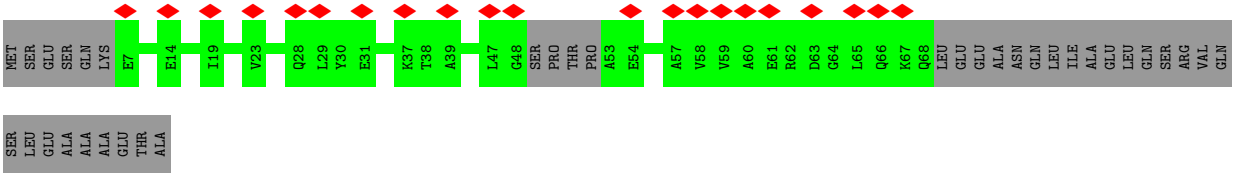
• Molecule 11: Flagellar WD repeat-containing protein Pf20

Chain T:



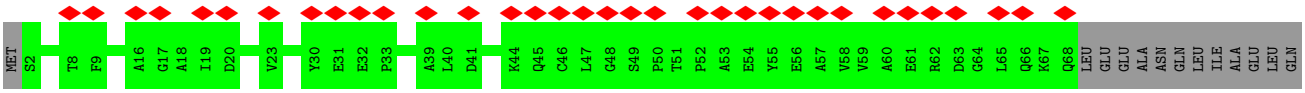
• Molecule 11: Flagellar WD repeat-containing protein Pf20

Chain U:



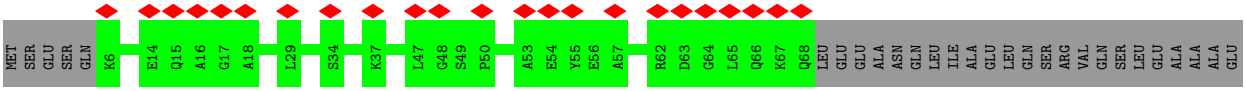
• Molecule 11: Flagellar WD repeat-containing protein Pf20

Chain V:



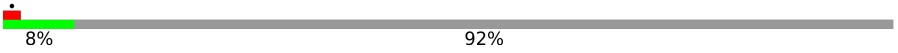
• Molecule 11: Flagellar WD repeat-containing protein Pf20

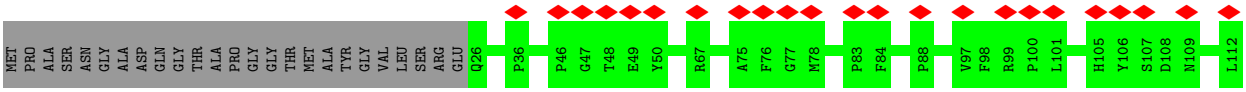
Chain W:

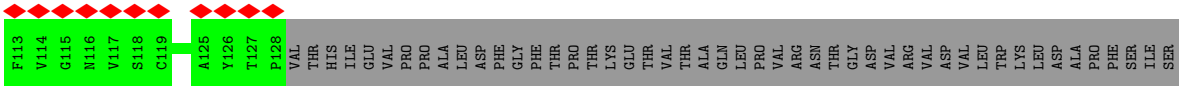


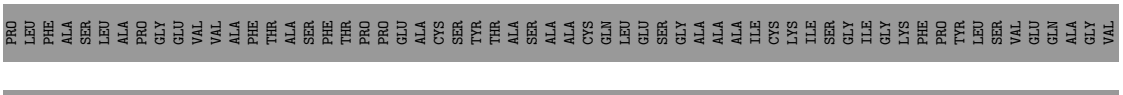
• Molecule 12: Flagellar associated protein

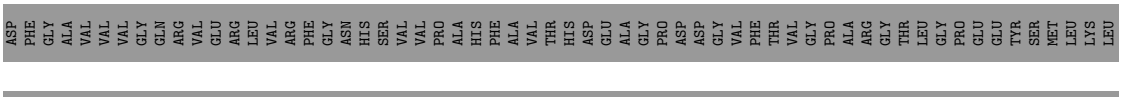
Chain bb:

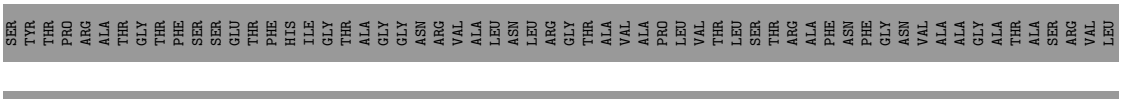


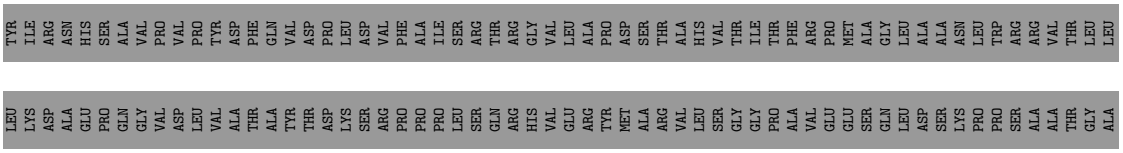


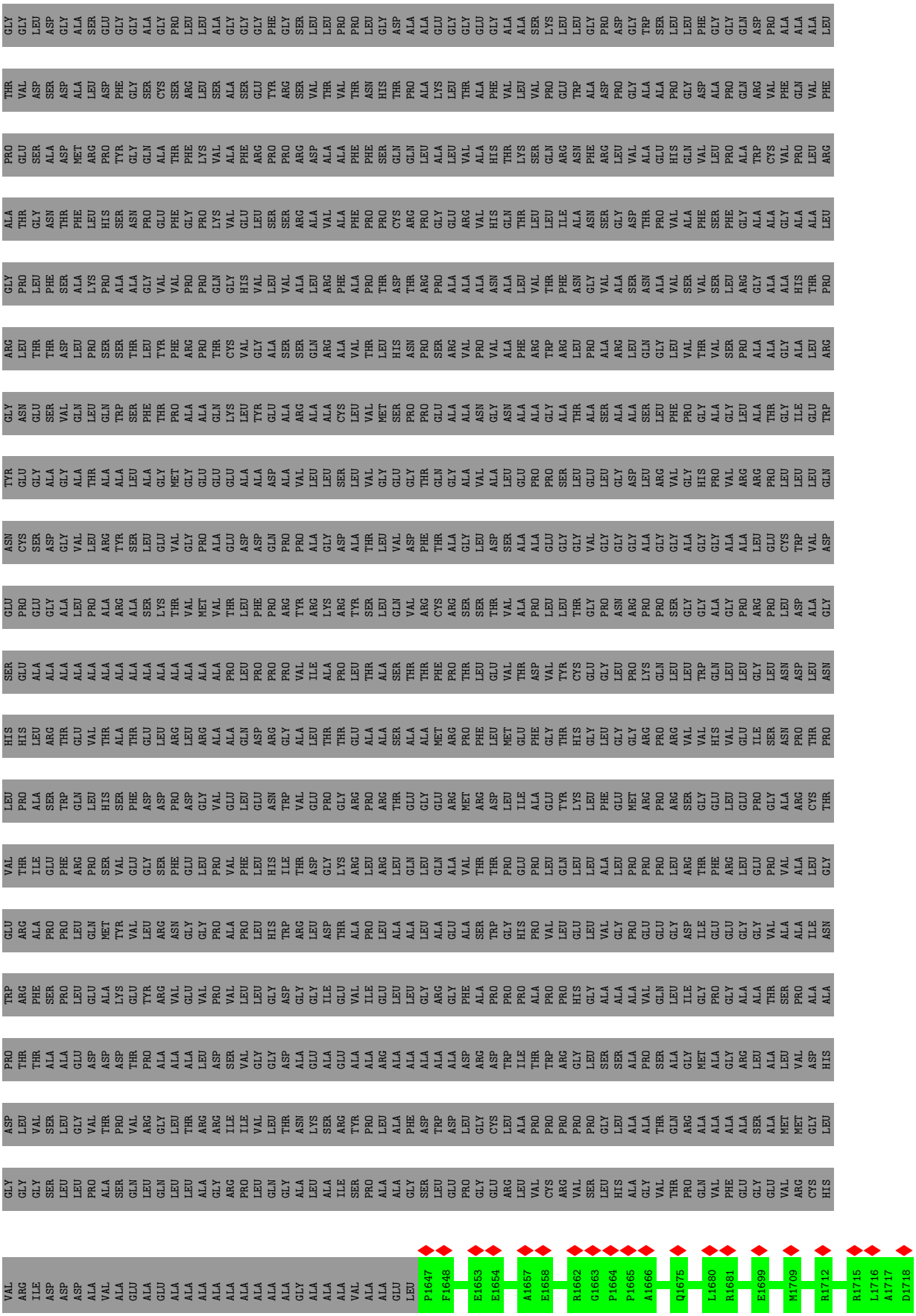








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R1681
E1699
M1709
R1712
R1715
L1716
A1717
D1718

ALA THR ARG PRO PRO SER TRP PRO GLU PRO GLN SER ILE SER VAL THR LEU ARG GLY ARG ILE LEU ASP GLU ARG GLN LEU GLY ALA LEU ARG TYR VAL PRO PRO HIS GLU ARG ALA ALA ALA ARG ALA ALA VAL VAL ALA GLY ALA ALA TRP VAL PRO PRO ALA MET VAL PRO PHE TRP

GLU GLU GLU GLY ARG SER THR PRO ALA VAL SER ALA GLN PRO SER SER GLN GLY GLY GLY GLY TYR GLY VAL GLY GLY TYR GLY GLY GLY TYR GLY SER GLY GLY SER GLN GLY GLY GLU ALA SER VAL ALA PRO SER GLY GLY ASP PRO GLY GLY TYR SER PRO ARG GLY GLY MET ALA

ASP SER TRP PRO SER LEU GLU PRO GLY LEU GLY MET GLU GLU THR VAL VAL GLY PRO PRO THR VAL GLY LEU ASP LEU SER LEU SER LEU GLN HIS ALA GLY GLY ALA GLY GLY ALA PRO GLY GLY ASP GLY ASP SER ASP SER ARG PRO GLY THR PRO SER MET THR ALA ALA ALA HIS

HIS HIS HIS HIS HIS PRO ARG HIS ALA GLY PRO ALA PRO GLY SER GLY THR ALA GLU VAL MET GLU VAL THR PHE SER GLY ASP GLN GLN PRO THR GLY GLY PRO MET PRO SER PRO PRO SER ILE SER GLY ALA PRO ASP PRO ASP SER ALA THR PRO ASP ASP ASP PHE ALA THR SER

ASP ALA ALA VAL ASN ALA ALA ALA ALA VAL ARG ALA ALA GLY GLY GLY MET GLY SER PRO GLN PRO VAL ASP PRO GLY GLY SER ALA ALA ALA ALA ALA SER GLU LEU ALA PRO PRO ALA LEU PRO PRO ALA PRO PRO ARG GLY GLY ASP ILE GLU TYR ASP ALA LEU VAL SER ALA ARG

GLU VAL LEU ALA GLY LEU PHE ALA GLU LEU MET GLU ASP ALA ASP VAL VAL ARG ALA VAL ALA PHE LEU PRO GLU HIS GLU VAL PRO SER PHE ALA GLU VAL ARG ALA THR PRO PRO PRO CYS TYR ASP PRO ALA VAL ARG ALA ALA ALA GLU ALA ALA ARG ALA GLU ALA GLU ALA ARG

ALA ALA ALA GLU ALA ALA THR LYS ALA ALA ALA GLU ALA GLU ALA VAL ALA ALA ARG ALA ALA ALA MET LEU GLY PRO LYS HIS GLU ALA SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER SER ALA ALA SER SER PRO GLY ALA SER

PRO THR GLY LYS ALA PRO VAL VAL GLU ALA ALA THR PRO ARG LEU VAL SER ALA VAL GLY GLY MET ALA PRO SER GLN PRO ALA LEU ALA LEU ARG PRO ALA PRO SER THR PRO PRO ARG THR PRO PRO LYS PRO SER GLN GLY ALA ALA PHE ALA ILE PRO ALA ALA ALA ALA GLN ALA

ALA THR GLU PRO PRO ALA LEU GLU ASP GLU LEU ALA ALA ASP THR GLU LEU ALA ARG VAL LEU VAL ALA PRO GLU TRP ARG ALA PHE ALA ASP PHE VAL LEU GLU SER ALA VAL LEU GLY LEU MET GLN GLU SER ALA ALA GLY ASP TRP GLU MET PRO GLU GLU GLU VAL GLY ARG

- Molecule 12: Flagellar associated protein

Chain D: 20% 67% 33%

MET PRO ALA SER ASN GLY ALA ASP GLN GLY THR ALA PRO GLY GLY THR MET A18 Y19 G20 V21 L22 G47 T48 T72 G77 M78 V97 P100 L101 L112 G115 N116 V117 S118 C119 A125 Y126 T127 P128 V129 T130 H131 I132 E133 A137 L138 D139 F140 G141 F142

T143 P144 T145 K146 E147 T148 V149 T150 A151 P154 V155 R156 N157 T158 G159 D160 V163 D164 V165 K168 L169 D170 S174 P177 L178 F179 A180 S181 L182 V187 V188 A189 A192 S193 F194 T195 P196 A199 C200 S201 Y202 A206 A207 C208 Q209 L210 G213 A214 A215 A216

I217 I220 S221 G222 I223 G224 K225 F226 P227 Q233 A234 G235 V236 D237 F238 V242 V243 G244 Q245 R246 V251 R252 F253 G254 N255 H256 H262 F263 A270 D274 A282 R283 G284 E289 E290 Y291 S292 M293 A302 T303 G304 S307 S308 E309 G314 T315 A316 G317

G318 N319 R320 V321 A322 R326 G327 T328 P332 S337 T338 A347 A348 G349 S353 R354 V355 L356 Y357 I358 R359 N360 H361 S362 A363 P367 Y368 D369 F378 R382 T383 D390 S391 T392 A393 A403 G404 L405 A406 A407 W410 R411 R412 V413 T414 L415 L416 L417 K418

D419 Q423 G424 D434 K435 S436 L441 S442 Q443 V446 M450 V453 V460 GLU GLU SER GLN LEU ASP SER LYS PRO PRO SER ALA ALA THR GLY ALA GLY GLY LEU ASP GLY ALA SER GLU GLY GLY ALA GLY PRO LEU LEU ALA GLY GLY GLY PHE GLY SER LEU LEU

PRO PRO LEU GLY ASP ALA ALA GLU GLY GLY GLU GLY ALA ALA S515 L518 G519 P520 D521 G522 G528 G529 Q530 D531 P532 A533 L536 A542 L543 D544 F545 G546 S547 C548 S549 R550 L551 S552 A553 S554 E555 Y556 R557 S558 V559 N563 K568 F572 V573 L574 E577 W578

A579 D580 P581 GLY ALA ALA PRO GLY ASP ALA P589 Q590 P597 E598 S599 A600 D601 M602 A608 T609 F610 K611 V612 A613 F614 R615 P616 P617 R618 D619 F623 S624 L627 A628 L629 V630 A631 R637 L641 V647 L648 P649 A650 W651 S665 N666 P667 E668 F669 G670 P671 K672

V673 E674 L675 S676 P683 P684 C685 R686 P687 G688 E689 R690 V691 H692 Q693 L696 I697 A698 N699 S700 G701 D702 T703 P704 V705 A706 F707 S708 F709 GLY ALA ALA GLY ALA ALA L716 G717 P718 L719 A722 K723 P724 A725 A726 G727 V728 Q732 G733 H734 V735 L736 V737 R740 F741 A742

P743 T744 D745 T746 A750 L754 V755 T756 F757 N758 G759 V760 A761 S762 N763 A764 V765 S766 V767 S768 L769 R770 G771 A772 A773 H774 T775 P776 R777 L778 T779 T780 D781 S785 F789 R790 C793 A796 S797 S798 Q799 R800 A801 S808 R809 V810 P811 V812 A813 F814 R815 W816 R817

A820 V826 T827 V828 A831 A832 G833 A834 N838 E839 Q842 L843 Q844 W845 S846 F847 A850 A851 A857 L862 V863 M864 SER PRO PRO GLU ALA ALA ASN GLY ASN ALA ALA GLY ALA THR ALA SER ALA ALA SER LEU PHE PRO GLY ALA GLY LEU ALA THR GLY ILE

GLU TRP TYR GLU GLY ALA GLY ALA THR ALA ALA LEU ALA GLY MET GLY GLU GLU GLU ALA ALA ASP ALA VAL LEU LEU SER LEU VAL GLY GLU GLY T927 Q928 G929 A932 L933 S937 G941 V945 G946 H947 L955 Q956 N957 D960 G961 R964 Y965 V969 G970 P971

A972 E973 D974 G980 D981 A982 T983 D986 F987 T988 ALA GLY LEU ASP SER ALA ALA GLU GLY GLY VAL GLY GLY GLY ALA GLY GLY ALA GLY GLY ALA ALA L1011 D1016 E1019 A1024 R1025 A1026 S1027 T1033 L1034 K1040 S1043 C1048 R1049 S1050 S1051 THR VAL ALA PRO

LEU LEU THR GLY PRO ASN ARG PRO PRO SER GLY GLY ALA GLY PRO ARG PRO LEU ASP ALA GLY SER GLU ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA PRO LEU PRO P1096 I1099 A1104 S1105 F1108 A1164 D1210 G1211 E1219 V1265 K1281

A1314 L1315 G1316 N1329 G1330 G1331 L1335 A1345 G1370 G1371 W1377 A1384 L1406 G1407 V1423 GLN LEU ILE GLY PRO GLY ALA ALA THR SER PRO ALA ALA PRO THR THR ALA ALA GLU ASP ASP ASP THR PRO ALA ALA A1450 S1453 V1454 D1457 A1468 A1469 I1474

T1475 W1476 R1477 V1506 S1520 P1536 PRO PRO PRO GLY LEU ALA ALA THR GLN ARG ALA ALA ALA ALA SER ALA MET MET GLY LEU GLY GLY GLY SER LEU L1562 L1567 Q1568 R1573 G1577 A1585 C1596 A1602 R1614 C1615 H1616 E1628 A1634 A1635 A1636 A1637 G1638

A1639 A1640 A1641 V1642 A1643 A1644 E1653 A1657 G1663 P1664 P1665 A1666 D1718 A1719 T1720 R1721 L1740 V1751 A1765 G1766 A1767 E1779 GLU GLU GLY ARG SER THR PRO ALA VAL SER ALA GLN PRO SER SER GLN GLY GLY GLY GLY TYR GLY VAL GLY GLY TYR GLY GLY GLY TYR

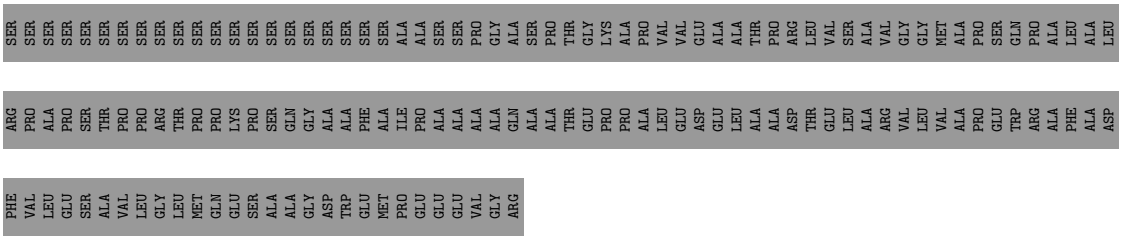
GLY SER GLY GLY SER GLN GLY GLY GLU ALA SER VAL ALA PRO SER GLY GLY ASP PRO GLY GLY TYR SER PRO ARG GLY GLY MET ALA ASP SER TRP PRO SER LEU GLU PRO GLY LEU GLY MET GLU GLU THR VAL VAL GLY PRO PRO THR VAL GLY LEU ASP LEU SER LEU SER LEU GLN

HIS ALA GLY GLY ALA GLY GLY ALA PRO GLY GLY ASP GLY ASP SER ASP SER ARG PRO GLY THR PRO SER MET THR ALA ALA ALA HIS HIS HIS HIS HIS HIS PRO ARG HIS ALA GLY PRO ALA PRO GLY SER GLY THR ALA GLU VAL MET GLU VAL THR PHE SER GLY ASP GLN GLN PRO

THR GLY GLY PRO MET PRO SER PRO PRO SER ILE SER GLY ALA PRO ASP PRO ASP SER ALA THR PRO ASP ASP ASP PHE ALA THR SER ASP ALA ALA VAL ASN ALA ALA ALA ALA VAL ARG ALA ALA GLY GLY GLY MET GLY SER PRO GLN PRO VAL ASP PRO GLY GLY SER ALA ALA ALA

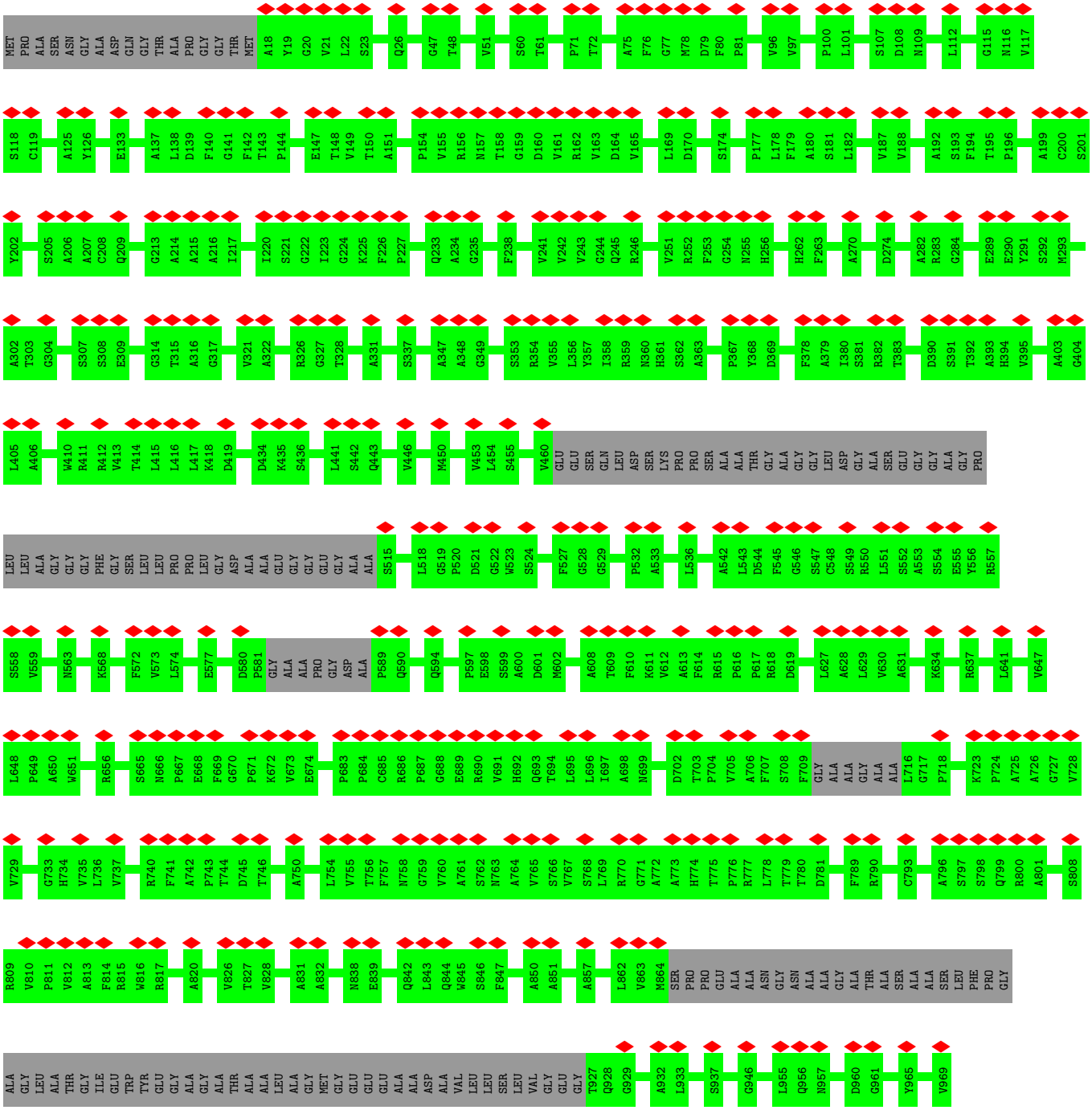
ALA ALA SER GLU LEU ALA PRO PRO ALA LEU PRO PRO ALA PRO PRO ARG GLY GLY ASP ILE GLU TYR ASP ALA LEU VAL SER ALA ARG GLU VAL LEU ALA GLY LEU PHE ALA GLU LEU MET GLU ASP ALA ASP VAL VAL ARG ALA VAL ALA PHE LEU PRO GLU HIS GLU VAL PRO SER PHE

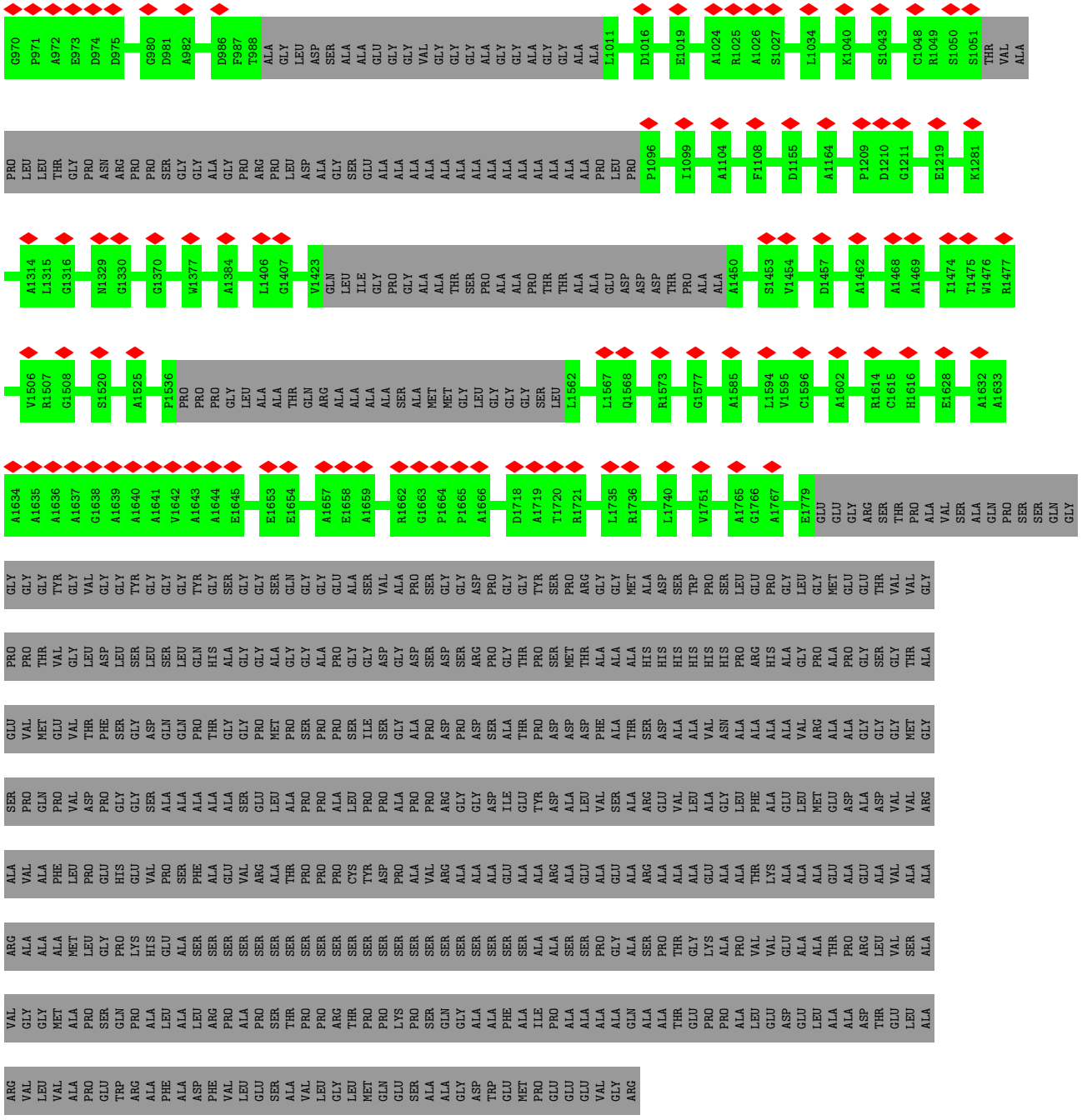
ALA GLU VAL ARG ALA THR PRO PRO PRO CYS TYR ASP PRO ALA VAL ARG ALA ALA ALA GLU ALA ALA ARG ALA GLU ALA GLU ALA ARG ALA ALA ALA GLU ALA ALA THR LYS ALA ALA ALA GLU ALA GLU ALA VAL ALA ALA ARG ALA ALA ALA MET LEU GLY PRO LYS HIS GLU ALA SER



• Molecule 12: Flagellar associated protein

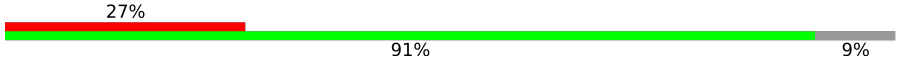
Chain E:

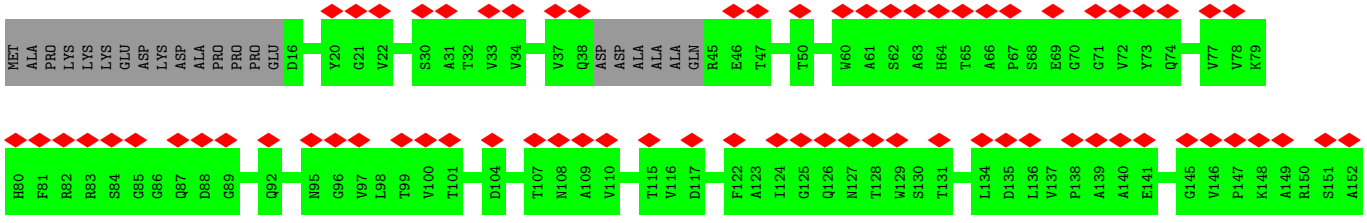


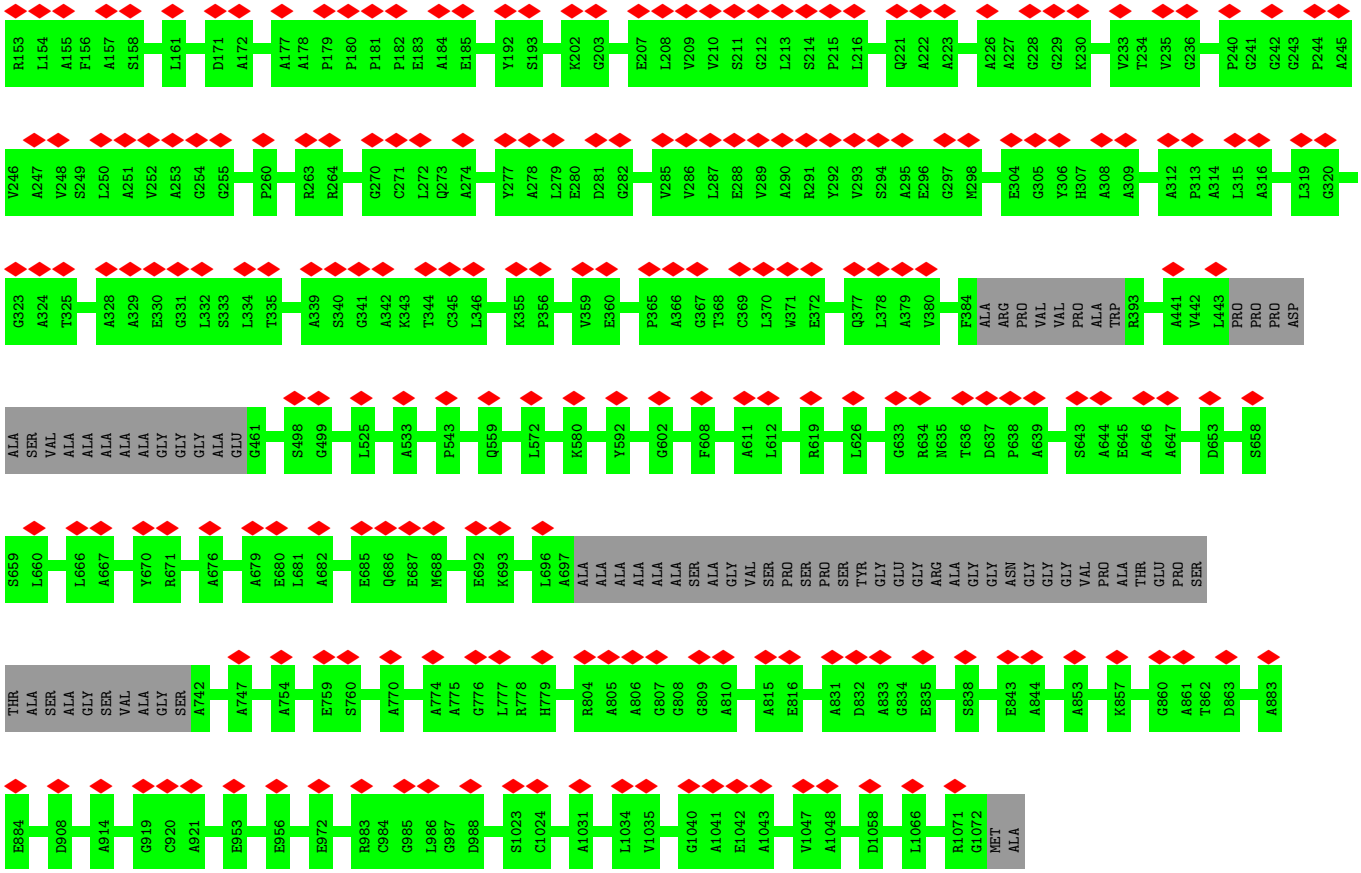


• Molecule 13: FAP196

Chain F:

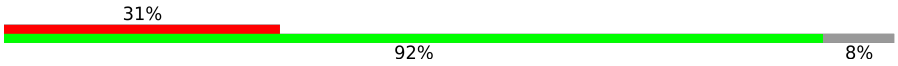


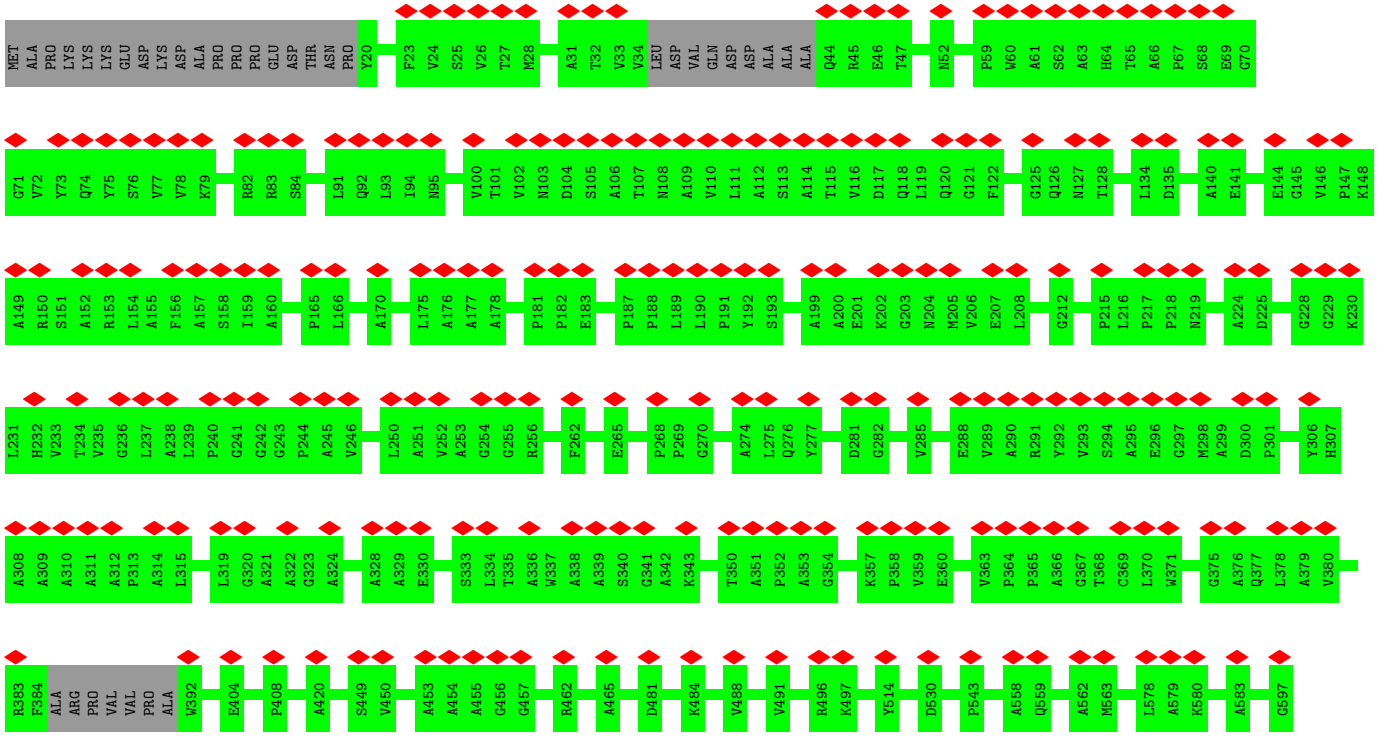


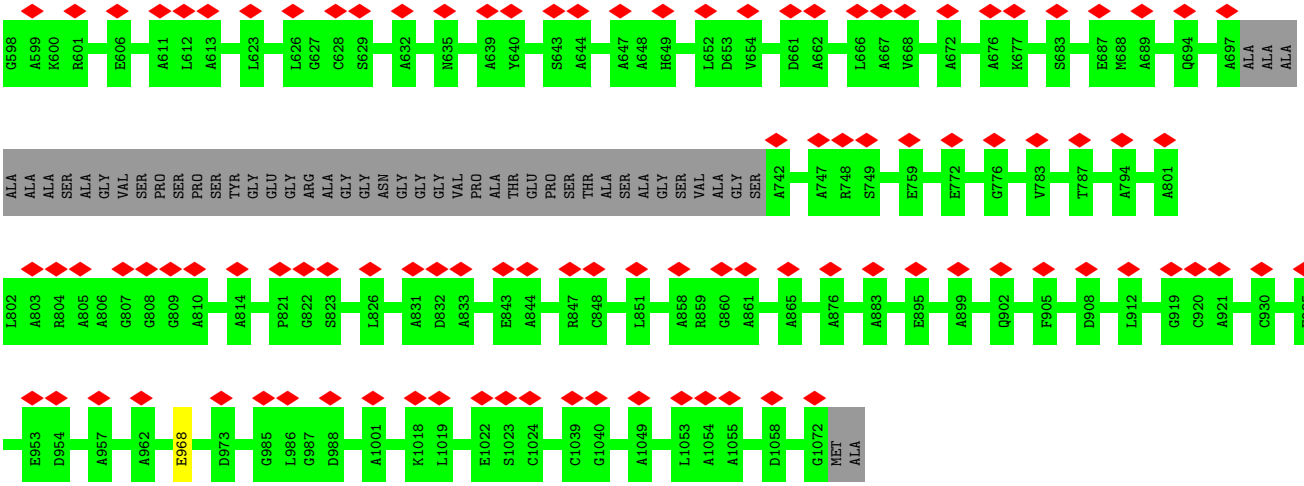


- Molecule 13: FAP196

Chain G:

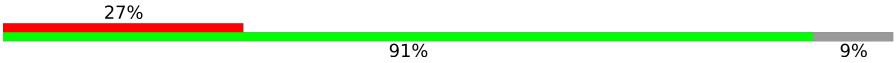


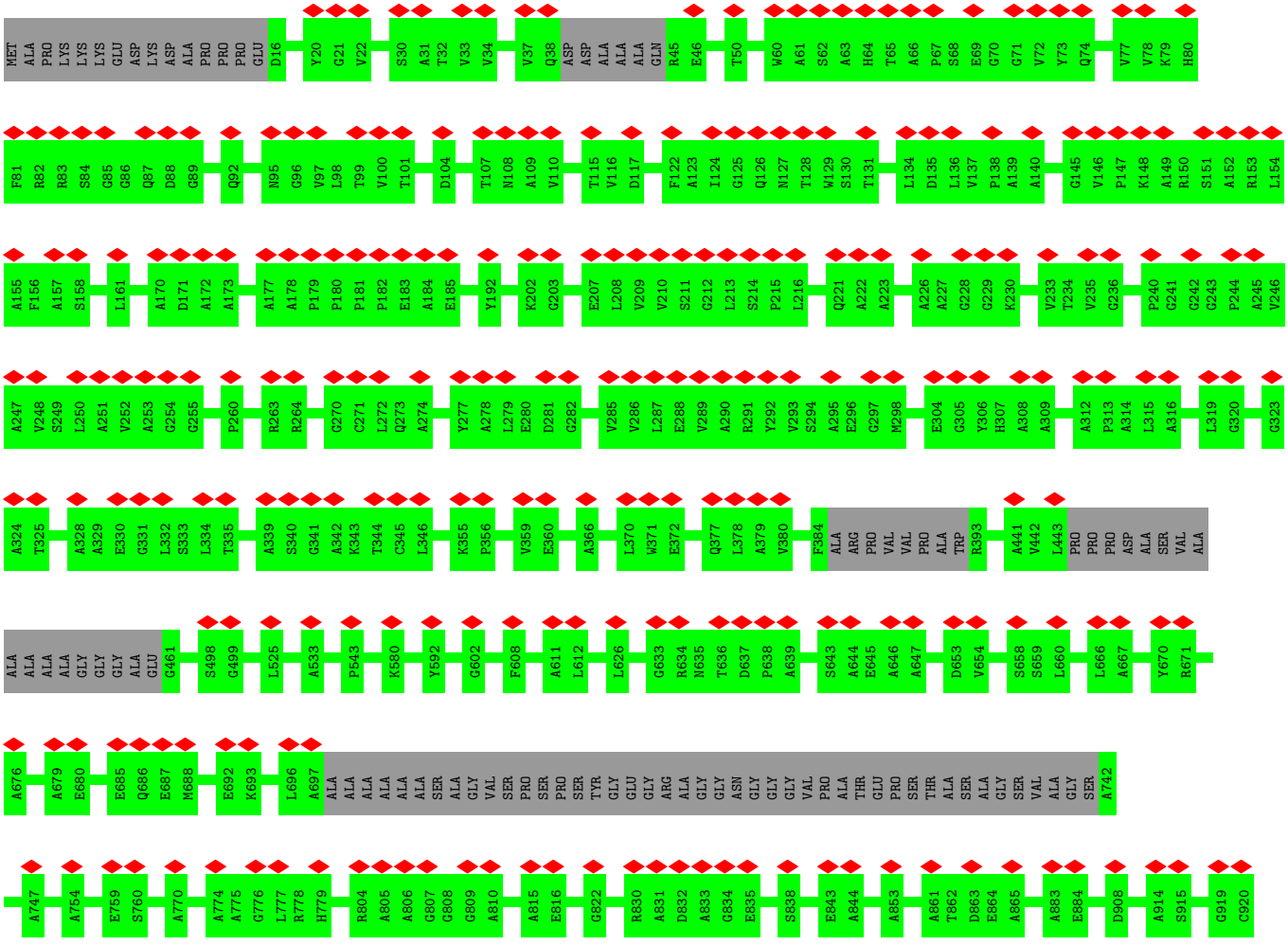


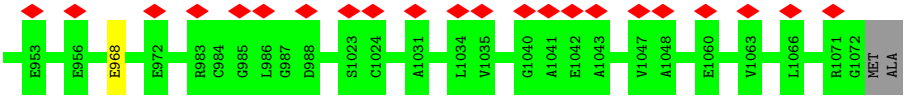


• Molecule 13: FAP196

Chain H:

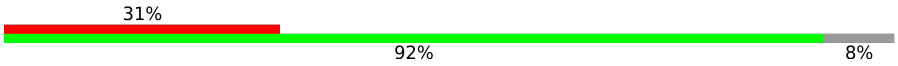


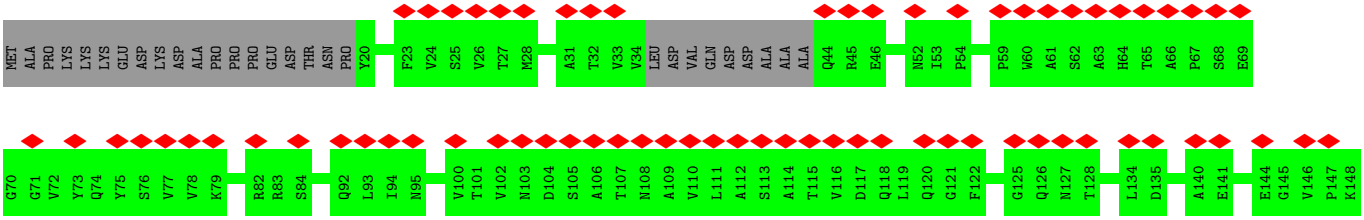




• Molecule 13: FAP196

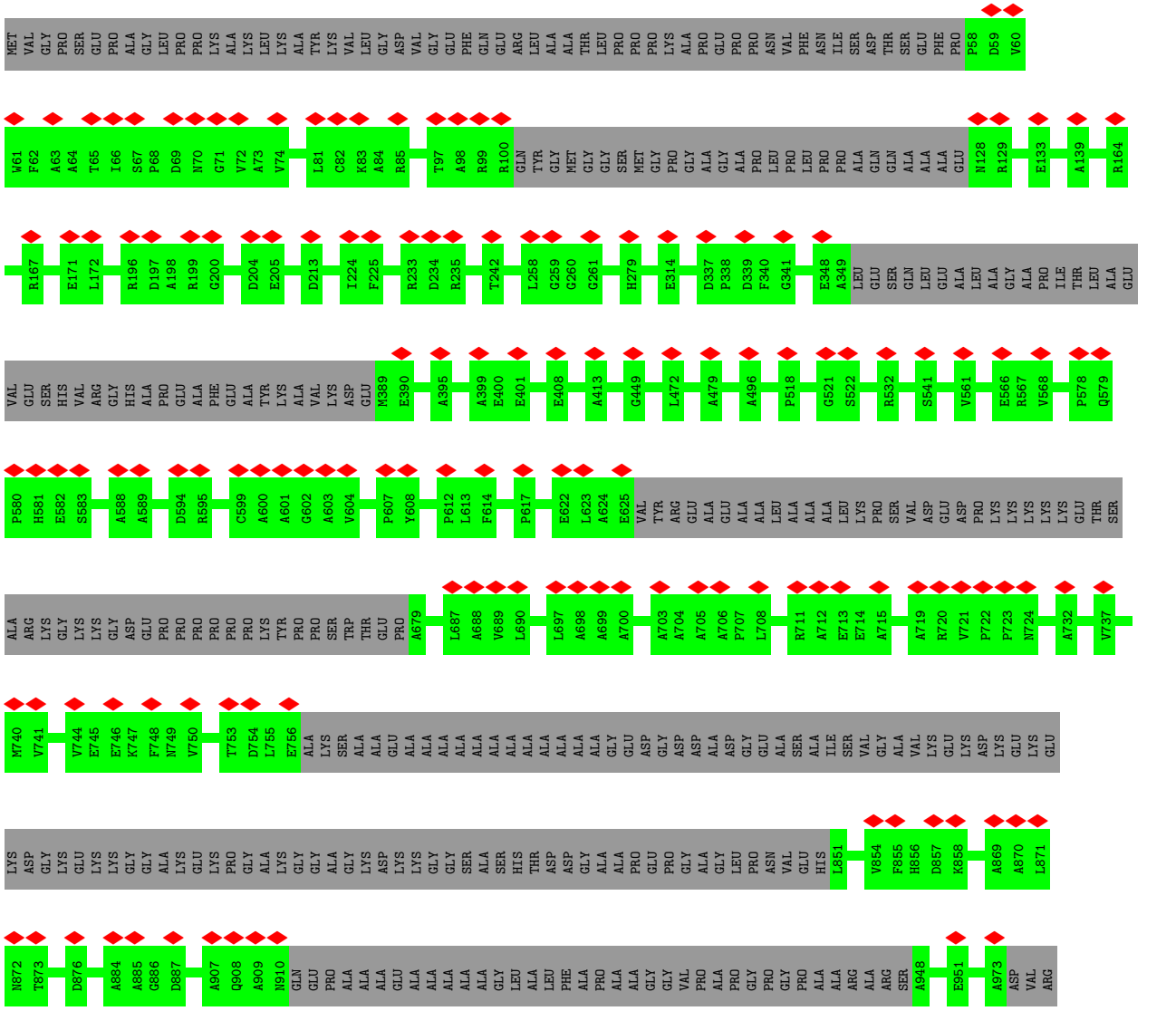
Chain I:





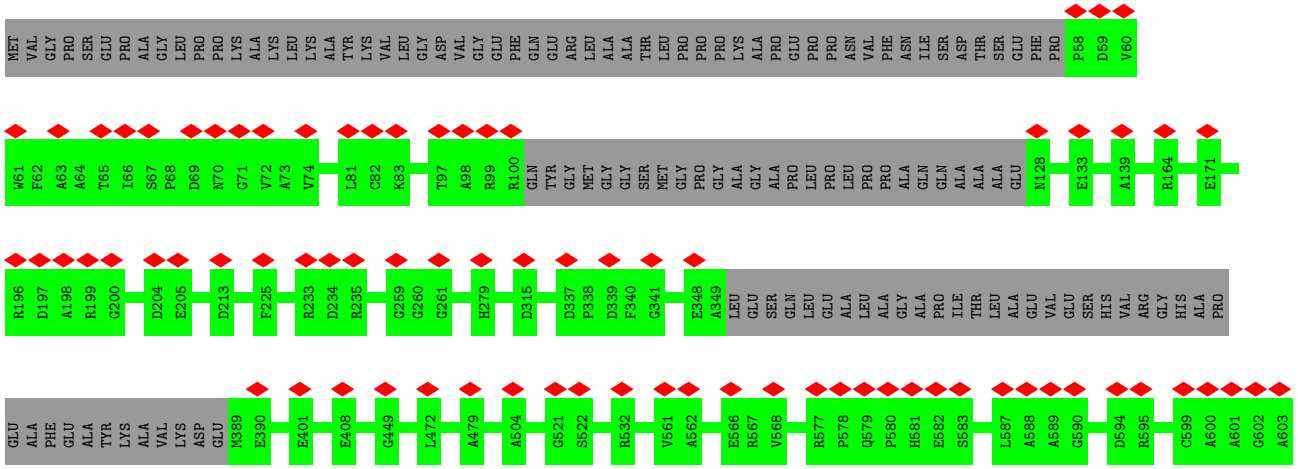
• Molecule 14: FAP213

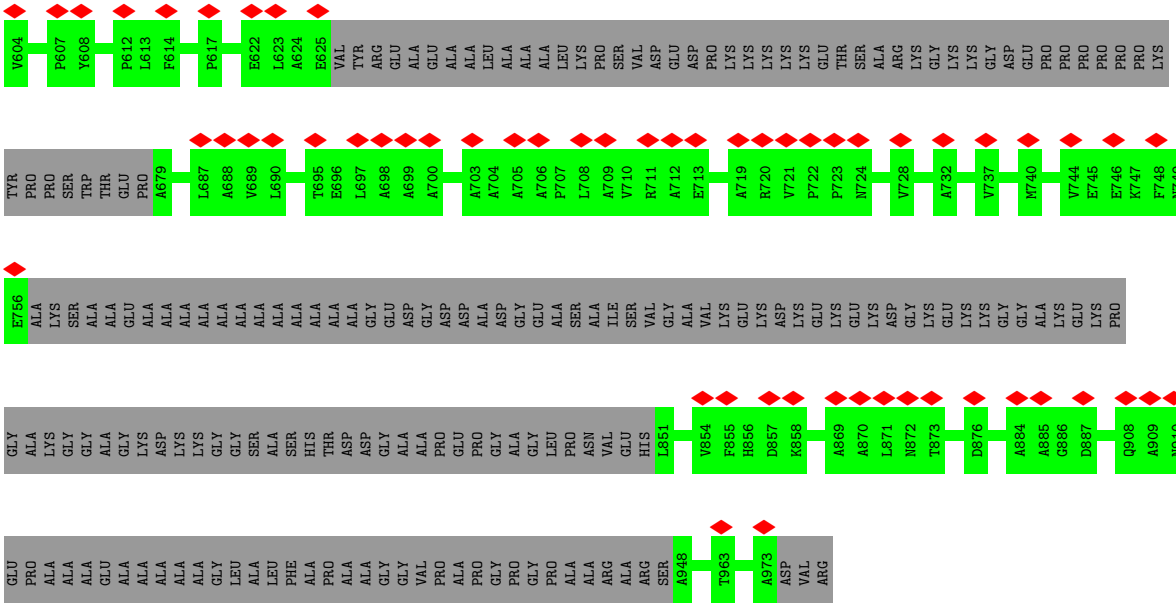
Chain J:



• Molecule 14: FAP213

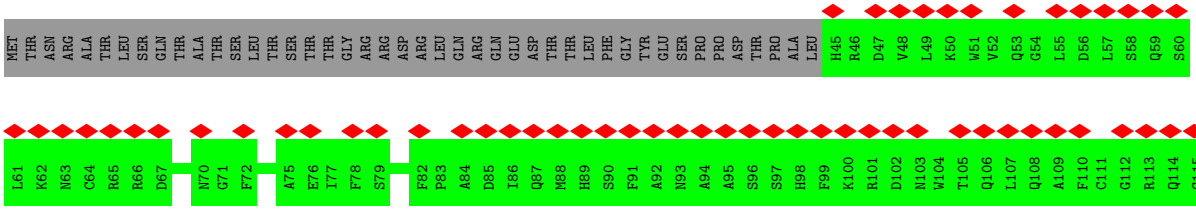
Chain K:





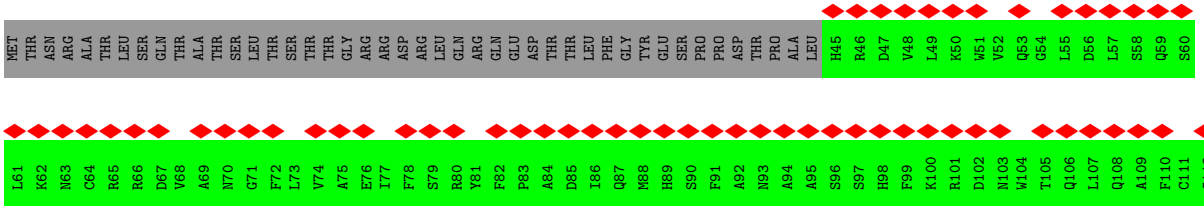
• Molecule 15: FAP225

Chain O:



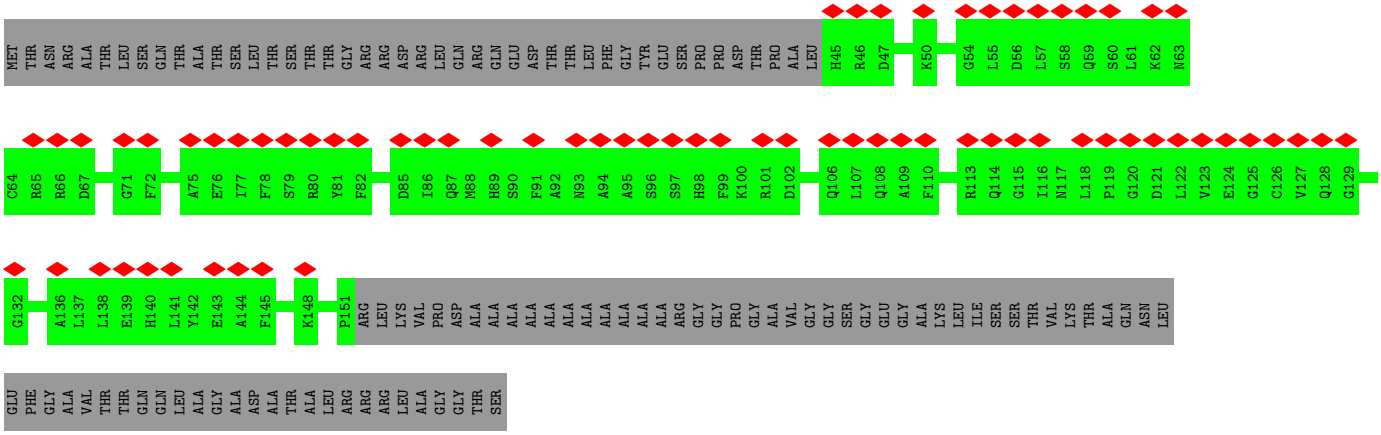
• Molecule 15: FAP225

Chain Y:



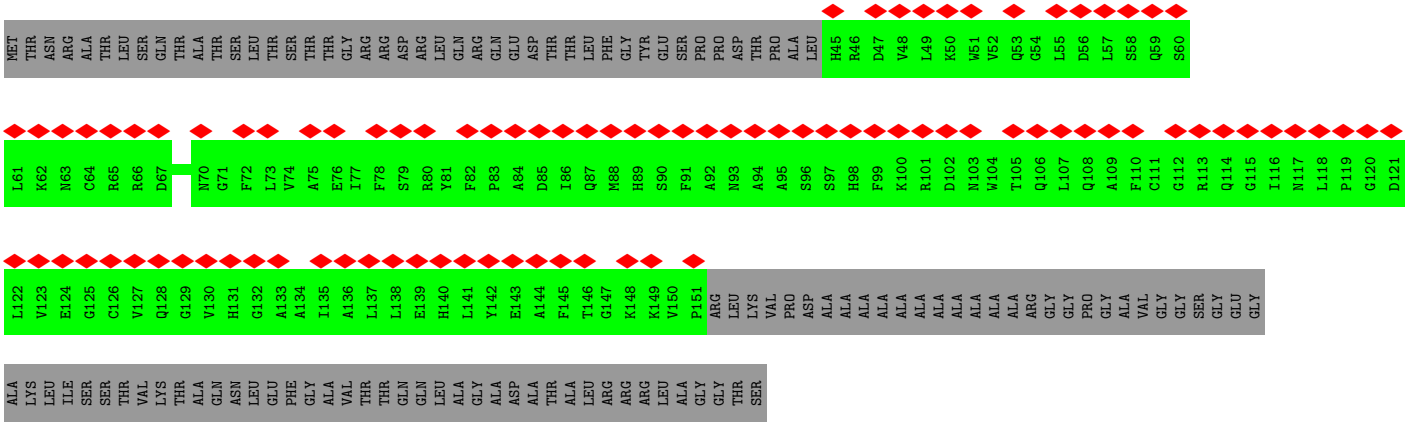
• Molecule 15: FAP225

Chain L:



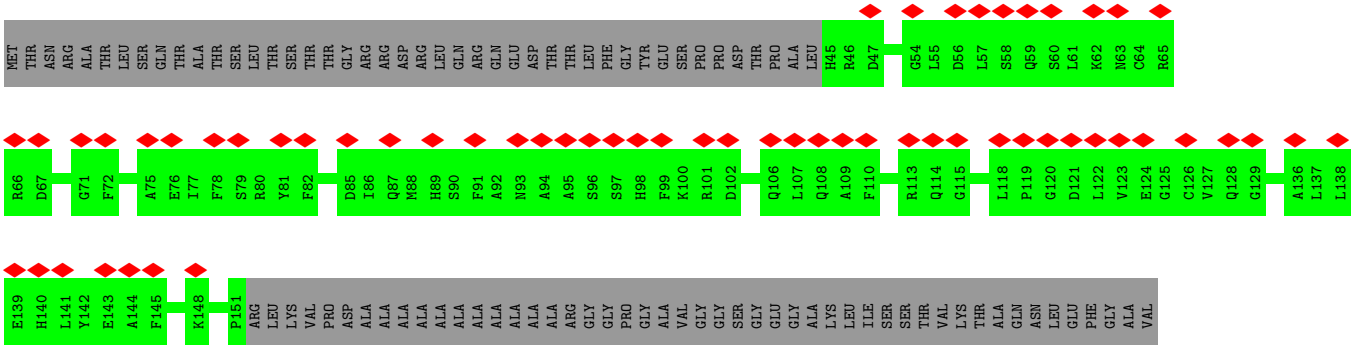
• Molecule 15: FAP225

Chain M:

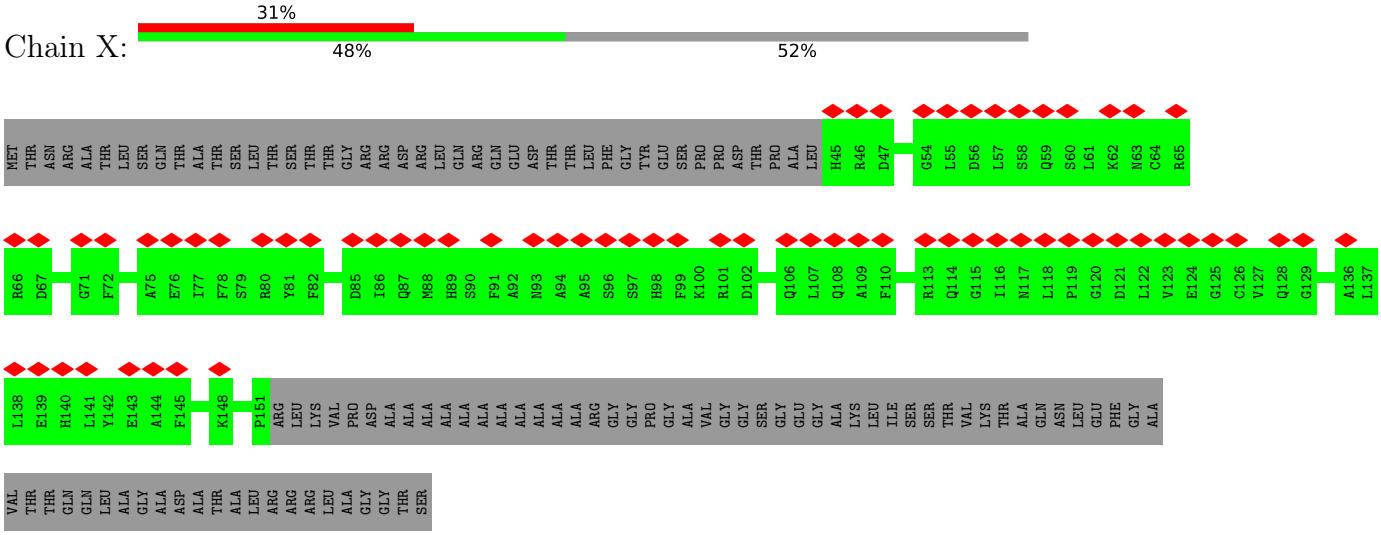


• Molecule 15: FAP225

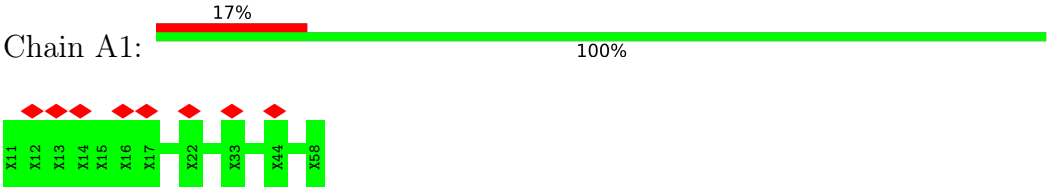
Chain N:



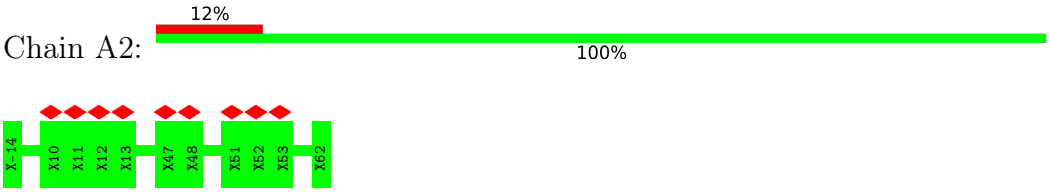
• Molecule 15: FAP225



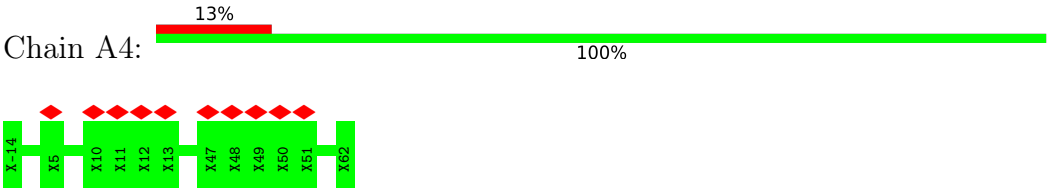
• Molecule 16: FAP239



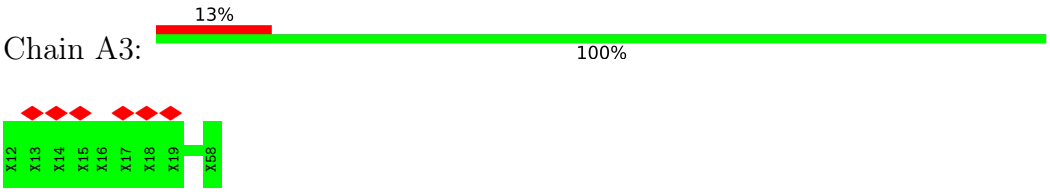
• Molecule 17: FAP388



• Molecule 17: FAP388



• Molecule 18: FAP424



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.998	Depositor
Minimum map value	0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	711.68, 711.68, 711.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	0.27	0/3453	0.52	1/4673 (0.0%)
1	AC	0.27	0/3444	0.53	1/4661 (0.0%)
1	AE	0.28	0/3453	0.54	1/4673 (0.0%)
1	AG	0.29	0/3453	0.54	1/4673 (0.0%)
1	AI	0.27	0/3453	0.52	0/4673
1	AK	0.26	0/3453	0.52	0/4673
1	BA	0.27	0/3462	0.52	0/4685
1	BC	0.27	0/3428	0.53	0/4639
1	BE	0.28	0/3462	0.52	0/4685
1	BG	0.28	0/3428	0.54	0/4639
1	BI	0.27	0/3462	0.51	0/4685
1	BK	0.27	0/3428	0.53	0/4639
1	CA	0.26	0/3428	0.51	1/4639 (0.0%)
1	CC	0.28	0/3428	0.52	0/4639
1	CE	0.28	0/3428	0.53	1/4639 (0.0%)
1	CG	0.28	0/3428	0.52	0/4639
1	CI	0.27	0/3428	0.53	1/4639 (0.0%)
1	CK	0.27	0/3428	0.52	0/4639
1	DC	0.27	0/3428	0.51	0/4639
1	DE	0.27	0/3428	0.51	0/4639
1	DG	0.29	0/3428	0.51	0/4639
1	DI	0.28	0/3428	0.52	0/4639
1	DK	0.27	0/3428	0.52	0/4639
1	EA	0.27	0/3428	0.51	0/4639
1	EC	0.27	0/3428	0.52	0/4639
1	EE	0.28	0/3428	0.52	0/4639
1	EG	0.29	0/3428	0.53	0/4639
1	EI	0.27	0/3428	0.51	0/4639
1	EK	0.27	0/3428	0.52	0/4639
1	FA	0.27	0/3428	0.52	0/4639
1	FC	0.26	0/3428	0.52	1/4639 (0.0%)
1	FE	0.28	0/3428	0.54	0/4639

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	FG	0.27	0/3428	0.53	1/4639 (0.0%)
1	FI	0.27	0/3428	0.52	0/4639
1	FK	0.27	0/3428	0.53	0/4639
1	GC	0.27	0/3428	0.52	1/4639 (0.0%)
1	GE	0.27	0/3428	0.52	0/4639
1	GG	0.27	0/3428	0.53	0/4639
1	GI	0.28	0/3428	0.52	0/4639
1	GK	0.27	0/3428	0.52	1/4639 (0.0%)
1	GM	0.27	0/3428	0.53	1/4639 (0.0%)
1	HC	0.26	0/3428	0.52	0/4639
1	HE	0.27	0/3428	0.53	1/4639 (0.0%)
1	HG	0.28	0/3428	0.54	0/4639
1	HI	0.26	0/3428	0.54	1/4639 (0.0%)
1	HK	0.26	0/3428	0.53	1/4639 (0.0%)
1	HM	0.26	0/3428	0.54	1/4639 (0.0%)
1	IC	0.26	0/3428	0.52	0/4639
1	IE	0.26	0/3428	0.53	0/4639
1	IG	0.27	0/3428	0.53	0/4639
1	II	0.27	0/3428	0.54	0/4639
1	IK	0.27	0/3428	0.53	0/4639
1	IM	0.27	0/3428	0.52	0/4639
1	JC	0.26	0/3428	0.52	1/4639 (0.0%)
1	JE	0.27	0/3428	0.53	1/4639 (0.0%)
1	JG	0.27	0/3428	0.53	1/4639 (0.0%)
1	JI	0.29	0/3420	0.55	1/4628 (0.0%)
1	JK	0.27	0/3428	0.54	1/4639 (0.0%)
1	JM	0.26	0/3420	0.52	0/4628
1	KC	0.27	0/3428	0.52	0/4639
1	KE	0.28	0/3428	0.54	1/4639 (0.0%)
1	KG	0.28	0/3428	0.53	0/4639
1	KI	0.28	0/3428	0.55	1/4639 (0.0%)
1	KK	0.27	0/3428	0.52	0/4639
1	LC	0.27	0/3428	0.51	0/4639
1	LE	0.27	0/3428	0.53	0/4639
1	LG	0.28	0/3428	0.52	0/4639
1	LI	0.28	0/3428	0.53	0/4639
1	LK	0.26	0/3428	0.52	0/4639
1	MC	0.27	0/3453	0.52	0/4673
1	ME	0.28	0/3428	0.53	0/4639
1	MG	0.29	0/3453	0.52	0/4673
1	MI	0.28	0/3428	0.52	0/4639
1	MK	0.28	0/3453	0.52	0/4673
2	AB	0.27	0/3426	0.53	0/4644

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	AD	0.26	0/3426	0.52	0/4644
2	AF	0.28	0/3426	0.53	0/4644
2	AH	0.29	0/3412	0.54	0/4625
2	AJ	0.26	0/3426	0.51	0/4644
2	AL	0.26	0/3412	0.52	0/4625
2	BB	0.26	0/3465	0.53	0/4697
2	BD	0.28	0/3412	0.52	0/4625
2	BF	0.28	0/3465	0.55	0/4697
2	BH	0.28	0/3412	0.53	0/4625
2	BJ	0.27	0/3465	0.53	0/4697
2	BL	0.26	0/3412	0.52	0/4625
2	CB	0.28	0/3406	0.53	0/4617
2	CD	0.28	0/3406	0.53	0/4617
2	CF	0.28	0/3406	0.52	0/4617
2	CH	0.28	0/3406	0.54	0/4617
2	CJ	0.27	0/3412	0.52	0/4625
2	DB	0.28	0/3412	0.54	0/4625
2	DD	0.28	0/3406	0.53	0/4617
2	DF	0.28	0/3412	0.55	0/4625
2	DH	0.28	0/3412	0.52	0/4625
2	DJ	0.27	0/3412	0.52	0/4625
2	DL	0.27	0/3412	0.53	0/4625
2	EB	0.27	0/3465	0.53	0/4697
2	ED	0.27	0/3406	0.53	0/4617
2	EF	0.29	0/3471	0.54	1/4705 (0.0%)
2	EH	0.28	0/3406	0.54	0/4617
2	EJ	0.27	0/3465	0.53	0/4697
2	EL	0.27	0/3406	0.52	0/4617
2	FB	0.27	0/3412	0.52	0/4625
2	FD	0.26	0/3412	0.51	0/4625
2	FF	0.28	0/3412	0.53	0/4625
2	FH	0.29	0/3412	0.56	2/4625 (0.0%)
2	FJ	0.27	0/3412	0.52	0/4625
2	FL	0.26	0/3412	0.52	0/4625
2	GD	0.27	0/3412	0.54	1/4625 (0.0%)
2	GF	0.27	0/3412	0.55	0/4625
2	GH	0.28	0/3412	0.53	1/4625 (0.0%)
2	GJ	0.28	0/3412	0.53	0/4625
2	GL	0.27	0/3412	0.53	0/4625
2	HD	0.27	0/3412	0.54	0/4625
2	HF	0.27	0/3412	0.55	0/4625
2	HH	0.27	0/3412	0.53	0/4625
2	HJ	0.27	0/3397	0.54	0/4605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	HL	0.26	0/3412	0.52	0/4625
2	ID	0.27	0/3406	0.54	1/4617 (0.0%)
2	IF	0.27	0/3412	0.55	2/4625 (0.0%)
2	IH	0.27	0/3406	0.52	0/4617
2	IJ	0.27	0/3412	0.54	0/4625
2	IL	0.27	0/3406	0.54	1/4617 (0.0%)
2	JB	0.26	0/3412	0.54	0/4625
2	JD	0.27	0/3412	0.52	0/4625
2	JF	0.27	0/3412	0.55	0/4625
2	JH	0.28	0/3412	0.52	0/4625
2	JJ	0.27	0/3406	0.53	0/4617
2	JL	0.27	0/3406	0.53	1/4617 (0.0%)
2	KB	0.27	0/3406	0.52	0/4617
2	KD	0.27	0/3412	0.53	0/4625
2	KF	0.28	0/3406	0.54	1/4617 (0.0%)
2	KH	0.28	0/3412	0.54	0/4625
2	KJ	0.27	0/3406	0.53	0/4617
2	KL	0.27	0/3412	0.53	0/4625
2	LB	0.26	0/3412	0.52	0/4625
2	LD	0.27	0/3412	0.53	1/4625 (0.0%)
2	LF	0.28	0/3412	0.54	1/4625 (0.0%)
2	LH	0.27	0/3412	0.54	0/4625
2	LJ	0.27	0/3412	0.53	0/4625
2	LL	0.26	0/3412	0.51	0/4625
2	MB	0.27	0/3412	0.52	0/4625
2	MD	0.27	0/3471	0.51	0/4705
2	MF	0.28	0/3412	0.53	1/4625 (0.0%)
2	MH	0.28	0/3476	0.53	0/4712
2	MJ	0.28	0/3412	0.52	0/4625
2	ML	0.27	0/3476	0.52	0/4712
3	a	0.27	0/2428	0.58	0/3300
3	b	0.28	0/4634	0.61	1/6298 (0.0%)
3	c	0.28	0/4634	0.64	3/6298 (0.0%)
3	d	0.27	0/2228	0.62	0/3026
4	e	0.26	0/1484	0.57	0/1994
4	f	0.27	0/1484	0.54	0/1994
4	g	0.28	0/1154	0.52	0/1553
5	h	0.26	0/4608	0.56	0/6234
5	i	0.27	0/4608	0.58	0/6234
5	j	0.26	0/4608	0.56	0/6234
6	k	0.26	0/3072	0.58	0/4147
6	l	0.27	0/3072	0.58	2/4147 (0.0%)
6	s	0.26	0/2253	0.56	0/3048

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	m	0.27	0/2808	0.60	1/3798 (0.0%)
7	n	0.27	0/2808	0.63	1/3798 (0.0%)
7	o	0.26	0/2808	0.60	1/3798 (0.0%)
8	p	0.25	0/714	0.58	0/962
8	q	0.26	0/714	0.58	0/962
8	r	0.25	0/714	0.58	0/962
9	A	0.26	0/1564	0.58	0/2113
9	B	0.26	0/1564	0.57	0/2113
9	C	0.26	0/1564	0.58	0/2113
10	P	0.27	0/2503	0.51	0/3420
10	Q	0.26	0/2498	0.52	1/3413 (0.0%)
10	R	0.27	0/2503	0.53	0/3420
10	S	0.26	0/2498	0.53	1/3413 (0.0%)
10	Z	0.23	0/786	0.47	0/1041
10	aa	0.24	0/1434	0.47	0/1989
10	cc	0.23	0/769	0.48	0/1018
11	T	0.24	0/310	0.33	0/429
11	U	0.24	0/285	0.30	0/394
11	V	0.25	0/331	0.39	0/460
11	W	0.23	0/311	0.34	0/432
12	D	0.26	0/7465	0.45	0/10373
12	E	0.26	0/7465	0.45	0/10373
12	bb	0.27	0/1076	0.57	0/1482
13	F	0.26	0/4827	0.40	0/6703
13	G	0.26	0/4880	0.40	0/6777
13	H	0.26	0/4827	0.40	0/6703
13	I	0.26	0/4880	0.40	0/6777
14	J	0.26	0/3904	0.49	0/5372
14	K	0.26	0/3904	0.49	0/5372
15	L	0.26	0/861	0.47	0/1163
15	M	0.26	0/861	0.47	0/1163
15	N	0.27	0/861	0.47	0/1163
15	O	0.26	0/861	0.48	0/1163
15	X	0.27	0/861	0.47	0/1163
15	Y	0.26	0/861	0.48	0/1163
All	All	0.27	0/625065	0.53	48/848033 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	DB	0	1
2	DF	0	1
2	GD	0	1
2	HD	0	1
2	HL	0	1
2	KD	0	1
2	KH	0	1
2	KL	0	1
3	c	0	1
3	d	0	1
13	G	0	1
13	H	0	1
13	I	0	1
All	All	0	13

