wwPDB EM Validation Summary Report ⓘ

Oct 10, 2022 – 04:18 PM EDT

PDB ID	:	7UN1
EMDB ID	:	EMD-26611
Title	:	8-nm repeat of the human sperm tip singlet microtubule
Authors	:	Gui, M.; Croft, J.T.; Zabeo, D.; Acharya, V.; Kollman, J.M.; Burgoyne, T.; Hoog, J.L.; Brown, A.
Deposited on	:	2022-04-08
Resolution	:	6.00 Å(reported)

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

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

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

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

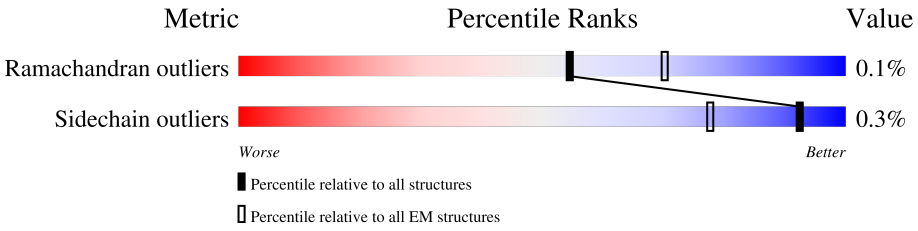
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	222	44% 72% 28%
1	B	222	23% 72% 28%
1	C	222	13% 71% 29%
1	D	222	13% 71% 28%
1	E	222	9% 72% 28%
1	F	222	5% 69% 29%
1	G	222	8% 72% 28%
1	H	222	6% 72% 28%
1	I	222	7% 72% 28%

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Mol	Chain	Length	Quality of chain
1	J	222	7% 72% 28%
1	K	222	18% 72% 28%
1	L	222	41% 72% 28%
1	M	222	38% 72% 28%
1	N	222	13% 70% 30%
1	O	222	13% 72% 28%
1	P	222	11% 72% 28%
1	Q	222	10% 71% 29%
1	R	222	5% 72% 28%
1	S	222	6% 70% 30%
1	T	222	5% 72% 28%
1	U	222	9% 72% 28%
1	V	222	9% 72% 28%
1	W	222	17% 70% 30%
1	X	222	50% 72% 28%
1	d	222	8% 69% 30%
1	e	222	7% 70% 29%
1	f	222	6% 72% 28%
1	g	222	5% 72% 28%
1	h	222	5% 70% 30%
1	i	222	8% 71% 28%
1	j	222	7% 72% 28%
1	k	222	14% 70% 30%
1	l	222	36% 68% 32%
2	AB	445	96%

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Mol	Chain	Length	Quality of chain
2	AD	445	95%
2	AF	445	95%
2	BA	445	95%
2	BD	445	95%
2	BF	445	95%
2	CB	445	95%
2	CD	445	96%
2	CF	445	95%
2	DB	445	96%
2	DD	445	96%
2	DF	445	95%
2	EB	445	91% 8%
2	ED	445	95%
2	EF	445	95%
2	FD	445	95%
2	FF	445	95%
2	FH	445	5% 85% 15%
2	GD	445	96%
2	GF	445	95%
2	GH	445	96%
2	HD	445	95%
2	HF	445	96%
2	HH	445	5% 95%
2	ID	445	5% 95%
2	IF	445	7% 95%

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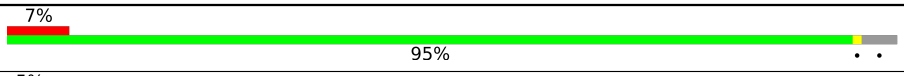
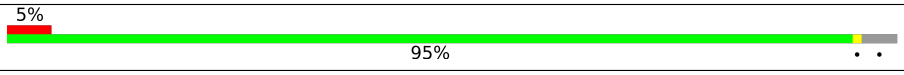
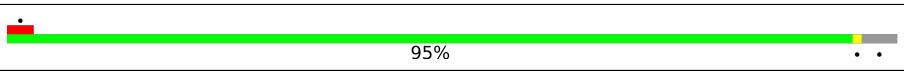
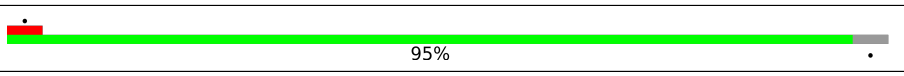
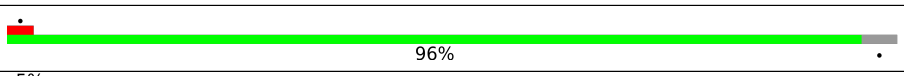
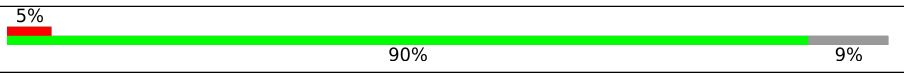
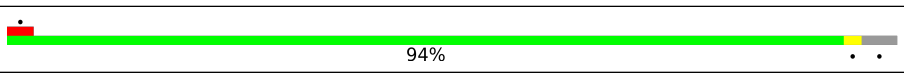
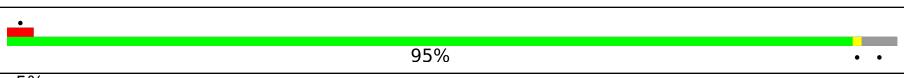
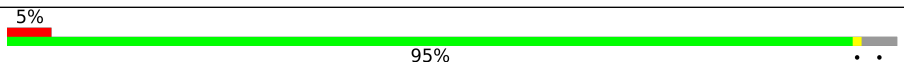
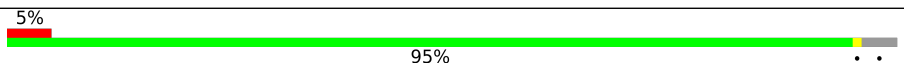
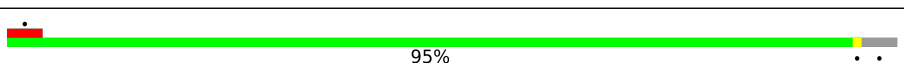
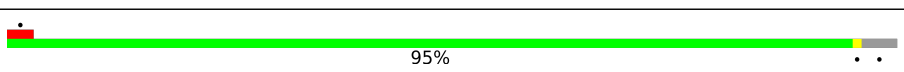
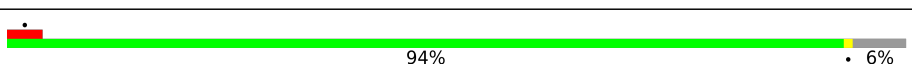
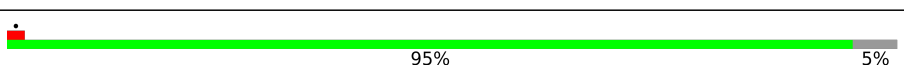
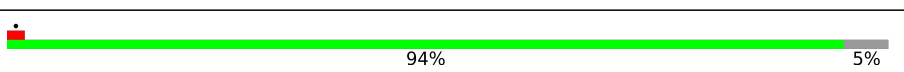
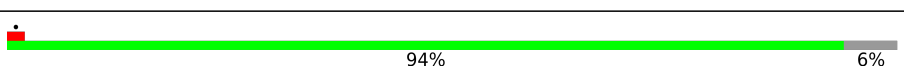
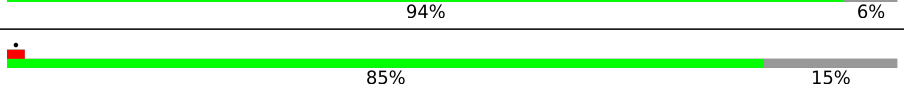
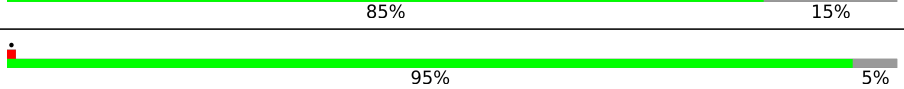
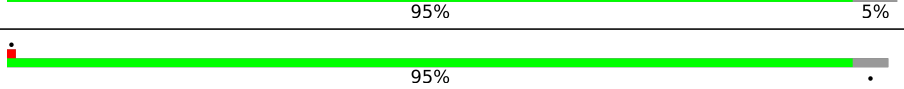
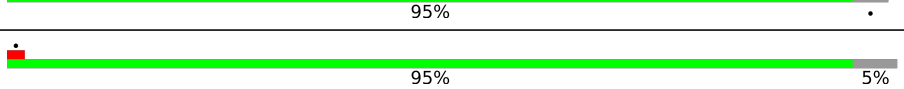
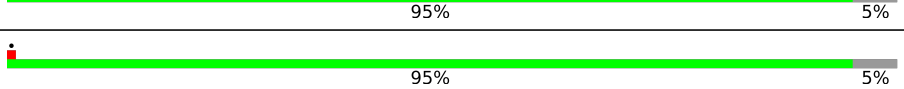
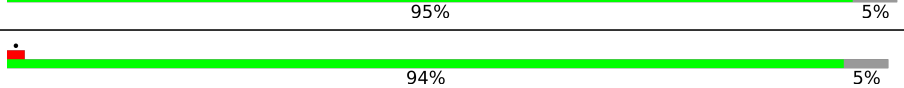
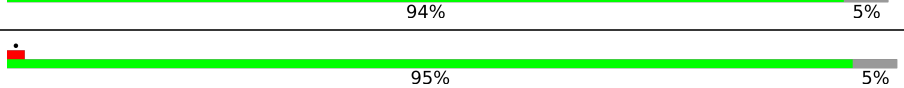
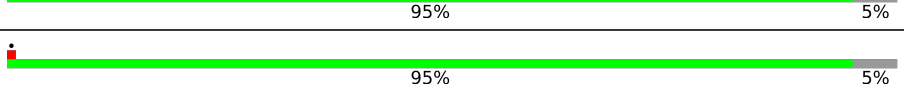
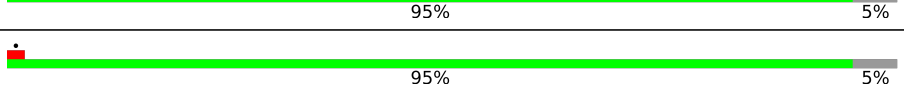
Mol	Chain	Length	Quality of chain
2	IH	445	
2	JD	445	
2	JF	445	
2	KD	445	
2	KF	445	
2	KH	445	
2	LB	445	
2	LD	445	
2	LF	445	
2	MB	445	
2	MD	445	
2	MF	445	
3	AC	451	
3	AE	451	
3	BC	451	
3	BE	451	
3	BG	451	
3	CC	451	
3	CE	451	
3	CG	451	
3	DC	451	
3	DE	451	
3	DG	451	
3	EC	451	
3	EE	451	

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Mol	Chain	Length	Quality of chain
3	EG	451	95% 5%
3	FC	451	95% 5%
3	FE	451	94% 5%
3	FG	451	95% 5%
3	GC	451	94% 5%
3	GE	451	94% 5%
3	GG	451	94% 5%
3	HC	451	94% 5%
3	HE	451	95% 5%
3	HG	451	94% 6%
3	IC	451	7% 92% 8%
3	IE	451	5% 95% 5%
3	IG	451	5% 94% 5%
3	JC	451	5% 95% 5%
3	JE	451	5% 94% 5%
3	JG	451	95% 5%
3	KC	451	94% 6%
3	KE	451	94% 6%
3	KG	451	94% 6%
3	LA	451	95% 5%
3	LC	451	95% 5%
3	LE	451	95% 5%
3	MA	451	5% 94% 6%
3	MC	451	5% 94% 5%
3	ME	451	94% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 290845 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 Sperm acrosome-associated protein 9.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	160	Total C N O 796 476 160 160	0	0
1	B	160	Total C N O 796 476 160 160	0	0
1	C	158	Total C N O 786 470 158 158	0	0
1	D	160	Total C N O S 1289 805 231 243 10	0	0
1	E	160	Total C N O S 1289 805 231 243 10	0	0
1	F	157	Total C N O S 1263 788 225 240 10	0	0
1	G	159	Total C N O S 1278 799 227 242 10	0	0
1	H	159	Total C N O S 1278 799 227 242 10	0	0
1	I	159	Total C N O S 1278 799 227 242 10	0	0
1	J	159	Total C N O 791 473 159 159	0	0
1	K	159	Total C N O 791 473 159 159	0	0
1	L	159	Total C N O 791 473 159 159	0	0
1	M	160	Total C N O 796 476 160 160	0	0
1	N	156	Total C N O 776 464 156 156	0	0
1	O	160	Total C N O 796 476 160 160	0	0
1	P	160	Total C N O S 1289 805 231 243 10	0	0
1	Q	157	Total C N O S 1263 788 225 240 10	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	R	160	Total C N O S 1289 805 231 243 10	0	0
1	S	156	Total C N O S 1254 782 223 239 10	0	0
1	T	159	Total C N O S 1278 799 227 242 10	0	0
1	U	159	Total C N O S 1278 799 227 242 10	0	0
1	V	159	Total C N O 791 473 159 159	0	0
1	W	155	Total C N O 771 461 155 155	0	0
1	X	160	Total C N O 796 476 160 160	0	0
1	d	156	Total C N O S 1254 782 223 239 10	0	0
1	e	157	Total C N O S 1263 788 225 240 10	0	0
1	f	160	Total C N O S 1289 805 231 243 10	0	0
1	g	159	Total C N O S 1278 799 227 242 10	0	0
1	h	156	Total C N O S 1254 782 223 239 10	0	0
1	i	159	Total C N O S 1278 799 227 242 10	0	0
1	j	159	Total C N O 791 473 159 159	0	0
1	k	155	Total C N O 771 461 155 155	0	0
1	l	152	Total C N O 756 452 152 152	0	0

- Molecule 2 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	AB	427	Total C N O S 3356 2109 575 646 26	0	0
2	AD	427	Total C N O S 3356 2109 575 646 26	0	0
2	AF	426	Total C N O S 3348 2105 574 643 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	BD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	BF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	CB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	CD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	CF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	DB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	DD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	DF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	EB	411	Total	C	N	O	S	0	0
			3214	2015	549	626	24		
2	ED	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	EF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	FD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	FF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	FH	379	Total	C	N	O	S	0	0
			2971	1871	508	570	22		
2	GD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	GF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	GH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	HD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	HF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	HH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	ID	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	IF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	IH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	JD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	JF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	KD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	KF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	KH	403	Total	C	N	O	S	0	0
			3165	1996	539	607	23		
2	LB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	LD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	LF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	MB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	MD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	MF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

- Molecule 3 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	426	Total	C	N	O	S	0	0
			3343	2123	569	629	22		
3	AE	427	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
3	BC	427	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
3	BE	426	Total	C	N	O	S	0	0
			3343	2123	569	629	22		
3	BG	385	Total	C	N	O	S	0	0
			3026	1914	516	575	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	CC	430	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
3	CE	431	Total	C	N	O	S	0	0
			3377	2140	574	641	22		
3	CG	429	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
3	DC	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	DE	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	DG	429	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
3	EC	429	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
3	EE	428	Total	C	N	O	S	0	0
			3356	2128	571	635	22		
3	EG	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	FC	429	Total	C	N	O	S	0	0
			3365	2134	572	637	22		
3	FE	430	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
3	FG	429	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
3	GC	430	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
3	GE	429	Total	C	N	O	S	0	0
			3364	2132	572	638	22		
3	GG	428	Total	C	N	O	S	0	0
			3356	2127	571	637	21		
3	HC	427	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
3	HE	427	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
3	HG	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
3	IC	414	Total	C	N	O	S	0	0
			3239	2051	550	617	21		
3	IE	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	IG	427	Total	C	N	O	S	0	0
			3350	2125	570	633	22		

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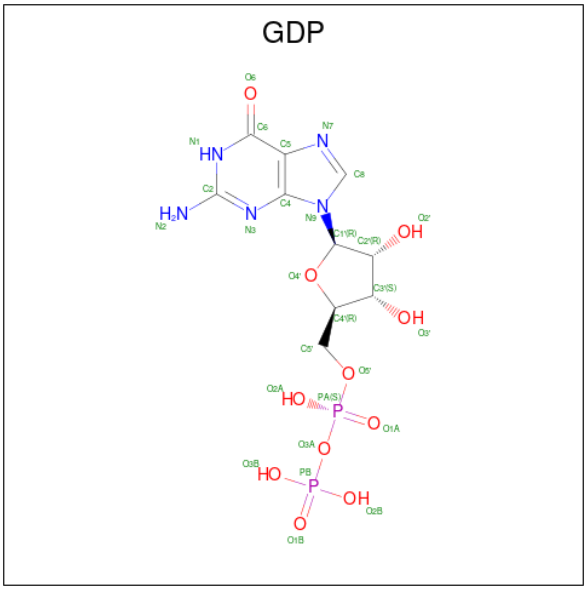
Mol	Chain	Residues	Atoms					AltConf	Trace
3	JC	429	Total	C	N	O	S	0	0
			3365	2134	572	637	22		
3	JE	428	Total	C	N	O	S	0	0
			3358	2129	571	636	22		
3	JG	427	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
3	KC	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
3	KE	425	Total	C	N	O	S	0	0
			3335	2116	568	629	22		
3	KG	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
3	LA	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	LC	427	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
3	LE	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	MA	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
3	MC	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	ME	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	AB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	BA	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	DB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	DF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	EB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	ED	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	FH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	GH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	

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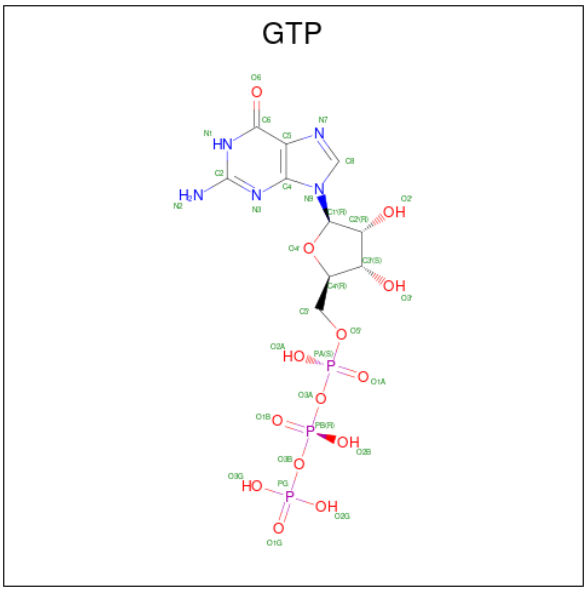
Mol	Chain	Residues	Atoms					AltConf
4	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	HH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	IH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	JD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	JF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	KD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	KF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	KH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	LD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	LF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	MB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	MD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	MF	1	Total	C	N	O	P	0
			28	10	5	11	2	

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



Mol	Chain	Residues	Atoms					AltConf
5	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	CC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	CE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	CG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	DC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	DE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	DG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	EC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	EE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	EG	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
5	FC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	FE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	FG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	GC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	GE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	GG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	HC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	HE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	HG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	IC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	IE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	IG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	JC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	JE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	JG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	KC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	KE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	KG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	LA	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	LC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	LE	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
5	MA	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	MC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	ME	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	AC	1	Total	Mg	0
			1	1	
6	AE	1	Total	Mg	0
			1	1	
6	BC	1	Total	Mg	0
			1	1	
6	BE	1	Total	Mg	0
			1	1	
6	BG	1	Total	Mg	0
			1	1	
6	CC	1	Total	Mg	0
			1	1	
6	CE	1	Total	Mg	0
			1	1	
6	CG	1	Total	Mg	0
			1	1	
6	DC	1	Total	Mg	0
			1	1	
6	DE	1	Total	Mg	0
			1	1	
6	DG	1	Total	Mg	0
			1	1	
6	EC	1	Total	Mg	0
			1	1	
6	EE	1	Total	Mg	0
			1	1	
6	EG	1	Total	Mg	0
			1	1	
6	FC	1	Total	Mg	0
			1	1	
6	FE	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
6	FG	1	Total Mg 1 1	0
6	GC	1	Total Mg 1 1	0
6	GE	1	Total Mg 1 1	0
6	GG	1	Total Mg 1 1	0
6	HC	1	Total Mg 1 1	0
6	HE	1	Total Mg 1 1	0
6	HG	1	Total Mg 1 1	0
6	IC	1	Total Mg 1 1	0
6	IE	1	Total Mg 1 1	0
6	IG	1	Total Mg 1 1	0
6	JC	1	Total Mg 1 1	0
6	JE	1	Total Mg 1 1	0
6	JG	1	Total Mg 1 1	0
6	KC	1	Total Mg 1 1	0
6	KE	1	Total Mg 1 1	0
6	KG	1	Total Mg 1 1	0
6	LA	1	Total Mg 1 1	0
6	LC	1	Total Mg 1 1	0
6	LE	1	Total Mg 1 1	0
6	MA	1	Total Mg 1 1	0
6	MC	1	Total Mg 1 1	0

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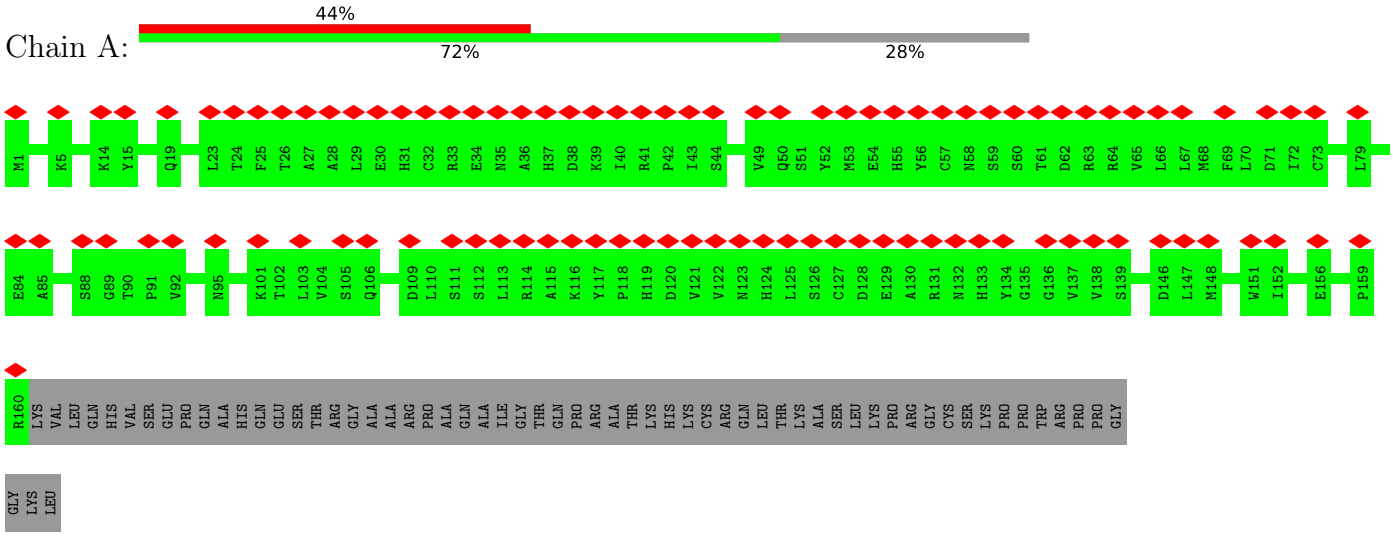
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	ME	1	1	1	0

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.