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	o	173	LEU	CA-CB-CG	6.77	130.88	115.30
3	c	277	LEU	CA-CB-CG	6.68	130.68	115.30
7	m	173	LEU	CA-CB-CG	6.59	130.46	115.30
1	CE	284	LEU	CA-CB-CG	6.44	130.10	115.30
1	AG	284	LEU	CA-CB-CG	6.27	129.71	115.30
2	ID	218	ASP	CB-CG-OD1	6.18	123.87	118.30
1	JK	284	LEU	CA-CB-CG	6.14	129.43	115.30
1	FG	284	LEU	CA-CB-CG	6.07	129.25	115.30
1	JI	284	LEU	CA-CB-CG	5.93	128.95	115.30
1	CI	284	LEU	CA-CB-CG	5.88	128.81	115.30
1	FC	284	LEU	CA-CB-CG	5.85	128.75	115.30
1	JE	284	LEU	CA-CB-CG	5.82	128.69	115.30
1	HK	284	LEU	CA-CB-CG	5.71	128.44	115.30
1	HM	284	LEU	CA-CB-CG	5.70	128.42	115.30
1	KE	284	LEU	CA-CB-CG	5.68	128.37	115.30
7	n	341	LEU	CA-CB-CG	5.68	128.36	115.30
2	IL	218	ASP	CB-CG-OD1	5.63	123.36	118.30
2	IF	217	LEU	CA-CB-CG	5.61	128.20	115.30
1	CA	284	LEU	CA-CB-CG	5.60	128.19	115.30
1	GM	284	LEU	CA-CB-CG	5.58	128.12	115.30
1	JC	284	LEU	CA-CB-CG	5.52	127.99	115.30
1	AE	284	LEU	CA-CB-CG	5.51	127.98	115.30
10	Q	124	LEU	CA-CB-CG	5.50	127.95	115.30
1	JG	284	LEU	CA-CB-CG	5.49	127.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	HE	284	LEU	CA-CB-CG	5.47	127.89	115.30
6	l	105	LEU	CA-CB-CG	5.46	127.86	115.30
2	GH	218	ASP	CB-CG-OD1	5.44	123.19	118.30
1	KI	284	LEU	CA-CB-CG	5.41	127.75	115.30
1	AC	284	LEU	CA-CB-CG	5.38	127.68	115.30
1	GK	284	LEU	CA-CB-CG	5.35	127.61	115.30
2	LF	218	ASP	CB-CG-OD1	5.35	123.12	118.30
2	KF	218	ASP	CB-CG-OD1	5.35	123.12	118.30
2	LD	218	ASP	CB-CG-OD1	5.33	123.09	118.30
1	AA	284	LEU	CA-CB-CG	5.30	127.49	115.30
6	l	486	LEU	CA-CB-CG	5.29	127.48	115.30
2	MF	218	ASP	CB-CG-OD1	5.27	123.04	118.30
2	FH	357	TYR	C-N-CA	-5.26	108.55	121.70
3	c	444	LEU	CA-CB-CG	5.23	127.34	115.30
2	GD	273	ALA	C-N-CD	-5.23	109.10	120.60
2	FH	218	ASP	CB-CG-OD1	5.22	123.00	118.30
1	HI	284	LEU	CA-CB-CG	5.21	127.28	115.30
10	S	124	LEU	CA-CB-CG	5.18	127.22	115.30
1	GC	284	LEU	CA-CB-CG	5.11	127.06	115.30
3	c	535	PRO	C-N-CA	5.10	134.45	121.70
2	JL	218	ASP	CB-CG-OD1	5.08	122.87	118.30
2	EF	68	LEU	CA-CB-CG	5.05	126.92	115.30
2	IF	218	ASP	CB-CG-OD1	5.03	122.83	118.30
3	b	143	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	DB	401	LYS	Peptide
2	DF	273	ALA	Peptide
13	G	968	GLU	Peptide
2	GD	273	ALA	Peptide
13	H	968	GLU	Peptide
2	HD	273	ALA	Peptide
2	HL	273	ALA	Peptide
13	I	968	GLU	Peptide
2	KD	273	ALA	Peptide
2	KH	273	ALA	Peptide
2	KL	273	ALA	Peptide
3	c	455	ALA	Peptide
3	d	593	ALA	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 222 ligands modelled in this entry, 74 are monoatomic - leaving 148 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	$\#\|Z\| > 2$
20	GTP	AB	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.64	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	GDP	DC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.27	4 (13%)
20	GTP	DB	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.67	8 (25%)
20	GTP	GF	501	21	26,34,34	1.16	2 (7%)	32,54,54	1.74	6 (18%)
20	GTP	LB	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.67	7 (21%)
19	GDP	EE	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.23	3 (10%)
19	GDP	BA	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.26	4 (13%)
19	GDP	JI	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.33	4 (13%)
20	GTP	IL	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
20	GTP	MJ	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.61	7 (21%)
19	GDP	HM	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.26	4 (13%)
20	GTP	EH	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.61	7 (21%)
20	GTP	KD	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.66	7 (21%)
20	GTP	EB	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.63	7 (21%)
19	GDP	CK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.29	4 (13%)
20	GTP	BL	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
20	GTP	BH	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.68	7 (21%)
19	GDP	HI	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.26	4 (13%)
20	GTP	AF	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.65	7 (21%)
20	GTP	JH	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.58	7 (21%)
19	GDP	BC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
19	GDP	HK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
20	GTP	DD	501	21	26,34,34	1.17	1 (3%)	32,54,54	1.63	7 (21%)
19	GDP	II	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.39	5 (16%)
20	GTP	LL	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
20	GTP	ED	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
20	GTP	LD	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
20	GTP	MD	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.78	7 (21%)
20	GTP	CD	501	21	26,34,34	1.19	2 (7%)	32,54,54	1.69	7 (21%)
19	GDP	AK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.23	3 (10%)
19	GDP	CE	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.26	4 (13%)
19	GDP	EA	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
19	GDP	FC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.27	4 (13%)
19	GDP	HE	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.25	4 (13%)
19	GDP	CA	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
19	GDP	GM	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	GDP	DE	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
20	GTP	GD	501	21	26,34,34	1.16	2 (7%)	32,54,54	1.71	7 (21%)
20	GTP	IH	501	21	26,34,34	1.19	2 (7%)	32,54,54	1.65	7 (21%)
20	GTP	JF	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.66	8 (25%)
20	GTP	IF	501	21	26,34,34	1.20	2 (7%)	32,54,54	1.69	7 (21%)
20	GTP	KB	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.70	7 (21%)
20	GTP	DJ	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.71	7 (21%)
19	GDP	LG	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
20	GTP	KF	501	21	26,34,34	1.19	2 (7%)	32,54,54	1.68	7 (21%)
19	GDP	JM	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
19	GDP	BK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
19	GDP	IE	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
19	GDP	DG	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.21	4 (13%)
20	GTP	HL	501	21	26,34,34	1.15	2 (7%)	32,54,54	1.71	7 (21%)
19	GDP	IM	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
20	GTP	HI	501	21	26,34,34	1.16	2 (7%)	32,54,54	1.70	6 (18%)
19	GDP	LI	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.27	4 (13%)
20	GTP	GL	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
19	GDP	GG	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
20	GTP	DF	501	21	26,34,34	1.20	2 (7%)	32,54,54	1.69	7 (21%)
19	GDP	MI	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	4 (13%)
19	GDP	FE	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
20	GTP	EL	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.66	7 (21%)
19	GDP	GI	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.26	4 (13%)
20	GTP	FH	501	21	26,34,34	1.19	2 (7%)	32,54,54	1.68	7 (21%)
19	GDP	GE	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	4 (13%)
20	GTP	GJ	501	21	26,34,34	1.16	2 (7%)	32,54,54	1.71	7 (21%)
20	GTP	CB	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.67	7 (21%)
20	GTP	JJ	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
19	GDP	EG	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.26	4 (13%)
20	GTP	BB	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.64	7 (21%)
19	GDP	FA	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
20	GTP	EF	501	21	26,34,34	1.20	2 (7%)	32,54,54	1.60	7 (21%)
20	GTP	AD	501	21	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
19	GDP	KC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	GDP	CI	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
19	GDP	KI	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
20	GTP	LF	501	21	26,34,34	1.19	2 (7%)	32,54,54	1.71	7 (21%)
19	GDP	BI	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.25	4 (13%)
20	GTP	ID	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.64	7 (21%)
19	GDP	JC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.25	4 (13%)
19	GDP	KG	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
19	GDP	EC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)
20	GTP	MB	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.62	7 (21%)
20	GTP	AJ	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.66	7 (21%)
20	GTP	BD	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.68	7 (21%)
19	GDP	AI	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
19	GDP	AE	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
19	GDP	JE	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.27	4 (13%)
20	GTP	CJ	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.68	7 (21%)
19	GDP	AA	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
20	GTP	FF	501	21	26,34,34	1.19	2 (7%)	32,54,54	1.63	7 (21%)
19	GDP	FI	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)
19	GDP	MG	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
20	GTP	FJ	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.73	7 (21%)
20	GTP	HJ	501	21	26,34,34	1.15	2 (7%)	32,54,54	1.71	6 (18%)
19	GDP	EK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
19	GDP	IK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.25	4 (13%)
19	GDP	ME	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)
19	GDP	GK	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.26	4 (13%)
19	GDP	MK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
20	GTP	FL	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.67	7 (21%)
19	GDP	FG	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.22	4 (13%)
19	GDP	LE	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.24	4 (13%)
20	GTP	MH	501	21	26,34,34	1.20	2 (7%)	32,54,54	1.69	7 (21%)
19	GDP	AC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.26	4 (13%)
20	GTP	HD	501	21	26,34,34	1.14	2 (7%)	32,54,54	1.68	7 (21%)
20	GTP	DL	501	21	26,34,34	1.20	2 (7%)	32,54,54	1.69	7 (21%)
19	GDP	DK	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.27	4 (13%)
20	GTP	FB	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.68	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	GTP	KH	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.67	7 (21%)
19	GDP	GC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	4 (13%)
19	GDP	JK	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	5 (16%)
20	GTP	KL	501	21	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
19	GDP	EI	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
19	GDP	MC	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
19	GDP	BG	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	5 (16%)
19	GDP	FK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
20	GTP	JL	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.69	7 (21%)
20	GTP	CH	501	21	26,34,34	1.19	2 (7%)	32,54,54	1.71	7 (21%)
19	GDP	CG	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.15	4 (13%)
19	GDP	IG	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.25	4 (13%)
20	GTP	AH	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.67	7 (21%)
20	GTP	CF	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.64	7 (21%)
20	GTP	IJ	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
19	GDP	KE	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
19	GDP	CC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
20	GTP	FD	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.66	7 (21%)
19	GDP	LC	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.30	4 (13%)
19	GDP	HC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.27	4 (13%)
20	GTP	JD	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.59	8 (25%)
19	GDP	KK	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
20	GTP	ML	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.73	7 (21%)
20	GTP	LJ	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.69	7 (21%)
20	GTP	HF	501	21	26,34,34	1.14	2 (7%)	32,54,54	1.67	7 (21%)
20	GTP	JB	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.66	7 (21%)
19	GDP	HG	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
19	GDP	LK	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.28	4 (13%)
20	GTP	BF	501	21	26,34,34	1.19	2 (7%)	32,54,54	1.62	7 (21%)
20	GTP	GH	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.71	7 (21%)
20	GTP	BJ	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.69	7 (21%)
20	GTP	AL	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
19	GDP	BE	501	-	24,30,30	1.00	1 (4%)	30,47,47	1.20	4 (13%)
20	GTP	DH	501	21	26,34,34	1.23	1 (3%)	32,54,54	1.78	8 (25%)
19	GDP	IC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	GTP	MF	501	21	26,34,34	1.20	2 (7%)	32,54,54	1.70	7 (21%)
19	GDP	DI	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
19	GDP	JG	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.27	5 (16%)
20	GTP	KJ	501	21	26,34,34	1.17	2 (7%)	32,54,54	1.67	7 (21%)
19	GDP	AG	501	-	24,30,30	1.01	1 (4%)	30,47,47	1.21	4 (13%)
20	GTP	EJ	501	21	26,34,34	1.16	2 (7%)	32,54,54	1.60	7 (21%)
20	GTP	LH	501	21	26,34,34	1.18	2 (7%)	32,54,54	1.68	6 (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
20	GTP	AB	501	21	-	4/18/38/38	0/3/3/3
19	GDP	DC	501	-	-	2/12/32/32	0/3/3/3
20	GTP	DB	501	21	-	6/18/38/38	0/3/3/3
20	GTP	GF	501	21	-	6/18/38/38	0/3/3/3
20	GTP	LB	501	21	-	3/18/38/38	0/3/3/3
19	GDP	EE	502	-	-	7/12/32/32	0/3/3/3
19	GDP	BA	501	-	-	7/12/32/32	0/3/3/3
19	GDP	JI	501	-	-	2/12/32/32	0/3/3/3
20	GTP	IL	501	21	-	6/18/38/38	0/3/3/3
20	GTP	MJ	501	21	-	4/18/38/38	0/3/3/3
19	GDP	HM	501	-	-	5/12/32/32	0/3/3/3
20	GTP	EH	501	21	-	6/18/38/38	0/3/3/3
20	GTP	KD	501	21	-	5/18/38/38	0/3/3/3
20	GTP	EB	501	21	-	4/18/38/38	0/3/3/3
19	GDP	CK	501	-	-	6/12/32/32	0/3/3/3
20	GTP	BL	501	21	-	4/18/38/38	0/3/3/3
20	GTP	BH	501	21	-	5/18/38/38	0/3/3/3
19	GDP	HI	502	-	-	3/12/32/32	0/3/3/3
20	GTP	AF	501	21	-	3/18/38/38	0/3/3/3
20	GTP	JH	501	21	-	6/18/38/38	0/3/3/3
19	GDP	BC	501	-	-	4/12/32/32	0/3/3/3
19	GDP	HK	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GTP	DD	501	21	-	8/18/38/38	0/3/3/3
19	GDP	II	501	-	-	7/12/32/32	0/3/3/3
20	GTP	LL	501	21	-	6/18/38/38	0/3/3/3
20	GTP	ED	501	21	-	3/18/38/38	0/3/3/3
20	GTP	LD	501	21	-	7/18/38/38	0/3/3/3
20	GTP	MD	501	21	-	4/18/38/38	0/3/3/3
20	GTP	CD	501	21	-	7/18/38/38	0/3/3/3
19	GDP	AK	501	-	-	4/12/32/32	0/3/3/3
19	GDP	CE	501	-	-	0/12/32/32	0/3/3/3
19	GDP	EA	501	-	-	6/12/32/32	0/3/3/3
19	GDP	FC	501	-	-	0/12/32/32	0/3/3/3
19	GDP	HE	501	-	-	5/12/32/32	0/3/3/3
19	GDP	CA	501	-	-	0/12/32/32	0/3/3/3
19	GDP	GM	501	-	-	1/12/32/32	0/3/3/3
19	GDP	DE	501	-	-	2/12/32/32	0/3/3/3
20	GTP	GD	501	21	-	4/18/38/38	0/3/3/3
20	GTP	IH	501	21	-	5/18/38/38	0/3/3/3
20	GTP	JF	501	21	-	1/18/38/38	0/3/3/3
20	GTP	IF	501	21	-	5/18/38/38	0/3/3/3
20	GTP	KB	501	21	-	4/18/38/38	0/3/3/3
20	GTP	DJ	501	21	-	5/18/38/38	0/3/3/3
19	GDP	LG	501	-	-	0/12/32/32	0/3/3/3
20	GTP	KF	501	21	-	5/18/38/38	0/3/3/3
19	GDP	JM	501	-	-	0/12/32/32	0/3/3/3
19	GDP	BK	501	-	-	4/12/32/32	0/3/3/3
19	GDP	IE	501	-	-	3/12/32/32	0/3/3/3
19	GDP	DG	501	-	-	2/12/32/32	0/3/3/3
20	GTP	HL	501	21	-	5/18/38/38	0/3/3/3
19	GDP	IM	501	-	-	4/12/32/32	0/3/3/3
20	GTP	HI	501	21	-	3/18/38/38	0/3/3/3
19	GDP	LI	501	-	-	0/12/32/32	0/3/3/3
20	GTP	GL	501	21	-	6/18/38/38	0/3/3/3
19	GDP	GG	501	-	-	0/12/32/32	0/3/3/3
20	GTP	DF	501	21	-	4/18/38/38	0/3/3/3
19	GDP	MI	501	-	-	4/12/32/32	0/3/3/3
19	GDP	FE	501	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GTP	EL	501	21	-	5/18/38/38	0/3/3/3
19	GDP	GI	501	-	-	2/12/32/32	0/3/3/3
20	GTP	FH	501	21	-	4/18/38/38	0/3/3/3
19	GDP	GE	501	-	-	2/12/32/32	0/3/3/3
20	GTP	GJ	501	21	-	6/18/38/38	0/3/3/3
20	GTP	CB	501	21	-	5/18/38/38	0/3/3/3
20	GTP	JJ	501	21	-	6/18/38/38	0/3/3/3
19	GDP	EG	501	-	-	4/12/32/32	0/3/3/3
20	GTP	BB	501	21	-	3/18/38/38	0/3/3/3
19	GDP	FA	501	-	-	1/12/32/32	0/3/3/3
20	GTP	EF	501	21	-	7/18/38/38	0/3/3/3
20	GTP	AD	501	21	-	5/18/38/38	0/3/3/3
19	GDP	KC	501	-	-	2/12/32/32	0/3/3/3
19	GDP	CI	501	-	-	2/12/32/32	0/3/3/3
19	GDP	KI	502	-	-	5/12/32/32	0/3/3/3
20	GTP	LF	501	21	-	3/18/38/38	0/3/3/3
19	GDP	BI	501	-	-	3/12/32/32	0/3/3/3
20	GTP	ID	501	21	-	3/18/38/38	0/3/3/3
19	GDP	JC	501	-	-	1/12/32/32	0/3/3/3
19	GDP	KG	501	-	-	1/12/32/32	0/3/3/3
19	GDP	EC	501	-	-	1/12/32/32	0/3/3/3
20	GTP	MB	501	21	-	5/18/38/38	0/3/3/3
20	GTP	AJ	501	21	-	6/18/38/38	0/3/3/3
20	GTP	BD	501	21	-	5/18/38/38	0/3/3/3
19	GDP	AI	501	-	-	1/12/32/32	0/3/3/3
19	GDP	AE	501	-	-	0/12/32/32	0/3/3/3
19	GDP	JE	501	-	-	4/12/32/32	0/3/3/3
20	GTP	CJ	501	21	-	4/18/38/38	0/3/3/3
19	GDP	AA	501	-	-	0/12/32/32	0/3/3/3
20	GTP	FF	501	21	-	5/18/38/38	0/3/3/3
19	GDP	FI	501	-	-	0/12/32/32	0/3/3/3
19	GDP	MG	501	-	-	0/12/32/32	0/3/3/3
20	GTP	FJ	501	21	-	4/18/38/38	0/3/3/3
20	GTP	HJ	501	21	-	3/18/38/38	0/3/3/3
19	GDP	EK	501	-	-	1/12/32/32	0/3/3/3
19	GDP	IK	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GDP	ME	501	-	-	3/12/32/32	0/3/3/3
19	GDP	GK	501	-	-	0/12/32/32	0/3/3/3
19	GDP	MK	501	-	-	0/12/32/32	0/3/3/3
20	GTP	FL	501	21	-	4/18/38/38	0/3/3/3
19	GDP	FG	501	-	-	1/12/32/32	0/3/3/3
19	GDP	LE	501	-	-	1/12/32/32	0/3/3/3
20	GTP	MH	501	21	-	6/18/38/38	0/3/3/3
19	GDP	AC	501	-	-	0/12/32/32	0/3/3/3
20	GTP	HD	501	21	-	4/18/38/38	0/3/3/3
20	GTP	DL	501	21	-	6/18/38/38	0/3/3/3
19	GDP	DK	501	-	-	2/12/32/32	0/3/3/3
20	GTP	FB	501	21	-	4/18/38/38	0/3/3/3
20	GTP	KH	501	21	-	3/18/38/38	0/3/3/3
19	GDP	GC	501	-	-	0/12/32/32	0/3/3/3
19	GDP	JK	501	-	-	2/12/32/32	0/3/3/3
20	GTP	KL	501	21	-	7/18/38/38	0/3/3/3
19	GDP	EI	501	-	-	0/12/32/32	0/3/3/3
19	GDP	MC	501	-	-	0/12/32/32	0/3/3/3
19	GDP	BG	501	-	-	1/12/32/32	0/3/3/3
19	GDP	FK	501	-	-	2/12/32/32	0/3/3/3
20	GTP	JL	501	21	-	7/18/38/38	0/3/3/3
20	GTP	CH	501	21	-	5/18/38/38	0/3/3/3
19	GDP	CG	501	-	-	3/12/32/32	0/3/3/3
19	GDP	IG	501	-	-	0/12/32/32	0/3/3/3
20	GTP	AH	501	21	-	7/18/38/38	0/3/3/3
20	GTP	CF	501	21	-	3/18/38/38	0/3/3/3
20	GTP	IJ	501	21	-	2/18/38/38	0/3/3/3
19	GDP	KE	501	-	-	7/12/32/32	0/3/3/3
19	GDP	CC	501	-	-	5/12/32/32	0/3/3/3
20	GTP	FD	501	21	-	3/18/38/38	0/3/3/3
19	GDP	LC	501	-	-	0/12/32/32	0/3/3/3
19	GDP	HC	501	-	-	3/12/32/32	0/3/3/3
20	GTP	JD	501	21	-	4/18/38/38	0/3/3/3
19	GDP	KK	501	-	-	0/12/32/32	0/3/3/3
20	GTP	ML	501	21	-	4/18/38/38	0/3/3/3
20	GTP	LJ	501	21	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GTP	HF	501	21	-	4/18/38/38	0/3/3/3
20	GTP	JB	501	21	-	7/18/38/38	0/3/3/3
19	GDP	HG	501	-	-	1/12/32/32	0/3/3/3
19	GDP	LK	501	-	-	0/12/32/32	0/3/3/3
20	GTP	BF	501	21	-	3/18/38/38	0/3/3/3
20	GTP	GH	501	21	-	6/18/38/38	0/3/3/3
20	GTP	BJ	501	21	-	2/18/38/38	0/3/3/3
20	GTP	AL	501	21	-	3/18/38/38	0/3/3/3
19	GDP	BE	501	-	-	2/12/32/32	0/3/3/3
20	GTP	DH	501	21	-	7/18/38/38	0/3/3/3
19	GDP	IC	501	-	-	5/12/32/32	0/3/3/3
20	GTP	MF	501	21	-	5/18/38/38	0/3/3/3
19	GDP	DI	501	-	-	2/12/32/32	0/3/3/3
19	GDP	JG	501	-	-	5/12/32/32	0/3/3/3
20	GTP	KJ	501	21	-	5/18/38/38	0/3/3/3
19	GDP	AG	501	-	-	0/12/32/32	0/3/3/3
20	GTP	EJ	501	21	-	6/18/38/38	0/3/3/3
20	GTP	LH	501	21	-	4/18/38/38	0/3/3/3

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	DH	501	GTP	C5-C6	-4.39	1.38	1.47
20	IF	501	GTP	C5-C6	-4.32	1.38	1.47
20	AF	501	GTP	C5-C6	-4.30	1.38	1.47
20	FH	501	GTP	C5-C6	-4.29	1.38	1.47
20	EF	501	GTP	C5-C6	-4.27	1.38	1.47
20	IH	501	GTP	C5-C6	-4.26	1.38	1.47
20	FF	501	GTP	C5-C6	-4.25	1.38	1.47
20	MF	501	GTP	C5-C6	-4.24	1.38	1.47
20	DL	501	GTP	C5-C6	-4.23	1.38	1.47
20	DF	501	GTP	C5-C6	-4.23	1.38	1.47
20	LH	501	GTP	C5-C6	-4.23	1.38	1.47
20	BF	501	GTP	C5-C6	-4.22	1.38	1.47
20	MH	501	GTP	C5-C6	-4.22	1.38	1.47
20	JF	501	GTP	C5-C6	-4.21	1.38	1.47
20	EH	501	GTP	C5-C6	-4.21	1.38	1.47
20	FJ	501	GTP	C5-C6	-4.21	1.38	1.47
20	FD	501	GTP	C5-C6	-4.21	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	AB	501	GTP	C5-C6	-4.21	1.38	1.47
20	CF	501	GTP	C5-C6	-4.20	1.38	1.47
20	EB	501	GTP	C5-C6	-4.20	1.38	1.47
20	IJ	501	GTP	C5-C6	-4.20	1.38	1.47
20	LF	501	GTP	C5-C6	-4.20	1.38	1.47
20	FL	501	GTP	C5-C6	-4.20	1.38	1.47
20	CH	501	GTP	C5-C6	-4.20	1.38	1.47
20	DB	501	GTP	C5-C6	-4.19	1.38	1.47
20	CD	501	GTP	C5-C6	-4.18	1.38	1.47
20	DJ	501	GTP	C5-C6	-4.18	1.38	1.47
20	DD	501	GTP	C5-C6	-4.18	1.38	1.47
20	IL	501	GTP	C5-C6	-4.18	1.38	1.47
20	AH	501	GTP	C5-C6	-4.18	1.38	1.47
20	JL	501	GTP	C5-C6	-4.18	1.38	1.47
20	KD	501	GTP	C5-C6	-4.18	1.38	1.47
20	ML	501	GTP	C5-C6	-4.18	1.38	1.47
20	BJ	501	GTP	C5-C6	-4.18	1.38	1.47
20	HI	501	GTP	C5-C6	-4.18	1.38	1.47
20	ID	501	GTP	C5-C6	-4.17	1.38	1.47
20	KF	501	GTP	C5-C6	-4.17	1.38	1.47
20	MB	501	GTP	C5-C6	-4.17	1.38	1.47
20	LD	501	GTP	C5-C6	-4.17	1.38	1.47
20	BB	501	GTP	C5-C6	-4.17	1.38	1.47
20	MJ	501	GTP	C5-C6	-4.17	1.38	1.47
20	LL	501	GTP	C5-C6	-4.17	1.38	1.47
20	KB	501	GTP	C5-C6	-4.17	1.38	1.47
20	AJ	501	GTP	C5-C6	-4.16	1.39	1.47
20	AL	501	GTP	C5-C6	-4.16	1.39	1.47
20	LB	501	GTP	C5-C6	-4.16	1.39	1.47
20	GH	501	GTP	C5-C6	-4.16	1.39	1.47
20	ED	501	GTP	C5-C6	-4.15	1.39	1.47
20	JJ	501	GTP	C5-C6	-4.15	1.39	1.47
20	EL	501	GTP	C5-C6	-4.15	1.39	1.47
20	GL	501	GTP	C5-C6	-4.15	1.39	1.47
20	FB	501	GTP	C5-C6	-4.14	1.39	1.47
20	KJ	501	GTP	C5-C6	-4.14	1.39	1.47
20	JB	501	GTP	C5-C6	-4.13	1.39	1.47
20	CJ	501	GTP	C5-C6	-4.13	1.39	1.47
20	EJ	501	GTP	C5-C6	-4.13	1.39	1.47
20	JH	501	GTP	C5-C6	-4.12	1.39	1.47
20	LJ	501	GTP	C5-C6	-4.12	1.39	1.47
20	JD	501	GTP	C5-C6	-4.12	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CB	501	GTP	C5-C6	-4.12	1.39	1.47
20	KL	501	GTP	C5-C6	-4.12	1.39	1.47
20	KH	501	GTP	C5-C6	-4.11	1.39	1.47
20	GD	501	GTP	C5-C6	-4.11	1.39	1.47
20	BH	501	GTP	C5-C6	-4.10	1.39	1.47
20	MD	501	GTP	C5-C6	-4.10	1.39	1.47
20	BL	501	GTP	C5-C6	-4.09	1.39	1.47
20	HL	501	GTP	C5-C6	-4.08	1.39	1.47
20	AD	501	GTP	C5-C6	-4.07	1.39	1.47
20	HJ	501	GTP	C5-C6	-4.06	1.39	1.47
20	GJ	501	GTP	C5-C6	-4.06	1.39	1.47
20	BD	501	GTP	C5-C6	-4.05	1.39	1.47
20	GF	501	GTP	C5-C6	-4.04	1.39	1.47
20	HD	501	GTP	C5-C6	-4.00	1.39	1.47
20	HF	501	GTP	C5-C6	-3.98	1.39	1.47
19	BE	501	GDP	C6-N1	-2.93	1.33	1.37
19	AG	501	GDP	C6-N1	-2.79	1.33	1.37
19	GI	501	GDP	C6-N1	-2.73	1.33	1.37
19	IM	501	GDP	C6-N1	-2.67	1.33	1.37
19	LC	501	GDP	C6-N1	-2.65	1.33	1.37
19	DE	501	GDP	C6-N1	-2.65	1.33	1.37
19	EE	502	GDP	C6-N1	-2.64	1.33	1.37
19	AE	501	GDP	C6-N1	-2.64	1.33	1.37
19	BG	501	GDP	C6-N1	-2.63	1.34	1.37
19	HI	502	GDP	C6-N1	-2.62	1.34	1.37
19	CA	501	GDP	C6-N1	-2.62	1.34	1.37
19	II	501	GDP	C6-N1	-2.62	1.34	1.37
19	HC	501	GDP	C6-N1	-2.61	1.34	1.37
19	FE	501	GDP	C6-N1	-2.61	1.34	1.37
19	HM	501	GDP	C6-N1	-2.60	1.34	1.37
19	CE	501	GDP	C6-N1	-2.60	1.34	1.37
19	EG	501	GDP	C6-N1	-2.60	1.34	1.37
19	GC	501	GDP	C6-N1	-2.59	1.34	1.37
19	GE	501	GDP	C6-N1	-2.59	1.34	1.37
19	HG	501	GDP	C6-N1	-2.59	1.34	1.37
19	EI	501	GDP	C6-N1	-2.59	1.34	1.37
19	GM	501	GDP	C6-N1	-2.59	1.34	1.37
19	JI	501	GDP	C6-N1	-2.59	1.34	1.37
19	KI	502	GDP	C6-N1	-2.59	1.34	1.37
19	BC	501	GDP	C6-N1	-2.58	1.34	1.37
19	KG	501	GDP	C6-N1	-2.58	1.34	1.37
19	MI	501	GDP	C6-N1	-2.58	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	LE	501	GDP	C6-N1	-2.58	1.34	1.37
19	LK	501	GDP	C6-N1	-2.58	1.34	1.37
19	EK	501	GDP	C6-N1	-2.58	1.34	1.37
19	CG	501	GDP	C6-N1	-2.57	1.34	1.37
19	AC	501	GDP	C6-N1	-2.57	1.34	1.37
19	GG	501	GDP	C6-N1	-2.57	1.34	1.37
19	ME	501	GDP	C6-N1	-2.57	1.34	1.37
19	LI	501	GDP	C6-N1	-2.56	1.34	1.37
19	BI	501	GDP	C6-N1	-2.56	1.34	1.37
19	GK	501	GDP	C6-N1	-2.56	1.34	1.37
19	EA	501	GDP	C6-N1	-2.56	1.34	1.37
19	EC	501	GDP	C6-N1	-2.56	1.34	1.37
19	FC	501	GDP	C6-N1	-2.56	1.34	1.37
19	DI	501	GDP	C6-N1	-2.56	1.34	1.37
19	AI	501	GDP	C6-N1	-2.55	1.34	1.37
19	FG	501	GDP	C6-N1	-2.55	1.34	1.37
19	CC	501	GDP	C6-N1	-2.55	1.34	1.37
19	KE	501	GDP	C6-N1	-2.55	1.34	1.37
19	MG	501	GDP	C6-N1	-2.55	1.34	1.37
19	DC	501	GDP	C6-N1	-2.53	1.34	1.37
19	CI	501	GDP	C6-N1	-2.53	1.34	1.37
19	IC	501	GDP	C6-N1	-2.53	1.34	1.37
19	FA	501	GDP	C6-N1	-2.52	1.34	1.37
19	HK	501	GDP	C6-N1	-2.52	1.34	1.37
19	MC	501	GDP	C6-N1	-2.52	1.34	1.37
19	BK	501	GDP	C6-N1	-2.52	1.34	1.37
19	DG	501	GDP	C6-N1	-2.52	1.34	1.37
19	IG	501	GDP	C6-N1	-2.52	1.34	1.37
19	LG	501	GDP	C6-N1	-2.51	1.34	1.37
19	AA	501	GDP	C6-N1	-2.51	1.34	1.37
19	JM	501	GDP	C6-N1	-2.51	1.34	1.37
19	CK	501	GDP	C6-N1	-2.51	1.34	1.37
19	FI	501	GDP	C6-N1	-2.51	1.34	1.37
19	IK	501	GDP	C6-N1	-2.50	1.34	1.37
19	JC	501	GDP	C6-N1	-2.50	1.34	1.37
19	FK	501	GDP	C6-N1	-2.50	1.34	1.37
19	KC	501	GDP	C6-N1	-2.50	1.34	1.37
19	IE	501	GDP	C6-N1	-2.48	1.34	1.37
19	MK	501	GDP	C6-N1	-2.48	1.34	1.37
19	JK	501	GDP	C6-N1	-2.48	1.34	1.37
19	AK	501	GDP	C6-N1	-2.47	1.34	1.37
19	HE	501	GDP	C6-N1	-2.47	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	KK	501	GDP	C6-N1	-2.46	1.34	1.37
19	DK	501	GDP	C6-N1	-2.42	1.34	1.37
19	JG	501	GDP	C6-N1	-2.41	1.34	1.37
19	JE	501	GDP	C6-N1	-2.40	1.34	1.37
19	BA	501	GDP	C6-N1	-2.36	1.34	1.37
20	EB	501	GTP	C2-N3	2.20	1.38	1.33
20	DL	501	GTP	C2-N3	2.20	1.38	1.33
20	GL	501	GTP	C2-N3	2.19	1.38	1.33
20	FF	501	GTP	C2-N3	2.19	1.38	1.33
20	AJ	501	GTP	C2-N3	2.18	1.38	1.33
20	EF	501	GTP	C2-N3	2.18	1.38	1.33
20	HD	501	GTP	C2-N3	2.18	1.38	1.33
20	FD	501	GTP	C2-N3	2.17	1.38	1.33
20	LJ	501	GTP	C2-N3	2.17	1.38	1.33
20	HJ	501	GTP	C2-N3	2.17	1.38	1.33
20	GD	501	GTP	C2-N3	2.17	1.38	1.33
20	JD	501	GTP	C2-N3	2.17	1.38	1.33
20	KH	501	GTP	C2-N3	2.17	1.38	1.33
20	LB	501	GTP	C2-N3	2.17	1.38	1.33
20	FJ	501	GTP	C2-N3	2.17	1.38	1.33
20	MB	501	GTP	C2-N3	2.16	1.38	1.33
20	DJ	501	GTP	C2-N3	2.16	1.38	1.33
20	CJ	501	GTP	C2-N3	2.16	1.38	1.33
20	GH	501	GTP	C2-N3	2.16	1.38	1.33
20	AD	501	GTP	C2-N3	2.15	1.38	1.33
20	HL	501	GTP	C2-N3	2.15	1.38	1.33
20	MJ	501	GTP	C2-N3	2.15	1.38	1.33
20	JJ	501	GTP	C2-N3	2.15	1.38	1.33
20	MD	501	GTP	C2-N3	2.15	1.38	1.33
20	LD	501	GTP	C2-N3	2.15	1.38	1.33
20	FB	501	GTP	C2-N3	2.15	1.38	1.33
20	KL	501	GTP	C2-N3	2.15	1.38	1.33
20	EJ	501	GTP	C2-N3	2.15	1.38	1.33
20	EL	501	GTP	C2-N3	2.14	1.38	1.33
20	BB	501	GTP	C2-N3	2.14	1.38	1.33
20	CB	501	GTP	C2-N3	2.14	1.38	1.33
20	MF	501	GTP	C2-N3	2.14	1.38	1.33
20	CH	501	GTP	C2-N3	2.13	1.38	1.33
20	ED	501	GTP	C2-N3	2.13	1.38	1.33
20	IF	501	GTP	C2-N3	2.13	1.38	1.33
20	JF	501	GTP	C2-N3	2.12	1.38	1.33
20	BL	501	GTP	C2-N3	2.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	FL	501	GTP	C2-N3	2.11	1.38	1.33
20	IH	501	GTP	C2-N3	2.11	1.38	1.33
20	FH	501	GTP	C2-N3	2.11	1.38	1.33
20	LL	501	GTP	C2-N3	2.11	1.38	1.33
20	ID	501	GTP	C2-N3	2.11	1.38	1.33
20	BJ	501	GTP	C2-N3	2.11	1.38	1.33
20	LF	501	GTP	C2-N3	2.11	1.38	1.33
20	CF	501	GTP	C2-N3	2.10	1.38	1.33
20	ML	501	GTP	C2-N3	2.10	1.38	1.33
20	KJ	501	GTP	C2-N3	2.10	1.38	1.33
20	JH	501	GTP	C2-N3	2.10	1.38	1.33
20	JL	501	GTP	C2-N3	2.10	1.38	1.33
20	HF	501	GTP	C2-N3	2.09	1.38	1.33
20	AB	501	GTP	C2-N3	2.09	1.38	1.33
20	IL	501	GTP	C2-N3	2.09	1.38	1.33
20	MH	501	GTP	C2-N3	2.09	1.38	1.33
20	JB	501	GTP	C2-N3	2.09	1.38	1.33
20	BD	501	GTP	C2-N3	2.09	1.38	1.33
20	BH	501	GTP	C2-N3	2.08	1.38	1.33
20	AL	501	GTP	C2-N3	2.08	1.38	1.33
20	KD	501	GTP	C2-N3	2.08	1.38	1.33
20	BF	501	GTP	C2-N3	2.07	1.38	1.33
20	GF	501	GTP	C2-N3	2.07	1.38	1.33
20	KB	501	GTP	C2-N3	2.06	1.38	1.33
20	DB	501	GTP	C2-N3	2.06	1.38	1.33
20	AH	501	GTP	C2-N3	2.06	1.38	1.33
20	EH	501	GTP	C2-N3	2.06	1.38	1.33
20	CD	501	GTP	C2-N3	2.05	1.38	1.33
20	IJ	501	GTP	C2-N3	2.05	1.38	1.33
20	HI	501	GTP	C2-N3	2.04	1.38	1.33
20	LH	501	GTP	C2-N3	2.04	1.38	1.33
20	DF	501	GTP	C2-N3	2.03	1.38	1.33
20	GJ	501	GTP	C2-N3	2.03	1.38	1.33
20	AF	501	GTP	C2-N3	2.02	1.38	1.33
20	KF	501	GTP	C2-N3	2.01	1.38	1.33

All (816) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	DH	501	GTP	PB-O3B-PG	-4.74	116.55	132.83
20	MD	501	GTP	PB-O3B-PG	-4.64	116.91	132.83
20	ML	501	GTP	PB-O3B-PG	-4.63	116.92	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	DE	501	GDP	PA-O3A-PB	-4.62	116.98	132.83
20	IH	501	GTP	PB-O3B-PG	-4.56	117.17	132.83
20	MD	501	GTP	PA-O3A-PB	-4.56	117.18	132.83
20	DJ	501	GTP	PA-O3A-PB	-4.53	117.28	132.83
20	DF	501	GTP	PA-O3A-PB	-4.50	117.37	132.83
20	DH	501	GTP	PA-O3A-PB	-4.50	117.38	132.83
20	LH	501	GTP	PA-O3A-PB	-4.48	117.45	132.83
20	KB	501	GTP	PA-O3A-PB	-4.47	117.47	132.83
20	CD	501	GTP	PB-O3B-PG	-4.46	117.51	132.83
20	AH	501	GTP	PB-O3B-PG	-4.46	117.51	132.83
20	KH	501	GTP	PA-O3A-PB	-4.46	117.52	132.83
20	DB	501	GTP	PA-O3A-PB	-4.43	117.61	132.83
20	KJ	501	GTP	PA-O3A-PB	-4.43	117.63	132.83
20	EL	501	GTP	PB-O3B-PG	-4.43	117.64	132.83
20	HI	501	GTP	PA-O3A-PB	-4.42	117.67	132.83
20	FL	501	GTP	PB-O3B-PG	-4.42	117.67	132.83
20	FJ	501	GTP	PA-O3A-PB	-4.40	117.72	132.83
20	LF	501	GTP	PA-O3A-PB	-4.40	117.73	132.83
20	CH	501	GTP	PB-O3B-PG	-4.39	117.75	132.83
20	FH	501	GTP	PB-O3B-PG	-4.39	117.76	132.83
20	BL	501	GTP	PB-O3B-PG	-4.39	117.77	132.83
20	HJ	501	GTP	PB-O3B-PG	-4.39	117.78	132.83
20	GD	501	GTP	PA-O3A-PB	-4.38	117.80	132.83
20	DL	501	GTP	PB-O3B-PG	-4.38	117.80	132.83
20	EB	501	GTP	PB-O3B-PG	-4.37	117.83	132.83
20	JF	501	GTP	PA-O3A-PB	-4.36	117.86	132.83
20	BH	501	GTP	PB-O3B-PG	-4.36	117.86	132.83
20	BF	501	GTP	PB-O3B-PG	-4.35	117.89	132.83
20	GF	501	GTP	PA-O3A-PB	-4.32	118.00	132.83
20	GJ	501	GTP	PA-O3A-PB	-4.32	118.02	132.83
20	IF	501	GTP	PA-O3A-PB	-4.31	118.05	132.83
20	LJ	501	GTP	PA-O3A-PB	-4.31	118.05	132.83
20	FD	501	GTP	PB-O3B-PG	-4.30	118.07	132.83
20	GF	501	GTP	PB-O3B-PG	-4.30	118.07	132.83
19	MI	501	GDP	PA-O3A-PB	-4.29	118.11	132.83
20	BJ	501	GTP	PB-O3B-PG	-4.28	118.14	132.83
20	HD	501	GTP	PA-O3A-PB	-4.28	118.14	132.83
20	FB	501	GTP	PA-O3A-PB	-4.28	118.15	132.83
19	DI	501	GDP	PA-O3A-PB	-4.28	118.16	132.83
20	MF	501	GTP	PA-O3A-PB	-4.27	118.16	132.83
19	JI	501	GDP	PA-O3A-PB	-4.27	118.17	132.83
20	ED	501	GTP	PA-O3A-PB	-4.25	118.23	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	HL	501	GTP	PB-O3B-PG	-4.25	118.24	132.83
20	CF	501	GTP	PB-O3B-PG	-4.24	118.27	132.83
20	BB	501	GTP	PB-O3B-PG	-4.24	118.27	132.83
20	FJ	501	GTP	PB-O3B-PG	-4.24	118.28	132.83
20	JB	501	GTP	PB-O3B-PG	-4.23	118.31	132.83
20	MJ	501	GTP	PB-O3B-PG	-4.23	118.32	132.83
20	BD	501	GTP	PB-O3B-PG	-4.22	118.35	132.83
20	CJ	501	GTP	PB-O3B-PG	-4.22	118.36	132.83
20	GH	501	GTP	PB-O3B-PG	-4.22	118.36	132.83
20	LL	501	GTP	PB-O3B-PG	-4.20	118.41	132.83
20	AL	501	GTP	PA-O3A-PB	-4.20	118.43	132.83
20	EH	501	GTP	PB-O3B-PG	-4.19	118.43	132.83
20	GJ	501	GTP	PB-O3B-PG	-4.18	118.47	132.83
20	KF	501	GTP	PA-O3A-PB	-4.18	118.49	132.83
19	ME	501	GDP	PA-O3A-PB	-4.17	118.50	132.83
20	LF	501	GTP	PB-O3B-PG	-4.17	118.51	132.83
20	AF	501	GTP	PB-O3B-PG	-4.17	118.51	132.83
20	IJ	501	GTP	PB-O3B-PG	-4.17	118.51	132.83
20	HF	501	GTP	PA-O3A-PB	-4.17	118.52	132.83
20	IF	501	GTP	PB-O3B-PG	-4.17	118.52	132.83
20	KD	501	GTP	PA-O3A-PB	-4.17	118.52	132.83
20	AD	501	GTP	PA-O3A-PB	-4.17	118.53	132.83
20	CH	501	GTP	PA-O3A-PB	-4.16	118.57	132.83
20	LB	501	GTP	PB-O3B-PG	-4.16	118.57	132.83
20	JL	501	GTP	PA-O3A-PB	-4.15	118.57	132.83
19	BC	501	GDP	PA-O3A-PB	-4.14	118.61	132.83
20	GL	501	GTP	PB-O3B-PG	-4.14	118.61	132.83
20	ID	501	GTP	PA-O3A-PB	-4.14	118.62	132.83
20	IL	501	GTP	PA-O3A-PB	-4.14	118.63	132.83
20	FB	501	GTP	PB-O3B-PG	-4.13	118.66	132.83
20	MH	501	GTP	PA-O3A-PB	-4.12	118.68	132.83
20	LJ	501	GTP	PB-O3B-PG	-4.12	118.69	132.83
20	MB	501	GTP	PB-O3B-PG	-4.12	118.69	132.83
20	GH	501	GTP	PA-O3A-PB	-4.11	118.71	132.83
20	CB	501	GTP	PB-O3B-PG	-4.10	118.77	132.83
20	MF	501	GTP	PB-O3B-PG	-4.09	118.80	132.83
20	EJ	501	GTP	PB-O3B-PG	-4.08	118.82	132.83
20	AJ	501	GTP	PA-O3A-PB	-4.07	118.85	132.83
20	JL	501	GTP	PB-O3B-PG	-4.07	118.85	132.83
19	AE	501	GDP	PA-O3A-PB	-4.07	118.86	132.83
20	LB	501	GTP	PA-O3A-PB	-4.07	118.87	132.83
19	JM	501	GDP	PA-O3A-PB	-4.06	118.91	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	KB	501	GTP	PB-O3B-PG	-4.05	118.91	132.83
20	GD	501	GTP	PB-O3B-PG	-4.05	118.94	132.83
20	AJ	501	GTP	PB-O3B-PG	-4.04	118.95	132.83
20	KJ	501	GTP	PB-O3B-PG	-4.03	119.00	132.83
20	IL	501	GTP	PB-O3B-PG	-4.03	119.00	132.83
20	JJ	501	GTP	PA-O3A-PB	-4.03	119.00	132.83
20	ML	501	GTP	PA-O3A-PB	-4.02	119.02	132.83
19	KE	501	GDP	PA-O3A-PB	-4.02	119.02	132.83
20	EF	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
19	GE	501	GDP	PA-O3A-PB	-4.02	119.02	132.83
19	BK	501	GDP	PA-O3A-PB	-4.02	119.02	132.83
20	AD	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
20	ED	501	GTP	PB-O3B-PG	-4.02	119.03	132.83
20	MH	501	GTP	PB-O3B-PG	-4.02	119.04	132.83
20	LH	501	GTP	PB-O3B-PG	-4.01	119.06	132.83
19	IE	501	GDP	PA-O3A-PB	-4.00	119.11	132.83
20	JB	501	GTP	PA-O3A-PB	-4.00	119.12	132.83
20	KF	501	GTP	PB-O3B-PG	-3.99	119.12	132.83
20	HJ	501	GTP	PA-O3A-PB	-3.99	119.13	132.83
20	DL	501	GTP	PA-O3A-PB	-3.99	119.14	132.83
20	IJ	501	GTP	PA-O3A-PB	-3.97	119.20	132.83
20	ID	501	GTP	PB-O3B-PG	-3.97	119.20	132.83
20	CJ	501	GTP	PA-O3A-PB	-3.96	119.22	132.83
19	MK	501	GDP	PA-O3A-PB	-3.96	119.23	132.83
20	AL	501	GTP	PB-O3B-PG	-3.95	119.27	132.83
20	HI	501	GTP	PB-O3B-PG	-3.95	119.27	132.83
20	DJ	501	GTP	PB-O3B-PG	-3.93	119.34	132.83
20	KD	501	GTP	PB-O3B-PG	-3.92	119.36	132.83
20	AB	501	GTP	PB-O3B-PG	-3.92	119.37	132.83
19	BG	501	GDP	PA-O3A-PB	-3.92	119.38	132.83
20	BD	501	GTP	PA-O3A-PB	-3.92	119.38	132.83
20	HL	501	GTP	PA-O3A-PB	-3.91	119.40	132.83
19	MG	501	GDP	PA-O3A-PB	-3.91	119.40	132.83
20	EL	501	GTP	PA-O3A-PB	-3.89	119.47	132.83
19	II	501	GDP	PA-O3A-PB	-3.87	119.55	132.83
19	AI	501	GDP	PA-O3A-PB	-3.87	119.56	132.83
20	FF	501	GTP	PB-O3B-PG	-3.86	119.58	132.83
20	BJ	501	GTP	PA-O3A-PB	-3.86	119.60	132.83
19	GM	501	GDP	PA-O3A-PB	-3.84	119.66	132.83
19	MC	501	GDP	PA-O3A-PB	-3.83	119.69	132.83
20	LD	501	GTP	PB-O3B-PG	-3.83	119.70	132.83
19	LG	501	GDP	PA-O3A-PB	-3.82	119.71	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	KK	501	GDP	PA-O3A-PB	-3.82	119.72	132.83
19	KG	501	GDP	PA-O3A-PB	-3.81	119.73	132.83
20	DD	501	GTP	PB-O3B-PG	-3.81	119.75	132.83
20	AB	501	GTP	PA-O3A-PB	-3.76	119.91	132.83
19	JK	501	GDP	PA-O3A-PB	-3.76	119.92	132.83
20	HD	501	GTP	PB-O3B-PG	-3.76	119.93	132.83
20	JJ	501	GTP	PB-O3B-PG	-3.75	119.95	132.83
19	AK	501	GDP	PA-O3A-PB	-3.73	120.01	132.83
20	JH	501	GTP	PB-O3B-PG	-3.73	120.04	132.83
19	FE	501	GDP	PA-O3A-PB	-3.72	120.05	132.83
19	GC	501	GDP	PA-O3A-PB	-3.72	120.05	132.83
20	AF	501	GTP	PA-O3A-PB	-3.71	120.11	132.83
20	KL	501	GTP	PA-O3A-PB	-3.69	120.15	132.83
19	GG	501	GDP	PA-O3A-PB	-3.69	120.16	132.83
20	BH	501	GTP	PA-O3A-PB	-3.69	120.17	132.83
19	HG	501	GDP	PA-O3A-PB	-3.67	120.24	132.83
19	GK	501	GDP	PA-O3A-PB	-3.66	120.25	132.83
19	AA	501	GDP	PA-O3A-PB	-3.66	120.27	132.83
19	HI	502	GDP	PA-O3A-PB	-3.66	120.27	132.83
19	CA	501	GDP	PA-O3A-PB	-3.66	120.28	132.83
19	FC	501	GDP	PA-O3A-PB	-3.63	120.36	132.83
19	LK	501	GDP	PA-O3A-PB	-3.63	120.38	132.83
19	EE	502	GDP	PA-O3A-PB	-3.62	120.39	132.83
19	EI	501	GDP	PA-O3A-PB	-3.62	120.39	132.83
20	FF	501	GTP	PA-O3A-PB	-3.62	120.39	132.83
20	KL	501	GTP	PB-O3B-PG	-3.61	120.45	132.83
19	JE	501	GDP	PA-O3A-PB	-3.61	120.45	132.83
19	KI	502	GDP	PA-O3A-PB	-3.60	120.47	132.83
19	EA	501	GDP	PA-O3A-PB	-3.59	120.51	132.83
20	CB	501	GTP	PA-O3A-PB	-3.58	120.53	132.83
20	KH	501	GTP	PB-O3B-PG	-3.57	120.59	132.83
19	FK	501	GDP	PA-O3A-PB	-3.56	120.62	132.83
19	CI	501	GDP	PA-O3A-PB	-3.54	120.68	132.83
19	EC	501	GDP	PA-O3A-PB	-3.54	120.68	132.83
19	FA	501	GDP	PA-O3A-PB	-3.53	120.70	132.83
20	DD	501	GTP	PA-O3A-PB	-3.53	120.70	132.83
20	HF	501	GTP	PB-O3B-PG	-3.53	120.70	132.83
19	AC	501	GDP	PA-O3A-PB	-3.53	120.72	132.83
19	BI	501	GDP	PA-O3A-PB	-3.52	120.75	132.83
20	JF	501	GTP	PB-O3B-PG	-3.52	120.75	132.83
20	DF	501	GTP	PB-O3B-PG	-3.52	120.75	132.83
19	IG	501	GDP	PA-O3A-PB	-3.52	120.76	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	CK	501	GDP	PA-O3A-PB	-3.51	120.77	132.83
20	FH	501	GTP	PA-O3A-PB	-3.51	120.77	132.83
20	FD	501	GTP	PA-O3A-PB	-3.51	120.78	132.83
19	CC	501	GDP	PA-O3A-PB	-3.51	120.78	132.83
20	CF	501	GTP	PA-O3A-PB	-3.50	120.81	132.83
19	FI	501	GDP	PA-O3A-PB	-3.47	120.91	132.83
19	LC	501	GDP	PA-O3A-PB	-3.47	120.92	132.83
19	JC	501	GDP	PA-O3A-PB	-3.47	120.93	132.83
19	HC	501	GDP	PA-O3A-PB	-3.46	120.94	132.83
19	KC	501	GDP	PA-O3A-PB	-3.46	120.96	132.83
19	BA	501	GDP	PA-O3A-PB	-3.45	120.97	132.83
19	DK	501	GDP	PA-O3A-PB	-3.45	120.99	132.83
19	LE	501	GDP	PA-O3A-PB	-3.44	121.03	132.83
19	IM	501	GDP	PA-O3A-PB	-3.43	121.05	132.83
19	DC	501	GDP	PA-O3A-PB	-3.42	121.08	132.83
20	JD	501	GTP	PA-O3A-PB	-3.42	121.10	132.83
20	EF	501	GTP	C5-C6-N1	3.41	119.97	113.95
19	HE	501	GDP	PA-O3A-PB	-3.41	121.12	132.83
19	EG	501	GDP	PA-O3A-PB	-3.40	121.17	132.83
20	FL	501	GTP	PA-O3A-PB	-3.39	121.19	132.83
20	CD	501	GTP	PA-O3A-PB	-3.39	121.20	132.83
20	AH	501	GTP	PA-O3A-PB	-3.39	121.21	132.83
19	BE	501	GDP	PA-O3A-PB	-3.38	121.21	132.83
20	BB	501	GTP	PA-O3A-PB	-3.38	121.23	132.83
19	CE	501	GDP	PA-O3A-PB	-3.36	121.30	132.83
20	HL	501	GTP	C5-C6-N1	3.36	119.88	113.95
20	CB	501	GTP	C5-C6-N1	3.35	119.87	113.95
20	HI	501	GTP	C5-C6-N1	3.35	119.87	113.95
19	IC	501	GDP	PA-O3A-PB	-3.35	121.33	132.83
19	AA	501	GDP	C3'-C2'-C1'	3.35	106.02	100.98
20	GD	501	GTP	C5-C6-N1	3.35	119.86	113.95
19	EK	501	GDP	PA-O3A-PB	-3.34	121.35	132.83
20	EH	501	GTP	PA-O3A-PB	-3.34	121.36	132.83
19	IK	501	GDP	PA-O3A-PB	-3.34	121.38	132.83
20	GL	501	GTP	PA-O3A-PB	-3.33	121.39	132.83
20	FF	501	GTP	C5-C6-N1	3.33	119.83	113.95
20	JH	501	GTP	C5-C6-N1	3.33	119.83	113.95
20	GH	501	GTP	C5-C6-N1	3.33	119.83	113.95
20	DJ	501	GTP	C5-C6-N1	3.33	119.83	113.95
20	DL	501	GTP	C5-C6-N1	3.32	119.82	113.95
20	IH	501	GTP	C5-C6-N1	3.32	119.81	113.95
20	LD	501	GTP	PA-O3A-PB	-3.32	121.43	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	MD	501	GTP	C5-C6-N1	3.32	119.81	113.95
20	HL	501	GTP	C3'-C2'-C1'	3.32	105.97	100.98
20	GL	501	GTP	C5-C6-N1	3.32	119.81	113.95
20	MJ	501	GTP	C5-C6-N1	3.32	119.81	113.95
20	EJ	501	GTP	C5-C6-N1	3.32	119.81	113.95
20	BL	501	GTP	PA-O3A-PB	-3.31	121.46	132.83
20	IF	501	GTP	C5-C6-N1	3.31	119.80	113.95
20	CD	501	GTP	C5-C6-N1	3.31	119.79	113.95
20	JD	501	GTP	PB-O3B-PG	-3.30	121.49	132.83
20	CJ	501	GTP	C5-C6-N1	3.30	119.78	113.95
20	LD	501	GTP	C5-C6-N1	3.30	119.78	113.95
19	LI	501	GDP	PA-O3A-PB	-3.30	121.51	132.83
20	LL	501	GTP	PA-O3A-PB	-3.30	121.52	132.83
20	JL	501	GTP	C5-C6-N1	3.29	119.77	113.95
20	IH	501	GTP	PA-O3A-PB	-3.29	121.53	132.83
20	BD	501	GTP	C5-C6-N1	3.29	119.76	113.95
20	LF	501	GTP	C5-C6-N1	3.29	119.76	113.95
20	CH	501	GTP	C5-C6-N1	3.29	119.76	113.95
20	MH	501	GTP	C5-C6-N1	3.29	119.76	113.95
20	MF	501	GTP	C5-C6-N1	3.29	119.76	113.95
20	ML	501	GTP	C5-C6-N1	3.29	119.75	113.95
20	KD	501	GTP	C5-C6-N1	3.28	119.75	113.95
20	MB	501	GTP	C5-C6-N1	3.28	119.74	113.95
20	CF	501	GTP	C5-C6-N1	3.28	119.74	113.95
20	DD	501	GTP	C5-C6-N1	3.28	119.74	113.95
19	DG	501	GDP	PA-O3A-PB	-3.27	121.59	132.83
20	FH	501	GTP	C5-C6-N1	3.27	119.73	113.95
20	EB	501	GTP	C5-C6-N1	3.27	119.73	113.95
20	FJ	501	GTP	C5-C6-N1	3.27	119.73	113.95
19	HM	501	GDP	PA-O3A-PB	-3.27	121.61	132.83
20	LB	501	GTP	C5-C6-N1	3.26	119.71	113.95
19	BK	501	GDP	C3'-C2'-C1'	3.26	105.89	100.98
20	AB	501	GTP	C5-C6-N1	3.26	119.71	113.95
20	BB	501	GTP	C5-C6-N1	3.26	119.71	113.95
20	CD	501	GTP	C3'-C2'-C1'	3.26	105.88	100.98
20	LJ	501	GTP	C5-C6-N1	3.25	119.69	113.95
20	KL	501	GTP	C5-C6-N1	3.25	119.69	113.95
19	GI	501	GDP	PA-O3A-PB	-3.25	121.69	132.83
19	AG	501	GDP	PA-O3A-PB	-3.24	121.69	132.83
20	HJ	501	GTP	C5-C6-N1	3.24	119.68	113.95
20	GF	501	GTP	C3'-C2'-C1'	3.24	105.86	100.98
20	BJ	501	GTP	C5-C6-N1	3.24	119.67	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	GJ	501	GTP	C5-C6-N1	3.24	119.67	113.95
20	HD	501	GTP	C5-C6-N1	3.24	119.67	113.95
20	FD	501	GTP	C5-C6-N1	3.23	119.66	113.95
20	BH	501	GTP	C5-C6-N1	3.23	119.66	113.95
20	DH	501	GTP	C5-C6-N1	3.23	119.66	113.95
20	KH	501	GTP	C5-C6-N1	3.23	119.66	113.95
20	AH	501	GTP	C5-C6-N1	3.23	119.66	113.95
20	AF	501	GTP	C5-C6-N1	3.23	119.66	113.95
20	JJ	501	GTP	C5-C6-N1	3.23	119.65	113.95
20	GF	501	GTP	C5-C6-N1	3.23	119.65	113.95
20	FL	501	GTP	C5-C6-N1	3.22	119.64	113.95
20	MD	501	GTP	C3'-C2'-C1'	3.22	105.83	100.98
20	KB	501	GTP	C5-C6-N1	3.22	119.64	113.95
20	AJ	501	GTP	C5-C6-N1	3.22	119.63	113.95
20	JD	501	GTP	C5-C6-N1	3.22	119.63	113.95
20	AD	501	GTP	C5-C6-N1	3.21	119.63	113.95
20	EH	501	GTP	C5-C6-N1	3.21	119.62	113.95
19	IM	501	GDP	C3'-C2'-C1'	3.21	105.81	100.98
20	FB	501	GTP	C5-C6-N1	3.21	119.62	113.95
20	HF	501	GTP	C5-C6-N1	3.21	119.62	113.95
19	EK	501	GDP	C3'-C2'-C1'	3.21	105.81	100.98
20	DF	501	GTP	C5-C6-N1	3.20	119.61	113.95
20	IL	501	GTP	C5-C6-N1	3.20	119.60	113.95
20	JF	501	GTP	C5-C6-N1	3.20	119.60	113.95
20	IJ	501	GTP	C5-C6-N1	3.20	119.59	113.95
20	BF	501	GTP	C5-C6-N1	3.19	119.59	113.95
20	LH	501	GTP	C5-C6-N1	3.19	119.58	113.95
20	DB	501	GTP	C5-C6-N1	3.18	119.57	113.95
19	FA	501	GDP	C3'-C2'-C1'	3.18	105.77	100.98
20	KF	501	GTP	C5-C6-N1	3.18	119.57	113.95
20	LL	501	GTP	C5-C6-N1	3.18	119.57	113.95
20	ED	501	GTP	C5-C6-N1	3.18	119.56	113.95
19	HK	501	GDP	PA-O3A-PB	-3.17	121.94	132.83
20	KF	501	GTP	C8-N7-C5	3.17	109.04	102.99
20	EL	501	GTP	C5-C6-N1	3.17	119.54	113.95
20	KJ	501	GTP	C5-C6-N1	3.16	119.54	113.95
20	JB	501	GTP	C5-C6-N1	3.15	119.52	113.95
20	AL	501	GTP	C5-C6-N1	3.15	119.51	113.95
20	HF	501	GTP	C3'-C2'-C1'	3.15	105.71	100.98
20	CH	501	GTP	C3'-C2'-C1'	3.14	105.71	100.98
20	BL	501	GTP	C5-C6-N1	3.14	119.50	113.95
20	FH	501	GTP	C3'-C2'-C1'	3.13	105.69	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	MB	501	GTP	C3'-C2'-C1'	3.13	105.69	100.98
19	JM	501	GDP	C3'-C2'-C1'	3.13	105.69	100.98
20	ID	501	GTP	C5-C6-N1	3.12	119.46	113.95
20	LF	501	GTP	C3'-C2'-C1'	3.12	105.67	100.98
19	GC	501	GDP	C3'-C2'-C1'	3.11	105.65	100.98
19	HM	501	GDP	C3'-C2'-C1'	3.11	105.65	100.98
20	BD	501	GTP	C8-N7-C5	3.11	108.91	102.99
20	GJ	501	GTP	C8-N7-C5	3.10	108.90	102.99
20	HJ	501	GTP	C3'-C2'-C1'	3.10	105.64	100.98
20	GD	501	GTP	C8-N7-C5	3.09	108.88	102.99
19	CA	501	GDP	C3'-C2'-C1'	3.09	105.63	100.98
20	FL	501	GTP	C3'-C2'-C1'	3.09	105.63	100.98
20	GF	501	GTP	C8-N7-C5	3.08	108.86	102.99
20	GH	501	GTP	C3'-C2'-C1'	3.08	105.61	100.98
20	FD	501	GTP	C3'-C2'-C1'	3.07	105.60	100.98
20	GH	501	GTP	C8-N7-C5	3.07	108.83	102.99
20	GL	501	GTP	C3'-C2'-C1'	3.06	105.59	100.98
19	KI	502	GDP	C3'-C2'-C1'	3.06	105.59	100.98
20	EJ	501	GTP	PA-O3A-PB	-3.06	122.32	132.83
20	JH	501	GTP	C8-N7-C5	3.06	108.82	102.99
20	KB	501	GTP	C8-N7-C5	3.06	108.81	102.99
20	DH	501	GTP	C8-N7-C5	3.06	108.81	102.99
20	BH	501	GTP	C8-N7-C5	3.05	108.80	102.99
20	JJ	501	GTP	C3'-C2'-C1'	3.05	105.57	100.98
19	CK	501	GDP	C3'-C2'-C1'	3.05	105.57	100.98
20	BL	501	GTP	C3'-C2'-C1'	3.05	105.57	100.98
20	BL	501	GTP	C8-N7-C5	3.05	108.80	102.99
20	KL	501	GTP	C3'-C2'-C1'	3.05	105.57	100.98
20	LF	501	GTP	C8-N7-C5	3.04	108.79	102.99
20	DB	501	GTP	C3'-C2'-C1'	3.04	105.56	100.98
20	MH	501	GTP	C8-N7-C5	3.04	108.79	102.99
20	HF	501	GTP	C8-N7-C5	3.04	108.79	102.99
20	CF	501	GTP	C8-N7-C5	3.04	108.78	102.99
20	HL	501	GTP	C2-N1-C6	-3.04	119.50	125.10
20	LB	501	GTP	C8-N7-C5	3.04	108.78	102.99
20	MB	501	GTP	C8-N7-C5	3.04	108.78	102.99
20	ML	501	GTP	C8-N7-C5	3.04	108.78	102.99
19	II	501	GDP	C3'-C2'-C1'	3.04	105.55	100.98
20	LH	501	GTP	C8-N7-C5	3.04	108.77	102.99
20	GD	501	GTP	C3'-C2'-C1'	3.03	105.55	100.98
20	HI	501	GTP	C3'-C2'-C1'	3.03	105.54	100.98
20	HD	501	GTP	C3'-C2'-C1'	3.03	105.54	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	EH	501	GTP	C8-N7-C5	3.03	108.76	102.99
20	EJ	501	GTP	C8-N7-C5	3.03	108.76	102.99
20	KH	501	GTP	C8-N7-C5	3.03	108.75	102.99
20	LD	501	GTP	C8-N7-C5	3.02	108.75	102.99
20	GL	501	GTP	C8-N7-C5	3.02	108.75	102.99
20	HD	501	GTP	C8-N7-C5	3.02	108.75	102.99
20	HF	501	GTP	C2-N1-C6	-3.02	119.54	125.10
20	EF	501	GTP	C2-N1-C6	-3.02	119.54	125.10
20	MJ	501	GTP	C8-N7-C5	3.02	108.74	102.99
20	CB	501	GTP	C3'-C2'-C1'	3.02	105.52	100.98
20	AD	501	GTP	C8-N7-C5	3.02	108.74	102.99
20	KL	501	GTP	C8-N7-C5	3.02	108.74	102.99
20	AL	501	GTP	C8-N7-C5	3.02	108.74	102.99
20	HJ	501	GTP	C8-N7-C5	3.02	108.74	102.99
20	GD	501	GTP	C2-N1-C6	-3.01	119.55	125.10
20	KD	501	GTP	C8-N7-C5	3.01	108.73	102.99
20	IH	501	GTP	C8-N7-C5	3.01	108.73	102.99
20	DD	501	GTP	C8-N7-C5	3.01	108.73	102.99
20	KJ	501	GTP	C8-N7-C5	3.01	108.73	102.99
20	HI	501	GTP	C8-N7-C5	3.01	108.73	102.99
20	CD	501	GTP	C8-N7-C5	3.01	108.73	102.99
20	CJ	501	GTP	C8-N7-C5	3.01	108.72	102.99
20	HL	501	GTP	C8-N7-C5	3.01	108.72	102.99
20	MB	501	GTP	PA-O3A-PB	-3.01	122.51	132.83
20	CB	501	GTP	C8-N7-C5	3.00	108.71	102.99
20	IL	501	GTP	C8-N7-C5	3.00	108.71	102.99
20	JL	501	GTP	C8-N7-C5	3.00	108.71	102.99
20	LJ	501	GTP	C8-N7-C5	3.00	108.71	102.99
20	AF	501	GTP	C8-N7-C5	3.00	108.71	102.99
20	EF	501	GTP	C8-N7-C5	3.00	108.71	102.99
20	MD	501	GTP	C8-N7-C5	3.00	108.71	102.99
20	JD	501	GTP	C8-N7-C5	3.00	108.70	102.99
20	JF	501	GTP	C8-N7-C5	3.00	108.70	102.99
20	BF	501	GTP	C8-N7-C5	2.99	108.69	102.99
20	DB	501	GTP	PB-O3B-PG	-2.99	122.56	132.83
20	ED	501	GTP	C8-N7-C5	2.99	108.69	102.99
19	LC	501	GDP	C3'-C2'-C1'	2.99	105.48	100.98
20	FJ	501	GTP	C3'-C2'-C1'	2.99	105.48	100.98
20	HI	501	GTP	C2-N1-C6	-2.99	119.60	125.10
20	KH	501	GTP	C3'-C2'-C1'	2.99	105.47	100.98
20	GH	501	GTP	C2-N1-C6	-2.99	119.60	125.10
20	MH	501	GTP	C3'-C2'-C1'	2.98	105.47	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BB	501	GTP	C8-N7-C5	2.98	108.67	102.99
20	BB	501	GTP	C3'-C2'-C1'	2.98	105.47	100.98
20	AH	501	GTP	C8-N7-C5	2.98	108.67	102.99
20	FB	501	GTP	C8-N7-C5	2.98	108.67	102.99
20	FF	501	GTP	C2-N1-C6	-2.98	119.61	125.10
20	AH	501	GTP	C3'-C2'-C1'	2.98	105.46	100.98
20	CH	501	GTP	C8-N7-C5	2.98	108.66	102.99
20	GJ	501	GTP	C3'-C2'-C1'	2.98	105.46	100.98
20	DJ	501	GTP	C8-N7-C5	2.98	108.66	102.99
20	JB	501	GTP	C8-N7-C5	2.97	108.66	102.99
20	MF	501	GTP	C8-N7-C5	2.97	108.66	102.99
20	HJ	501	GTP	C2-N1-C6	-2.97	119.62	125.10
20	FB	501	GTP	C3'-C2'-C1'	2.97	105.45	100.98
20	AJ	501	GTP	C8-N7-C5	2.97	108.65	102.99
20	GL	501	GTP	C2-N1-C6	-2.97	119.63	125.10
20	JH	501	GTP	C2-N1-C6	-2.97	119.63	125.10
20	FF	501	GTP	C8-N7-C5	2.97	108.65	102.99
20	LL	501	GTP	C8-N7-C5	2.97	108.64	102.99
20	CJ	501	GTP	C3'-C2'-C1'	2.97	105.45	100.98
19	FE	501	GDP	C3'-C2'-C1'	2.97	105.45	100.98
19	FG	501	GDP	PA-O3A-PB	-2.97	122.64	132.83
20	IJ	501	GTP	C8-N7-C5	2.96	108.64	102.99
20	JJ	501	GTP	C8-N7-C5	2.96	108.64	102.99
20	AD	501	GTP	C3'-C2'-C1'	2.96	105.44	100.98
20	EH	501	GTP	C2-N1-C6	-2.96	119.65	125.10
20	JF	501	GTP	C2-N1-C6	-2.96	119.65	125.10
20	EB	501	GTP	PA-O3A-PB	-2.96	122.67	132.83
20	BB	501	GTP	C2-N1-C6	-2.96	119.65	125.10
20	CB	501	GTP	C2-N1-C6	-2.96	119.65	125.10
20	CD	501	GTP	C2-N1-C6	-2.96	119.65	125.10
20	HD	501	GTP	C2-N1-C6	-2.96	119.65	125.10
20	BJ	501	GTP	C3'-C2'-C1'	2.96	105.43	100.98
20	MF	501	GTP	C3'-C2'-C1'	2.96	105.43	100.98
20	DB	501	GTP	C8-N7-C5	2.96	108.62	102.99
20	CH	501	GTP	C2-N1-C6	-2.96	119.66	125.10
20	EL	501	GTP	C8-N7-C5	2.95	108.62	102.99
20	BJ	501	GTP	C8-N7-C5	2.95	108.62	102.99
20	DF	501	GTP	C8-N7-C5	2.95	108.62	102.99
20	ML	501	GTP	C3'-C2'-C1'	2.95	105.42	100.98
20	ID	501	GTP	C8-N7-C5	2.95	108.61	102.99
20	MB	501	GTP	C2-N1-C6	-2.95	119.66	125.10
20	IH	501	GTP	C2-N1-C6	-2.95	119.67	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	GI	501	GDP	C3'-C2'-C1'	2.95	105.42	100.98
20	GJ	501	GTP	C2-N1-C6	-2.95	119.67	125.10
20	BD	501	GTP	C2-N1-C6	-2.95	119.67	125.10
20	AB	501	GTP	C8-N7-C5	2.95	108.60	102.99
20	LJ	501	GTP	C3'-C2'-C1'	2.95	105.41	100.98
19	BC	501	GDP	C3'-C2'-C1'	2.94	105.41	100.98
20	JD	501	GTP	C3'-C2'-C1'	2.94	105.41	100.98
20	MD	501	GTP	C2-N1-C6	-2.94	119.68	125.10
20	EB	501	GTP	C8-N7-C5	2.94	108.60	102.99
20	FJ	501	GTP	C8-N7-C5	2.94	108.60	102.99
20	BH	501	GTP	C2-N1-C6	-2.94	119.68	125.10
20	BH	501	GTP	C3'-C2'-C1'	2.94	105.41	100.98
20	DL	501	GTP	C8-N7-C5	2.94	108.59	102.99
20	LB	501	GTP	C3'-C2'-C1'	2.94	105.41	100.98
20	IF	501	GTP	C2-N1-C6	-2.94	119.68	125.10
20	KB	501	GTP	C2-N1-C6	-2.94	119.69	125.10
20	LL	501	GTP	C3'-C2'-C1'	2.94	105.40	100.98
20	DD	501	GTP	C2-N1-C6	-2.93	119.69	125.10
20	KL	501	GTP	C2-N1-C6	-2.93	119.70	125.10
20	FD	501	GTP	C8-N7-C5	2.93	108.58	102.99
19	JG	501	GDP	PA-O3A-PB	-2.93	122.77	132.83
20	AJ	501	GTP	C3'-C2'-C1'	2.93	105.39	100.98
20	BF	501	GTP	C2-N1-C6	-2.93	119.71	125.10
20	FH	501	GTP	C8-N7-C5	2.92	108.56	102.99
20	EB	501	GTP	C2-N1-C6	-2.92	119.71	125.10
20	FL	501	GTP	C2-N1-C6	-2.92	119.72	125.10
20	BF	501	GTP	C3'-C2'-C1'	2.92	105.38	100.98
20	JJ	501	GTP	C2-N1-C6	-2.92	119.72	125.10
20	IJ	501	GTP	C3'-C2'-C1'	2.92	105.37	100.98
20	MJ	501	GTP	C2-N1-C6	-2.92	119.73	125.10
19	AE	501	GDP	C3'-C2'-C1'	2.92	105.37	100.98
20	CJ	501	GTP	C2-N1-C6	-2.91	119.73	125.10
20	EJ	501	GTP	C3'-C2'-C1'	2.91	105.37	100.98
20	BF	501	GTP	PA-O3A-PB	-2.91	122.83	132.83
20	AB	501	GTP	C2-N1-C6	-2.91	119.73	125.10
20	DJ	501	GTP	C2-N1-C6	-2.91	119.73	125.10
20	FJ	501	GTP	C2-N1-C6	-2.91	119.73	125.10
20	DL	501	GTP	C2-N1-C6	-2.91	119.74	125.10
19	IC	501	GDP	C3'-C2'-C1'	2.91	105.36	100.98
20	JL	501	GTP	C2-N1-C6	-2.91	119.74	125.10
19	LG	501	GDP	C3'-C2'-C1'	2.91	105.36	100.98
20	LJ	501	GTP	C2-N1-C6	-2.91	119.74	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	IF	501	GTP	C8-N7-C5	2.91	108.53	102.99
20	BJ	501	GTP	C2-N1-C6	-2.91	119.75	125.10
20	FD	501	GTP	C2-N1-C6	-2.91	119.75	125.10
20	KH	501	GTP	C2-N1-C6	-2.91	119.75	125.10
20	ED	501	GTP	C3'-C2'-C1'	2.91	105.35	100.98
20	JD	501	GTP	C2-N1-C6	-2.90	119.75	125.10
20	FH	501	GTP	C2-N1-C6	-2.90	119.75	125.10
20	EB	501	GTP	C3'-C2'-C1'	2.90	105.34	100.98
20	MH	501	GTP	C2-N1-C6	-2.90	119.76	125.10
20	EJ	501	GTP	C2-N1-C6	-2.90	119.76	125.10
20	ID	501	GTP	C3'-C2'-C1'	2.90	105.34	100.98
20	FL	501	GTP	C8-N7-C5	2.90	108.51	102.99
20	FB	501	GTP	C2-N1-C6	-2.90	119.76	125.10
20	DL	501	GTP	C3'-C2'-C1'	2.90	105.34	100.98
20	GF	501	GTP	C2-N1-C6	-2.89	119.77	125.10
20	JF	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
20	IF	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
20	IH	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
20	LD	501	GTP	C2-N1-C6	-2.89	119.78	125.10
20	JL	501	GTP	C3'-C2'-C1'	2.89	105.32	100.98
20	LB	501	GTP	C2-N1-C6	-2.89	119.78	125.10
20	EL	501	GTP	C3'-C2'-C1'	2.89	105.32	100.98
20	EH	501	GTP	C3'-C2'-C1'	2.88	105.32	100.98
20	JB	501	GTP	C3'-C2'-C1'	2.88	105.32	100.98
20	KD	501	GTP	C2-N1-C6	-2.88	119.79	125.10
20	AD	501	GTP	C2-N1-C6	-2.88	119.79	125.10
20	DB	501	GTP	C2-N1-C6	-2.88	119.80	125.10
20	LF	501	GTP	C2-N1-C6	-2.88	119.80	125.10
20	KF	501	GTP	C2-N1-C6	-2.88	119.80	125.10
19	CI	501	GDP	C3'-C2'-C1'	2.87	105.30	100.98
20	LD	501	GTP	C3'-C2'-C1'	2.87	105.30	100.98
20	ML	501	GTP	C2-N1-C6	-2.87	119.82	125.10
19	EC	501	GDP	C3'-C2'-C1'	2.87	105.30	100.98
20	CF	501	GTP	C2-N1-C6	-2.87	119.82	125.10
20	EF	501	GTP	C3'-C2'-C1'	2.86	105.29	100.98
20	AF	501	GTP	C2-N1-C6	-2.86	119.83	125.10
20	DF	501	GTP	C2-N1-C6	-2.86	119.84	125.10
20	DH	501	GTP	C2-N1-C6	-2.86	119.84	125.10
19	EG	501	GDP	C3'-C2'-C1'	2.86	105.28	100.98
20	MF	501	GTP	C2-N1-C6	-2.85	119.84	125.10
19	CC	501	GDP	C3'-C2'-C1'	2.85	105.28	100.98
20	IL	501	GTP	C2-N1-C6	-2.85	119.85	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	AH	501	GTP	C2-N1-C6	-2.85	119.85	125.10
20	IJ	501	GTP	C2-N1-C6	-2.84	119.86	125.10
20	AB	501	GTP	C3'-C2'-C1'	2.84	105.25	100.98
20	IL	501	GTP	C3'-C2'-C1'	2.84	105.25	100.98
20	JB	501	GTP	C2-N1-C6	-2.83	119.88	125.10
20	AL	501	GTP	C3'-C2'-C1'	2.83	105.24	100.98
19	GK	501	GDP	C3'-C2'-C1'	2.83	105.24	100.98
20	AJ	501	GTP	C2-N1-C6	-2.83	119.89	125.10
19	DK	501	GDP	C3'-C2'-C1'	2.82	105.23	100.98
20	LL	501	GTP	C2-N1-C6	-2.82	119.90	125.10
20	MJ	501	GTP	PA-O3A-PB	-2.82	123.16	132.83
20	KD	501	GTP	C3'-C2'-C1'	2.82	105.22	100.98
20	LH	501	GTP	C3'-C2'-C1'	2.81	105.22	100.98
19	JG	501	GDP	C3'-C2'-C1'	2.81	105.21	100.98
20	KB	501	GTP	C3'-C2'-C1'	2.81	105.21	100.98
20	AF	501	GTP	C3'-C2'-C1'	2.81	105.21	100.98
20	ED	501	GTP	C2-N1-C6	-2.80	119.93	125.10
20	BL	501	GTP	C2-N1-C6	-2.80	119.94	125.10
20	DJ	501	GTP	C3'-C2'-C1'	2.80	105.19	100.98
20	JH	501	GTP	PA-O3A-PB	-2.80	123.23	132.83
19	EI	501	GDP	C3'-C2'-C1'	2.80	105.19	100.98
20	KJ	501	GTP	C2-N1-C6	-2.79	119.95	125.10
20	DH	501	GTP	C3'-C2'-C1'	2.79	105.18	100.98
20	EL	501	GTP	C2-N1-C6	-2.79	119.95	125.10
19	JE	501	GDP	C3'-C2'-C1'	2.79	105.18	100.98
19	MC	501	GDP	C3'-C2'-C1'	2.79	105.18	100.98
20	FF	501	GTP	C3'-C2'-C1'	2.78	105.17	100.98
20	JH	501	GTP	C3'-C2'-C1'	2.78	105.17	100.98
19	IK	501	GDP	C3'-C2'-C1'	2.78	105.16	100.98
19	GG	501	GDP	C3'-C2'-C1'	2.78	105.16	100.98
20	DF	501	GTP	C3'-C2'-C1'	2.77	105.16	100.98
19	GE	501	GDP	C3'-C2'-C1'	2.77	105.15	100.98
20	ID	501	GTP	C2-N1-C6	-2.77	120.00	125.10
20	AL	501	GTP	C2-N1-C6	-2.76	120.01	125.10
19	FI	501	GDP	C3'-C2'-C1'	2.76	105.14	100.98
19	FK	501	GDP	C3'-C2'-C1'	2.76	105.13	100.98
20	DD	501	GTP	C3'-C2'-C1'	2.75	105.11	100.98
19	GM	501	GDP	C3'-C2'-C1'	2.75	105.11	100.98
20	KJ	501	GTP	C3'-C2'-C1'	2.75	105.11	100.98
20	CF	501	GTP	C3'-C2'-C1'	2.74	105.11	100.98
19	LI	501	GDP	C3'-C2'-C1'	2.74	105.11	100.98
19	HK	501	GDP	C3'-C2'-C1'	2.74	105.10	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	KK	501	GDP	C3'-C2'-C1'	2.73	105.09	100.98
20	MJ	501	GTP	C3'-C2'-C1'	2.73	105.09	100.98
19	KC	501	GDP	C3'-C2'-C1'	2.72	105.08	100.98
19	EA	501	GDP	C3'-C2'-C1'	2.72	105.07	100.98
20	KF	501	GTP	C3'-C2'-C1'	2.72	105.07	100.98
19	HG	501	GDP	C3'-C2'-C1'	2.71	105.06	100.98
19	FG	501	GDP	C3'-C2'-C1'	2.70	105.05	100.98
20	LH	501	GTP	C2-N1-C6	-2.70	120.12	125.10
20	EF	501	GTP	PA-O3A-PB	-2.70	123.58	132.83
20	BD	501	GTP	C3'-C2'-C1'	2.69	105.03	100.98
19	BI	501	GDP	C3'-C2'-C1'	2.69	105.02	100.98
19	CG	501	GDP	PA-O3A-PB	-2.69	123.61	132.83
19	CE	501	GDP	C3'-C2'-C1'	2.66	104.98	100.98
19	KE	501	GDP	C3'-C2'-C1'	2.65	104.96	100.98
19	MK	501	GDP	C3'-C2'-C1'	2.64	104.95	100.98
19	LK	501	GDP	C3'-C2'-C1'	2.61	104.91	100.98
19	BG	501	GDP	C3'-C2'-C1'	2.60	104.89	100.98
19	AI	501	GDP	C3'-C2'-C1'	2.59	104.87	100.98
19	DC	501	GDP	C3'-C2'-C1'	2.59	104.87	100.98
19	JG	501	GDP	O3B-PB-O3A	2.58	113.30	104.64
19	HE	501	GDP	C3'-C2'-C1'	2.57	104.85	100.98
19	LI	501	GDP	C8-N7-C5	2.55	107.84	102.99
19	JK	501	GDP	C3'-C2'-C1'	2.54	104.81	100.98
19	HC	501	GDP	C5-C6-N1	2.52	118.41	113.95
19	IE	501	GDP	C3'-C2'-C1'	2.51	104.76	100.98
19	AC	501	GDP	C3'-C2'-C1'	2.51	104.75	100.98
19	KG	501	GDP	C3'-C2'-C1'	2.49	104.73	100.98
19	JK	501	GDP	C5-C6-N1	2.48	118.33	113.95
19	LC	501	GDP	C8-N7-C5	2.47	107.70	102.99
19	BA	501	GDP	C3'-C2'-C1'	2.46	104.68	100.98
19	DE	501	GDP	C5-C6-N1	2.45	118.28	113.95
19	HI	502	GDP	C3'-C2'-C1'	2.45	104.67	100.98
19	MG	501	GDP	C3'-C2'-C1'	2.44	104.66	100.98
19	DE	501	GDP	C3'-C2'-C1'	2.43	104.64	100.98
19	AG	501	GDP	C8-N7-C5	2.43	107.61	102.99
19	DE	501	GDP	C8-N7-C5	2.42	107.59	102.99
19	GM	501	GDP	C5-C6-N1	2.41	118.22	113.95
19	LK	501	GDP	C8-N7-C5	2.41	107.58	102.99
19	DI	501	GDP	C3'-C2'-C1'	2.41	104.61	100.98
19	CE	501	GDP	C5-C6-N1	2.41	118.21	113.95
19	EA	501	GDP	C5-C6-N1	2.40	118.20	113.95
19	MI	501	GDP	C8-N7-C5	2.40	107.57	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	FC	501	GDP	C5-C6-N1	2.40	118.19	113.95
19	KE	501	GDP	C8-N7-C5	2.39	107.54	102.99
19	EI	501	GDP	C5-C6-N1	2.39	118.17	113.95
19	HI	502	GDP	C5-C6-N1	2.39	118.17	113.95
19	JI	501	GDP	C8-N7-C5	2.38	107.52	102.99
19	AC	501	GDP	C8-N7-C5	2.37	107.51	102.99
19	MG	501	GDP	C8-N7-C5	2.37	107.51	102.99
19	EI	501	GDP	C8-N7-C5	2.37	107.50	102.99
19	GC	501	GDP	C8-N7-C5	2.37	107.50	102.99
19	ME	501	GDP	C8-N7-C5	2.37	107.50	102.99
19	AI	501	GDP	C8-N7-C5	2.37	107.50	102.99
19	HM	501	GDP	C5-C6-N1	2.37	118.13	113.95
19	CI	501	GDP	C5-C6-N1	2.36	118.12	113.95
19	AK	501	GDP	C8-N7-C5	2.36	107.49	102.99
19	JC	501	GDP	C8-N7-C5	2.36	107.49	102.99
19	MK	501	GDP	C8-N7-C5	2.36	107.49	102.99
19	GG	501	GDP	C8-N7-C5	2.36	107.49	102.99
19	JE	501	GDP	C8-N7-C5	2.36	107.49	102.99
19	GE	501	GDP	C8-N7-C5	2.36	107.49	102.99
19	HC	501	GDP	C3'-C2'-C1'	2.36	104.53	100.98
19	DG	501	GDP	C8-N7-C5	2.36	107.48	102.99
19	MI	501	GDP	C5-C6-N1	2.36	118.11	113.95
19	AI	501	GDP	C5-C6-N1	2.36	118.11	113.95
19	IE	501	GDP	C8-N7-C5	2.35	107.47	102.99
19	BC	501	GDP	C8-N7-C5	2.35	107.47	102.99
19	KG	501	GDP	C5-C6-N1	2.35	118.10	113.95
19	HG	501	GDP	C8-N7-C5	2.35	107.46	102.99
19	CG	501	GDP	C5-C6-N1	2.35	118.10	113.95
19	DC	501	GDP	C8-N7-C5	2.35	107.46	102.99
19	MG	501	GDP	C5-C6-N1	2.35	118.09	113.95
19	LI	501	GDP	C5-C6-N1	2.34	118.09	113.95
19	LE	501	GDP	C5-C6-N1	2.34	118.09	113.95
19	CE	501	GDP	C8-N7-C5	2.34	107.45	102.99
19	CC	501	GDP	C8-N7-C5	2.34	107.45	102.99
19	FA	501	GDP	C5-C6-N1	2.34	118.08	113.95
19	HK	501	GDP	C8-N7-C5	2.34	107.44	102.99
19	DI	501	GDP	C8-N7-C5	2.34	107.44	102.99
19	GG	501	GDP	C5-C6-N1	2.33	118.07	113.95
19	MC	501	GDP	C8-N7-C5	2.33	107.43	102.99
20	IF	501	GTP	O6-C6-C5	-2.33	119.82	124.37
19	CA	501	GDP	C8-N7-C5	2.33	107.43	102.99
19	EA	501	GDP	C8-N7-C5	2.33	107.43	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	501	GDP	C8-N7-C5	2.33	107.42	102.99
19	KC	501	GDP	C8-N7-C5	2.33	107.42	102.99
19	IC	501	GDP	C8-N7-C5	2.33	107.42	102.99
19	HK	501	GDP	C5-C6-N1	2.33	118.06	113.95
19	JK	501	GDP	O6-C6-C5	-2.33	119.83	124.37
19	IK	501	GDP	C5-C6-N1	2.33	118.06	113.95
19	HI	502	GDP	C8-N7-C5	2.32	107.42	102.99
19	AA	501	GDP	C5-C6-N1	2.32	118.06	113.95
19	EE	502	GDP	C8-N7-C5	2.32	107.42	102.99
19	GC	501	GDP	C5-C6-N1	2.32	118.06	113.95
19	HE	501	GDP	C8-N7-C5	2.32	107.41	102.99
19	BI	501	GDP	C8-N7-C5	2.32	107.41	102.99
19	IG	501	GDP	C8-N7-C5	2.32	107.41	102.99
20	DH	501	GTP	O6-C6-C5	-2.32	119.85	124.37
19	AE	501	GDP	C8-N7-C5	2.32	107.40	102.99
19	FG	501	GDP	C8-N7-C5	2.32	107.40	102.99
19	FI	501	GDP	C8-N7-C5	2.32	107.40	102.99
19	LC	501	GDP	C5-C6-N1	2.32	118.04	113.95
19	AC	501	GDP	C5-C6-N1	2.32	118.04	113.95
19	CK	501	GDP	C8-N7-C5	2.32	107.40	102.99
19	GE	501	GDP	C5-C6-N1	2.32	118.04	113.95
19	EC	501	GDP	C8-N7-C5	2.31	107.40	102.99
19	FA	501	GDP	C8-N7-C5	2.31	107.40	102.99
19	CA	501	GDP	C5-C6-N1	2.31	118.04	113.95
19	FK	501	GDP	C8-N7-C5	2.31	107.40	102.99
19	GM	501	GDP	C8-N7-C5	2.31	107.40	102.99
19	GI	501	GDP	C8-N7-C5	2.31	107.40	102.99
19	ME	501	GDP	C5-C6-N1	2.31	118.03	113.95
19	CI	501	GDP	C8-N7-C5	2.31	107.39	102.99
19	JM	501	GDP	C8-N7-C5	2.31	107.39	102.99
19	IC	501	GDP	C5-C6-N1	2.31	118.03	113.95
19	IK	501	GDP	C8-N7-C5	2.31	107.39	102.99
19	MK	501	GDP	C5-C6-N1	2.31	118.03	113.95
19	LE	501	GDP	C8-N7-C5	2.31	107.39	102.99
19	AG	501	GDP	C5-C6-N1	2.31	118.03	113.95
19	GI	501	GDP	C5-C6-N1	2.31	118.03	113.95
19	HM	501	GDP	C8-N7-C5	2.31	107.39	102.99
19	FC	501	GDP	C3'-C2'-C1'	2.31	104.45	100.98
19	IG	501	GDP	C5-C6-N1	2.31	118.03	113.95
19	DC	501	GDP	C5-C6-N1	2.31	118.03	113.95
19	HG	501	GDP	C5-C6-N1	2.30	118.02	113.95
19	BE	501	GDP	C5-C6-N1	2.30	118.02	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	KG	501	GDP	C8-N7-C5	2.30	107.38	102.99
19	HC	501	GDP	C8-N7-C5	2.30	107.37	102.99
20	FF	501	GTP	O6-C6-C5	-2.30	119.88	124.37
19	EE	502	GDP	C5-C6-N1	2.30	118.01	113.95
19	BE	501	GDP	C8-N7-C5	2.30	107.36	102.99
19	KI	502	GDP	C5-C6-N1	2.30	118.00	113.95
19	DK	501	GDP	C8-N7-C5	2.29	107.36	102.99
19	KK	501	GDP	C8-N7-C5	2.29	107.36	102.99
19	BK	501	GDP	C5-C6-N1	2.29	118.00	113.95
19	II	501	GDP	C5-C6-N1	2.29	118.00	113.95
19	BG	501	GDP	C8-N7-C5	2.29	107.36	102.99
19	BC	501	GDP	C5-C6-N1	2.29	118.00	113.95
20	EB	501	GTP	O6-C6-C5	-2.29	119.89	124.37
19	BI	501	GDP	C5-C6-N1	2.29	118.00	113.95
19	JI	501	GDP	C5-C6-N1	2.29	118.00	113.95
19	BK	501	GDP	C8-N7-C5	2.29	107.36	102.99
19	CC	501	GDP	C5-C6-N1	2.29	117.99	113.95
19	FK	501	GDP	C5-C6-N1	2.29	117.99	113.95
19	LK	501	GDP	C5-C6-N1	2.29	117.99	113.95
19	KI	502	GDP	C8-N7-C5	2.29	107.34	102.99
19	AK	501	GDP	C5-C6-N1	2.28	117.98	113.95
19	CG	501	GDP	C8-N7-C5	2.28	107.33	102.99
19	EK	501	GDP	C8-N7-C5	2.28	107.33	102.99
19	IM	501	GDP	C8-N7-C5	2.28	107.33	102.99
19	JG	501	GDP	C8-N7-C5	2.28	107.33	102.99
19	MC	501	GDP	C5-C6-N1	2.28	117.97	113.95
19	FC	501	GDP	C8-N7-C5	2.28	107.33	102.99
19	JM	501	GDP	C5-C6-N1	2.28	117.97	113.95
20	EF	501	GTP	O6-C6-C5	-2.27	119.93	124.37
19	JC	501	GDP	C5-C6-N1	2.27	117.96	113.95
19	KC	501	GDP	C5-C6-N1	2.27	117.96	113.95
19	FE	501	GDP	C8-N7-C5	2.27	107.31	102.99
19	GK	501	GDP	C8-N7-C5	2.26	107.29	102.99
19	FI	501	GDP	C5-C6-N1	2.26	117.94	113.95
19	EG	501	GDP	C8-N7-C5	2.26	107.29	102.99
20	FH	501	GTP	O6-C6-C5	-2.25	119.97	124.37
20	DF	501	GTP	O6-C6-C5	-2.25	119.98	124.37
19	JE	501	GDP	C5-C6-N1	2.25	117.92	113.95
20	KB	501	GTP	O6-C6-C5	-2.24	119.99	124.37
20	FJ	501	GTP	O6-C6-C5	-2.24	119.99	124.37
19	AE	501	GDP	C5-C6-N1	2.24	117.91	113.95
19	JC	501	GDP	C3'-C2'-C1'	2.24	104.35	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	DB	501	GTP	O6-C6-C5	-2.24	120.00	124.37
19	FE	501	GDP	C5-C6-N1	2.24	117.90	113.95
20	ML	501	GTP	O6-C6-C5	-2.24	120.00	124.37
19	IG	501	GDP	C3'-C2'-C1'	2.24	104.34	100.98
19	KK	501	GDP	C5-C6-N1	2.23	117.89	113.95
19	DG	501	GDP	C5-C6-N1	2.23	117.88	113.95
20	AB	501	GTP	O6-C6-C5	-2.22	120.04	124.37
19	IE	501	GDP	C5-C6-N1	2.22	117.87	113.95
19	JG	501	GDP	C5-C6-N1	2.22	117.87	113.95
20	DJ	501	GTP	O6-C6-C5	-2.21	120.05	124.37
20	JF	501	GTP	O6-C6-C5	-2.21	120.05	124.37
19	CK	501	GDP	C5-C6-N1	2.21	117.86	113.95
20	CH	501	GTP	O6-C6-C5	-2.21	120.06	124.37
19	KE	501	GDP	C5-C6-N1	2.21	117.85	113.95
20	DL	501	GTP	O6-C6-C5	-2.21	120.06	124.37
19	FG	501	GDP	C5-C6-N1	2.20	117.84	113.95
19	LG	501	GDP	C5-C6-N1	2.20	117.84	113.95
20	MD	501	GTP	O6-C6-C5	-2.20	120.08	124.37
19	IM	501	GDP	C5-C6-N1	2.20	117.84	113.95
19	JK	501	GDP	C8-N7-C5	2.20	107.18	102.99
20	FD	501	GTP	O6-C6-C5	-2.20	120.08	124.37
19	EG	501	GDP	C5-C6-N1	2.19	117.83	113.95
20	MF	501	GTP	O6-C6-C5	-2.19	120.09	124.37
20	LJ	501	GTP	O6-C6-C5	-2.19	120.09	124.37
20	MH	501	GTP	O6-C6-C5	-2.19	120.09	124.37
19	LG	501	GDP	C8-N7-C5	2.19	107.17	102.99
19	DK	501	GDP	C5-C6-N1	2.19	117.82	113.95
19	EK	501	GDP	C5-C6-N1	2.19	117.82	113.95
20	FB	501	GTP	O6-C6-C5	-2.19	120.10	124.37
20	JD	501	GTP	O6-C6-C5	-2.19	120.10	124.37
19	II	501	GDP	C8-N7-C5	2.19	107.16	102.99
20	AF	501	GTP	O6-C6-C5	-2.19	120.10	124.37
20	MB	501	GTP	O6-C6-C5	-2.19	120.10	124.37
20	KD	501	GTP	O6-C6-C5	-2.18	120.11	124.37
19	EC	501	GDP	C5-C6-N1	2.18	117.80	113.95
20	LB	501	GTP	O6-C6-C5	-2.18	120.12	124.37
20	DB	501	GTP	O3G-PG-O3B	2.18	111.94	104.64
20	LF	501	GTP	O6-C6-C5	-2.18	120.12	124.37
19	BE	501	GDP	C3'-C2'-C1'	2.18	104.25	100.98
20	HL	501	GTP	O6-C6-C5	-2.17	120.13	124.37
20	CJ	501	GTP	O6-C6-C5	-2.17	120.13	124.37
20	BD	501	GTP	O6-C6-C5	-2.17	120.13	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BA	501	GDP	C5-C6-N1	2.17	117.78	113.95
20	FL	501	GTP	O6-C6-C5	-2.16	120.14	124.37
20	AJ	501	GTP	O6-C6-C5	-2.16	120.15	124.37
20	GL	501	GTP	O6-C6-C5	-2.16	120.15	124.37
19	MI	501	GDP	C3'-C2'-C1'	2.16	104.23	100.98
20	IJ	501	GTP	O6-C6-C5	-2.16	120.16	124.37
19	GK	501	GDP	C5-C6-N1	2.15	117.76	113.95
20	JJ	501	GTP	O6-C6-C5	-2.15	120.16	124.37
20	BJ	501	GTP	O6-C6-C5	-2.15	120.17	124.37
20	JB	501	GTP	O6-C6-C5	-2.15	120.17	124.37
19	HE	501	GDP	C5-C6-N1	2.15	117.75	113.95
20	JH	501	GTP	O6-C6-C5	-2.15	120.18	124.37
20	BB	501	GTP	O6-C6-C5	-2.15	120.18	124.37
20	GH	501	GTP	O6-C6-C5	-2.15	120.18	124.37
20	LL	501	GTP	O6-C6-C5	-2.14	120.18	124.37
20	JL	501	GTP	O6-C6-C5	-2.14	120.19	124.37
20	IH	501	GTP	O6-C6-C5	-2.14	120.19	124.37
20	GD	501	GTP	O6-C6-C5	-2.14	120.19	124.37
20	LD	501	GTP	O6-C6-C5	-2.14	120.19	124.37
20	ID	501	GTP	O6-C6-C5	-2.14	120.20	124.37
20	MJ	501	GTP	O6-C6-C5	-2.14	120.20	124.37
20	KL	501	GTP	O6-C6-C5	-2.13	120.21	124.37
19	DI	501	GDP	C5-C6-N1	2.13	117.70	113.95
20	CD	501	GTP	O6-C6-C5	-2.12	120.23	124.37
20	BF	501	GTP	O6-C6-C5	-2.12	120.23	124.37
19	BA	501	GDP	C8-N7-C5	2.12	107.03	102.99
20	IL	501	GTP	O6-C6-C5	-2.12	120.24	124.37
20	KJ	501	GTP	O6-C6-C5	-2.11	120.24	124.37
20	AD	501	GTP	O6-C6-C5	-2.11	120.25	124.37
20	CB	501	GTP	O6-C6-C5	-2.10	120.27	124.37
20	EJ	501	GTP	O6-C6-C5	-2.10	120.27	124.37
19	BG	501	GDP	C2'-C3'-C4'	2.10	106.72	102.64
20	ED	501	GTP	O6-C6-C5	-2.10	120.27	124.37
20	EL	501	GTP	O6-C6-C5	-2.10	120.27	124.37
20	CF	501	GTP	O6-C6-C5	-2.10	120.28	124.37
20	EH	501	GTP	O6-C6-C5	-2.09	120.29	124.37
19	LE	501	GDP	C3'-C2'-C1'	2.09	104.12	100.98
20	DD	501	GTP	O6-C6-C5	-2.09	120.30	124.37
20	HF	501	GTP	O6-C6-C5	-2.08	120.30	124.37
19	AG	501	GDP	C3'-C2'-C1'	2.08	104.11	100.98
20	HD	501	GTP	O6-C6-C5	-2.08	120.31	124.37
20	BL	501	GTP	O6-C6-C5	-2.08	120.31	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	AH	501	GTP	O6-C6-C5	-2.08	120.31	124.37
20	KF	501	GTP	O6-C6-C5	-2.06	120.34	124.37
20	JD	501	GTP	O3G-PG-O3B	2.06	111.55	104.64
19	BG	501	GDP	C5-C6-N1	2.06	117.58	113.95
20	JF	501	GTP	O3G-PG-O3B	2.05	111.52	104.64
20	BH	501	GTP	O6-C6-C5	-2.04	120.38	124.37
20	AL	501	GTP	O6-C6-C5	-2.04	120.39	124.37
20	KH	501	GTP	O6-C6-C5	-2.04	120.39	124.37
20	GJ	501	GTP	O6-C6-C5	-2.03	120.40	124.37
19	DG	501	GDP	C2'-C3'-C4'	2.03	106.58	102.64
20	DH	501	GTP	O2G-PG-O3B	2.03	111.43	104.64
19	CG	501	GDP	C3'-C2'-C1'	2.02	104.03	100.98
19	II	501	GDP	O6-C6-C5	-2.01	120.45	124.37
19	JI	501	GDP	C3'-C2'-C1'	2.01	104.00	100.98
19	ME	501	GDP	C3'-C2'-C1'	2.00	103.99	100.98