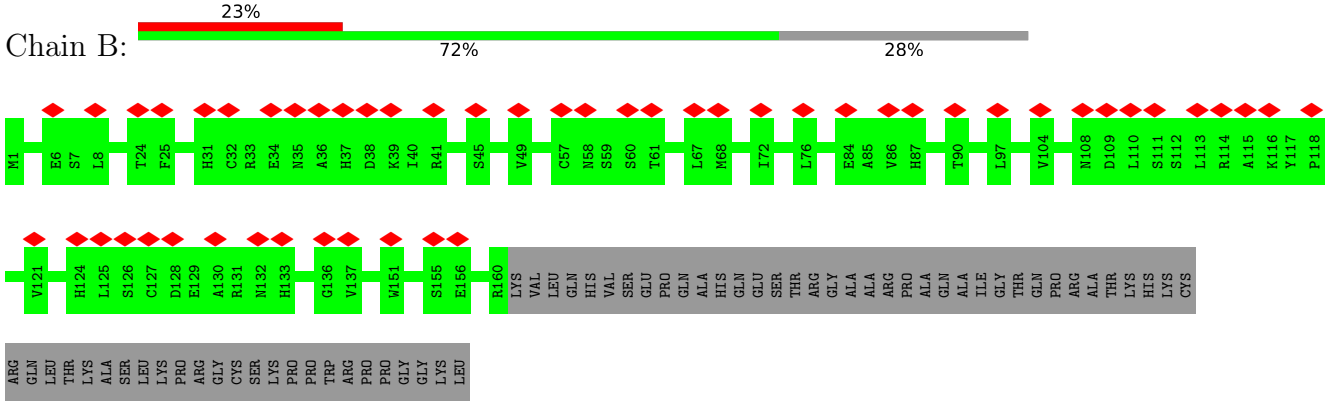
• Molecule 1: Sperm acrosome-associated protein 9

Chain A:



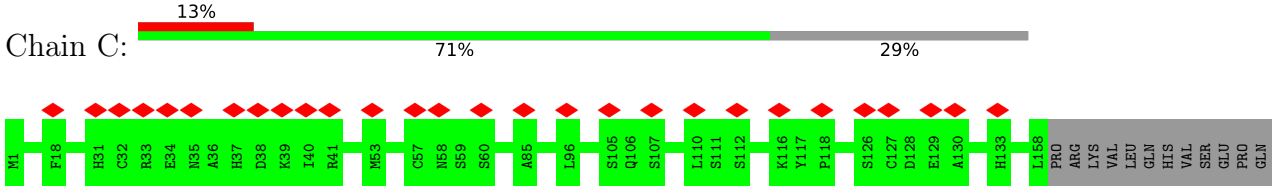
• Molecule 1: Sperm acrosome-associated protein 9

Chain B:



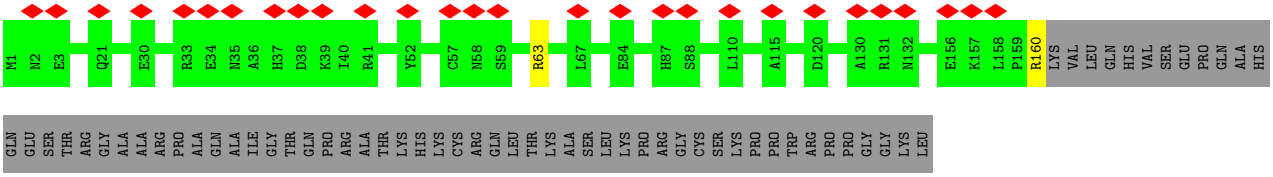
• Molecule 1: Sperm acrosome-associated protein 9

Chain C:



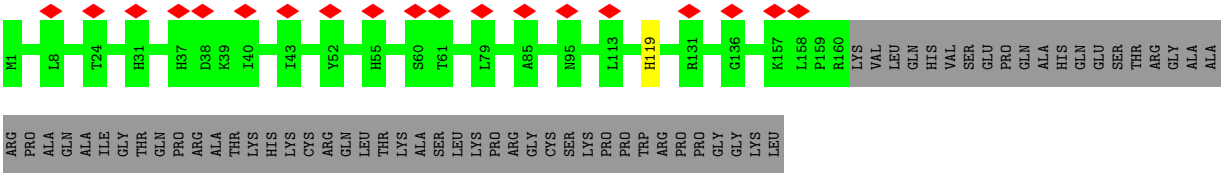
• Molecule 1: Sperm acrosome-associated protein 9

Chain D:



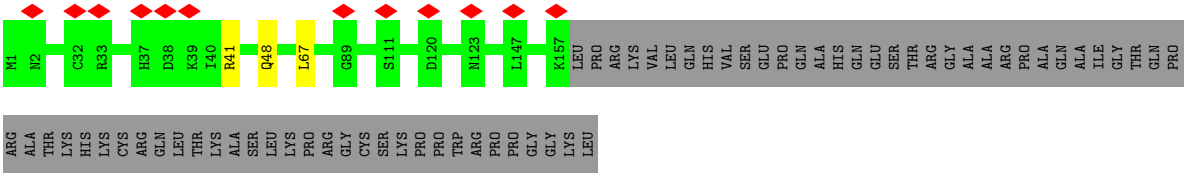
• Molecule 1: Sperm acrosome-associated protein 9

Chain E:



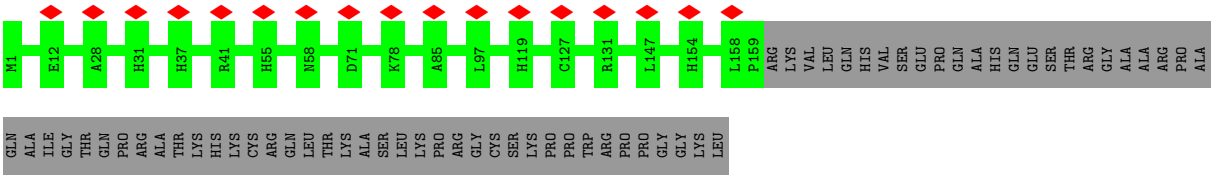
• Molecule 1: Sperm acrosome-associated protein 9

Chain F:



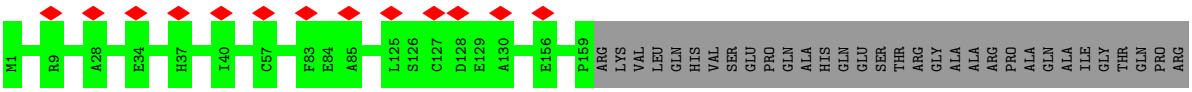
• Molecule 1: Sperm acrosome-associated protein 9

Chain G:



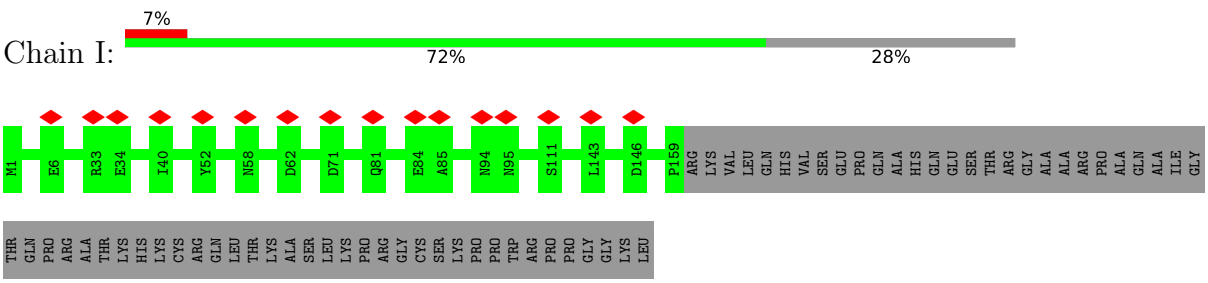
• Molecule 1: Sperm acrosome-associated protein 9

Chain H:



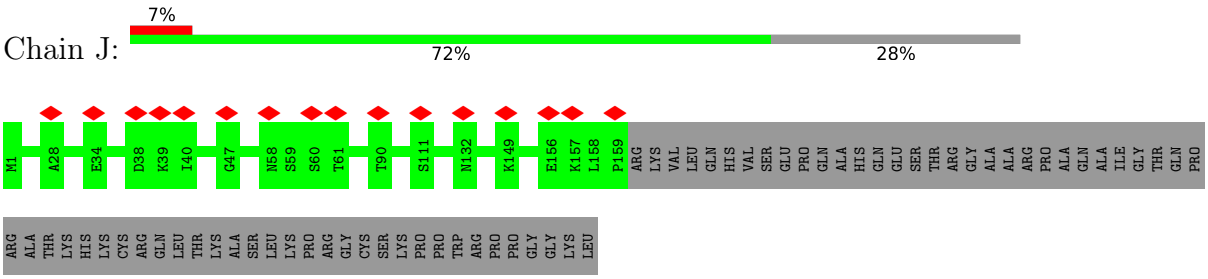
• Molecule 1: Sperm acrosome-associated protein 9

Chain I:



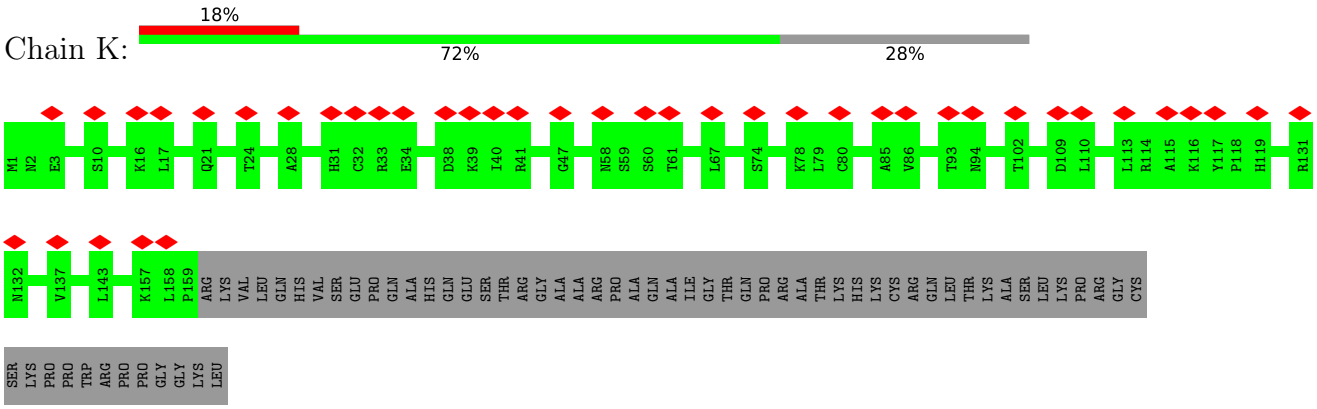
• Molecule 1: Sperm acrosome-associated protein 9

Chain J:



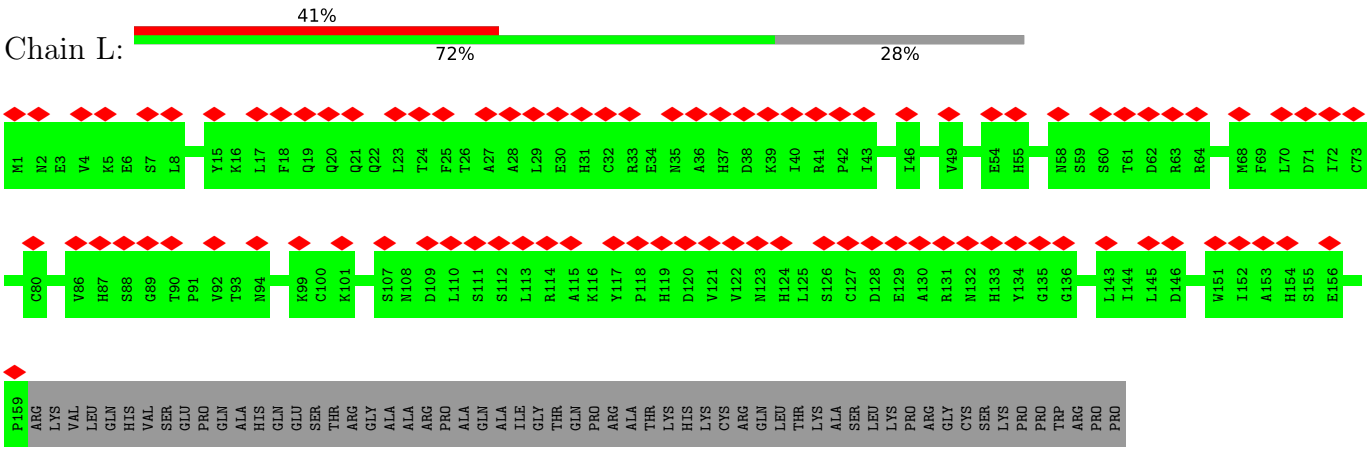
• Molecule 1: Sperm acrosome-associated protein 9

Chain K:



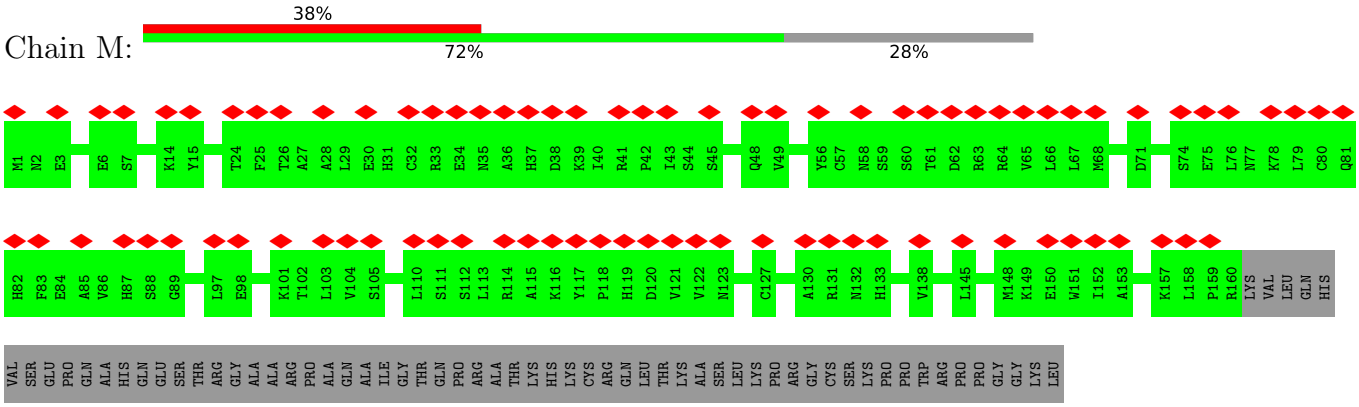
• Molecule 1: Sperm acrosome-associated protein 9

Chain L:



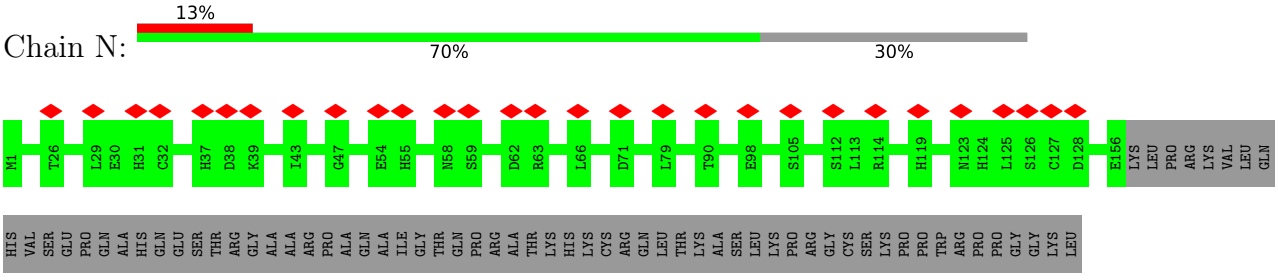
• Molecule 1: Sperm acrosome-associated protein 9

Chain M:



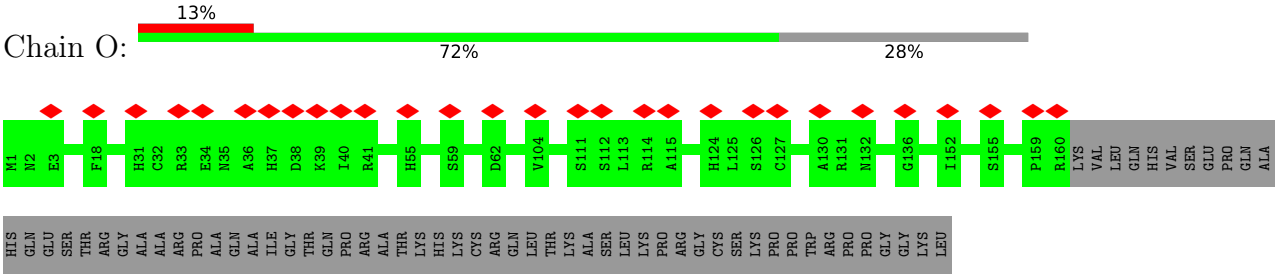
• Molecule 1: Sperm acrosome-associated protein 9

Chain N:



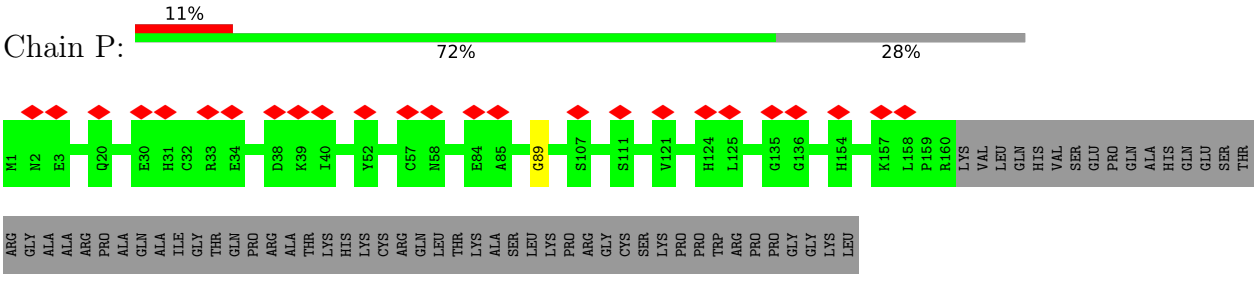
• Molecule 1: Sperm acrosome-associated protein 9

Chain O:



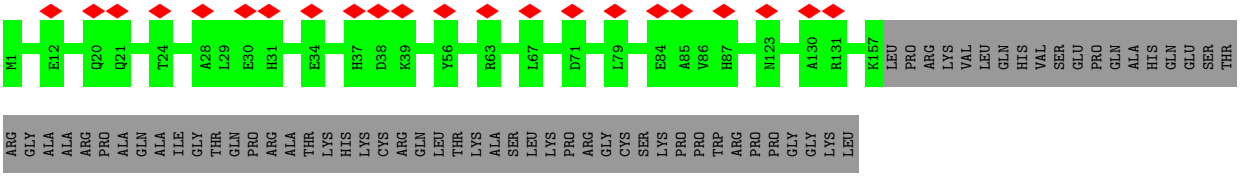
• Molecule 1: Sperm acrosome-associated protein 9

Chain P:

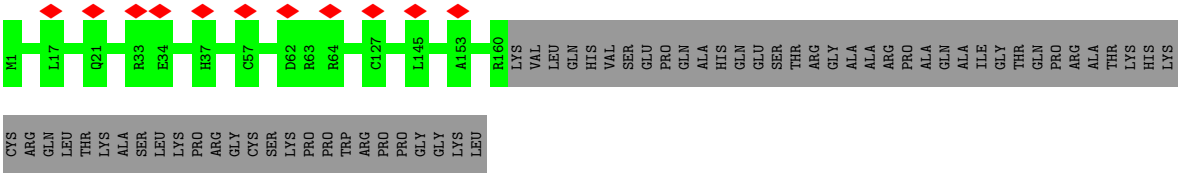


• Molecule 1: Sperm acrosome-associated protein 9

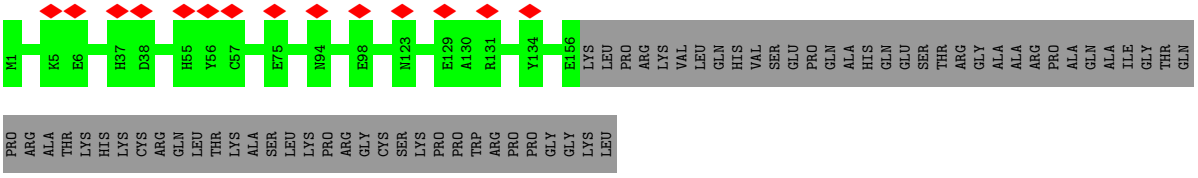
Chain Q:



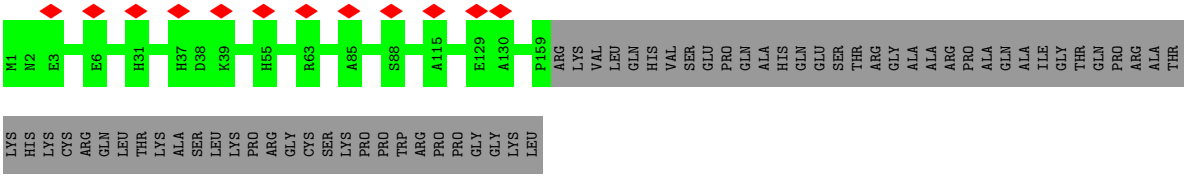
• Molecule 1: Sperm acrosome-associated protein 9



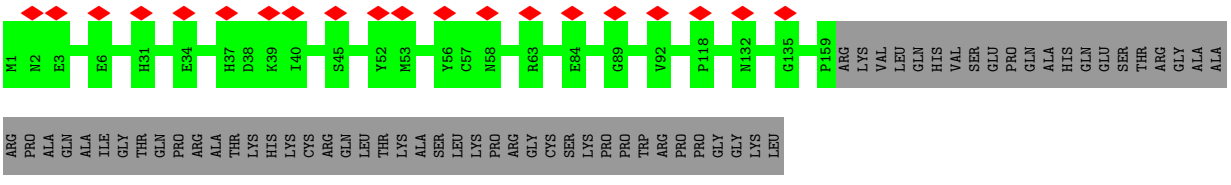
• Molecule 1: Sperm acrosome-associated protein 9



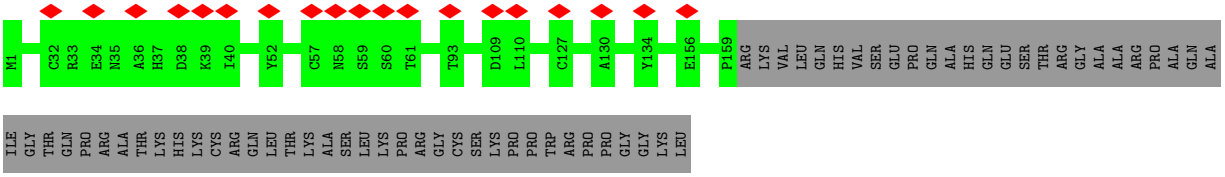
• Molecule 1: Sperm acrosome-associated protein 9



• Molecule 1: Sperm acrosome-associated protein 9



• Molecule 1: Sperm acrosome-associated protein 9



• Molecule 1: Sperm acrosome-associated protein 9

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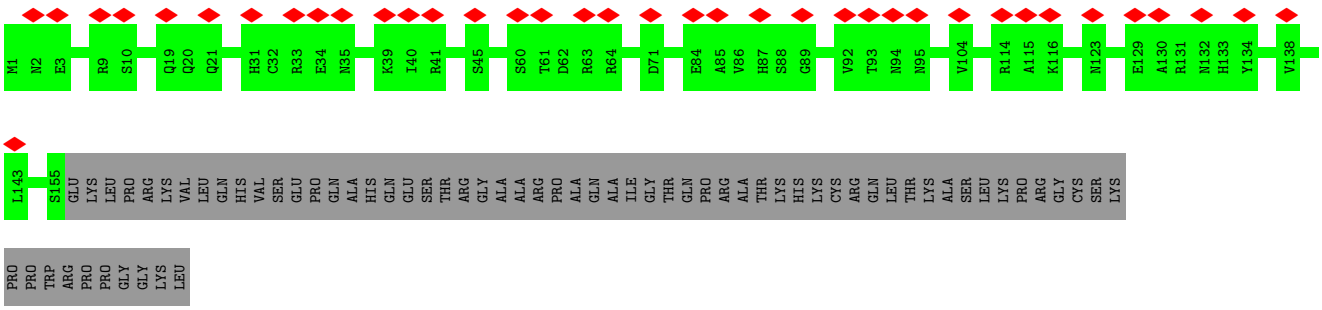
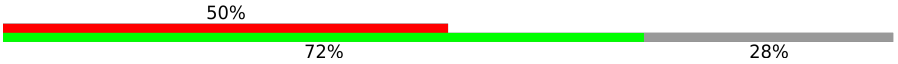
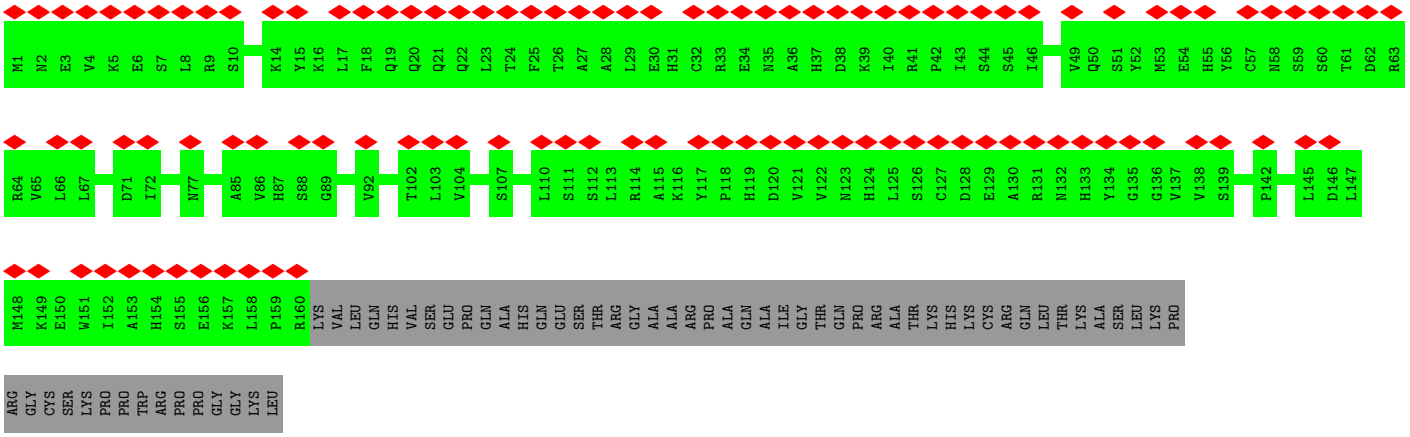


• Molecule 1: Sperm acrosome-associated protein 9

Chain X:





• Molecule 1: Sperm acrosome-associated protein 9

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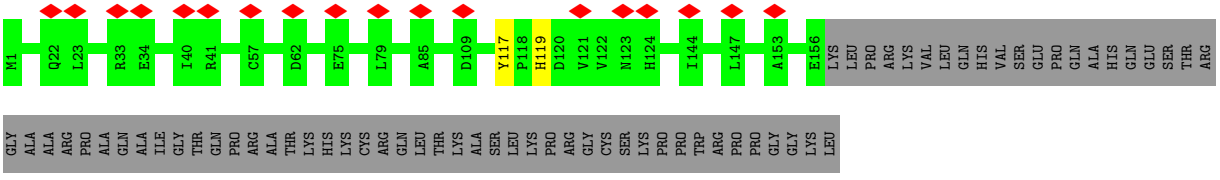

• Molecule 1: Sperm acrosome-associated protein 9

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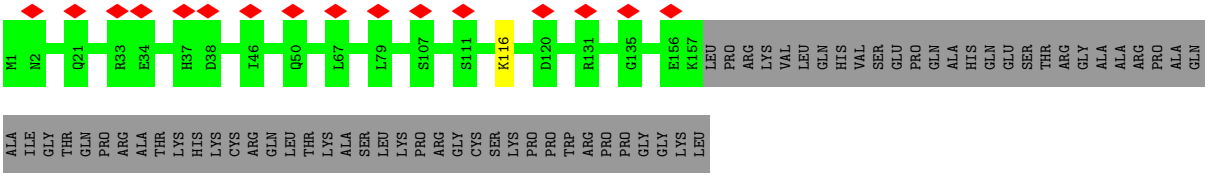
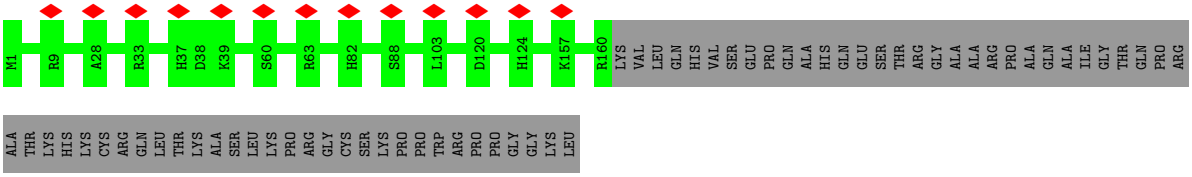


• Molecule 1: Sperm acrosome-associated protein 9



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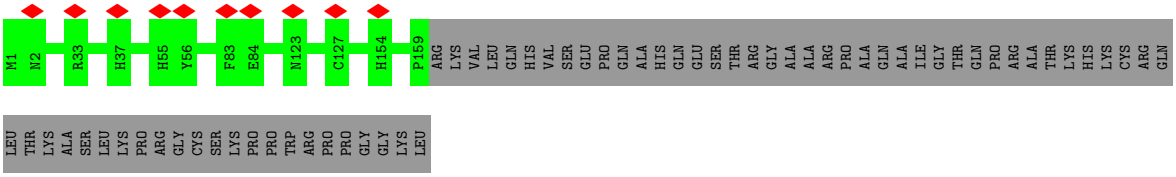

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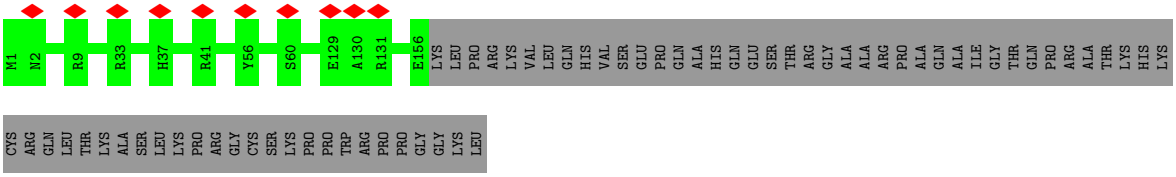

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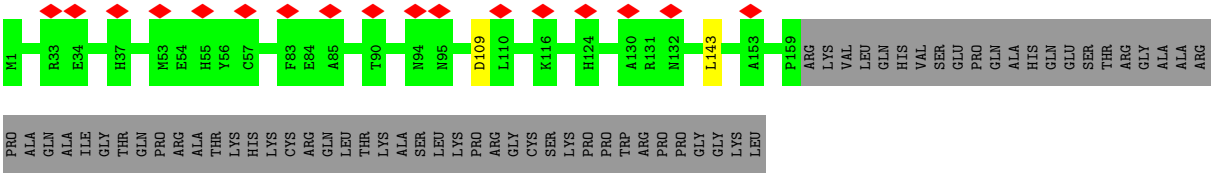

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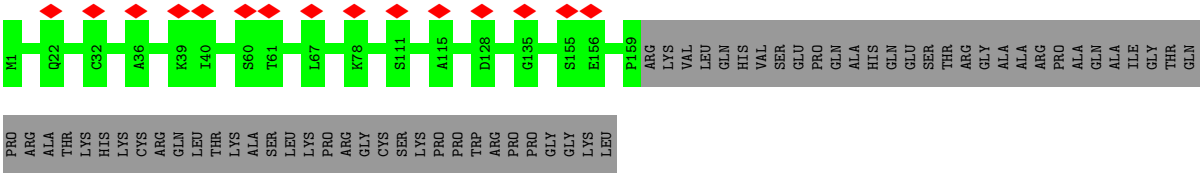

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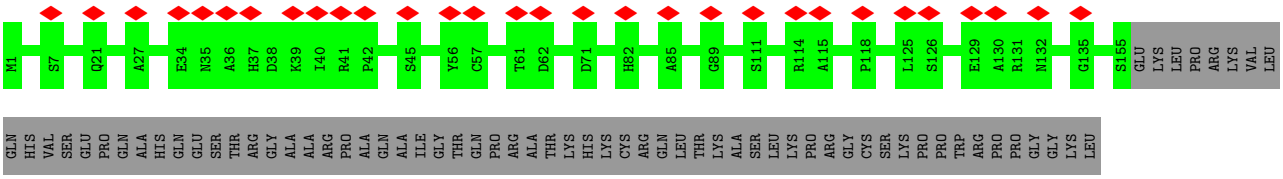
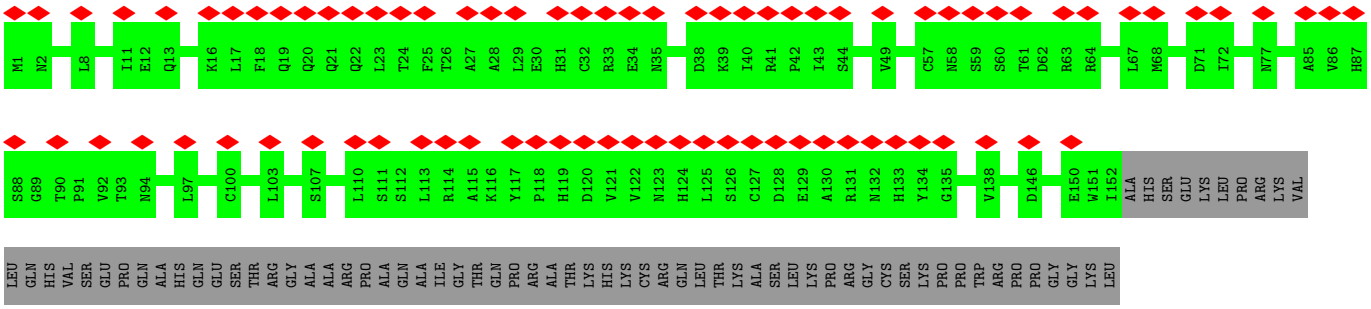
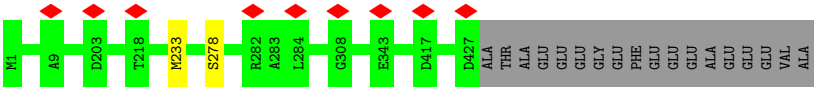


• Molecule 1: Sperm acrosome-associated protein 9



• Molecule 2: Tubulin beta-4B chain



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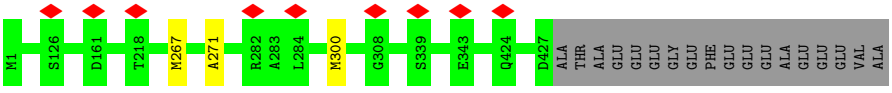
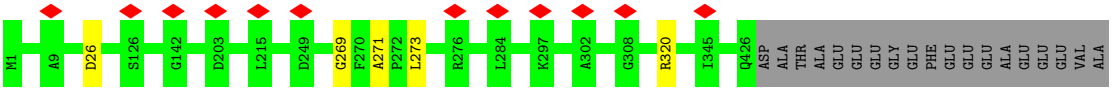
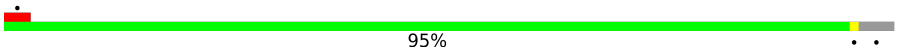


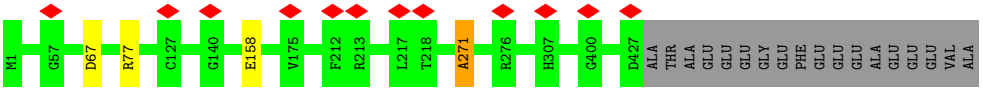
• Molecule 2: Tubulin beta-4B chain



• Molecule 2: Tubulin beta-4B chain

Chain BA:





• Molecule 2: Tubulin beta-4B chain

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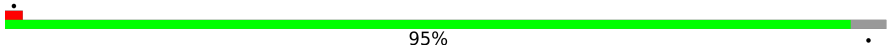
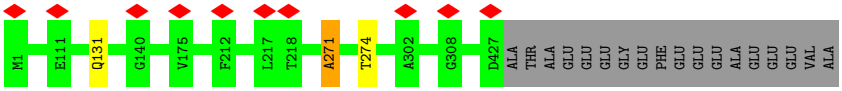
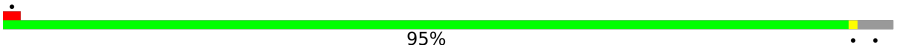
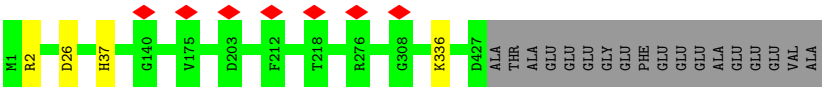




• Molecule 2: Tubulin beta-4B chain

Chain BF:





• Molecule 2: Tubulin beta-4B chain

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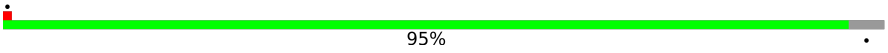

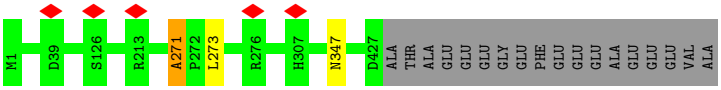

• Molecule 2: Tubulin beta-4B chain

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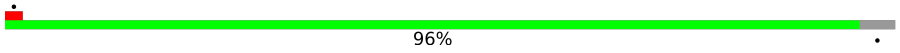

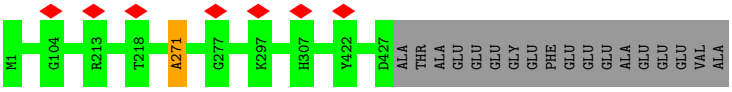

• Molecule 2: Tubulin beta-4B chain

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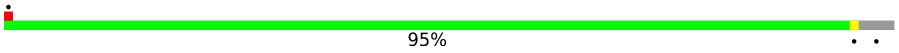

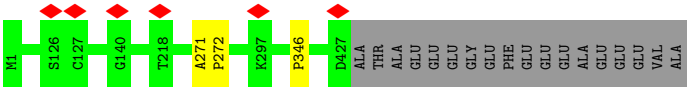

• Molecule 2: Tubulin beta-4B chain

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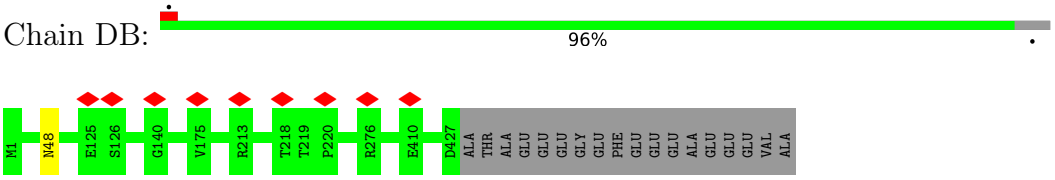
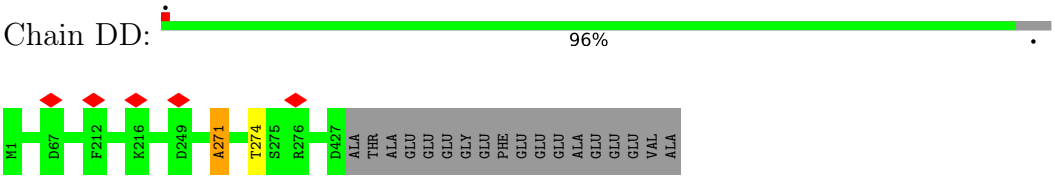


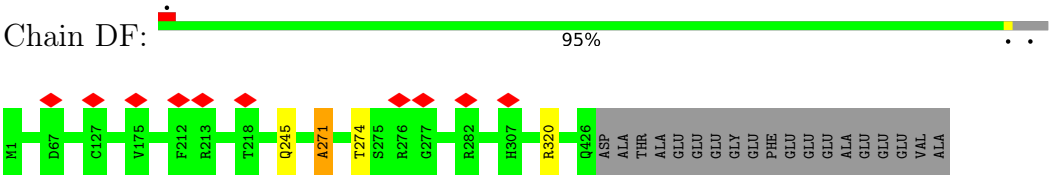
• Molecule 2: Tubulin beta-4B chain

Chain DD:



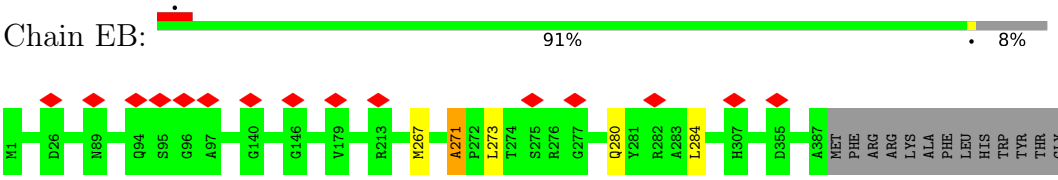
• Molecule 2: Tubulin beta-4B chain

Chain DF:



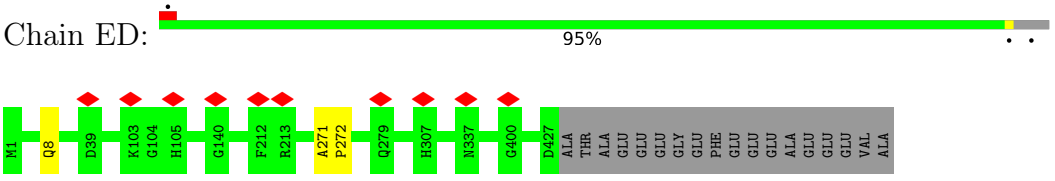
• Molecule 2: Tubulin beta-4B chain

Chain EB:



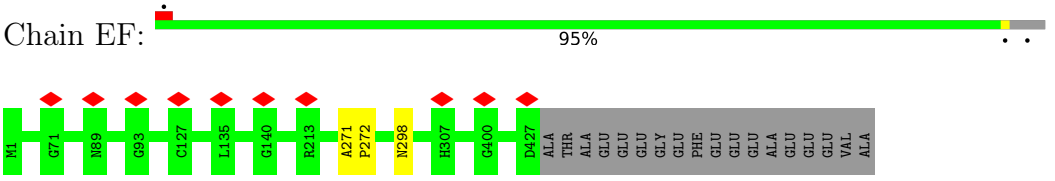
• Molecule 2: Tubulin beta-4B chain

Chain ED:



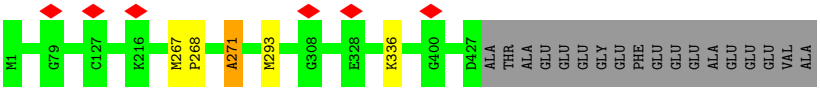
• Molecule 2: Tubulin beta-4B chain

Chain EF:



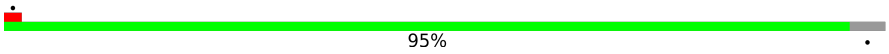
• Molecule 2: Tubulin beta-4B chain

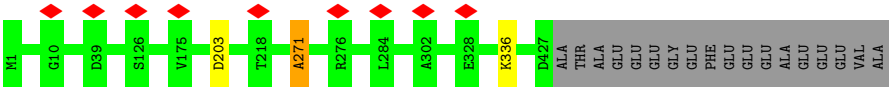
Chain FD:



• Molecule 2: Tubulin beta-4B chain

Chain FF:





• Molecule 2: Tubulin beta-4B chain

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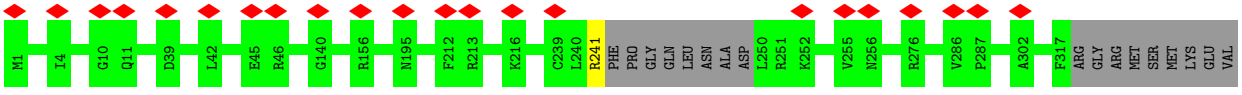

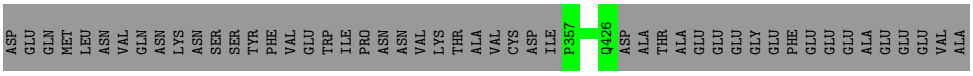

• Molecule 2: Tubulin beta-4B chain

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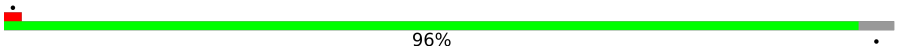

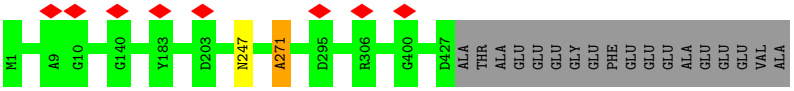

• Molecule 2: Tubulin beta-4B chain

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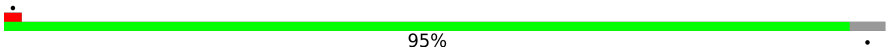

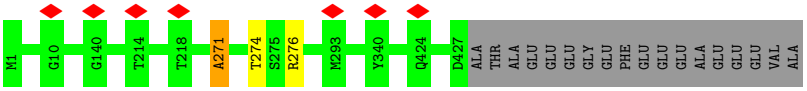

• Molecule 2: Tubulin beta-4B chain

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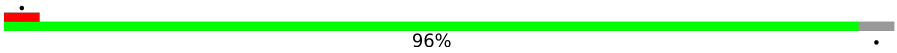
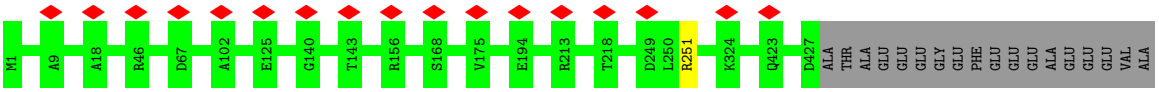
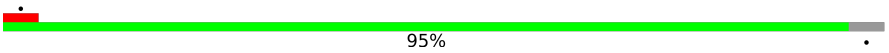
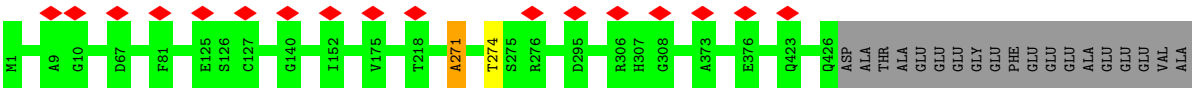




• Molecule 2: Tubulin beta-4B chain

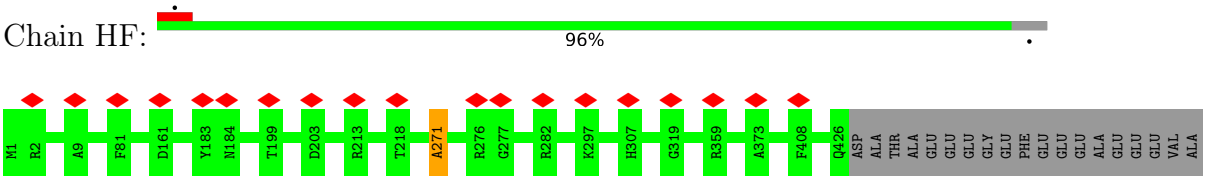
Chain HD:





• Molecule 2: Tubulin beta-4B chain

Chain HF:



• Molecule 2: Tubulin beta-4B chain

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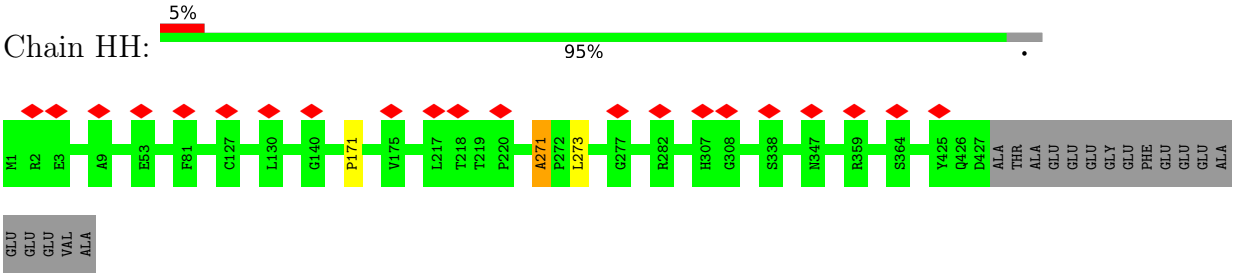

• Molecule 2: Tubulin beta-4B chain

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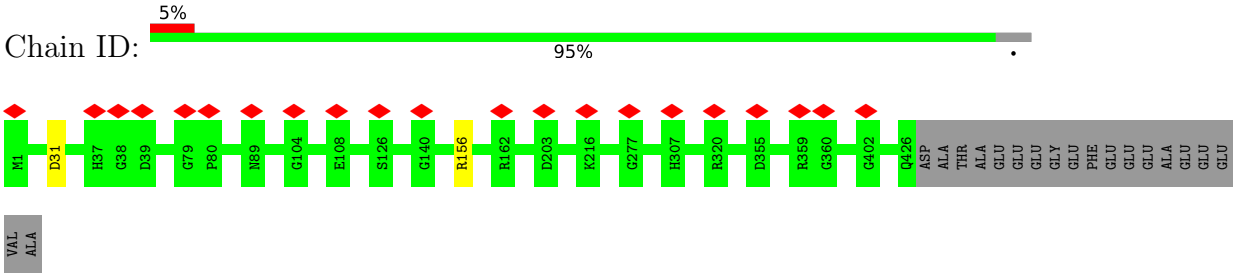

• Molecule 2: Tubulin beta-4B chain

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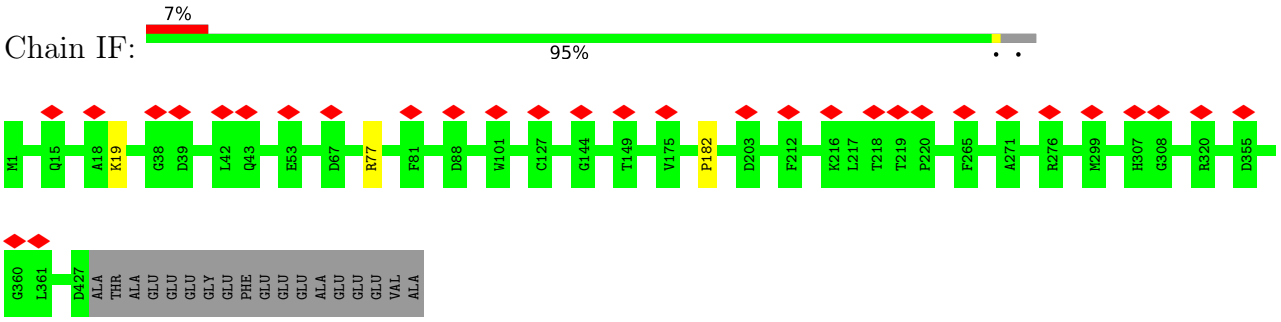

• Molecule 2: Tubulin beta-4B chain

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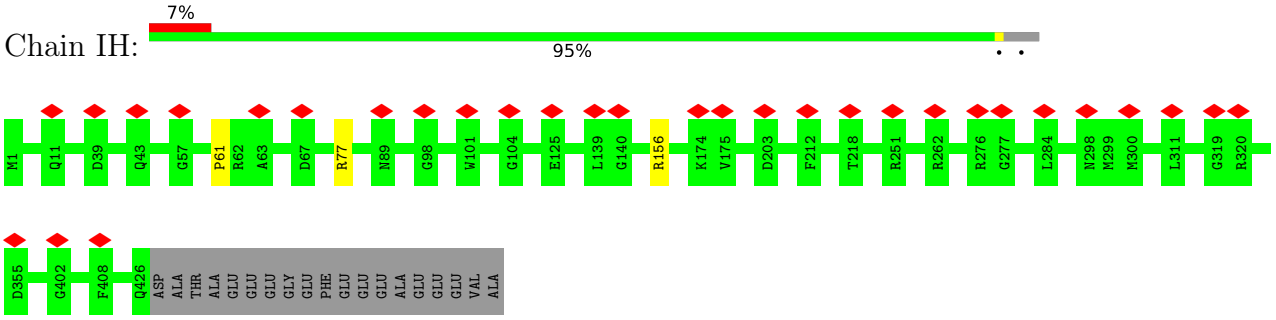

• Molecule 2: Tubulin beta-4B chain

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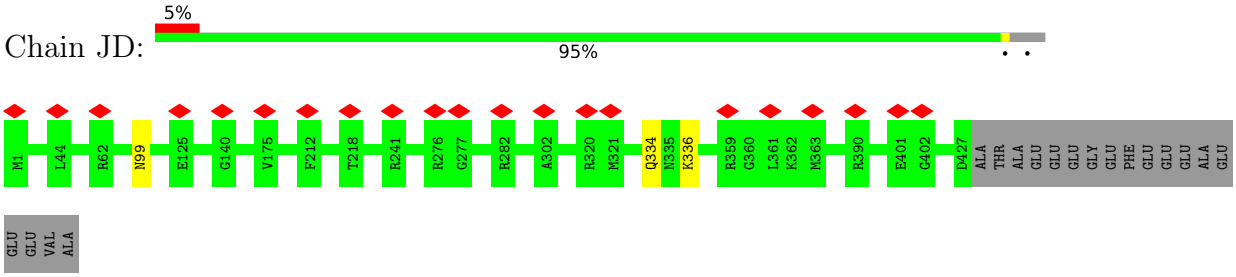
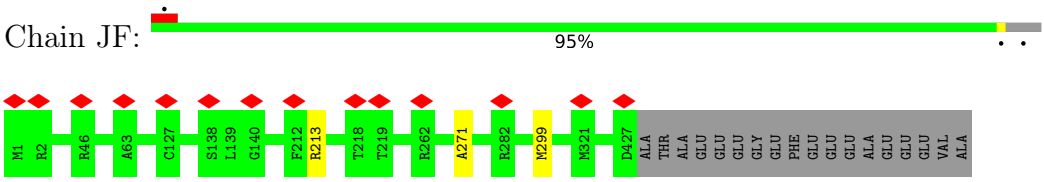