There are no chirality outliers.

All (507) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	BA	501	GDP	C5'-O5'-PA-O3A
19	BA	501	GDP	C5'-O5'-PA-O2A
19	BA	501	GDP	O4'-C4'-C5'-O5'
19	BA	501	GDP	C3'-C4'-C5'-O5'
19	BC	501	GDP	PA-O3A-PB-O2B
19	BC	501	GDP	O4'-C4'-C5'-O5'
19	BC	501	GDP	C3'-C4'-C5'-O5'
19	BI	501	GDP	PA-O3A-PB-O2B
19	BK	501	GDP	O4'-C4'-C5'-O5'
19	BK	501	GDP	C3'-C4'-C5'-O5'
19	CC	501	GDP	PA-O3A-PB-O2B
19	CG	501	GDP	C5'-O5'-PA-O3A
19	CG	501	GDP	C5'-O5'-PA-O2A
19	DC	501	GDP	C3'-C4'-C5'-O5'
19	EA	501	GDP	C5'-O5'-PA-O3A
19	EA	501	GDP	O4'-C4'-C5'-O5'
19	EA	501	GDP	C3'-C4'-C5'-O5'
19	EE	502	GDP	C5'-O5'-PA-O3A
19	EE	502	GDP	O4'-C4'-C5'-O5'
19	EE	502	GDP	C3'-C4'-C5'-O5'
19	EG	501	GDP	C5'-O5'-PA-O3A
19	GI	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
19	HI	502	GDP	PA-O3A-PB-O2B
19	HI	502	GDP	C5'-O5'-PA-O1A
19	HM	501	GDP	C5'-O5'-PA-O1A
19	IC	501	GDP	PA-O3A-PB-O3B
19	II	501	GDP	C5'-O5'-PA-O3A
19	II	501	GDP	C5'-O5'-PA-O2A
19	IM	501	GDP	PA-O3A-PB-O3B
19	IM	501	GDP	C5'-O5'-PA-O3A
19	JC	501	GDP	C5'-O5'-PA-O1A
19	JE	501	GDP	C3'-C4'-C5'-O5'
19	JG	501	GDP	PA-O3A-PB-O2B
19	JG	501	GDP	C5'-O5'-PA-O3A
19	JI	501	GDP	C3'-C4'-C5'-O5'
19	KC	501	GDP	C5'-O5'-PA-O1A
19	KE	501	GDP	C5'-O5'-PA-O3A
19	KE	501	GDP	C5'-O5'-PA-O2A
19	KE	501	GDP	O4'-C4'-C5'-O5'
19	KE	501	GDP	C3'-C4'-C5'-O5'
19	KI	502	GDP	C5'-O5'-PA-O3A
19	LE	501	GDP	C5'-O5'-PA-O1A
19	ME	501	GDP	O4'-C4'-C5'-O5'
19	ME	501	GDP	C3'-C4'-C5'-O5'
19	MI	501	GDP	C5'-O5'-PA-O3A
19	MI	501	GDP	O4'-C4'-C5'-O5'
19	MI	501	GDP	C3'-C4'-C5'-O5'
20	AB	501	GTP	C5'-O5'-PA-O1A
20	AB	501	GTP	C5'-O5'-PA-O2A
20	AD	501	GTP	C5'-O5'-PA-O1A
20	AF	501	GTP	C5'-O5'-PA-O3A
20	AH	501	GTP	C5'-O5'-PA-O3A
20	AH	501	GTP	C5'-O5'-PA-O2A
20	AH	501	GTP	C4'-C5'-O5'-PA
20	AJ	501	GTP	C5'-O5'-PA-O1A
20	AJ	501	GTP	C5'-O5'-PA-O2A
20	BB	501	GTP	C5'-O5'-PA-O3A
20	BB	501	GTP	C5'-O5'-PA-O2A
20	BD	501	GTP	C5'-O5'-PA-O1A
20	BD	501	GTP	C5'-O5'-PA-O2A
20	BF	501	GTP	C5'-O5'-PA-O3A
20	BH	501	GTP	C5'-O5'-PA-O1A
20	BH	501	GTP	C5'-O5'-PA-O2A
20	BL	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
20	BL	501	GTP	C5'-O5'-PA-O2A
20	CB	501	GTP	C5'-O5'-PA-O1A
20	CB	501	GTP	C5'-O5'-PA-O2A
20	CD	501	GTP	C5'-O5'-PA-O1A
20	CF	501	GTP	C5'-O5'-PA-O3A
20	CH	501	GTP	C5'-O5'-PA-O1A
20	CJ	501	GTP	C5'-O5'-PA-O3A
20	CJ	501	GTP	C5'-O5'-PA-O1A
20	CJ	501	GTP	C5'-O5'-PA-O2A
20	DB	501	GTP	C5'-O5'-PA-O3A
20	DB	501	GTP	C5'-O5'-PA-O1A
20	DB	501	GTP	C5'-O5'-PA-O2A
20	DD	501	GTP	C5'-O5'-PA-O1A
20	DD	501	GTP	C5'-O5'-PA-O2A
20	DF	501	GTP	C5'-O5'-PA-O3A
20	DH	501	GTP	C5'-O5'-PA-O1A
20	DJ	501	GTP	C5'-O5'-PA-O3A
20	DJ	501	GTP	C5'-O5'-PA-O1A
20	DJ	501	GTP	C5'-O5'-PA-O2A
20	DL	501	GTP	C5'-O5'-PA-O1A
20	EB	501	GTP	C5'-O5'-PA-O3A
20	EB	501	GTP	C5'-O5'-PA-O1A
20	EB	501	GTP	C5'-O5'-PA-O2A
20	EF	501	GTP	C5'-O5'-PA-O1A
20	EF	501	GTP	C5'-O5'-PA-O2A
20	EH	501	GTP	C5'-O5'-PA-O1A
20	EH	501	GTP	C5'-O5'-PA-O2A
20	EJ	501	GTP	C5'-O5'-PA-O1A
20	EL	501	GTP	C5'-O5'-PA-O1A
20	FD	501	GTP	C5'-O5'-PA-O3A
20	FF	501	GTP	C5'-O5'-PA-O1A
20	FF	501	GTP	C5'-O5'-PA-O2A
20	FH	501	GTP	C5'-O5'-PA-O3A
20	FH	501	GTP	C4'-C5'-O5'-PA
20	FJ	501	GTP	C5'-O5'-PA-O3A
20	FJ	501	GTP	C4'-C5'-O5'-PA
20	FL	501	GTP	C5'-O5'-PA-O3A
20	GF	501	GTP	C5'-O5'-PA-O1A
20	GH	501	GTP	C5'-O5'-PA-O1A
20	GL	501	GTP	C5'-O5'-PA-O1A
20	GL	501	GTP	C5'-O5'-PA-O2A
20	HD	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
20	HF	501	GTP	C5'-O5'-PA-O3A
20	HJ	501	GTP	C5'-O5'-PA-O3A
20	HL	501	GTP	C5'-O5'-PA-O1A
20	HL	501	GTP	C5'-O5'-PA-O2A
20	IF	501	GTP	C5'-O5'-PA-O1A
20	IF	501	GTP	C5'-O5'-PA-O2A
20	IH	501	GTP	C5'-O5'-PA-O1A
20	IH	501	GTP	C5'-O5'-PA-O2A
20	IL	501	GTP	C5'-O5'-PA-O1A
20	JB	501	GTP	C5'-O5'-PA-O1A
20	JB	501	GTP	C5'-O5'-PA-O2A
20	JD	501	GTP	C5'-O5'-PA-O1A
20	JH	501	GTP	C5'-O5'-PA-O1A
20	JH	501	GTP	C5'-O5'-PA-O2A
20	JJ	501	GTP	C5'-O5'-PA-O1A
20	JL	501	GTP	C5'-O5'-PA-O1A
20	KB	501	GTP	C5'-O5'-PA-O3A
20	KB	501	GTP	C5'-O5'-PA-O1A
20	KD	501	GTP	C5'-O5'-PA-O3A
20	KH	501	GTP	C5'-O5'-PA-O3A
20	KH	501	GTP	C5'-O5'-PA-O1A
20	KH	501	GTP	C5'-O5'-PA-O2A
20	KJ	501	GTP	C5'-O5'-PA-O3A
20	KL	501	GTP	C5'-O5'-PA-O3A
20	LD	501	GTP	C5'-O5'-PA-O3A
20	LD	501	GTP	O4'-C4'-C5'-O5'
20	LD	501	GTP	C3'-C4'-C5'-O5'
20	LJ	501	GTP	C5'-O5'-PA-O1A
20	LJ	501	GTP	C5'-O5'-PA-O2A
20	LL	501	GTP	C5'-O5'-PA-O1A
20	LL	501	GTP	C5'-O5'-PA-O2A
20	MD	501	GTP	C5'-O5'-PA-O1A
20	MD	501	GTP	C5'-O5'-PA-O2A
20	MF	501	GTP	C5'-O5'-PA-O1A
20	MH	501	GTP	C5'-O5'-PA-O1A
20	MJ	501	GTP	C5'-O5'-PA-O1A
20	MJ	501	GTP	C5'-O5'-PA-O2A
19	DC	501	GDP	O4'-C4'-C5'-O5'
19	DG	501	GDP	C3'-C4'-C5'-O5'
19	DI	501	GDP	C3'-C4'-C5'-O5'
19	HC	501	GDP	C3'-C4'-C5'-O5'
19	JE	501	GDP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
19	JI	501	GDP	O4'-C4'-C5'-O5'
19	KI	502	GDP	C3'-C4'-C5'-O5'
20	KL	501	GTP	O4'-C4'-C5'-O5'
20	KL	501	GTP	C3'-C4'-C5'-O5'
20	DF	501	GTP	C4'-C5'-O5'-PA
20	HD	501	GTP	C4'-C5'-O5'-PA
19	BI	501	GDP	O4'-C4'-C5'-O5'
19	BI	501	GDP	C3'-C4'-C5'-O5'
19	DG	501	GDP	O4'-C4'-C5'-O5'
19	DI	501	GDP	O4'-C4'-C5'-O5'
19	HC	501	GDP	O4'-C4'-C5'-O5'
19	II	501	GDP	O4'-C4'-C5'-O5'
19	II	501	GDP	C3'-C4'-C5'-O5'
19	KI	502	GDP	O4'-C4'-C5'-O5'
20	DJ	501	GTP	C4'-C5'-O5'-PA
20	FL	501	GTP	C4'-C5'-O5'-PA
19	JG	501	GDP	O4'-C4'-C5'-O5'
19	JG	501	GDP	C3'-C4'-C5'-O5'
20	DD	501	GTP	C3'-C4'-C5'-O5'
20	DB	501	GTP	C4'-C5'-O5'-PA
19	AK	501	GDP	C3'-C4'-C5'-O5'
19	CC	501	GDP	C3'-C4'-C5'-O5'
19	CK	501	GDP	C3'-C4'-C5'-O5'
19	DE	501	GDP	C3'-C4'-C5'-O5'
19	JK	501	GDP	C3'-C4'-C5'-O5'
20	AH	501	GTP	C3'-C4'-C5'-O5'
20	JB	501	GTP	C3'-C4'-C5'-O5'
20	LL	501	GTP	C3'-C4'-C5'-O5'
20	FD	501	GTP	C4'-C5'-O5'-PA
19	EG	501	GDP	C3'-C4'-C5'-O5'
20	DD	501	GTP	O4'-C4'-C5'-O5'
20	BB	501	GTP	C4'-C5'-O5'-PA
20	EB	501	GTP	C4'-C5'-O5'-PA
20	HF	501	GTP	C4'-C5'-O5'-PA
19	CC	501	GDP	O4'-C4'-C5'-O5'
19	CK	501	GDP	O4'-C4'-C5'-O5'
19	DE	501	GDP	O4'-C4'-C5'-O5'
19	DK	501	GDP	C3'-C4'-C5'-O5'
19	GE	501	GDP	C3'-C4'-C5'-O5'
19	JK	501	GDP	O4'-C4'-C5'-O5'
20	CD	501	GTP	C3'-C4'-C5'-O5'
20	LD	501	GTP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
20	MD	501	GTP	C4'-C5'-O5'-PA
20	AL	501	GTP	PA-O3A-PB-O1B
20	DH	501	GTP	PA-O3A-PB-O1B
20	KD	501	GTP	PA-O3A-PB-O1B
19	IE	501	GDP	C3'-C4'-C5'-O5'
20	AH	501	GTP	O4'-C4'-C5'-O5'
20	DJ	501	GTP	C3'-C4'-C5'-O5'
20	JL	501	GTP	C3'-C4'-C5'-O5'
20	AB	501	GTP	C4'-C5'-O5'-PA
20	AJ	501	GTP	C4'-C5'-O5'-PA
20	BJ	501	GTP	C4'-C5'-O5'-PA
20	BL	501	GTP	C4'-C5'-O5'-PA
20	CJ	501	GTP	C4'-C5'-O5'-PA
20	HJ	501	GTP	C4'-C5'-O5'-PA
20	HL	501	GTP	C4'-C5'-O5'-PA
19	AK	501	GDP	O4'-C4'-C5'-O5'
20	AD	501	GTP	C4'-C5'-O5'-PA
20	AF	501	GTP	C4'-C5'-O5'-PA
20	BF	501	GTP	C4'-C5'-O5'-PA
20	CB	501	GTP	C4'-C5'-O5'-PA
20	CD	501	GTP	C4'-C5'-O5'-PA
20	CF	501	GTP	C4'-C5'-O5'-PA
20	EH	501	GTP	C4'-C5'-O5'-PA
20	EJ	501	GTP	C4'-C5'-O5'-PA
20	GJ	501	GTP	C4'-C5'-O5'-PA
20	JB	501	GTP	C4'-C5'-O5'-PA
20	JJ	501	GTP	C4'-C5'-O5'-PA
20	JL	501	GTP	C4'-C5'-O5'-PA
20	LL	501	GTP	C4'-C5'-O5'-PA
20	MH	501	GTP	C4'-C5'-O5'-PA
20	MJ	501	GTP	C4'-C5'-O5'-PA
20	JB	501	GTP	O4'-C4'-C5'-O5'
19	BA	501	GDP	PA-O3A-PB-O1B
19	CK	501	GDP	PA-O3A-PB-O1B
19	II	501	GDP	PA-O3A-PB-O1B
19	IK	501	GDP	PA-O3A-PB-O1B
19	KE	501	GDP	PA-O3A-PB-O1B
20	BD	501	GTP	C4'-C5'-O5'-PA
20	FF	501	GTP	C4'-C5'-O5'-PA
20	GH	501	GTP	C4'-C5'-O5'-PA
20	IH	501	GTP	C4'-C5'-O5'-PA
20	LF	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
19	AK	501	GDP	PA-O3A-PB-O2B
19	BK	501	GDP	PA-O3A-PB-O2B
19	IE	501	GDP	PA-O3A-PB-O2B
19	JE	501	GDP	PA-O3A-PB-O2B
19	KI	502	GDP	PA-O3A-PB-O2B
19	CC	501	GDP	C5'-O5'-PA-O3A
19	IC	501	GDP	C5'-O5'-PA-O3A
20	AB	501	GTP	C5'-O5'-PA-O3A
20	AD	501	GTP	C5'-O5'-PA-O3A
20	CD	501	GTP	C5'-O5'-PA-O3A
20	CH	501	GTP	C5'-O5'-PA-O3A
20	DH	501	GTP	C5'-O5'-PA-O3A
20	EJ	501	GTP	C5'-O5'-PA-O3A
20	EL	501	GTP	C5'-O5'-PA-O3A
20	GF	501	GTP	C5'-O5'-PA-O3A
20	GH	501	GTP	C5'-O5'-PA-O3A
20	IH	501	GTP	C5'-O5'-PA-O3A
20	IL	501	GTP	C5'-O5'-PA-O3A
20	JD	501	GTP	C5'-O5'-PA-O3A
20	JJ	501	GTP	C5'-O5'-PA-O3A
20	JL	501	GTP	C5'-O5'-PA-O3A
20	MF	501	GTP	C5'-O5'-PA-O3A
20	MH	501	GTP	C5'-O5'-PA-O3A
19	BE	501	GDP	C3'-C4'-C5'-O5'
19	CI	501	GDP	C3'-C4'-C5'-O5'
19	EG	501	GDP	O4'-C4'-C5'-O5'
19	FK	501	GDP	C3'-C4'-C5'-O5'
20	FJ	501	GTP	C3'-C4'-C5'-O5'
20	LL	501	GTP	O4'-C4'-C5'-O5'
20	AD	501	GTP	PA-O3A-PB-O2B
20	CH	501	GTP	PA-O3A-PB-O2B
20	EL	501	GTP	PA-O3A-PB-O2B
20	GD	501	GTP	PA-O3A-PB-O2B
20	GF	501	GTP	PA-O3A-PB-O2B
20	GH	501	GTP	PA-O3A-PB-O2B
20	GJ	501	GTP	PA-O3A-PB-O2B
20	HF	501	GTP	PG-O3B-PB-O1B
20	HI	501	GTP	PA-O3A-PB-O1B
20	JJ	501	GTP	PA-O3A-PB-O2B
20	JL	501	GTP	PA-O3A-PB-O2B
20	KB	501	GTP	PA-O3A-PB-O1B
20	KL	501	GTP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
20	LB	501	GTP	PA-O3A-PB-O2B
20	LH	501	GTP	PA-O3A-PB-O1B
20	ML	501	GTP	PA-O3A-PB-O2B
20	BH	501	GTP	C4'-C5'-O5'-PA
20	CH	501	GTP	C4'-C5'-O5'-PA
20	DD	501	GTP	C4'-C5'-O5'-PA
20	DH	501	GTP	C4'-C5'-O5'-PA
20	DL	501	GTP	C4'-C5'-O5'-PA
20	EF	501	GTP	C4'-C5'-O5'-PA
20	EL	501	GTP	C4'-C5'-O5'-PA
20	GF	501	GTP	C4'-C5'-O5'-PA
20	GL	501	GTP	C4'-C5'-O5'-PA
20	IL	501	GTP	C4'-C5'-O5'-PA
20	JH	501	GTP	C4'-C5'-O5'-PA
20	LJ	501	GTP	C4'-C5'-O5'-PA
19	EA	501	GDP	C5'-O5'-PA-O2A
19	EE	502	GDP	C5'-O5'-PA-O2A
19	EG	501	GDP	C5'-O5'-PA-O2A
19	IC	501	GDP	C5'-O5'-PA-O2A
19	IM	501	GDP	C5'-O5'-PA-O2A
19	JG	501	GDP	C5'-O5'-PA-O2A
19	KI	502	GDP	C5'-O5'-PA-O2A
19	MI	501	GDP	C5'-O5'-PA-O2A
20	AD	501	GTP	C5'-O5'-PA-O2A
20	AF	501	GTP	C5'-O5'-PA-O2A
20	BF	501	GTP	C5'-O5'-PA-O2A
20	CD	501	GTP	C5'-O5'-PA-O2A
20	CF	501	GTP	C5'-O5'-PA-O2A
20	CH	501	GTP	C5'-O5'-PA-O2A
20	DF	501	GTP	C5'-O5'-PA-O2A
20	DH	501	GTP	C5'-O5'-PA-O2A
20	DL	501	GTP	C5'-O5'-PA-O2A
20	EJ	501	GTP	C5'-O5'-PA-O2A
20	EL	501	GTP	C5'-O5'-PA-O2A
20	FH	501	GTP	C5'-O5'-PA-O2A
20	FJ	501	GTP	C5'-O5'-PA-O2A
20	FL	501	GTP	C5'-O5'-PA-O2A
20	GF	501	GTP	C5'-O5'-PA-O2A
20	GH	501	GTP	C5'-O5'-PA-O2A
20	HD	501	GTP	C5'-O5'-PA-O2A
20	HF	501	GTP	C5'-O5'-PA-O2A
20	HJ	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
20	IL	501	GTP	C5'-O5'-PA-O2A
20	JD	501	GTP	C5'-O5'-PA-O2A
20	JJ	501	GTP	C5'-O5'-PA-O2A
20	JL	501	GTP	C5'-O5'-PA-O2A
20	KD	501	GTP	C5'-O5'-PA-O1A
20	KD	501	GTP	C5'-O5'-PA-O2A
20	KJ	501	GTP	C5'-O5'-PA-O1A
20	KJ	501	GTP	C5'-O5'-PA-O2A
20	KL	501	GTP	C5'-O5'-PA-O1A
20	KL	501	GTP	C5'-O5'-PA-O2A
20	LD	501	GTP	C5'-O5'-PA-O2A
20	MB	501	GTP	C5'-O5'-PA-O1A
20	MB	501	GTP	C5'-O5'-PA-O2A
20	MH	501	GTP	C5'-O5'-PA-O2A
19	HK	501	GDP	C3'-C4'-C5'-O5'
19	IC	501	GDP	C3'-C4'-C5'-O5'
20	DF	501	GTP	C3'-C4'-C5'-O5'
20	DH	501	GTP	C3'-C4'-C5'-O5'
20	JJ	501	GTP	C3'-C4'-C5'-O5'
20	KF	501	GTP	C3'-C4'-C5'-O5'
20	MH	501	GTP	C3'-C4'-C5'-O5'
20	IF	501	GTP	C4'-C5'-O5'-PA
20	MB	501	GTP	C4'-C5'-O5'-PA
19	BG	501	GDP	C3'-C4'-C5'-O5'
19	DK	501	GDP	O4'-C4'-C5'-O5'
19	GM	501	GDP	C3'-C4'-C5'-O5'
20	ED	501	GTP	C4'-C5'-O5'-PA
20	LB	501	GTP	C4'-C5'-O5'-PA
20	ML	501	GTP	C4'-C5'-O5'-PA
19	GE	501	GDP	O4'-C4'-C5'-O5'
20	IF	501	GTP	C3'-C4'-C5'-O5'
20	AJ	501	GTP	PA-O3A-PB-O2B
20	CD	501	GTP	PA-O3A-PB-O2B
20	ED	501	GTP	PA-O3A-PB-O2B
20	EH	501	GTP	PB-O3A-PA-O2A
20	FB	501	GTP	PA-O3A-PB-O2B
20	ID	501	GTP	PA-O3A-PB-O2B
20	IJ	501	GTP	PA-O3A-PB-O2B
20	IL	501	GTP	PA-O3A-PB-O2B
20	JH	501	GTP	PB-O3A-PA-O1A
20	KF	501	GTP	PA-O3A-PB-O1B
20	LF	501	GTP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
20	MF	501	GTP	PG-O3B-PB-O1B
20	MF	501	GTP	PA-O3A-PB-O2B
20	FB	501	GTP	C4'-C5'-O5'-PA
20	GD	501	GTP	C4'-C5'-O5'-PA
20	KF	501	GTP	C4'-C5'-O5'-PA
20	LH	501	GTP	C4'-C5'-O5'-PA
20	HI	501	GTP	C4'-C5'-O5'-PA
19	EE	502	GDP	PA-O3A-PB-O1B
19	HE	501	GDP	PA-O3A-PB-O1B
19	HM	501	GDP	PA-O3A-PB-O1B
20	CD	501	GTP	O4'-C4'-C5'-O5'
19	HG	501	GDP	C4'-C5'-O5'-PA
20	DH	501	GTP	PA-O3A-PB-O2B
20	EF	501	GTP	PA-O3A-PB-O2B
20	EF	501	GTP	PB-O3A-PA-O1A
20	GL	501	GTP	PB-O3A-PA-O2A
20	IH	501	GTP	PA-O3A-PB-O2B
20	IL	501	GTP	PA-O3A-PB-O1B
20	JD	501	GTP	C4'-C5'-O5'-PA
20	KJ	501	GTP	PA-O3A-PB-O1B
20	KL	501	GTP	PA-O3A-PB-O1B
20	LD	501	GTP	PA-O3A-PB-O1B
20	MB	501	GTP	PG-O3B-PB-O1B
20	MF	501	GTP	PA-O3A-PB-O1B
19	BE	501	GDP	O4'-C4'-C5'-O5'
19	FK	501	GDP	O4'-C4'-C5'-O5'
19	IE	501	GDP	O4'-C4'-C5'-O5'
19	CI	501	GDP	O4'-C4'-C5'-O5'
19	HK	501	GDP	O4'-C4'-C5'-O5'
19	IC	501	GDP	O4'-C4'-C5'-O5'
20	BD	501	GTP	C3'-C4'-C5'-O5'
20	KJ	501	GTP	C3'-C4'-C5'-O5'
19	EA	501	GDP	PA-O3A-PB-O1B
20	FF	501	GTP	C3'-C4'-C5'-O5'
20	FH	501	GTP	C3'-C4'-C5'-O5'
20	ML	501	GTP	C3'-C4'-C5'-O5'
19	BA	501	GDP	PA-O3A-PB-O2B
19	BA	501	GDP	PA-O3A-PB-O3B
19	CK	501	GDP	PA-O3A-PB-O2B
19	CK	501	GDP	PA-O3A-PB-O3B
19	EA	501	GDP	PA-O3A-PB-O3B
19	EE	502	GDP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
19	EE	502	GDP	PA-O3A-PB-O3B
19	HC	501	GDP	PA-O3A-PB-O3B
19	HE	501	GDP	PA-O3A-PB-O2B
19	HE	501	GDP	PA-O3A-PB-O3B
19	HM	501	GDP	PA-O3A-PB-O2B
19	HM	501	GDP	PA-O3A-PB-O3B
19	II	501	GDP	PA-O3A-PB-O2B
19	II	501	GDP	PA-O3A-PB-O3B
19	IK	501	GDP	PA-O3A-PB-O2B
19	IK	501	GDP	PA-O3A-PB-O3B
19	KE	501	GDP	PA-O3A-PB-O2B
19	KE	501	GDP	PA-O3A-PB-O3B
19	AK	501	GDP	C5'-O5'-PA-O3A
19	BC	501	GDP	C5'-O5'-PA-O3A
19	BK	501	GDP	C5'-O5'-PA-O3A
19	CK	501	GDP	C5'-O5'-PA-O3A
19	GI	501	GDP	C5'-O5'-PA-O3A
19	HI	502	GDP	C5'-O5'-PA-O3A
19	HM	501	GDP	C5'-O5'-PA-O3A
19	JE	501	GDP	C5'-O5'-PA-O3A
19	KC	501	GDP	C5'-O5'-PA-O3A
19	ME	501	GDP	C5'-O5'-PA-O3A
20	AJ	501	GTP	C5'-O5'-PA-O3A
20	BD	501	GTP	C5'-O5'-PA-O3A
20	BH	501	GTP	C5'-O5'-PA-O3A
20	BJ	501	GTP	C5'-O5'-PA-O3A
20	BL	501	GTP	C5'-O5'-PA-O3A
20	CB	501	GTP	C5'-O5'-PA-O3A
20	DD	501	GTP	C5'-O5'-PA-O3A
20	DL	501	GTP	C5'-O5'-PA-O3A
20	EF	501	GTP	C5'-O5'-PA-O3A
20	EH	501	GTP	C5'-O5'-PA-O3A
20	FF	501	GTP	C5'-O5'-PA-O3A
20	GL	501	GTP	C5'-O5'-PA-O3A
20	HL	501	GTP	C5'-O5'-PA-O3A
20	IF	501	GTP	C5'-O5'-PA-O3A
20	JB	501	GTP	C5'-O5'-PA-O3A
20	JH	501	GTP	C5'-O5'-PA-O3A
20	LJ	501	GTP	C5'-O5'-PA-O3A
20	LL	501	GTP	C5'-O5'-PA-O3A
20	MB	501	GTP	C5'-O5'-PA-O3A
20	MD	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
20	MJ	501	GTP	C5'-O5'-PA-O3A
19	AI	501	GDP	C3'-C4'-C5'-O5'
19	CG	501	GDP	C3'-C4'-C5'-O5'
19	HE	501	GDP	C3'-C4'-C5'-O5'
19	IM	501	GDP	C3'-C4'-C5'-O5'
20	DB	501	GTP	C3'-C4'-C5'-O5'
20	GF	501	GTP	C3'-C4'-C5'-O5'
20	AH	501	GTP	PA-O3A-PB-O1B
20	AH	501	GTP	PA-O3A-PB-O2B
20	AJ	501	GTP	PA-O3A-PB-O1B
20	AL	501	GTP	PA-O3A-PB-O2B
20	BH	501	GTP	PB-O3A-PA-O1A
20	DD	501	GTP	PA-O3A-PB-O1B
20	DD	501	GTP	PA-O3A-PB-O2B
20	DL	501	GTP	PA-O3A-PB-O1B
20	DL	501	GTP	PA-O3A-PB-O2B
20	ED	501	GTP	PA-O3A-PB-O1B
20	EF	501	GTP	PA-O3A-PB-O1B
20	EH	501	GTP	PB-O3A-PA-O1A
20	EJ	501	GTP	PB-O3A-PA-O1A
20	EJ	501	GTP	PB-O3A-PA-O2A
20	FB	501	GTP	PG-O3B-PB-O1B
20	FB	501	GTP	PA-O3A-PB-O1B
20	GD	501	GTP	PG-O3B-PB-O2B
20	GD	501	GTP	PA-O3A-PB-O1B
20	GH	501	GTP	PG-O3B-PB-O2B
20	GJ	501	GTP	PG-O3B-PB-O2B
20	GJ	501	GTP	PA-O3A-PB-O1B
20	GL	501	GTP	PB-O3A-PA-O1A
20	HI	501	GTP	PA-O3A-PB-O2B
20	HL	501	GTP	PA-O3A-PB-O2B
20	ID	501	GTP	PA-O3A-PB-O1B
20	IJ	501	GTP	PA-O3A-PB-O1B
20	JB	501	GTP	PA-O3A-PB-O2B
20	JF	501	GTP	PA-O3A-PB-O2B
20	JH	501	GTP	PA-O3A-PB-O2B
20	JL	501	GTP	PA-O3A-PB-O1B
20	KB	501	GTP	PG-O3B-PB-O1B
20	KD	501	GTP	PA-O3A-PB-O2B
20	KF	501	GTP	PG-O3B-PB-O2B
20	KF	501	GTP	PA-O3A-PB-O2B
20	LB	501	GTP	PA-O3A-PB-O1B

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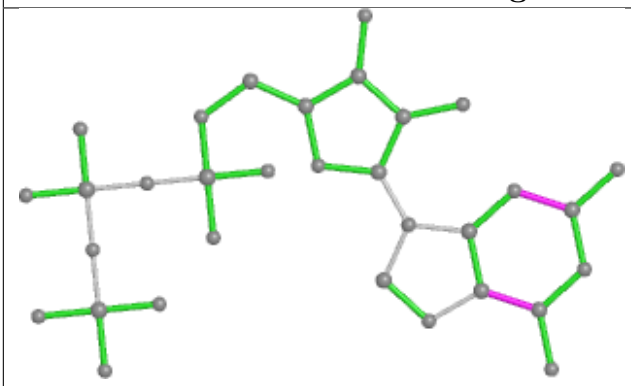
Mol	Chain	Res	Type	Atoms
20	LF	501	GTP	PA-O3A-PB-O1B
20	LH	501	GTP	PG-O3B-PB-O2B
20	LH	501	GTP	PA-O3A-PB-O2B
20	MH	501	GTP	PA-O3A-PB-O2B
20	ML	501	GTP	PA-O3A-PB-O1B
20	AL	501	GTP	C4'-C5'-O5'-PA
19	CC	501	GDP	C5'-O5'-PA-O2A
19	EC	501	GDP	C5'-O5'-PA-O1A
19	EK	501	GDP	C5'-O5'-PA-O1A
19	FA	501	GDP	C5'-O5'-PA-O1A
19	FE	501	GDP	C5'-O5'-PA-O1A
19	FG	501	GDP	C5'-O5'-PA-O1A
19	HE	501	GDP	C5'-O5'-PA-O1A
19	KG	501	GDP	C5'-O5'-PA-O1A
20	FD	501	GTP	C5'-O5'-PA-O2A
20	GJ	501	GTP	C5'-O5'-PA-O2A
20	ID	501	GTP	C5'-O5'-PA-O1A
20	LD	501	GTP	C5'-O5'-PA-O1A
20	GJ	501	GTP	C3'-C4'-C5'-O5'
20	DB	501	GTP	PB-O3B-PG-O1G
20	CB	501	GTP	C3'-C4'-C5'-O5'
20	FL	501	GTP	C3'-C4'-C5'-O5'
20	HD	501	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

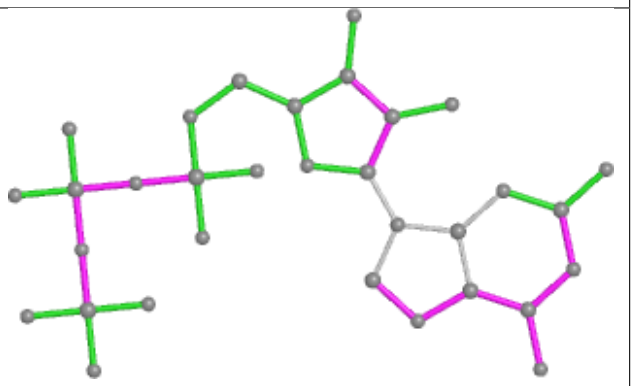
No monomer is involved in short contacts.

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.

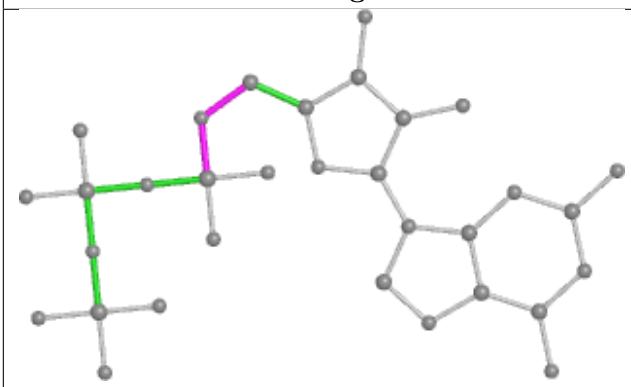
Ligand GTP AB 501



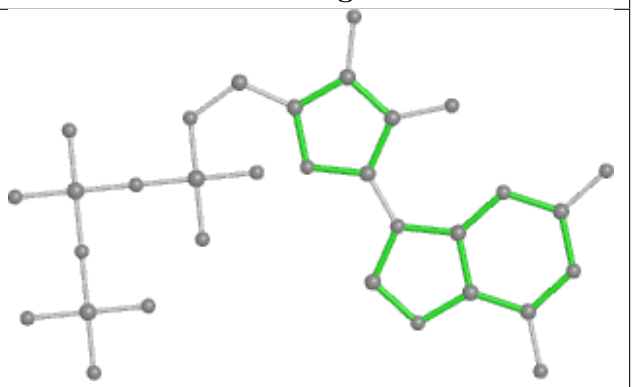
Bond lengths



Bond angles

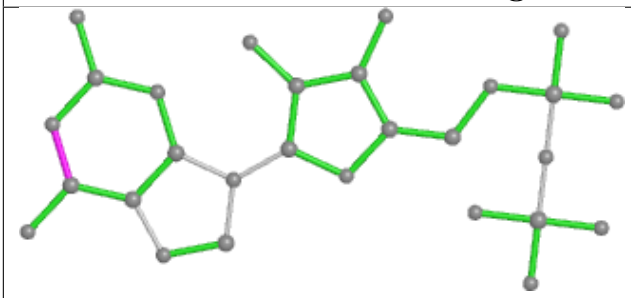


Torsions



Rings

Ligand GDP DC 501



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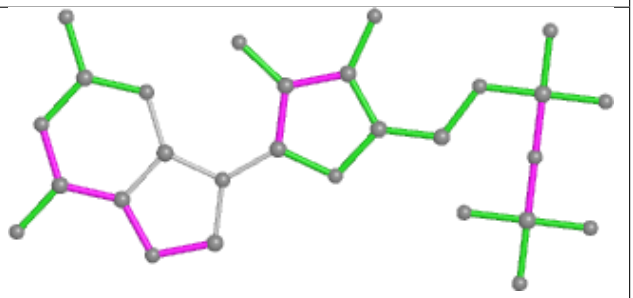
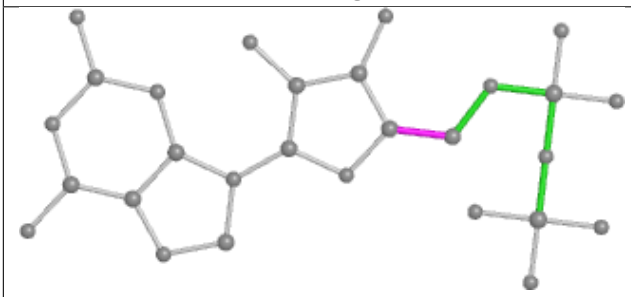


Bond angles



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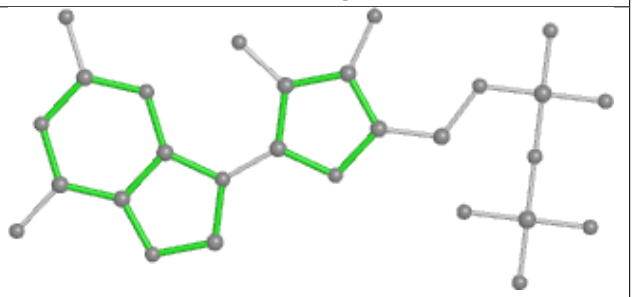

Rings

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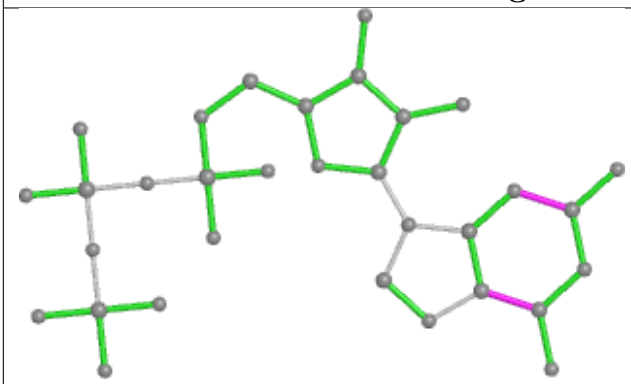

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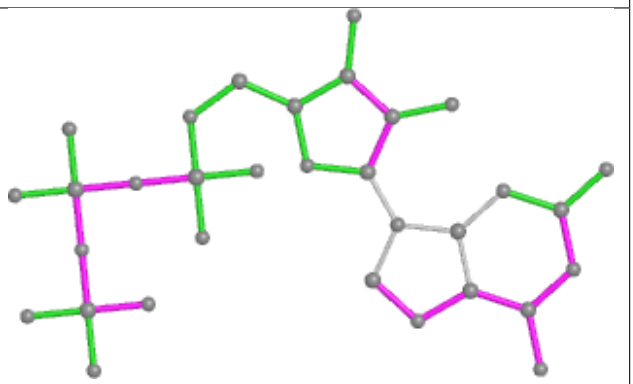
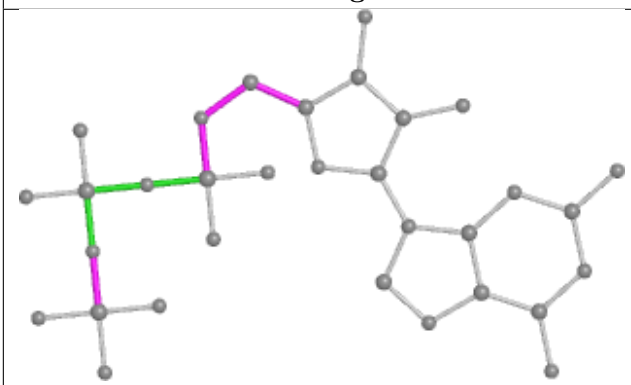


Bond angles



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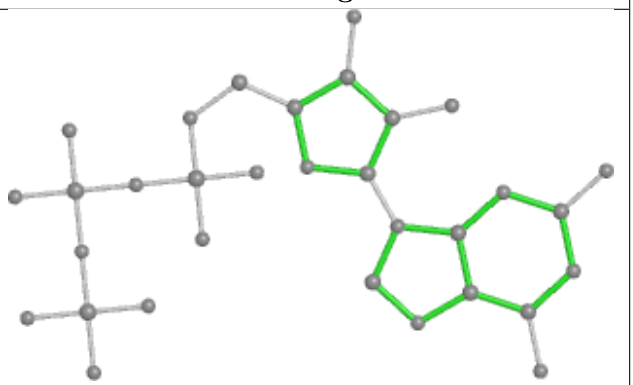

Rings

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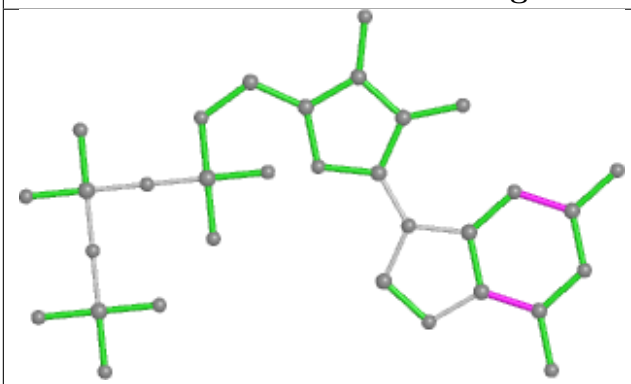

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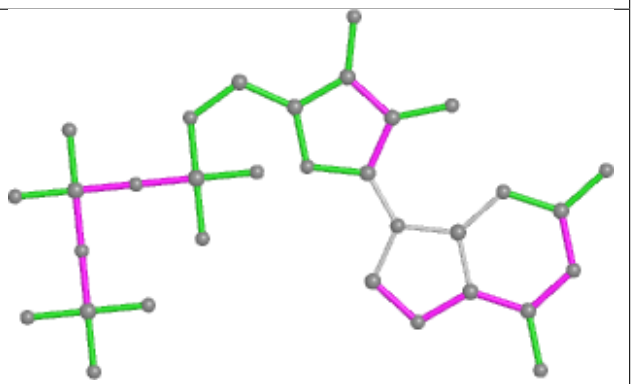

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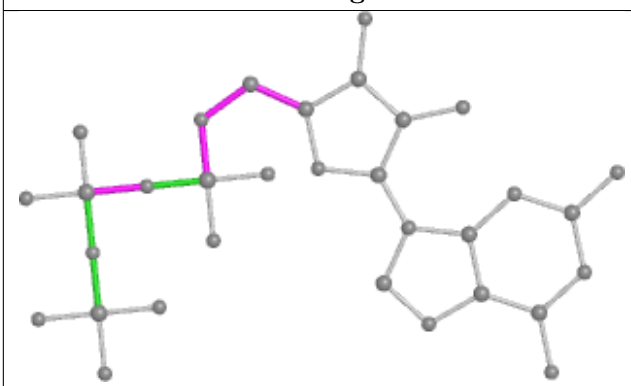

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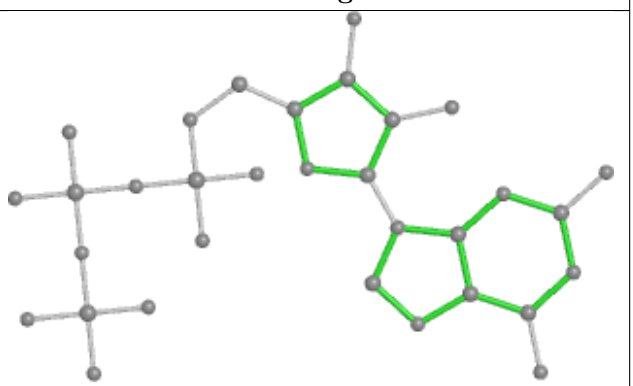
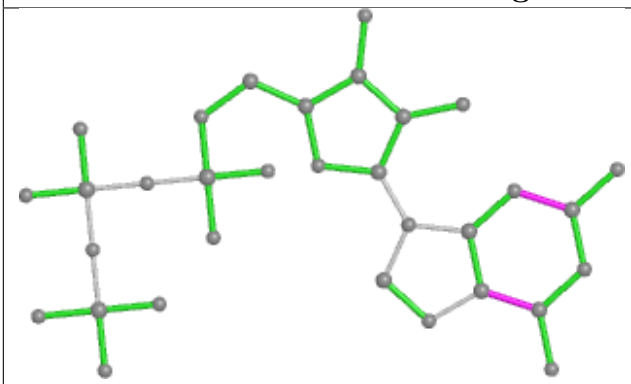


Rings

Ligand GTP LB 501



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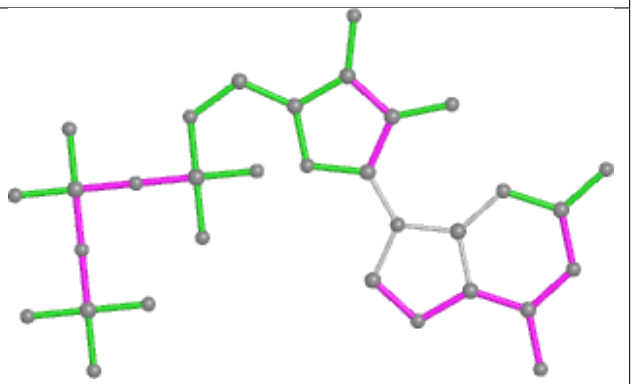
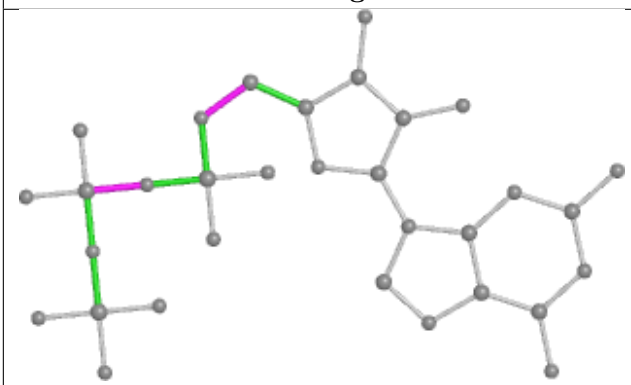


Bond angles



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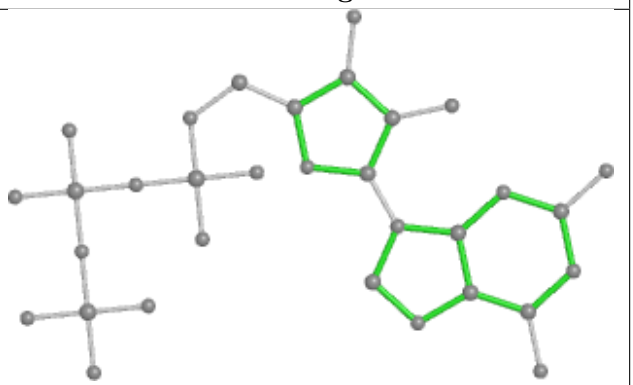

Rings

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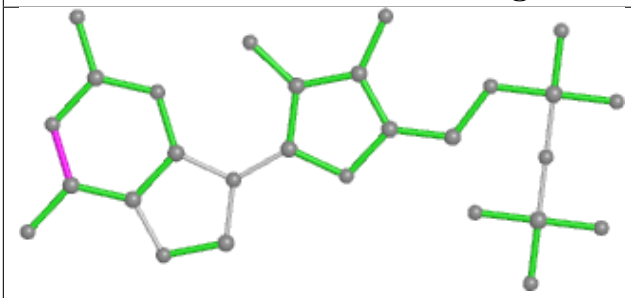

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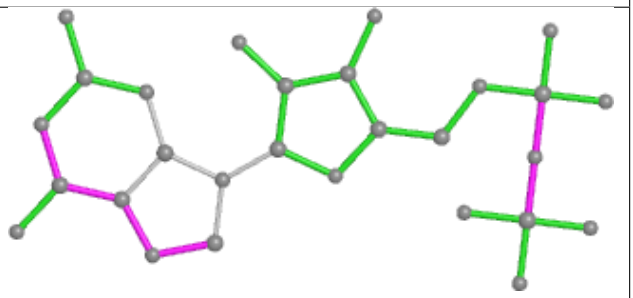

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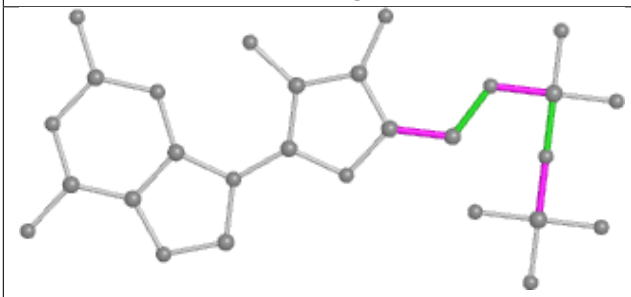

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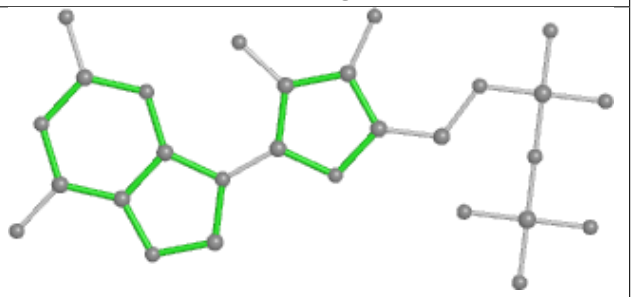

Rings

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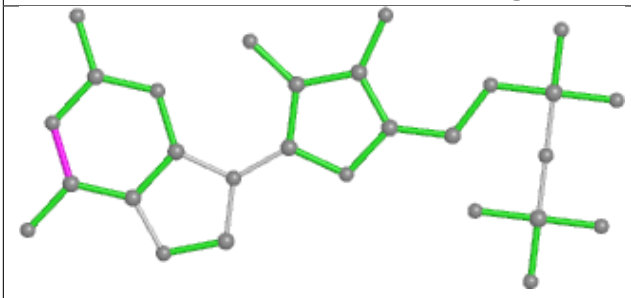
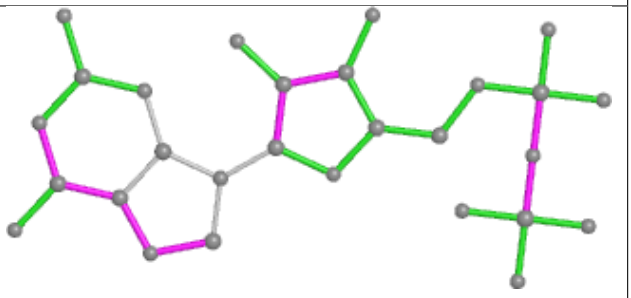
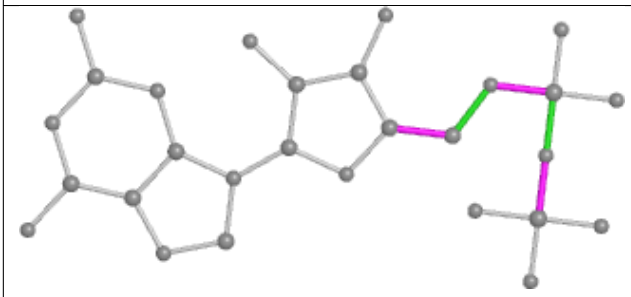
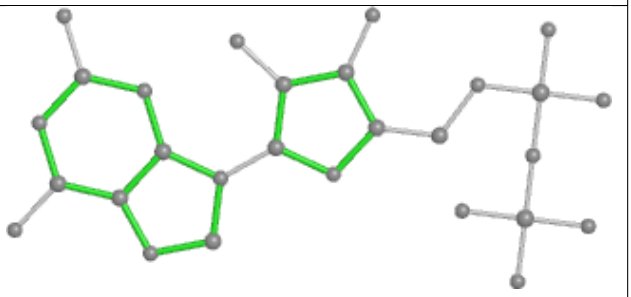
 Bond lengths	 Bond angles
 Torsions	 Rings

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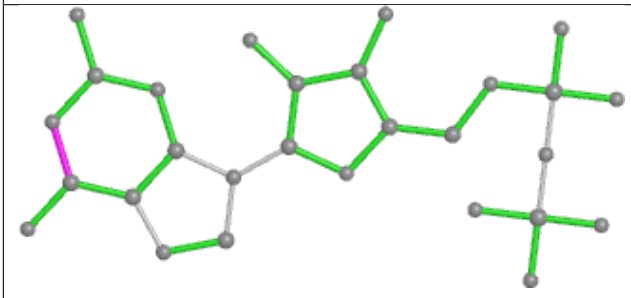
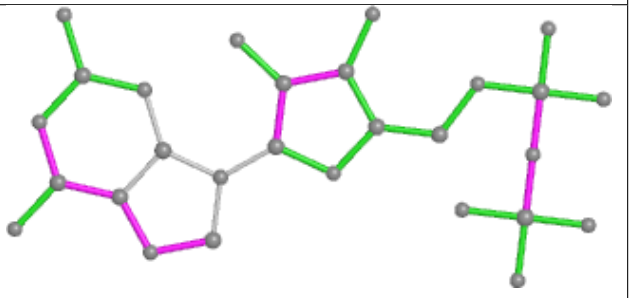
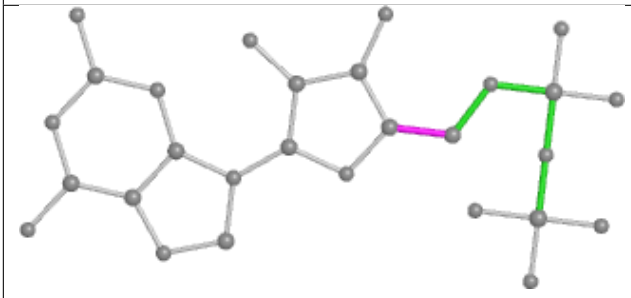
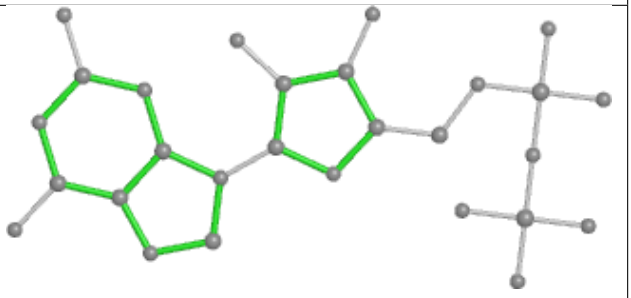
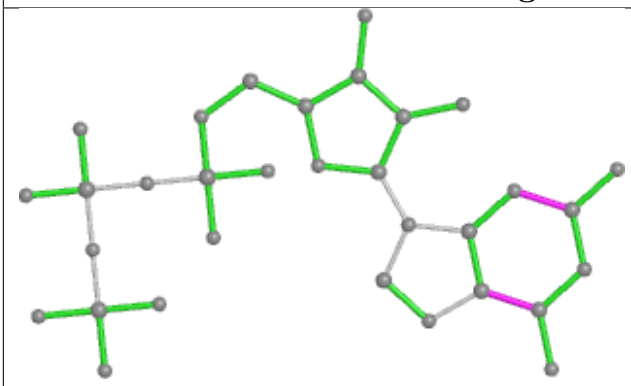
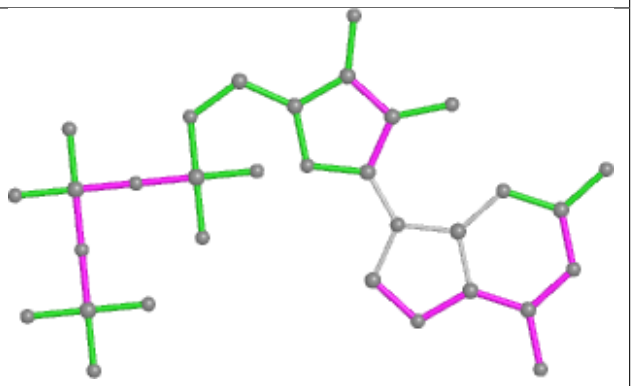
 Bond lengths	 Bond angles
 Torsions	 Rings

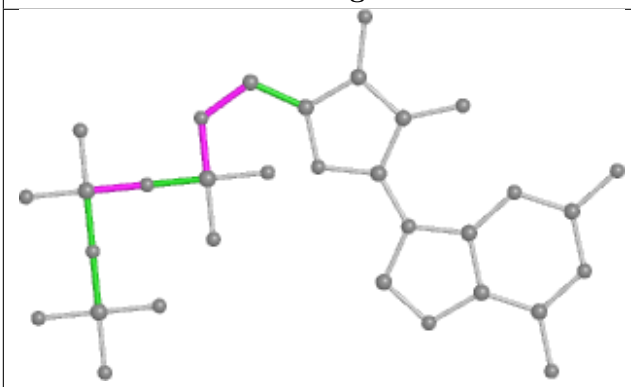
Ligand GTP IL 501



Bond lengths



Bond angles



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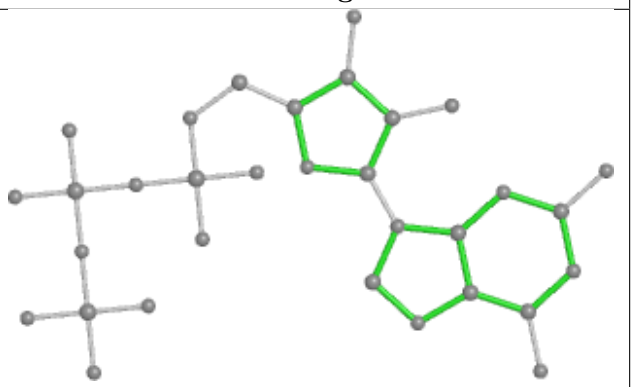
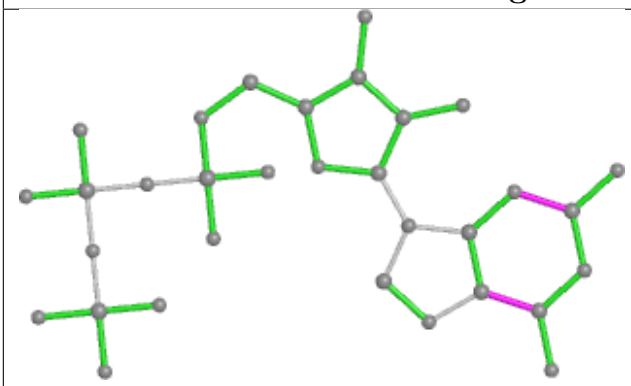


Rings

Ligand GTP MJ 501



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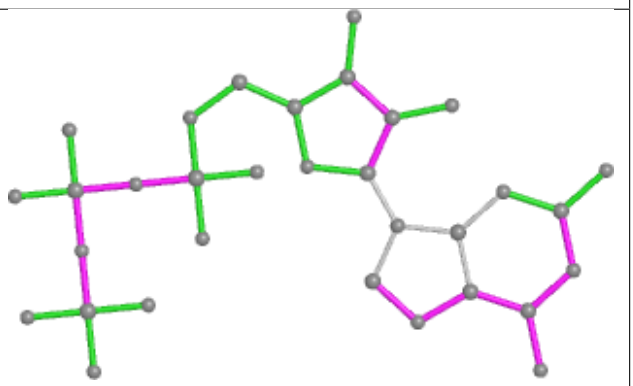

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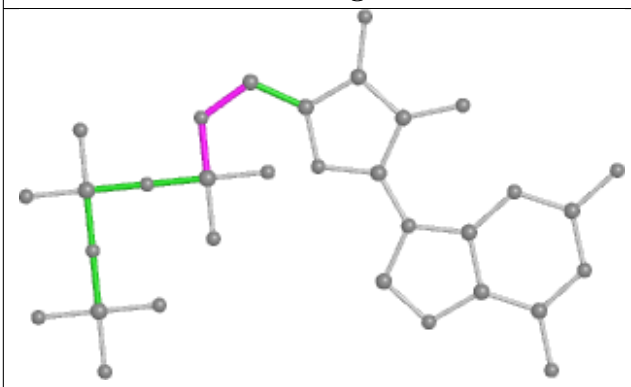

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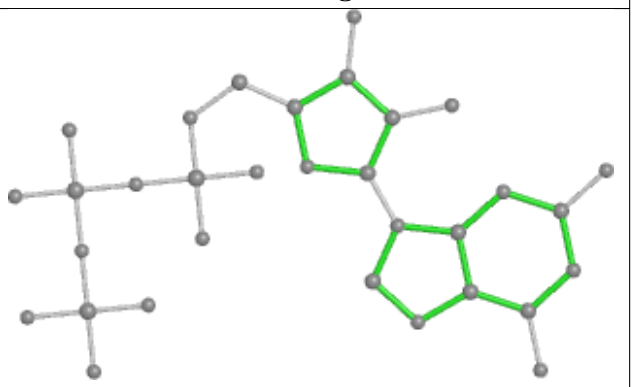

Rings

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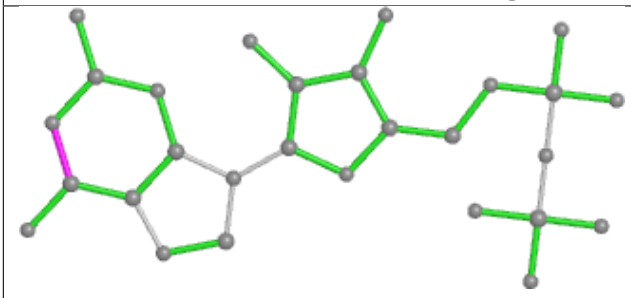

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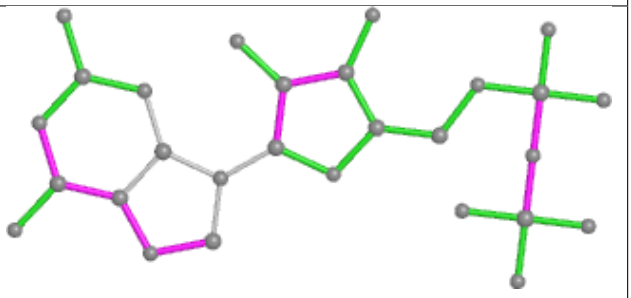

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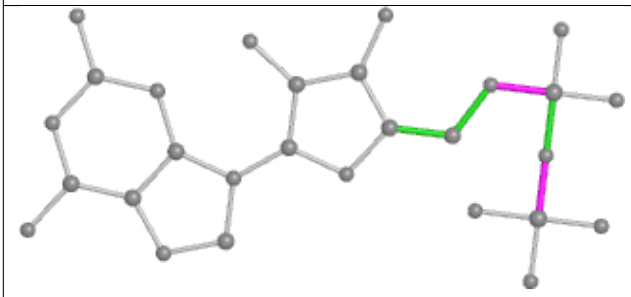

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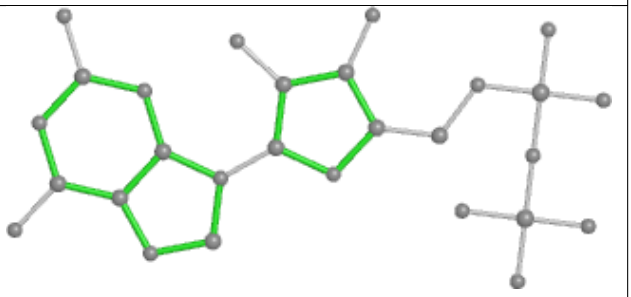
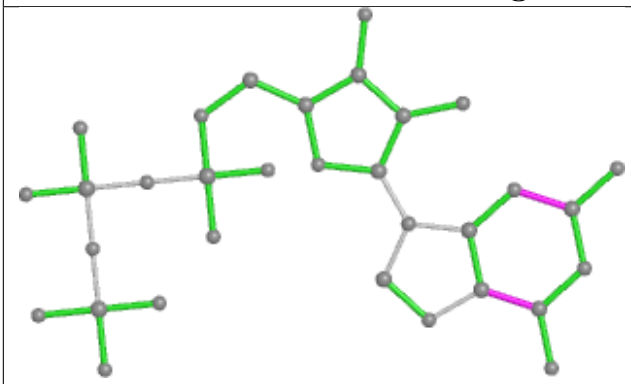
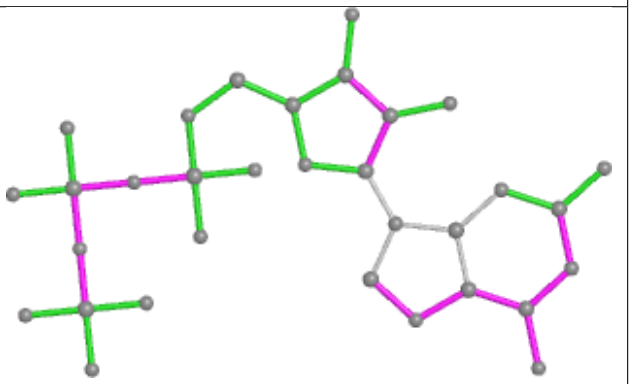


Rings

Ligand GTP EH 501



Bond lengths



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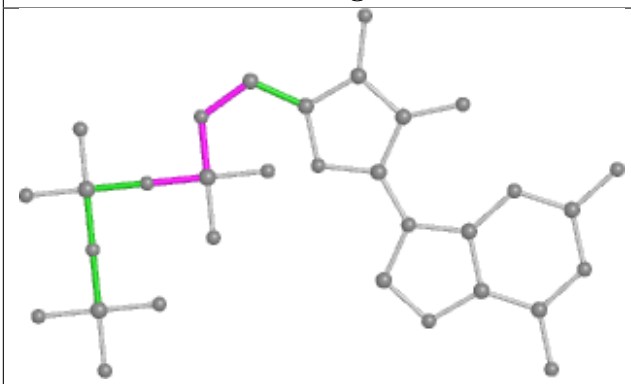

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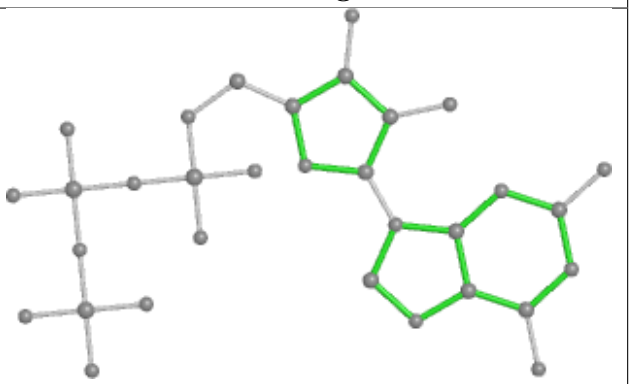
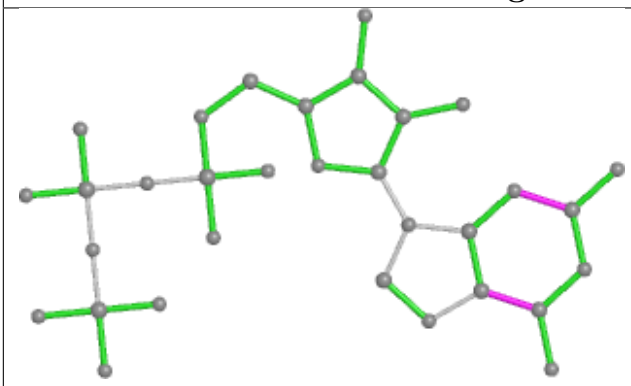


Rings

Ligand GTP KD 501



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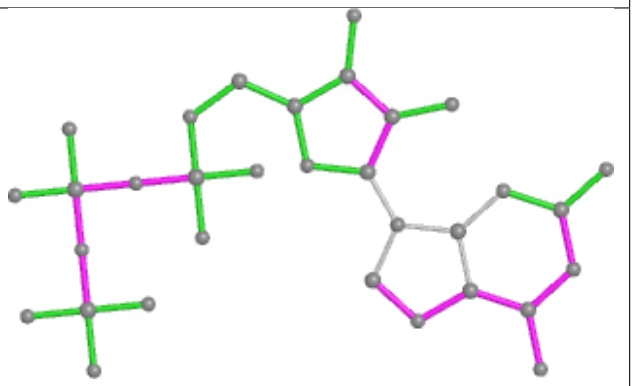
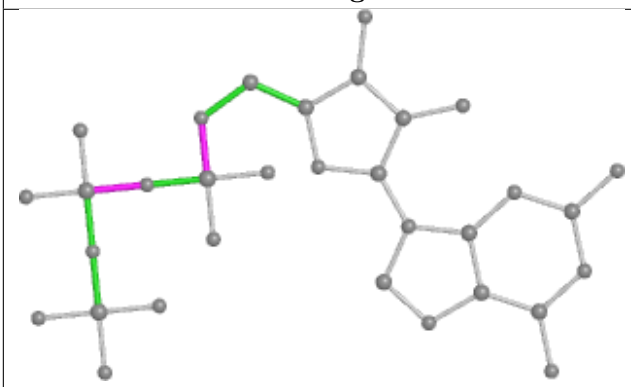
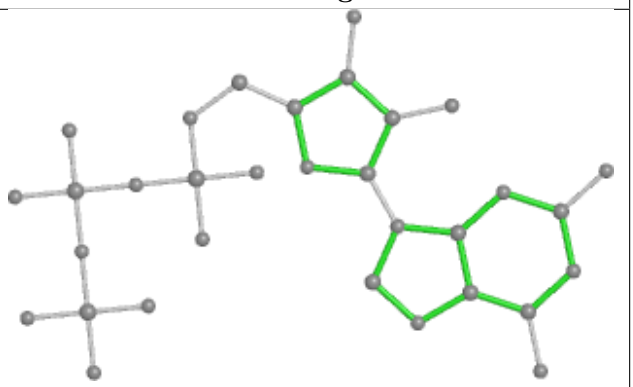