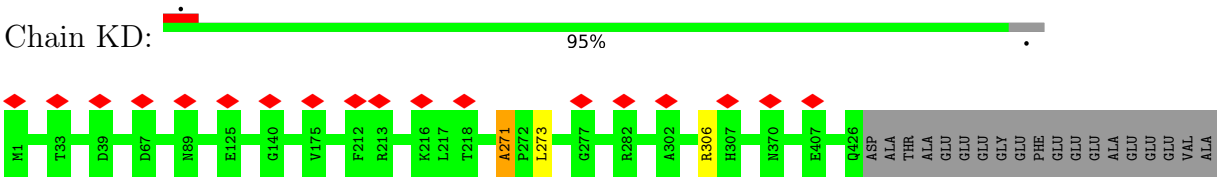
• Molecule 2: Tubulin beta-4B chain

Chain JF:



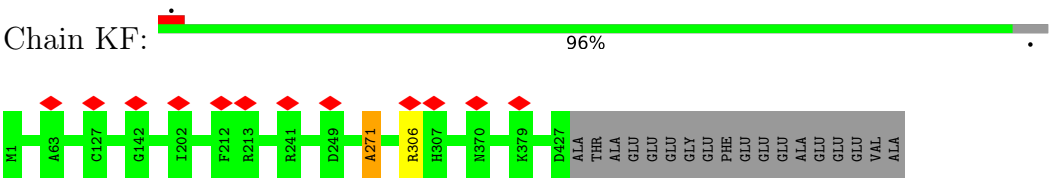
• Molecule 2: Tubulin beta-4B chain

Chain KD:



• Molecule 2: Tubulin beta-4B chain

Chain KF:



• Molecule 2: Tubulin beta-4B chain

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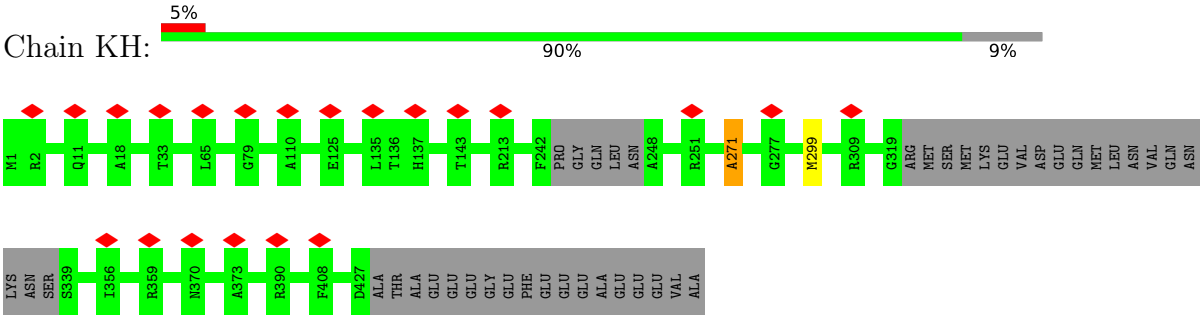
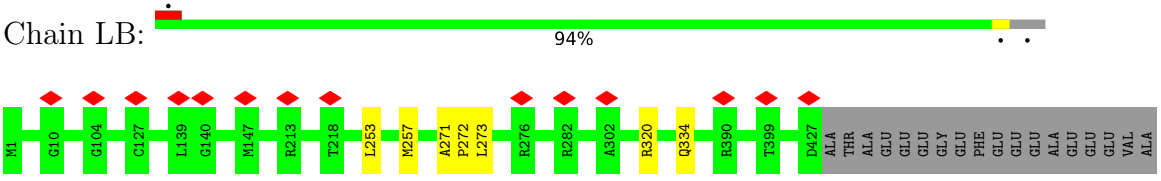


• Molecule 2: Tubulin beta-4B chain

Chain LB:



• Molecule 2: Tubulin beta-4B chain

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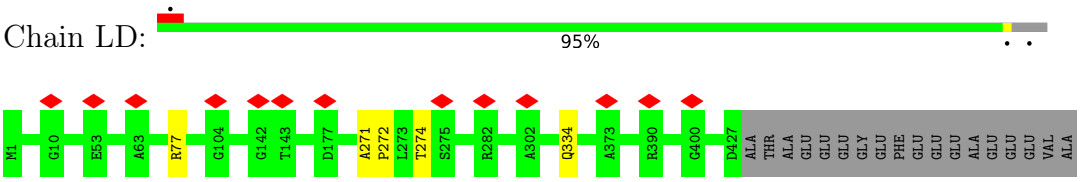
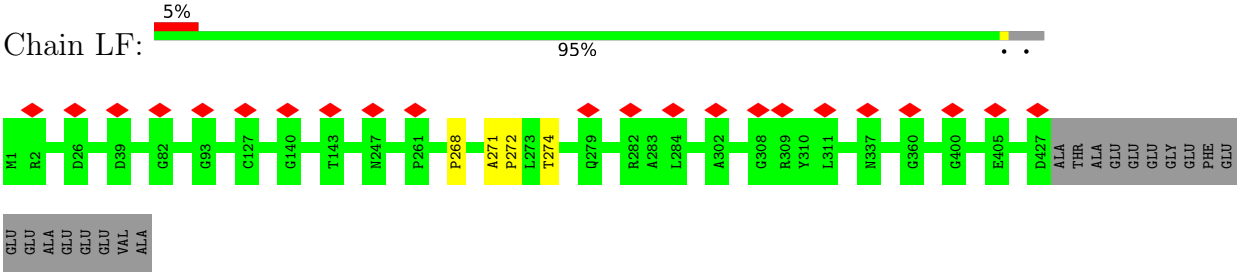


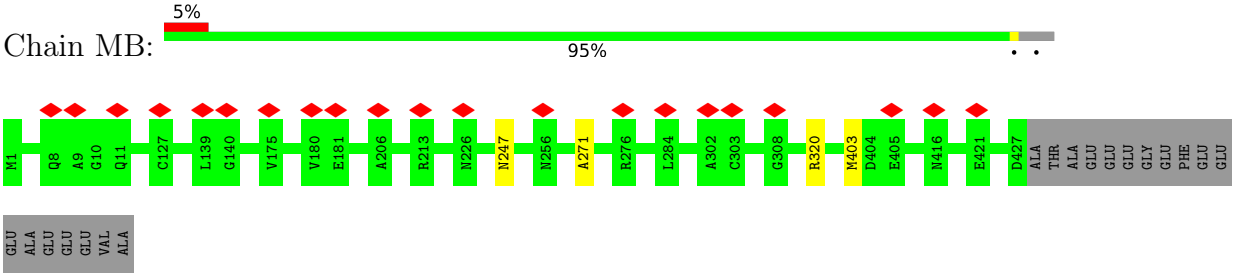
• Molecule 2: Tubulin beta-4B chain

Chain LF:



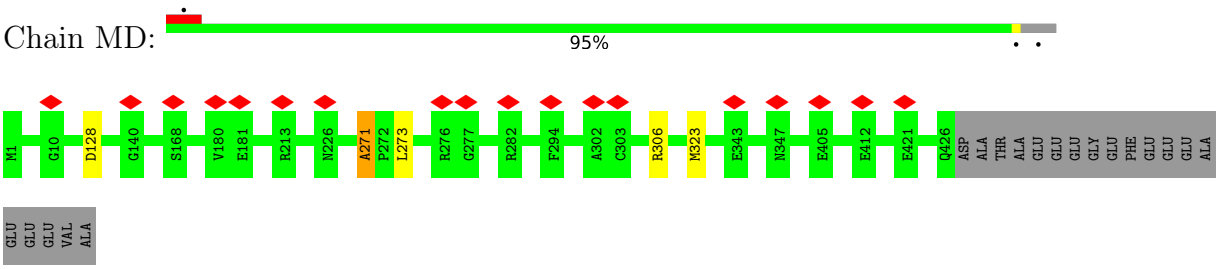
• Molecule 2: Tubulin beta-4B chain

Chain MB:



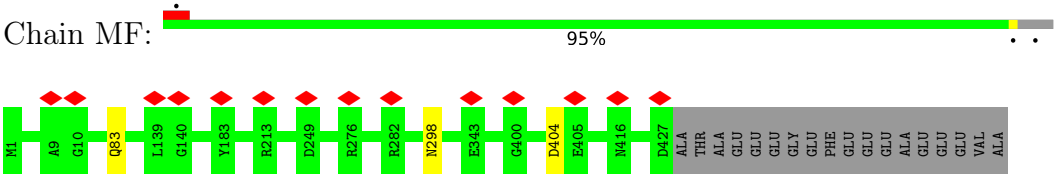
• Molecule 2: Tubulin beta-4B chain

Chain MD:



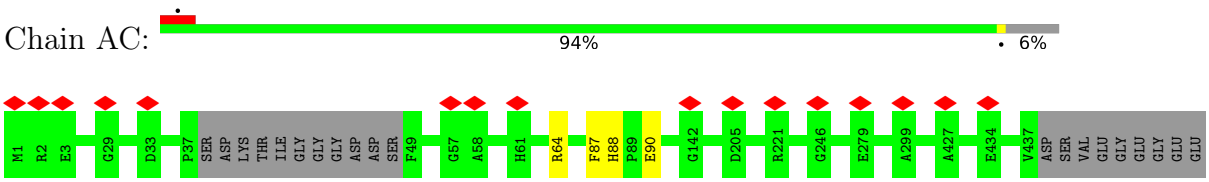
• Molecule 2: Tubulin beta-4B chain

Chain MF:



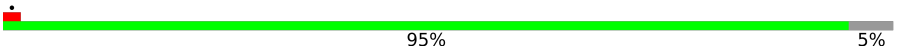
• Molecule 3: Tubulin alpha-1A chain

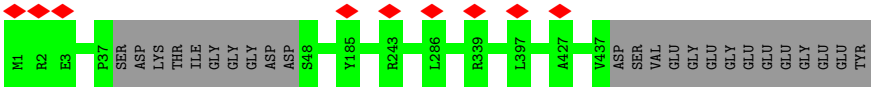
Chain AC:



• Molecule 3: Tubulin alpha-1A chain

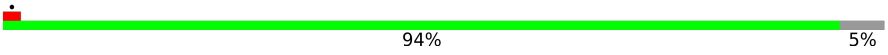
Chain AE:

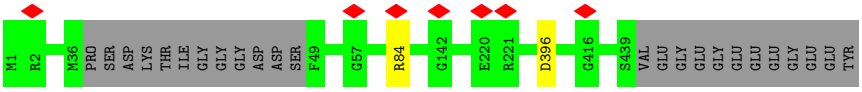




• Molecule 3: Tubulin alpha-1A chain

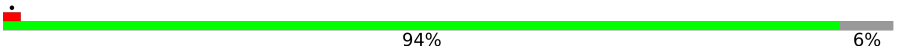
Chain BC:

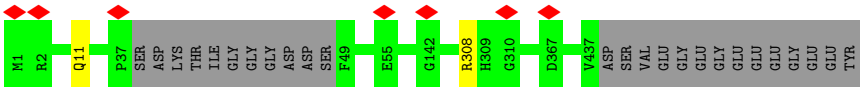




• Molecule 3: Tubulin alpha-1A chain

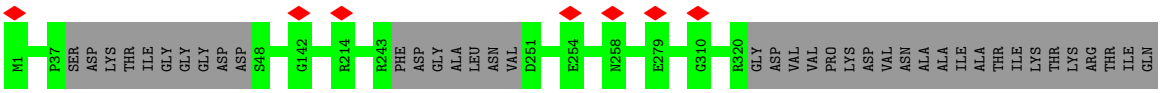
Chain BE:

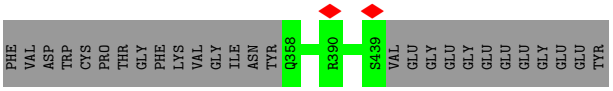




• Molecule 3: Tubulin alpha-1A chain

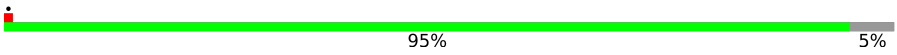
Chain BG:

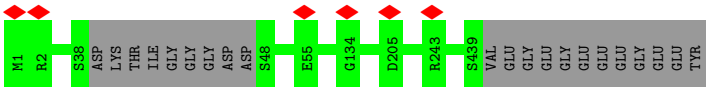




• Molecule 3: Tubulin alpha-1A chain

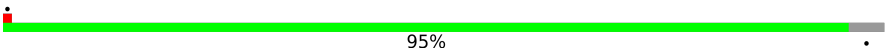
Chain CC:

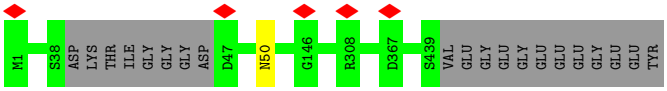




• Molecule 3: Tubulin alpha-1A chain

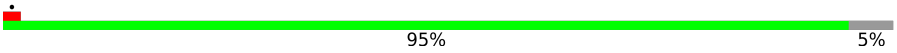
Chain CE:

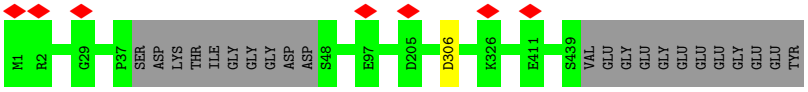




• Molecule 3: Tubulin alpha-1A chain

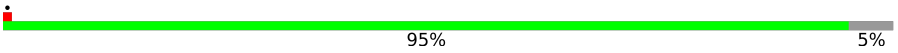
Chain CG:

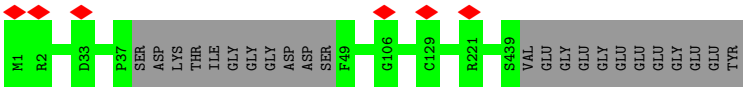




• Molecule 3: Tubulin alpha-1A chain

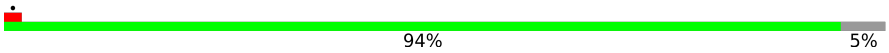
Chain DC:

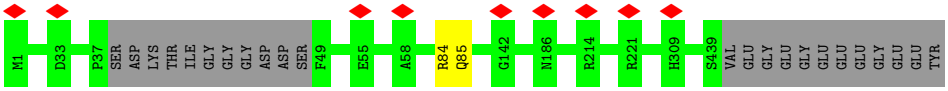




• Molecule 3: Tubulin alpha-1A chain

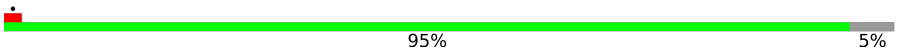
Chain DE:

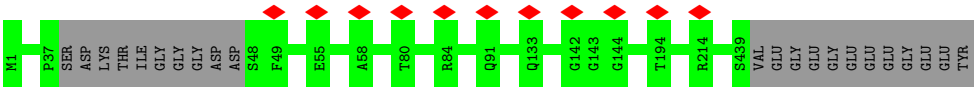




• Molecule 3: Tubulin alpha-1A chain

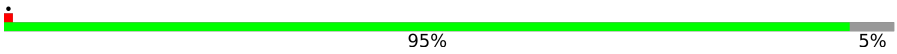
Chain DG:

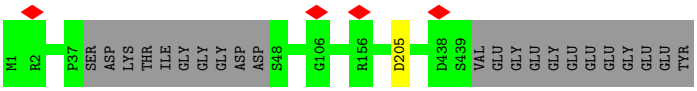




• Molecule 3: Tubulin alpha-1A chain

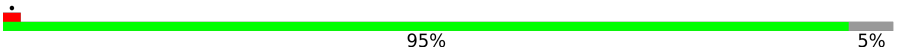
Chain EC:

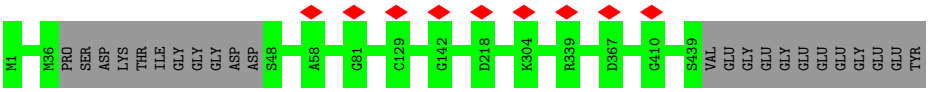




• Molecule 3: Tubulin alpha-1A chain

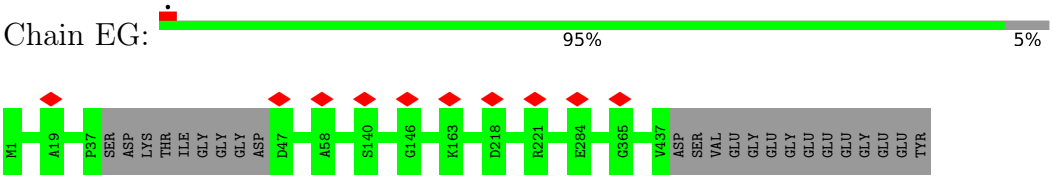
Chain EE:





• Molecule 3: Tubulin alpha-1A chain

Chain EG:



• Molecule 3: Tubulin alpha-1A chain

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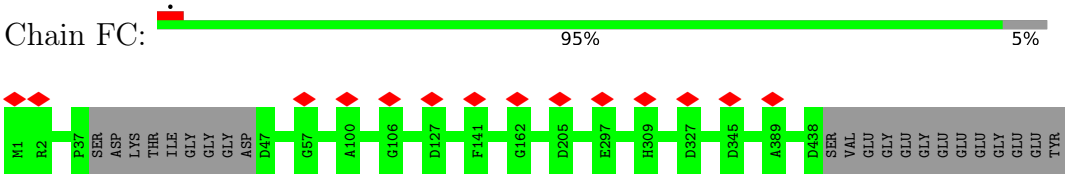
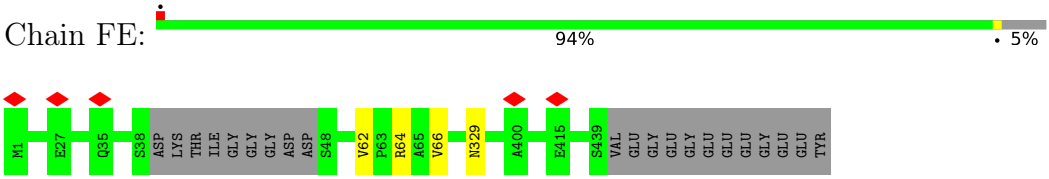


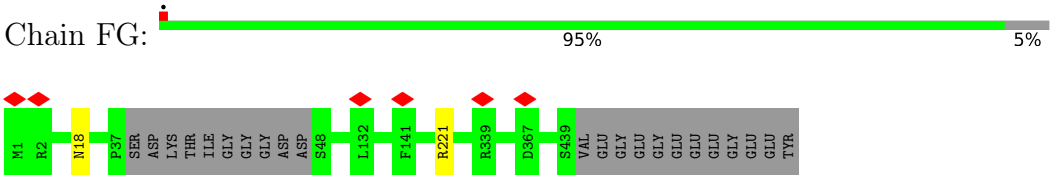
• Molecule 3: Tubulin alpha-1A chain

Chain FE:



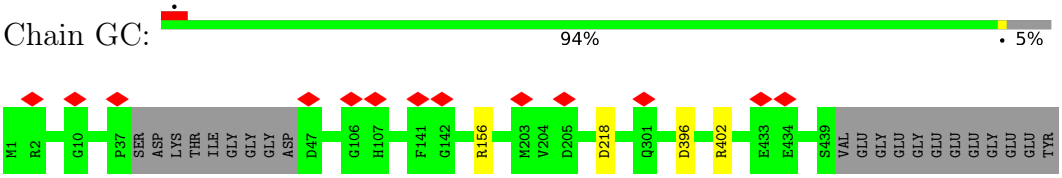
• Molecule 3: Tubulin alpha-1A chain

Chain FG:



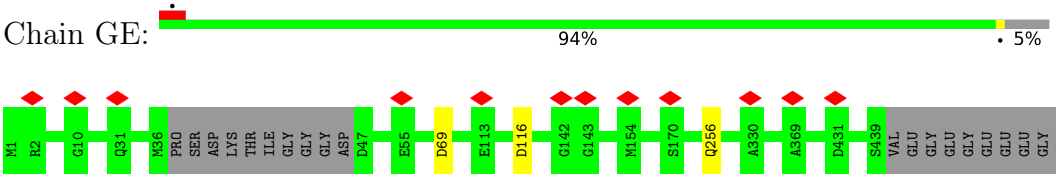
• Molecule 3: Tubulin alpha-1A chain

Chain GC:



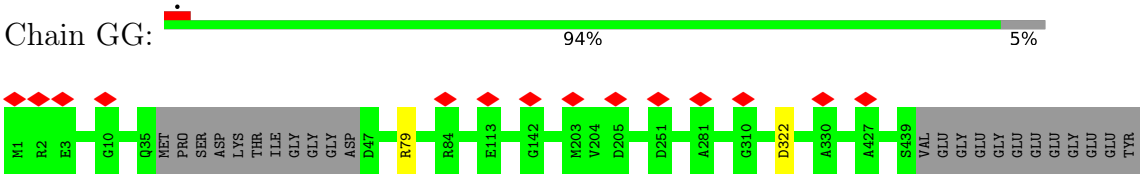
• Molecule 3: Tubulin alpha-1A chain

Chain GE:



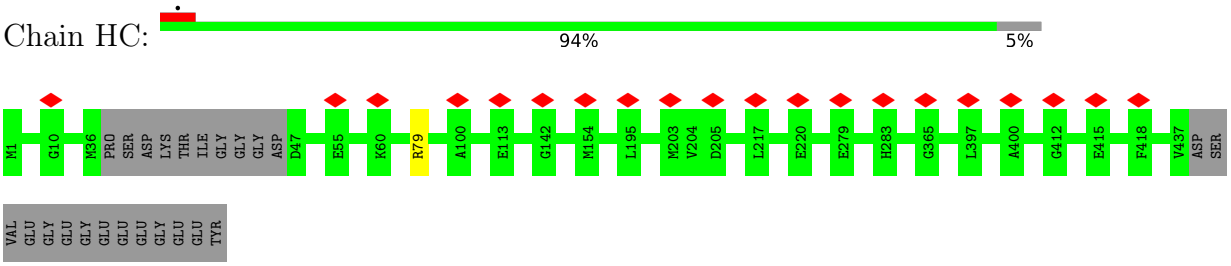
• Molecule 3: Tubulin alpha-1A chain

Chain GG:



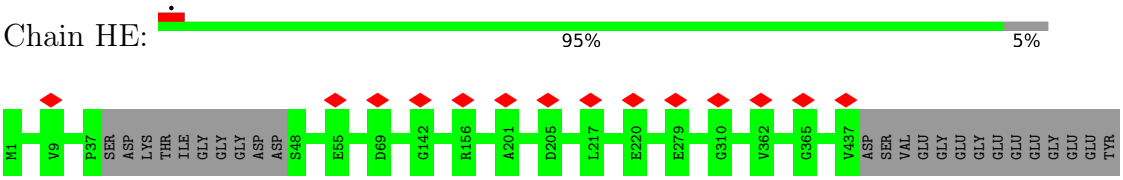
• Molecule 3: Tubulin alpha-1A chain

Chain HC:



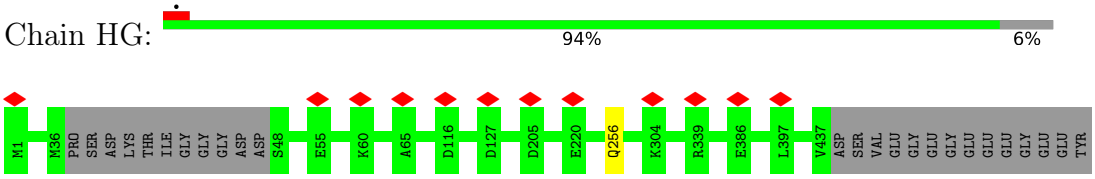
• Molecule 3: Tubulin alpha-1A chain

Chain HE:



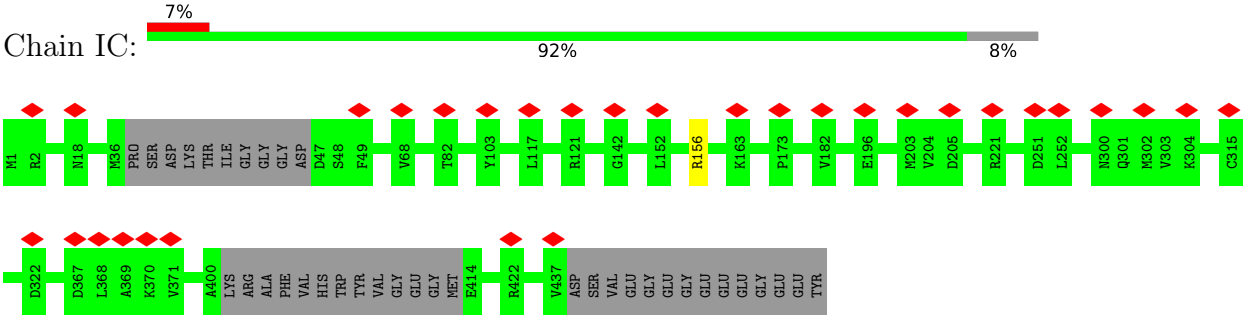
• Molecule 3: Tubulin alpha-1A chain

Chain HG:



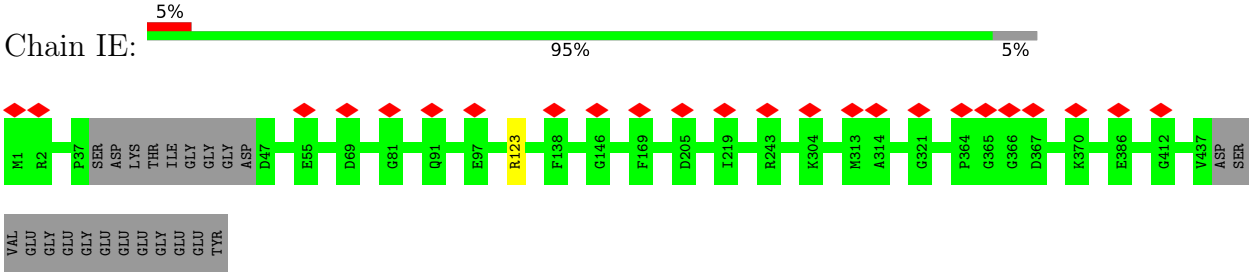
• Molecule 3: Tubulin alpha-1A chain

Chain IC:



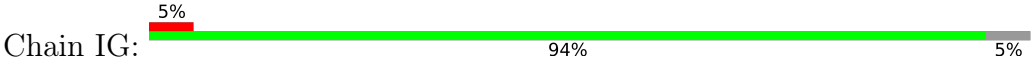
• Molecule 3: Tubulin alpha-1A chain

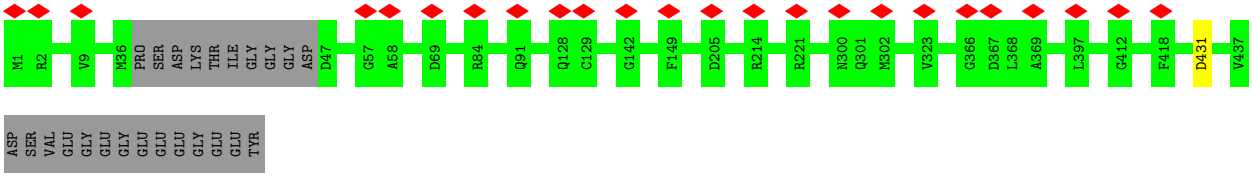
Chain IE:



• Molecule 3: Tubulin alpha-1A chain

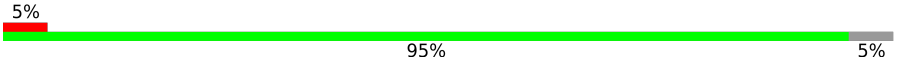
Chain IG:

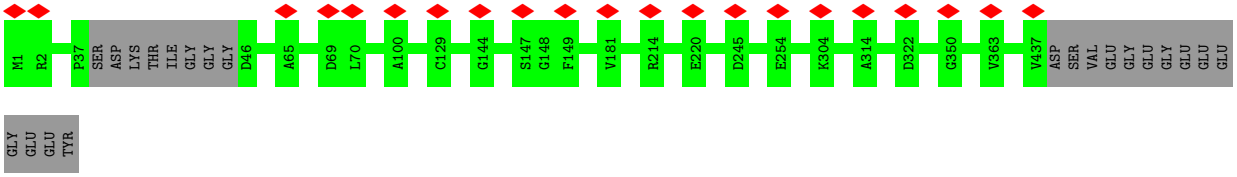




• Molecule 3: Tubulin alpha-1A chain

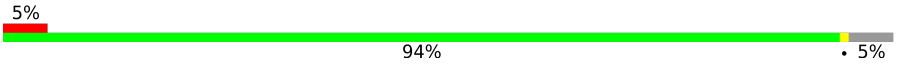
Chain JC:

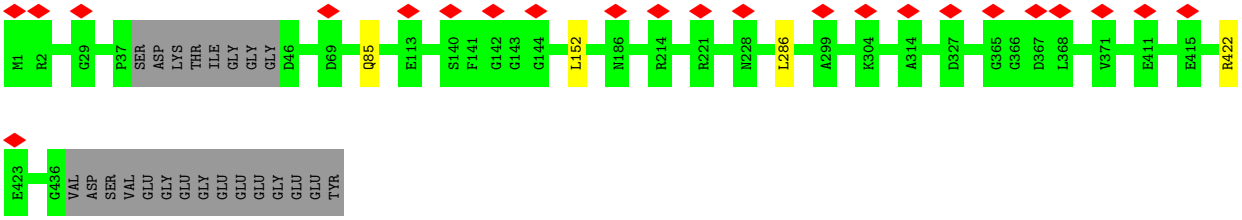




• Molecule 3: Tubulin alpha-1A chain

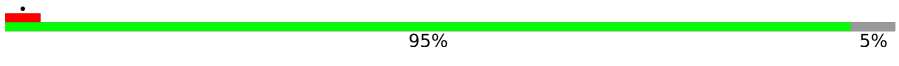
Chain JE:

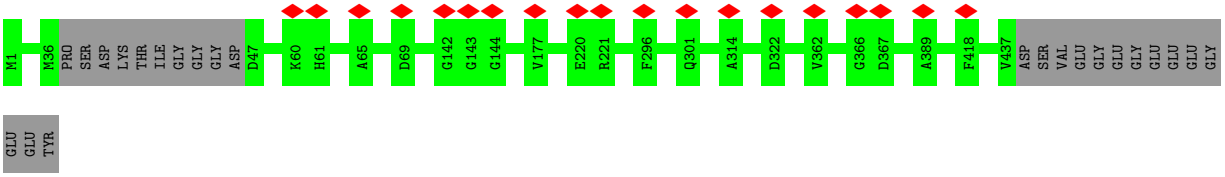




• Molecule 3: Tubulin alpha-1A chain

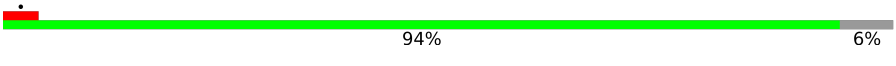
Chain JG:

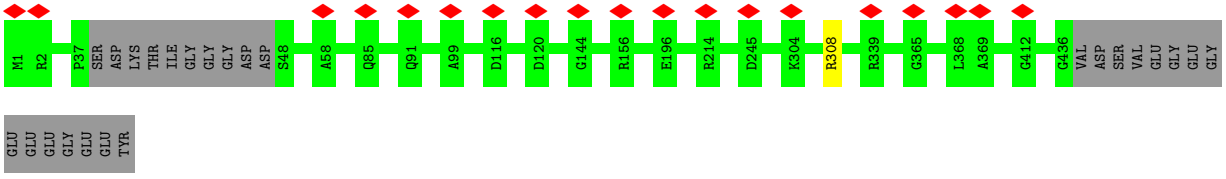




• Molecule 3: Tubulin alpha-1A chain

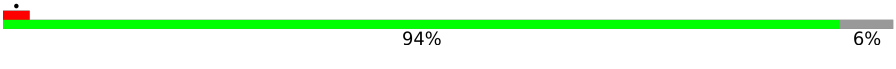
Chain KC:

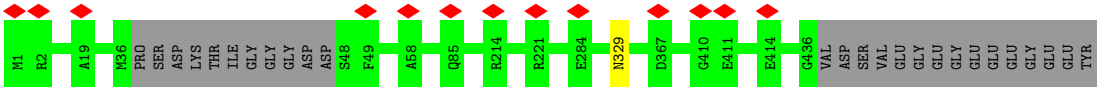




• Molecule 3: Tubulin alpha-1A chain

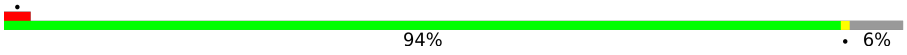
Chain KE:

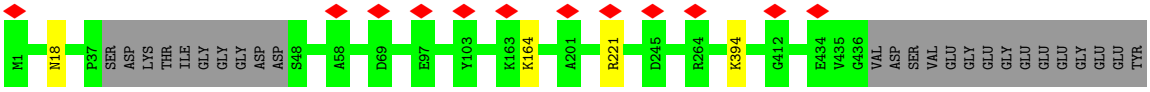




• Molecule 3: Tubulin alpha-1A chain

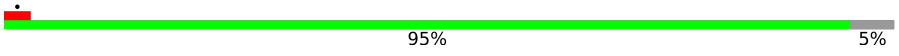
Chain KG:

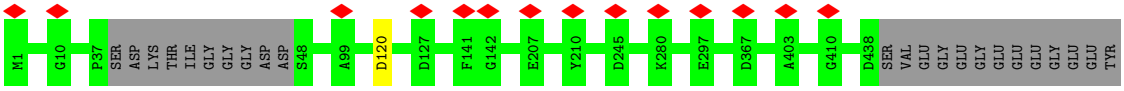




• Molecule 3: Tubulin alpha-1A chain

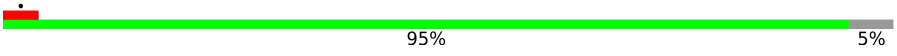
Chain LA:

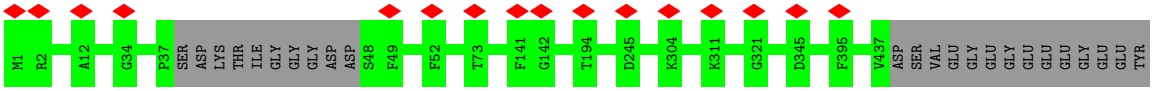




• Molecule 3: Tubulin alpha-1A chain

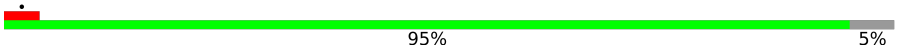
Chain LC:

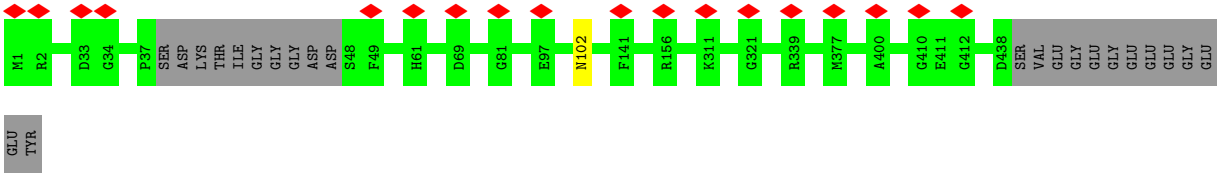




• Molecule 3: Tubulin alpha-1A chain

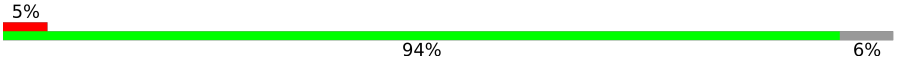
Chain LE:

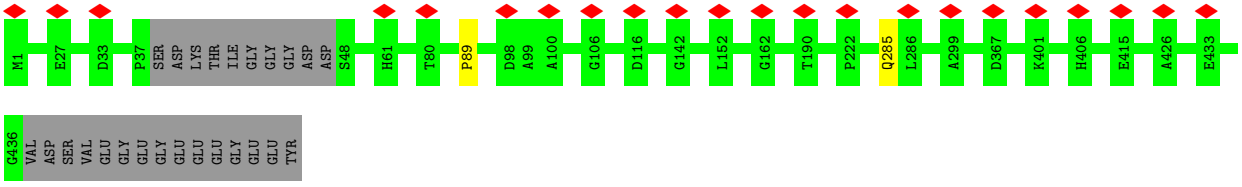




• Molecule 3: Tubulin alpha-1A chain

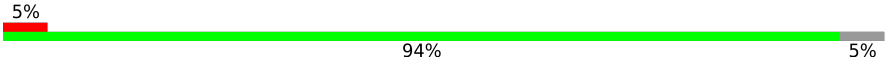
Chain MA:

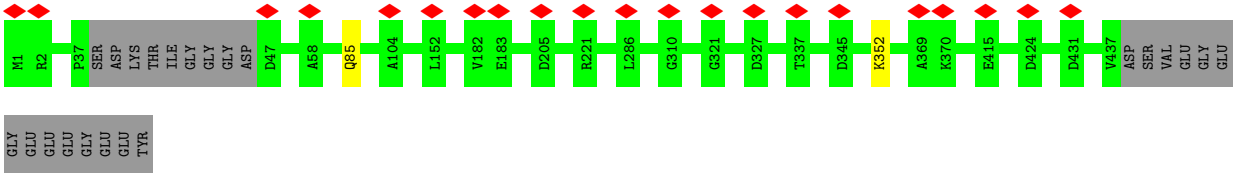




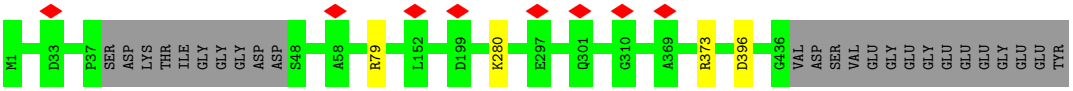
• Molecule 3: Tubulin alpha-1A chain

Chain MC:





• Molecule 3: Tubulin alpha-1A chain



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21990	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.386	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	404.63998, 404.63998, 404.63998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.843, 0.843, 0.843	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.23	0/795	0.36	0/1109
1	B	0.23	0/795	0.34	0/1109
1	C	0.23	0/785	0.35	0/1095
1	D	0.26	0/1313	0.52	0/1772
1	E	0.26	0/1313	0.52	0/1772
1	F	0.27	0/1286	0.51	1/1735 (0.1%)
1	G	0.27	0/1302	0.58	0/1758
1	H	0.25	0/1302	0.48	0/1758
1	I	0.26	0/1302	0.49	0/1758
1	J	0.24	0/790	0.36	0/1102
1	K	0.24	0/790	0.33	0/1102
1	L	0.23	0/790	0.35	0/1102
1	M	0.23	0/795	0.36	0/1109
1	N	0.24	0/775	0.38	0/1081
1	O	0.24	0/795	0.36	0/1109
1	P	0.28	0/1313	0.55	1/1772 (0.1%)
1	Q	0.27	0/1286	0.53	0/1735
1	R	0.27	0/1313	0.53	0/1772
1	S	0.27	0/1277	0.50	0/1724
1	T	0.27	0/1302	0.54	0/1758
1	U	0.27	0/1302	0.56	0/1758
1	V	0.24	0/790	0.36	0/1102
1	W	0.23	0/770	0.35	0/1074
1	X	0.23	0/795	0.36	0/1109
1	d	0.29	0/1277	0.57	1/1724 (0.1%)
1	e	0.27	0/1286	0.53	0/1735
1	f	0.26	0/1313	0.52	0/1772
1	g	0.28	0/1302	0.53	0/1758
1	h	0.27	0/1277	0.52	0/1724
1	i	0.28	0/1302	0.56	2/1758 (0.1%)
1	j	0.24	0/790	0.35	0/1102
1	k	0.24	0/770	0.37	0/1074

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	l	0.23	0/755	0.35	0/1053
2	AB	0.31	0/3431	0.59	1/4649 (0.0%)
2	AD	0.29	0/3431	0.59	3/4649 (0.1%)
2	AF	0.29	0/3423	0.59	3/4638 (0.1%)
2	BA	0.29	0/3431	0.60	2/4649 (0.0%)
2	BD	0.30	0/3431	0.57	1/4649 (0.0%)
2	BF	0.30	0/3431	0.60	1/4649 (0.0%)
2	CB	0.28	0/3431	0.58	1/4649 (0.0%)
2	CD	0.28	0/3431	0.57	1/4649 (0.0%)
2	CF	0.30	0/3431	0.61	2/4649 (0.0%)
2	DB	0.29	0/3431	0.58	0/4649
2	DD	0.30	0/3431	0.60	1/4649 (0.0%)
2	DF	0.29	0/3423	0.59	1/4638 (0.0%)
2	EB	0.28	0/3282	0.58	3/4449 (0.1%)
2	ED	0.31	0/3431	0.62	1/4649 (0.0%)
2	EF	0.31	0/3431	0.61	1/4649 (0.0%)
2	FD	0.30	0/3431	0.61	4/4649 (0.1%)
2	FF	0.29	0/3431	0.60	2/4649 (0.0%)
2	FH	0.28	0/3037	0.56	0/4112
2	GD	0.29	0/3431	0.57	1/4649 (0.0%)
2	GF	0.29	0/3431	0.56	1/4649 (0.0%)
2	GH	0.27	0/3431	0.56	0/4649
2	HD	0.29	0/3423	0.57	1/4638 (0.0%)
2	HF	0.29	0/3423	0.57	1/4638 (0.0%)
2	HH	0.29	0/3431	0.57	2/4649 (0.0%)
2	ID	0.28	0/3423	0.57	1/4638 (0.0%)
2	IF	0.29	0/3431	0.61	1/4649 (0.0%)
2	IH	0.29	0/3423	0.58	1/4638 (0.0%)
2	JD	0.29	0/3431	0.58	0/4649
2	JF	0.29	0/3431	0.59	1/4649 (0.0%)
2	KD	0.29	0/3423	0.58	1/4638 (0.0%)
2	KF	0.30	0/3431	0.59	1/4649 (0.0%)
2	KH	0.27	0/3237	0.59	1/4387 (0.0%)
2	LB	0.30	0/3431	0.58	2/4649 (0.0%)
2	LD	0.29	0/3431	0.58	2/4649 (0.0%)
2	LF	0.29	0/3431	0.60	1/4649 (0.0%)
2	MB	0.30	0/3431	0.58	0/4649
2	MD	0.29	0/3423	0.60	2/4638 (0.0%)
2	MF	0.29	0/3431	0.59	1/4649 (0.0%)
3	AC	0.31	0/3420	0.59	1/4643 (0.0%)
3	AE	0.30	0/3426	0.56	0/4651
3	BC	0.29	0/3426	0.56	1/4650 (0.0%)
3	BE	0.29	0/3420	0.53	0/4643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	BG	0.28	0/3093	0.55	0/4193
3	CC	0.29	0/3446	0.58	0/4678
3	CE	0.29	0/3454	0.57	0/4689
3	CG	0.28	0/3440	0.56	1/4670 (0.0%)
3	DC	0.29	0/3434	0.55	0/4662
3	DE	0.30	0/3434	0.55	0/4662
3	DG	0.28	0/3440	0.55	0/4670
3	EC	0.29	0/3440	0.57	1/4670 (0.0%)
3	EE	0.29	0/3432	0.56	0/4658
3	EG	0.28	0/3434	0.54	0/4662
3	FC	0.28	0/3442	0.54	0/4673
3	FE	0.30	0/3446	0.58	0/4678
3	FG	0.28	0/3440	0.57	0/4670
3	GC	0.28	0/3448	0.57	2/4681 (0.0%)
3	GE	0.28	0/3440	0.58	2/4669 (0.0%)
3	GG	0.28	0/3432	0.56	1/4659 (0.0%)
3	HC	0.28	0/3426	0.56	0/4650
3	HE	0.28	0/3426	0.54	0/4651
3	HG	0.28	0/3418	0.58	0/4639
3	IC	0.27	0/3309	0.54	0/4491
3	IE	0.27	0/3434	0.55	0/4662
3	IG	0.28	0/3426	0.54	1/4650 (0.0%)
3	JC	0.27	0/3442	0.54	0/4673
3	JE	0.29	0/3435	0.58	2/4663 (0.0%)
3	JG	0.28	0/3426	0.54	0/4650
3	KC	0.28	0/3419	0.56	0/4641
3	KE	0.27	0/3411	0.53	0/4629
3	KG	0.28	0/3419	0.53	0/4641
3	LA	0.27	0/3434	0.55	1/4662 (0.0%)
3	LC	0.29	0/3426	0.57	0/4651
3	LE	0.29	0/3434	0.55	0/4662
3	MA	0.28	0/3419	0.56	1/4641 (0.0%)
3	MC	0.29	0/3434	0.56	0/4662
3	ME	0.29	0/3419	0.60	1/4641 (0.0%)
All	All	0.28	0/294669	0.56	69/399940 (0.0%)

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	FF	271	ALA	N-CA-C	8.14	132.99	111.00
3	GG	322	ASP	CB-CG-OD2	7.32	124.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	IF	182	PRO	CA-N-CD	-7.30	101.27	111.50
2	KH	271	ALA	N-CA-C	7.28	130.65	111.00
2	LD	271	ALA	N-CA-C	7.18	130.40	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/222 (71%)	155 (98%)	3 (2%)	0	100	100
1	B	158/222 (71%)	155 (98%)	3 (2%)	0	100	100
1	C	156/222 (70%)	149 (96%)	7 (4%)	0	100	100
1	D	158/222 (71%)	150 (95%)	8 (5%)	0	100	100
1	E	158/222 (71%)	150 (95%)	8 (5%)	0	100	100
1	F	155/222 (70%)	150 (97%)	5 (3%)	0	100	100
1	G	157/222 (71%)	151 (96%)	6 (4%)	0	100	100
1	H	157/222 (71%)	153 (98%)	4 (2%)	0	100	100
1	I	157/222 (71%)	153 (98%)	4 (2%)	0	100	100
1	J	157/222 (71%)	147 (94%)	10 (6%)	0	100	100
1	K	157/222 (71%)	154 (98%)	3 (2%)	0	100	100
1	L	157/222 (71%)	153 (98%)	4 (2%)	0	100	100
1	M	158/222 (71%)	155 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	154/222 (69%)	146 (95%)	8 (5%)	0	100	100
1	O	158/222 (71%)	154 (98%)	4 (2%)	0	100	100
1	P	158/222 (71%)	158 (100%)	0	0	100	100
1	Q	155/222 (70%)	152 (98%)	3 (2%)	0	100	100
1	R	158/222 (71%)	151 (96%)	7 (4%)	0	100	100
1	S	154/222 (69%)	149 (97%)	5 (3%)	0	100	100
1	T	157/222 (71%)	152 (97%)	5 (3%)	0	100	100
1	U	157/222 (71%)	152 (97%)	5 (3%)	0	100	100
1	V	157/222 (71%)	150 (96%)	7 (4%)	0	100	100
1	W	153/222 (69%)	149 (97%)	4 (3%)	0	100	100
1	X	158/222 (71%)	152 (96%)	6 (4%)	0	100	100
1	d	154/222 (69%)	146 (95%)	8 (5%)	0	100	100
1	e	155/222 (70%)	148 (96%)	7 (4%)	0	100	100
1	f	158/222 (71%)	151 (96%)	7 (4%)	0	100	100
1	g	157/222 (71%)	150 (96%)	7 (4%)	0	100	100
1	h	154/222 (69%)	145 (94%)	9 (6%)	0	100	100
1	i	157/222 (71%)	152 (97%)	5 (3%)	0	100	100
1	j	157/222 (71%)	147 (94%)	10 (6%)	0	100	100
1	k	153/222 (69%)	149 (97%)	4 (3%)	0	100	100
1	l	150/222 (68%)	145 (97%)	5 (3%)	0	100	100
2	AB	425/445 (96%)	408 (96%)	17 (4%)	0	100	100
2	AD	425/445 (96%)	405 (95%)	20 (5%)	0	100	100
2	AF	424/445 (95%)	399 (94%)	25 (6%)	0	100	100
2	BA	425/445 (96%)	407 (96%)	16 (4%)	2 (0%)	29	69
2	BD	425/445 (96%)	406 (96%)	18 (4%)	1 (0%)	47	81
2	BF	425/445 (96%)	403 (95%)	22 (5%)	0	100	100
2	CB	425/445 (96%)	405 (95%)	19 (4%)	1 (0%)	47	81
2	CD	425/445 (96%)	398 (94%)	26 (6%)	1 (0%)	47	81
2	CF	425/445 (96%)	407 (96%)	17 (4%)	1 (0%)	47	81
2	DB	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
2	DD	425/445 (96%)	407 (96%)	17 (4%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DF	424/445 (95%)	397 (94%)	26 (6%)	1 (0%)	47	81
2	EB	407/445 (92%)	387 (95%)	19 (5%)	1 (0%)	47	81
2	ED	425/445 (96%)	408 (96%)	16 (4%)	1 (0%)	47	81
2	EF	425/445 (96%)	400 (94%)	24 (6%)	1 (0%)	47	81
2	FD	425/445 (96%)	405 (95%)	19 (4%)	1 (0%)	47	81
2	FF	425/445 (96%)	406 (96%)	18 (4%)	1 (0%)	47	81
2	FH	373/445 (84%)	353 (95%)	20 (5%)	0	100	100
2	GD	425/445 (96%)	409 (96%)	15 (4%)	1 (0%)	47	81
2	GF	425/445 (96%)	406 (96%)	18 (4%)	1 (0%)	47	81
2	GH	425/445 (96%)	402 (95%)	23 (5%)	0	100	100
2	HD	424/445 (95%)	400 (94%)	23 (5%)	1 (0%)	47	81
2	HF	424/445 (95%)	399 (94%)	24 (6%)	1 (0%)	47	81
2	HH	425/445 (96%)	407 (96%)	17 (4%)	1 (0%)	47	81
2	ID	424/445 (95%)	403 (95%)	21 (5%)	0	100	100
2	IF	425/445 (96%)	389 (92%)	36 (8%)	0	100	100
2	IH	424/445 (95%)	402 (95%)	22 (5%)	0	100	100
2	JD	425/445 (96%)	399 (94%)	26 (6%)	0	100	100
2	JF	425/445 (96%)	402 (95%)	23 (5%)	0	100	100
2	KD	424/445 (95%)	403 (95%)	20 (5%)	1 (0%)	47	81
2	KF	425/445 (96%)	403 (95%)	21 (5%)	1 (0%)	47	81
2	KH	397/445 (89%)	374 (94%)	22 (6%)	1 (0%)	41	76
2	LB	425/445 (96%)	402 (95%)	22 (5%)	1 (0%)	47	81
2	LD	425/445 (96%)	406 (96%)	19 (4%)	0	100	100
2	LF	425/445 (96%)	404 (95%)	19 (4%)	2 (0%)	29	69
2	MB	425/445 (96%)	405 (95%)	19 (4%)	1 (0%)	47	81
2	MD	424/445 (95%)	405 (96%)	18 (4%)	1 (0%)	47	81
2	MF	425/445 (96%)	404 (95%)	20 (5%)	1 (0%)	47	81
3	AC	422/451 (94%)	409 (97%)	13 (3%)	0	100	100
3	AE	423/451 (94%)	409 (97%)	14 (3%)	0	100	100
3	BC	423/451 (94%)	411 (97%)	12 (3%)	0	100	100
3	BE	422/451 (94%)	403 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BG	377/451 (84%)	367 (97%)	10 (3%)	0	100	100
3	CC	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
3	CE	427/451 (95%)	410 (96%)	17 (4%)	0	100	100
3	CG	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
3	DC	424/451 (94%)	411 (97%)	13 (3%)	0	100	100
3	DE	424/451 (94%)	404 (95%)	20 (5%)	0	100	100
3	DG	425/451 (94%)	407 (96%)	18 (4%)	0	100	100
3	EC	425/451 (94%)	418 (98%)	7 (2%)	0	100	100
3	EE	424/451 (94%)	410 (97%)	14 (3%)	0	100	100
3	EG	424/451 (94%)	402 (95%)	22 (5%)	0	100	100
3	FC	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
3	FE	426/451 (94%)	408 (96%)	18 (4%)	0	100	100
3	FG	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
3	GC	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
3	GE	425/451 (94%)	406 (96%)	19 (4%)	0	100	100
3	GG	424/451 (94%)	410 (97%)	14 (3%)	0	100	100
3	HC	423/451 (94%)	410 (97%)	13 (3%)	0	100	100
3	HE	423/451 (94%)	412 (97%)	11 (3%)	0	100	100
3	HG	422/451 (94%)	406 (96%)	16 (4%)	0	100	100
3	IC	408/451 (90%)	393 (96%)	15 (4%)	0	100	100
3	IE	424/451 (94%)	409 (96%)	15 (4%)	0	100	100
3	IG	423/451 (94%)	408 (96%)	15 (4%)	0	100	100
3	JC	425/451 (94%)	407 (96%)	18 (4%)	0	100	100
3	JE	424/451 (94%)	403 (95%)	21 (5%)	0	100	100
3	JG	423/451 (94%)	404 (96%)	19 (4%)	0	100	100
3	KC	422/451 (94%)	411 (97%)	11 (3%)	0	100	100
3	KE	421/451 (93%)	406 (96%)	15 (4%)	0	100	100
3	KG	422/451 (94%)	411 (97%)	11 (3%)	0	100	100
3	LA	424/451 (94%)	402 (95%)	22 (5%)	0	100	100
3	LC	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
3	LE	424/451 (94%)	409 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	MA	422/451 (94%)	407 (96%)	15 (4%)	0	100 100
3	MC	424/451 (94%)	405 (96%)	19 (4%)	0	100 100
3	ME	422/451 (94%)	408 (97%)	14 (3%)	0	100 100
All	All	37242/41374 (90%)	35680 (96%)	1535 (4%)	27 (0%)	54 85