Bond angles

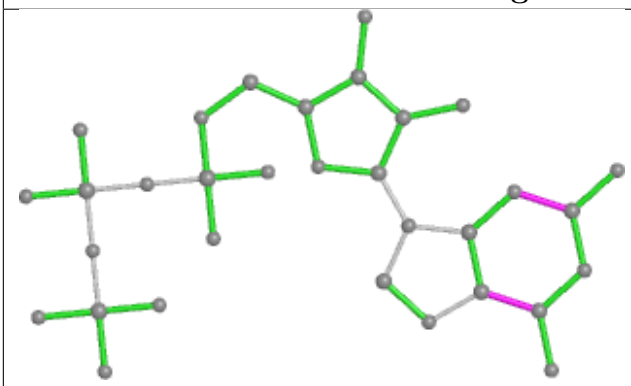


Torsions



Rings

Ligand GTP EB 501



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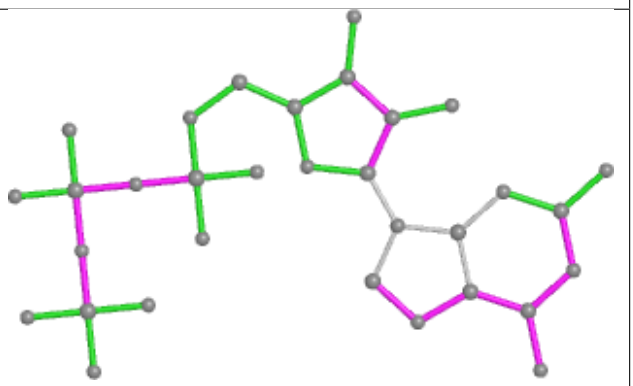

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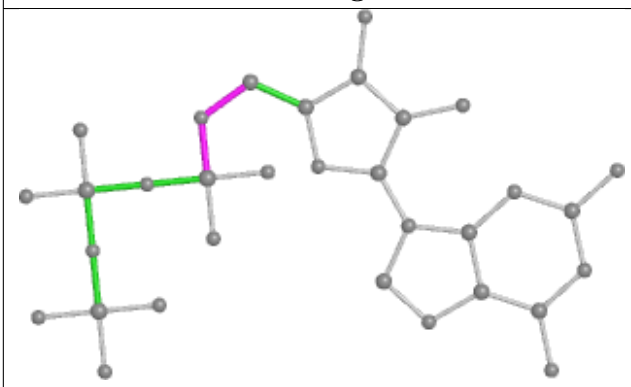

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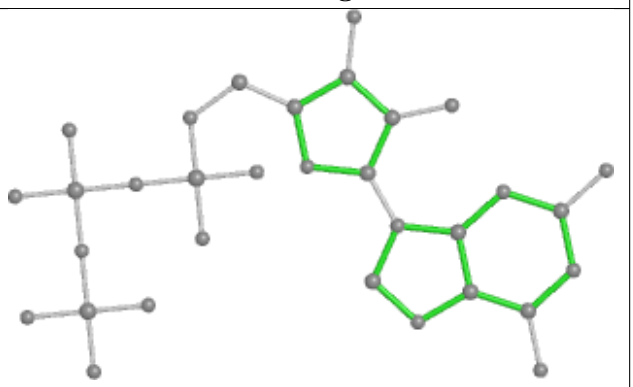
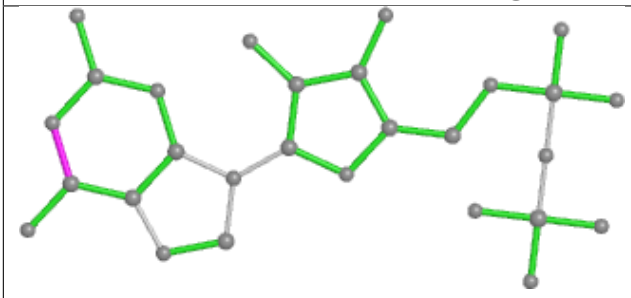


Rings

Ligand GDP CK 501



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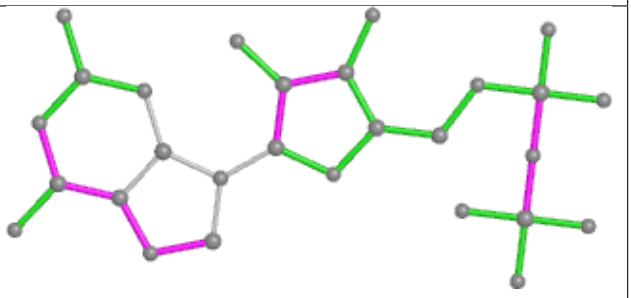

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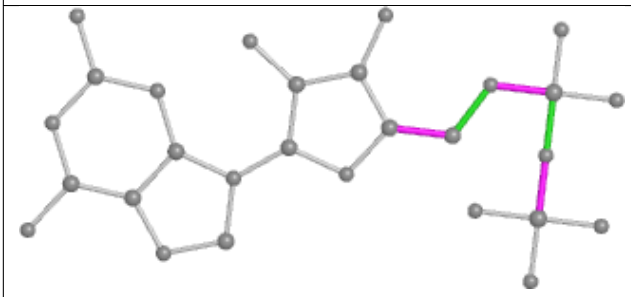

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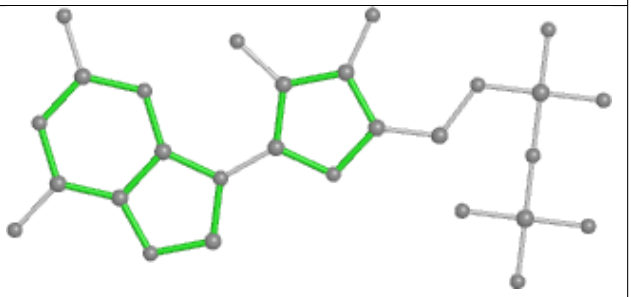

Rings

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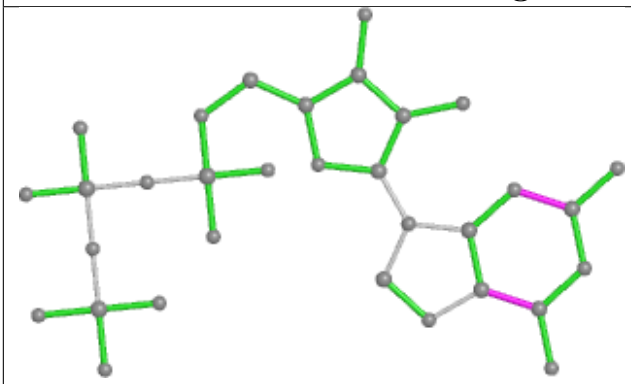

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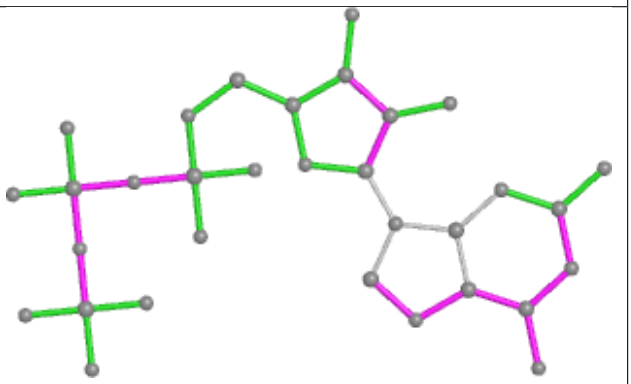

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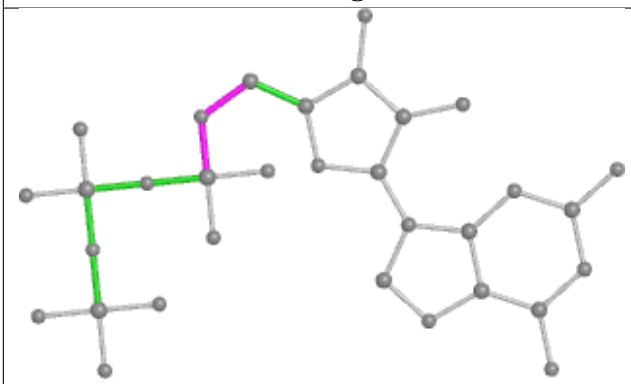

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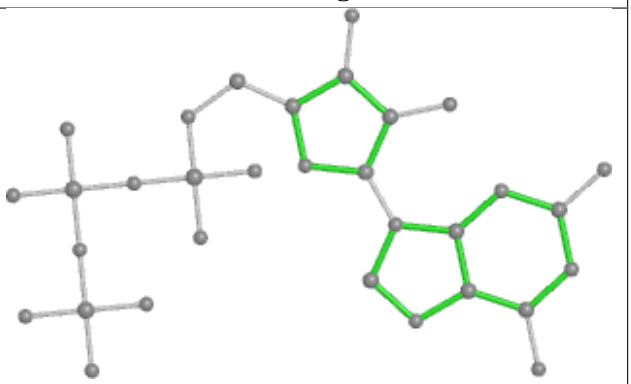
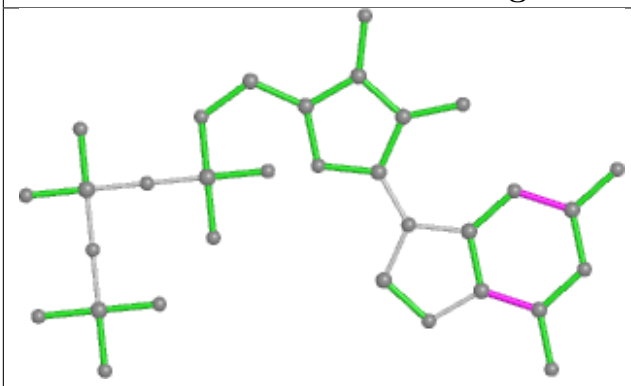


Rings

Ligand GTP BH 501



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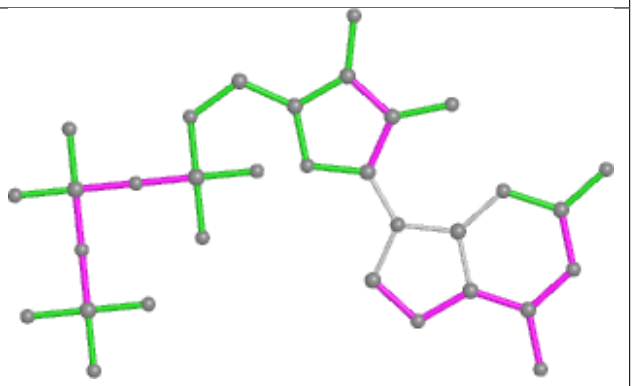

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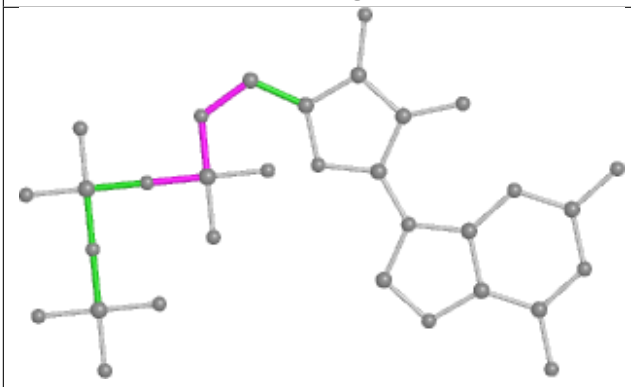

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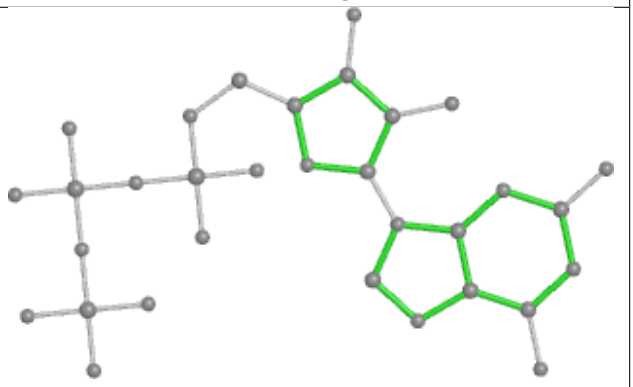

Rings

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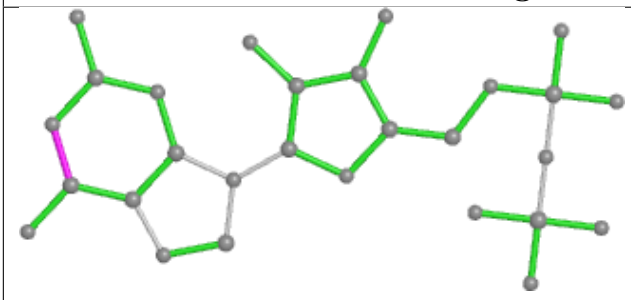

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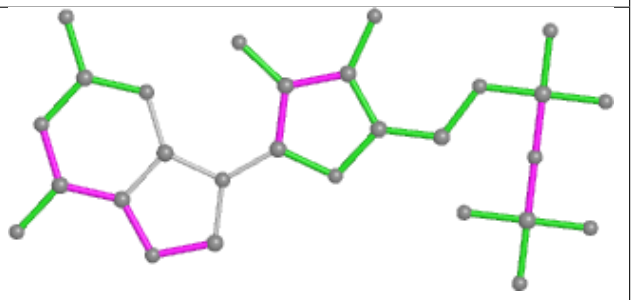

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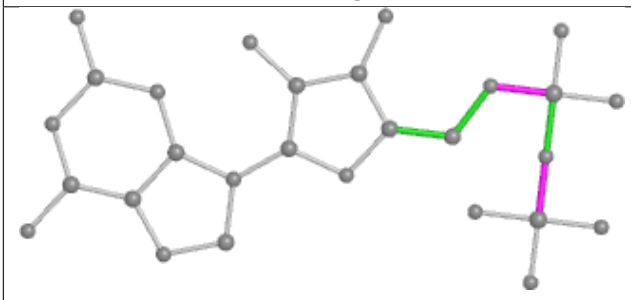

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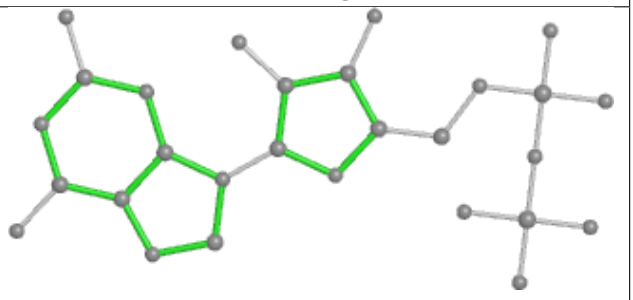

Rings

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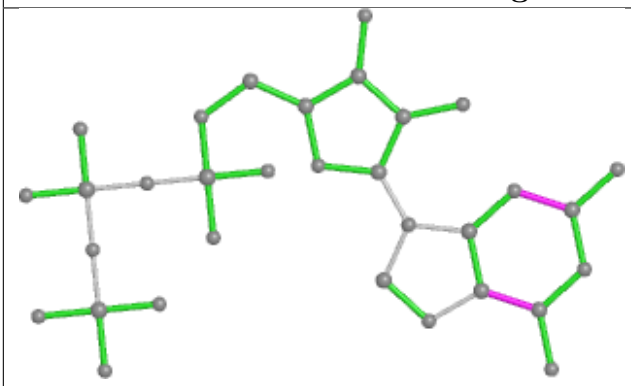

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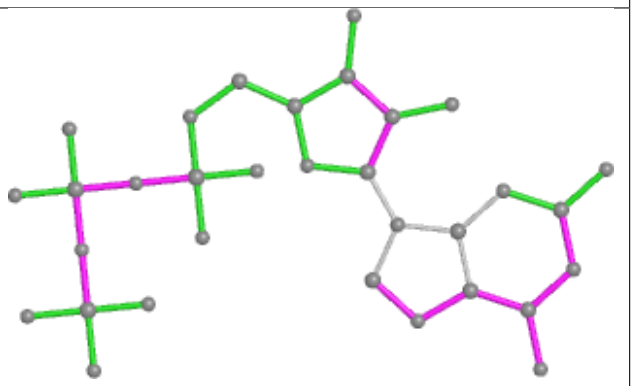

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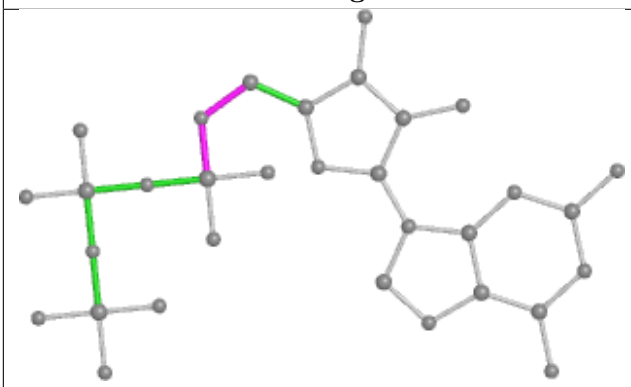

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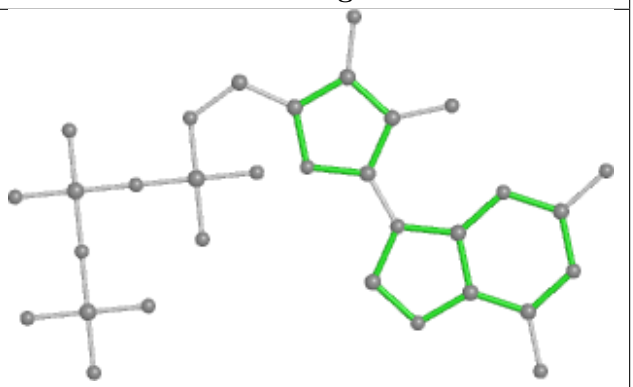

Rings

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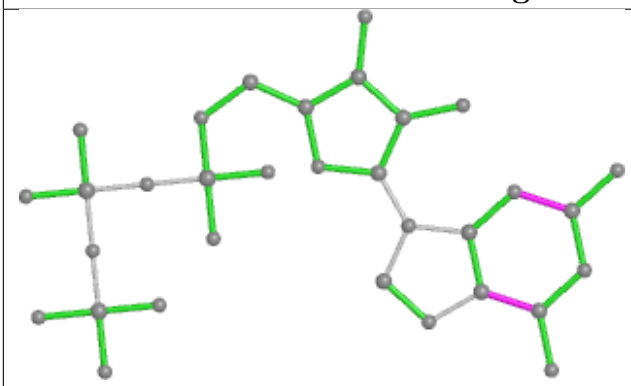

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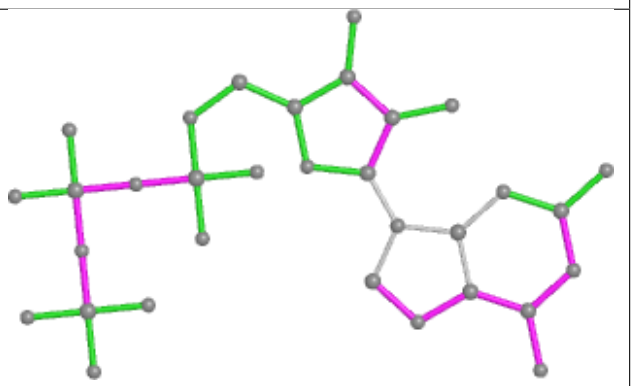

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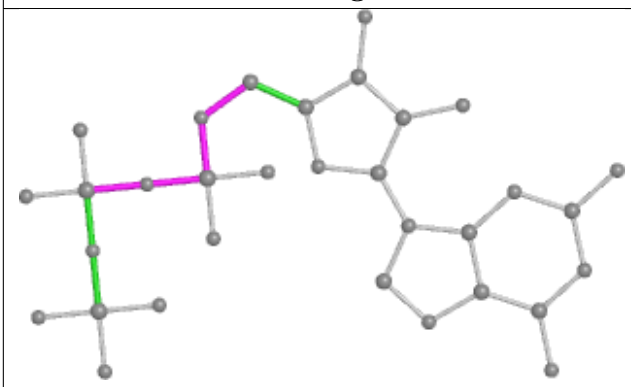

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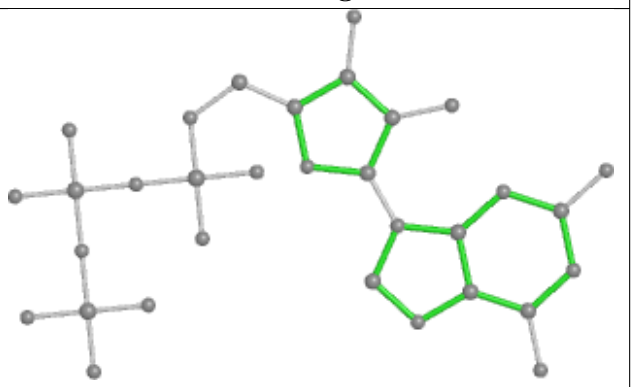
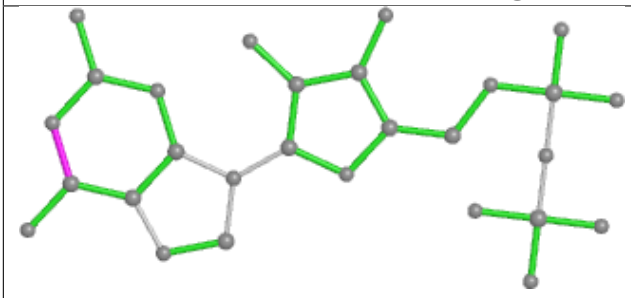
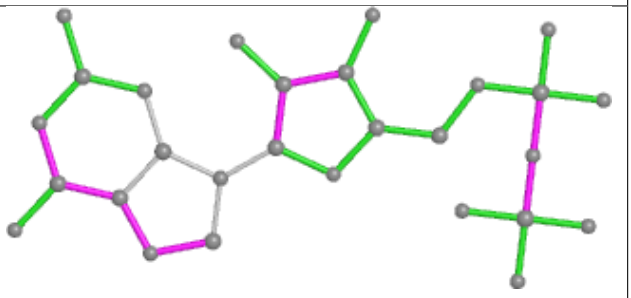
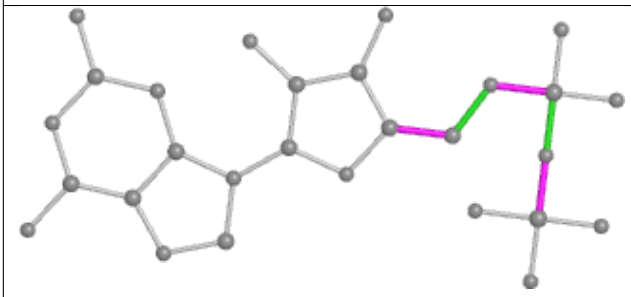
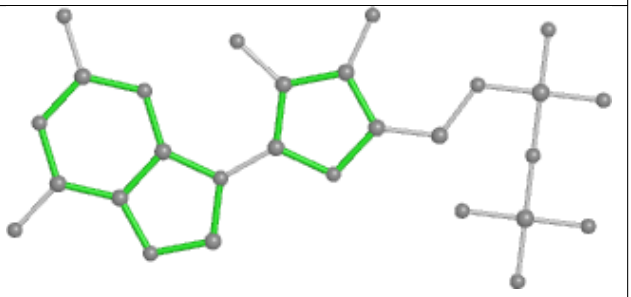


Rings

Ligand GDP BC 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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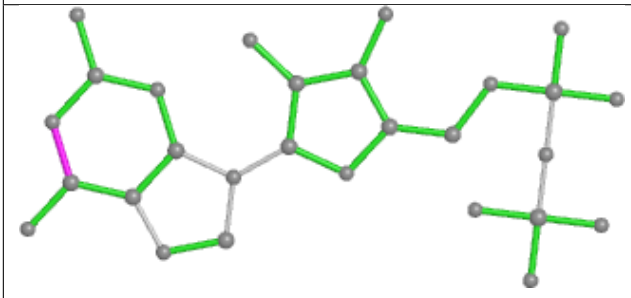
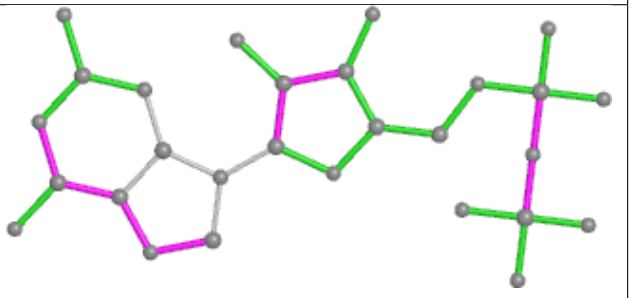
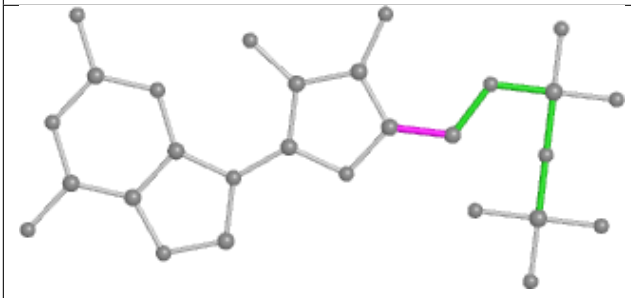
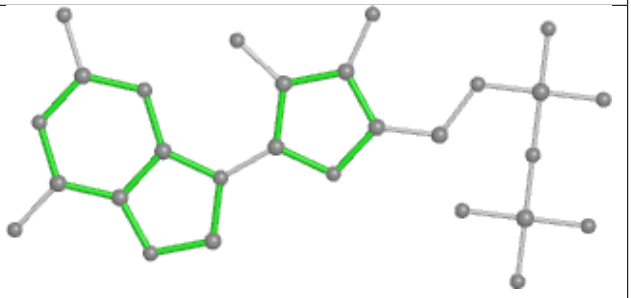
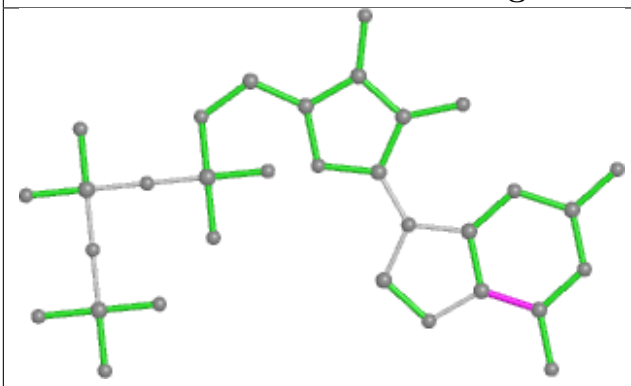
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP DD 501



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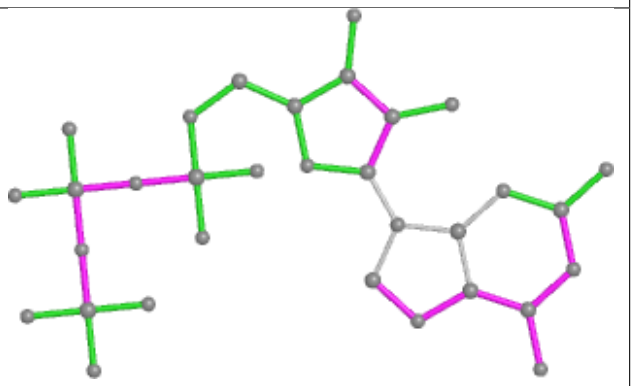

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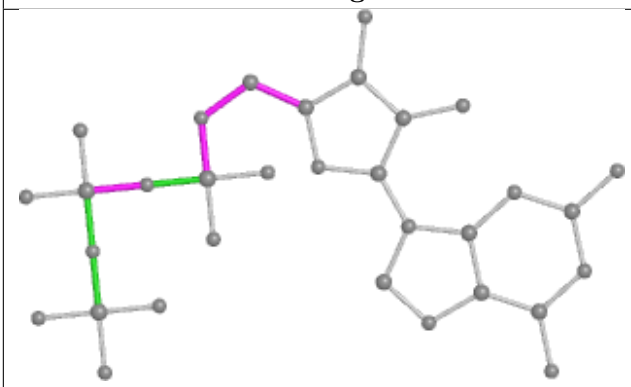

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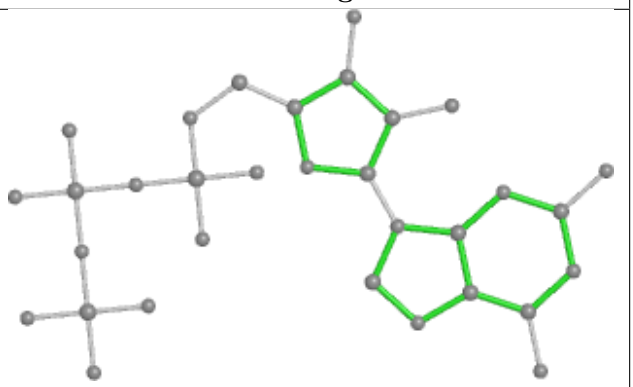
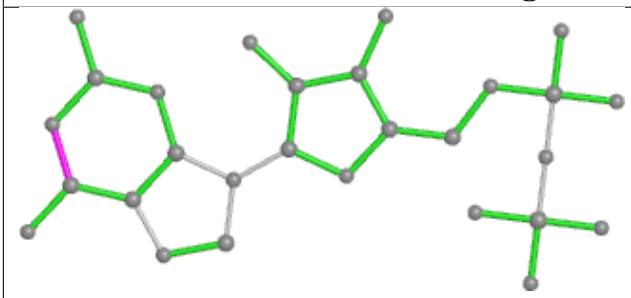


Rings

Ligand GDP II 501



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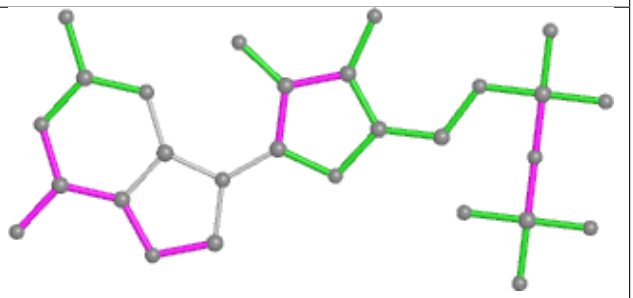
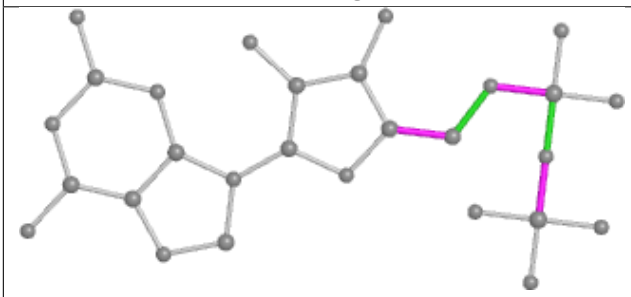


Bond angles



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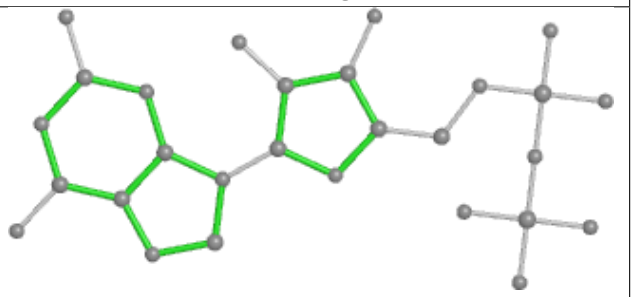

Rings

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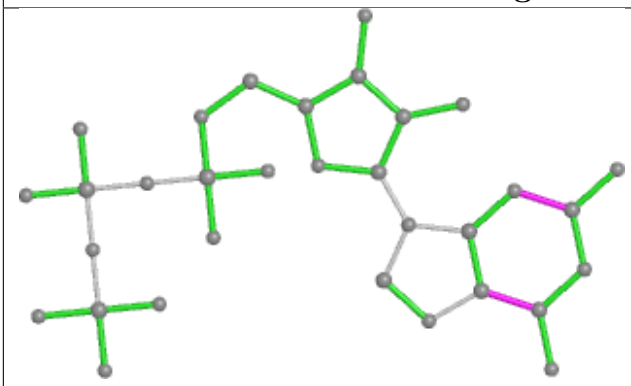

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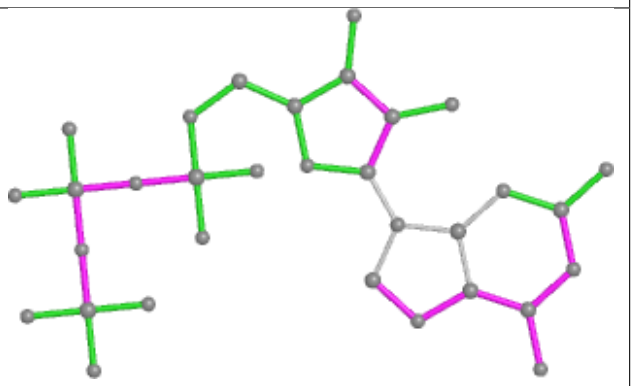

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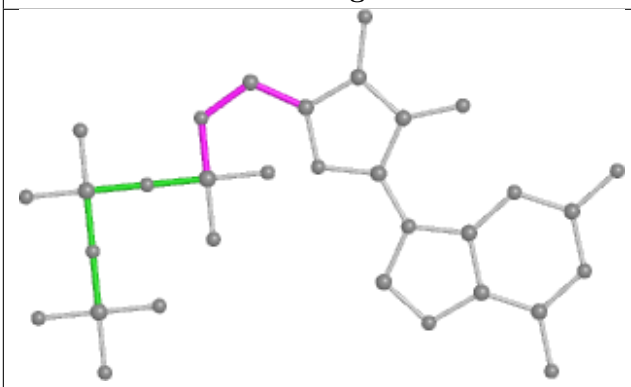

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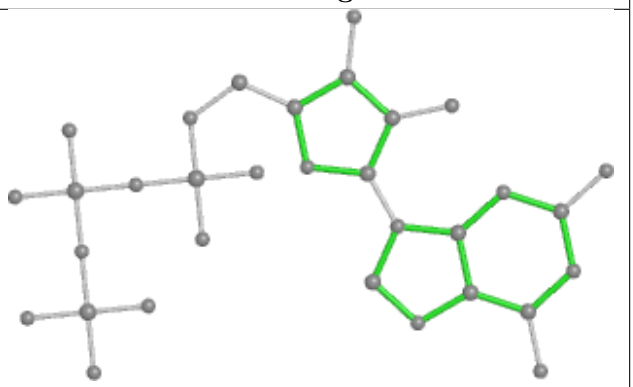

Rings

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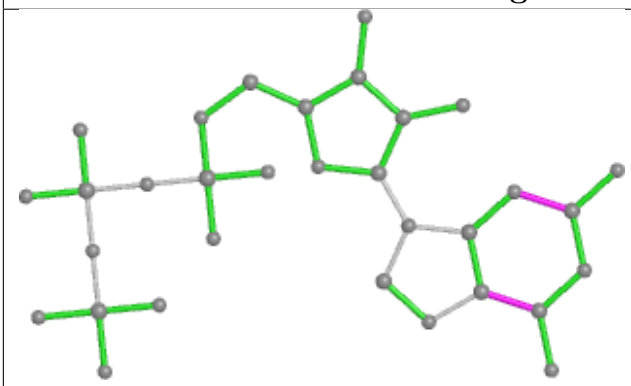

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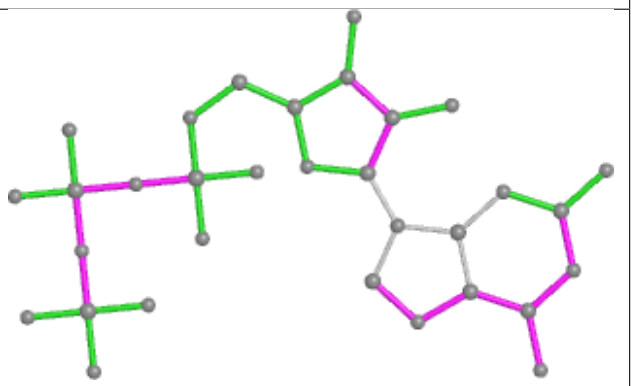
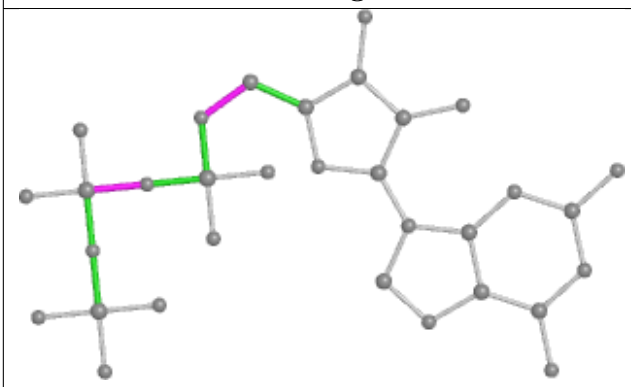


Bond angles



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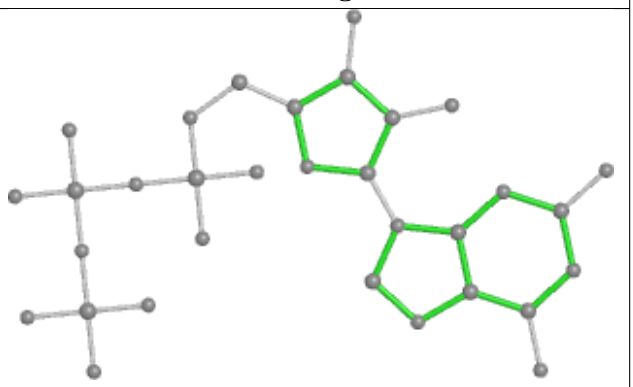
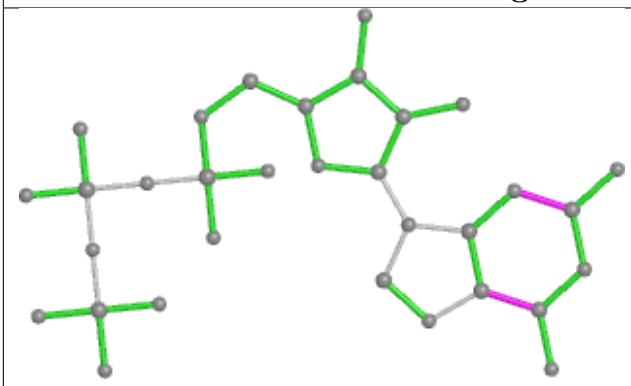


Rings

Ligand GTP LD 501



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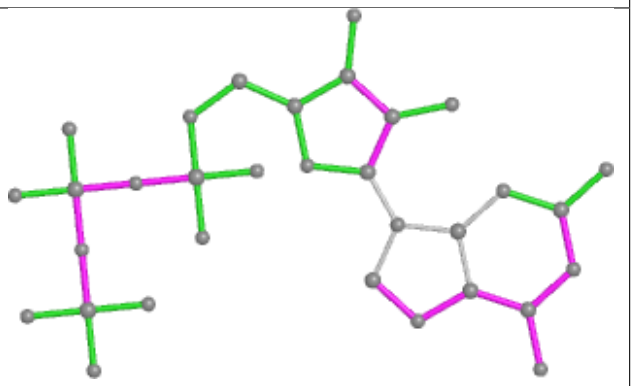

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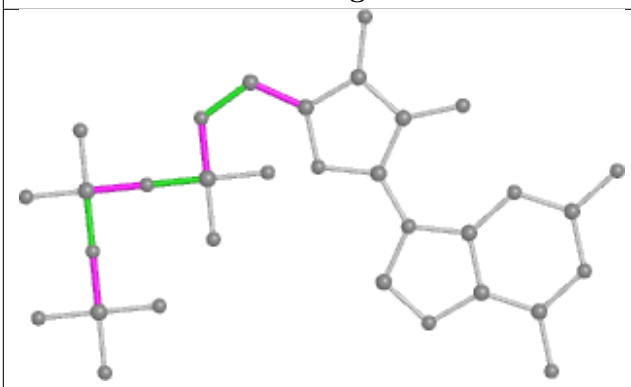

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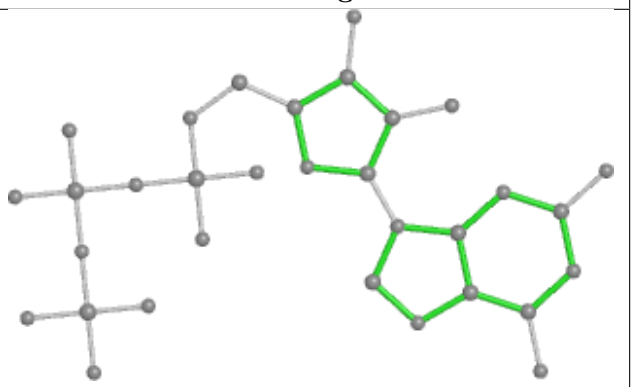
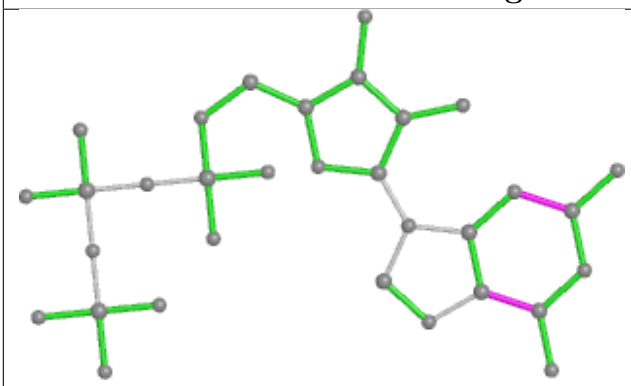
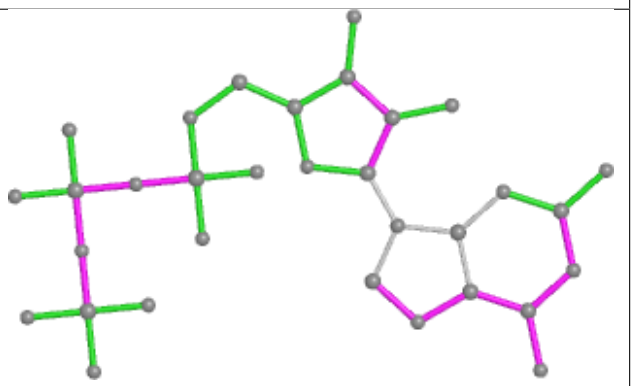


Rings

Ligand GTP MD 501



Bond lengths



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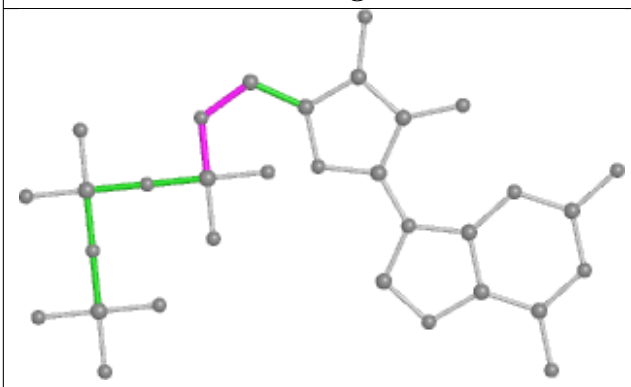
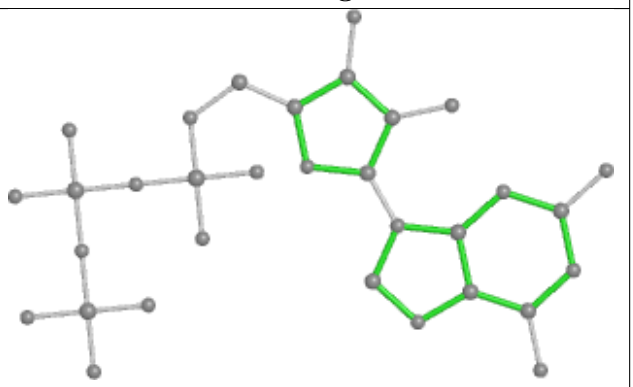
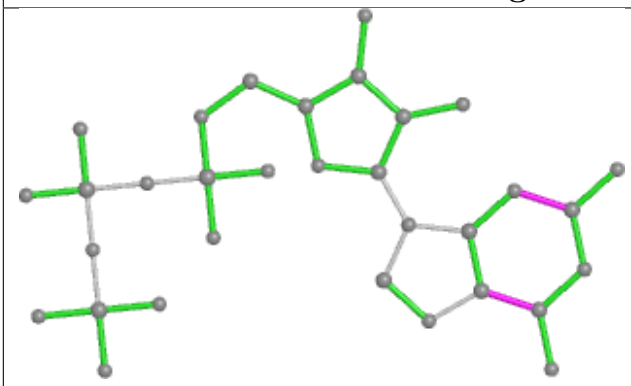


Torsions



Rings

Ligand GTP CD 501



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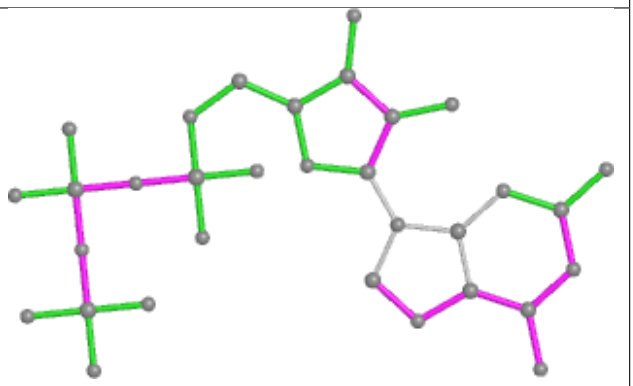

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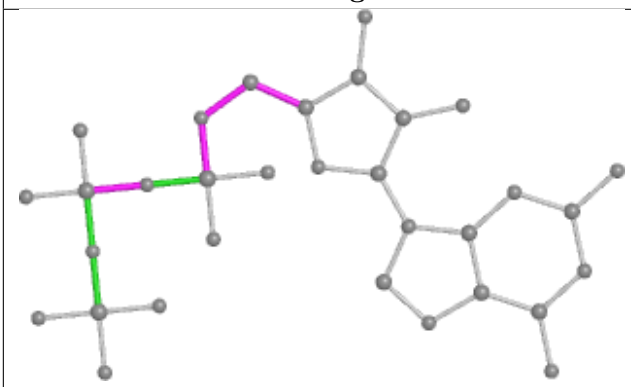

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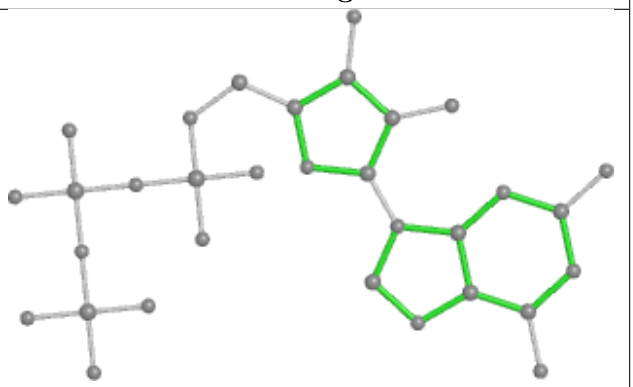
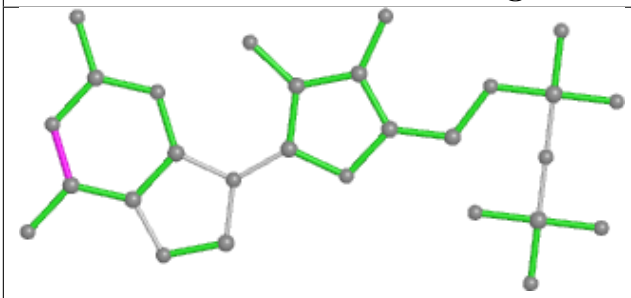


Rings

Ligand GDP AK 501



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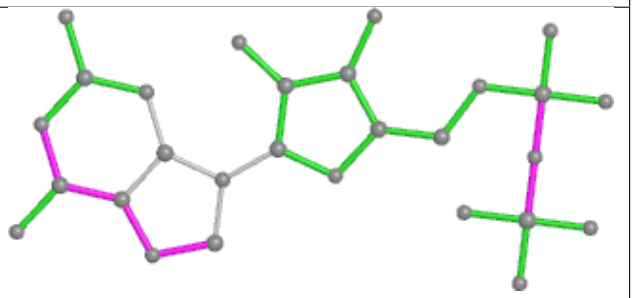

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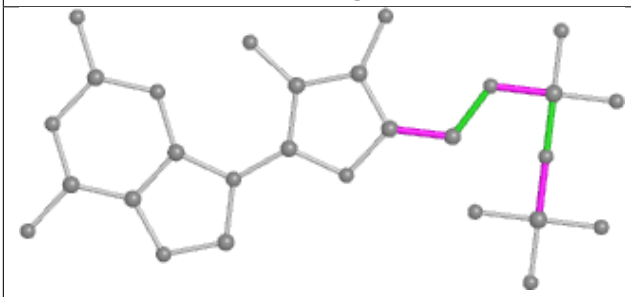

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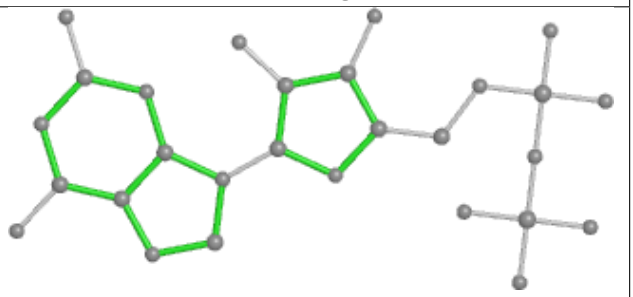

Rings

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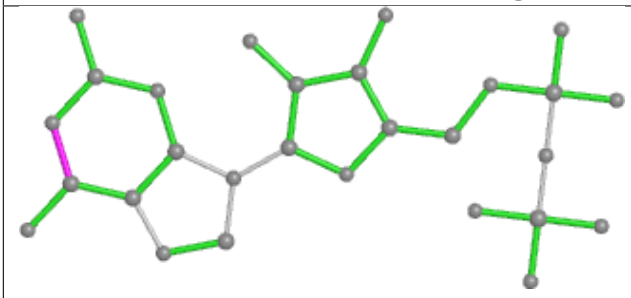

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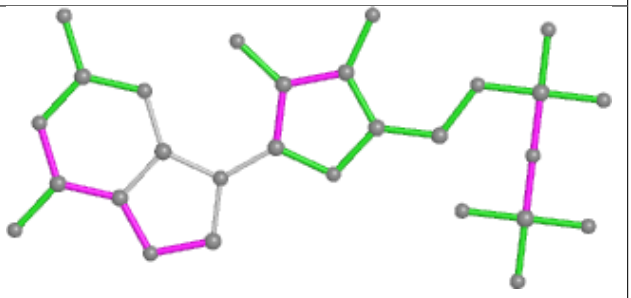

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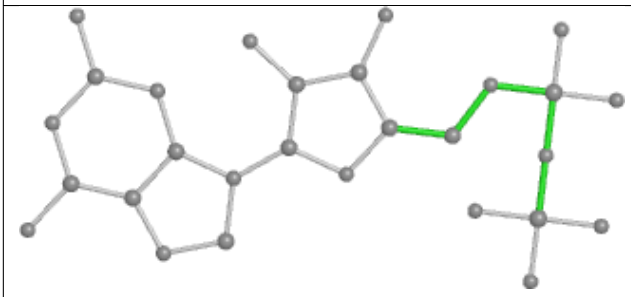

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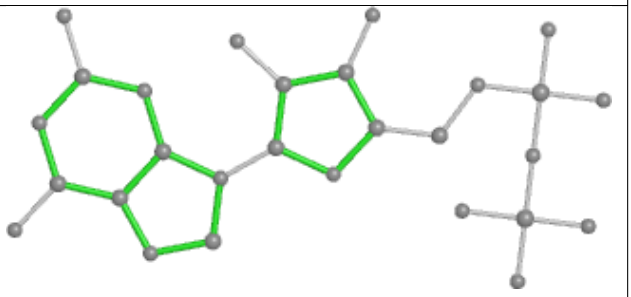
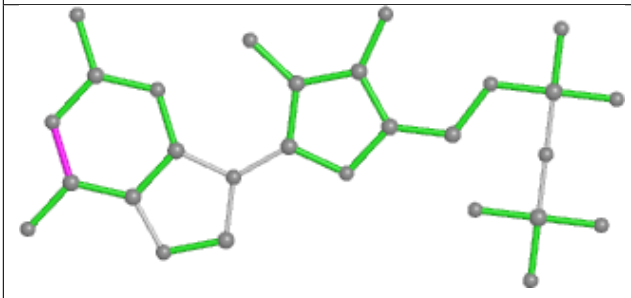


Rings

Ligand GDP EA 501



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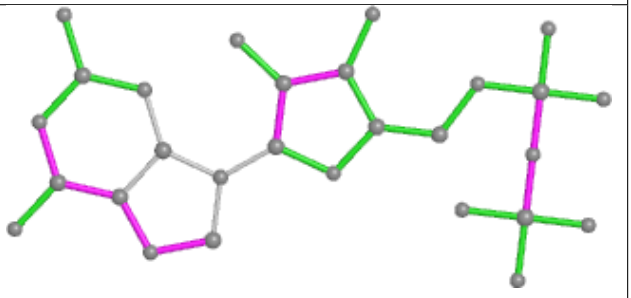

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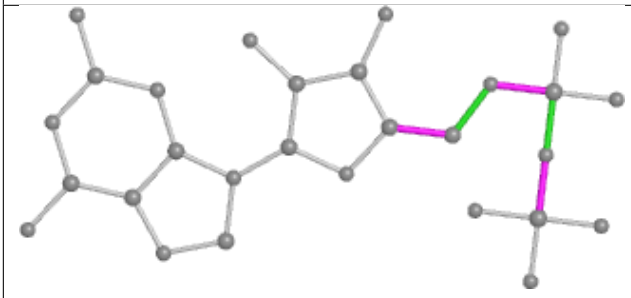

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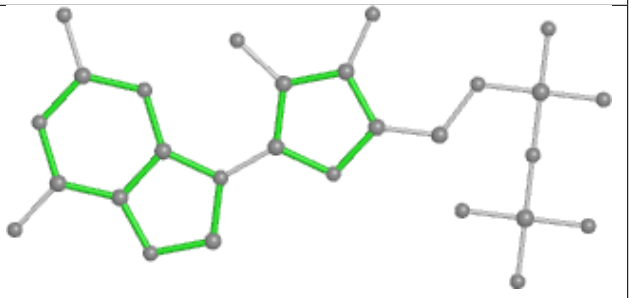

Rings

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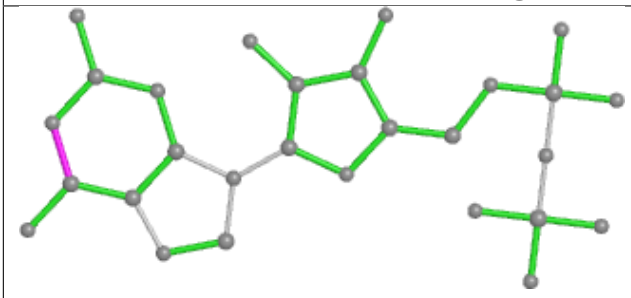

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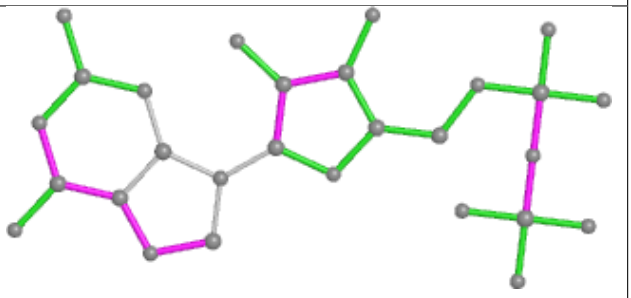

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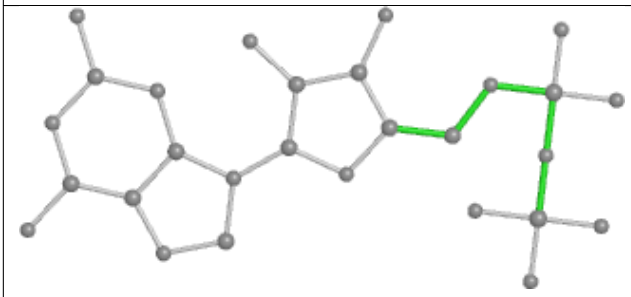

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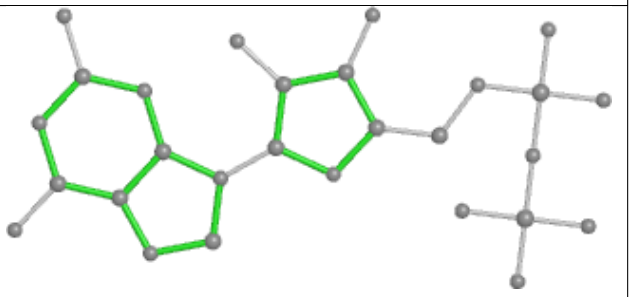
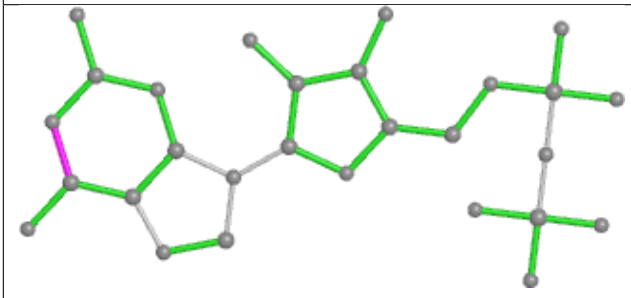


Rings

Ligand GDP HE 501



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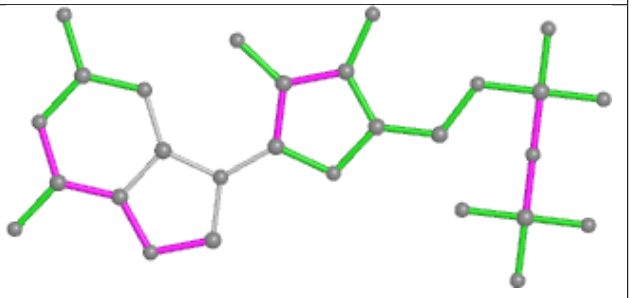

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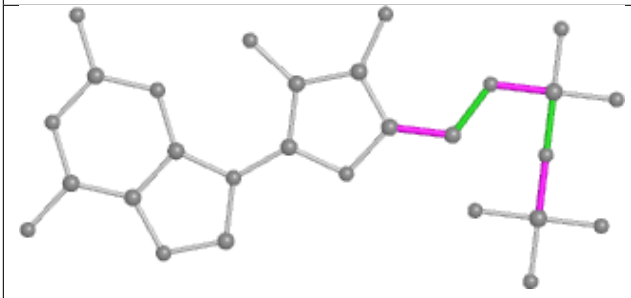

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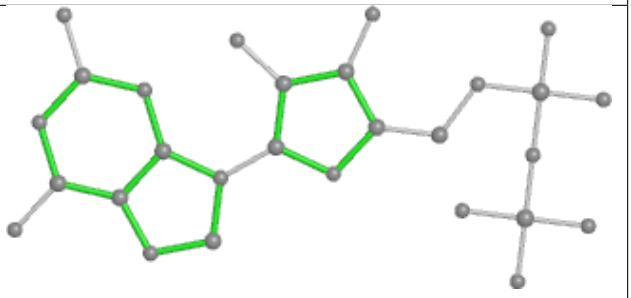
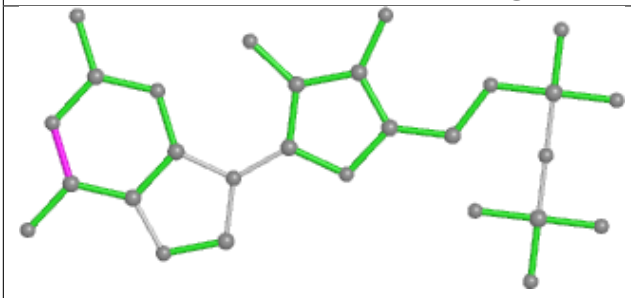
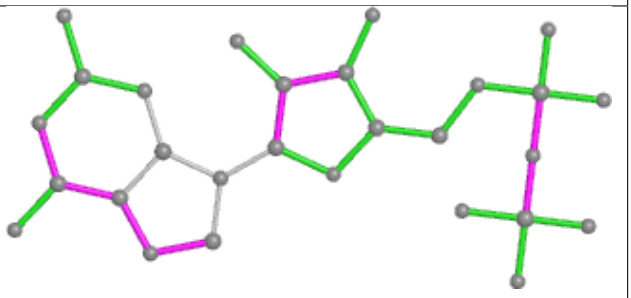
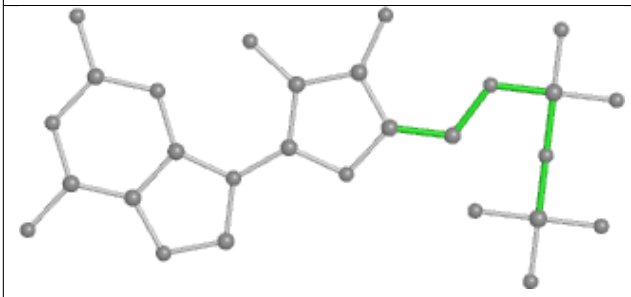
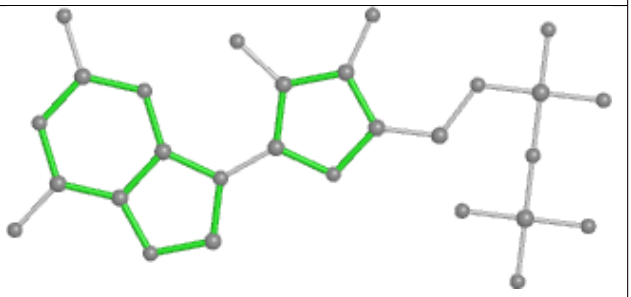


Rings

Ligand GDP CA 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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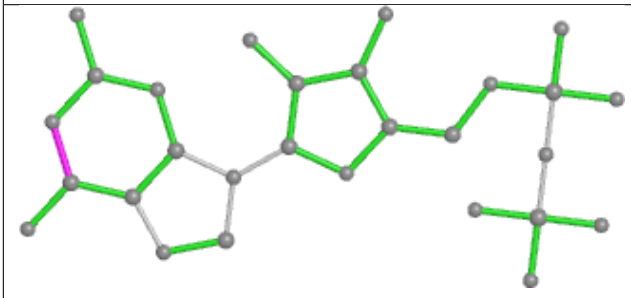
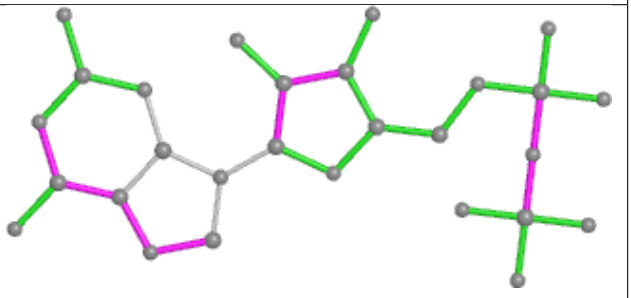
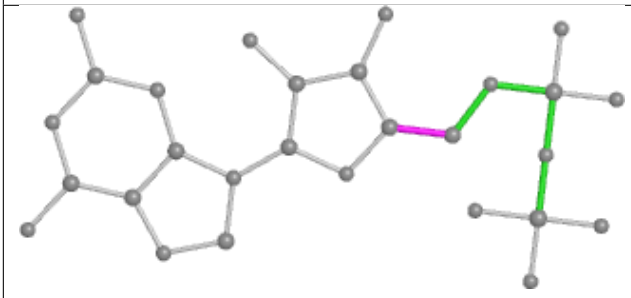
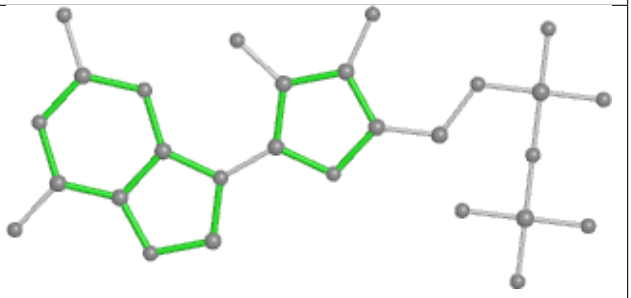
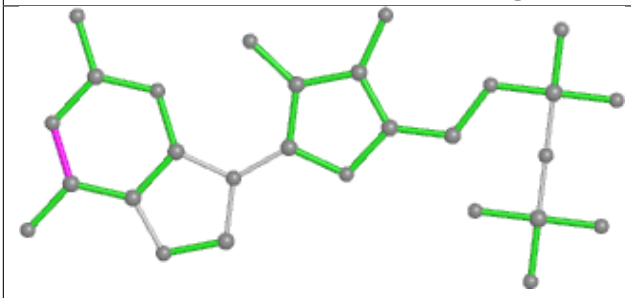
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP DE 501



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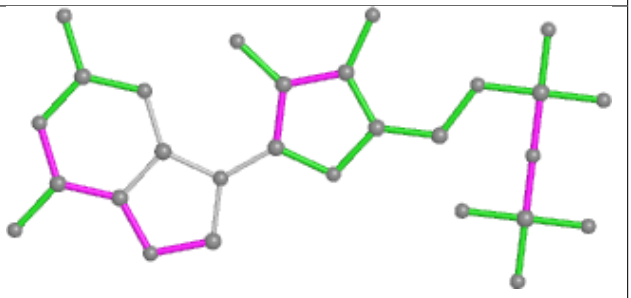

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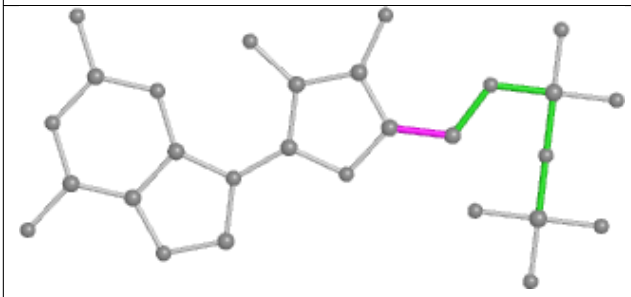

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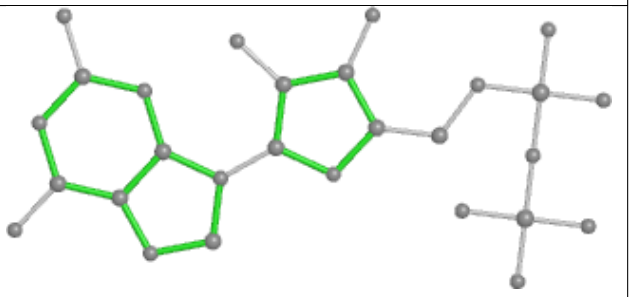
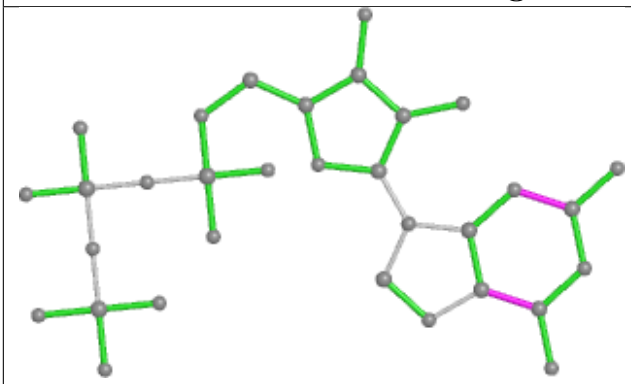


Rings

Ligand GTP GD 501



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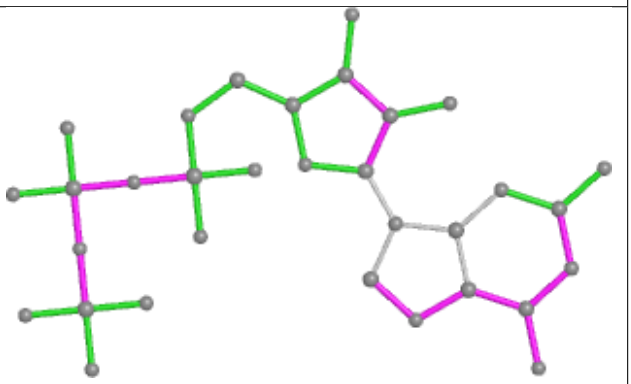

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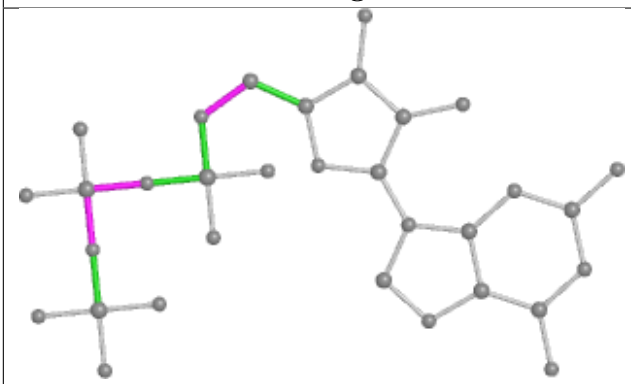

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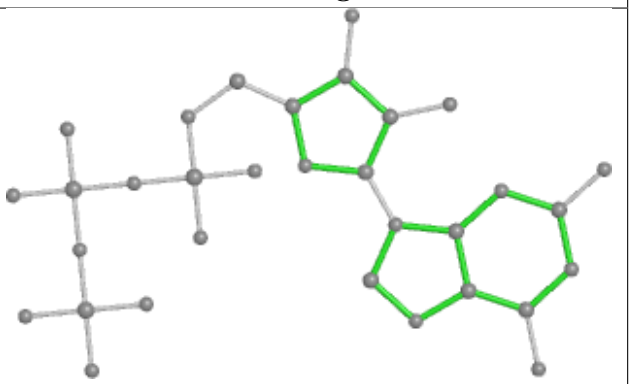
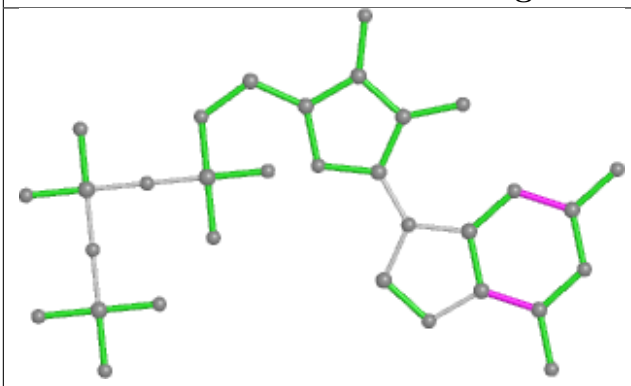


Rings

Ligand GTP IH 501



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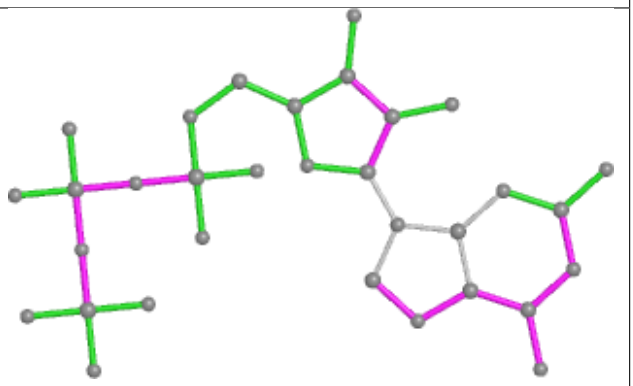

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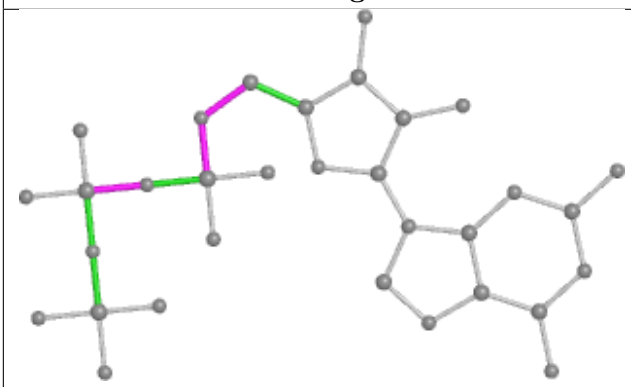

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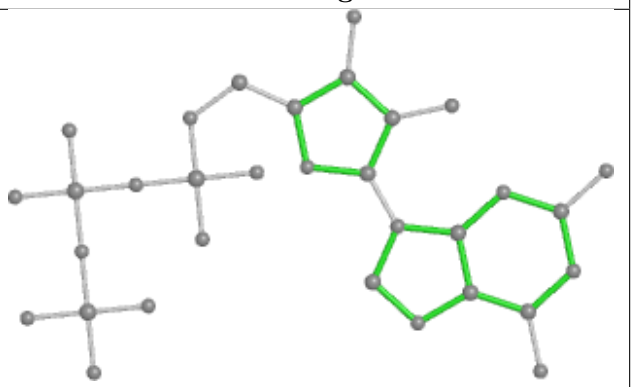
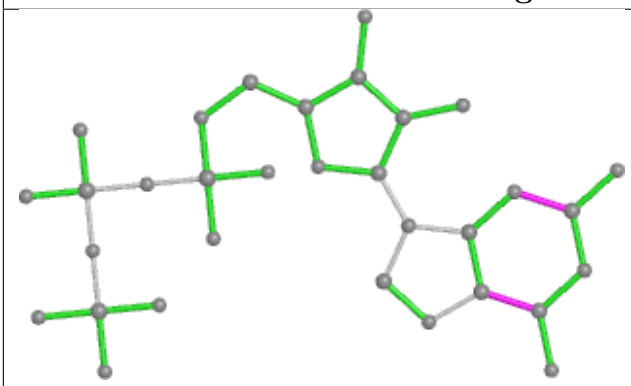


Rings

Ligand GTP JF 501



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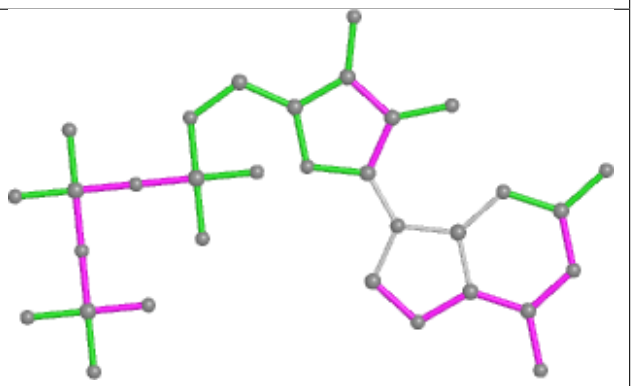

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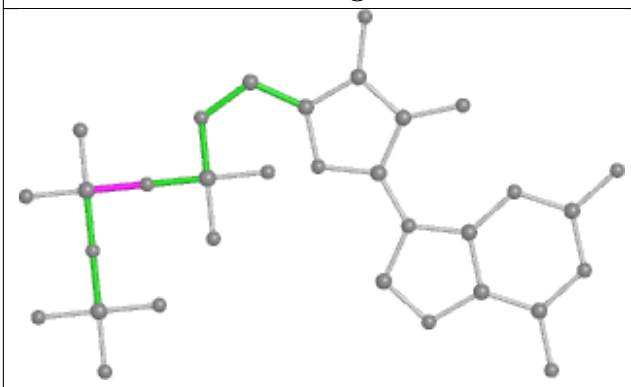

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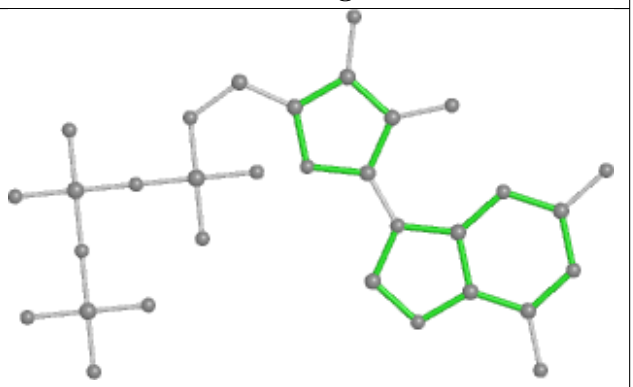
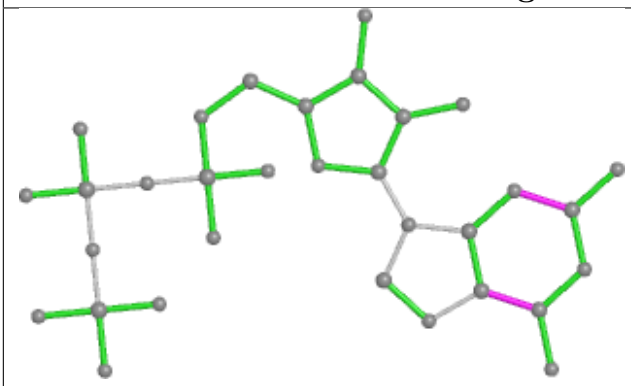


Rings

Ligand GTP IF 501



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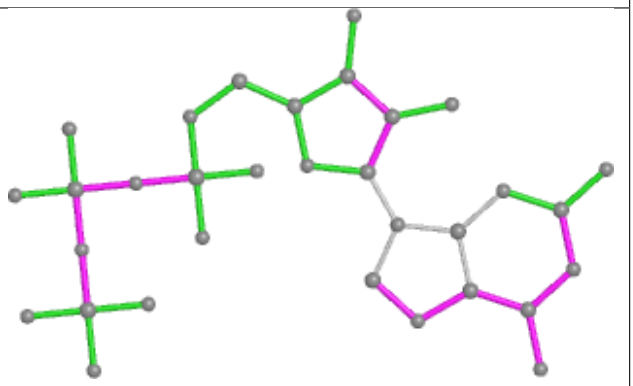

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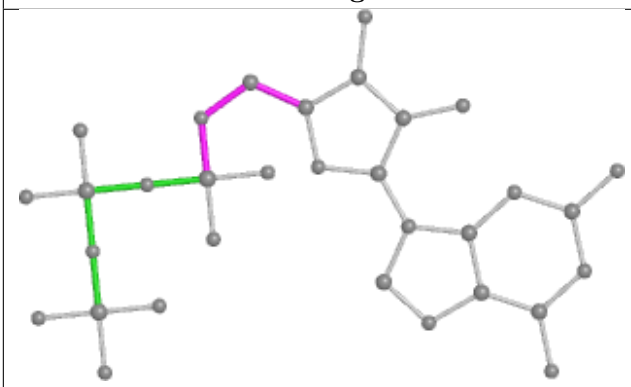

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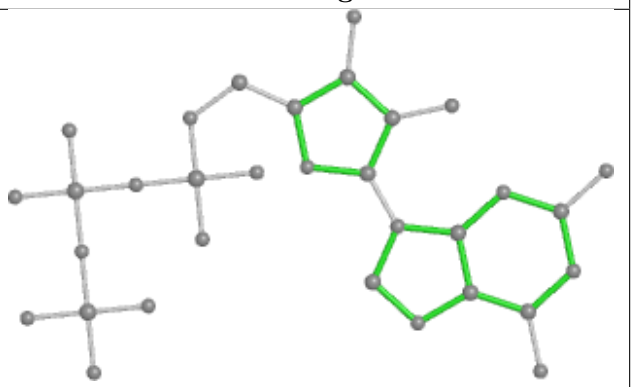

Rings

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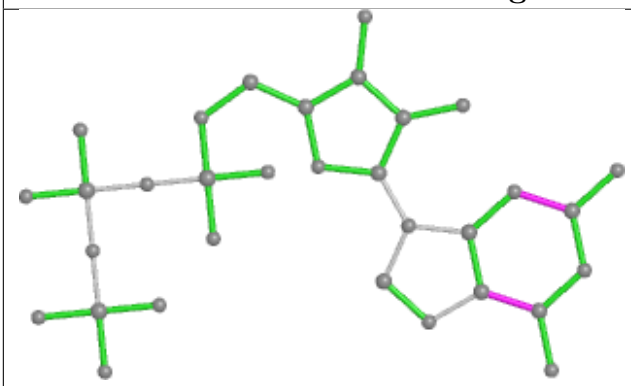

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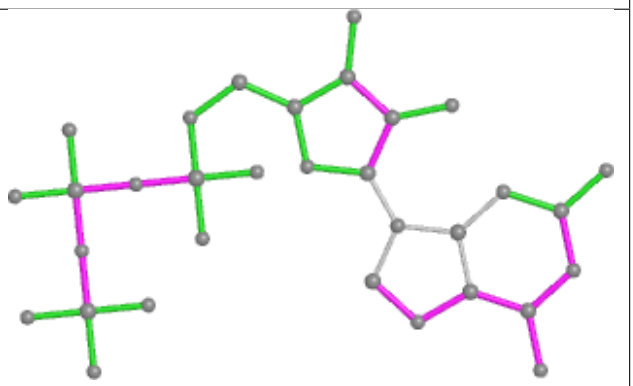

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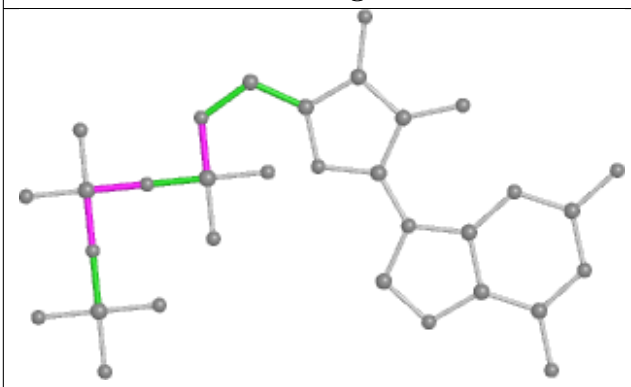

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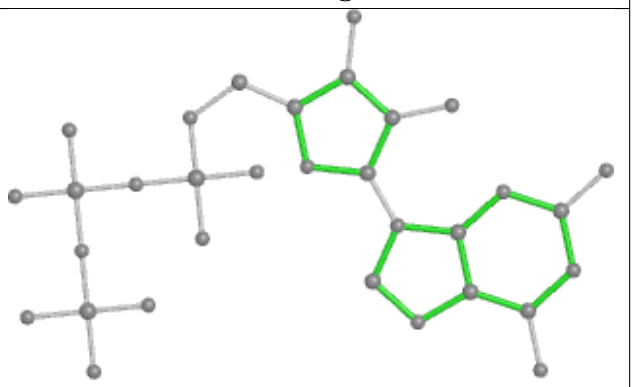
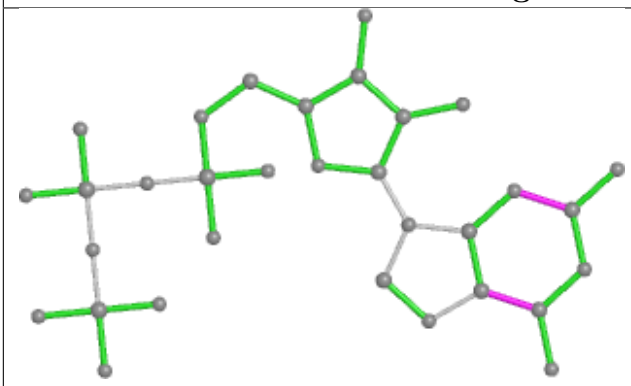
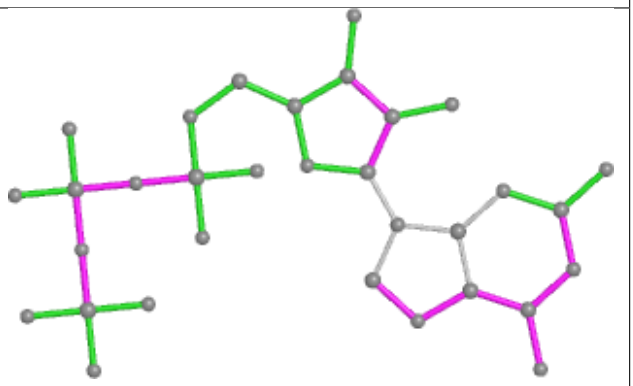


Rings

Ligand GTP DJ 501



Bond lengths



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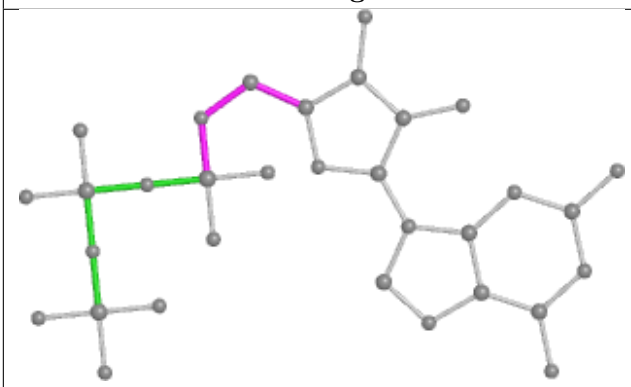
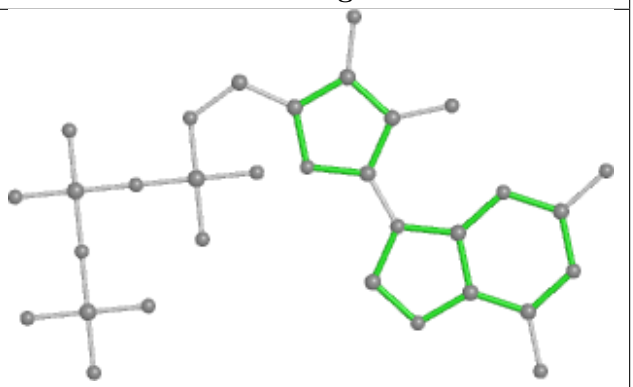
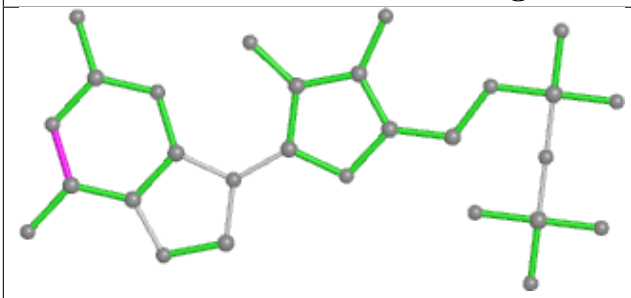


Torsions



Rings

Ligand GDP LG 501



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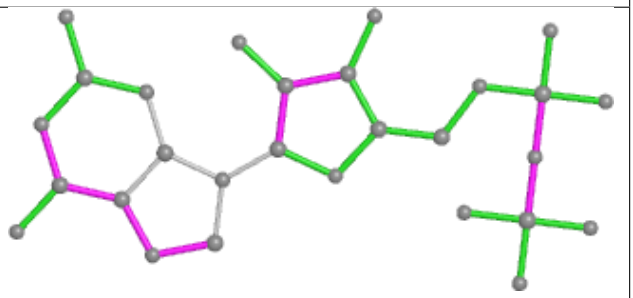

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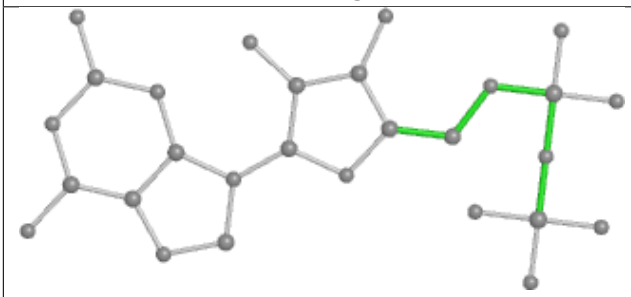

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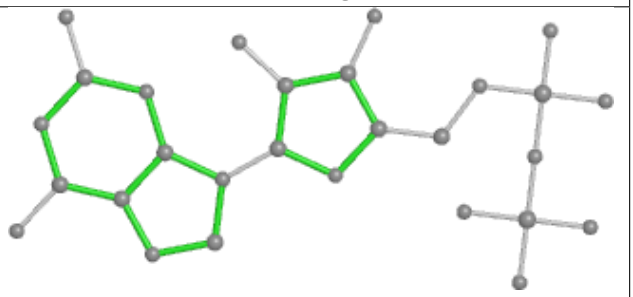
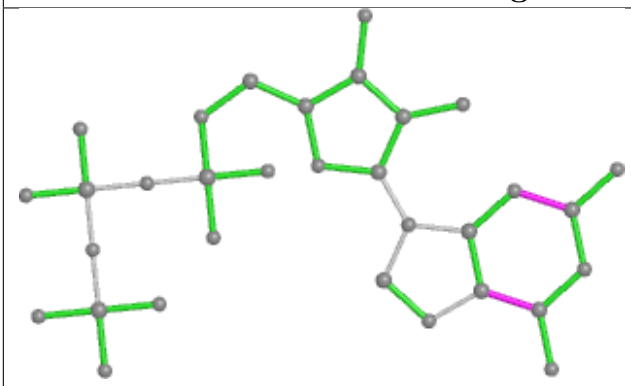


Rings

Ligand GTP KF 501



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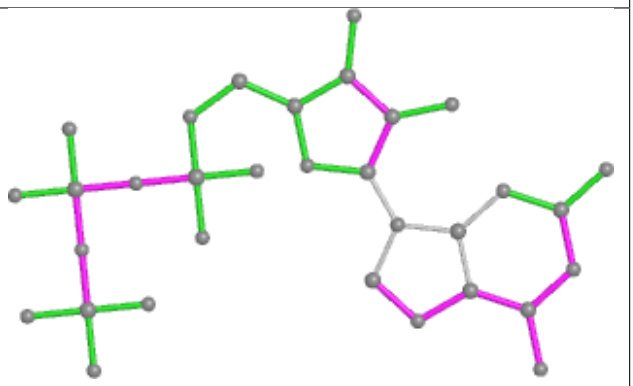

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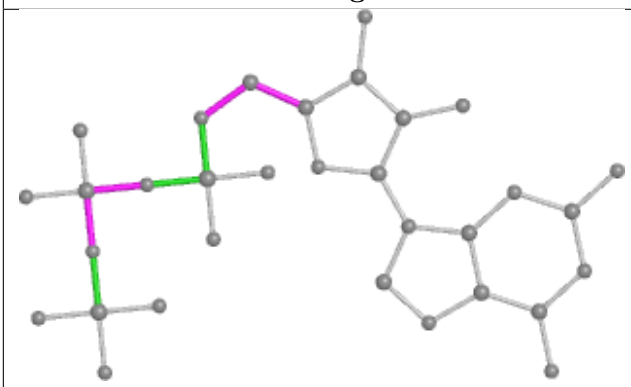

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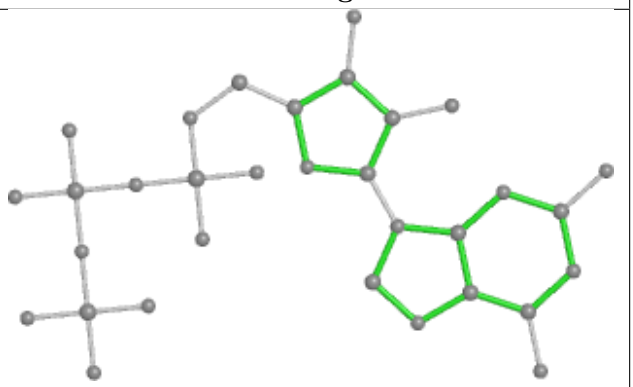
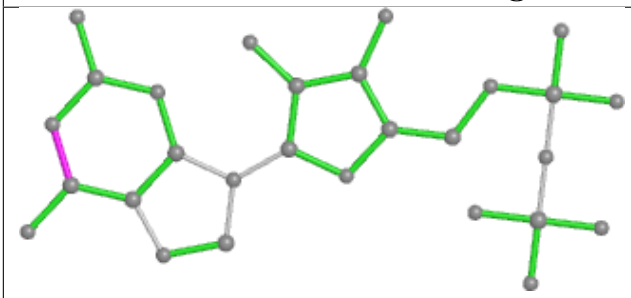


Rings

Ligand GDP JM 501



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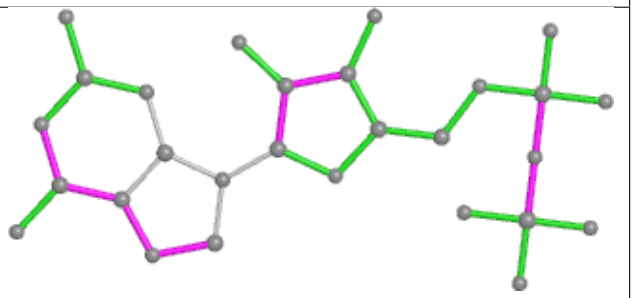

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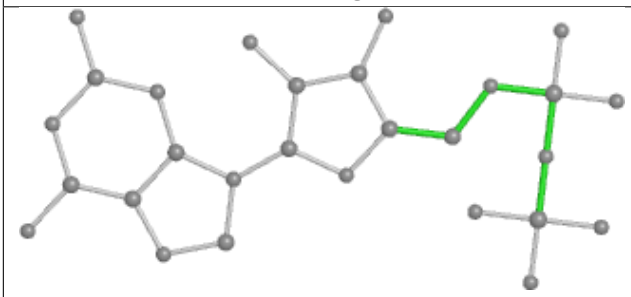

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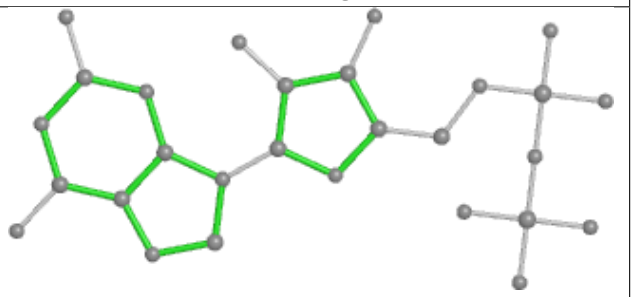
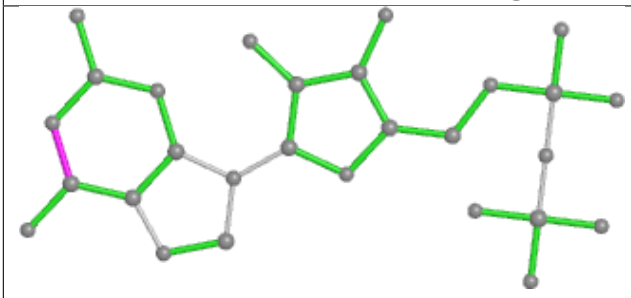
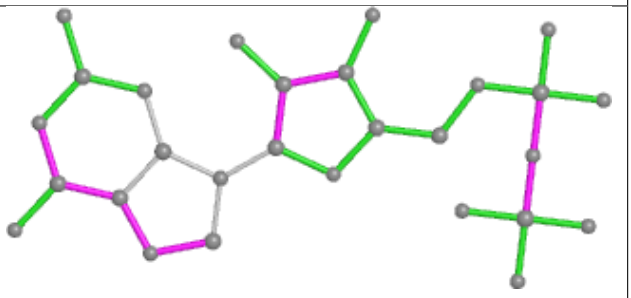
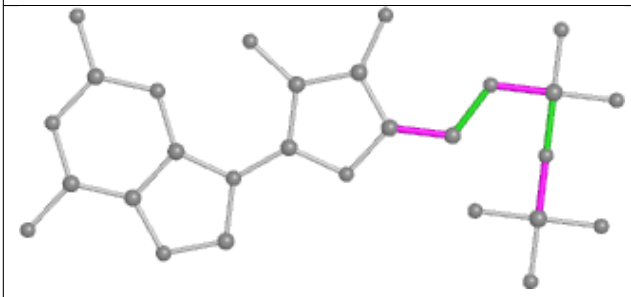
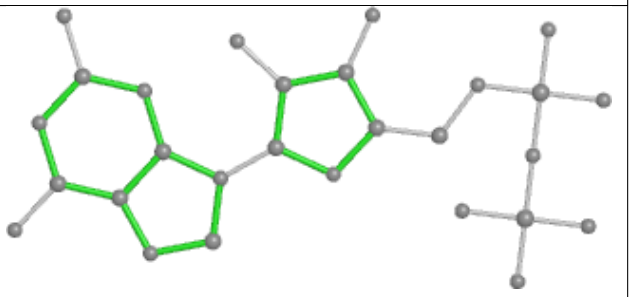


Rings

Ligand GDP BK 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

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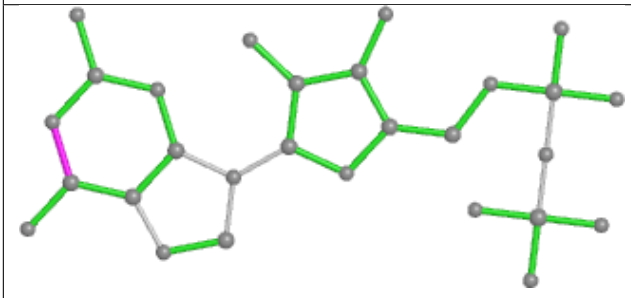
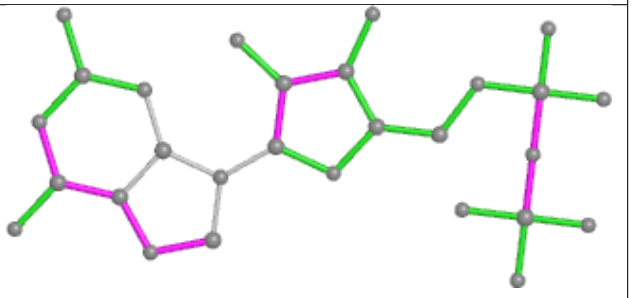
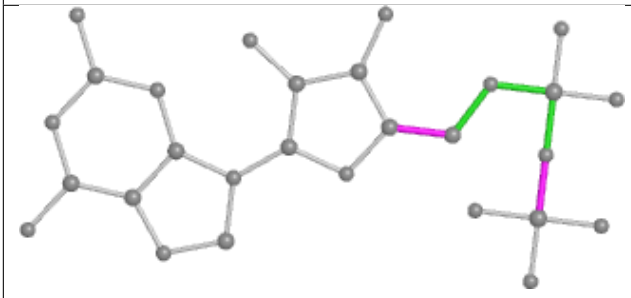
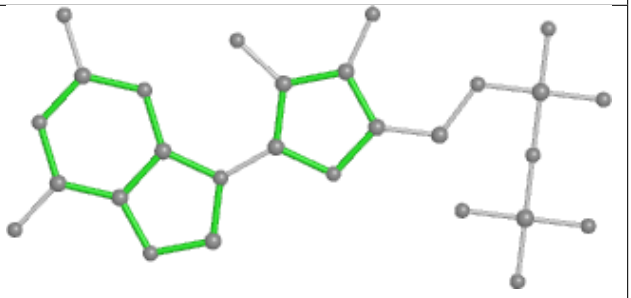
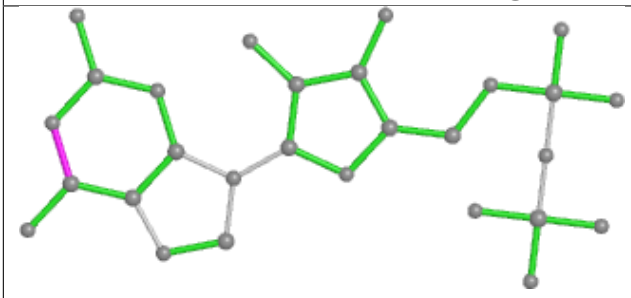
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP DG 501



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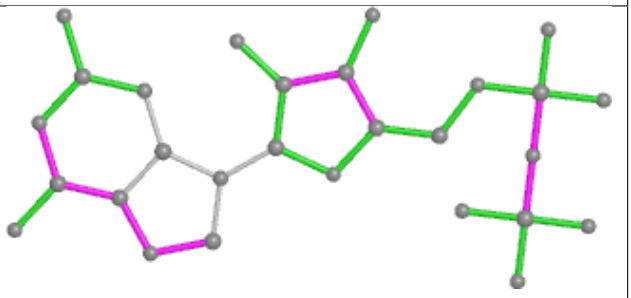

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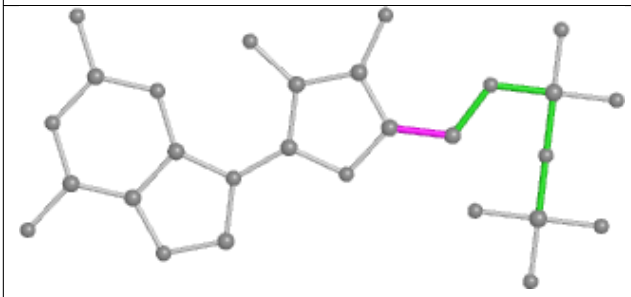

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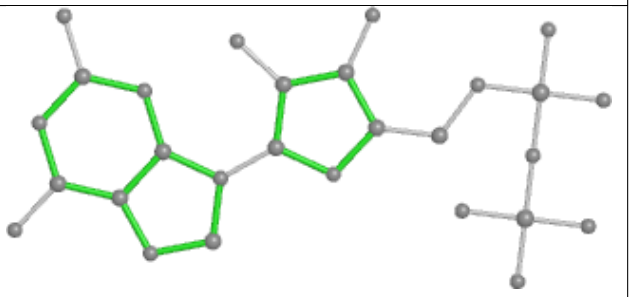
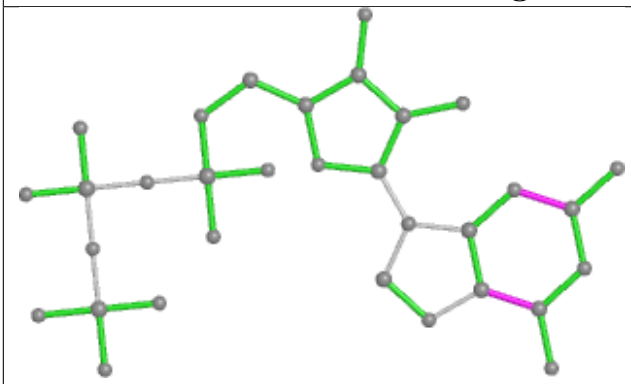


Rings

Ligand GTP HL 501



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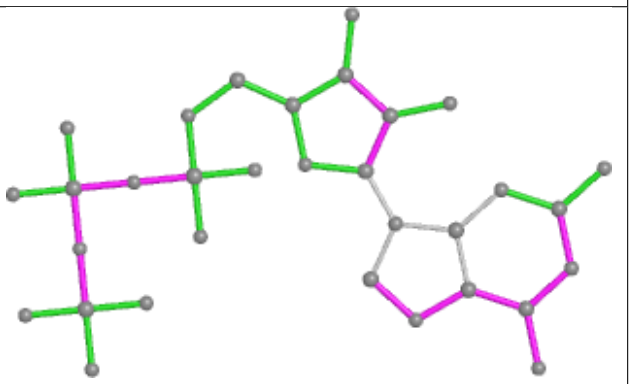

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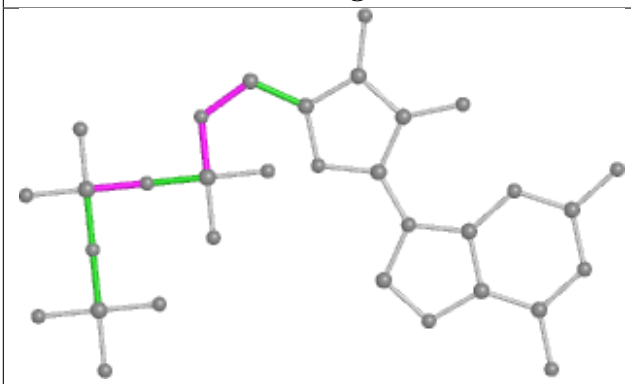

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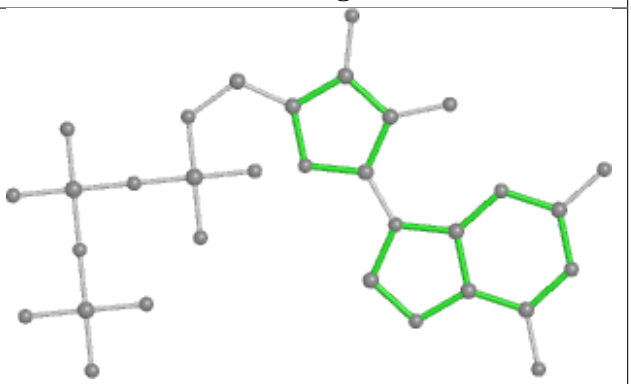
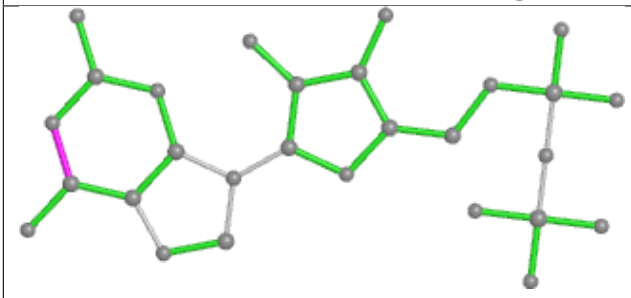


Rings

Ligand GDP IM 501



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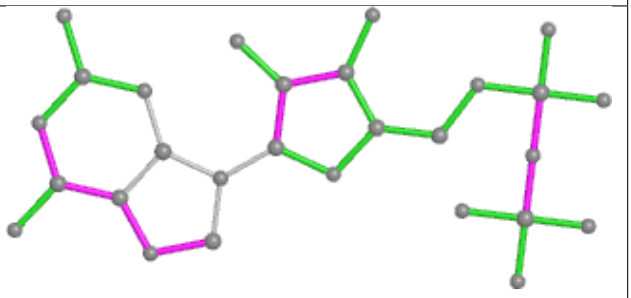

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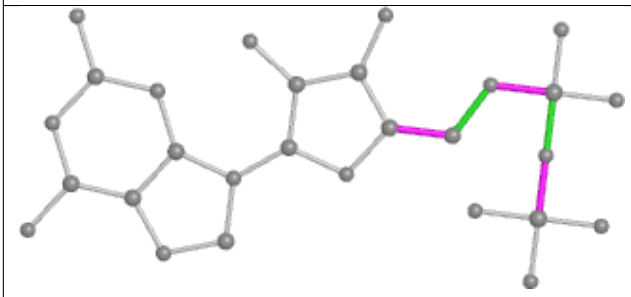

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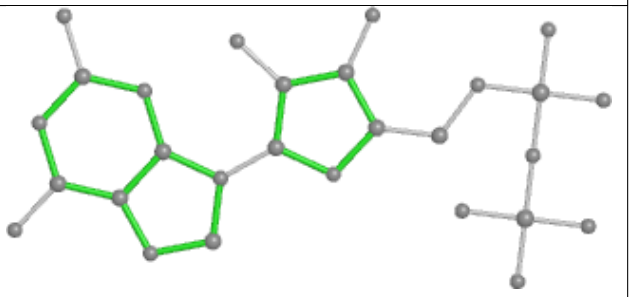
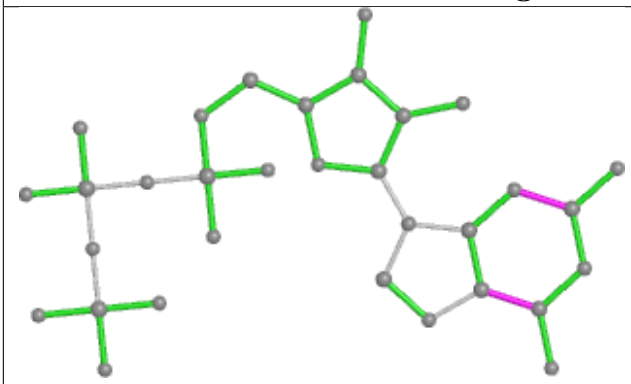


Rings

Ligand GTP HI 501



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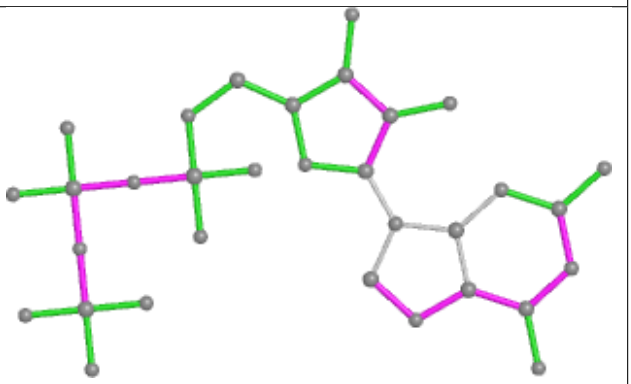

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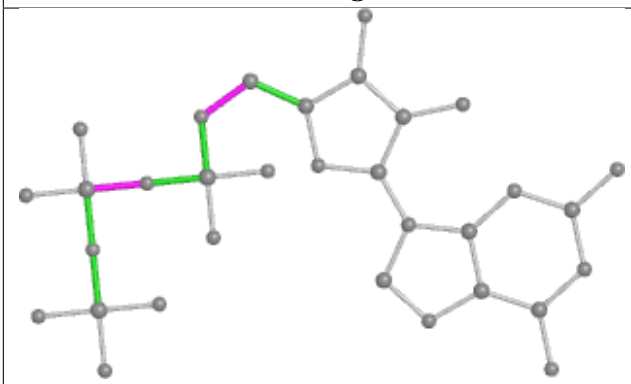

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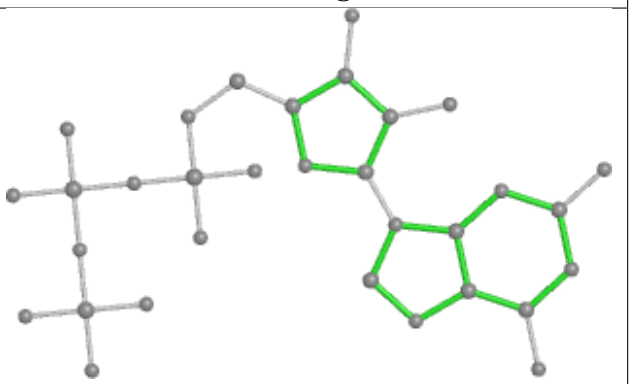
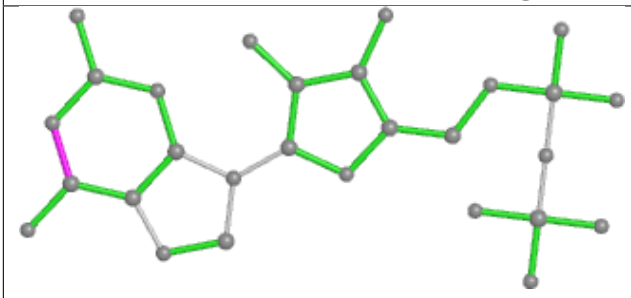
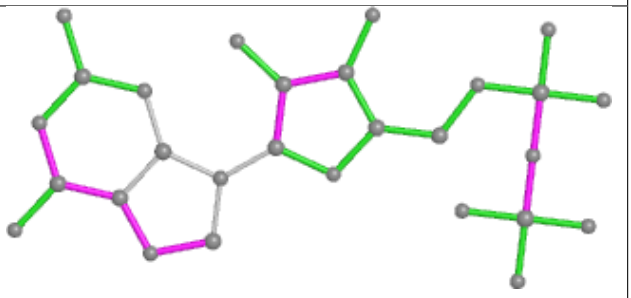
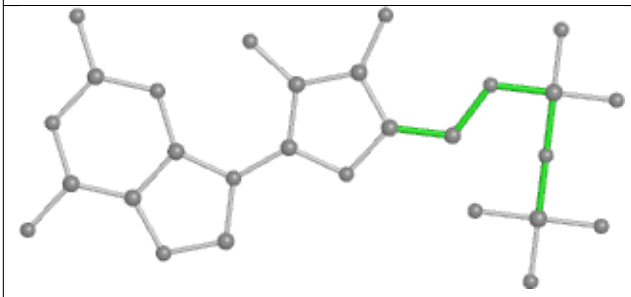
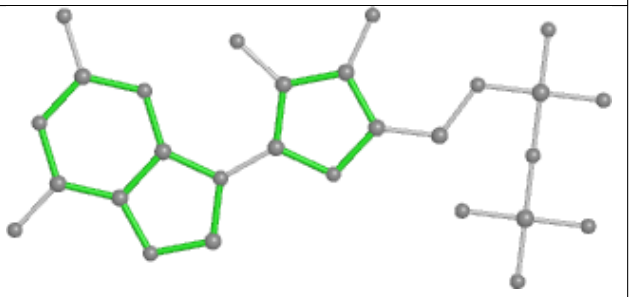
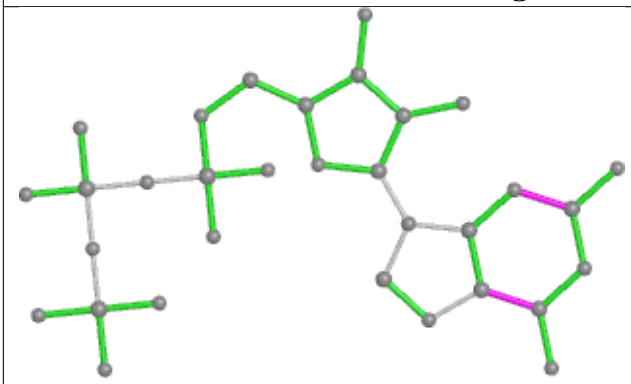
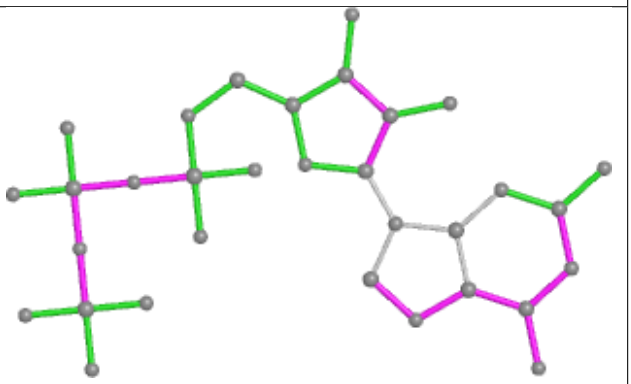
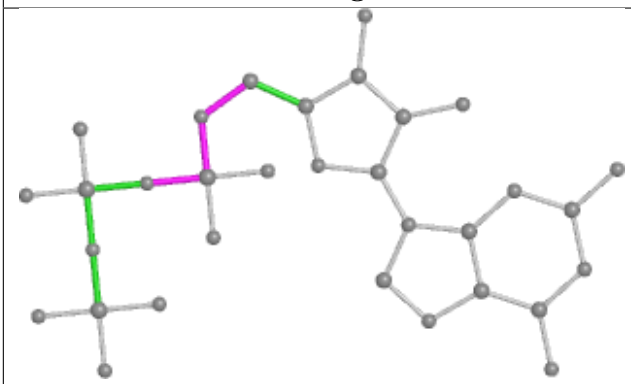
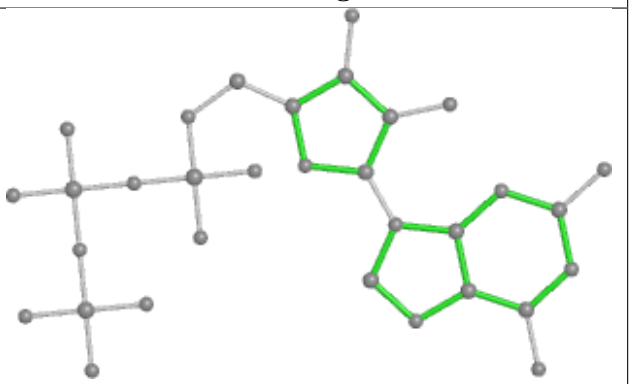
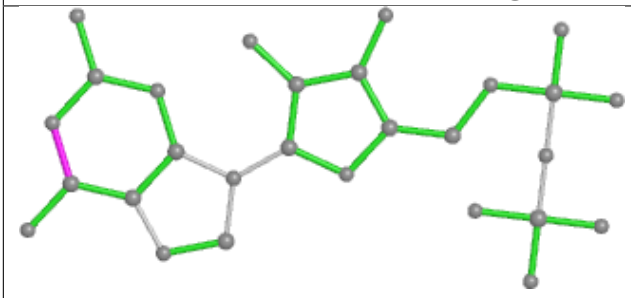


Rings

Ligand GDP LI 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP GL 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP GG 501



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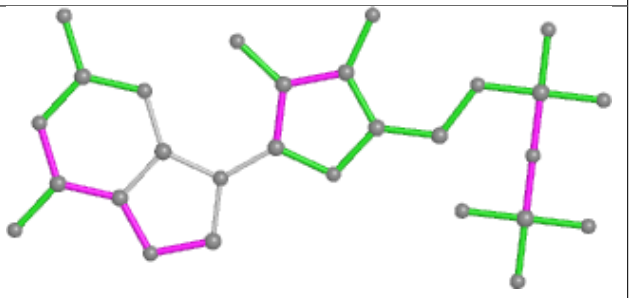

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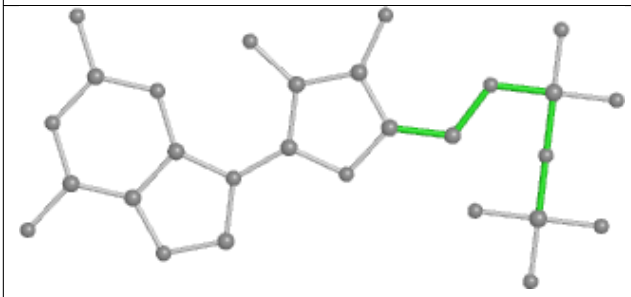

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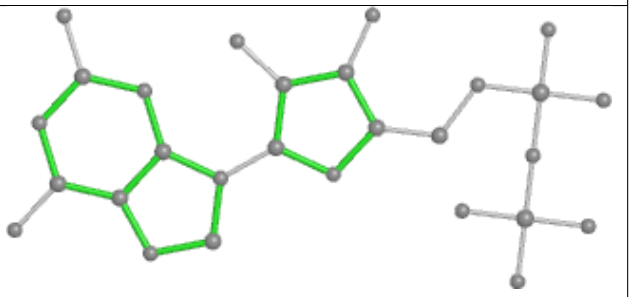
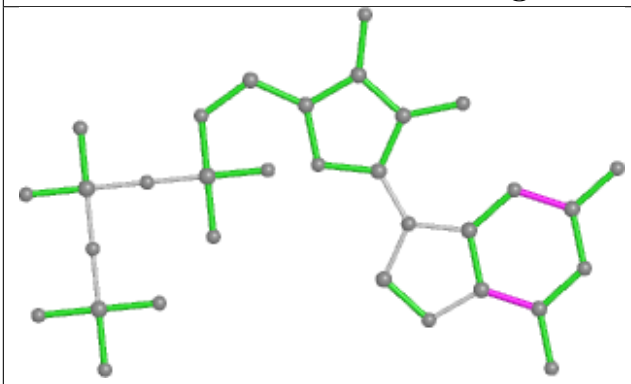


Rings

Ligand GTP DF 501



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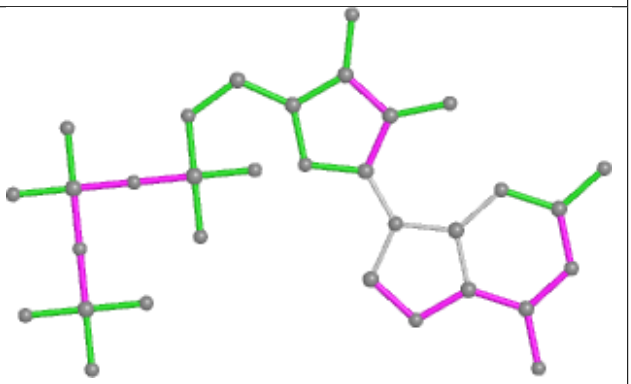
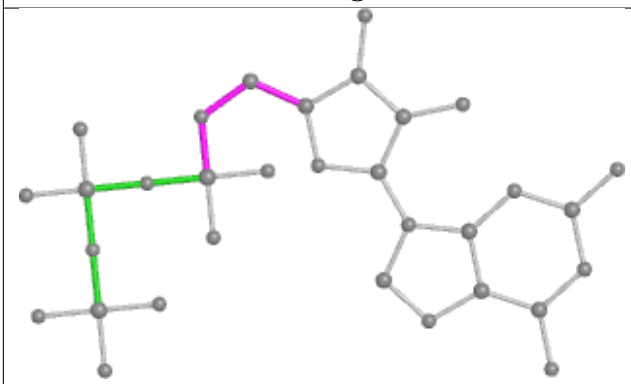


Bond angles



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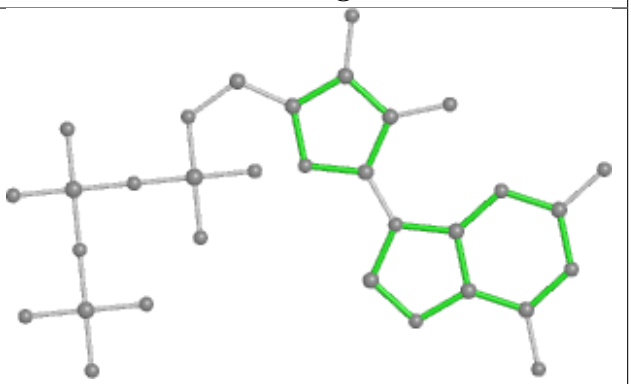
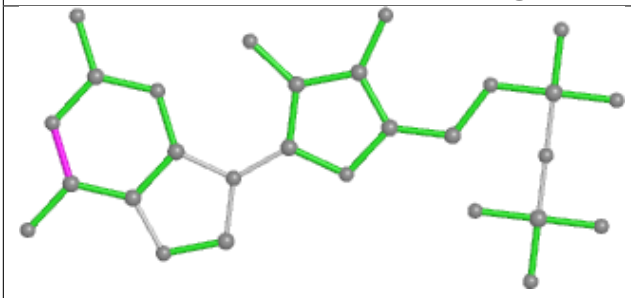
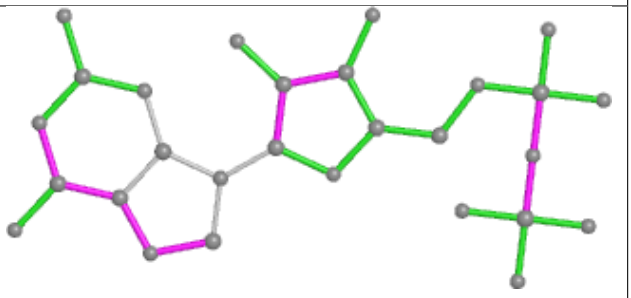
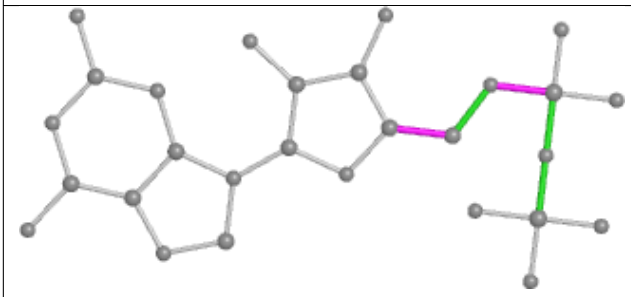
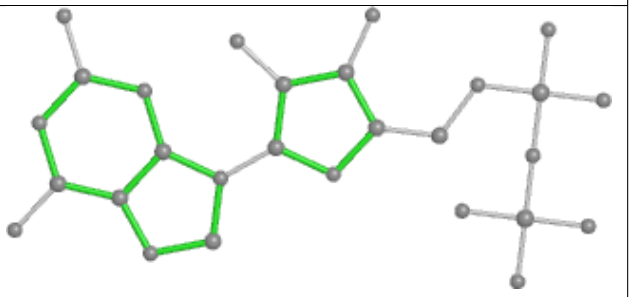
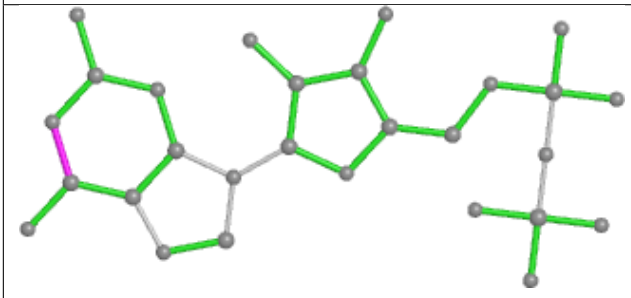
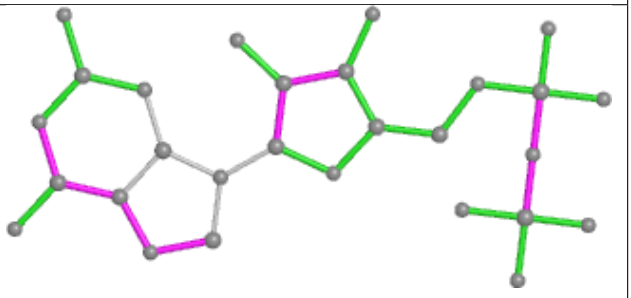
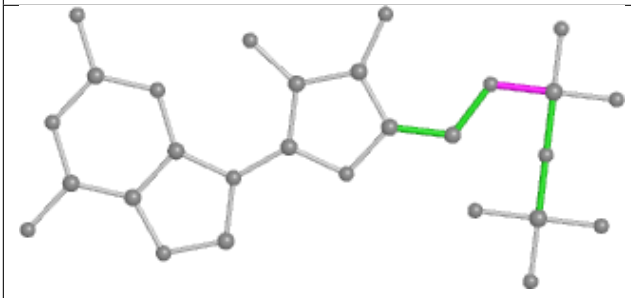
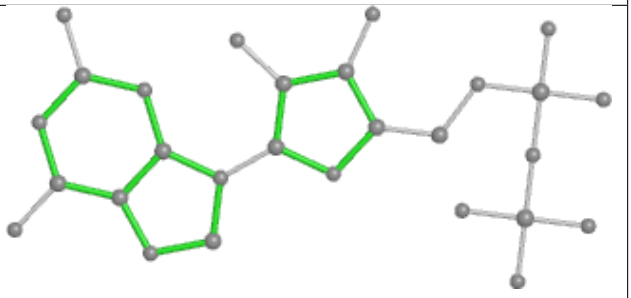


Rings

Ligand GDP MI 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP FE 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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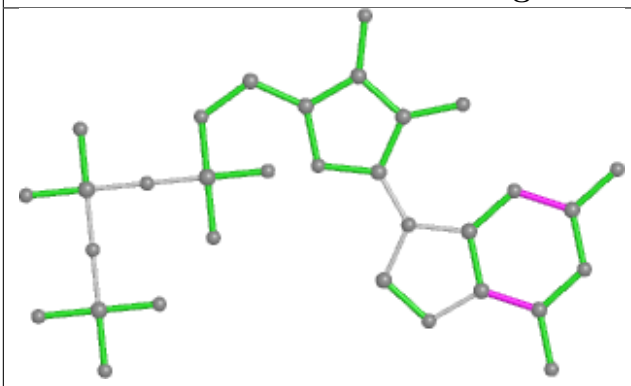

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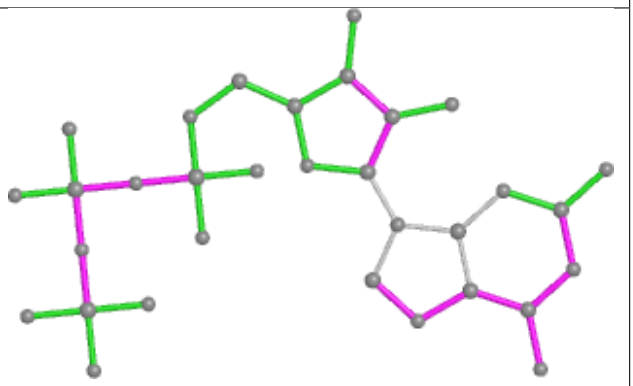

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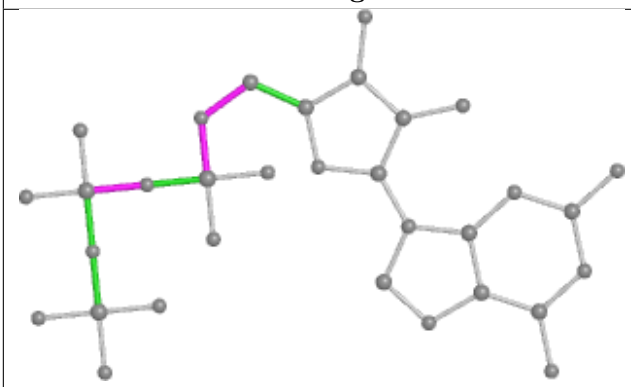

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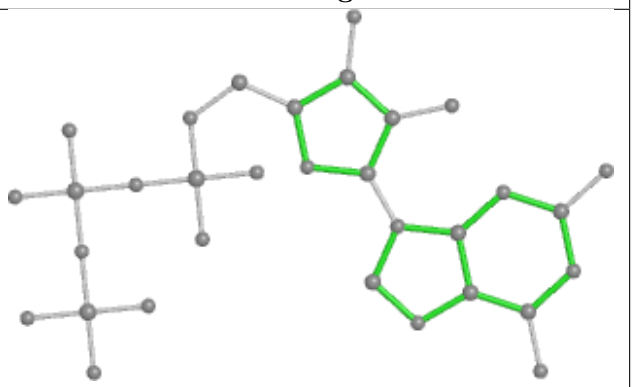

Rings

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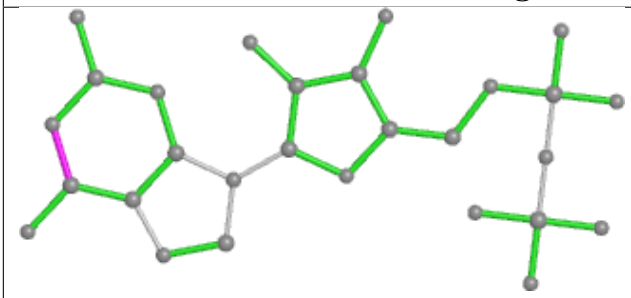

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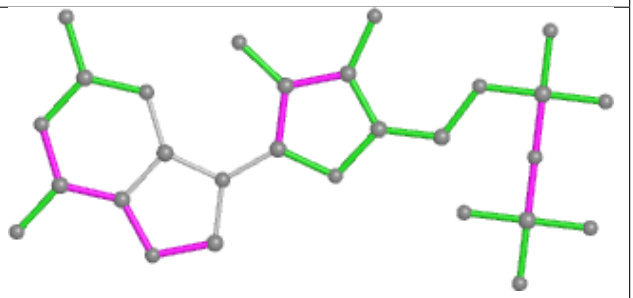

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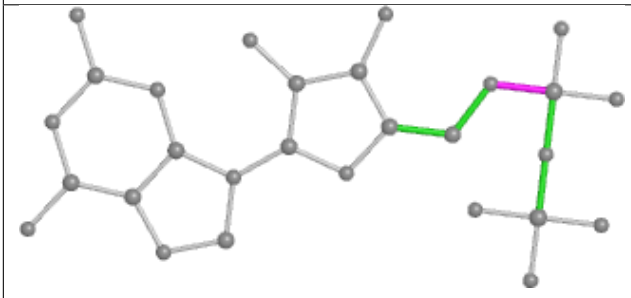

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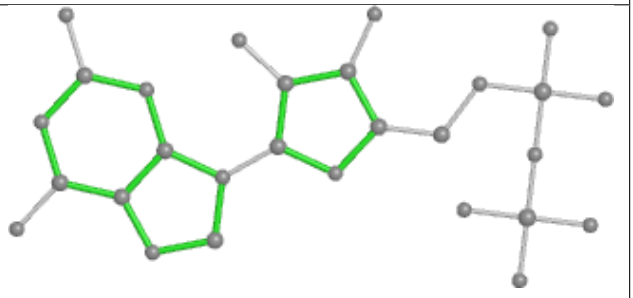

Rings

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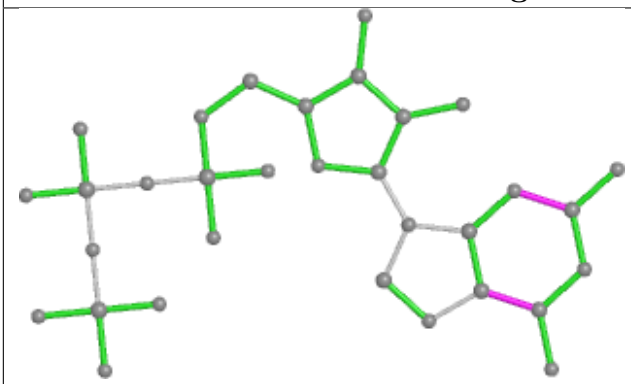

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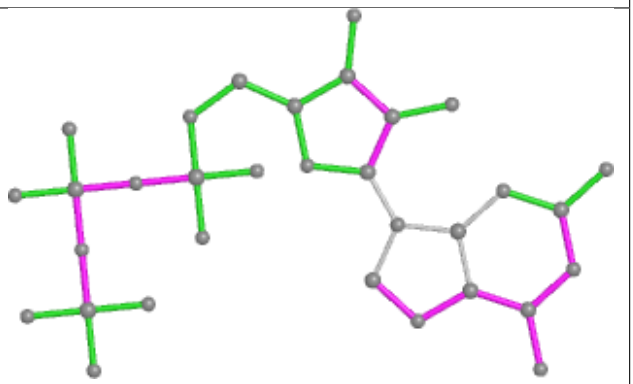

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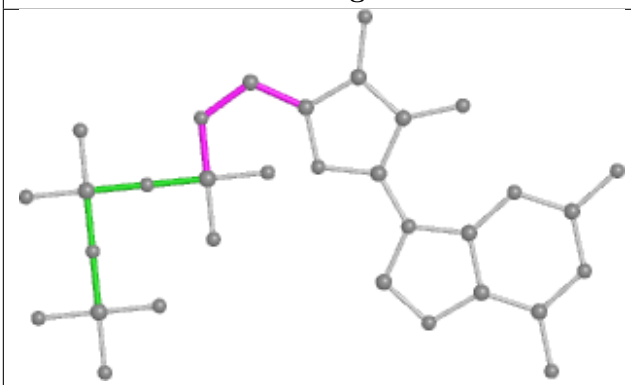

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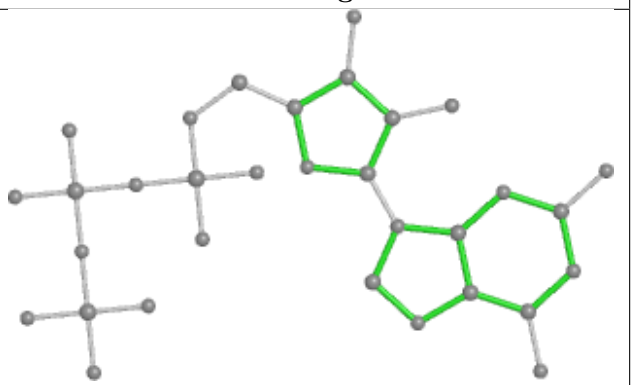

Rings

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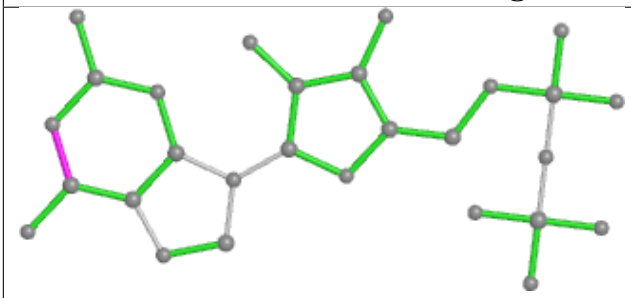

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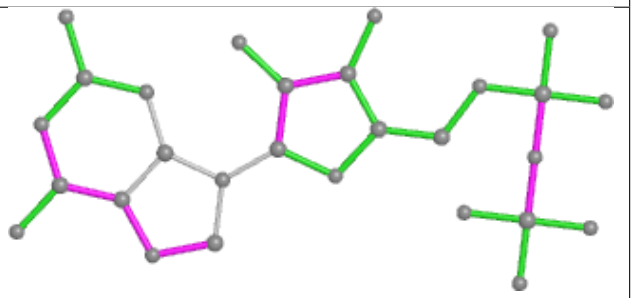

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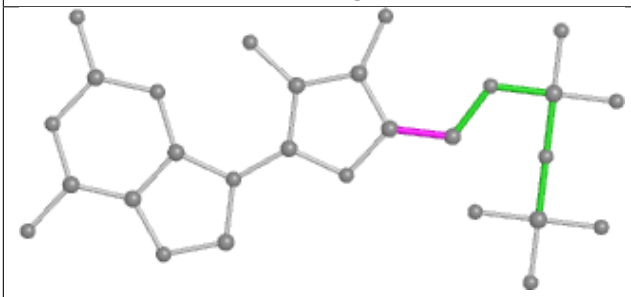

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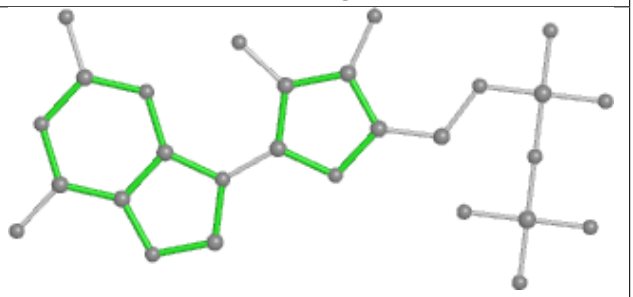

Rings

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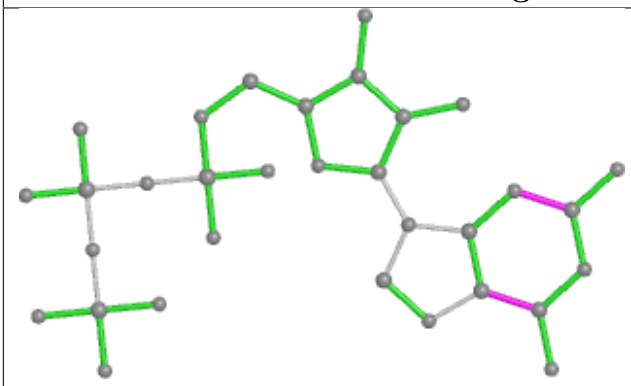

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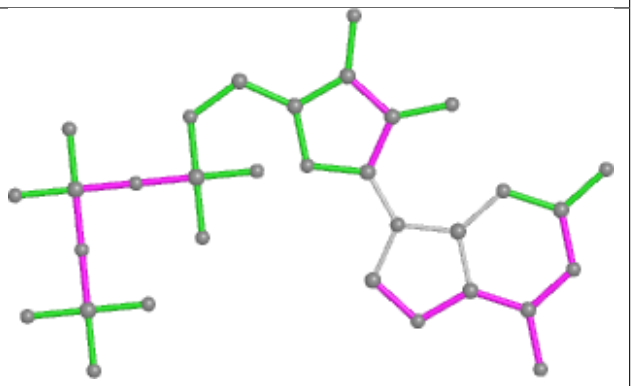

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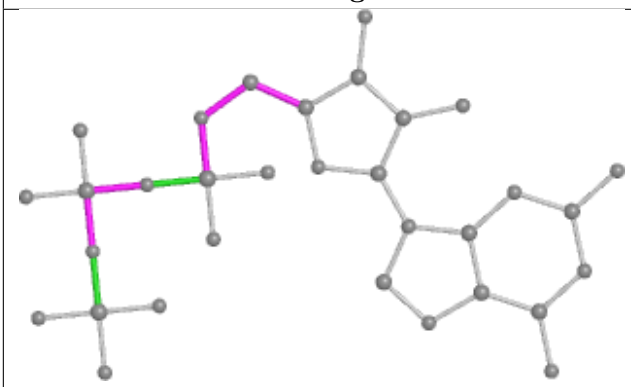

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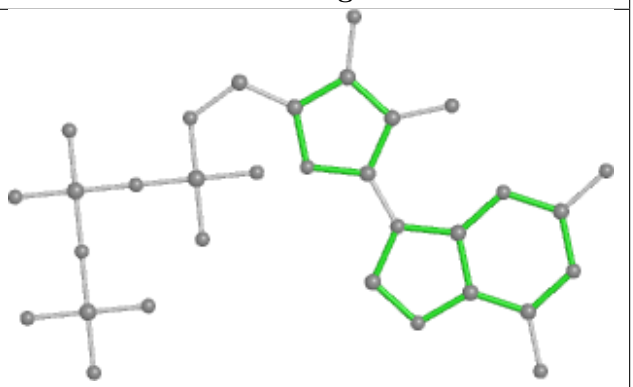

Rings

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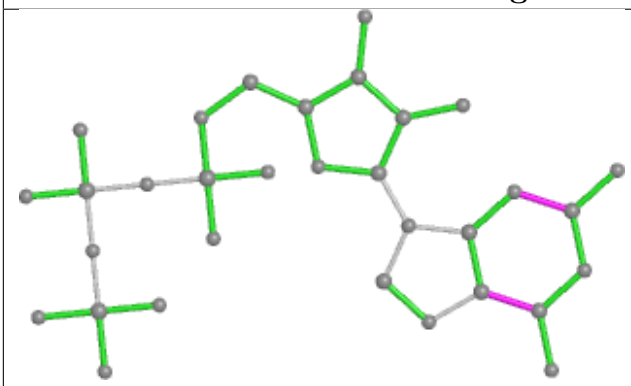

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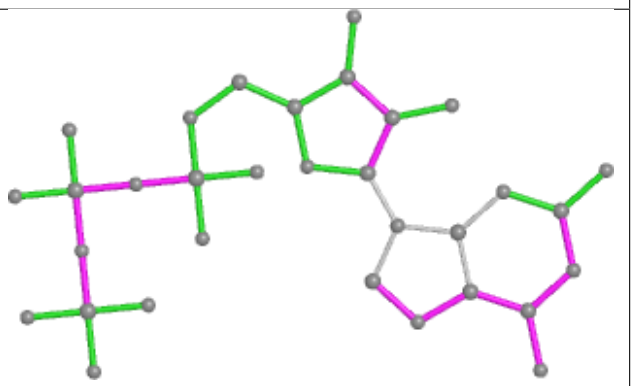

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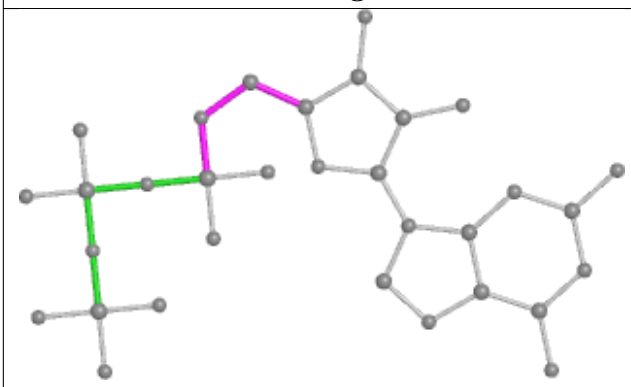

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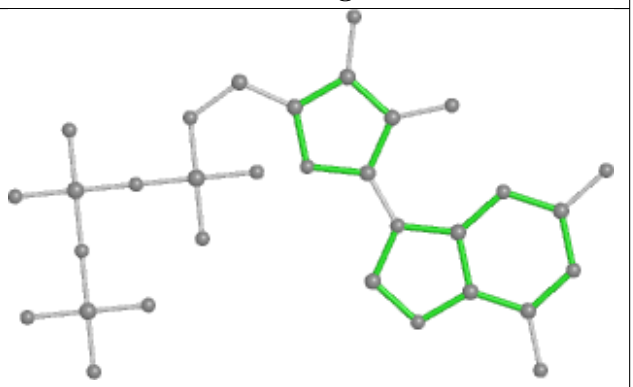

Rings

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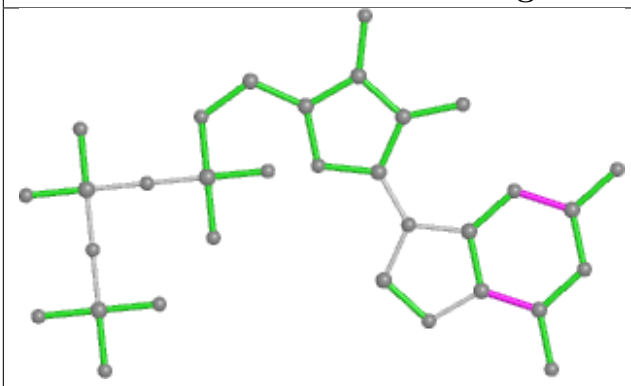

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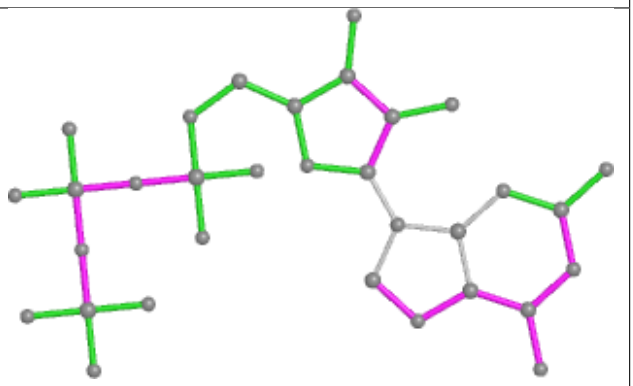

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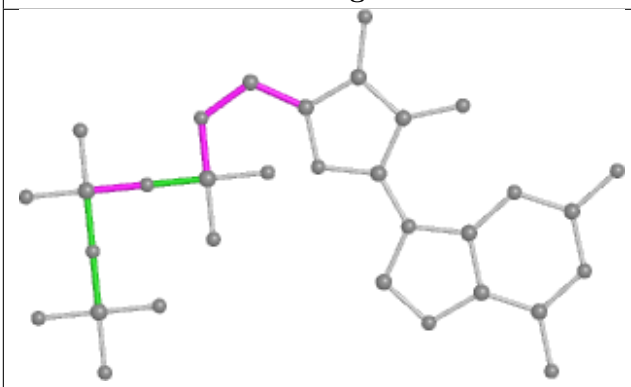

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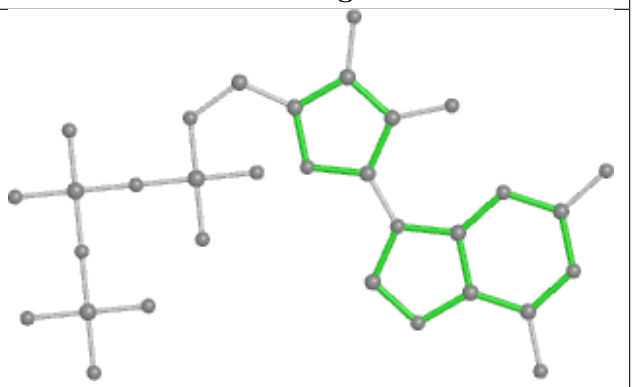

Rings

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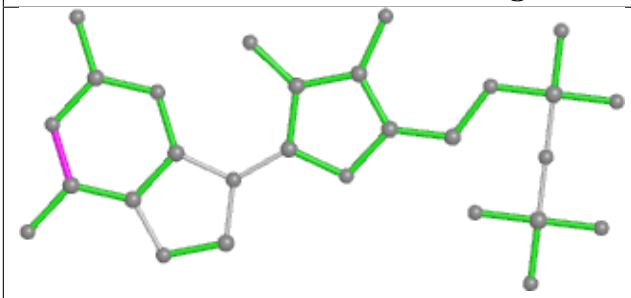

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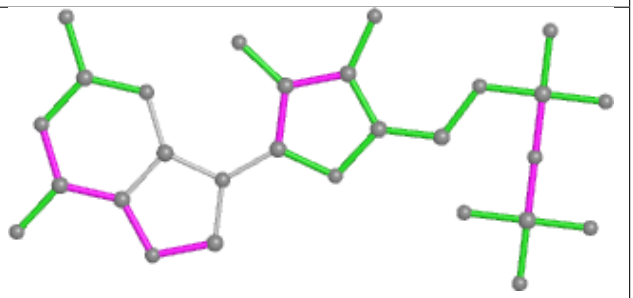

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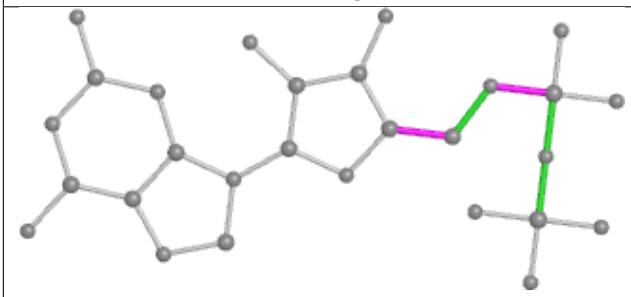

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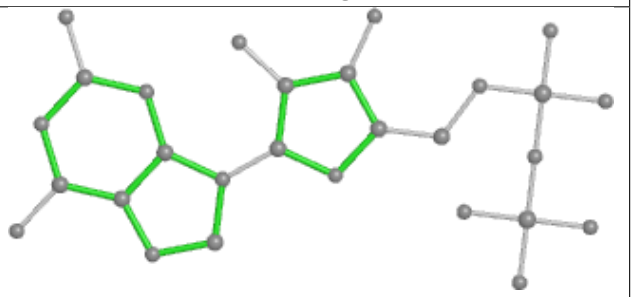

Rings

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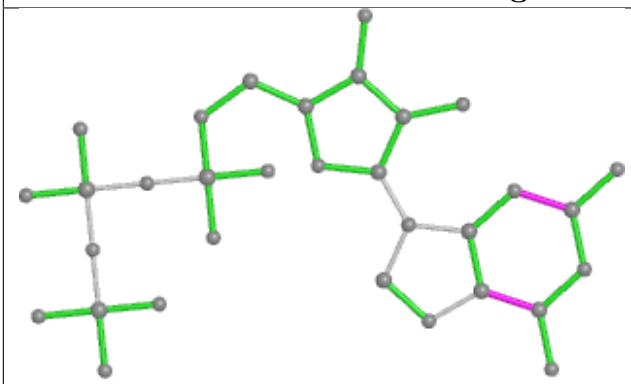

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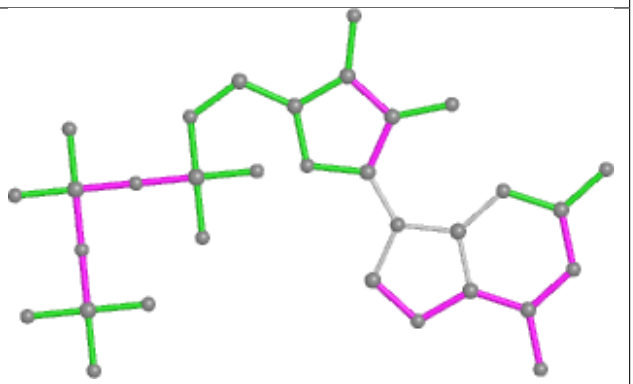

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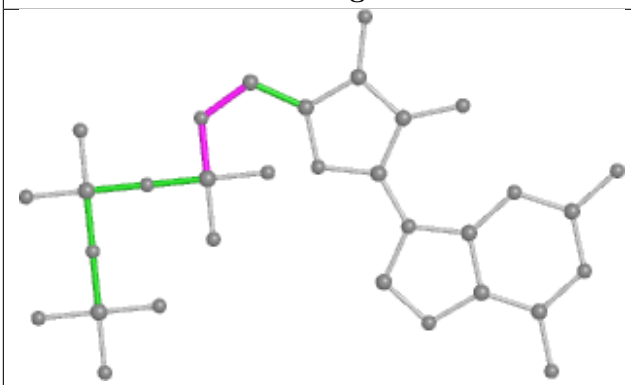

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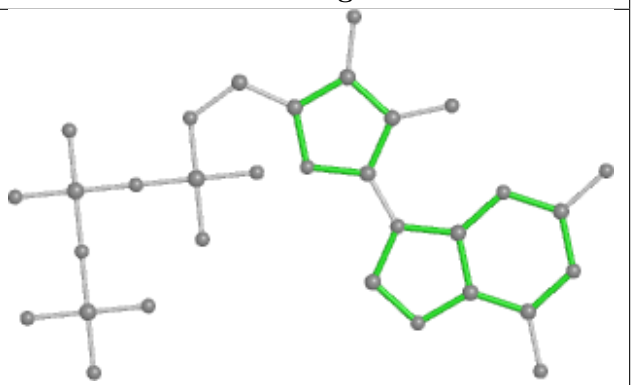

Rings

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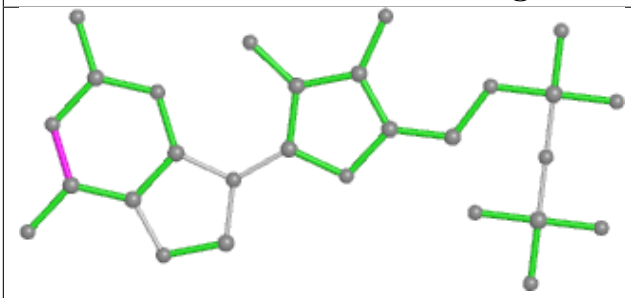

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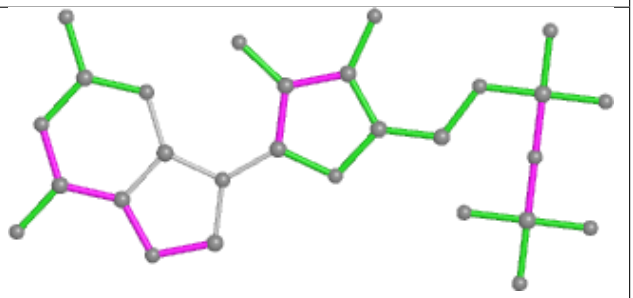

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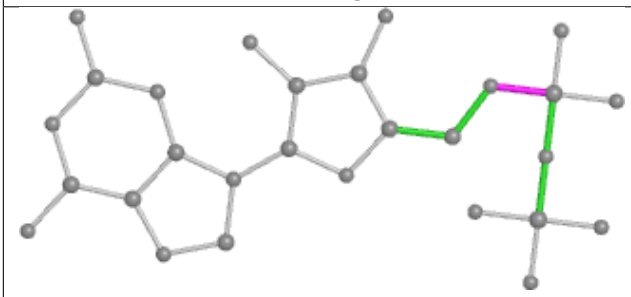

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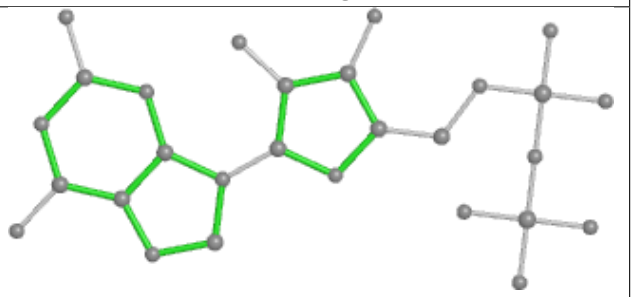

Rings

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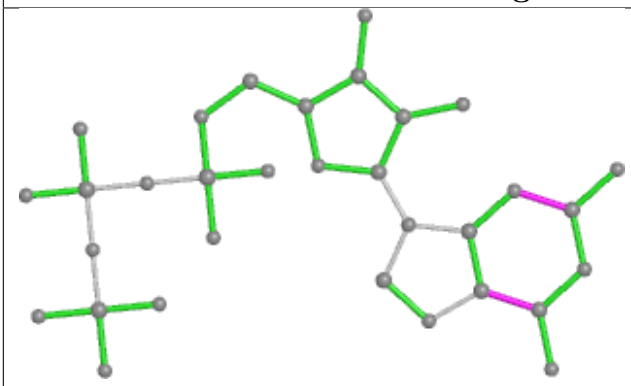

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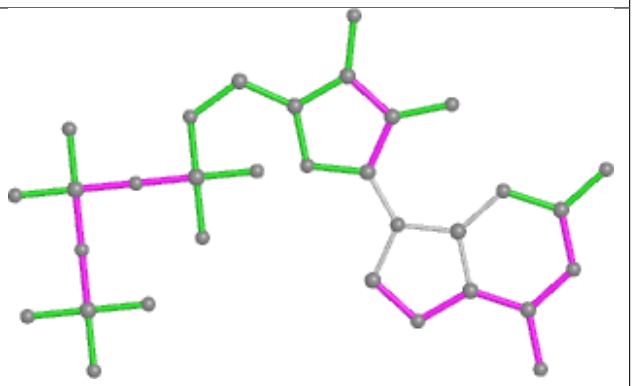

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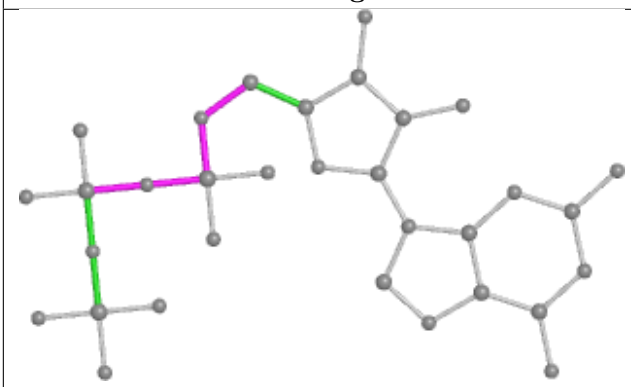

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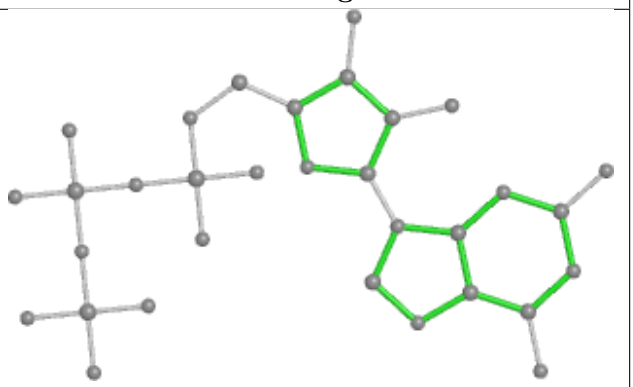

Rings

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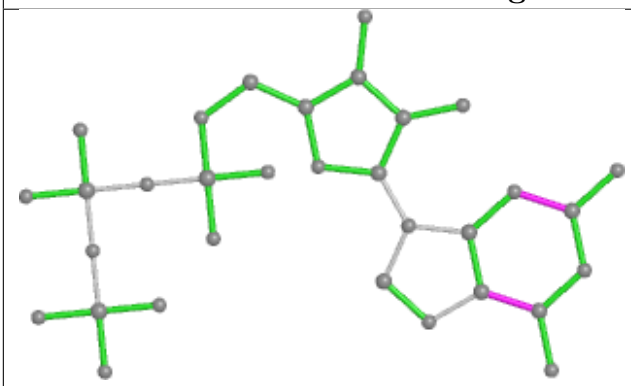

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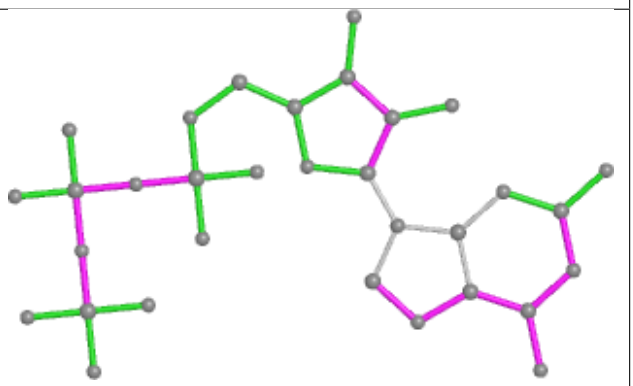

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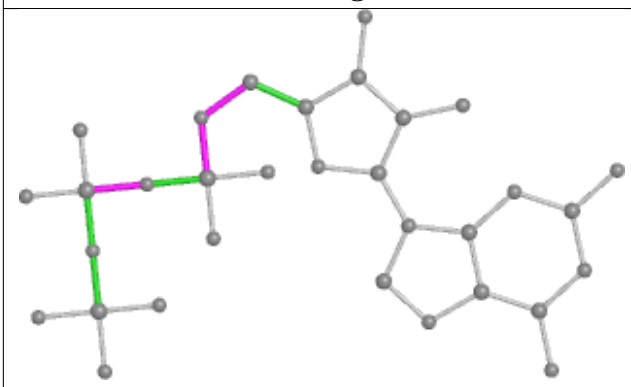

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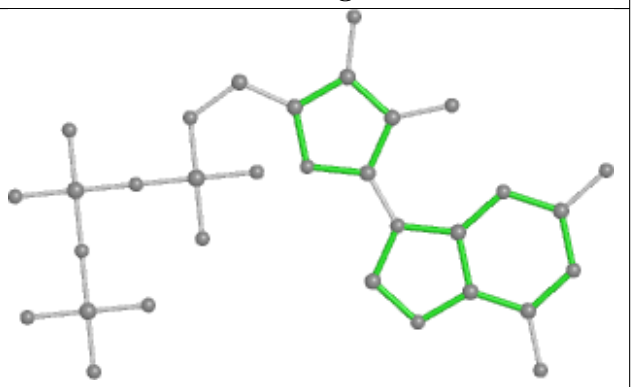

Rings

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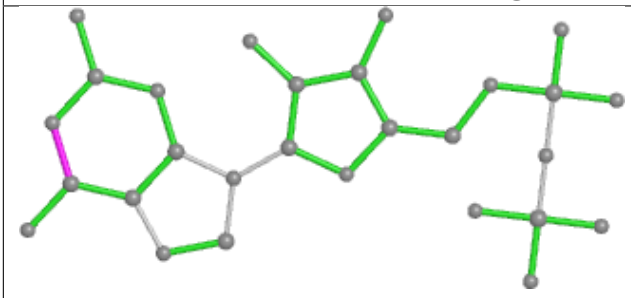
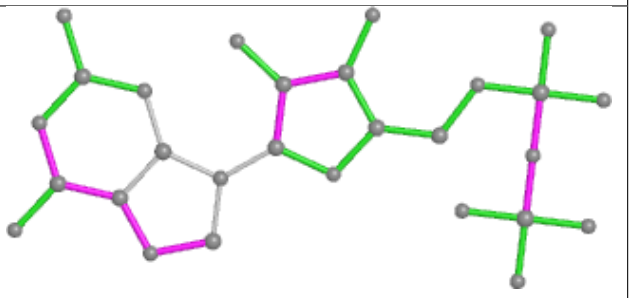
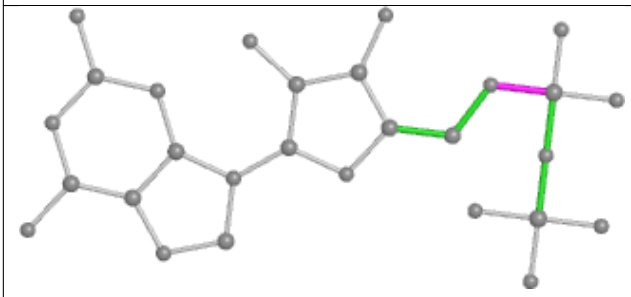
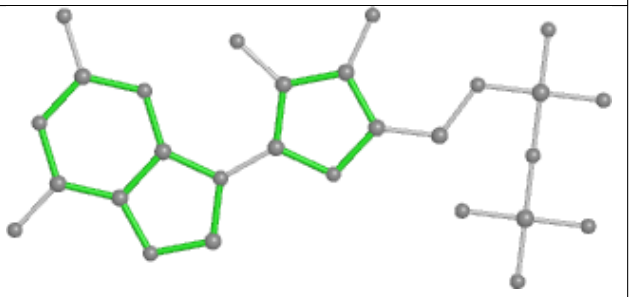
 Bond lengths	 Bond angles
 Torsions	 Rings

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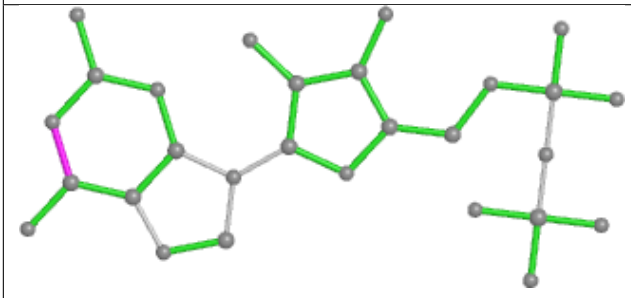
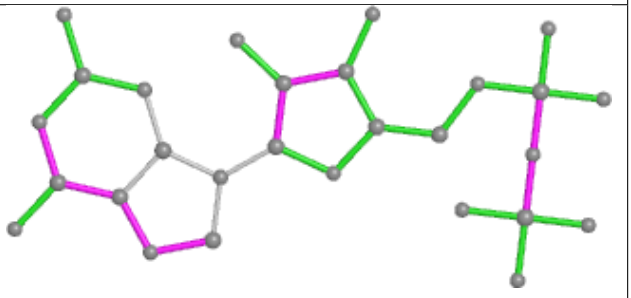
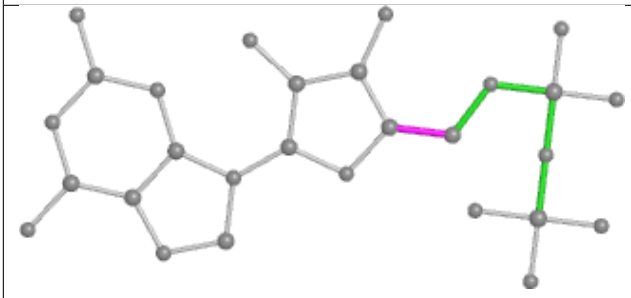
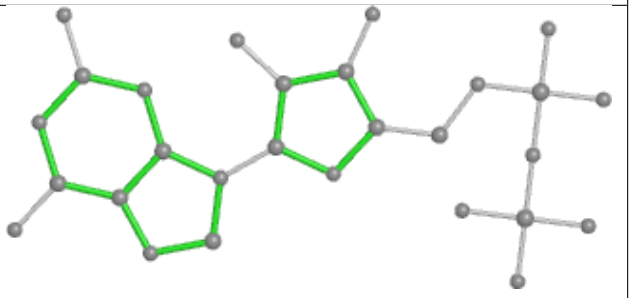
 Bond lengths	 Bond angles
 Torsions	 Rings