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BA	158	GLU
2	LF	268	PRO
2	ED	272	PRO
2	MF	83	GLN
2	CB	271	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	149/199 (75%)	147 (99%)	2 (1%)	69 82
1	E	149/199 (75%)	148 (99%)	1 (1%)	84 90
1	F	146/199 (73%)	144 (99%)	2 (1%)	67 80
1	G	148/199 (74%)	148 (100%)	0	100 100
1	H	148/199 (74%)	148 (100%)	0	100 100
1	I	148/199 (74%)	148 (100%)	0	100 100
1	P	149/199 (75%)	149 (100%)	0	100 100
1	Q	146/199 (73%)	146 (100%)	0	100 100
1	R	149/199 (75%)	149 (100%)	0	100 100
1	S	145/199 (73%)	145 (100%)	0	100 100
1	T	148/199 (74%)	148 (100%)	0	100 100
1	U	148/199 (74%)	148 (100%)	0	100 100
1	d	145/199 (73%)	144 (99%)	1 (1%)	84 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	e	146/199 (73%)	145 (99%)	1 (1%)	84 90
1	f	149/199 (75%)	149 (100%)	0	100 100
1	g	148/199 (74%)	148 (100%)	0	100 100
1	h	145/199 (73%)	145 (100%)	0	100 100
1	i	148/199 (74%)	148 (100%)	0	100 100
2	AB	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	AD	367/380 (97%)	367 (100%)	0	100 100
2	AF	366/380 (96%)	364 (100%)	2 (0%)	88 93
2	BA	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	BD	367/380 (97%)	365 (100%)	2 (0%)	88 93
2	BF	367/380 (97%)	364 (99%)	3 (1%)	81 89
2	CB	367/380 (97%)	365 (100%)	2 (0%)	88 93
2	CD	367/380 (97%)	367 (100%)	0	100 100
2	CF	367/380 (97%)	367 (100%)	0	100 100
2	DB	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	DD	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	DF	366/380 (96%)	363 (99%)	3 (1%)	81 89
2	EB	354/380 (93%)	352 (99%)	2 (1%)	86 92
2	ED	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	EF	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	FD	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	FF	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	FH	323/380 (85%)	322 (100%)	1 (0%)	92 94
2	GD	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	GF	367/380 (97%)	365 (100%)	2 (0%)	88 93
2	GH	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	HD	366/380 (96%)	365 (100%)	1 (0%)	92 94
2	HF	366/380 (96%)	366 (100%)	0	100 100
2	HH	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	ID	366/380 (96%)	365 (100%)	1 (0%)	92 94
2	IF	367/380 (97%)	365 (100%)	2 (0%)	88 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	IH	366/380 (96%)	364 (100%)	2 (0%)	88 93
2	JD	367/380 (97%)	364 (99%)	3 (1%)	81 89
2	JF	367/380 (97%)	365 (100%)	2 (0%)	88 93
2	KD	366/380 (96%)	364 (100%)	2 (0%)	88 93
2	KF	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	KH	344/380 (90%)	343 (100%)	1 (0%)	92 94
2	LB	367/380 (97%)	363 (99%)	4 (1%)	73 84
2	LD	367/380 (97%)	364 (99%)	3 (1%)	81 89
2	LF	367/380 (97%)	366 (100%)	1 (0%)	92 94
2	MB	367/380 (97%)	364 (99%)	3 (1%)	81 89
2	MD	366/380 (96%)	363 (99%)	3 (1%)	81 89
2	MF	367/380 (97%)	366 (100%)	1 (0%)	92 94
3	AC	359/378 (95%)	356 (99%)	3 (1%)	81 89
3	AE	360/378 (95%)	360 (100%)	0	100 100
3	BC	360/378 (95%)	359 (100%)	1 (0%)	92 94
3	BE	359/378 (95%)	357 (99%)	2 (1%)	86 92
3	BG	326/378 (86%)	326 (100%)	0	100 100
3	CC	363/378 (96%)	363 (100%)	0	100 100
3	CE	364/378 (96%)	363 (100%)	1 (0%)	92 94
3	CG	362/378 (96%)	362 (100%)	0	100 100
3	DC	361/378 (96%)	361 (100%)	0	100 100
3	DE	361/378 (96%)	359 (99%)	2 (1%)	86 92
3	DG	362/378 (96%)	362 (100%)	0	100 100
3	EC	362/378 (96%)	362 (100%)	0	100 100
3	EE	361/378 (96%)	361 (100%)	0	100 100
3	EG	361/378 (96%)	361 (100%)	0	100 100
3	FC	362/378 (96%)	362 (100%)	0	100 100
3	FE	363/378 (96%)	359 (99%)	4 (1%)	73 84
3	FG	362/378 (96%)	360 (99%)	2 (1%)	86 92
3	GC	363/378 (96%)	361 (99%)	2 (1%)	86 92
3	GE	362/378 (96%)	361 (100%)	1 (0%)	92 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	GG	361/378 (96%)	360 (100%)	1 (0%)	92 94
3	HC	360/378 (95%)	359 (100%)	1 (0%)	92 94
3	HE	360/378 (95%)	360 (100%)	0	100 100
3	HG	359/378 (95%)	358 (100%)	1 (0%)	92 94
3	IC	350/378 (93%)	349 (100%)	1 (0%)	92 94
3	IE	361/378 (96%)	360 (100%)	1 (0%)	92 94
3	IG	360/378 (95%)	360 (100%)	0	100 100
3	JC	362/378 (96%)	362 (100%)	0	100 100
3	JE	361/378 (96%)	359 (99%)	2 (1%)	86 92
3	JG	360/378 (95%)	360 (100%)	0	100 100
3	KC	359/378 (95%)	358 (100%)	1 (0%)	92 94
3	KE	358/378 (95%)	357 (100%)	1 (0%)	92 94
3	KG	359/378 (95%)	355 (99%)	4 (1%)	73 84
3	LA	361/378 (96%)	361 (100%)	0	100 100
3	LC	360/378 (95%)	360 (100%)	0	100 100
3	LE	361/378 (96%)	360 (100%)	1 (0%)	92 94
3	MA	359/378 (95%)	358 (100%)	1 (0%)	92 94
3	MC	361/378 (96%)	359 (99%)	2 (1%)	86 92
3	ME	359/378 (95%)	356 (99%)	3 (1%)	81 89
All	All	30176/32386 (93%)	30073 (100%)	103 (0%)	92 94

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	IE	123	ARG
2	KD	306	ARG
3	ME	373	ARG
2	IF	77	ARG
3	JE	85	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
2	IH	292	GLN

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Mol	Chain	Res	Type
2	KF	329	GLN
3	JC	342	GLN
3	JG	228	ASN
2	LD	329	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 114 ligands modelled in this entry, 38 are monoatomic - leaving 76 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	$\#\|Z\| > 2$
4	GDP	DF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	4 (13%)
4	GDP	AF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	3 (10%)
4	GDP	GF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.40	5 (16%)
4	GDP	GD	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.32	4 (13%)
4	GDP	BD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.29	4 (13%)
4	GDP	HH	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.41	4 (13%)
5	GTP	DC	501	6	26,34,34	1.24	2 (7%)	32,54,54	1.61	6 (18%)
5	GTP	CE	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.64	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GTP	IC	501	6	26,34,34	1.19	2 (7%)	32,54,54	1.57	7 (21%)
5	GTP	JE	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.58	6 (18%)
5	GTP	EE	501	6	26,34,34	1.25	2 (7%)	32,54,54	1.66	5 (15%)
4	GDP	JF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.32	4 (13%)
5	GTP	FG	501	6	26,34,34	1.25	1 (3%)	32,54,54	1.59	6 (18%)
5	GTP	JG	501	6	26,34,34	1.18	2 (7%)	32,54,54	1.55	6 (18%)
4	GDP	MD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	4 (13%)
5	GTP	LE	501	6	26,34,34	1.23	2 (7%)	32,54,54	1.63	7 (21%)
5	GTP	ME	501	6	26,34,34	1.26	2 (7%)	32,54,54	1.67	8 (25%)
5	GTP	CC	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.45	6 (18%)
5	GTP	EC	501	6	26,34,34	1.23	3 (11%)	32,54,54	1.68	6 (18%)
4	GDP	KD	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
4	GDP	ID	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.22	4 (13%)
5	GTP	BE	501	6	26,34,34	1.23	2 (7%)	32,54,54	1.65	7 (21%)
4	GDP	BA	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
4	GDP	HD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
5	GTP	FE	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.61	7 (21%)
4	GDP	EB	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.30	4 (13%)
5	GTP	LC	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.58	6 (18%)
5	GTP	AC	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.72	7 (21%)
4	GDP	LF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.26	6 (20%)
5	GTP	CG	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.63	7 (21%)
5	GTP	EG	501	6	26,34,34	1.29	2 (7%)	32,54,54	1.72	7 (21%)
4	GDP	CD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
5	GTP	GG	501	6	26,34,34	1.24	2 (7%)	32,54,54	1.74	7 (21%)
5	GTP	KE	501	6	26,34,34	1.25	2 (7%)	32,54,54	1.56	6 (18%)
4	GDP	MF	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.34	4 (13%)
4	GDP	DD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
4	GDP	BF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.27	4 (13%)
5	GTP	MA	501	6	26,34,34	1.23	2 (7%)	32,54,54	1.59	7 (21%)
5	GTP	DG	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.59	6 (18%)
5	GTP	IG	501	6	26,34,34	1.19	2 (7%)	32,54,54	1.63	7 (21%)
4	GDP	LB	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.23	4 (13%)
5	GTP	BG	501	6	26,34,34	1.19	1 (3%)	32,54,54	1.60	6 (18%)
4	GDP	KF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.19	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GTP	HC	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.56	7 (21%)
4	GDP	FF	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.32	4 (13%)
5	GTP	IE	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.58	7 (21%)
4	GDP	AD	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.38	3 (10%)
5	GTP	MC	501	6	26,34,34	1.25	2 (7%)	32,54,54	1.54	6 (18%)
4	GDP	LD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	5 (16%)
5	GTP	GC	501	6	26,34,34	1.24	2 (7%)	32,54,54	1.70	7 (21%)
5	GTP	KG	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.60	6 (18%)
4	GDP	IF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	4 (13%)
5	GTP	GE	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.67	6 (18%)
4	GDP	GH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
4	GDP	HF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
5	GTP	DE	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.63	7 (21%)
4	GDP	CB	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.25	4 (13%)
5	GTP	FC	501	6	26,34,34	1.19	2 (7%)	32,54,54	1.63	7 (21%)
4	GDP	DB	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.33	4 (13%)
4	GDP	FD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.27	4 (13%)
5	GTP	BC	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.51	7 (21%)
4	GDP	CF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
5	GTP	HG	501	6	26,34,34	1.28	2 (7%)	32,54,54	1.66	7 (21%)
4	GDP	MB	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.28	5 (16%)
5	GTP	KC	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.50	7 (21%)
4	GDP	KH	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.36	5 (16%)
4	GDP	IH	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.42	5 (16%)
5	GTP	LA	501	6	26,34,34	1.17	2 (7%)	32,54,54	1.62	7 (21%)
5	GTP	AE	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.55	7 (21%)
5	GTP	JC	501	6	26,34,34	1.17	2 (7%)	32,54,54	1.58	7 (21%)
4	GDP	FH	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.38	4 (13%)
4	GDP	JD	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
4	GDP	EF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	3 (10%)
4	GDP	AB	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.36	4 (13%)
5	GTP	HE	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.60	7 (21%)
4	GDP	ED	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)

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
4	GDP	DF	501	-	-	1/12/32/32	0/3/3/3
4	GDP	AF	501	-	-	5/12/32/32	0/3/3/3
4	GDP	GF	501	-	-	3/12/32/32	0/3/3/3
4	GDP	GD	501	-	-	4/12/32/32	0/3/3/3
4	GDP	BD	501	-	-	2/12/32/32	0/3/3/3
4	GDP	HH	501	-	-	2/12/32/32	0/3/3/3
5	GTP	DC	501	6	-	7/18/38/38	0/3/3/3
5	GTP	CE	501	6	-	5/18/38/38	0/3/3/3
5	GTP	IC	501	6	-	9/18/38/38	0/3/3/3
5	GTP	JE	501	6	-	7/18/38/38	0/3/3/3
5	GTP	EE	501	6	-	8/18/38/38	0/3/3/3
4	GDP	JF	501	-	-	4/12/32/32	0/3/3/3
5	GTP	FG	501	6	-	7/18/38/38	0/3/3/3
5	GTP	JG	501	6	-	1/18/38/38	0/3/3/3
4	GDP	MD	501	-	-	2/12/32/32	0/3/3/3
5	GTP	LE	501	6	-	5/18/38/38	0/3/3/3
5	GTP	ME	501	6	-	5/18/38/38	0/3/3/3
5	GTP	CC	501	6	-	4/18/38/38	0/3/3/3
5	GTP	EC	501	6	-	5/18/38/38	0/3/3/3
4	GDP	KD	501	-	-	1/12/32/32	0/3/3/3
4	GDP	ID	501	-	-	5/12/32/32	0/3/3/3
5	GTP	BE	501	6	-	4/18/38/38	0/3/3/3
4	GDP	BA	501	-	-	3/12/32/32	0/3/3/3
4	GDP	HD	501	-	-	2/12/32/32	0/3/3/3
5	GTP	FE	501	6	-	5/18/38/38	0/3/3/3
4	GDP	EB	501	-	-	3/12/32/32	0/3/3/3
5	GTP	LC	501	6	-	2/18/38/38	0/3/3/3
5	GTP	AC	501	6	-	3/18/38/38	0/3/3/3
4	GDP	LF	501	-	-	4/12/32/32	0/3/3/3
5	GTP	CG	501	6	-	5/18/38/38	0/3/3/3
5	GTP	EG	501	6	-	5/18/38/38	0/3/3/3
4	GDP	CD	501	-	-	1/12/32/32	0/3/3/3
5	GTP	GG	501	6	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	KE	501	6	-	4/18/38/38	0/3/3/3
4	GDP	MF	501	-	-	2/12/32/32	0/3/3/3
4	GDP	DD	501	-	-	2/12/32/32	0/3/3/3
4	GDP	BF	501	-	-	2/12/32/32	0/3/3/3
5	GTP	MA	501	6	-	1/18/38/38	0/3/3/3
5	GTP	DG	501	6	-	6/18/38/38	0/3/3/3
5	GTP	IG	501	6	-	2/18/38/38	0/3/3/3
4	GDP	LB	501	-	-	4/12/32/32	0/3/3/3
5	GTP	BG	501	6	-	6/18/38/38	0/3/3/3
4	GDP	KF	501	-	-	1/12/32/32	0/3/3/3
5	GTP	HC	501	6	-	7/18/38/38	0/3/3/3
4	GDP	FF	501	-	-	2/12/32/32	0/3/3/3
5	GTP	IE	501	6	-	8/18/38/38	0/3/3/3
4	GDP	AD	501	-	-	4/12/32/32	0/3/3/3
5	GTP	MC	501	6	-	5/18/38/38	0/3/3/3
4	GDP	LD	501	-	-	2/12/32/32	0/3/3/3
5	GTP	GC	501	6	-	6/18/38/38	0/3/3/3
5	GTP	KG	501	6	-	5/18/38/38	0/3/3/3
4	GDP	IF	501	-	-	5/12/32/32	0/3/3/3
5	GTP	GE	501	6	-	7/18/38/38	0/3/3/3
4	GDP	GH	501	-	-	3/12/32/32	0/3/3/3
4	GDP	HF	501	-	-	3/12/32/32	0/3/3/3
5	GTP	DE	501	6	-	7/18/38/38	0/3/3/3
4	GDP	CB	501	-	-	2/12/32/32	0/3/3/3
5	GTP	FC	501	6	-	4/18/38/38	0/3/3/3
4	GDP	DB	501	-	-	2/12/32/32	0/3/3/3
4	GDP	FD	501	-	-	1/12/32/32	0/3/3/3
5	GTP	BC	501	6	-	3/18/38/38	0/3/3/3
4	GDP	CF	501	-	-	1/12/32/32	0/3/3/3
5	GTP	HG	501	6	-	5/18/38/38	0/3/3/3
4	GDP	MB	501	-	-	2/12/32/32	0/3/3/3
5	GTP	KC	501	6	-	4/18/38/38	0/3/3/3
4	GDP	KH	501	-	-	3/12/32/32	0/3/3/3
4	GDP	IH	501	-	-	1/12/32/32	0/3/3/3
5	GTP	LA	501	6	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	AE	501	6	-	2/18/38/38	0/3/3/3
5	GTP	JC	501	6	-	6/18/38/38	0/3/3/3
4	GDP	FH	501	-	-	3/12/32/32	0/3/3/3
4	GDP	JD	501	-	-	2/12/32/32	0/3/3/3
4	GDP	EF	501	-	-	2/12/32/32	0/3/3/3
4	GDP	AB	501	-	-	1/12/32/32	0/3/3/3
5	GTP	HE	501	6	-	7/18/38/38	0/3/3/3
4	GDP	ED	501	-	-	2/12/32/32	0/3/3/3

The worst 5 of 113 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	HG	501	GTP	C5-C6	-4.69	1.37	1.47
5	EG	501	GTP	C5-C6	-4.59	1.38	1.47
5	ME	501	GTP	C5-C6	-4.52	1.38	1.47
5	GC	501	GTP	C5-C6	-4.52	1.38	1.47
5	MC	501	GTP	C5-C6	-4.52	1.38	1.47

The worst 5 of 407 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	HH	501	GDP	PA-O3A-PB	-4.64	116.91	132.83
4	GF	501	GDP	PA-O3A-PB	-4.61	117.01	132.83
5	IG	501	GTP	PB-O3B-PG	-4.60	117.06	132.83
5	EC	501	GTP	PA-O3A-PB	-4.57	117.14	132.83
5	GG	501	GTP	PB-O3B-PG	-4.55	117.22	132.83

There are no chirality outliers.

5 of 286 torsion outliers are listed below:

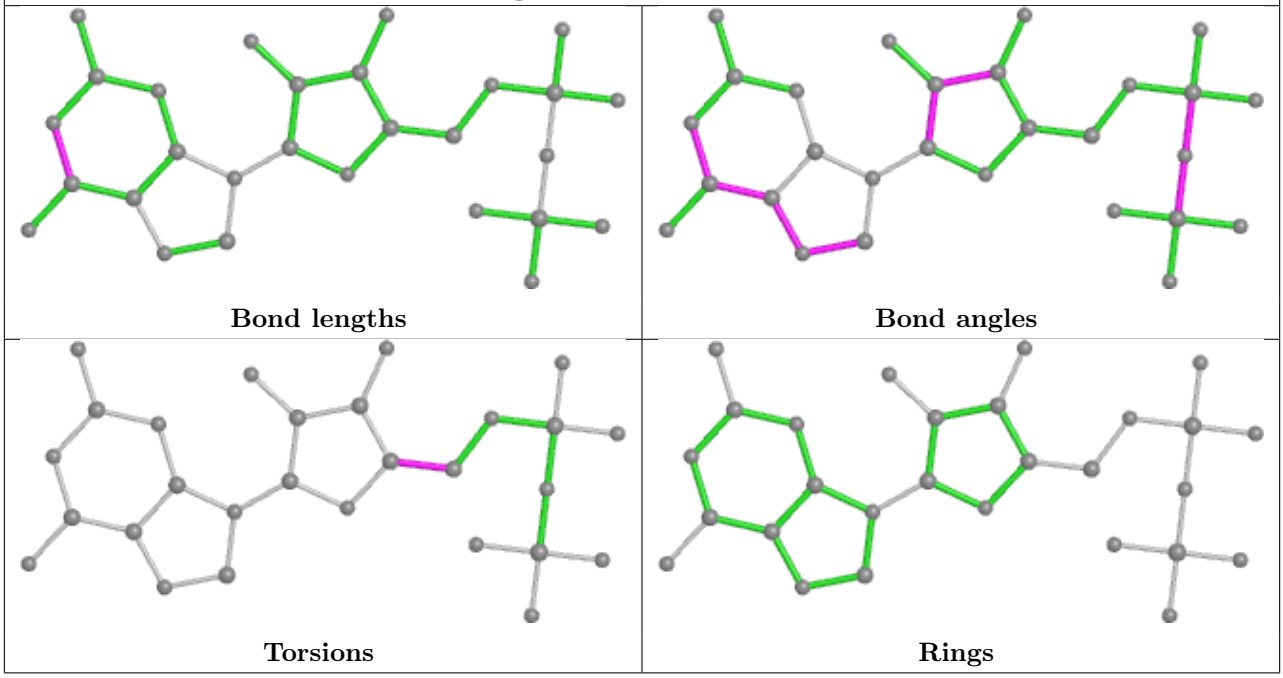
Mol	Chain	Res	Type	Atoms
4	AB	501	GDP	C5'-O5'-PA-O1A
4	AD	501	GDP	C5'-O5'-PA-O1A
4	AF	501	GDP	C5'-O5'-PA-O3A
4	AF	501	GDP	C5'-O5'-PA-O2A
4	AF	501	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

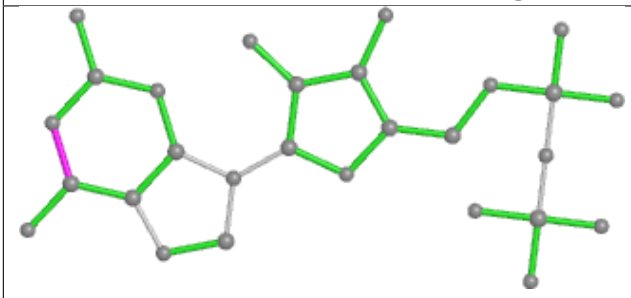
No monomer is involved in short contacts.

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.