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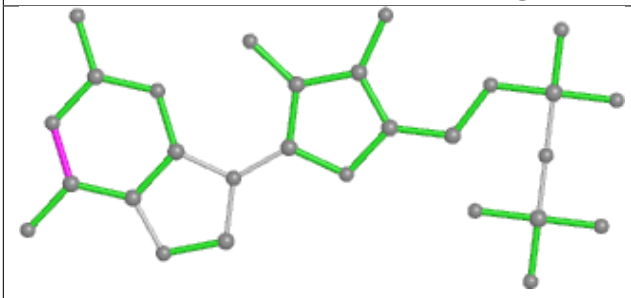
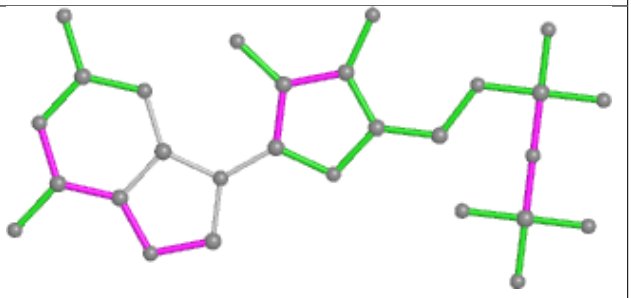
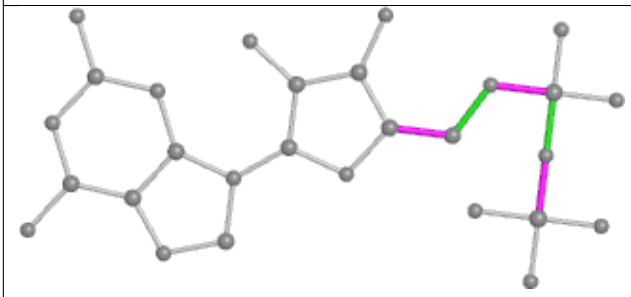
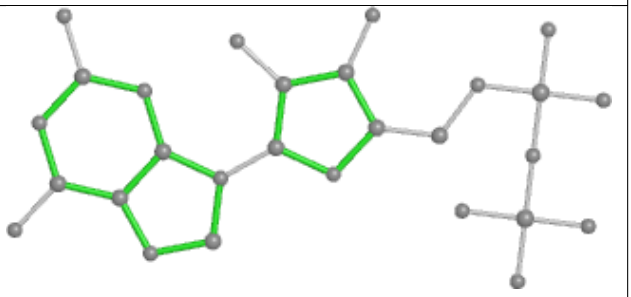
 Bond lengths	 Bond angles
 Torsions	 Rings

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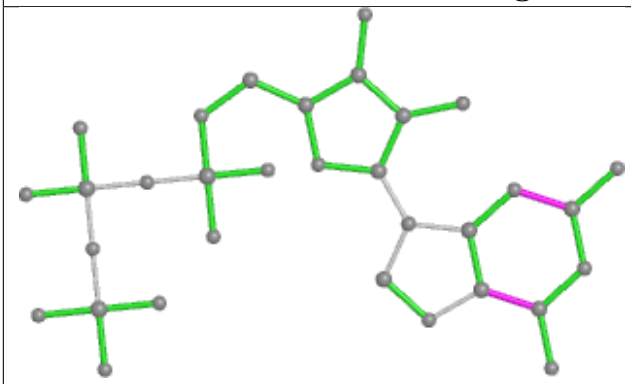
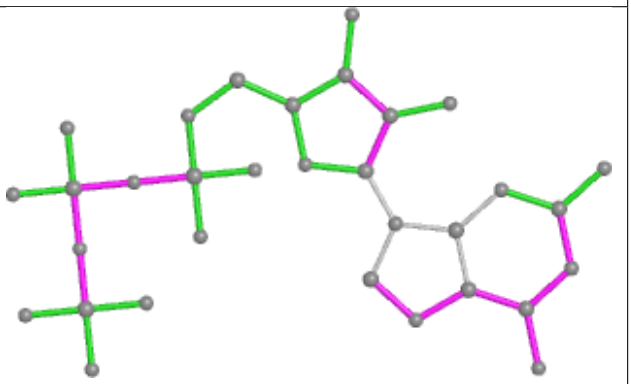
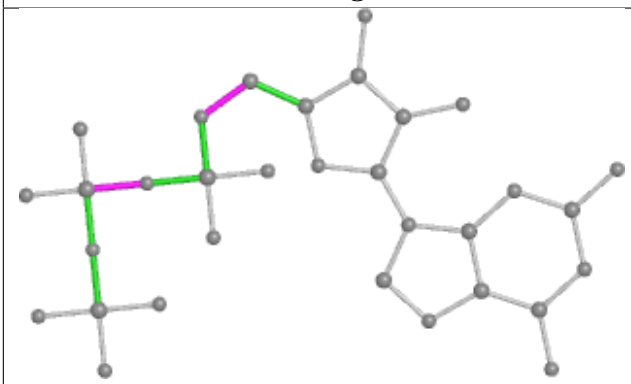
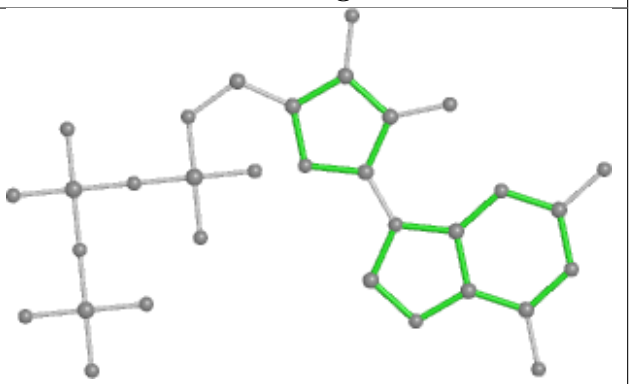
 Bond lengths	 Bond angles
 Torsions	 Rings

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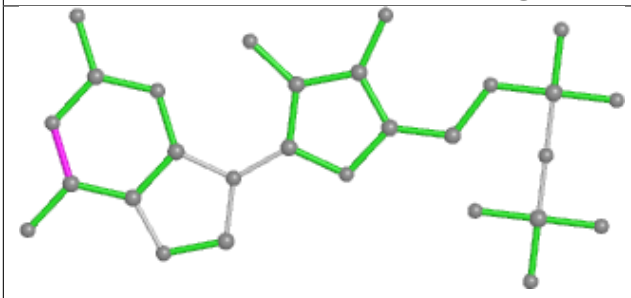

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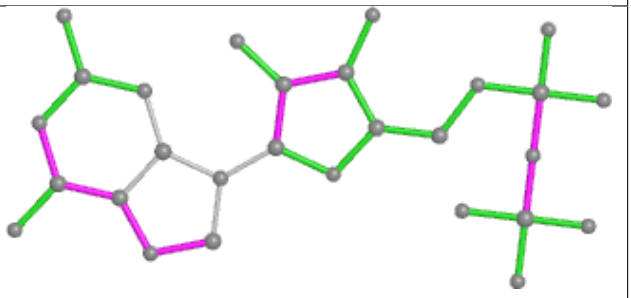

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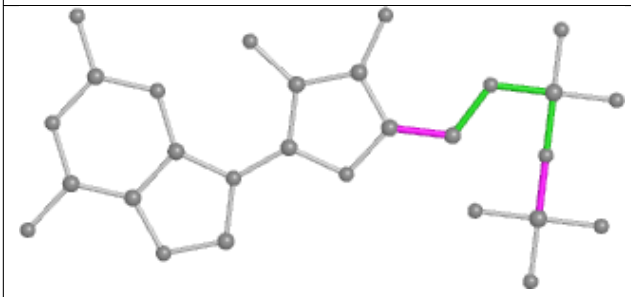

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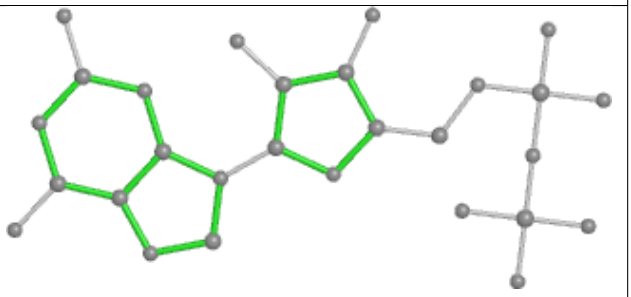

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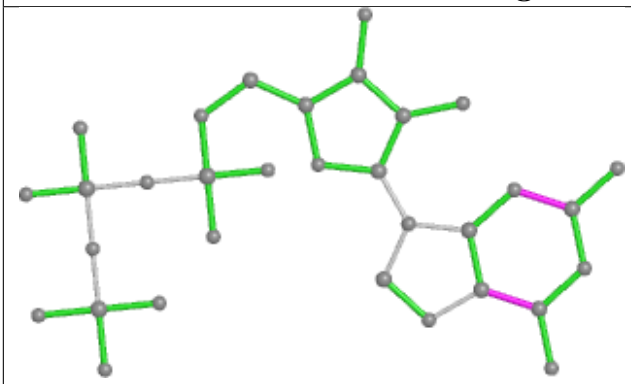

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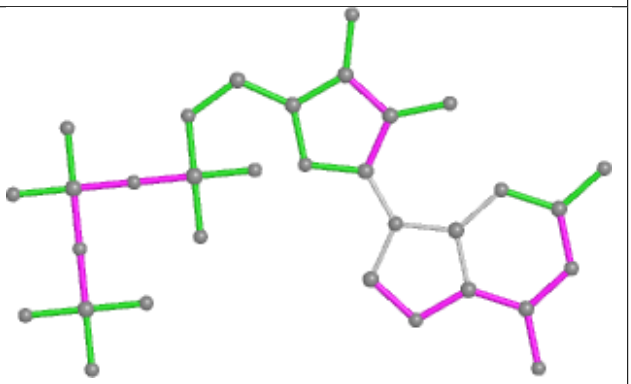

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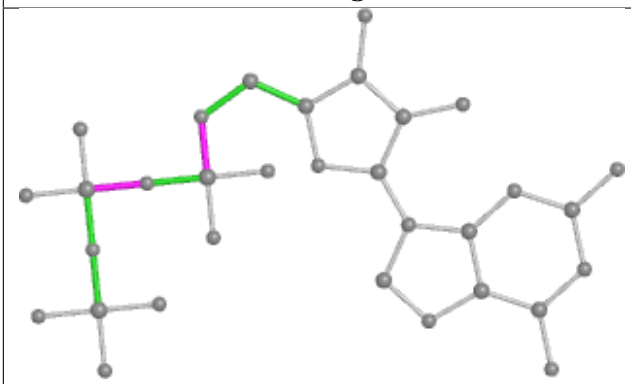

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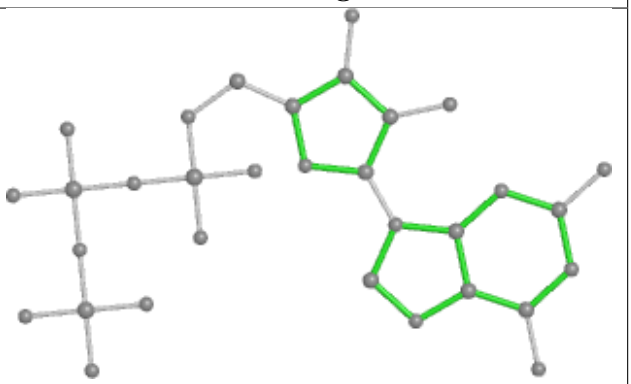

Rings

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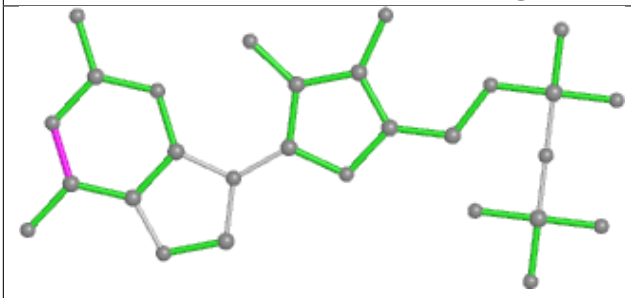

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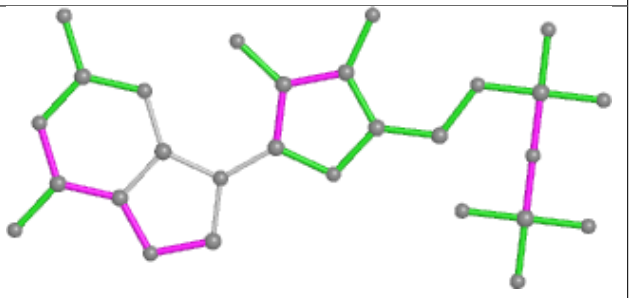

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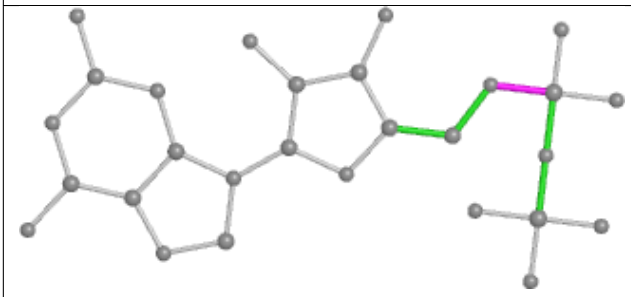

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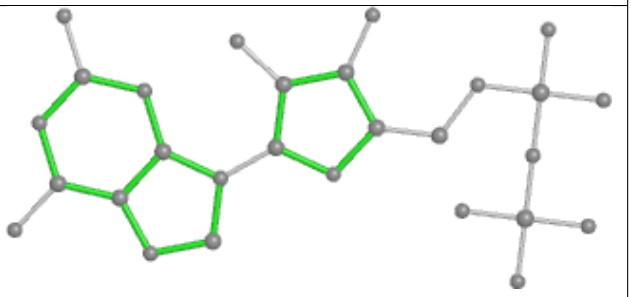

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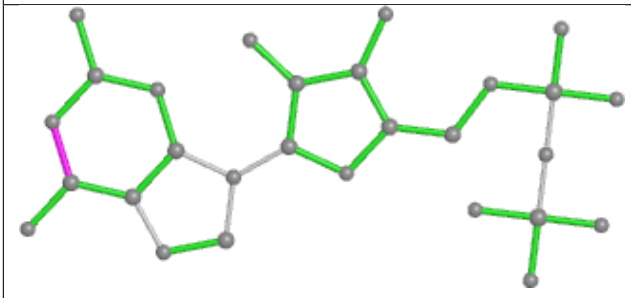

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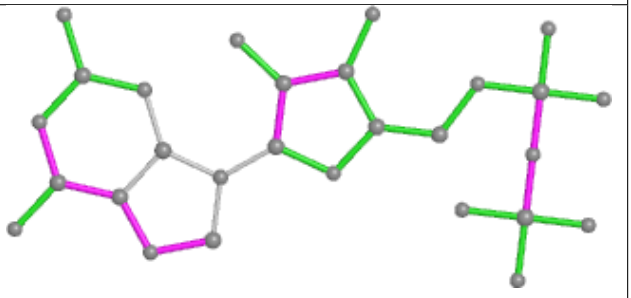

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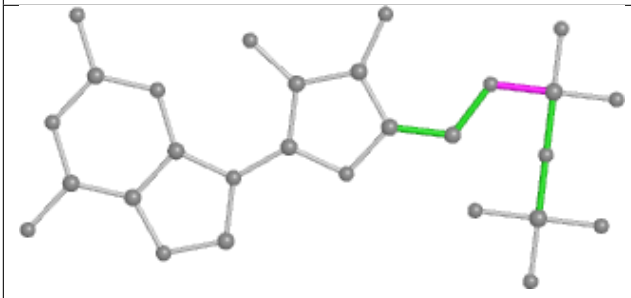

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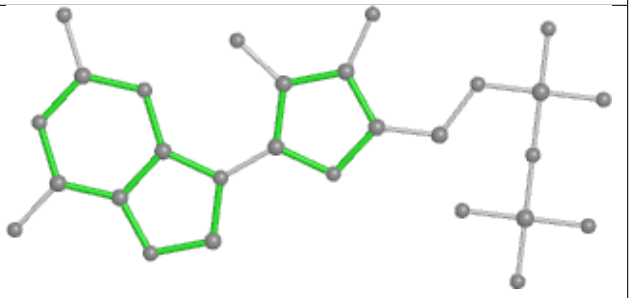

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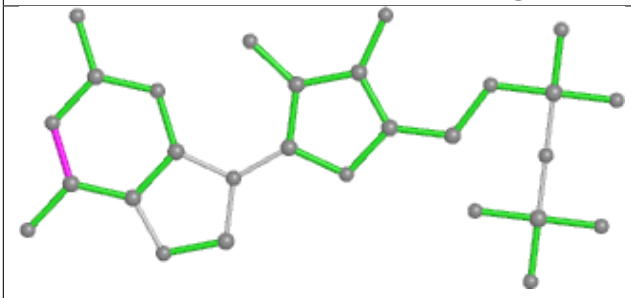

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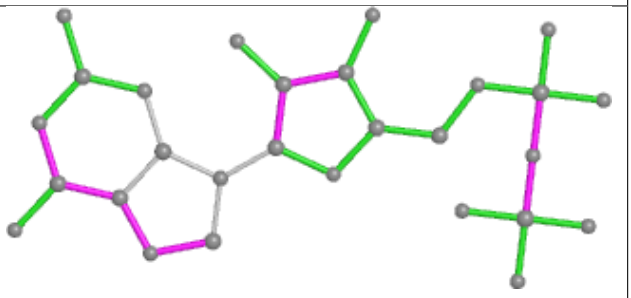

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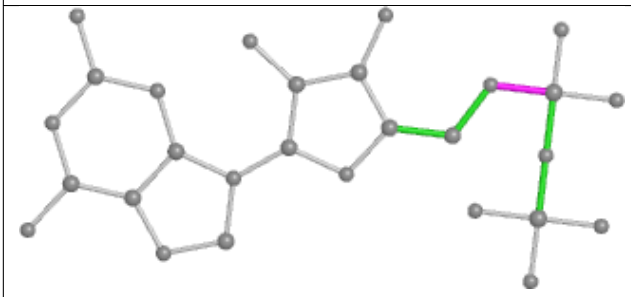

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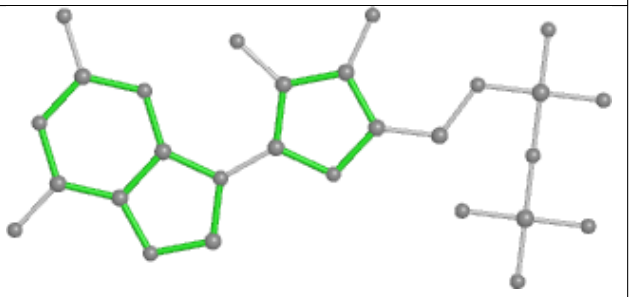

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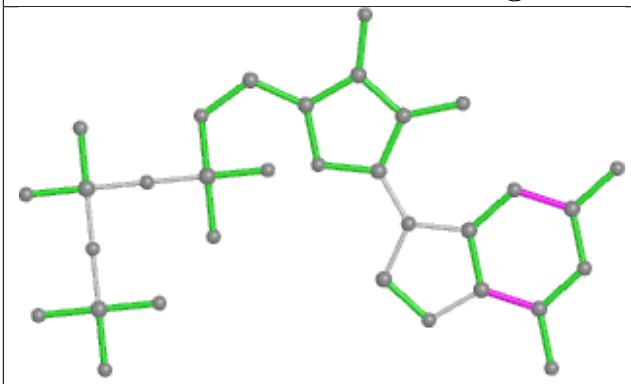

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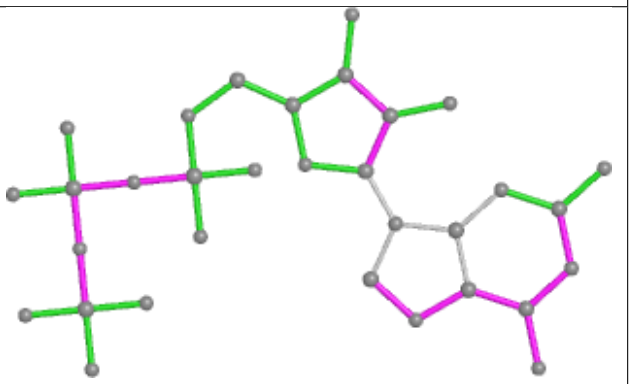

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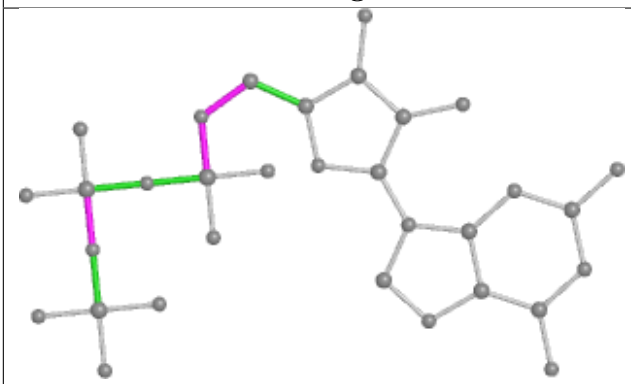

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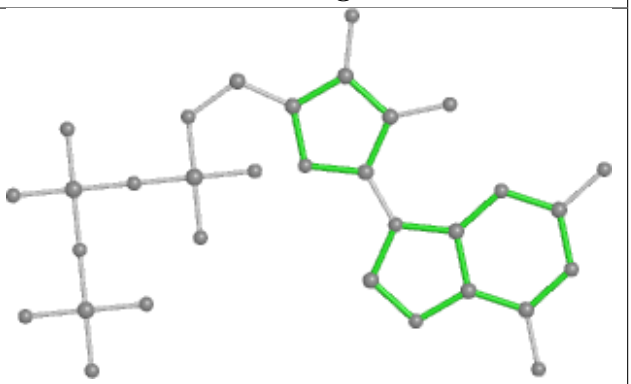

Rings

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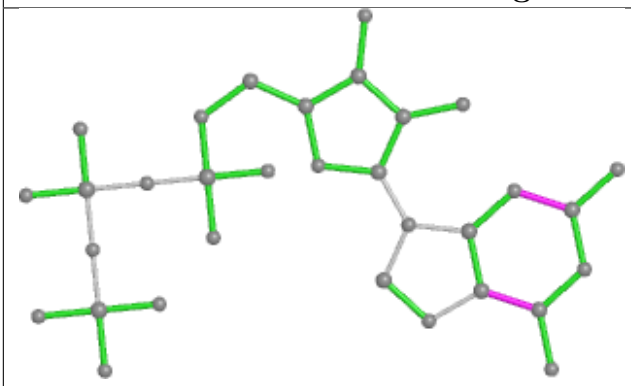

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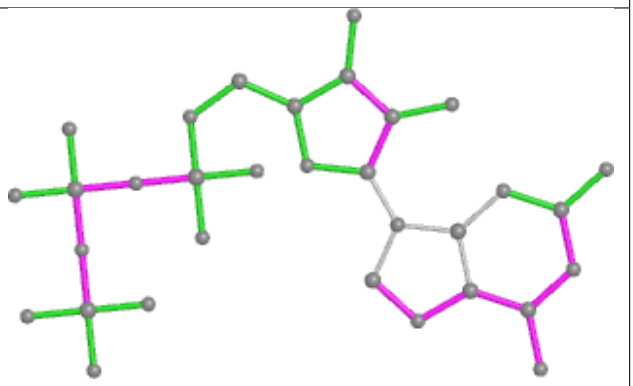

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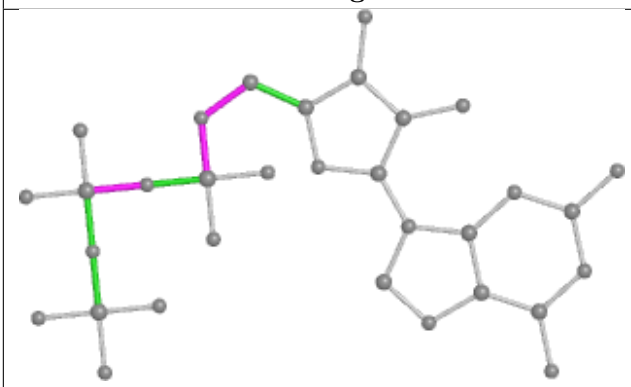

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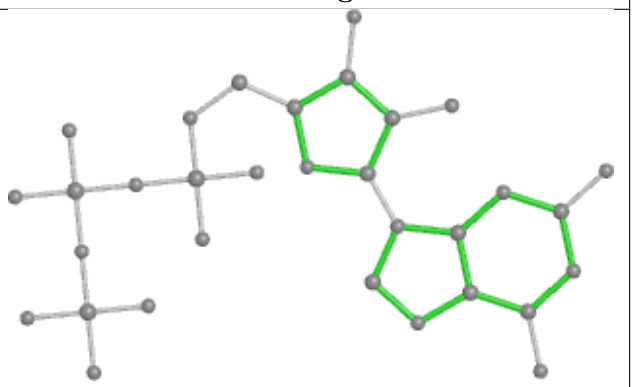

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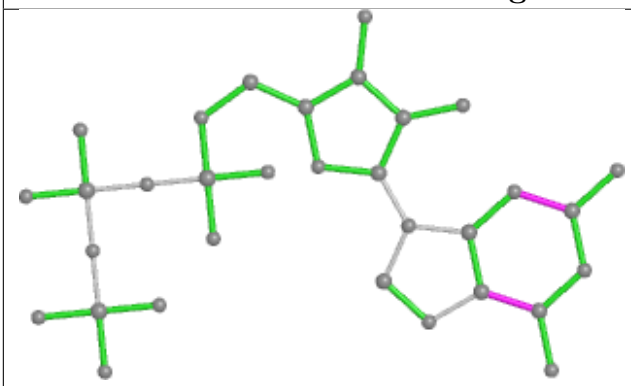

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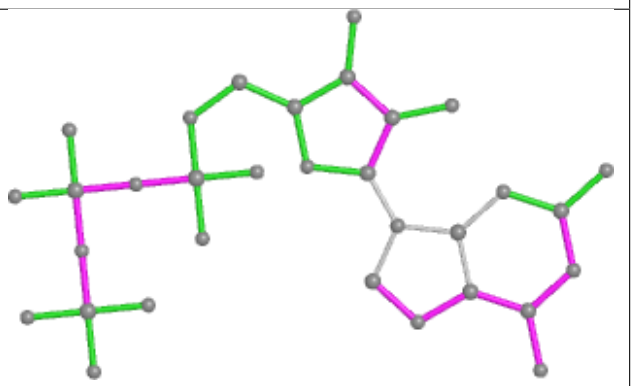

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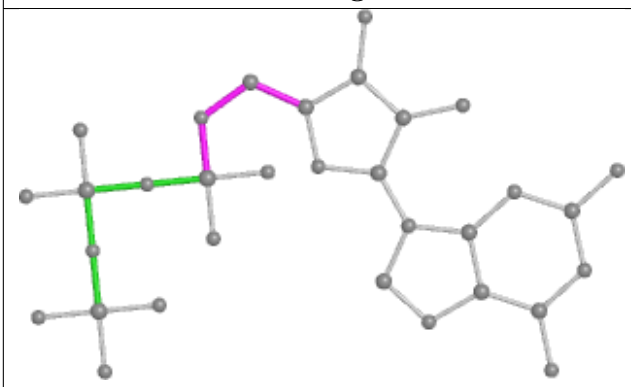

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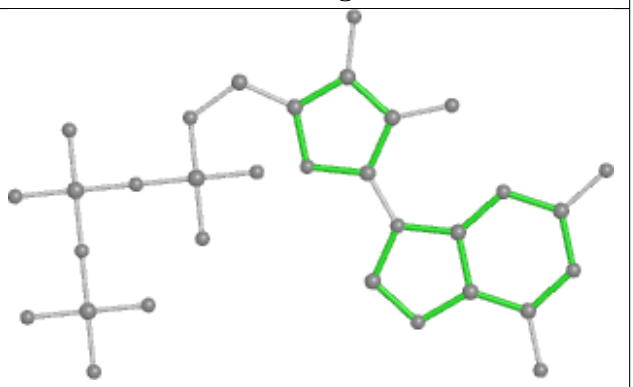

Rings

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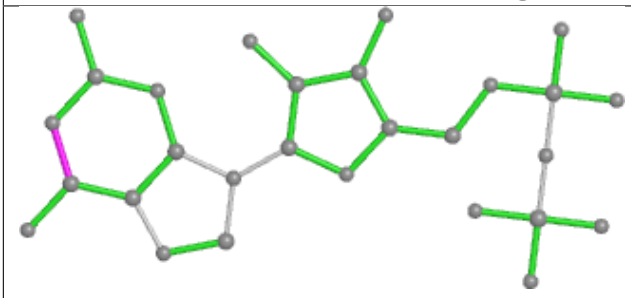
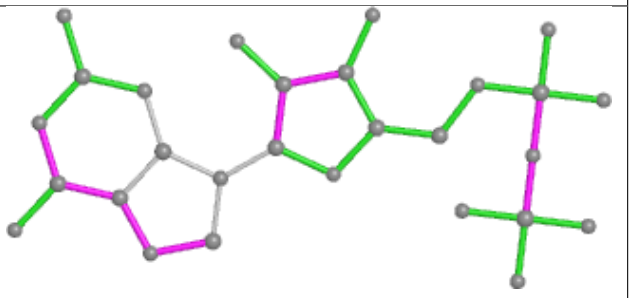
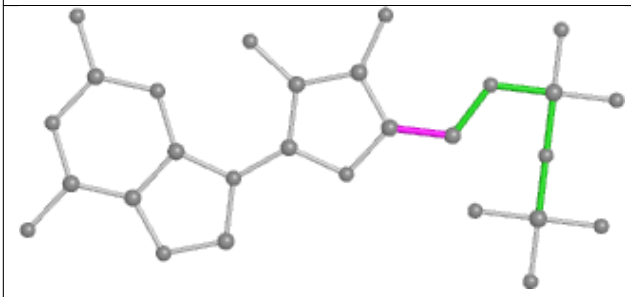
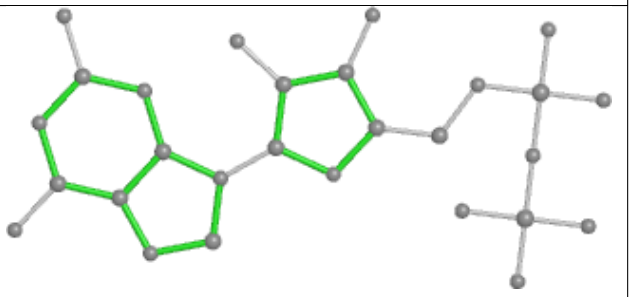
 Bond lengths	 Bond angles
 Torsions	 Rings

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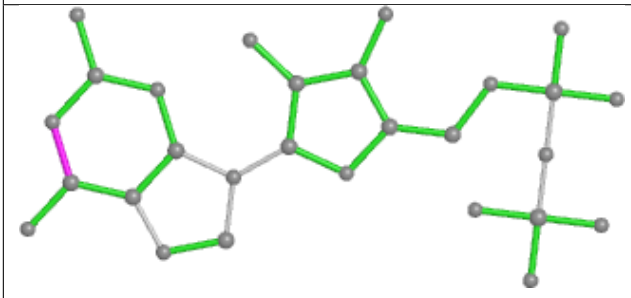
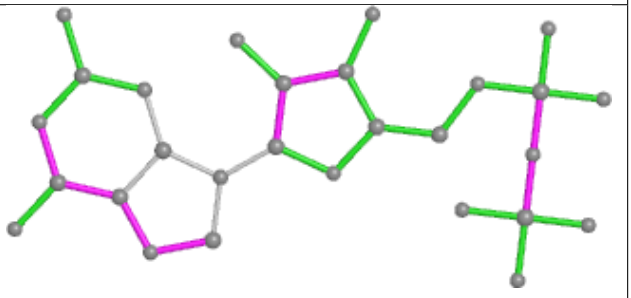
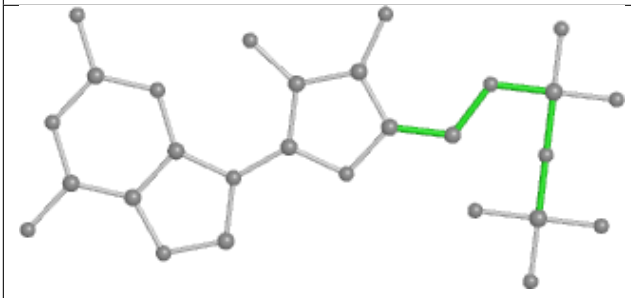
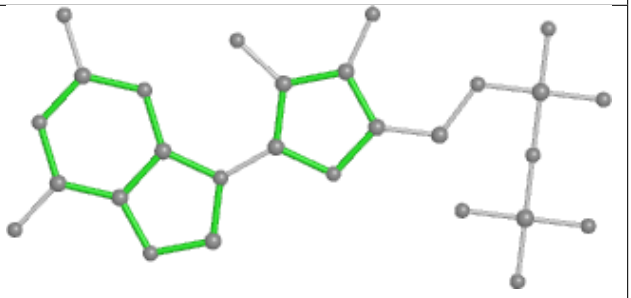
 Bond lengths	 Bond angles
 Torsions	 Rings

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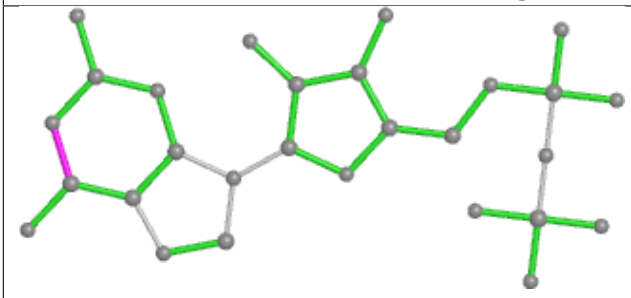

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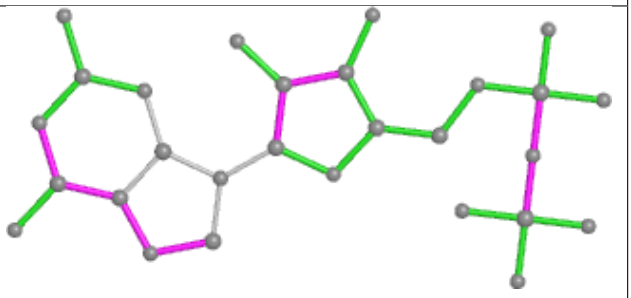

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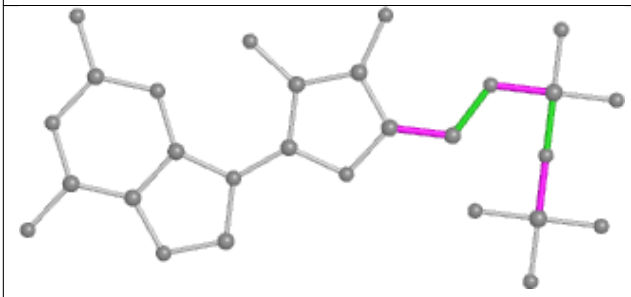

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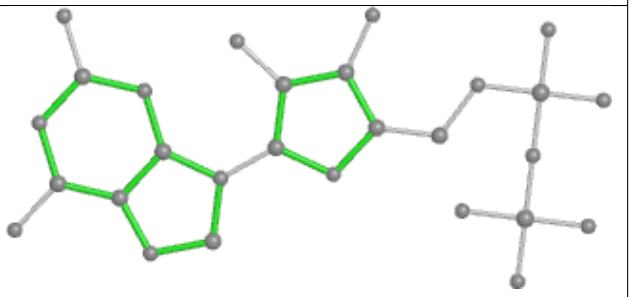

Rings

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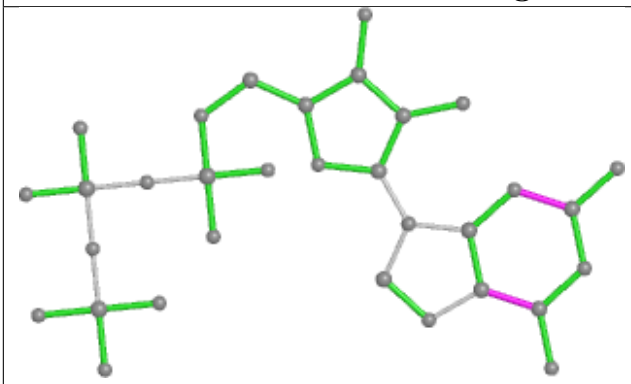

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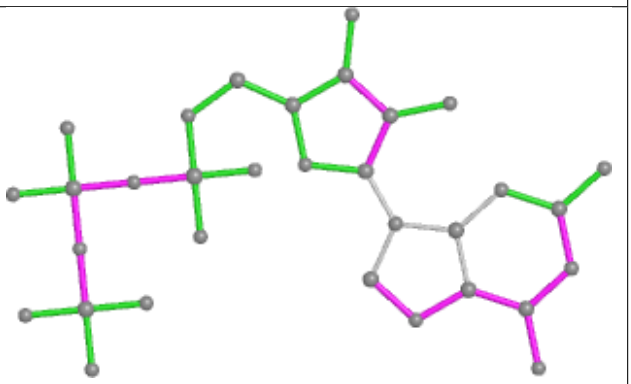

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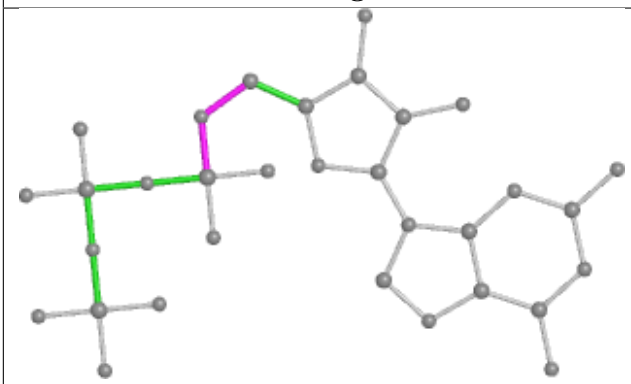

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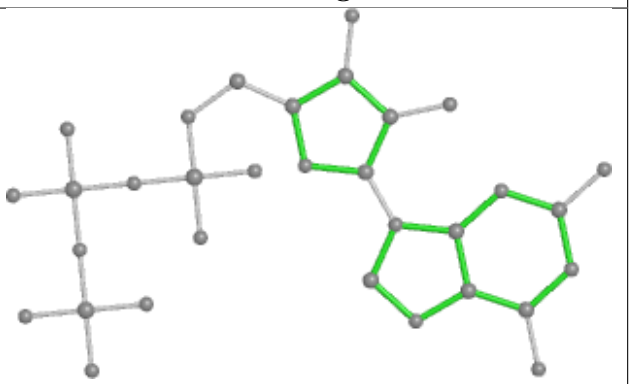
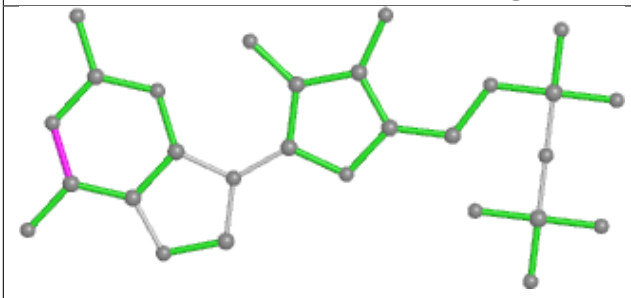


Rings

Ligand GDP AA 501



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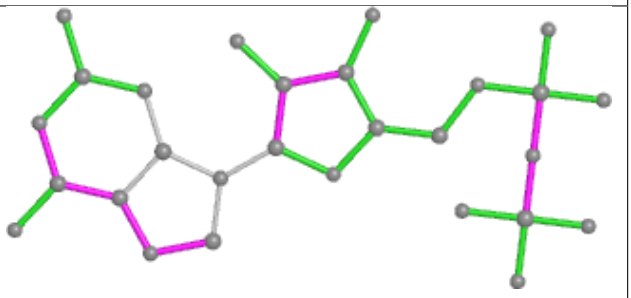

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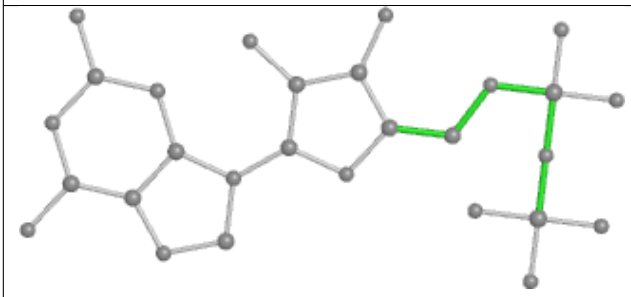
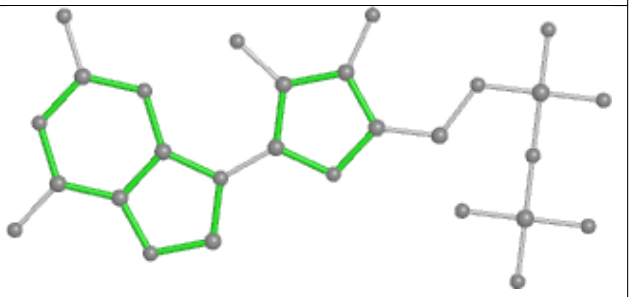
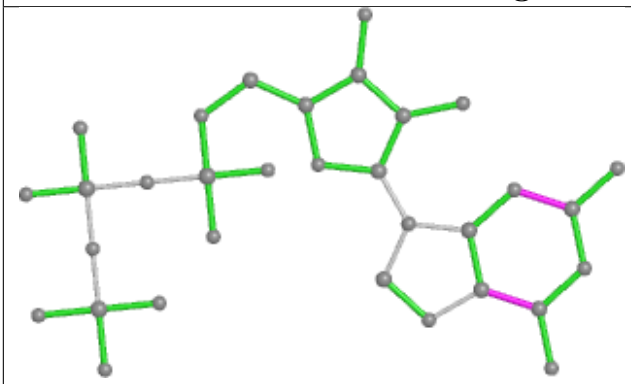


Torsions



Rings

Ligand GTP FF 501



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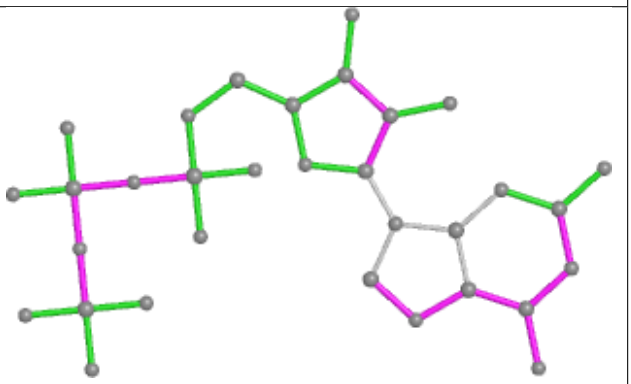

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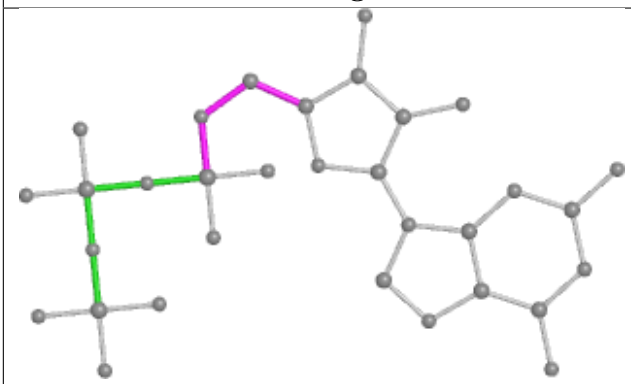

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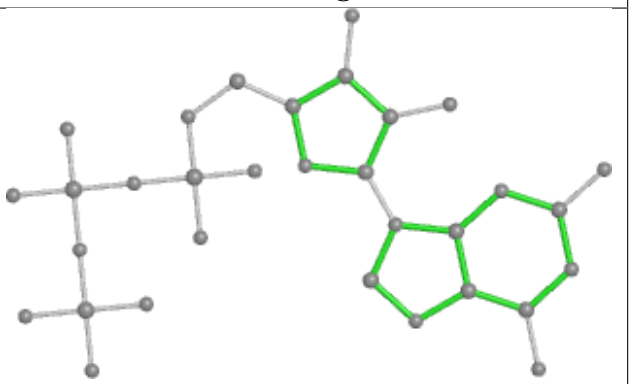

Rings

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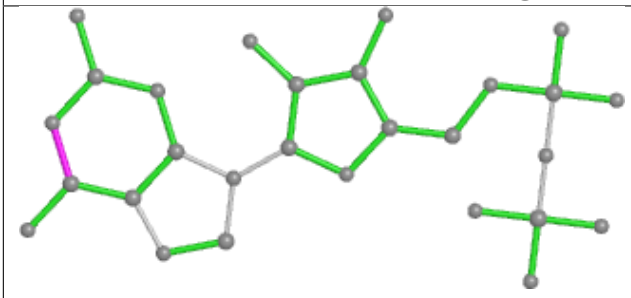

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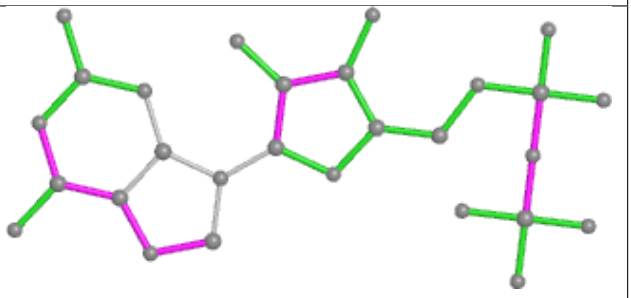

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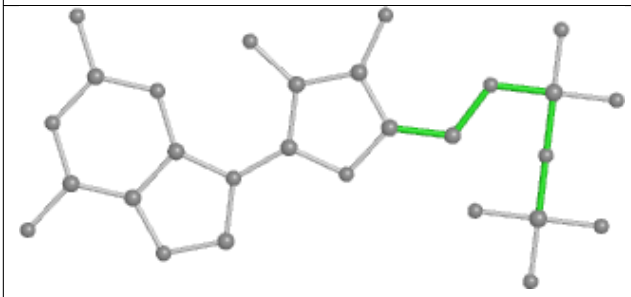

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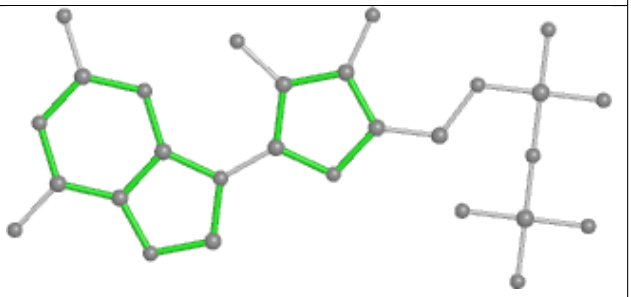

Rings

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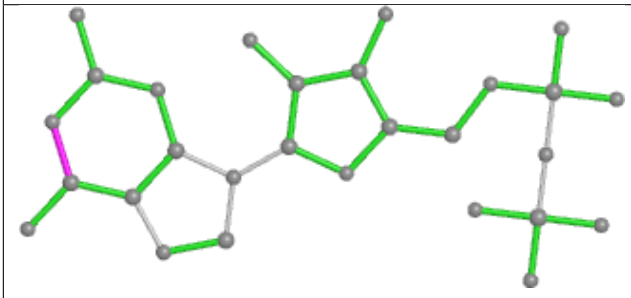

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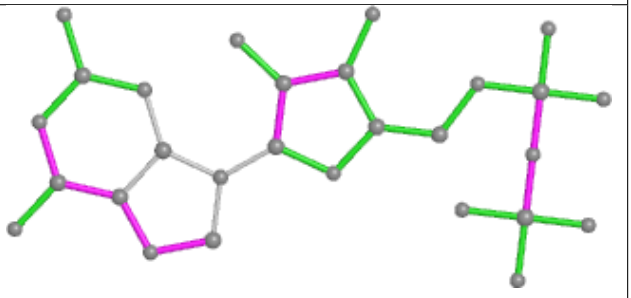

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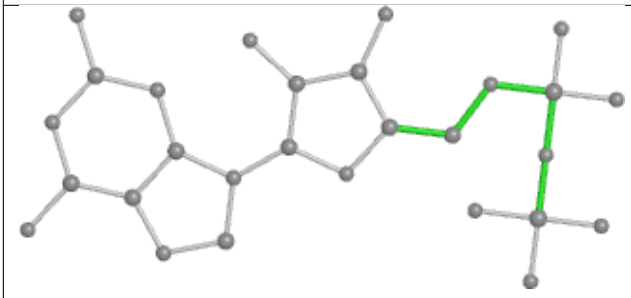

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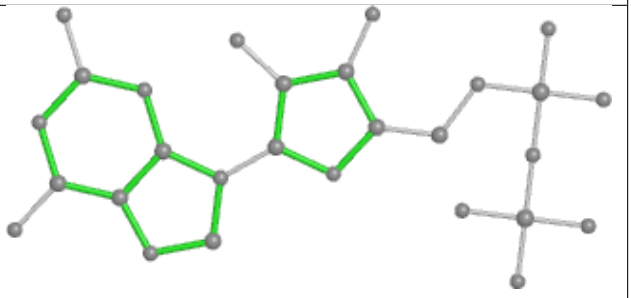
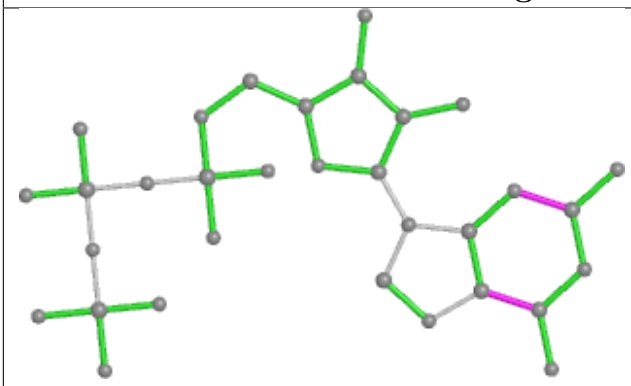


Rings

Ligand GTP FJ 501



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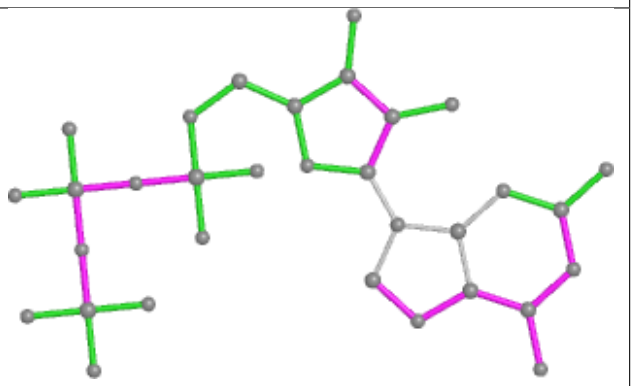

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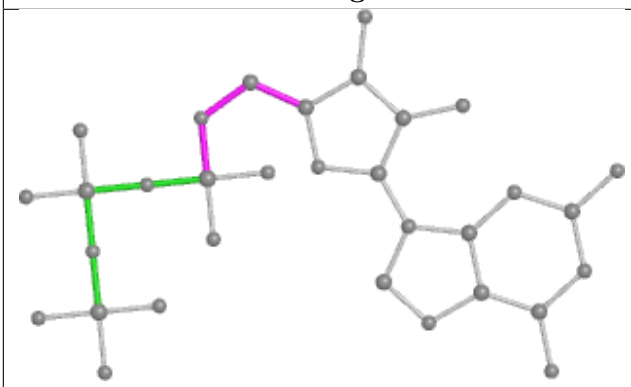

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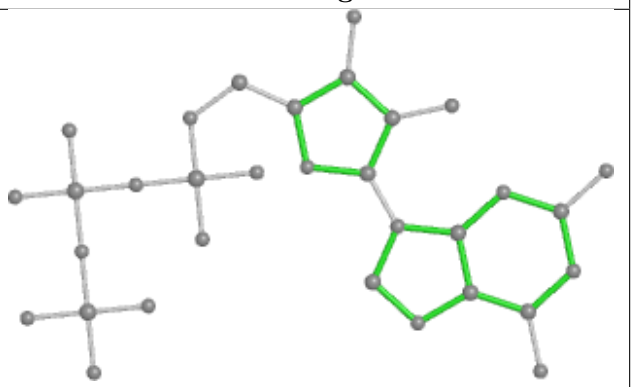

Rings

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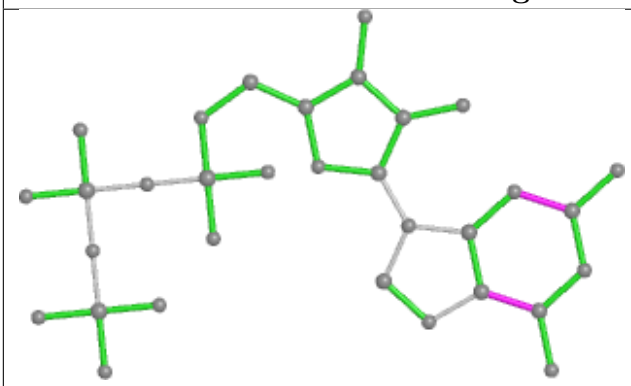

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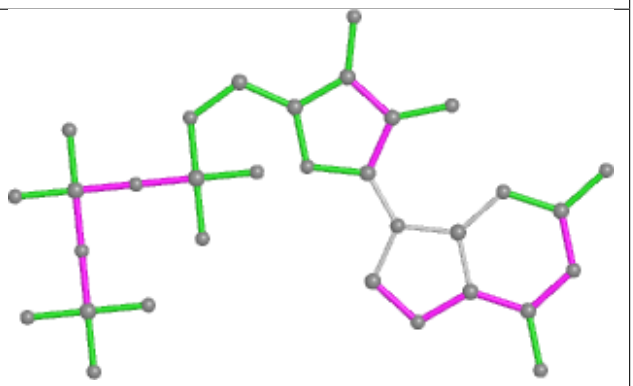

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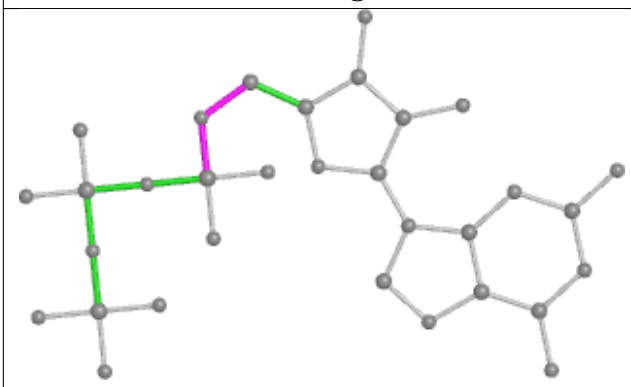

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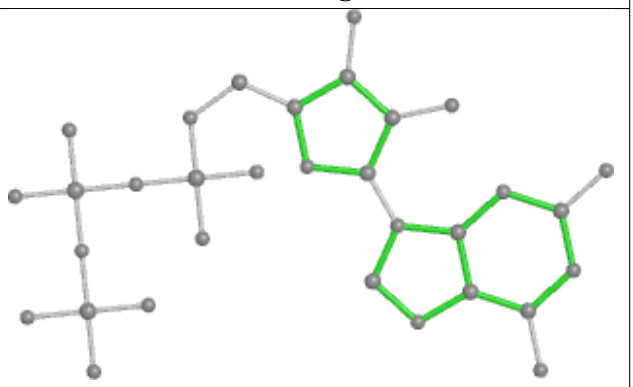
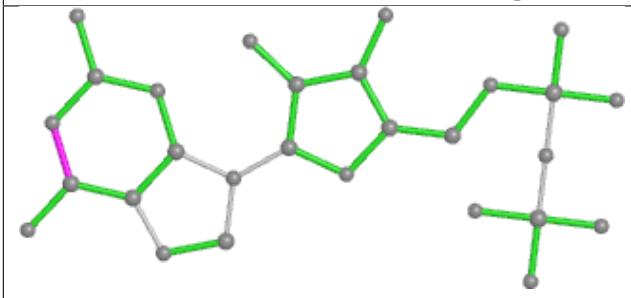
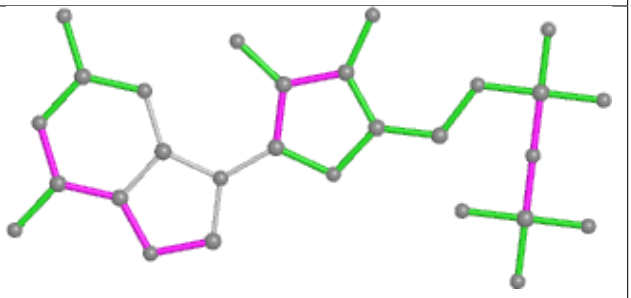
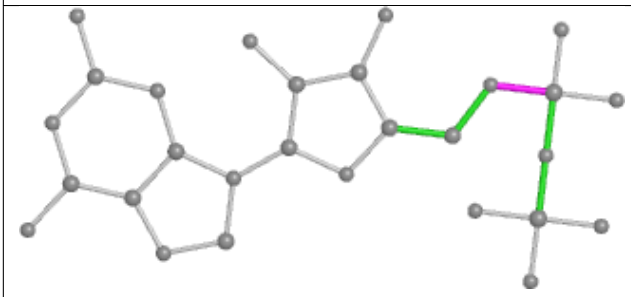
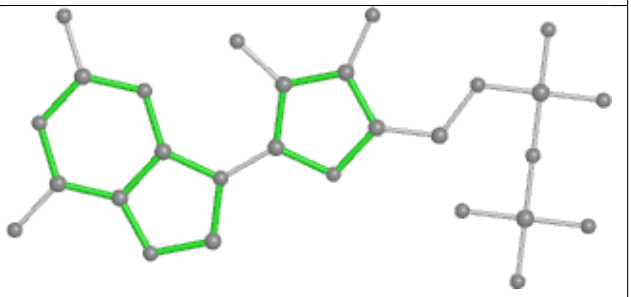


Rings

Ligand GDP EK 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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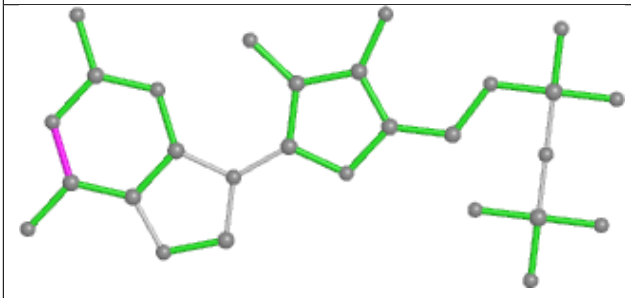
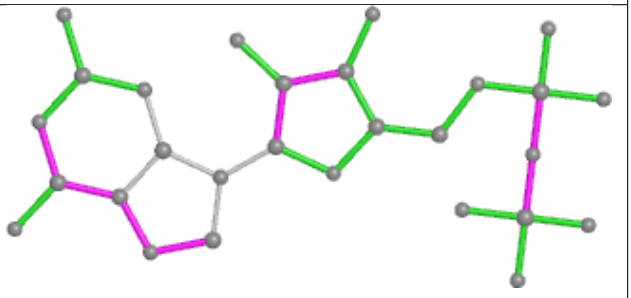
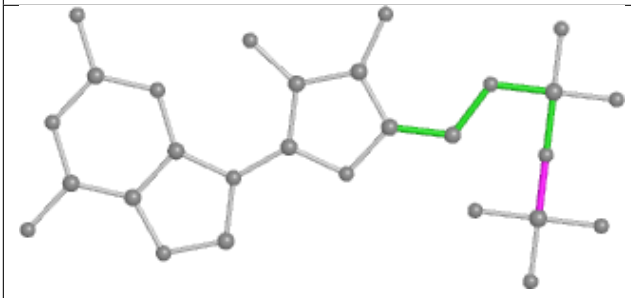
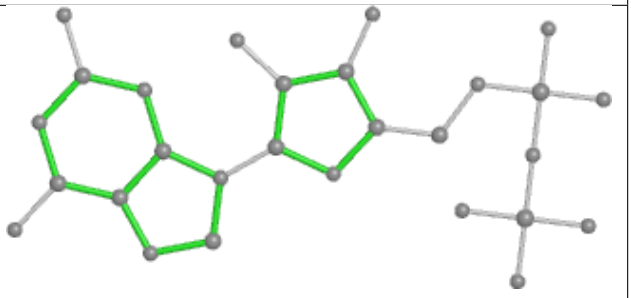
 Bond lengths	 Bond angles
 Torsions	 Rings

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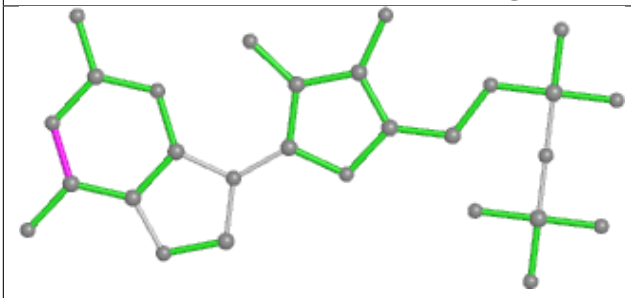

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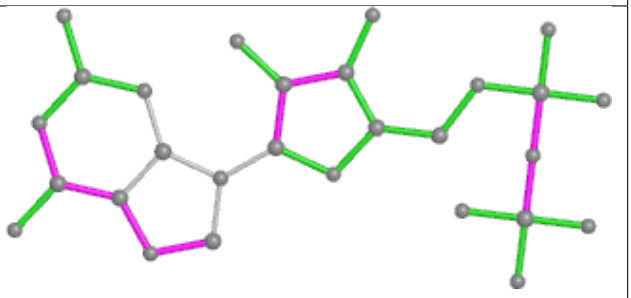

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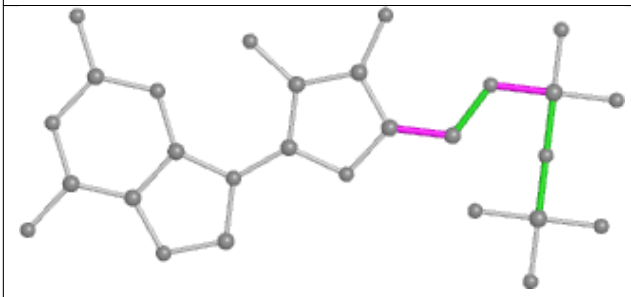

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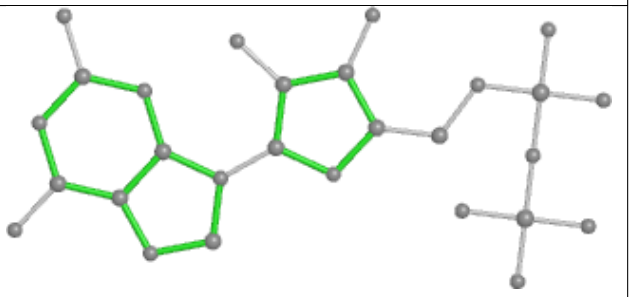
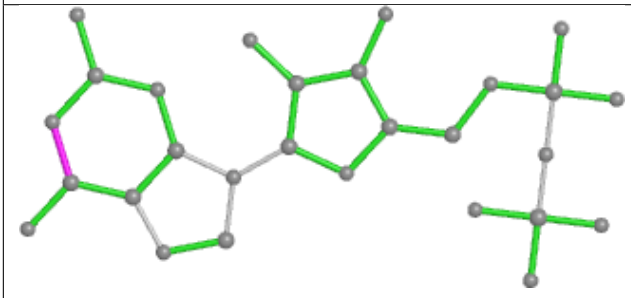


Rings

Ligand GDP GK 501



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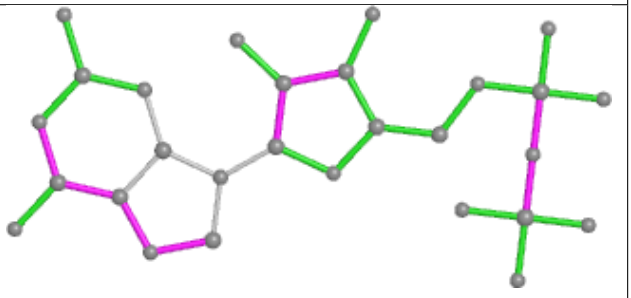

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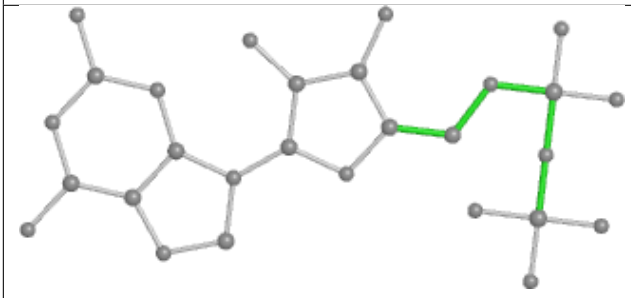

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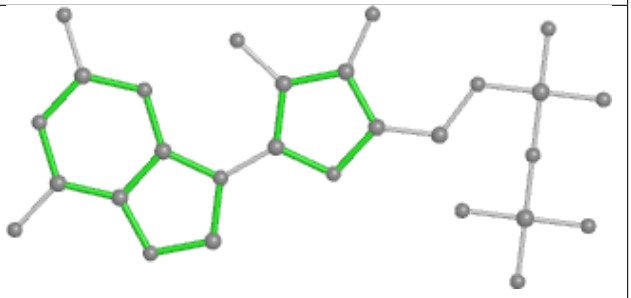

Rings

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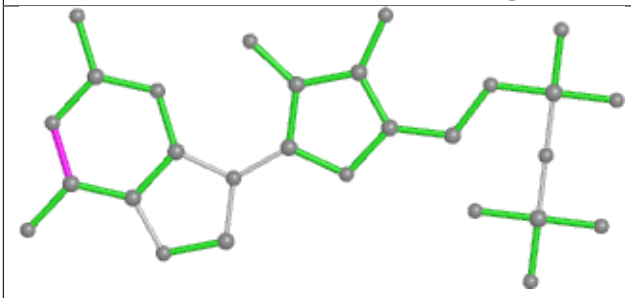

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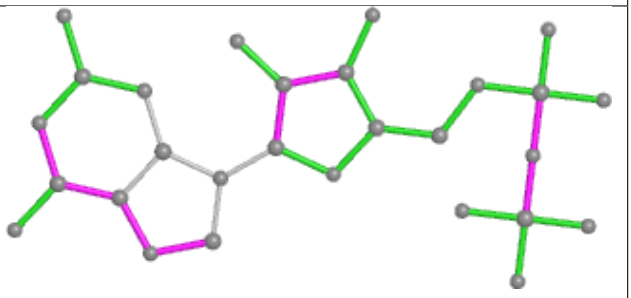

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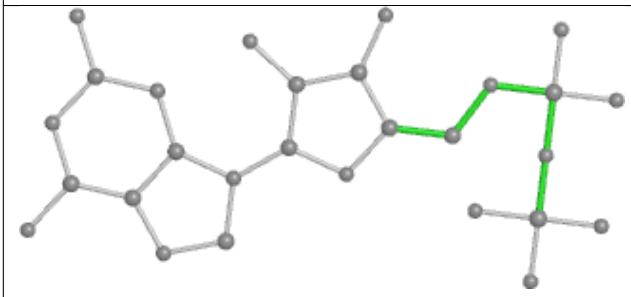

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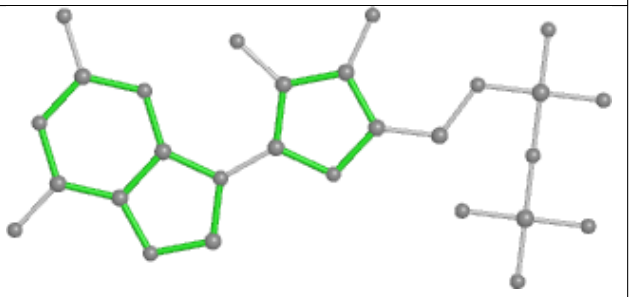
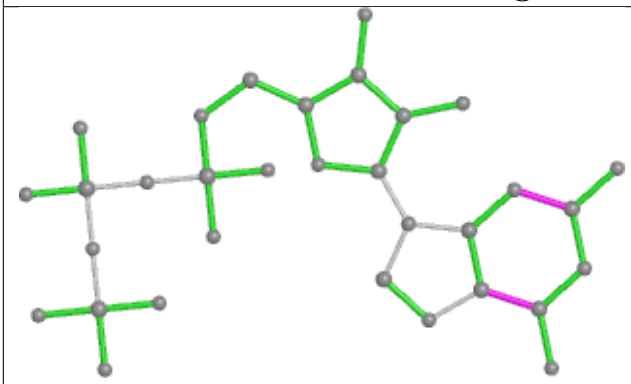


Rings

Ligand GTP FL 501



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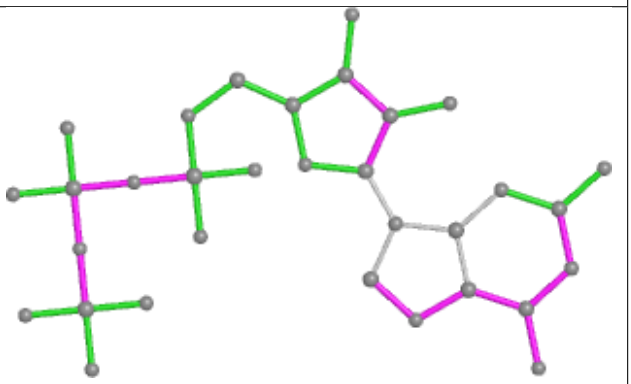

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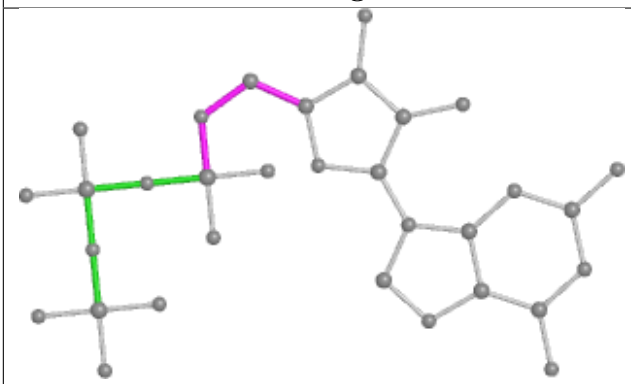

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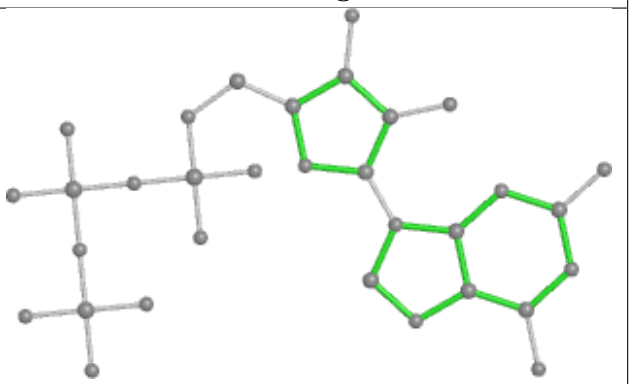
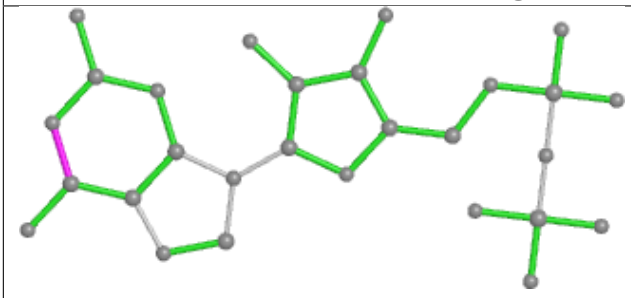


Rings

Ligand GDP FG 501



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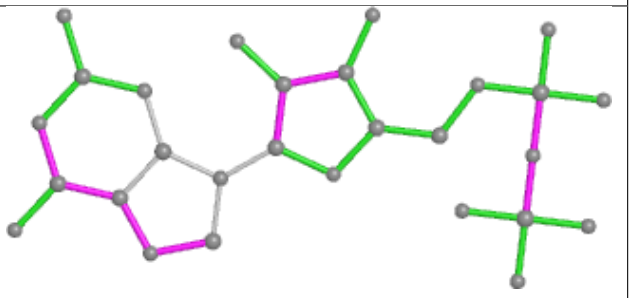

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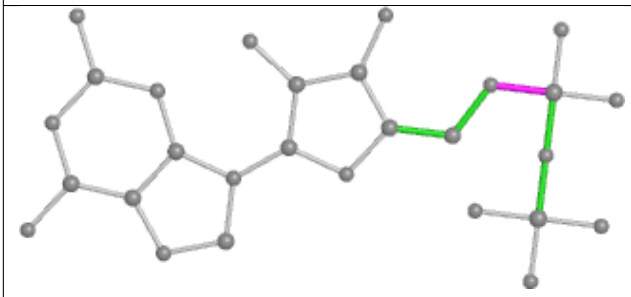

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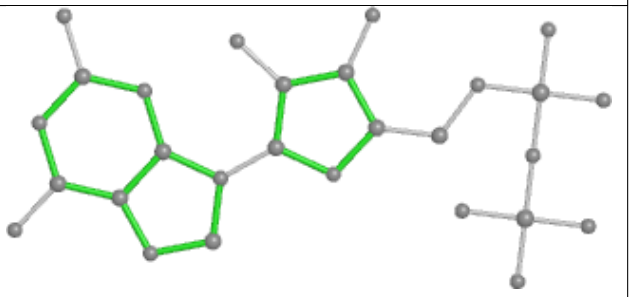
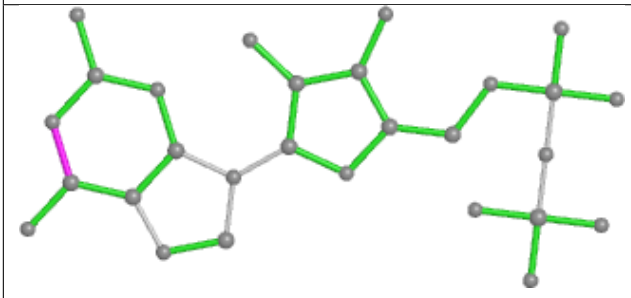


Rings

Ligand GDP LE 501



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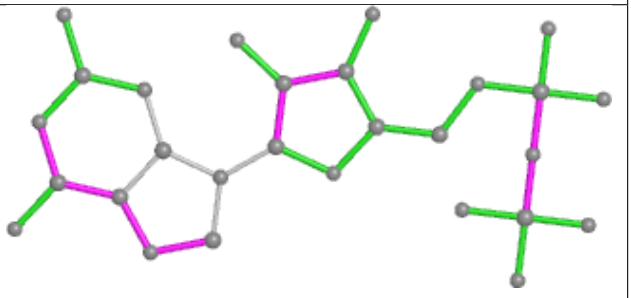

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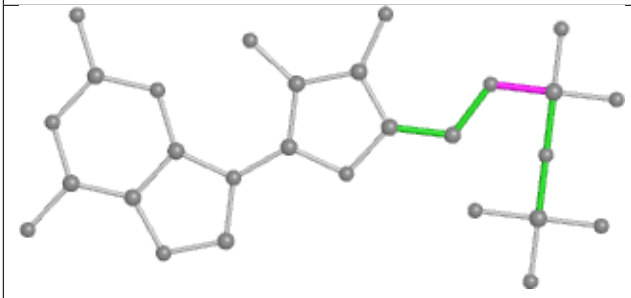

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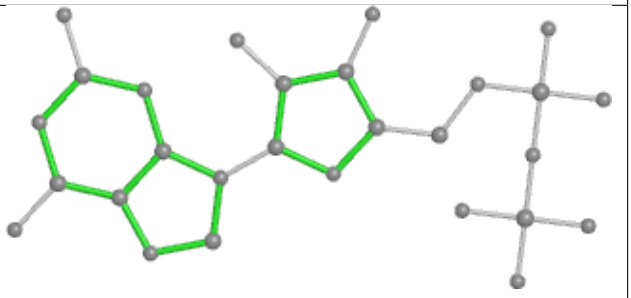
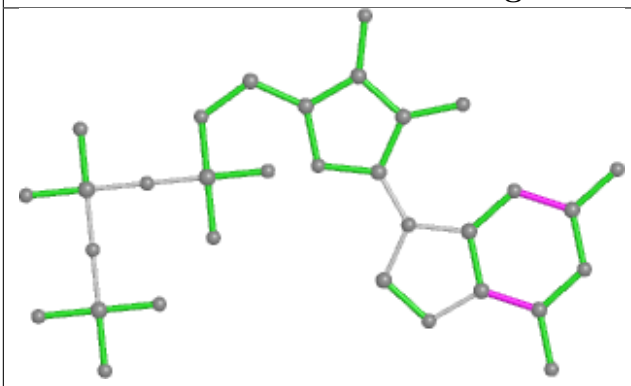


Rings

Ligand GTP MH 501



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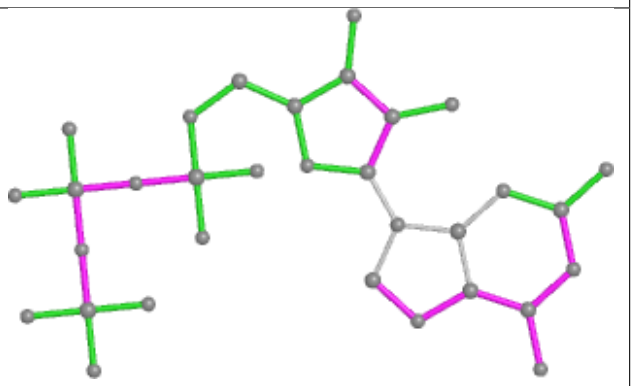

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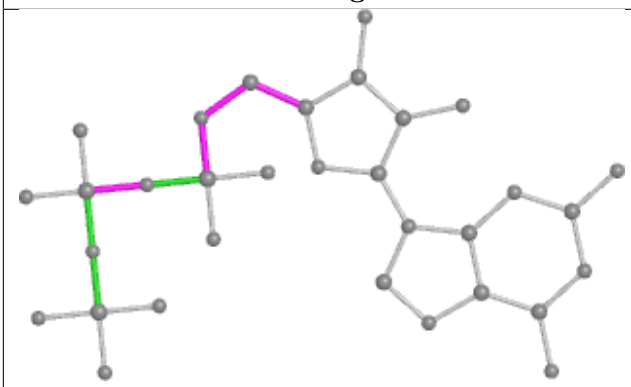

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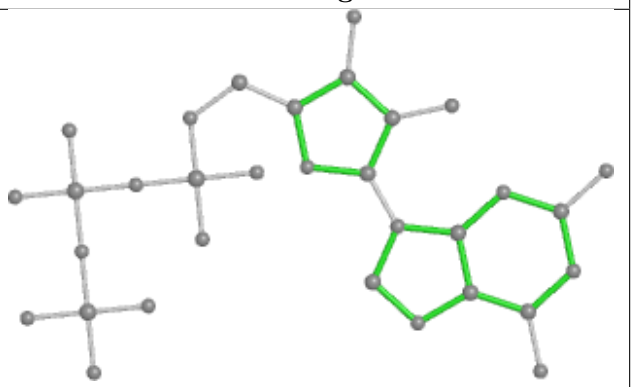
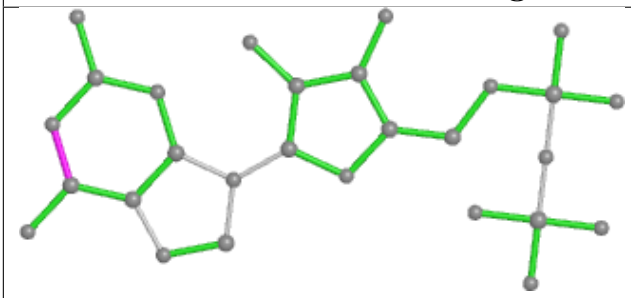


Rings

Ligand GDP AC 501



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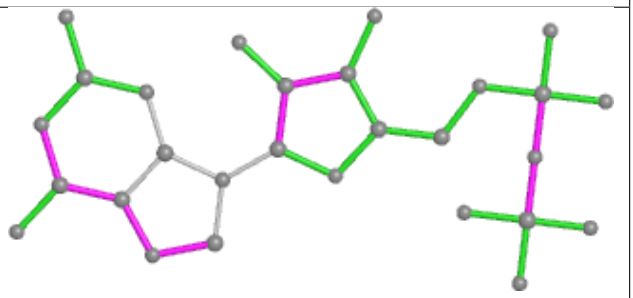

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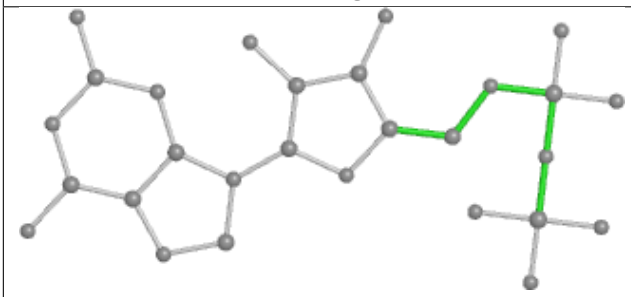
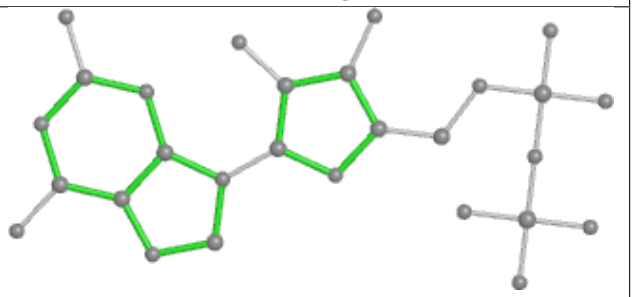
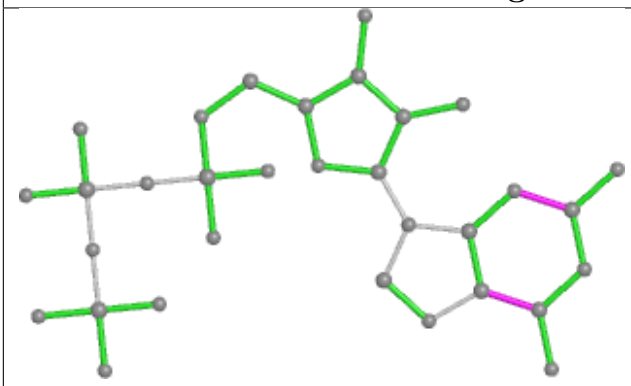


Torsions



Rings

Ligand GTP HD 501



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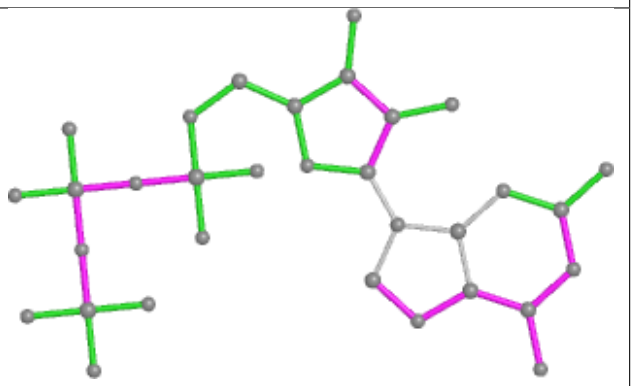

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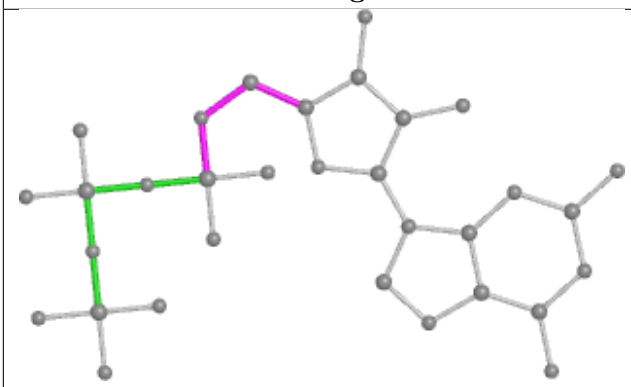

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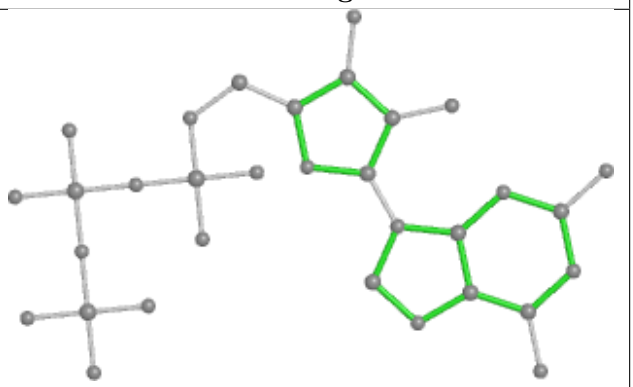

Rings

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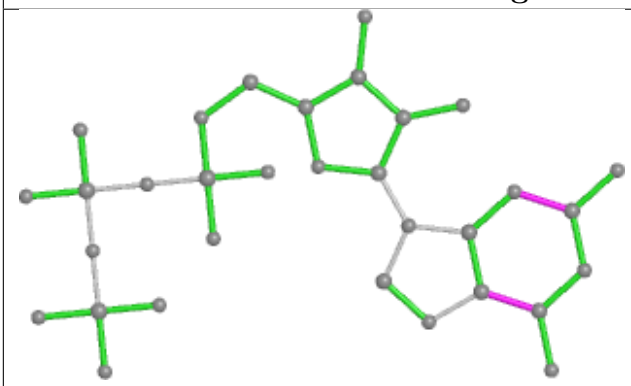

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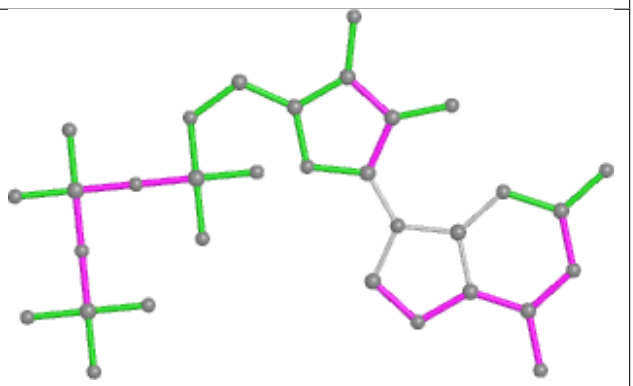

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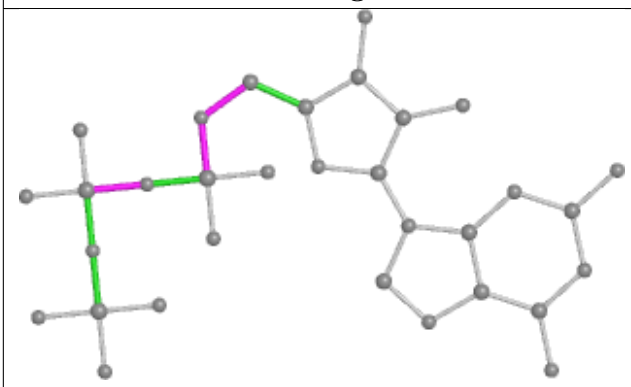

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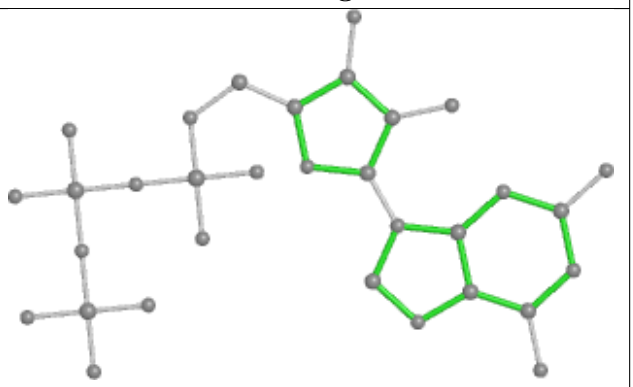

Rings

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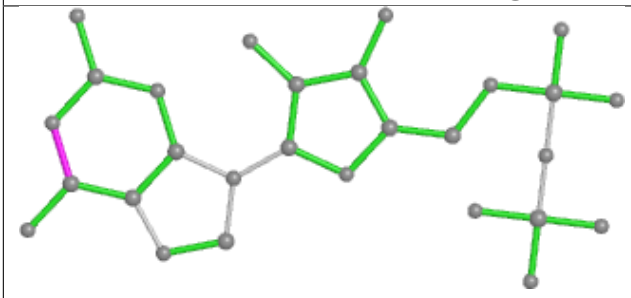

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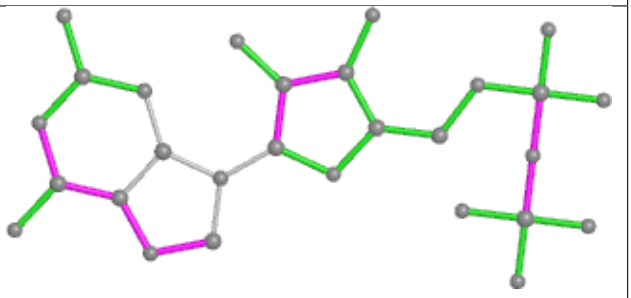

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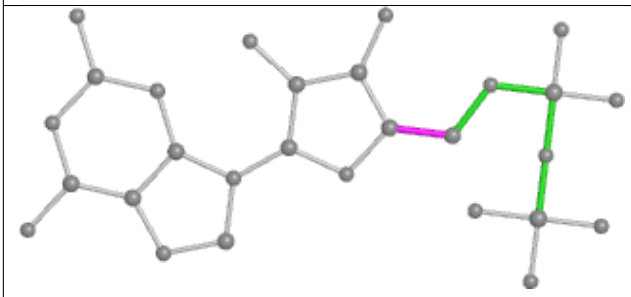

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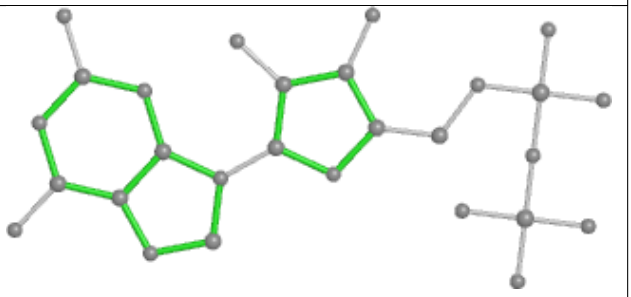
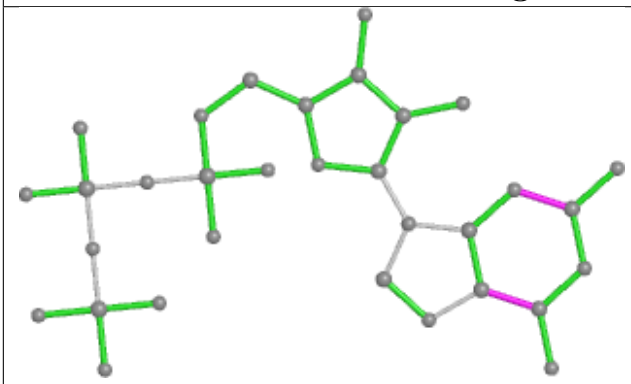


Rings

Ligand GTP FB 501



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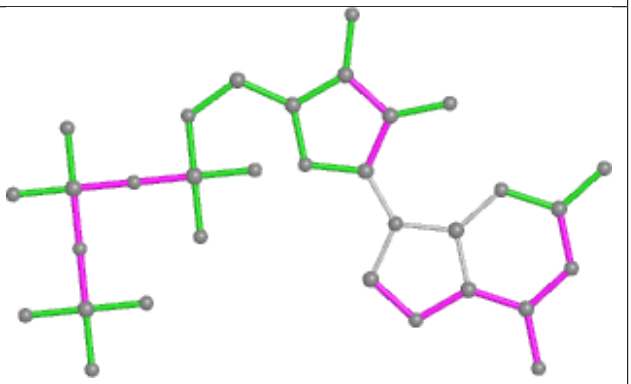

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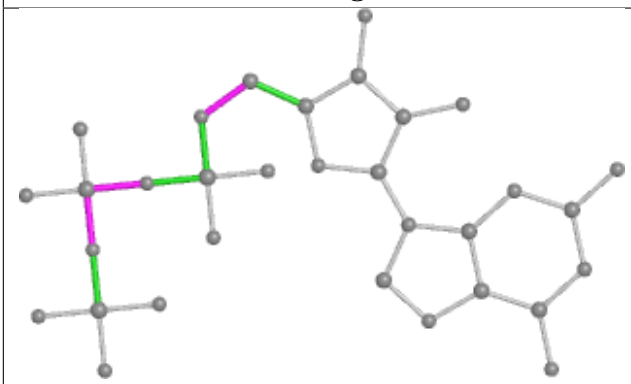

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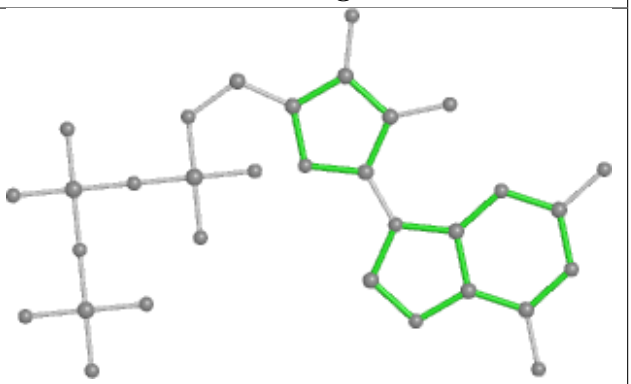

Rings

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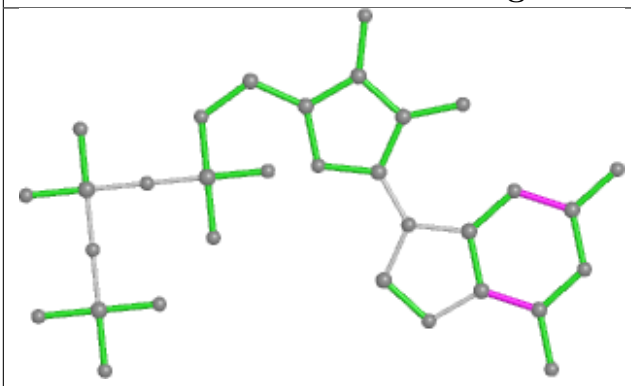

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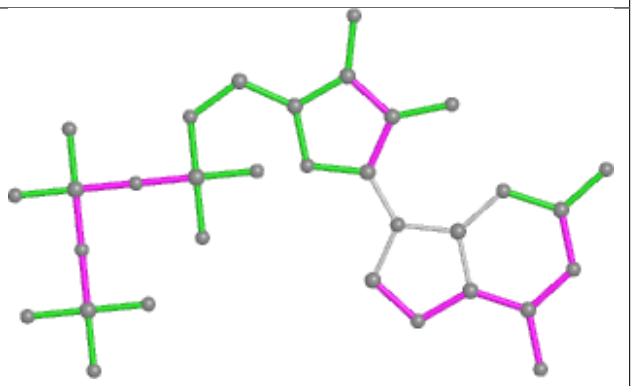

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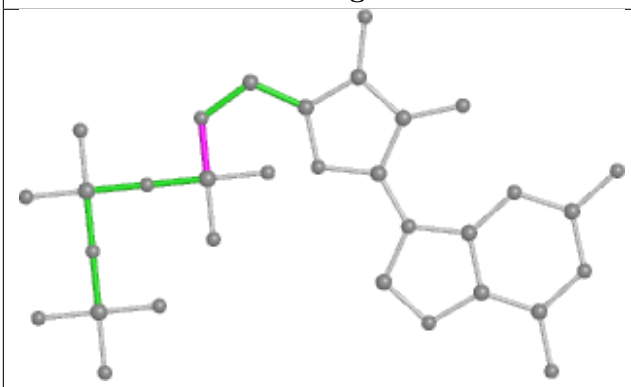

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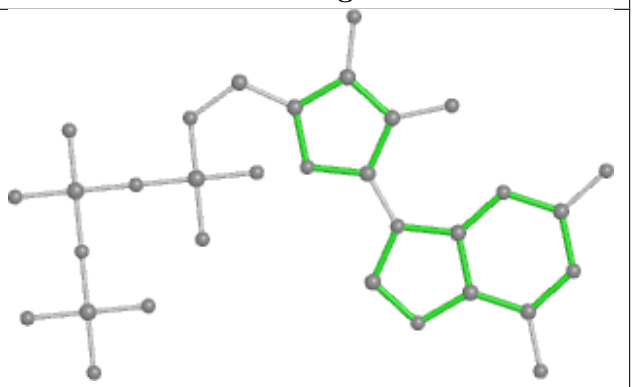

Rings

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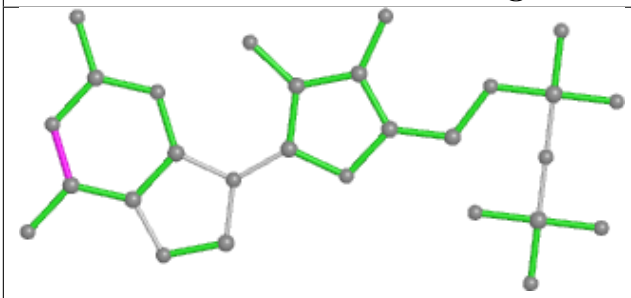

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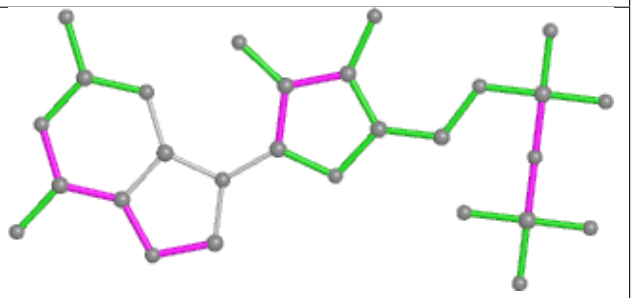

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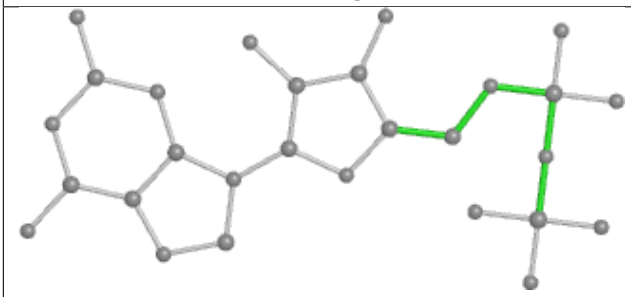

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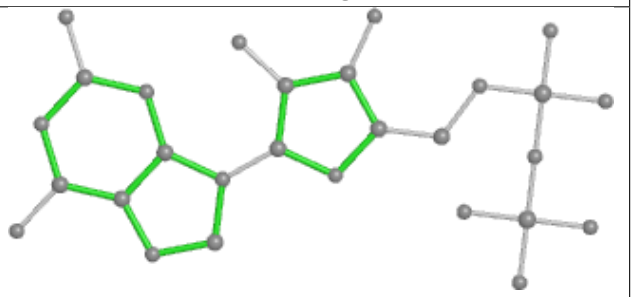

Rings

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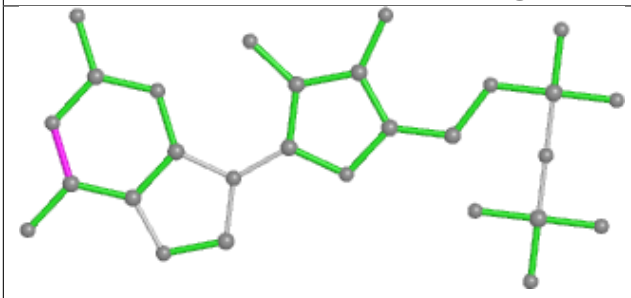

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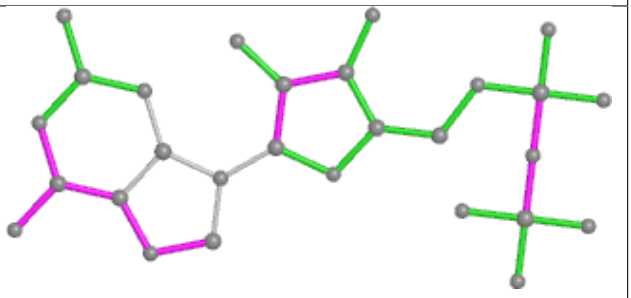

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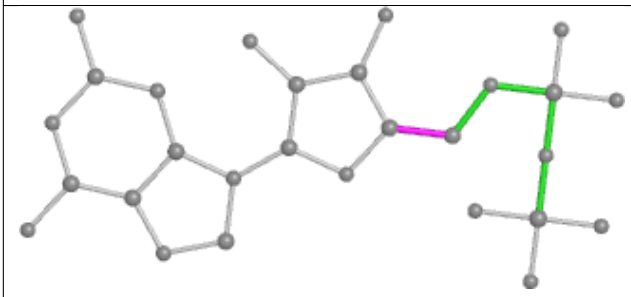

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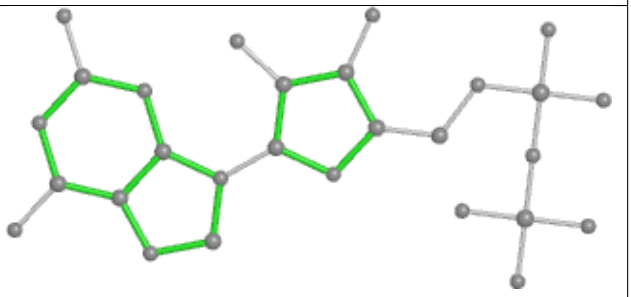

Rings

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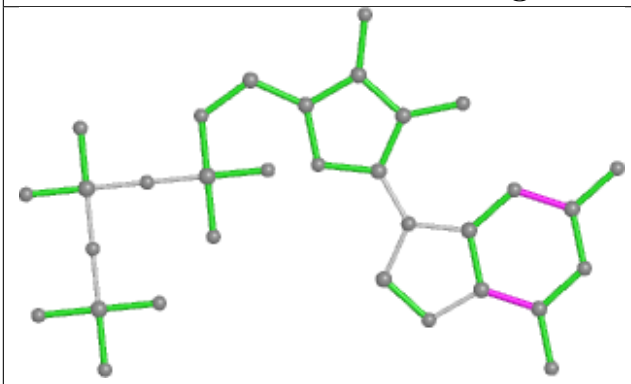

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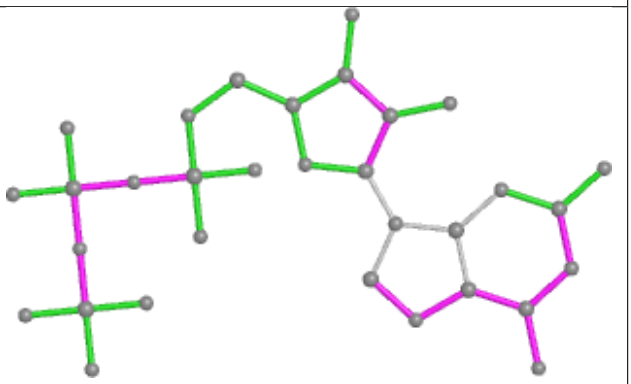

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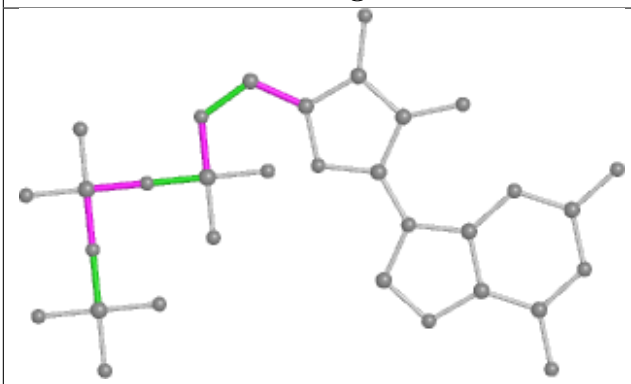

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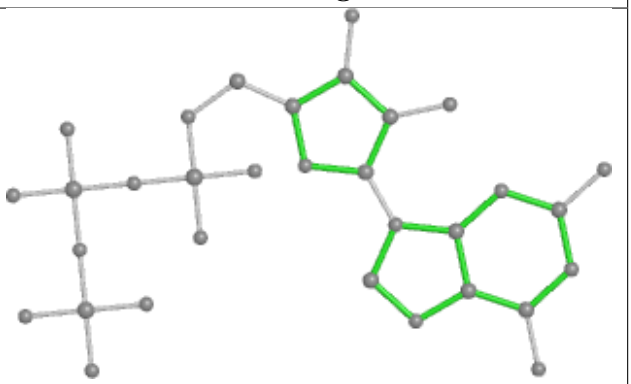
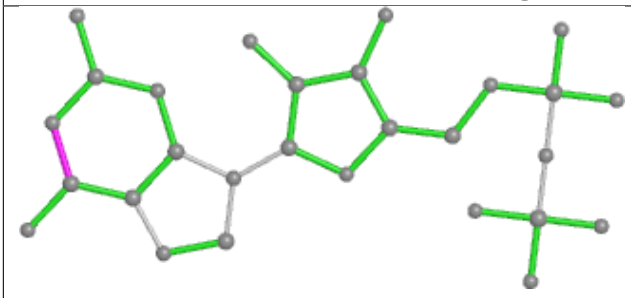
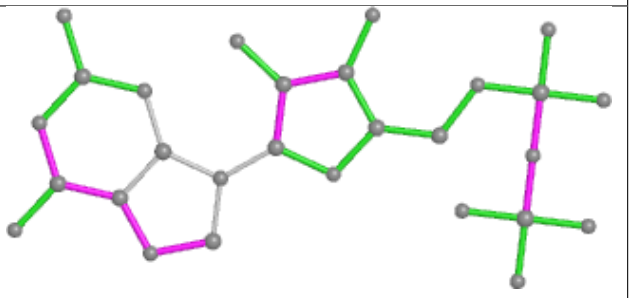
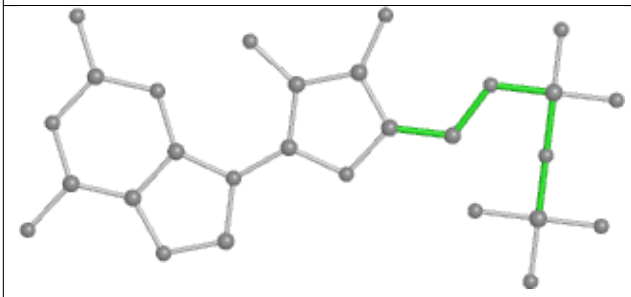
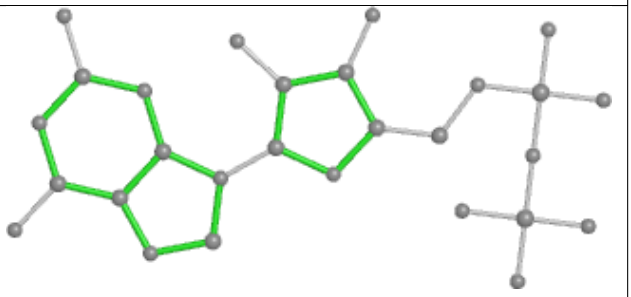
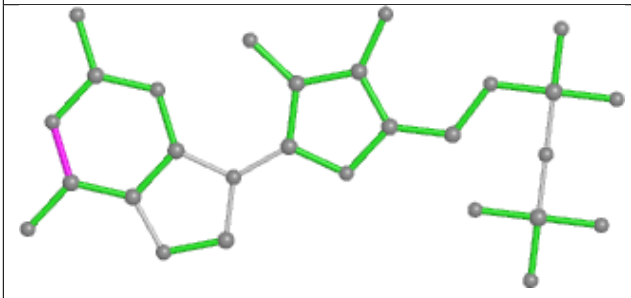
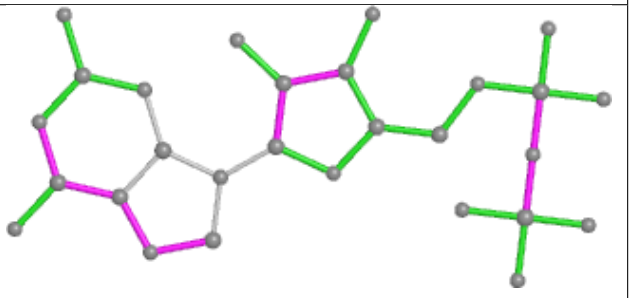
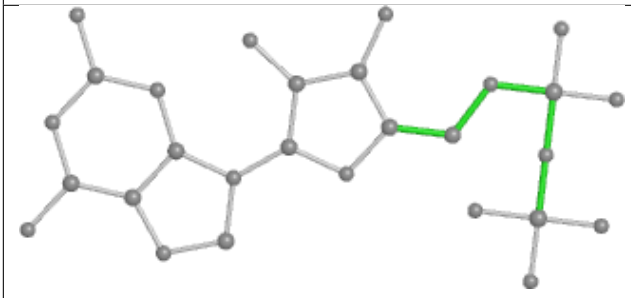
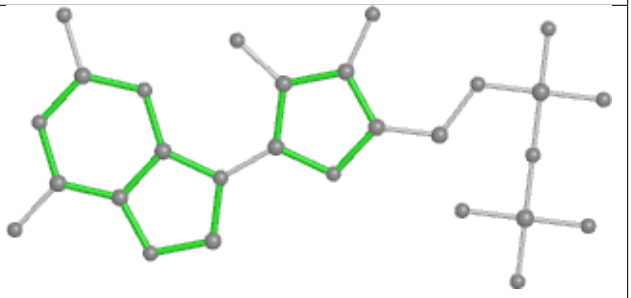
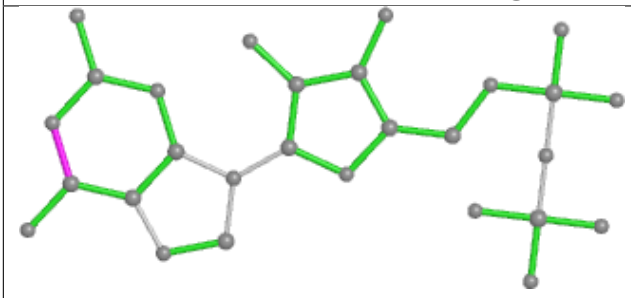


Rings

Ligand GDP EI 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP MC 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP BG 501



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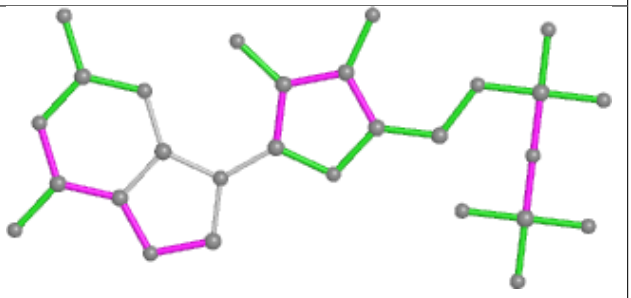

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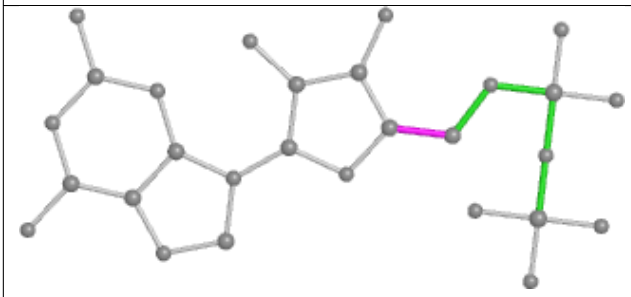

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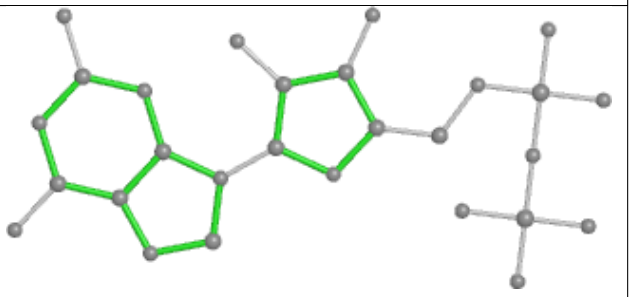

Rings

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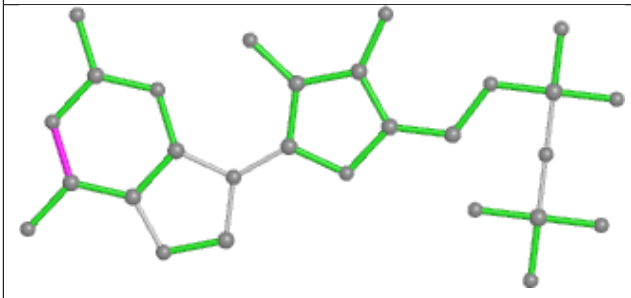

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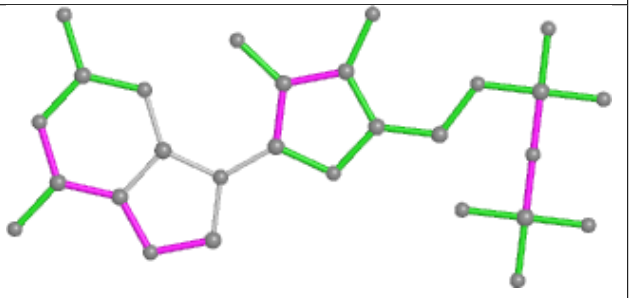

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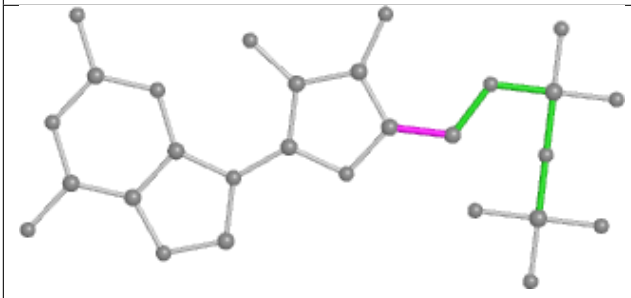

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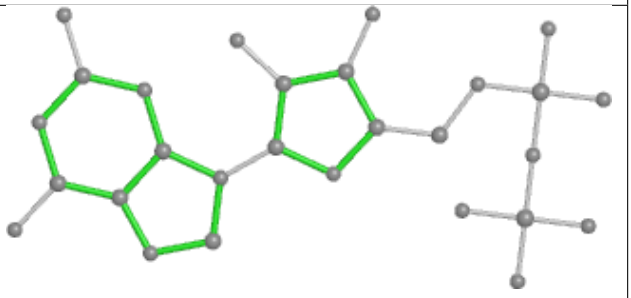

Rings

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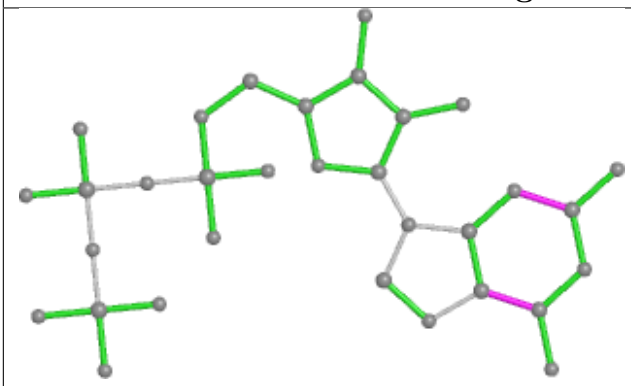

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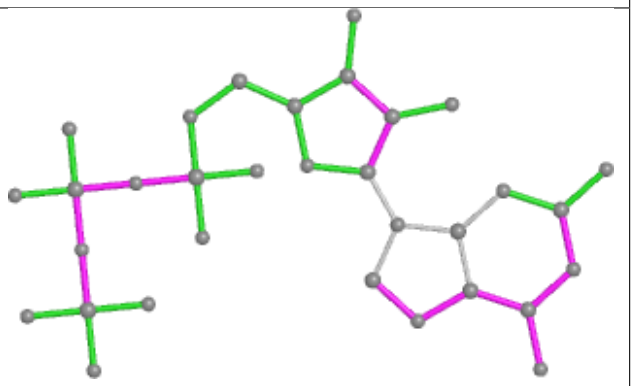
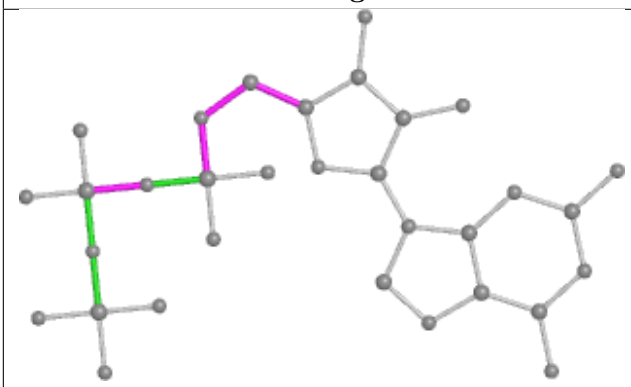


Bond angles



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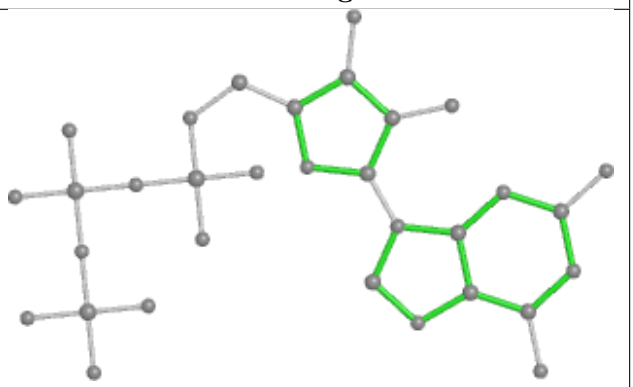
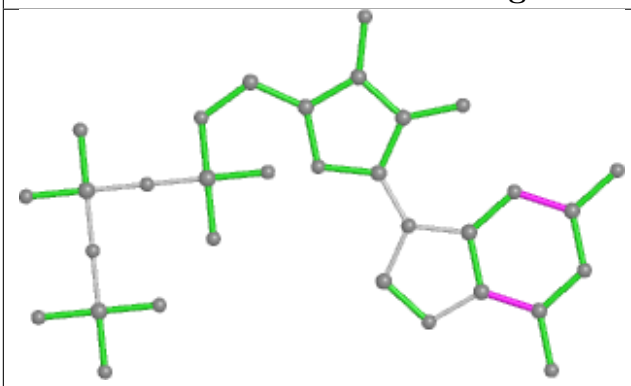


Rings

Ligand GTP CH 501



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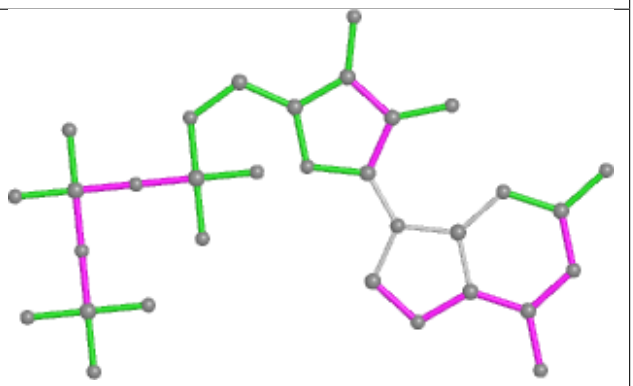
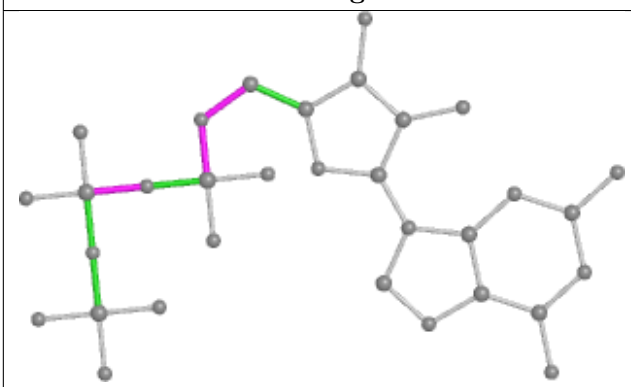


Bond angles



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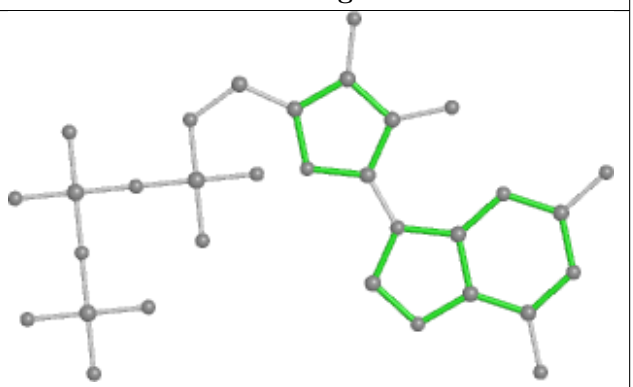
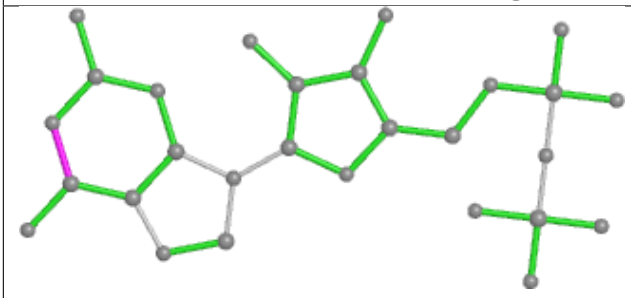
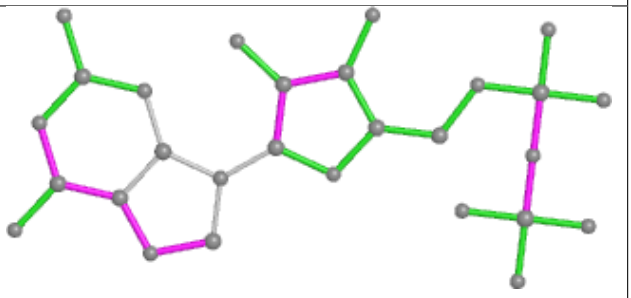
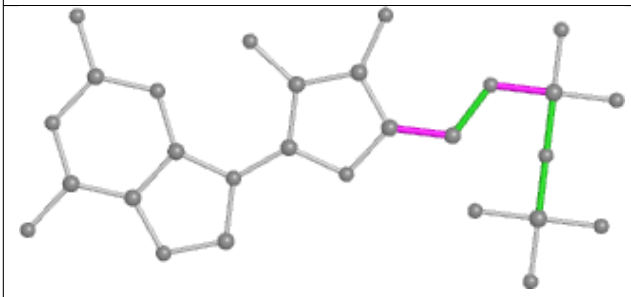
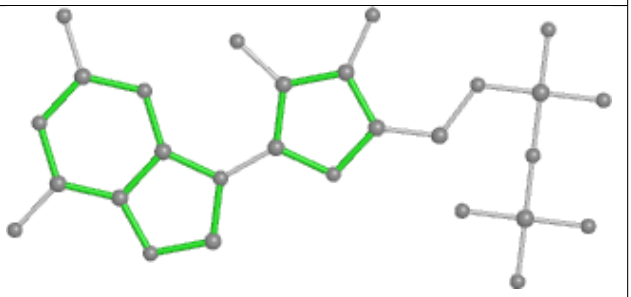


Rings

Ligand GDP CG 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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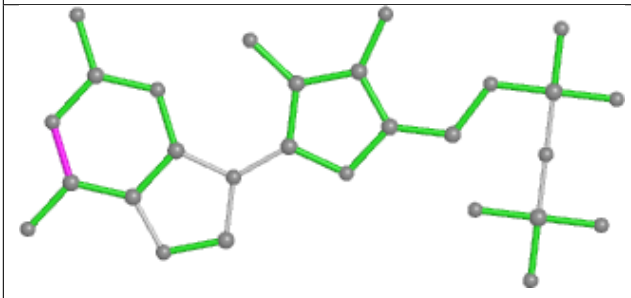
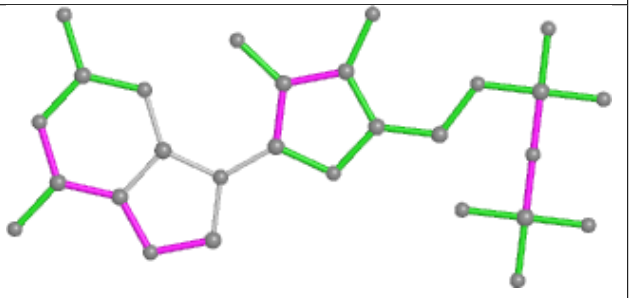
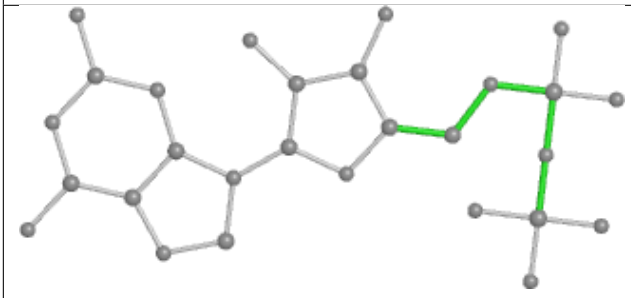
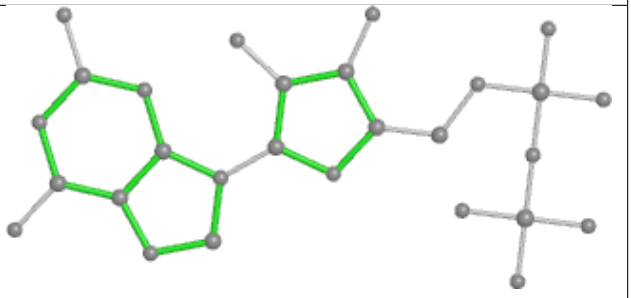
 Bond lengths	 Bond angles
 Torsions	 Rings

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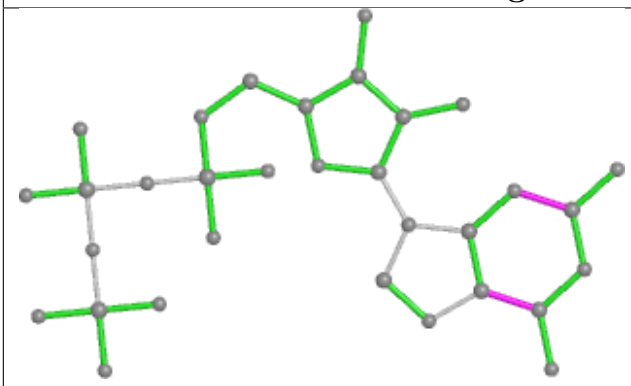

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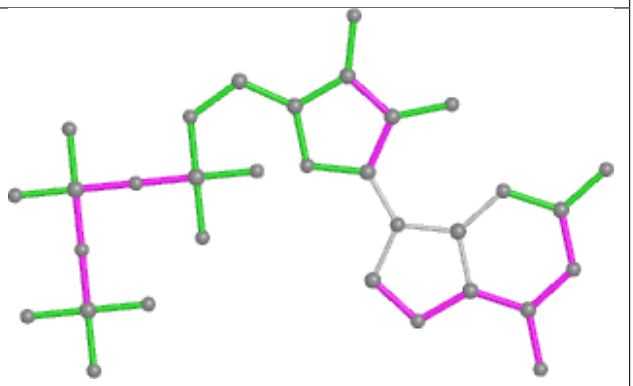

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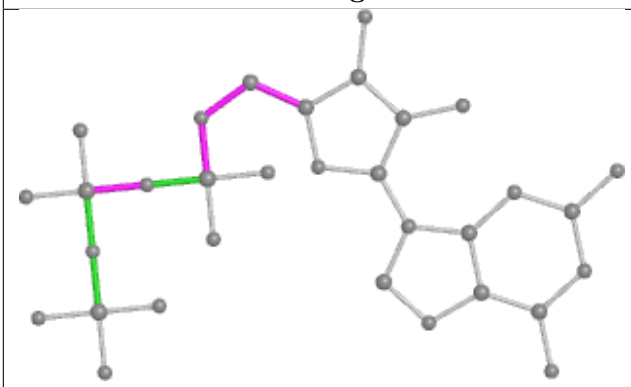

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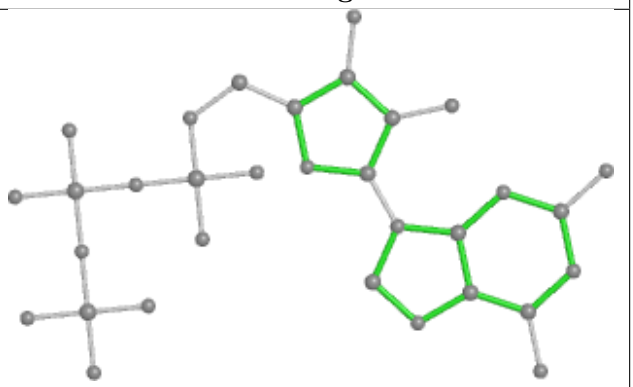

Rings

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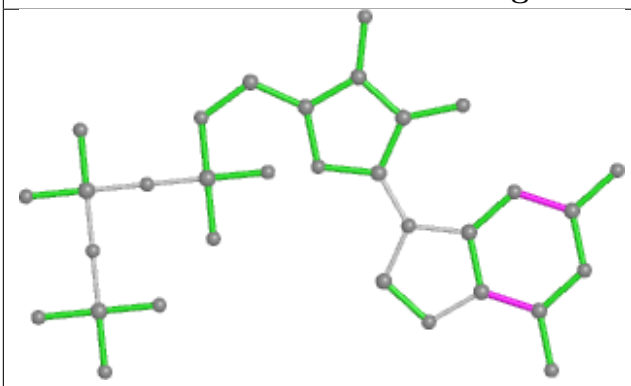

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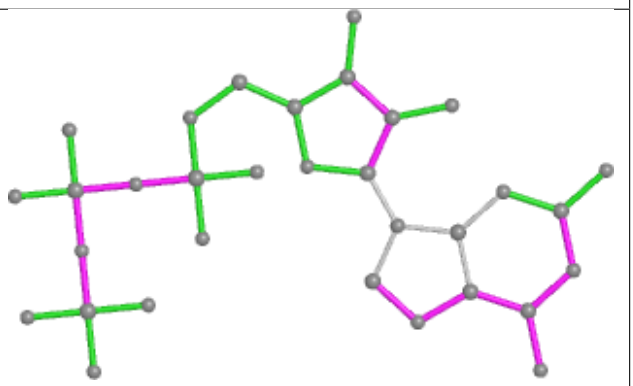

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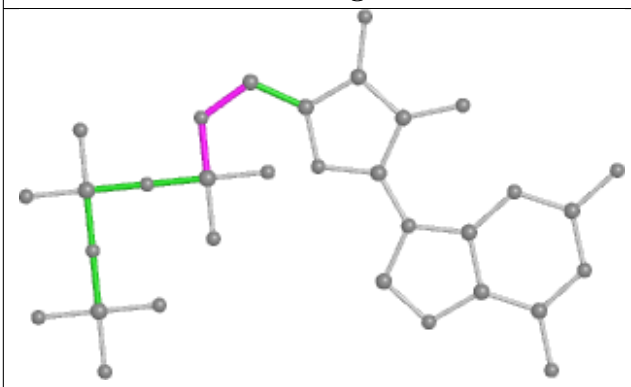

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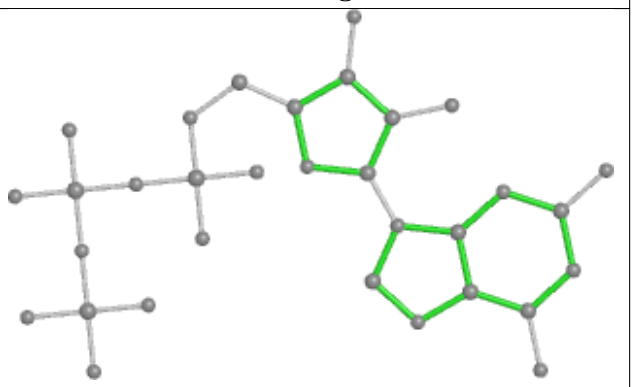
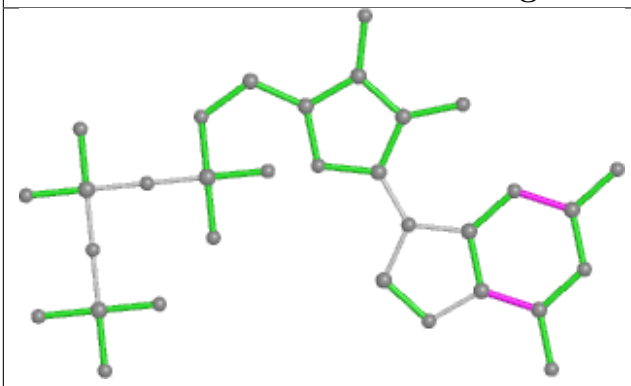


Rings

Ligand GTP IJ 501



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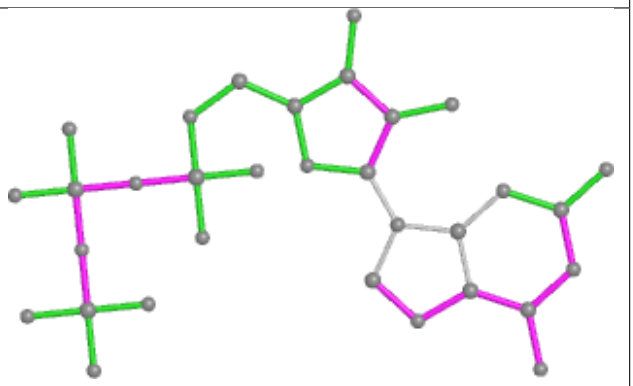

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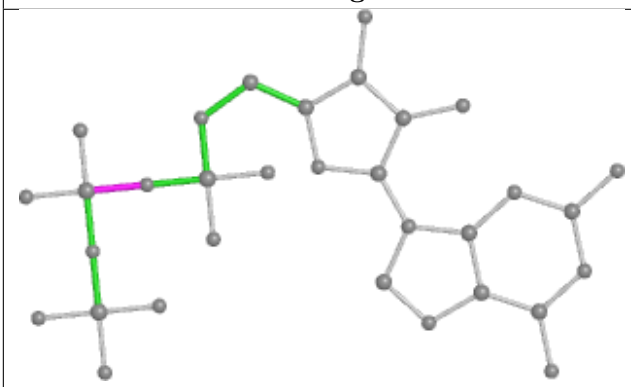

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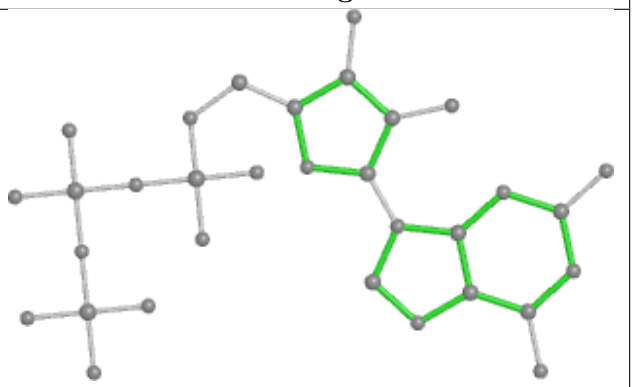

Rings

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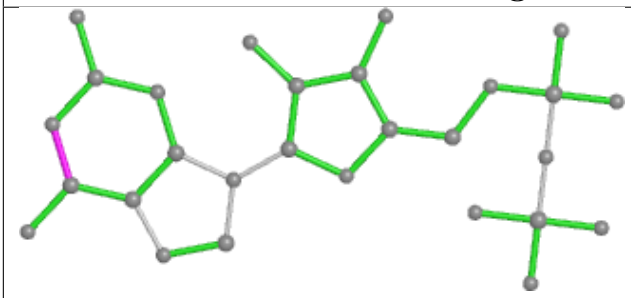

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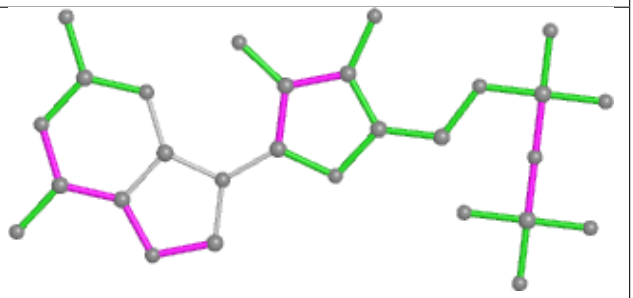

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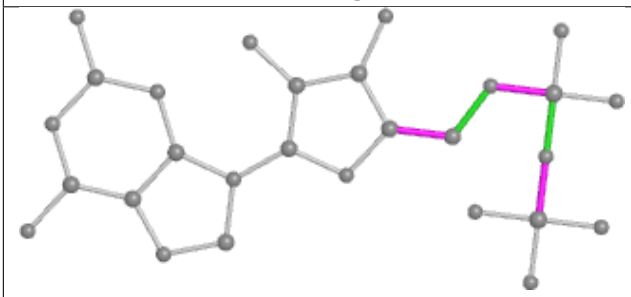

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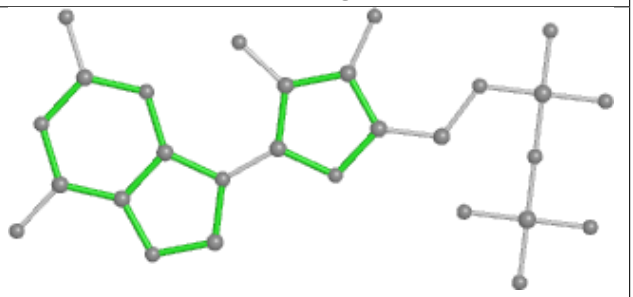
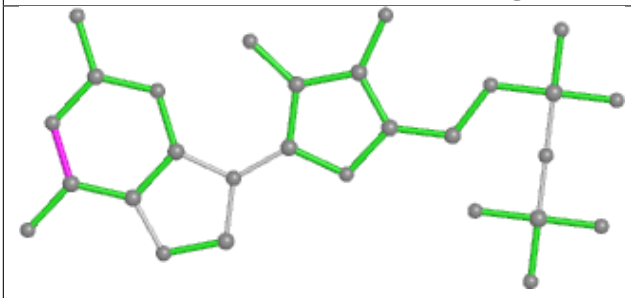


Rings

Ligand GDP CC 501



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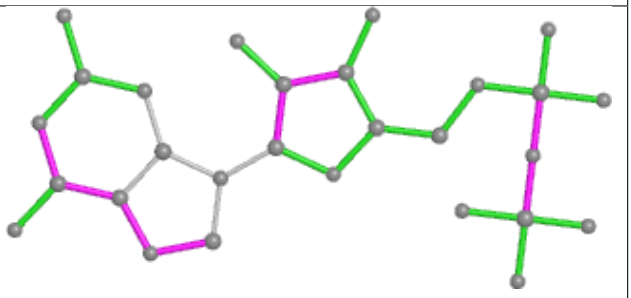

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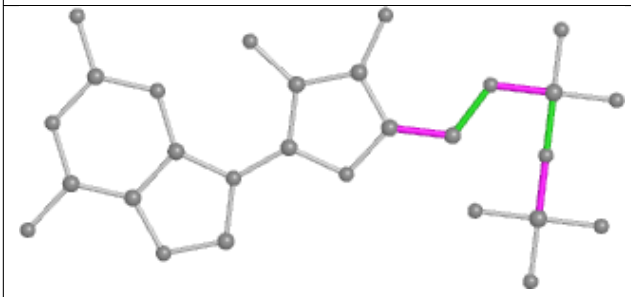

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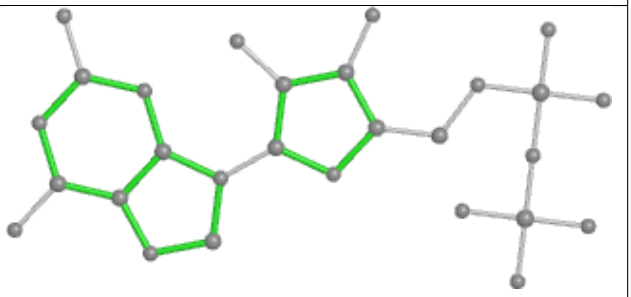

Rings

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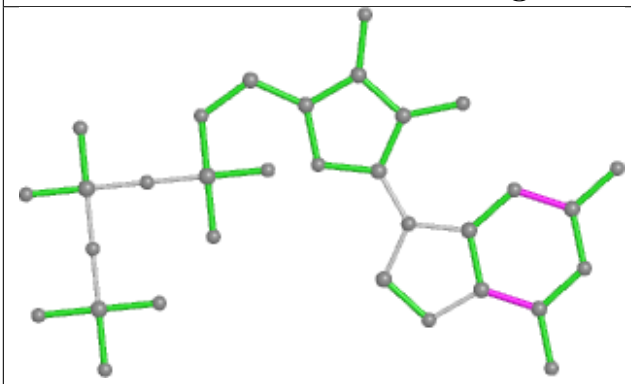

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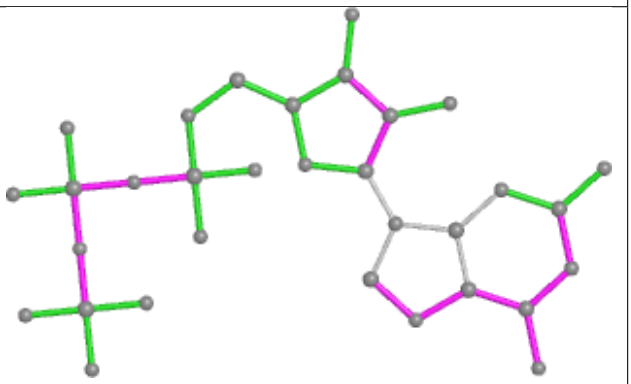

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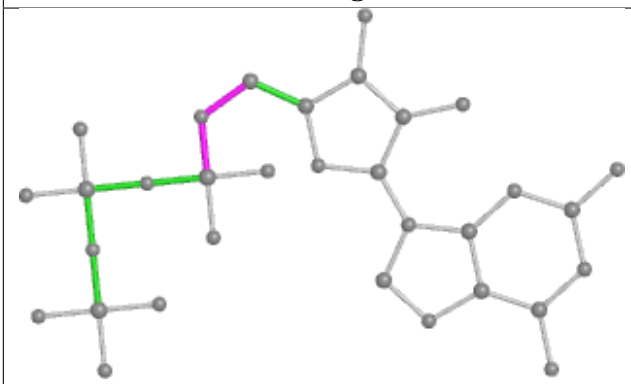

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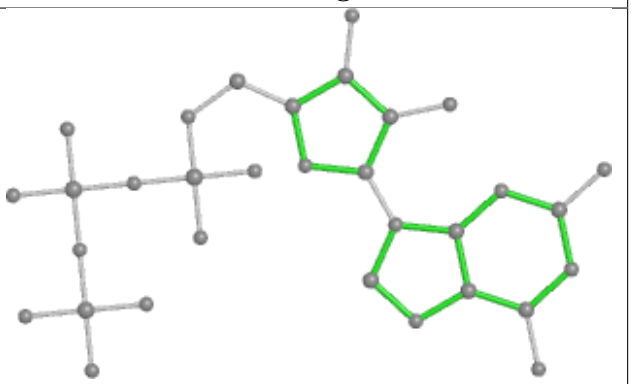

Rings

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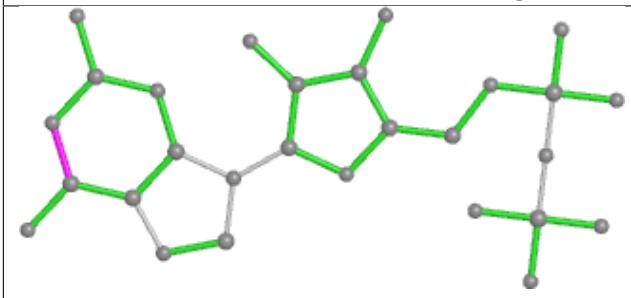

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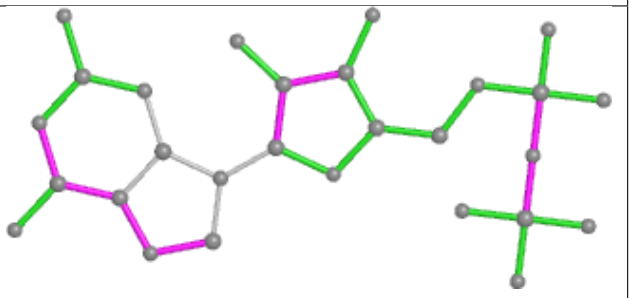

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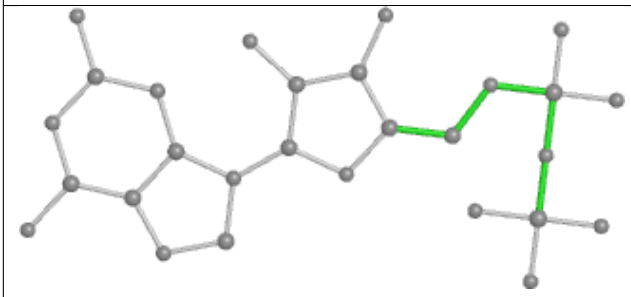

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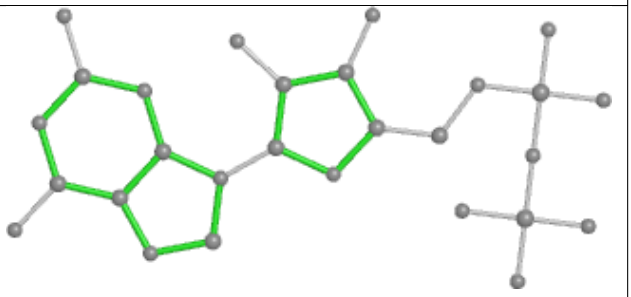

Rings

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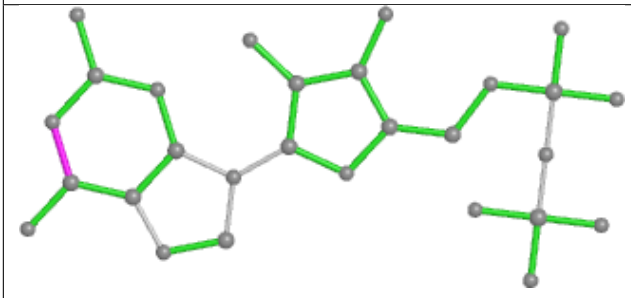

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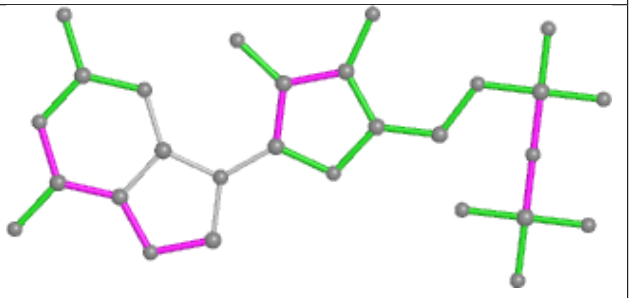

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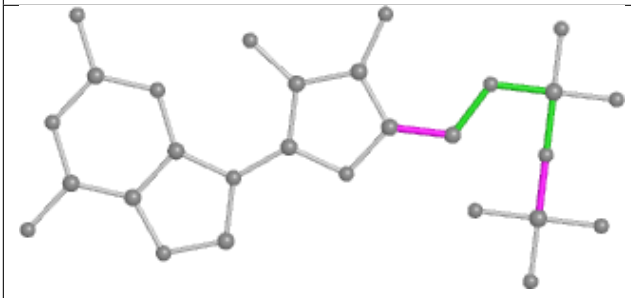

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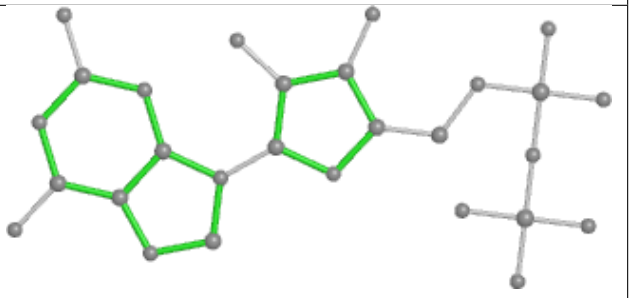

Rings

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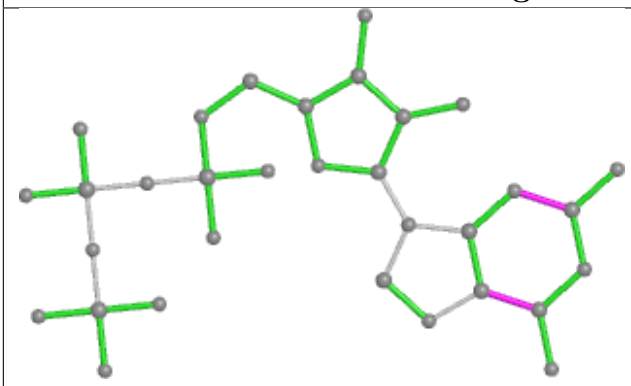

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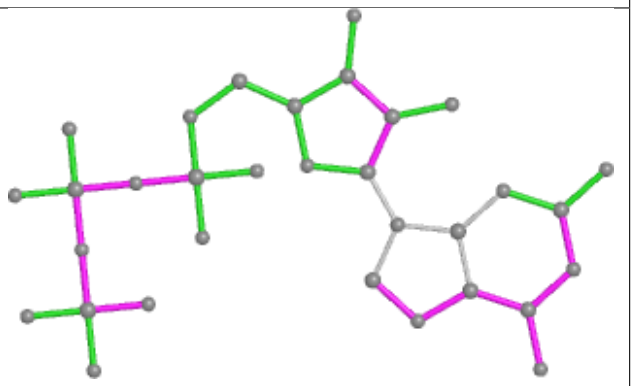

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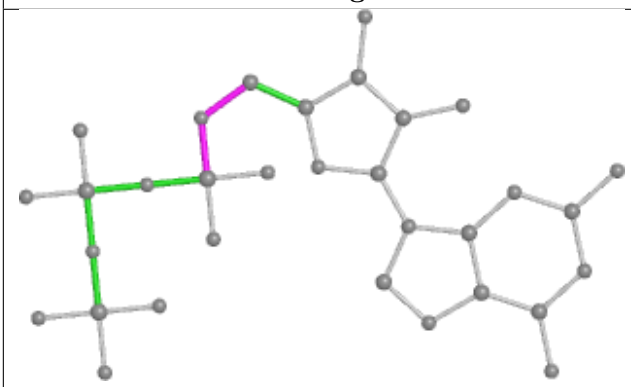

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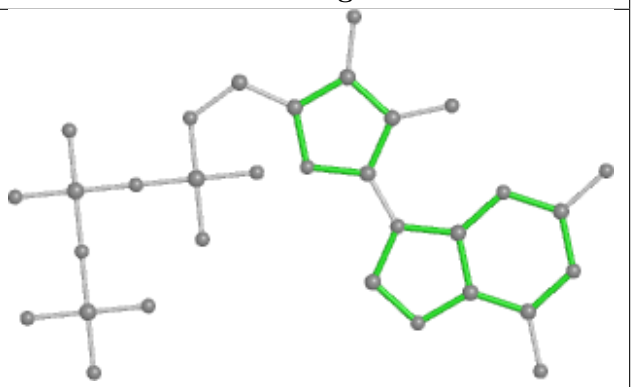

Rings

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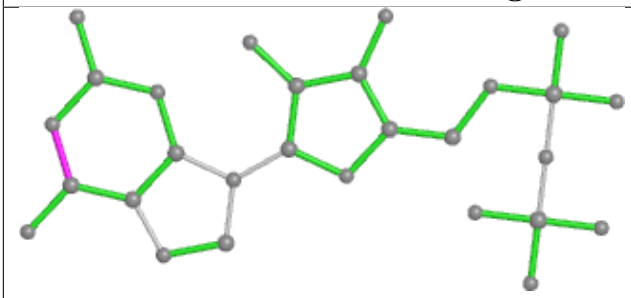

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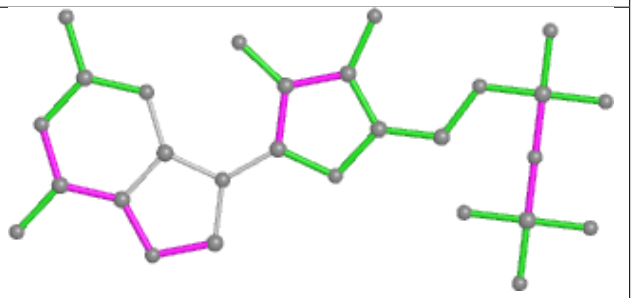

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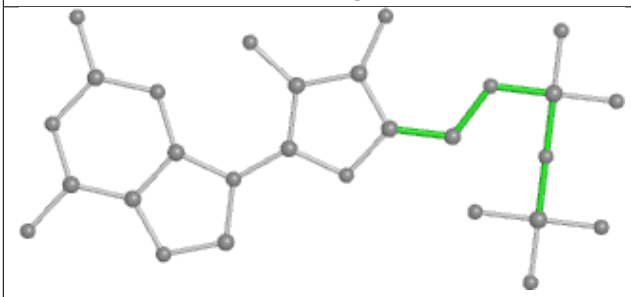

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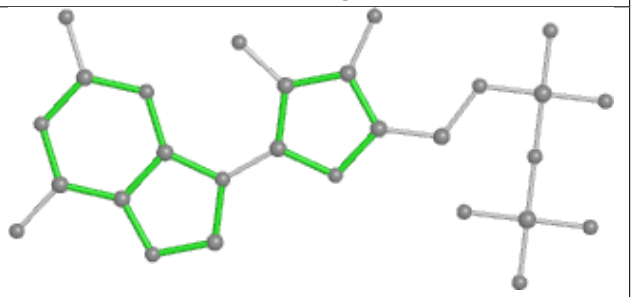

Rings

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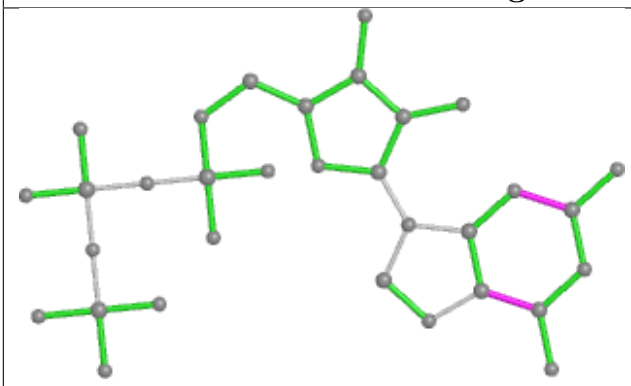

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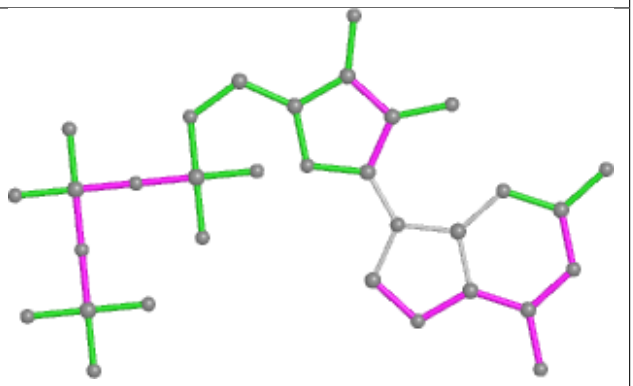

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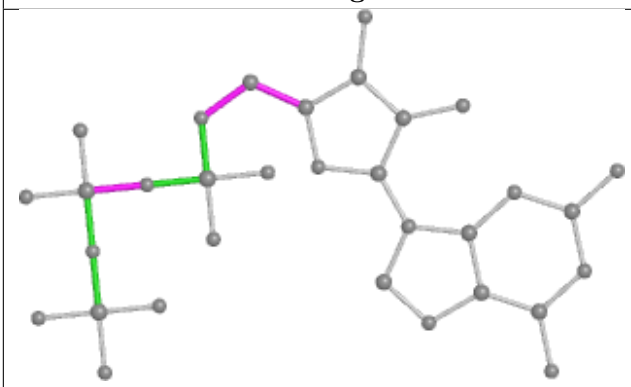

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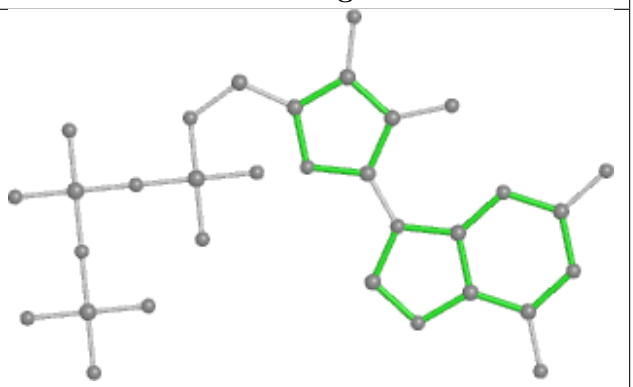
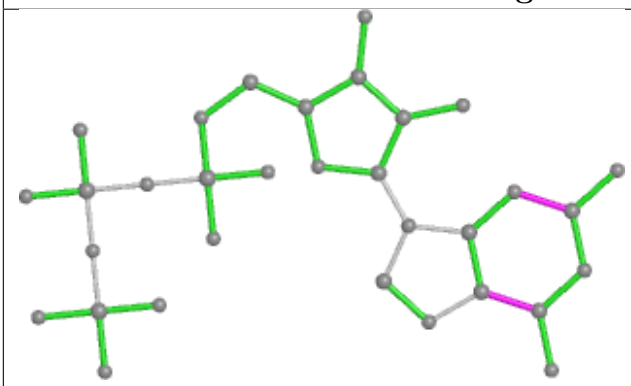


Rings

Ligand GTP LJ 501



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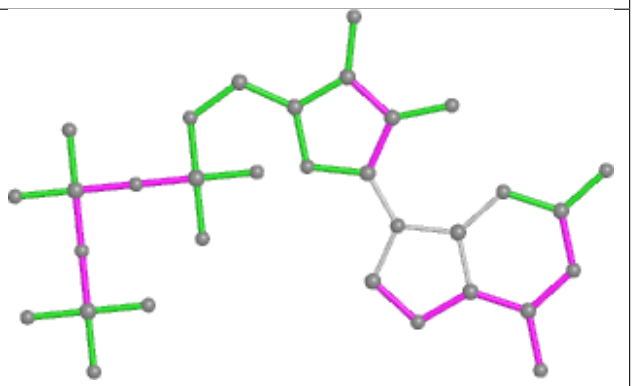

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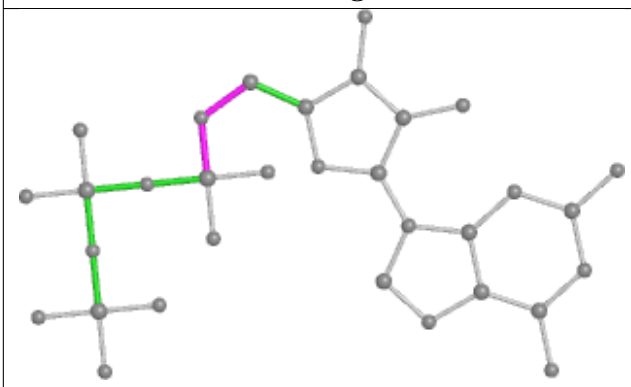

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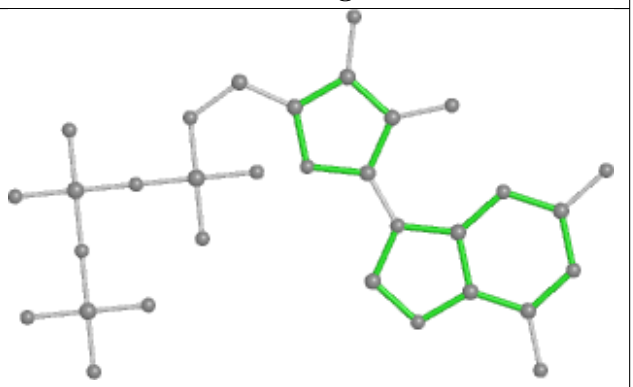

Rings

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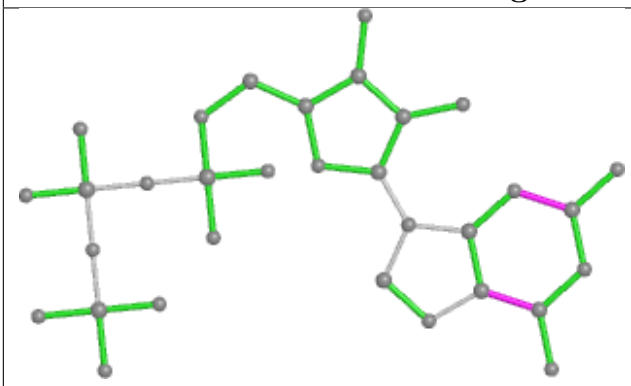

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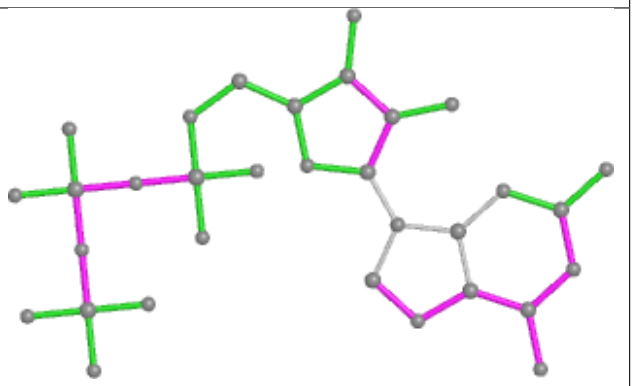

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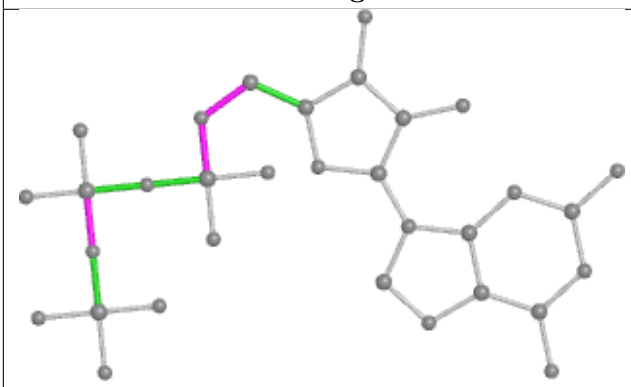

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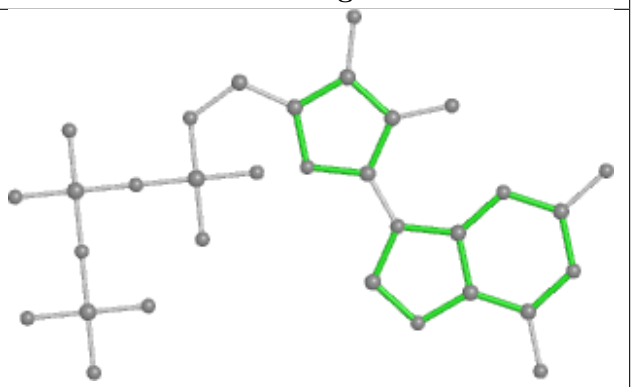
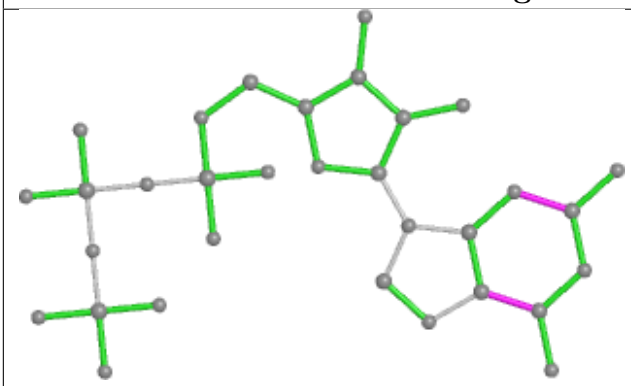


Rings

Ligand GTP JB 501



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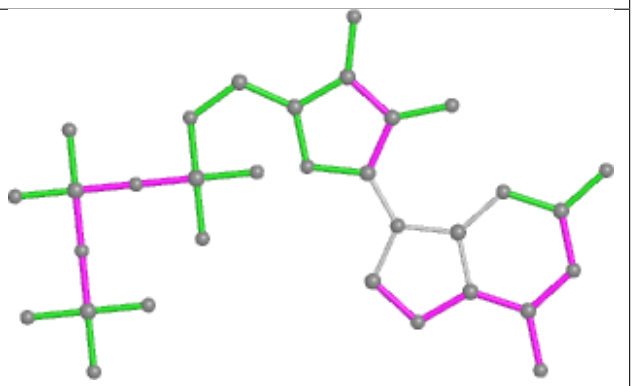
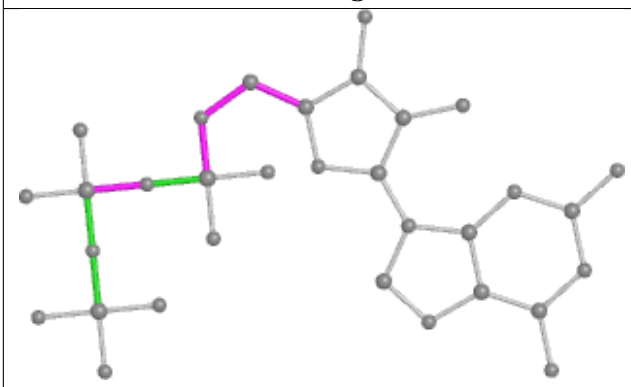
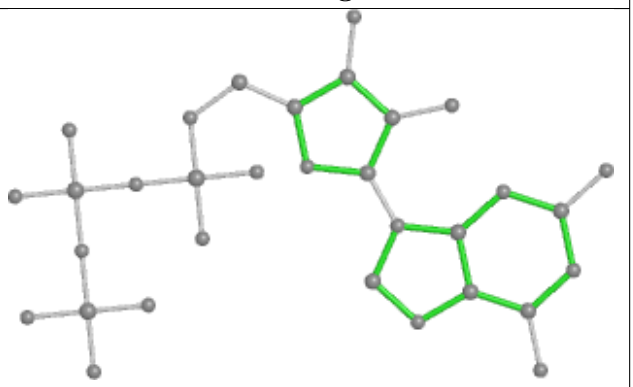