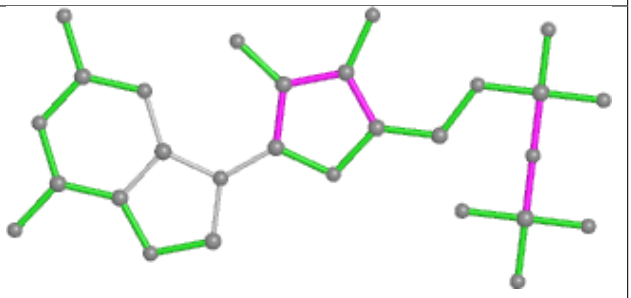
Ligand GDP DF 501



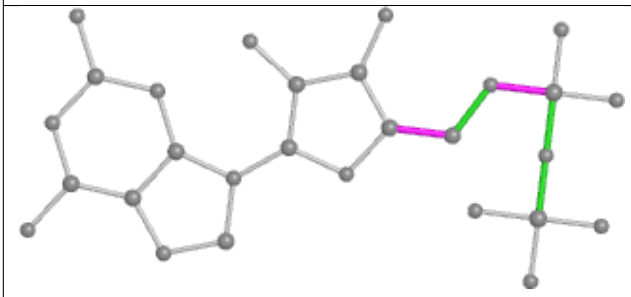
Ligand GDP AF 501



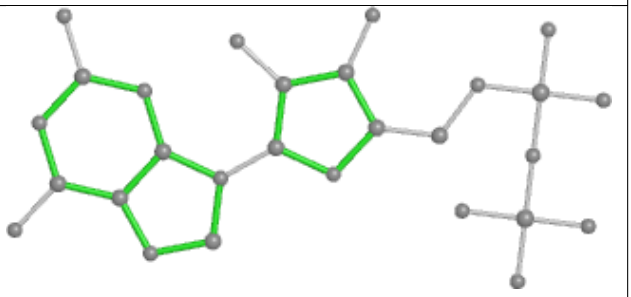
Bond lengths



Bond angles

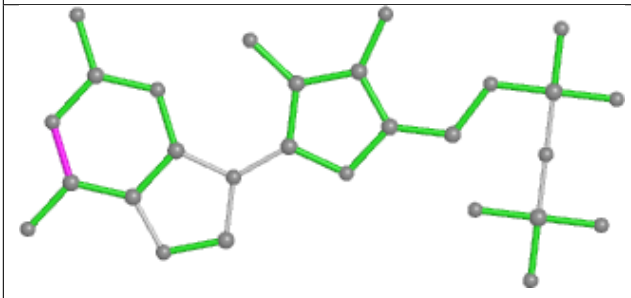


Torsions

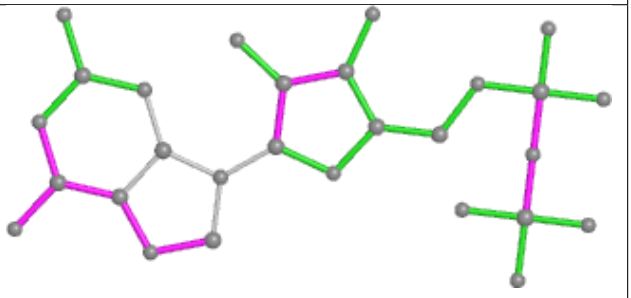


Rings

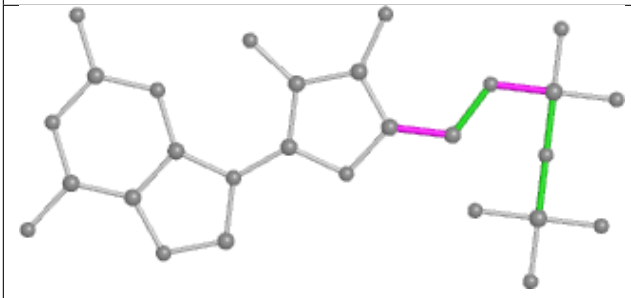
Ligand GDP GF 501



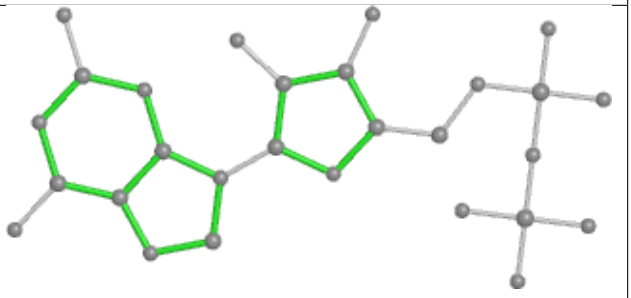
Bond lengths



Bond angles

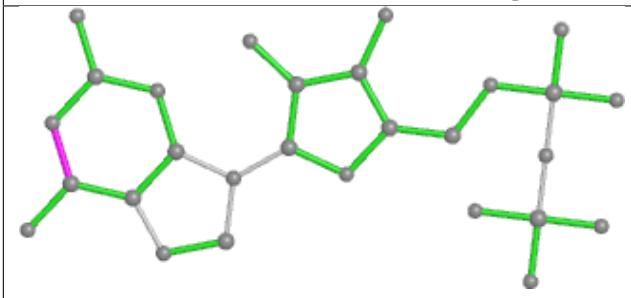


Torsions

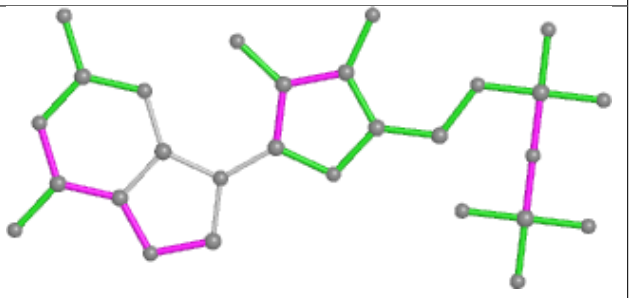


Rings

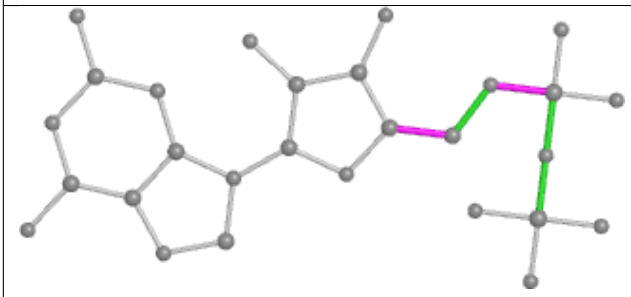
Ligand GDP GD 501



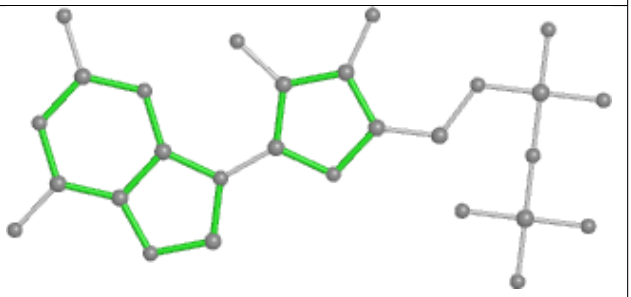
Bond lengths



Bond angles

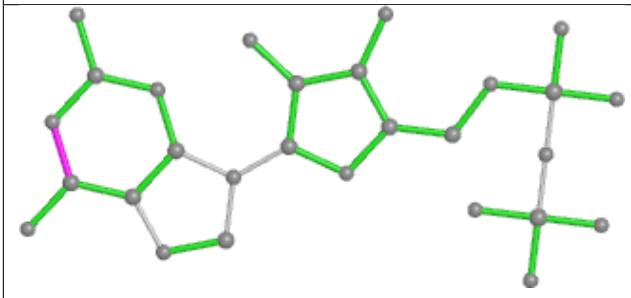


Torsions

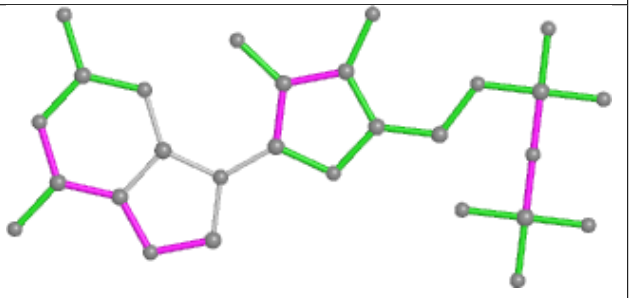


Rings

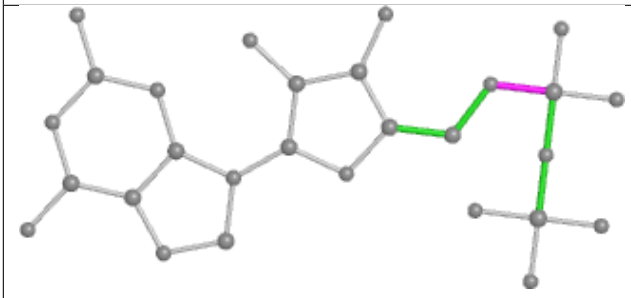
Ligand GDP BD 501



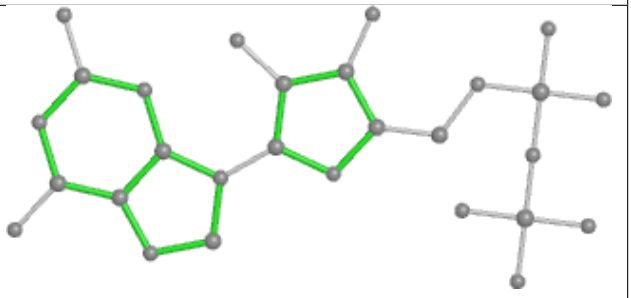
Bond lengths



Bond angles

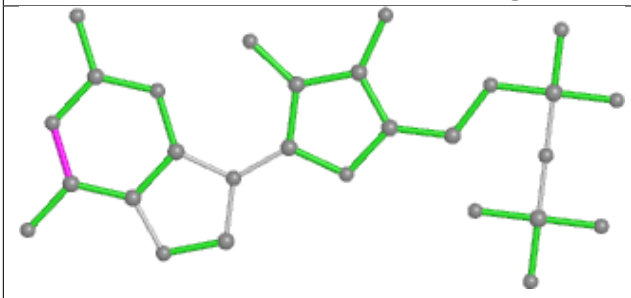


Torsions

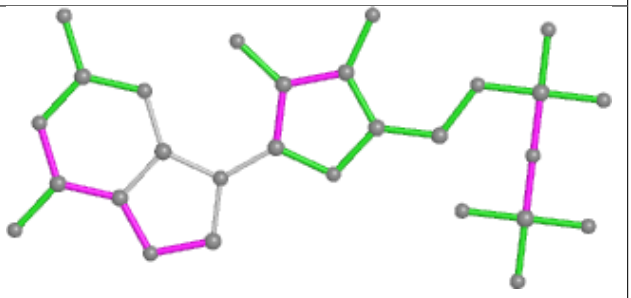


Rings

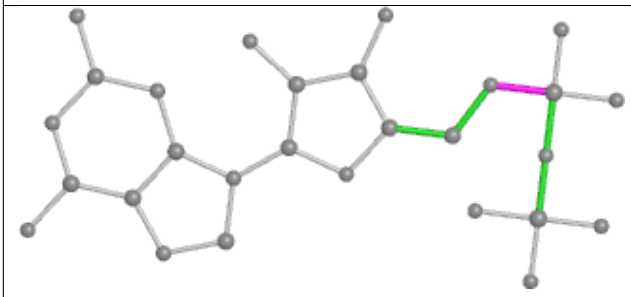
Ligand GDP HH 501



Bond lengths



Bond angles



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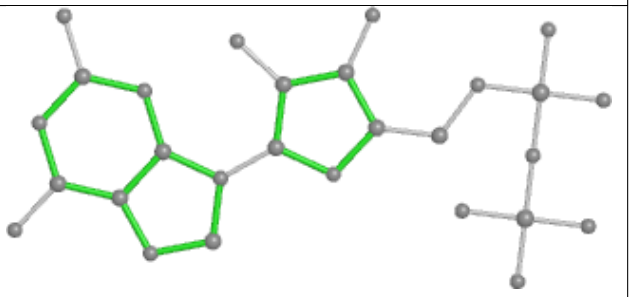
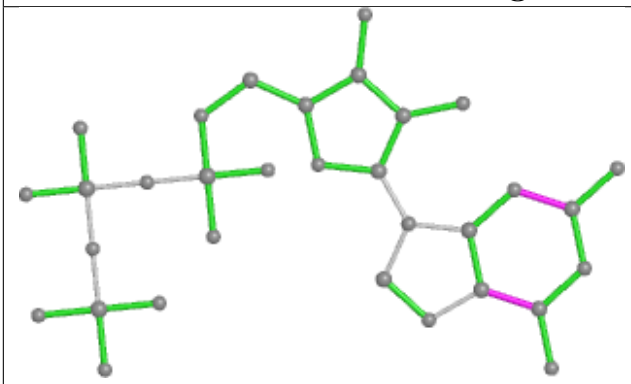
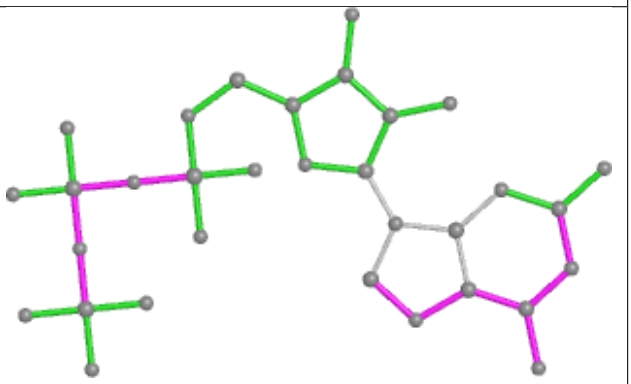


Rings

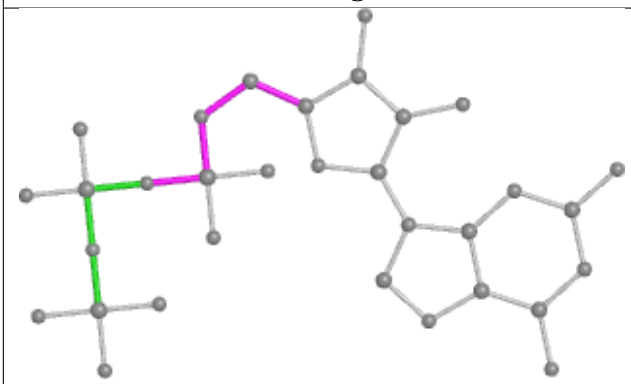
Ligand GTP DC 501



Bond lengths



Bond angles



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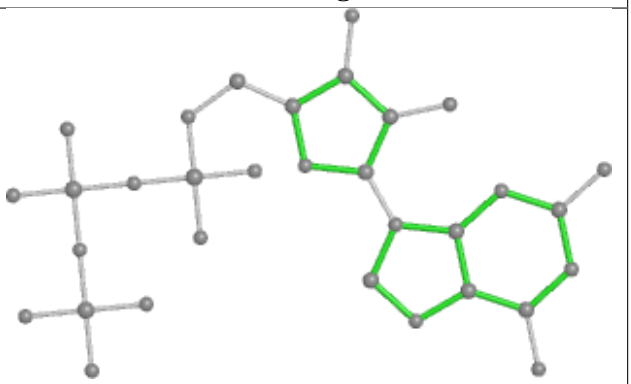
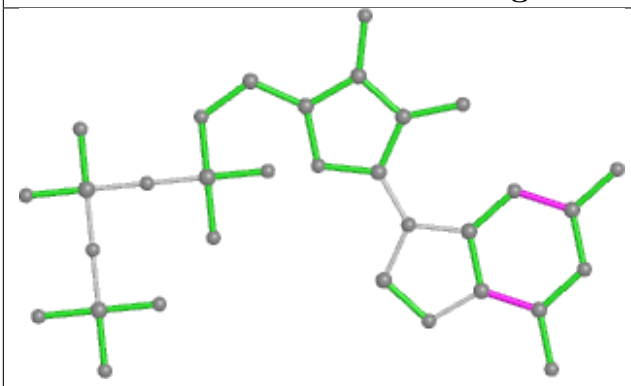
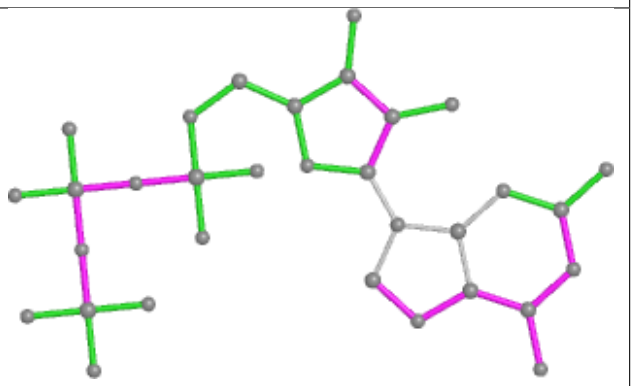


Rings

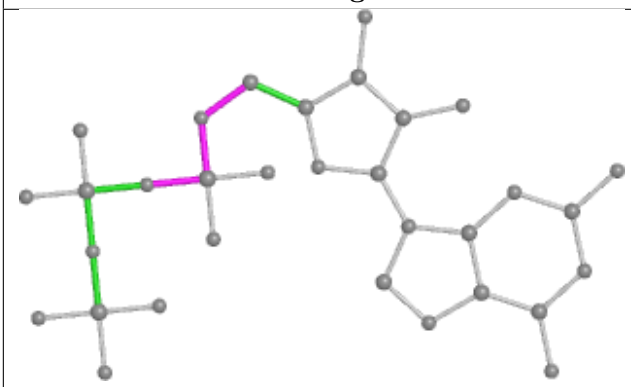
Ligand GTP CE 501



Bond lengths



Bond angles



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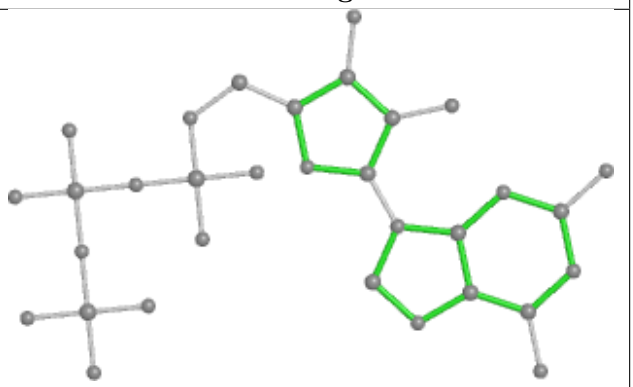
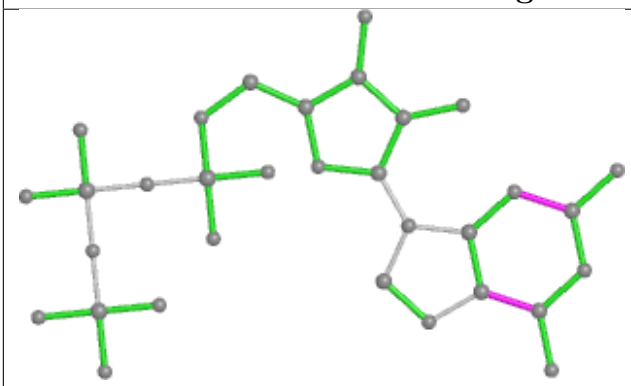


Rings

Ligand GTP IC 501



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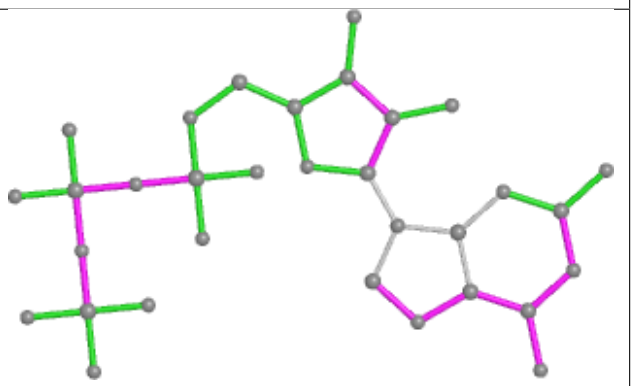

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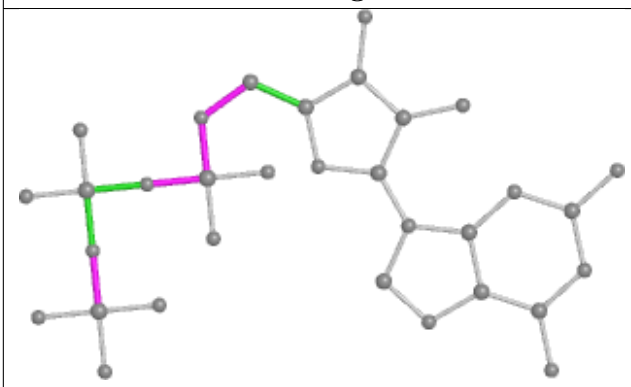

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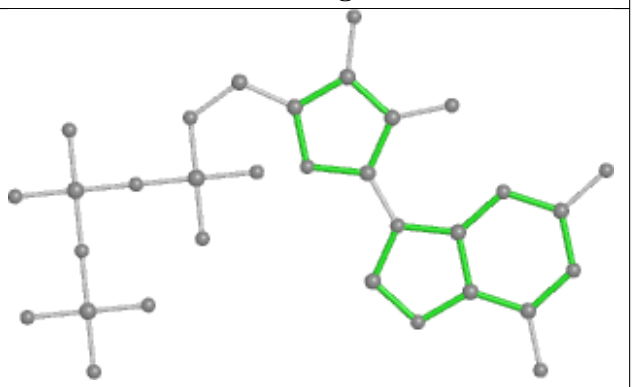
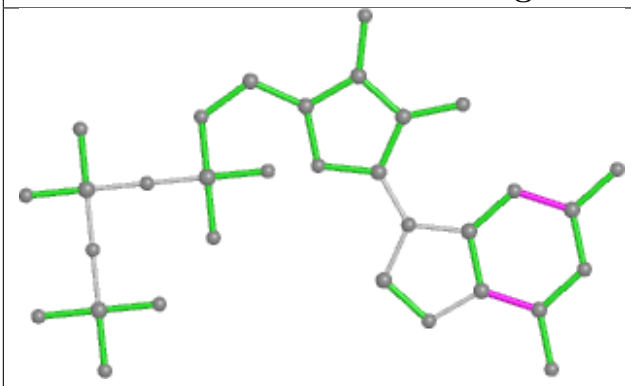
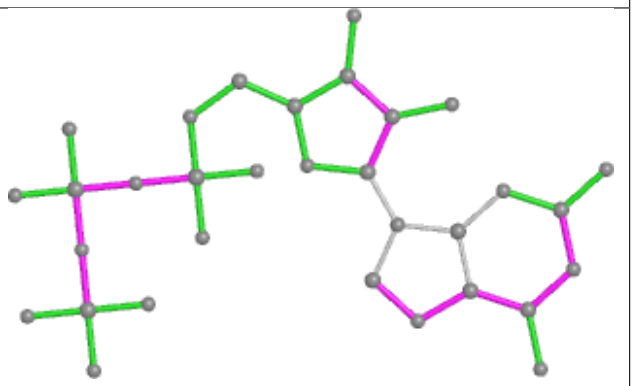


Rings

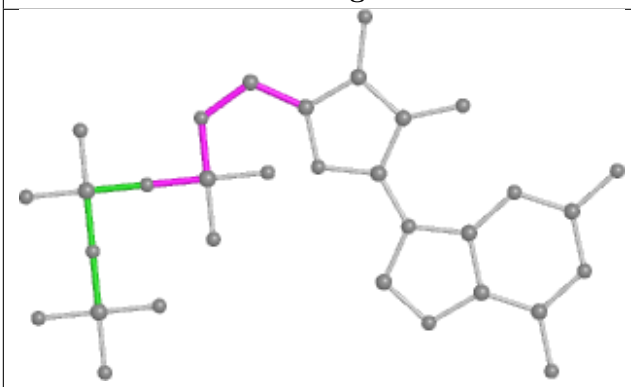
Ligand GTP JE 501



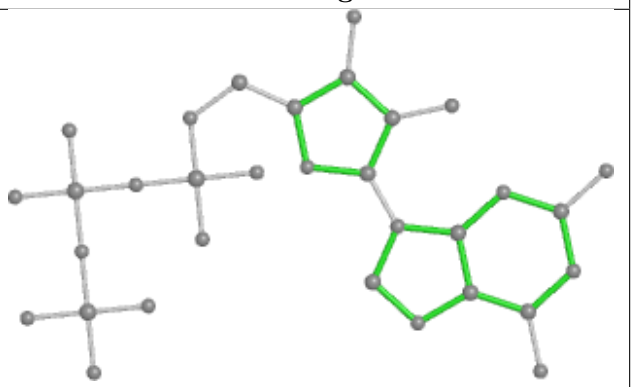
Bond lengths



Bond angles

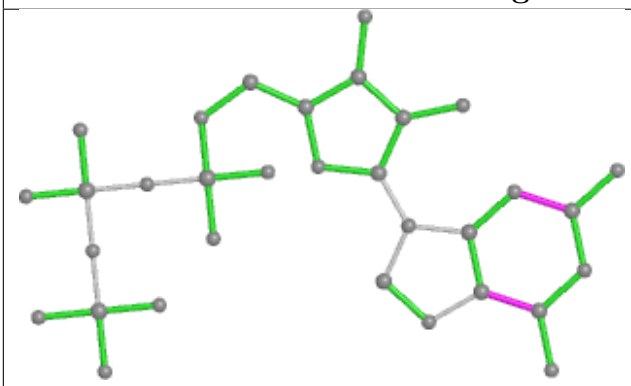


Torsions

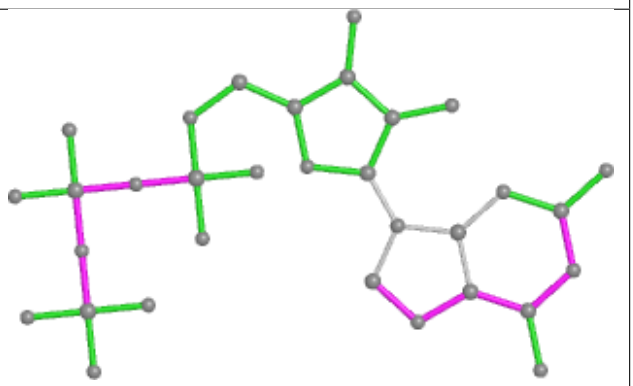


Rings

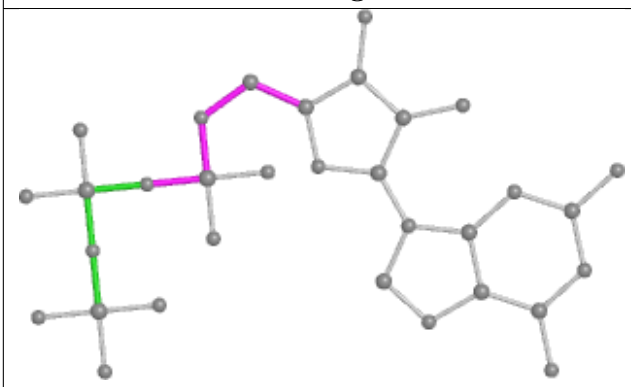
Ligand GTP EE 501



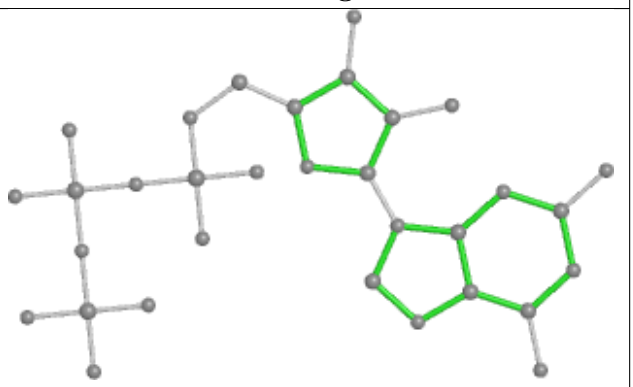
Bond lengths



Bond angles

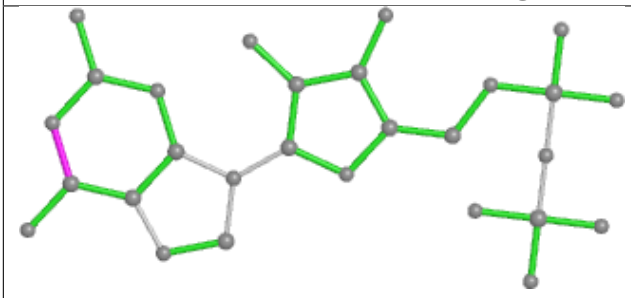


Torsions



Rings

Ligand GDP JF 501



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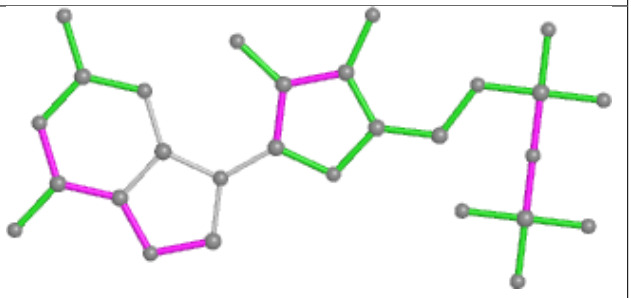