Bond angles

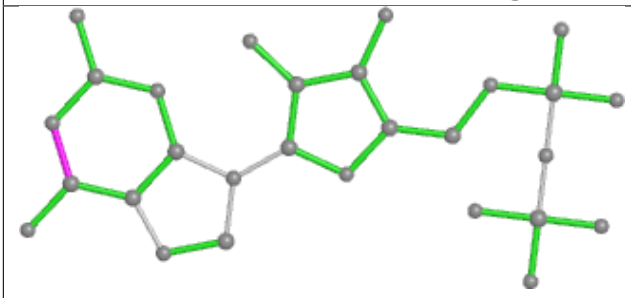


Torsions



Rings

Ligand GDP HG 501



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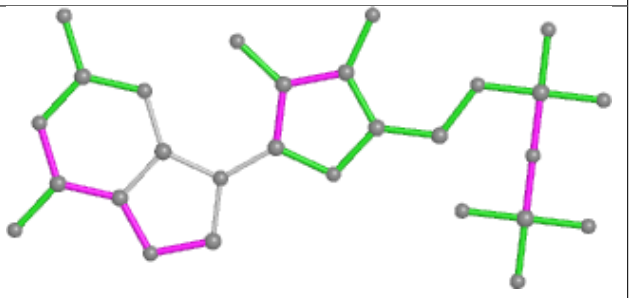

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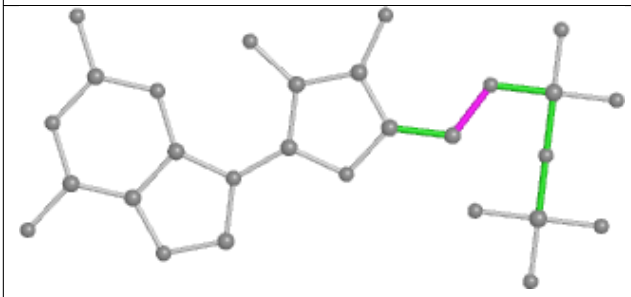

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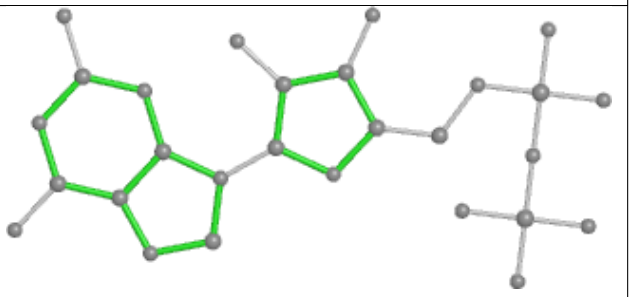
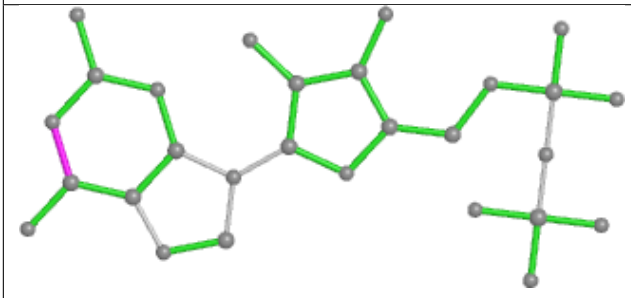


Rings

Ligand GDP LK 501



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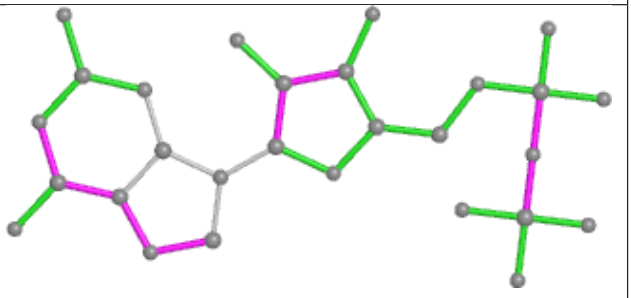

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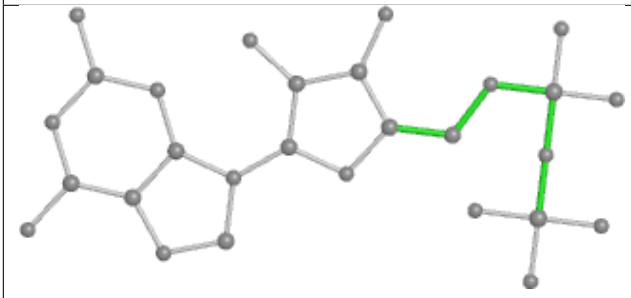

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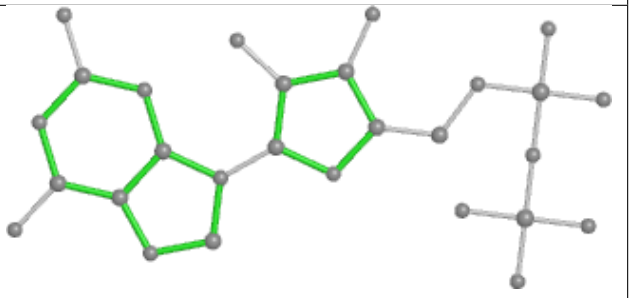
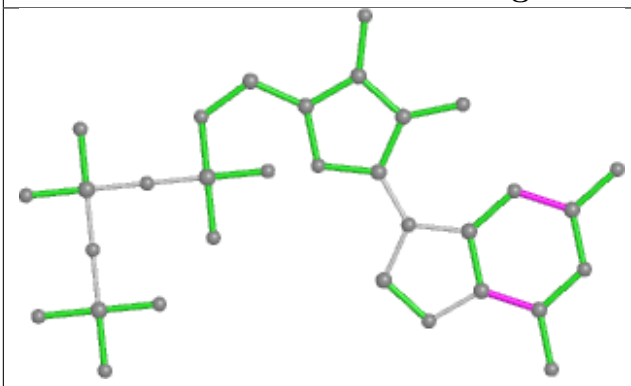


Rings

Ligand GTP BF 501



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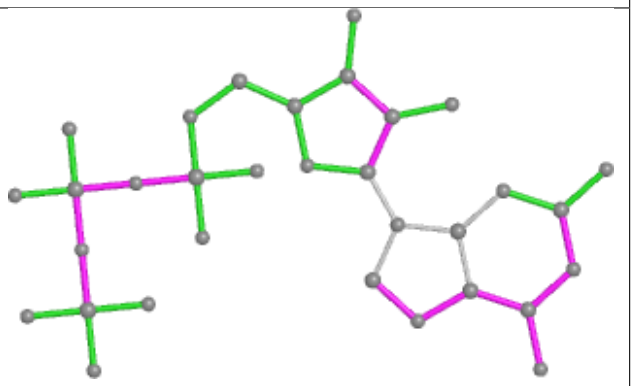

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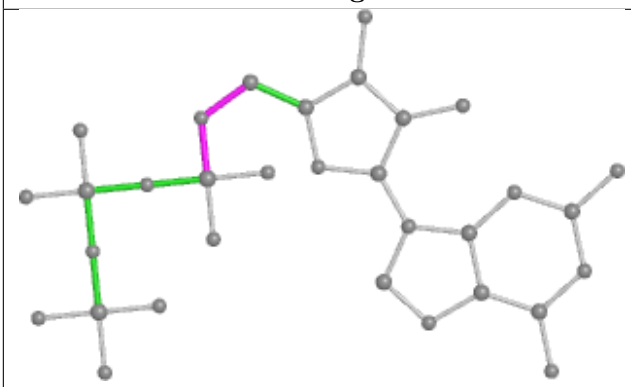

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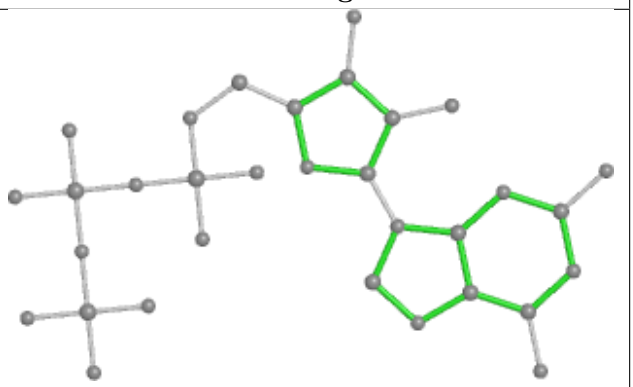
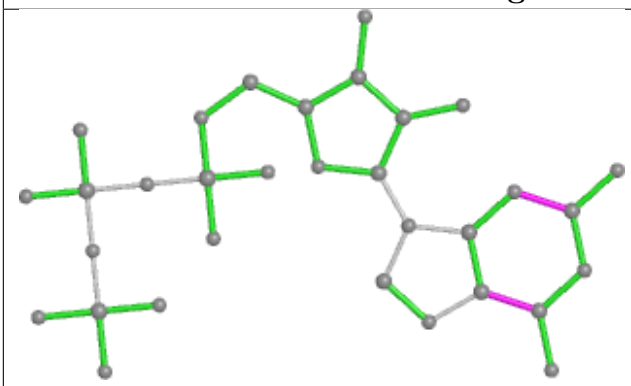


Rings

Ligand GTP GH 501



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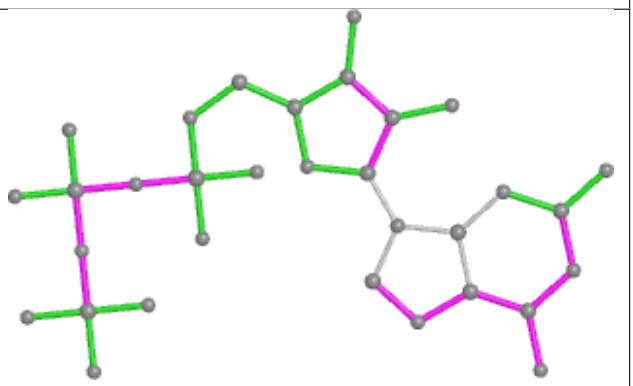

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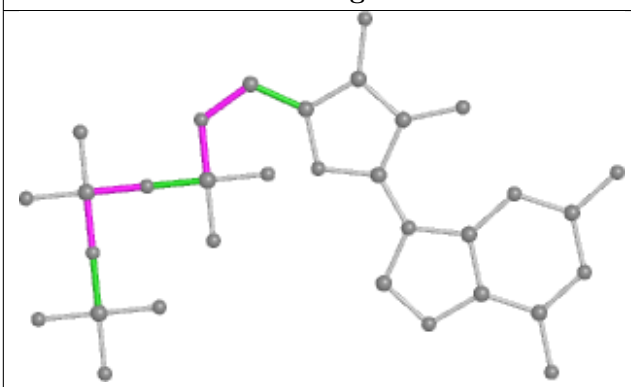

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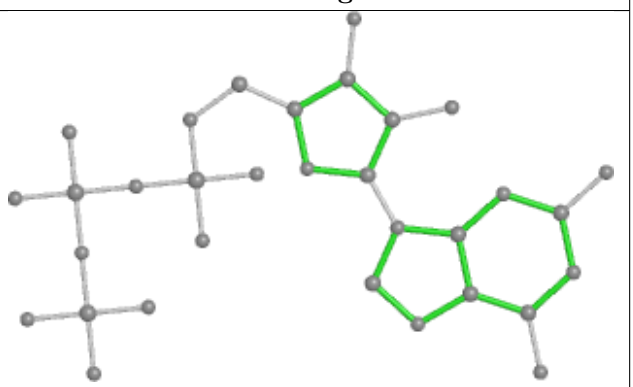

Rings

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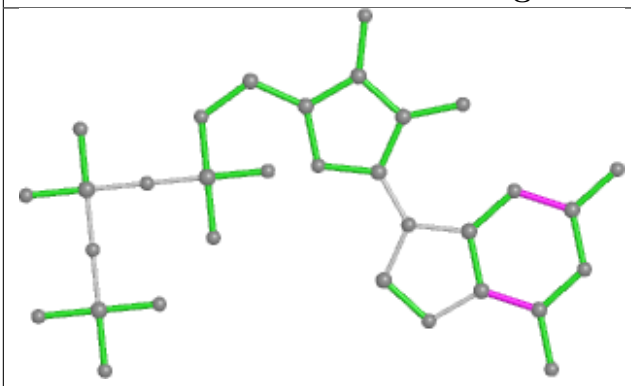

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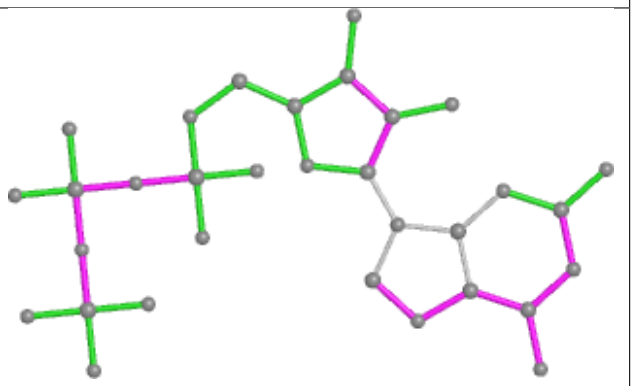

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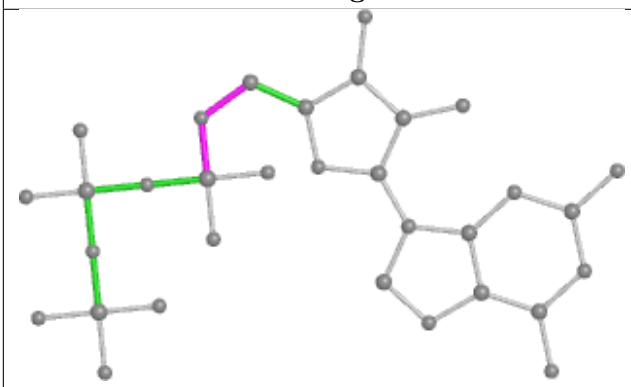

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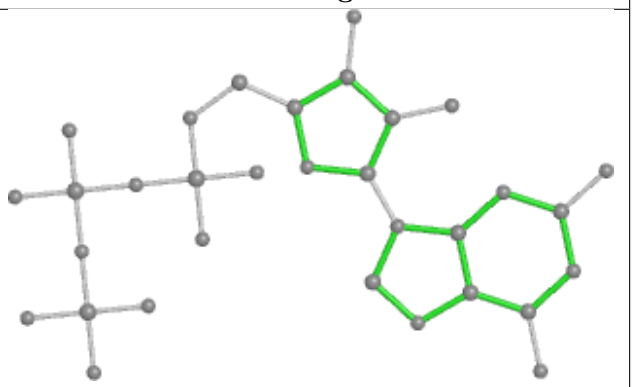

Rings

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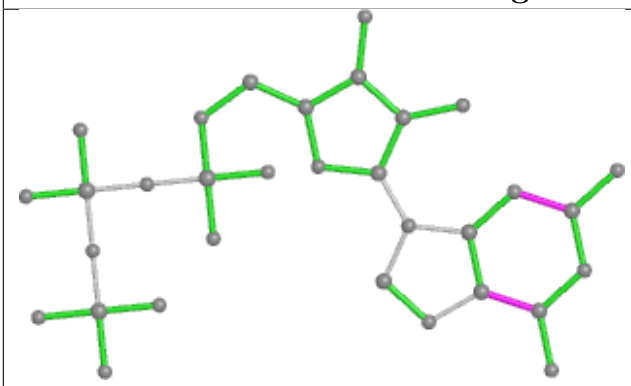

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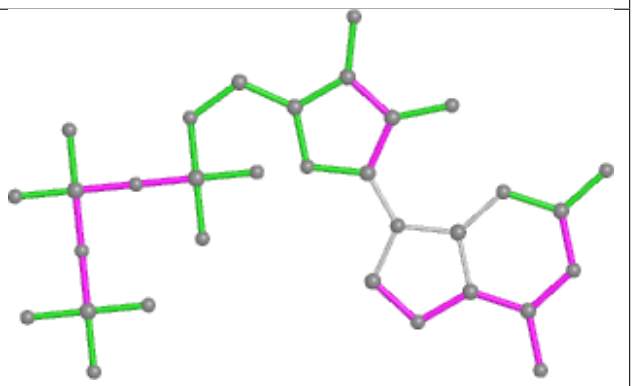

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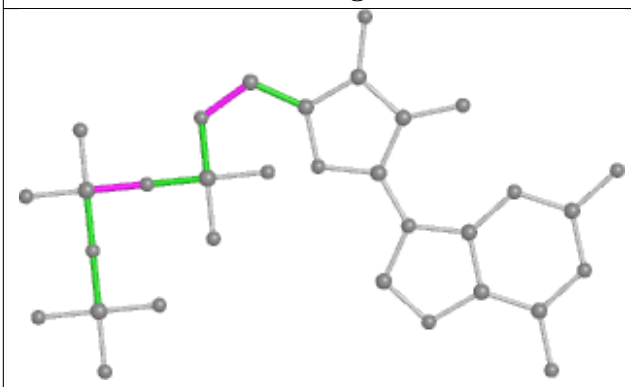

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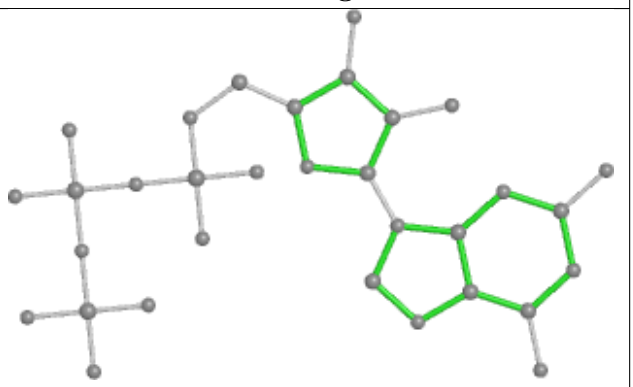

Rings

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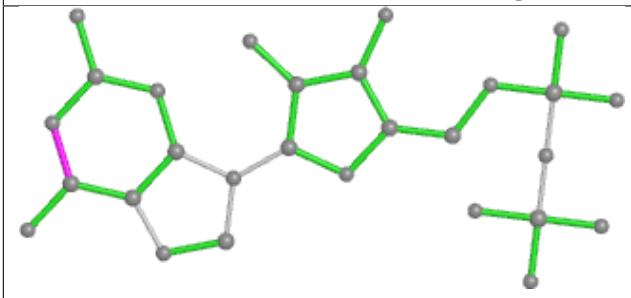

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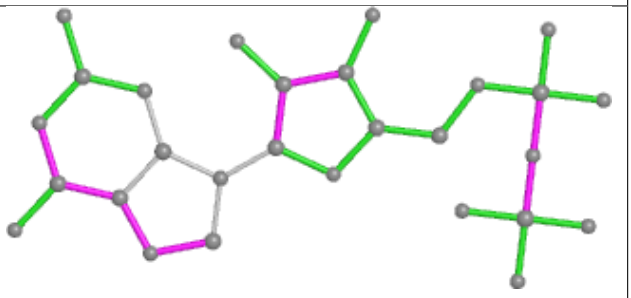

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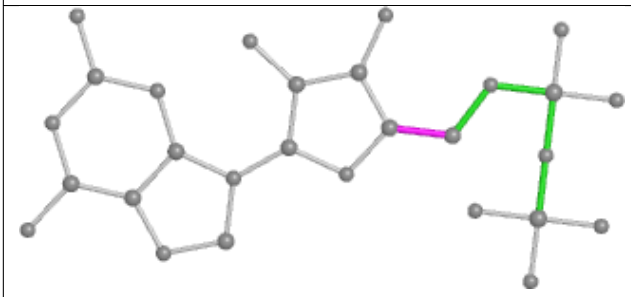

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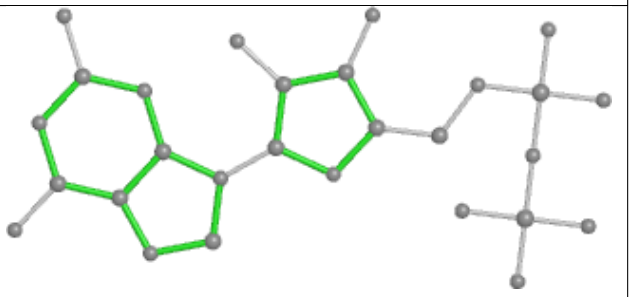

Rings

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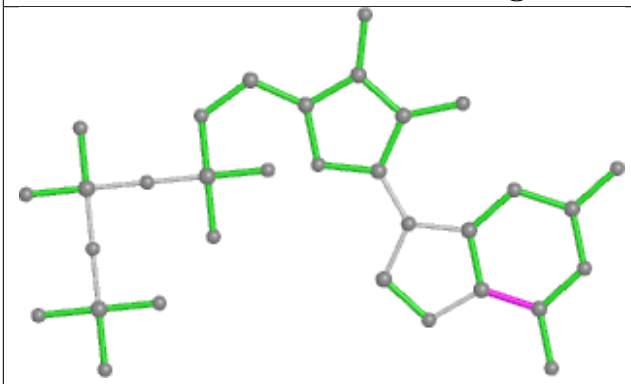

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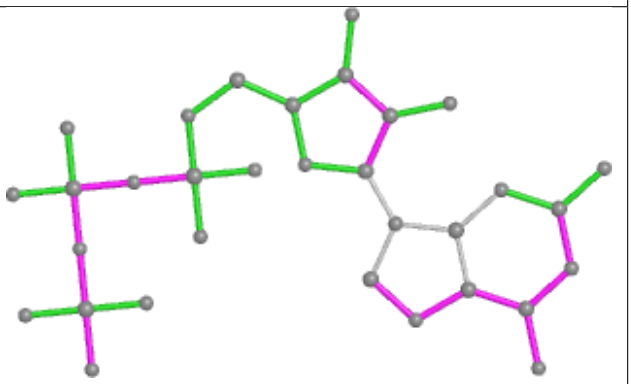

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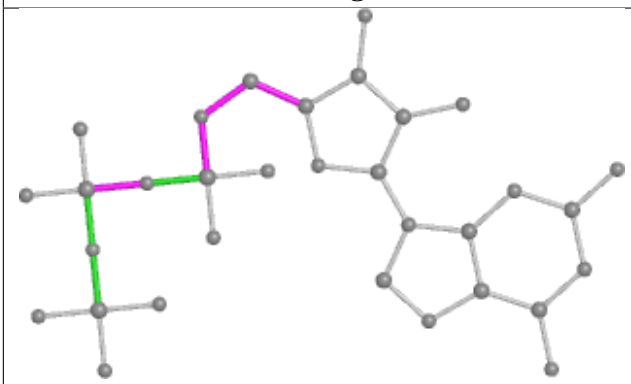

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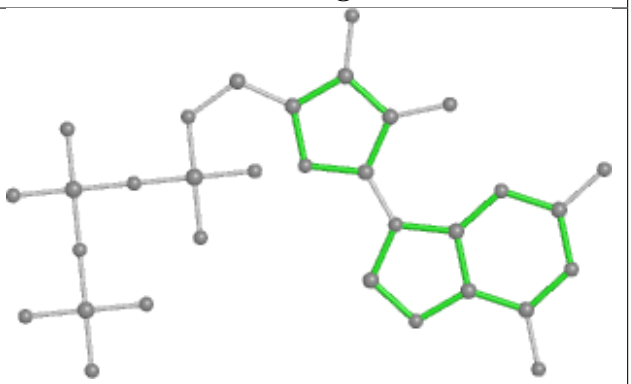
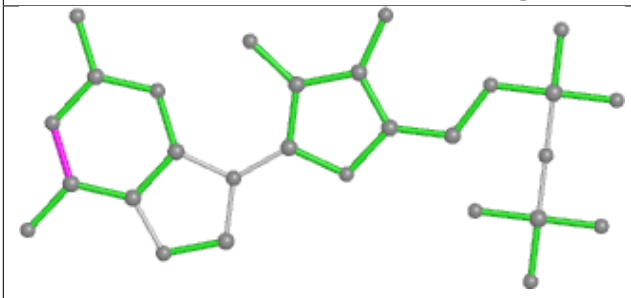


Rings

Ligand GDP IC 501



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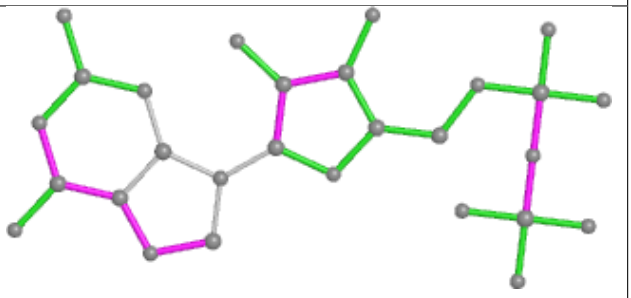

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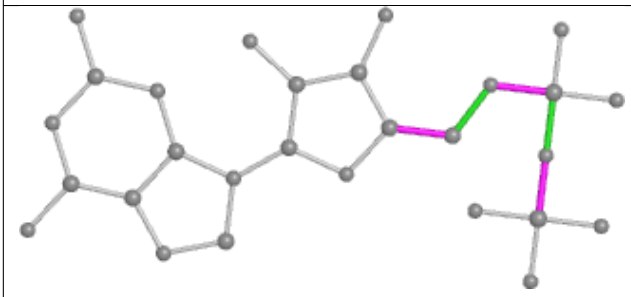

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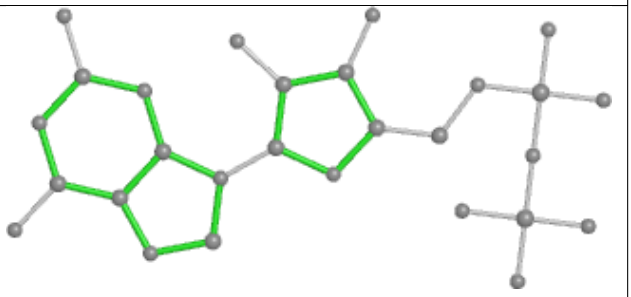

Rings

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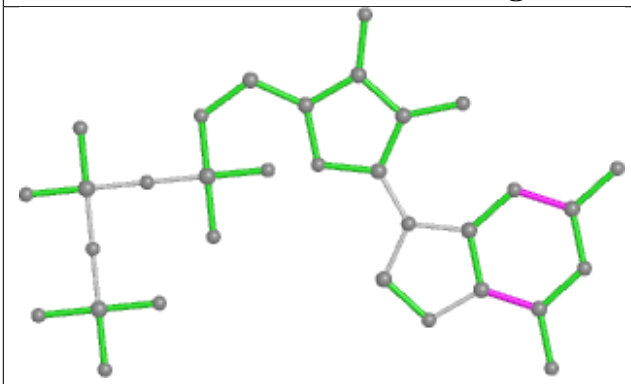

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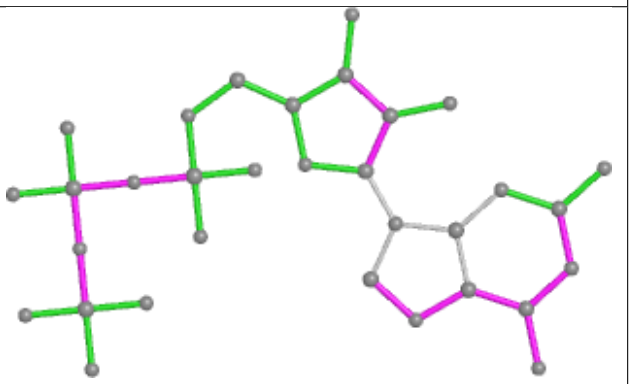

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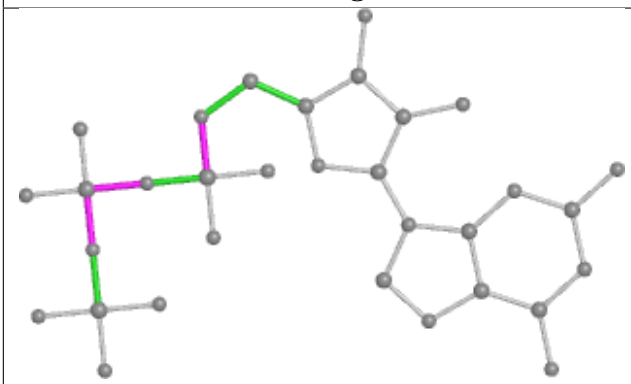

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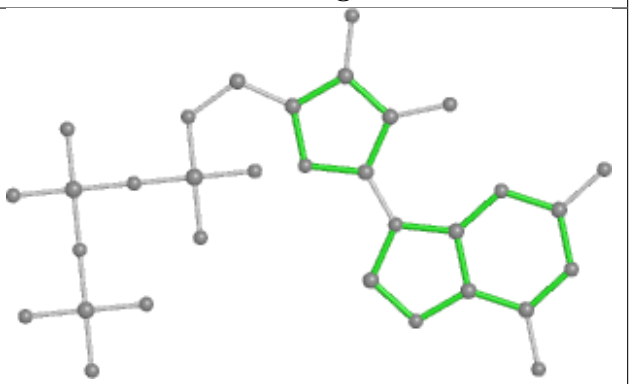
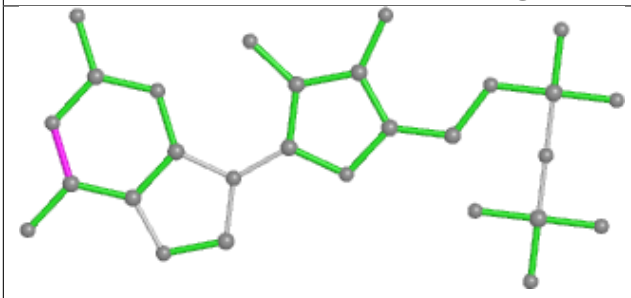
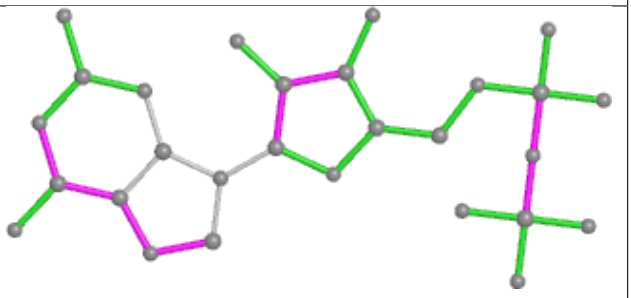
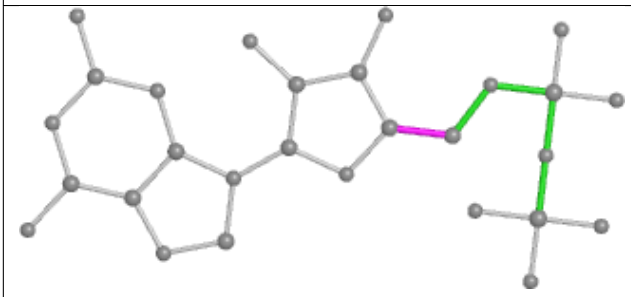
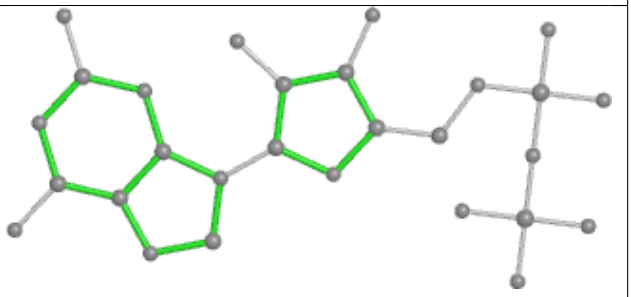


Rings

Ligand GDP DI 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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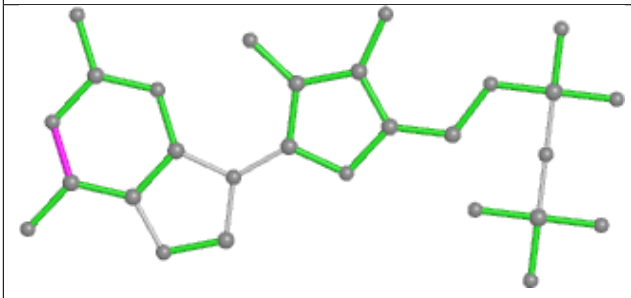
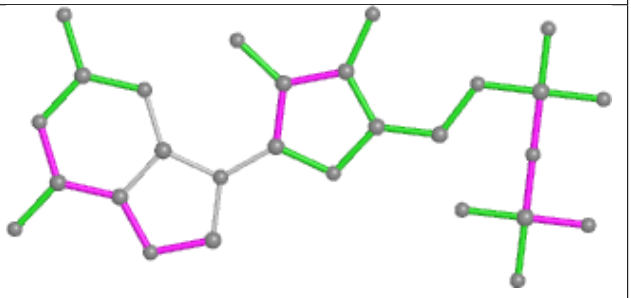
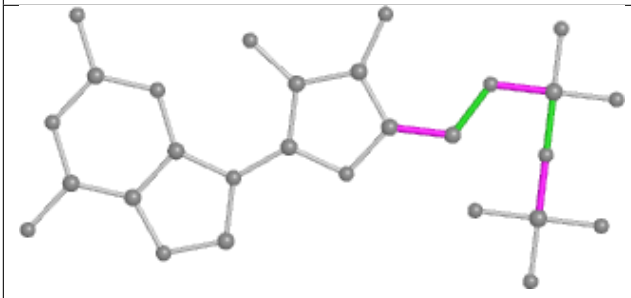
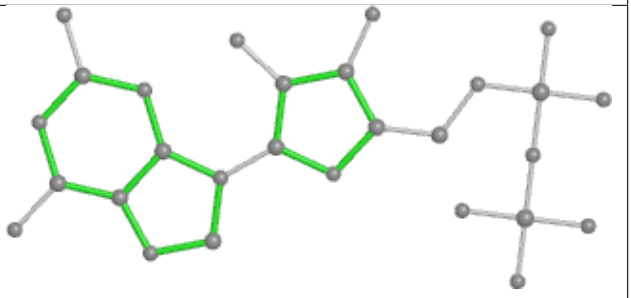
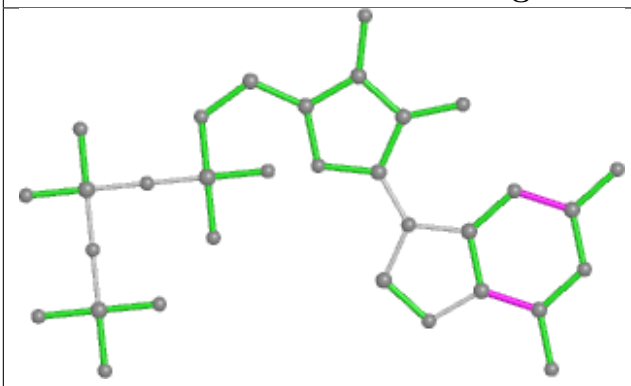
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP KJ 501



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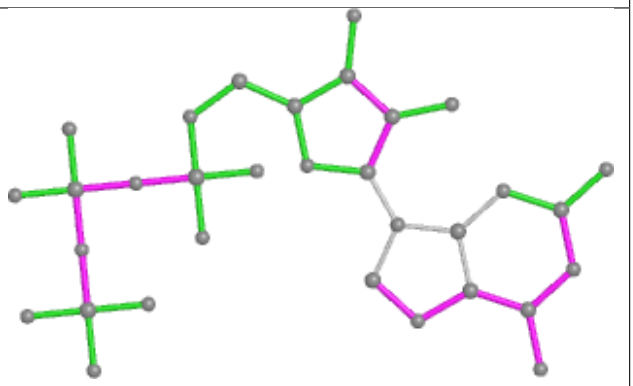
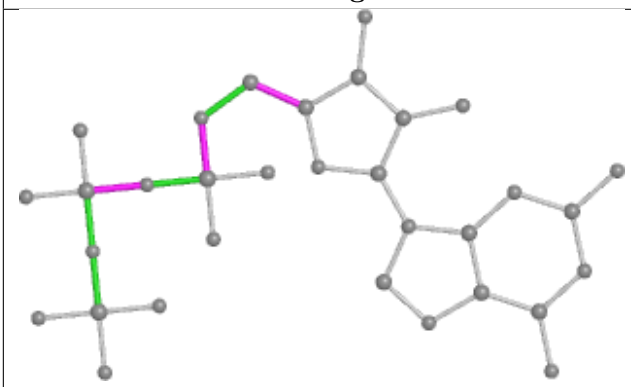


Bond angles



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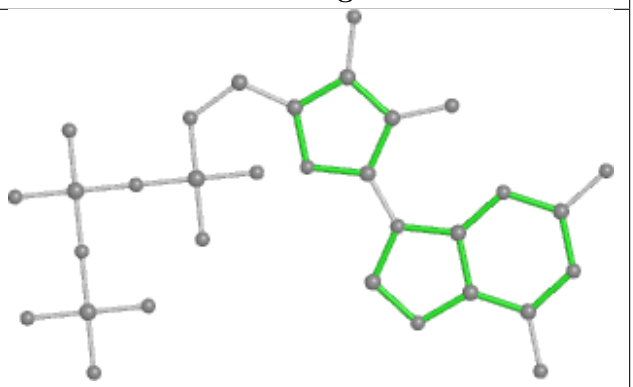
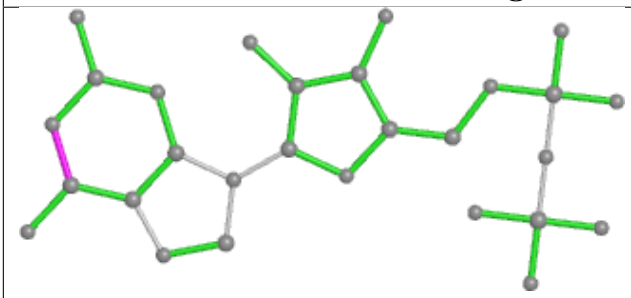


Rings

Ligand GDP AG 501



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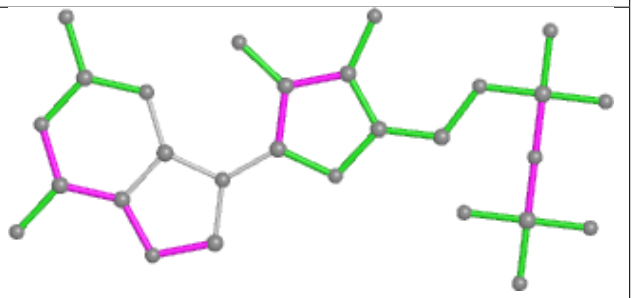

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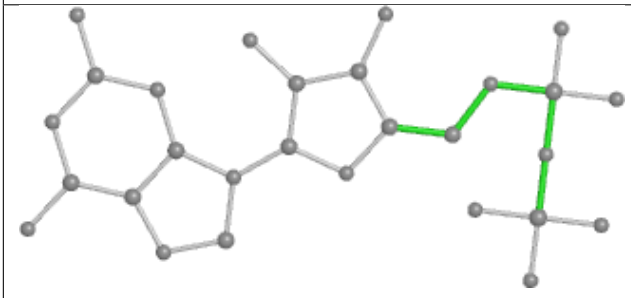

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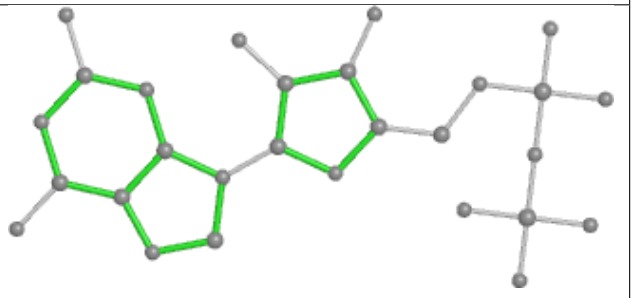
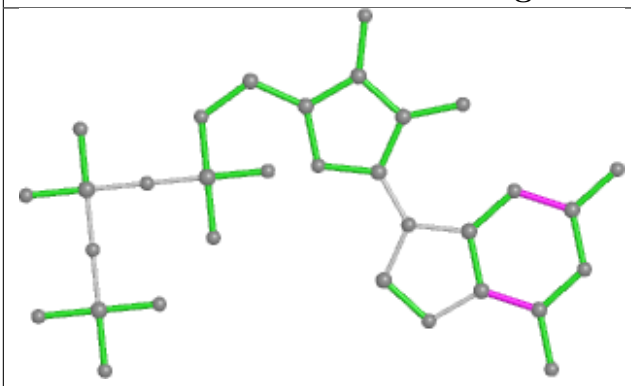
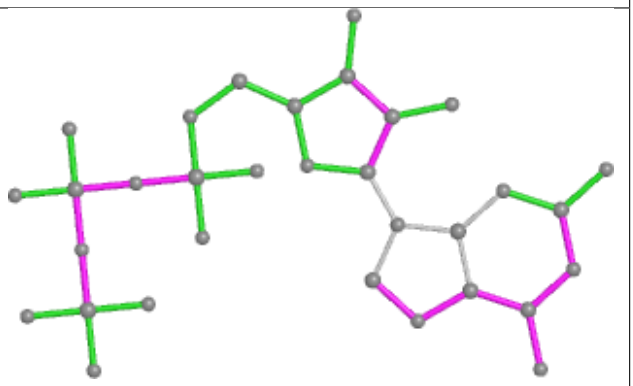


Rings

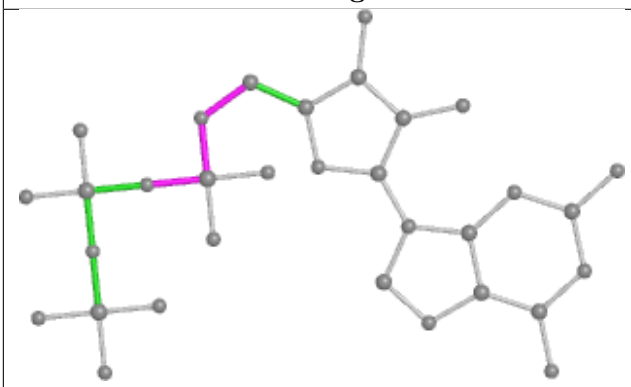
Ligand GTP EJ 501



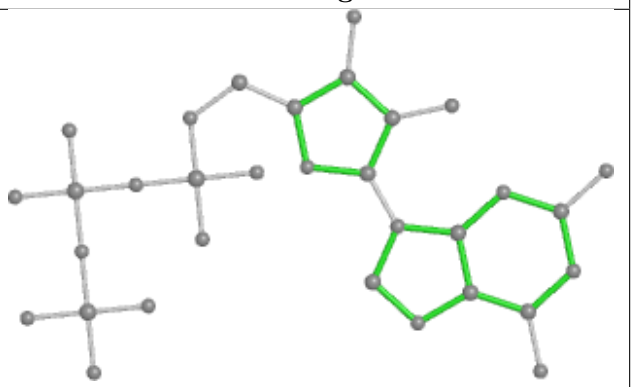
Bond lengths



Bond angles

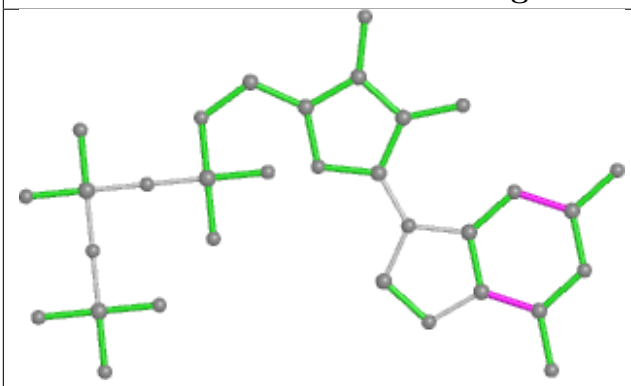


Torsions

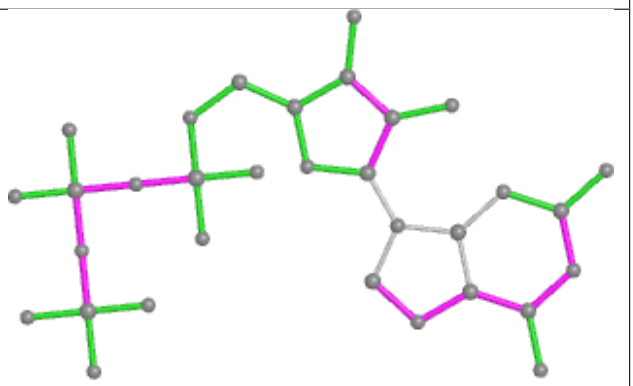


Rings

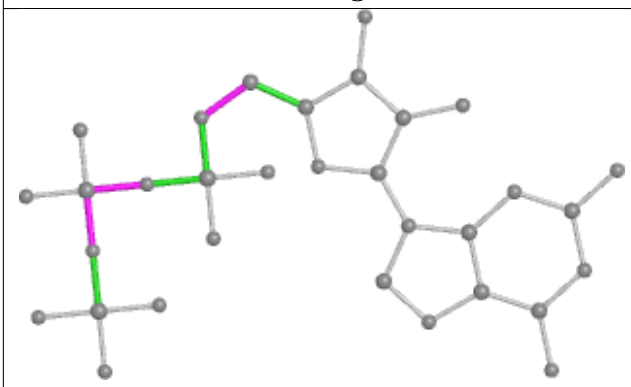
Ligand GTP LH 501



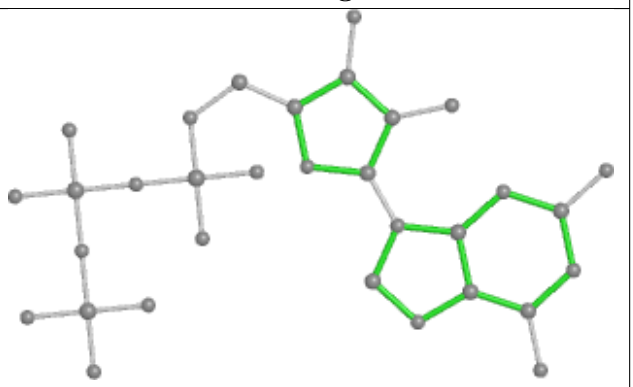
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

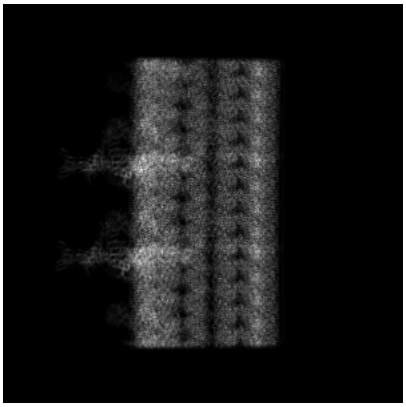
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25361. These allow visual inspection of the internal detail of the map and identification of artifacts.

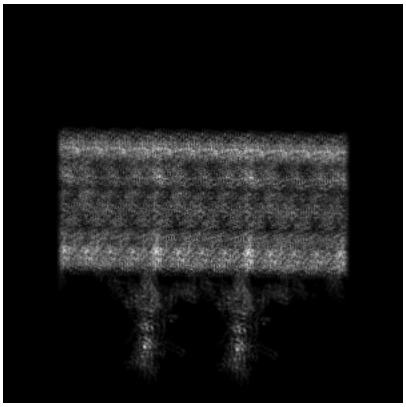
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

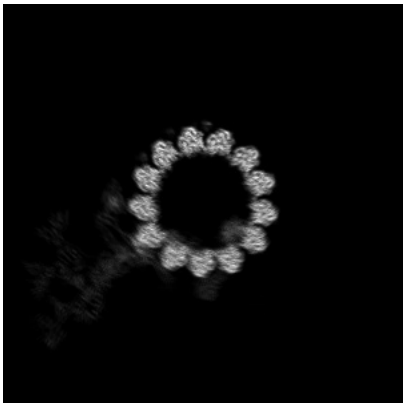
6.1.1 Primary map



X



Y



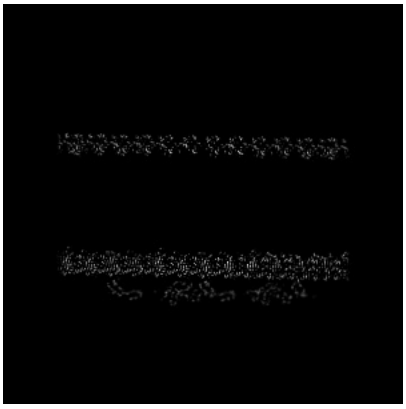
Z

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

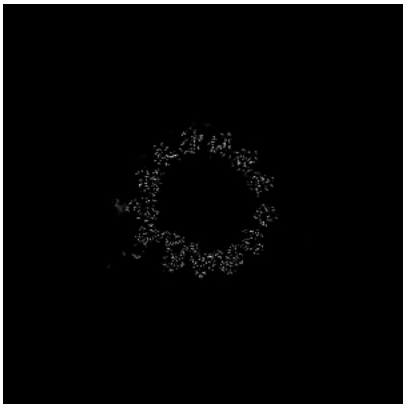
6.2 Central slices

6.2.1 Primary map

X Index: 256



Y Index: 256

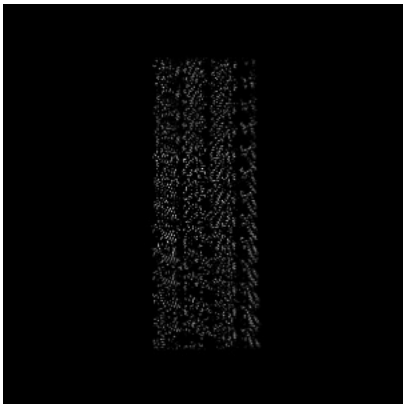


Z Index: 256

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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 324

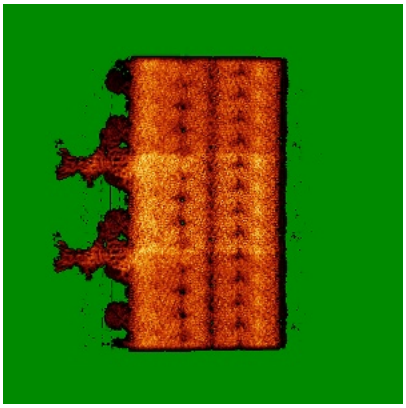
Y Index: 187

Z Index: 195

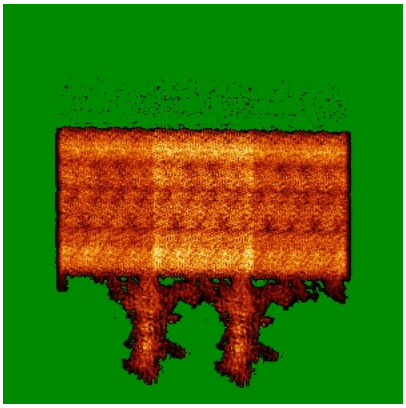
The images above show the largest variance slices of the map in three orthogonal directions.

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

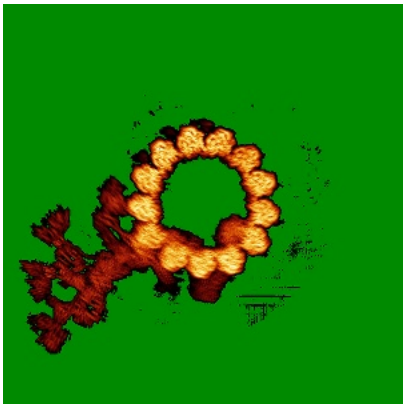
6.4.1 Primary map



X



Y

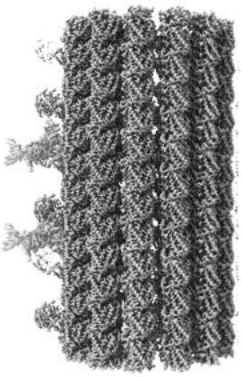


Z

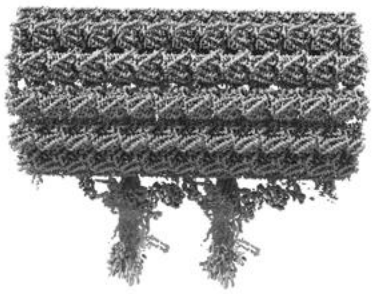
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

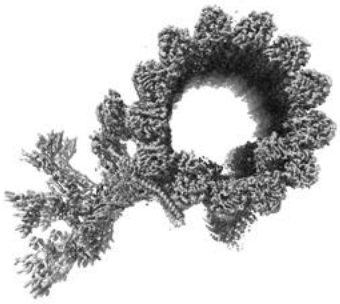
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

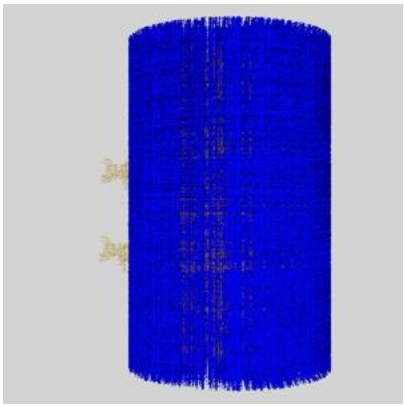
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

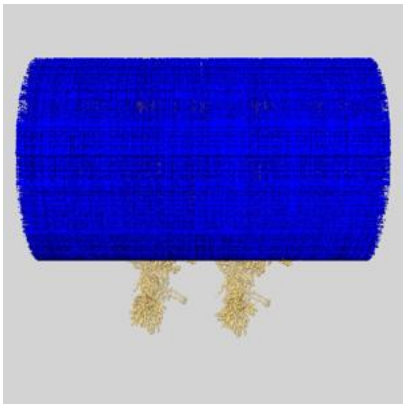
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

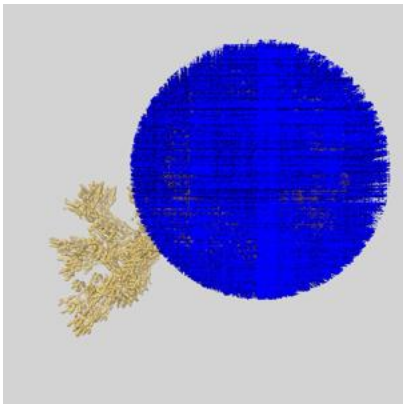
6.6.1 emd_25361_msk_1.map (i)



X



Y

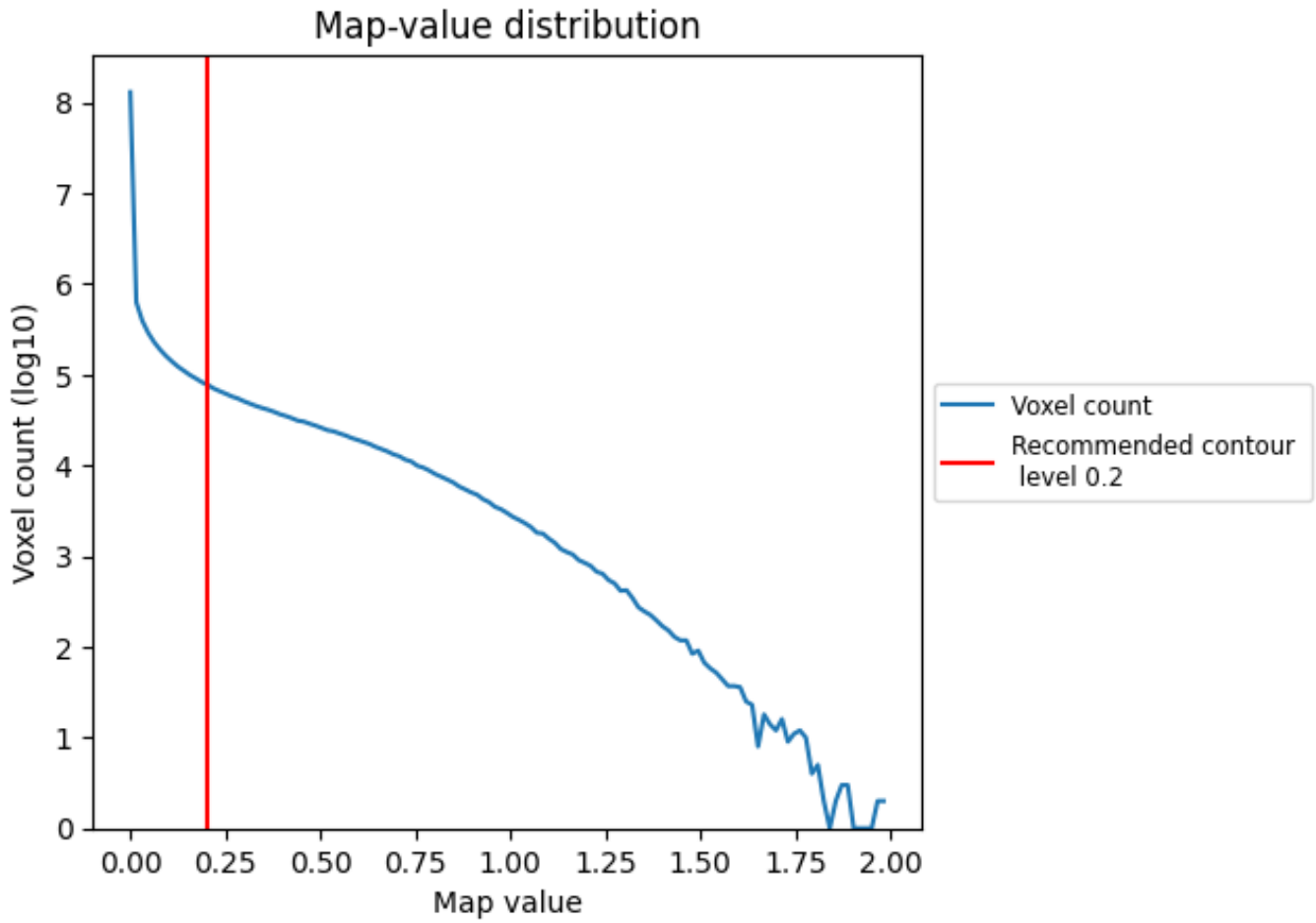


Z

7 Map analysis

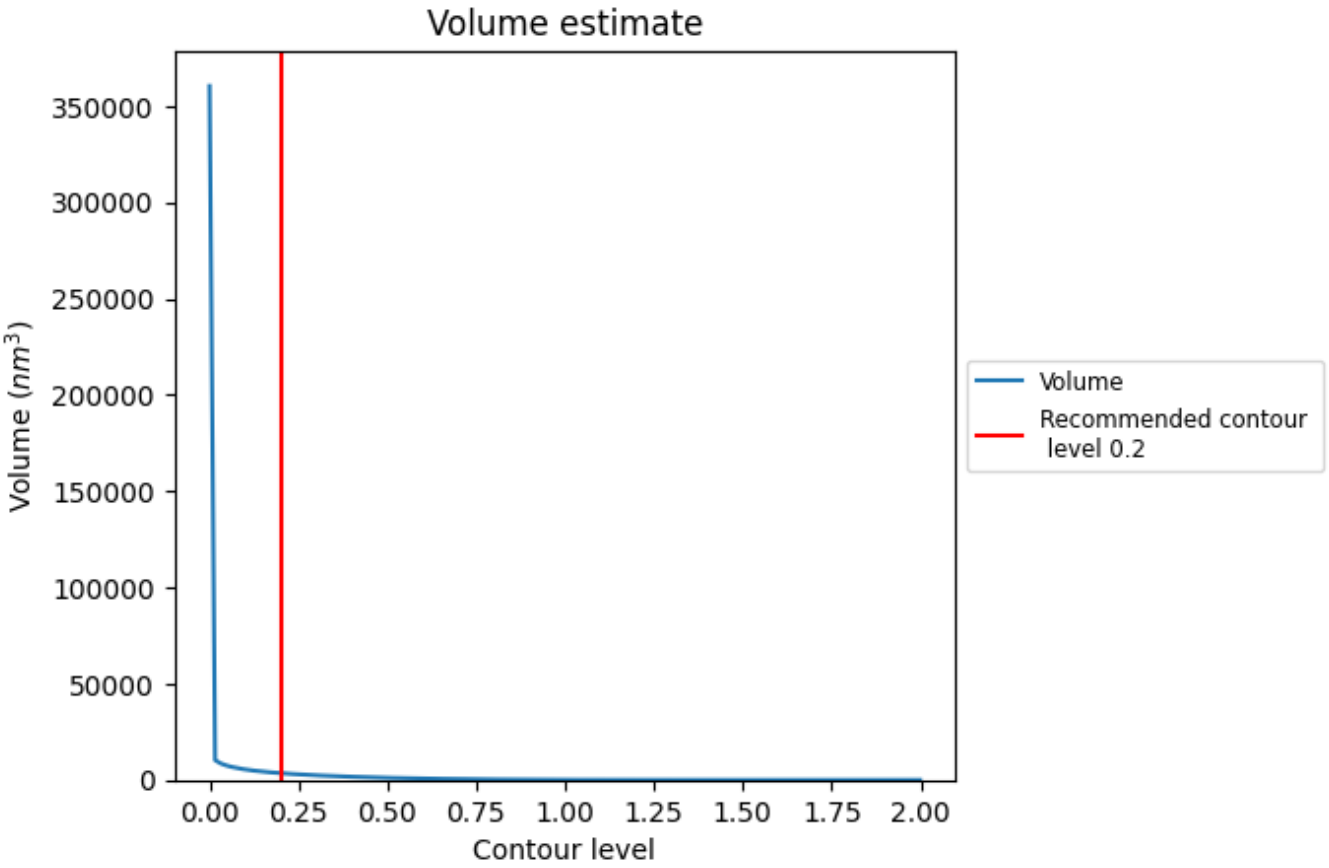
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

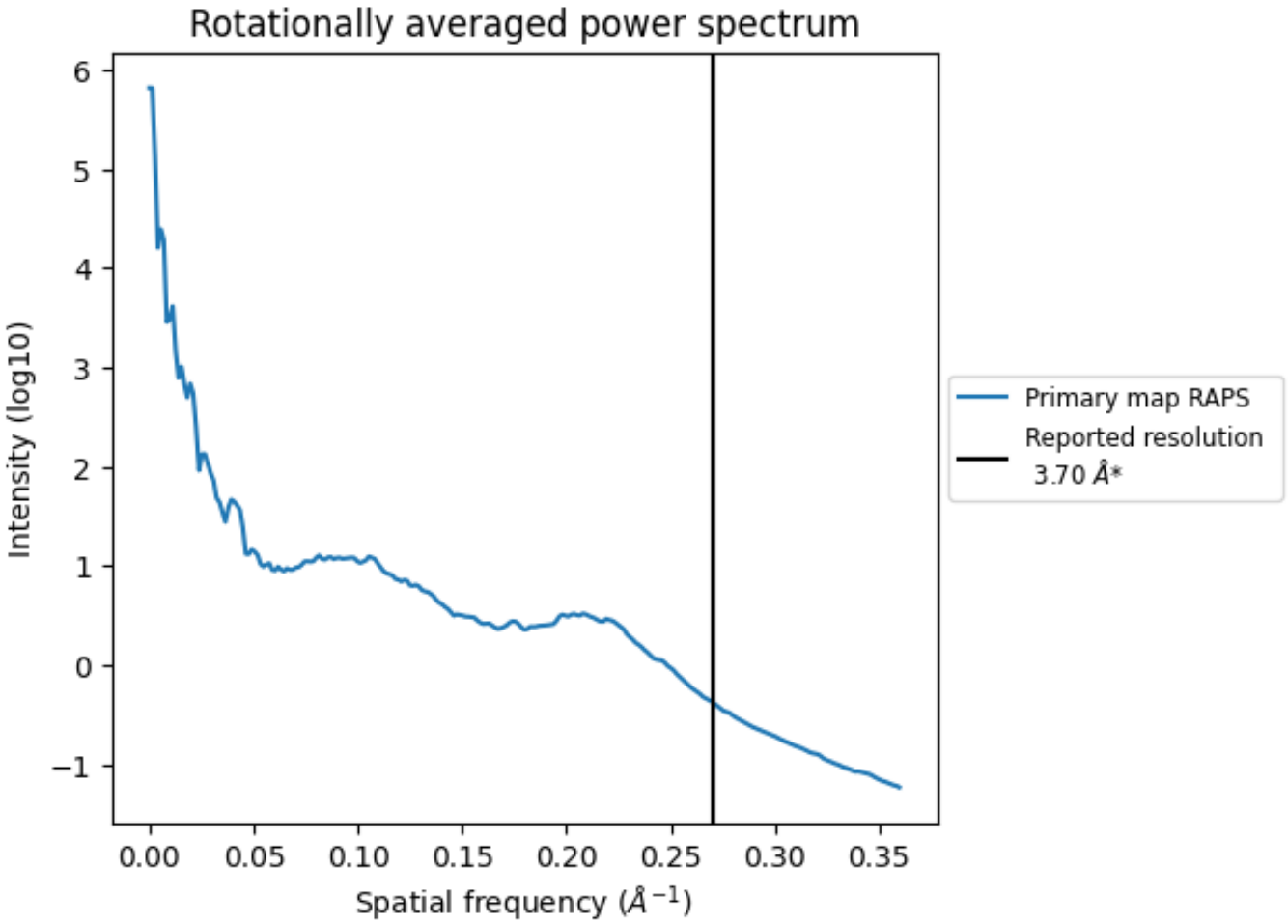
7.2 Volume estimate



The volume at the recommended contour level is 3525 nm^3; this corresponds to an approximate mass of 3184 kDa.

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

7.3 Rotationally averaged power spectrum (i)

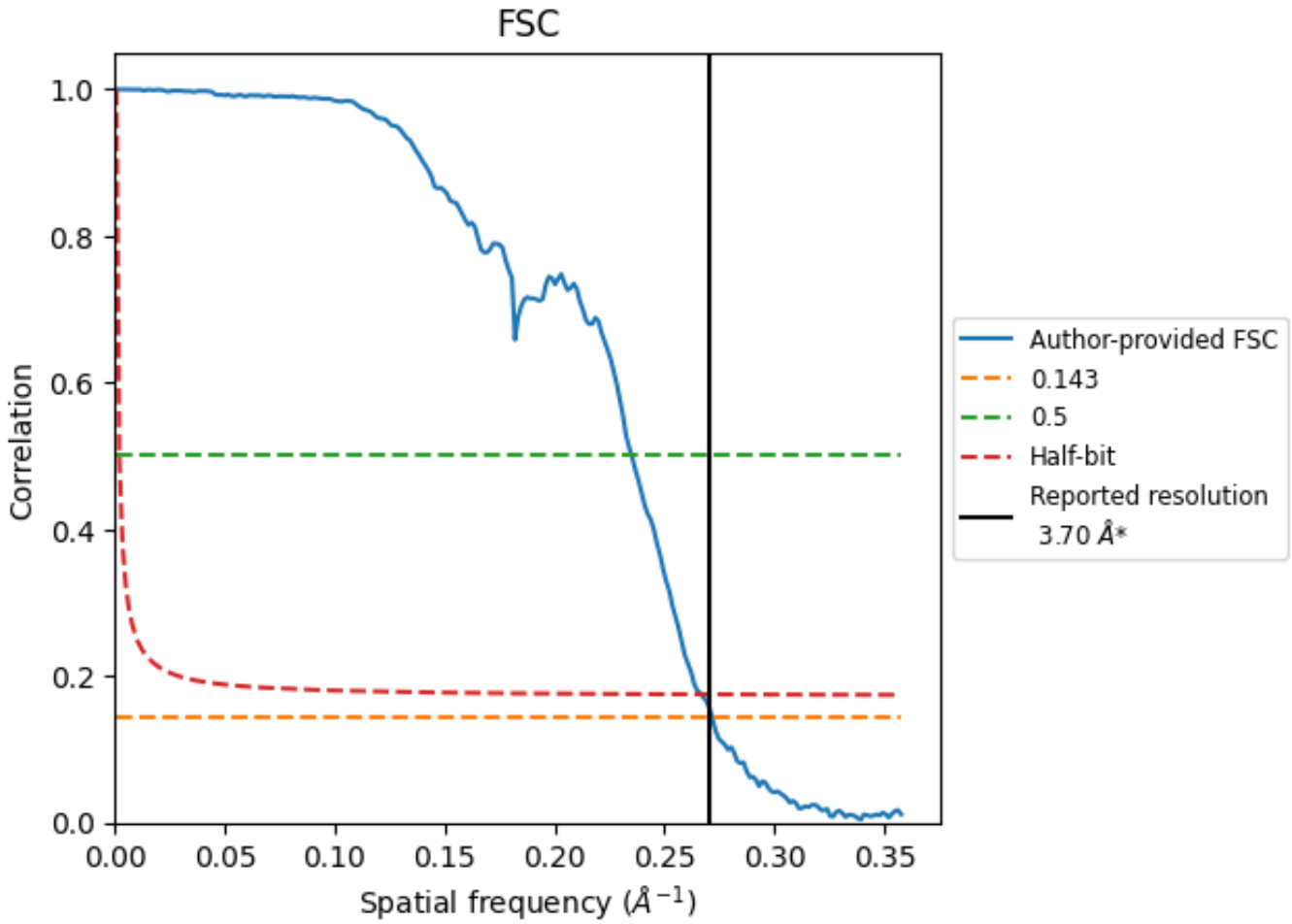


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

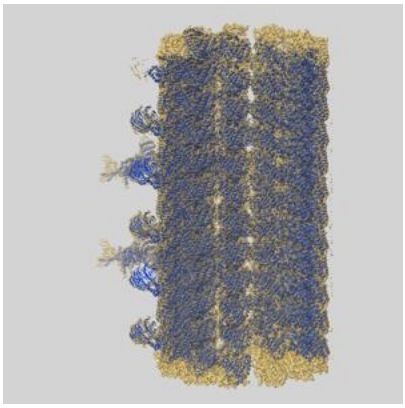
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.26	3.75
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

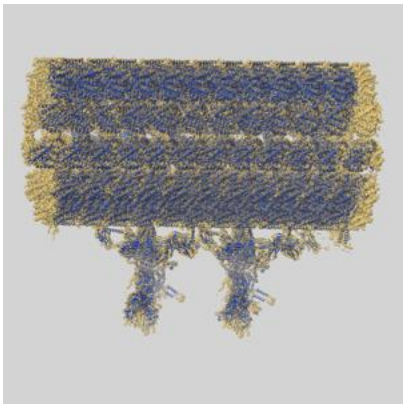
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25361 and PDB model 7SOM. Per-residue inclusion information can be found in section 3 on page 34.

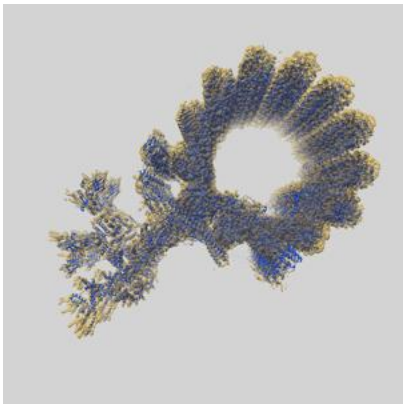
9.1 Map-model overlay



X



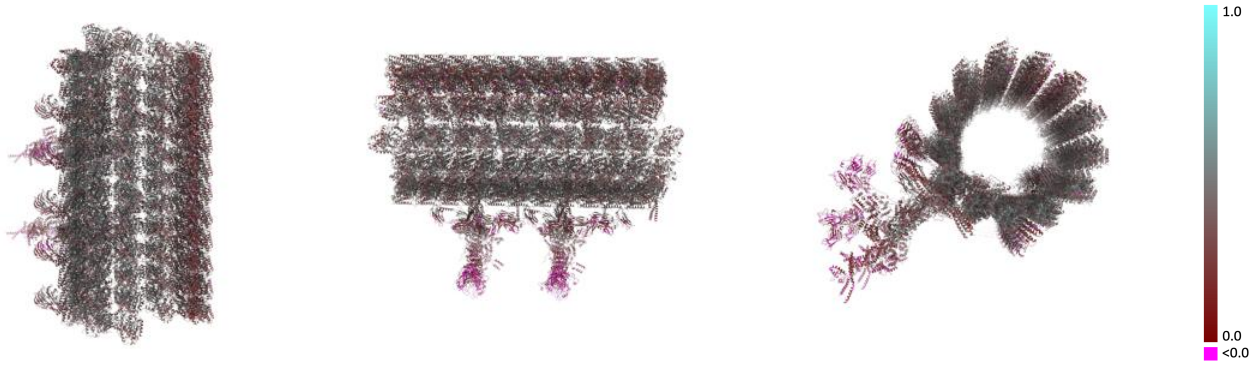
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

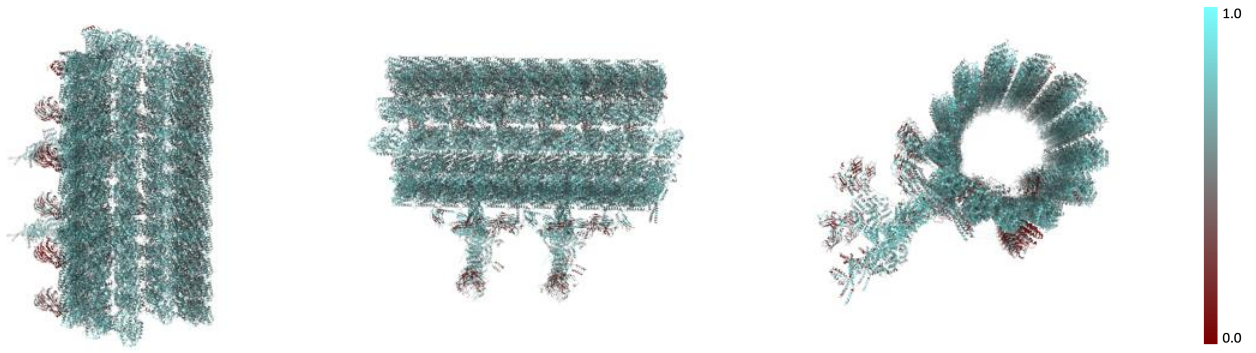
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

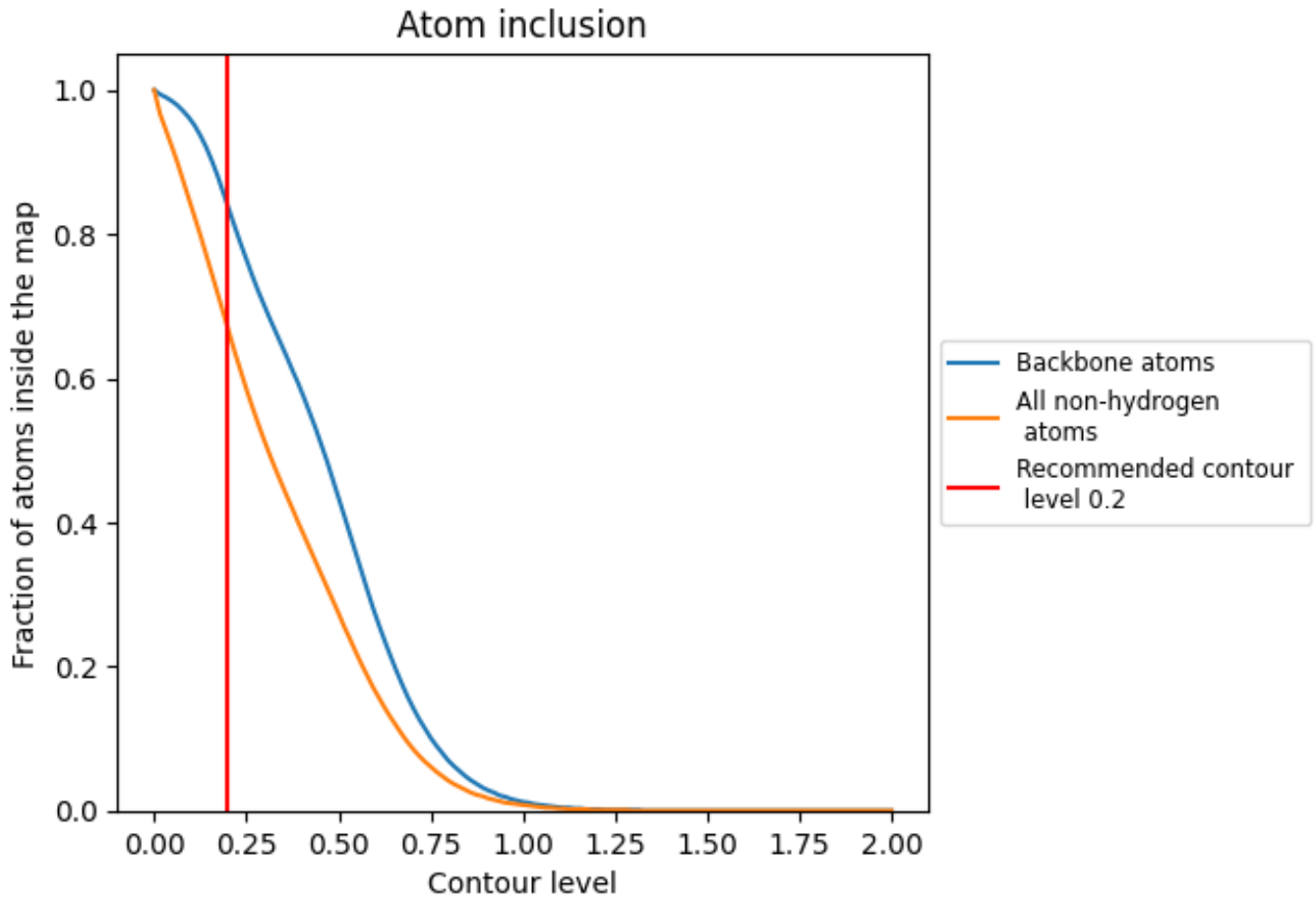
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6680	0.3970
A	0.5370	0.3720
A1	0.7080	0.3380
A2	0.7560	0.3430
A3	0.6890	0.3320
A4	0.7560	0.3440
AA	0.7110	0.4210
AB	0.6970	0.4310
AC	0.7070	0.4310
AD	0.6910	0.4120
AE	0.7460	0.4430
AF	0.7100	0.4510
AG	0.7180	0.4580
AH	0.7170	0.4440
AI	0.7320	0.4270
AJ	0.6910	0.4220
AK	0.7080	0.4340
AL	0.7050	0.4260
B	0.5720	0.3900
BA	0.6860	0.4220
BB	0.6850	0.4320
BC	0.7140	0.4210
BD	0.7180	0.4200
BE	0.6910	0.4320
BF	0.6950	0.4430
BG	0.7160	0.4420
BH	0.7270	0.4280
BI	0.6760	0.4110
BJ	0.6800	0.4190
BK	0.7040	0.4220
BL	0.6820	0.4060
C	0.5090	0.3720
CA	0.7170	0.4420
CB	0.7160	0.4480
CC	0.7270	0.4430

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Chain	Atom inclusion	Q-score
CD	0.7450	0.4440
CE	0.7270	0.4590
CF	0.7240	0.4630
CG	0.7350	0.4530
CH	0.7510	0.4430
CI	0.7100	0.4460
CJ	0.7020	0.4420
CK	0.7170	0.4290
D	0.6240	0.3360
DB	0.7140	0.4430
DC	0.7080	0.4470
DD	0.7130	0.4340
DE	0.7310	0.4370
DF	0.7240	0.4520
DG	0.7150	0.4540
DH	0.7160	0.4470
DI	0.7310	0.4380
DJ	0.7190	0.4380
DK	0.6990	0.4350
DL	0.7060	0.4300
E	0.6190	0.3340
EA	0.6710	0.4220
EB	0.6900	0.4320
EC	0.6740	0.4160
ED	0.6820	0.4240
EE	0.7230	0.4390
EF	0.6990	0.4510
EG	0.6860	0.4430
EH	0.7040	0.4480
EI	0.7140	0.4270
EJ	0.6880	0.4320
EK	0.6810	0.4180
EL	0.6890	0.4280
F	0.6240	0.2290
FA	0.6920	0.4160
FB	0.6900	0.4140
FC	0.6790	0.4070
FD	0.7000	0.4140
FE	0.7140	0.4310
FF	0.7050	0.4430
FG	0.6980	0.4370
FH	0.7180	0.4280

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Chain	Atom inclusion	Q-score
FI	0.7100	0.4180
FJ	0.7040	0.4260
FK	0.6930	0.4190
FL	0.6990	0.4110
G	0.5950	0.2040
GC	0.6890	0.4070
GD	0.6850	0.4050
GE	0.6800	0.4060
GF	0.6950	0.3960
GG	0.6920	0.4160
GH	0.6920	0.4210
GI	0.6940	0.4220
GJ	0.6990	0.3960
GK	0.6780	0.3990
GL	0.6900	0.4030
GM	0.6800	0.4050
H	0.6260	0.2310
HC	0.6110	0.3320
HD	0.6100	0.3270
HE	0.5890	0.3120
HF	0.6550	0.3230
HG	0.6290	0.3460
HH	0.6330	0.3450
HI	0.6210	0.3420
HJ	0.6490	0.3250
HK	0.6020	0.3200
HL	0.6070	0.3260
HM	0.6100	0.3170
I	0.5910	0.2010
IC	0.6260	0.3490
ID	0.6470	0.3550
IE	0.6300	0.3400
IF	0.6850	0.3480
IG	0.6490	0.3670
IH	0.6610	0.3670
II	0.6410	0.3520
IJ	0.6810	0.3490
IK	0.6320	0.3540
IL	0.6510	0.3560
IM	0.6360	0.3440
J	0.6390	0.3300
JB	0.6990	0.3940

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Chain	Atom inclusion	Q-score
JC	0.6740	0.3960
JD	0.6790	0.4000
JE	0.6950	0.4000
JF	0.7170	0.4050
JG	0.6930	0.4140
JH	0.6980	0.4220
JI	0.7040	0.4110
JJ	0.7100	0.3960
JK	0.6850	0.4040
JL	0.6900	0.4050
JM	0.6900	0.4000
K	0.6510	0.3350
KB	0.6990	0.4060
KC	0.6930	0.4190
KD	0.6820	0.4050
KE	0.6950	0.4000
KF	0.6990	0.4190
KG	0.7010	0.4300
KH	0.6890	0.4230
KI	0.7080	0.4110
KJ	0.6890	0.3970
KK	0.6890	0.4110
KL	0.6820	0.4090
L	0.3190	0.2810
LB	0.7060	0.4200
LC	0.6920	0.4230
LD	0.6880	0.4110
LE	0.7290	0.4170
LF	0.7110	0.4440
LG	0.6980	0.4350
LH	0.6890	0.4320
LI	0.7170	0.4200
LJ	0.6940	0.4140
LK	0.6770	0.4070
LL	0.6930	0.4100
M	0.1770	0.2360
MB	0.6920	0.4310
MC	0.6900	0.4310
MD	0.6950	0.4240
ME	0.7110	0.4310
MF	0.7030	0.4480
MG	0.6980	0.4410

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Chain	Atom inclusion	Q-score
MH	0.7010	0.4420
MI	0.7110	0.4360
MJ	0.6990	0.4350
MK	0.6900	0.4260
ML	0.7000	0.4310
N	0.3600	0.2880
O	0.2140	0.2400
P	0.3020	0.2320
Q	0.4590	0.3420
R	0.2880	0.2380
S	0.4960	0.3390
T	0.5320	0.1890
U	0.5680	0.2250
V	0.4640	0.1730
W	0.5580	0.2060
X	0.3150	0.2790
Y	0.1560	0.2320
Z	0.5670	0.3170
a	0.5900	0.3810
aa	0.3150	0.3660
b	0.6280	0.3910
bb	0.5450	0.3360
c	0.6250	0.3880
cc	0.5790	0.3280
d	0.6320	0.3820
e	0.5810	0.3700
f	0.5940	0.3940
g	0.6200	0.3830
h	0.5590	0.3980
i	0.6140	0.4150
j	0.5770	0.3990
k	0.5840	0.3510
l	0.5840	0.3420
m	0.5990	0.3980
n	0.6230	0.4130
o	0.5960	0.3970
p	0.5840	0.4030
q	0.6150	0.4130
r	0.6020	0.4180
s	0.5730	0.3570