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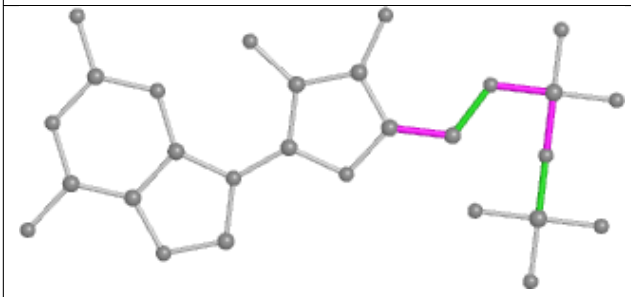

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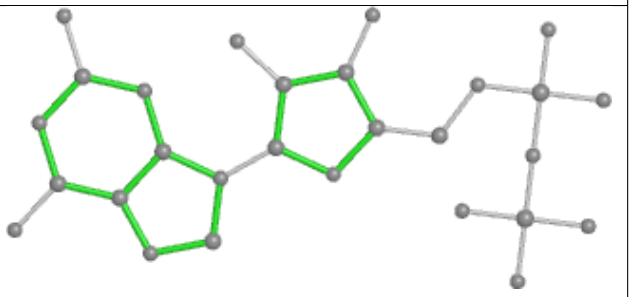

Rings

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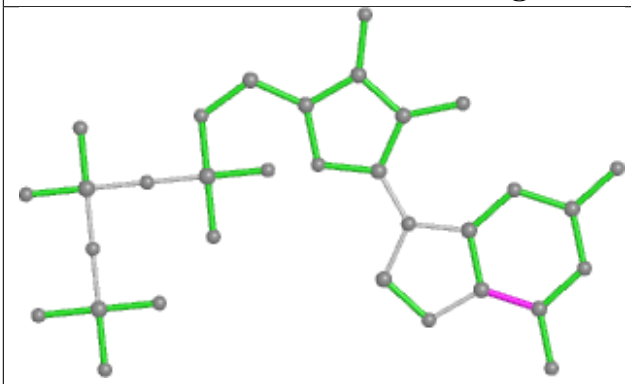

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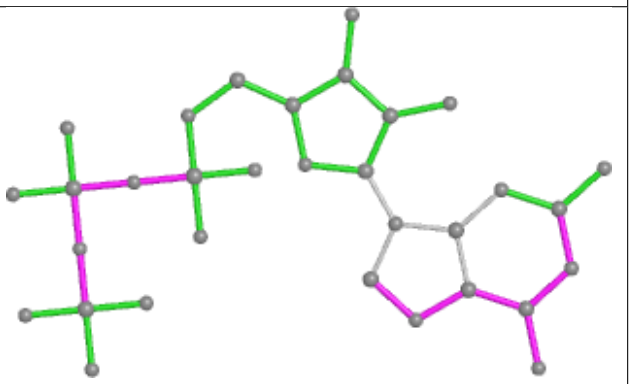

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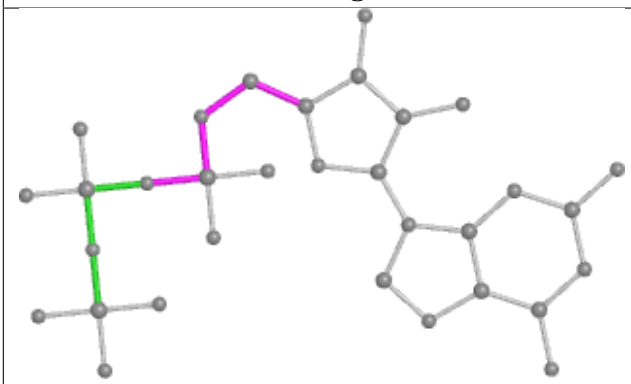

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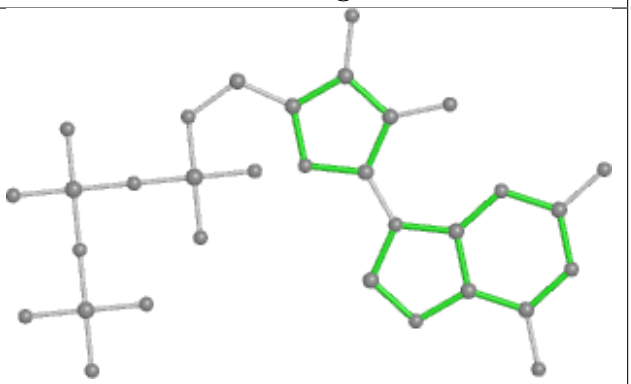

Rings

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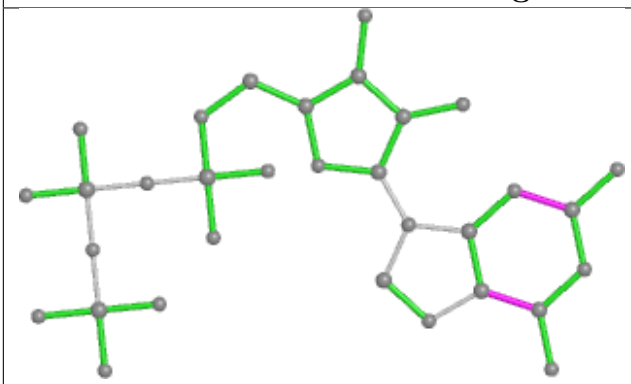

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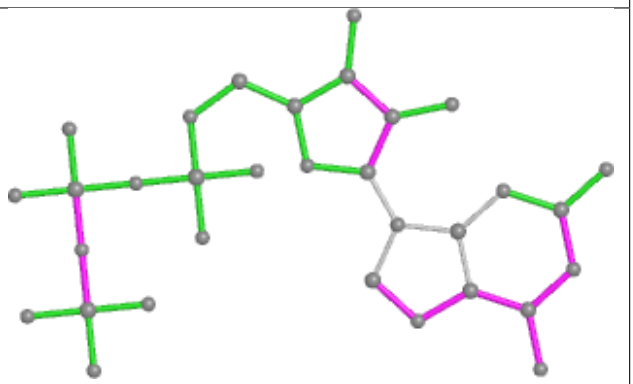

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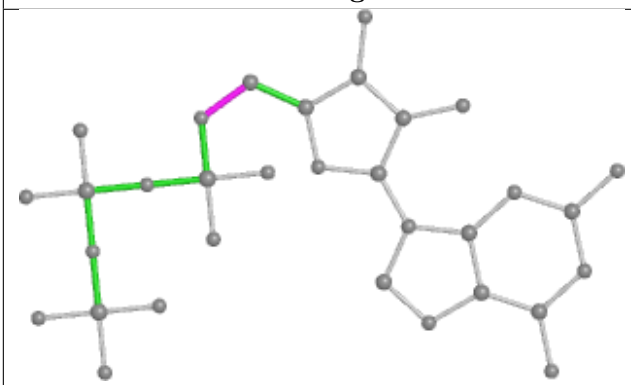

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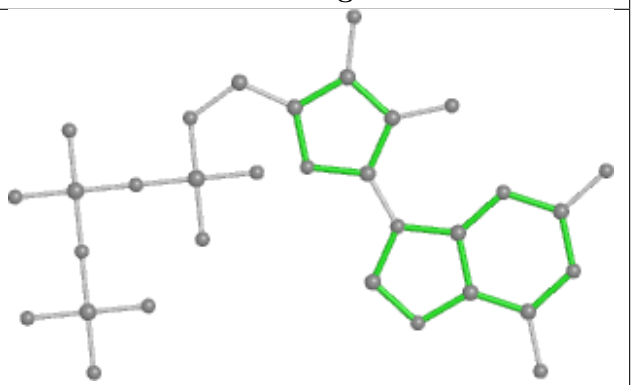
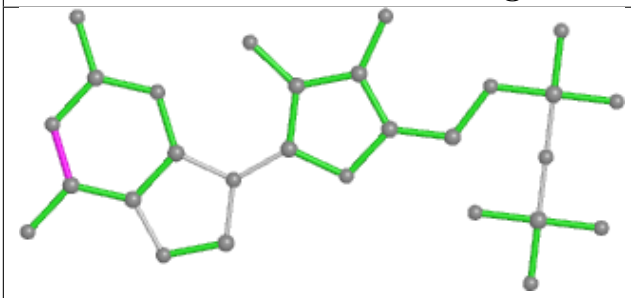


Rings

Ligand GDP MD 501



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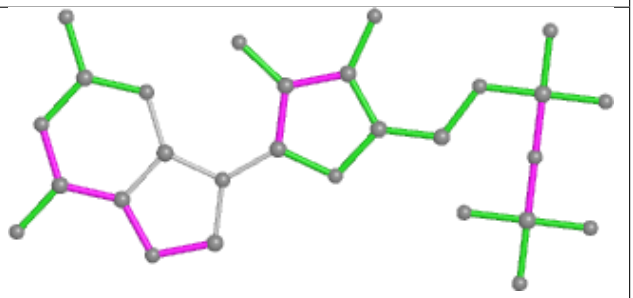

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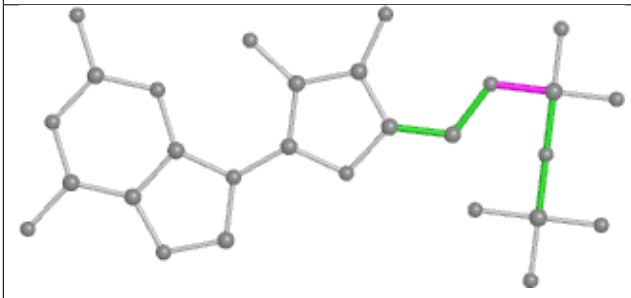

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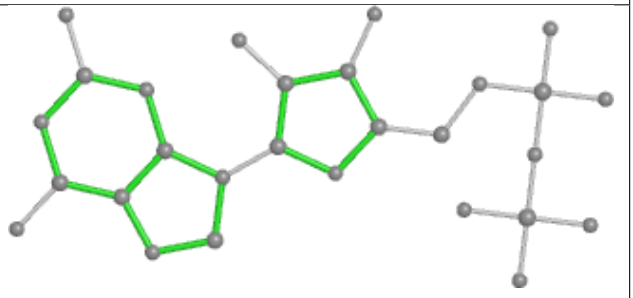
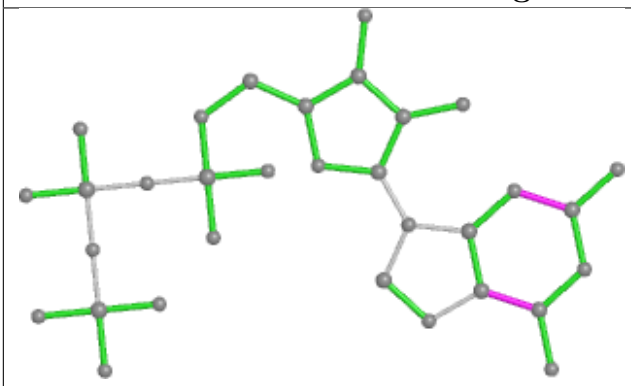


Rings

Ligand GTP LE 501



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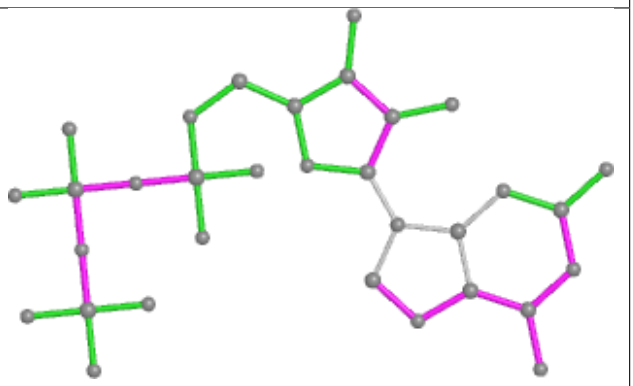

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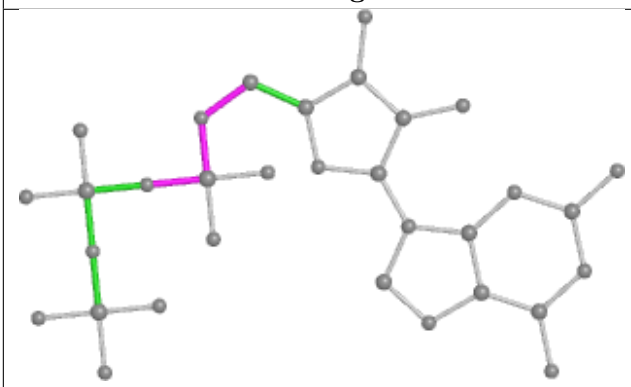

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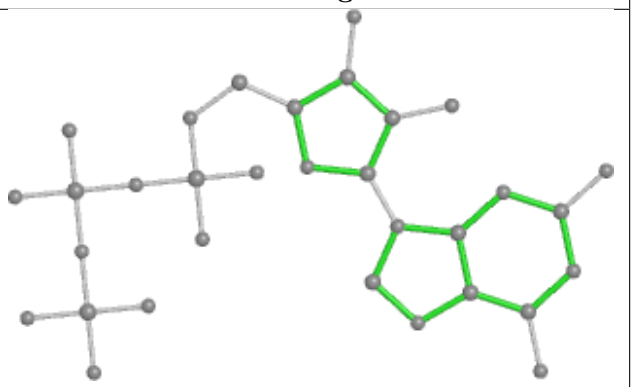

Rings

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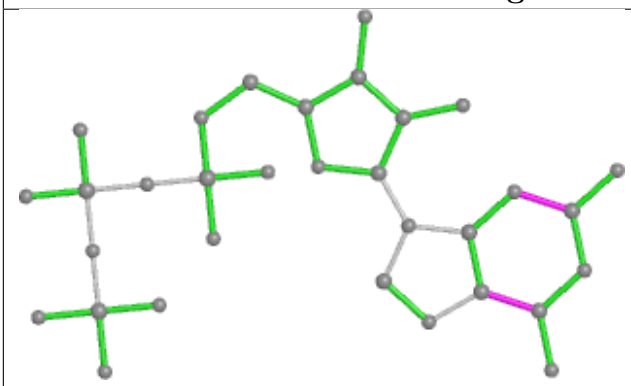

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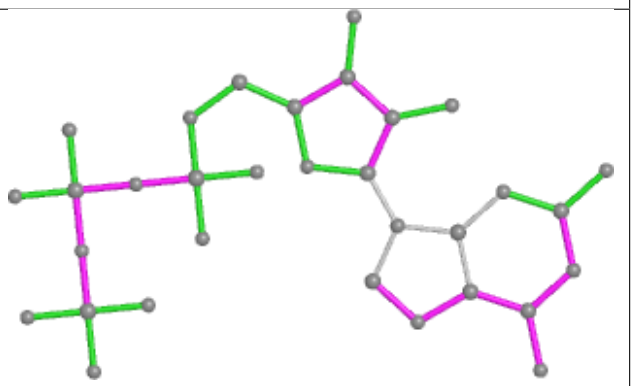

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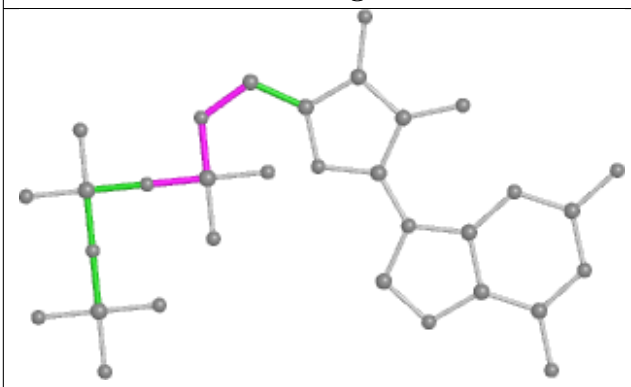

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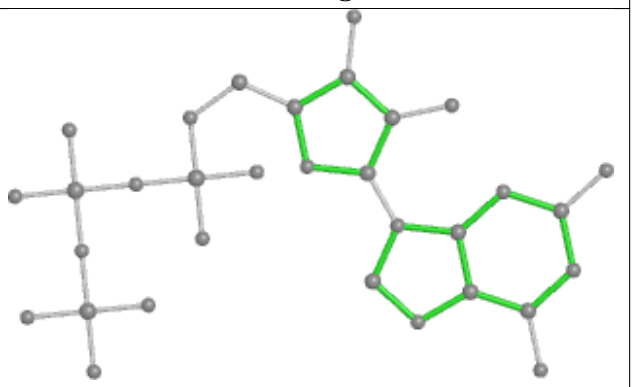
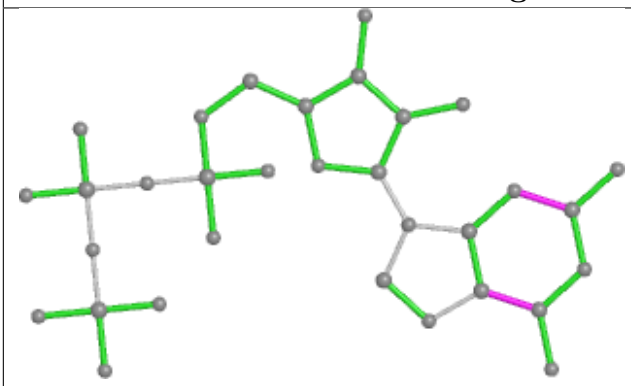


Rings

Ligand GTP CC 501



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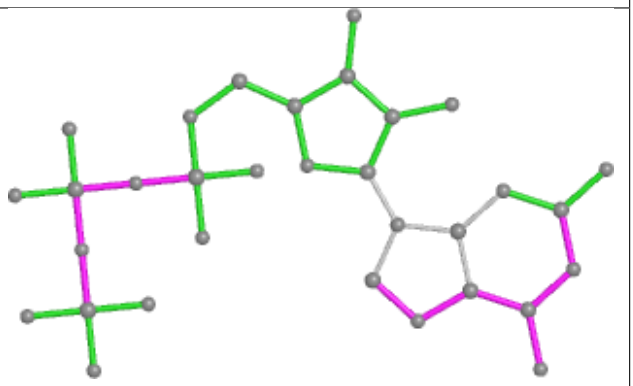

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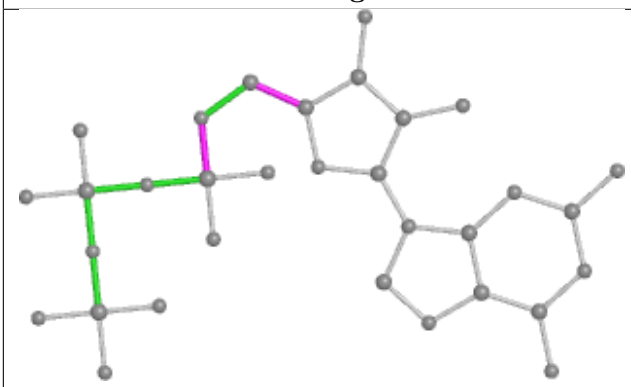

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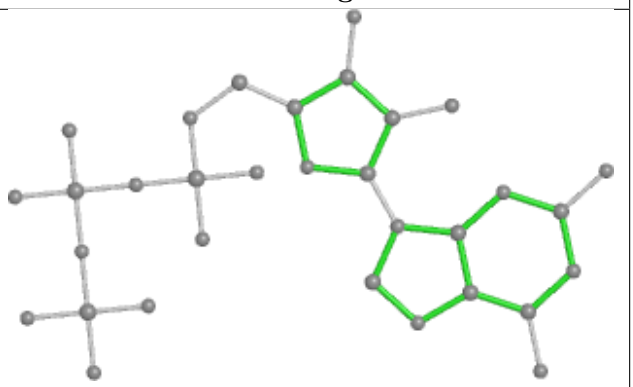

Rings

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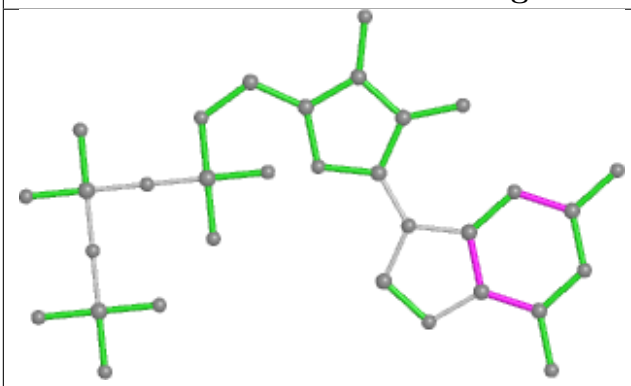

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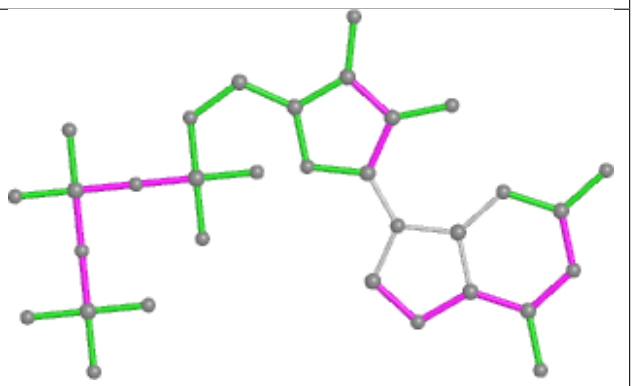

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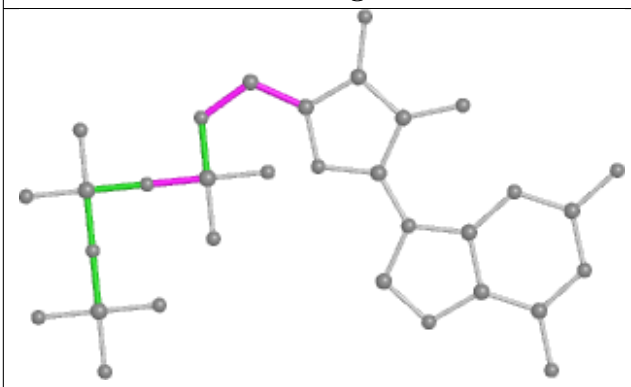

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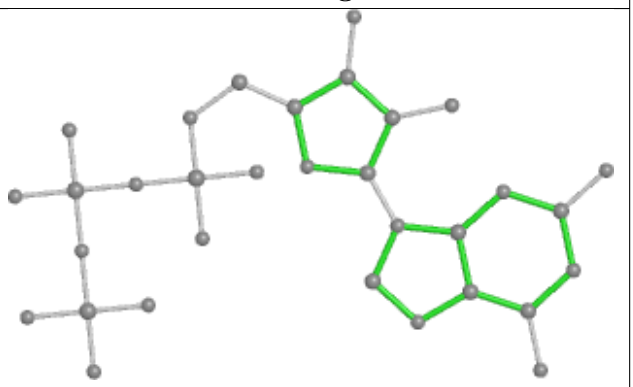

Rings

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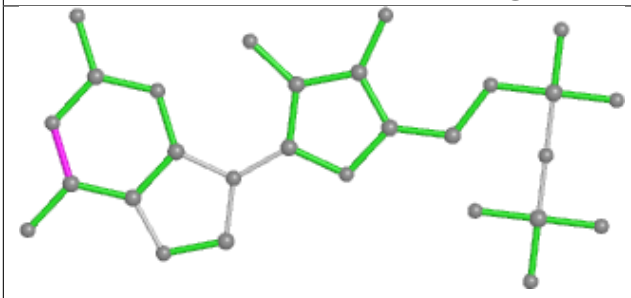

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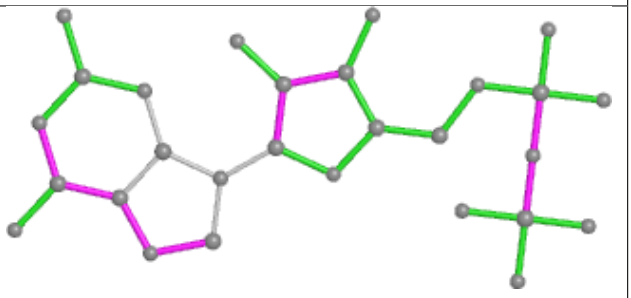

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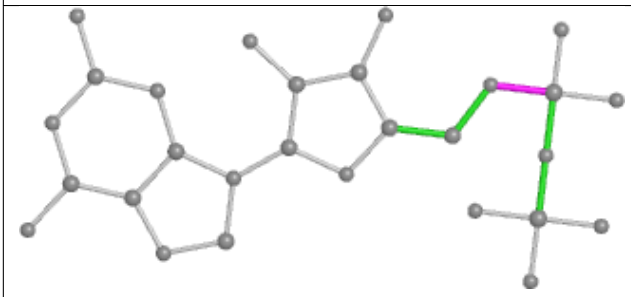

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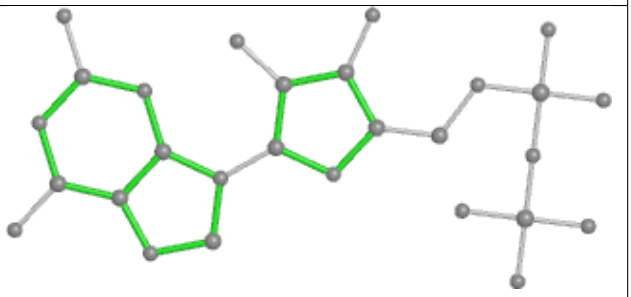

Rings

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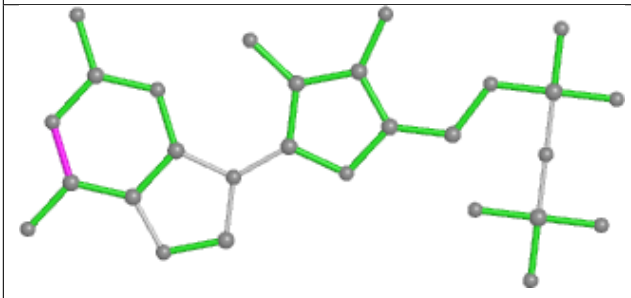

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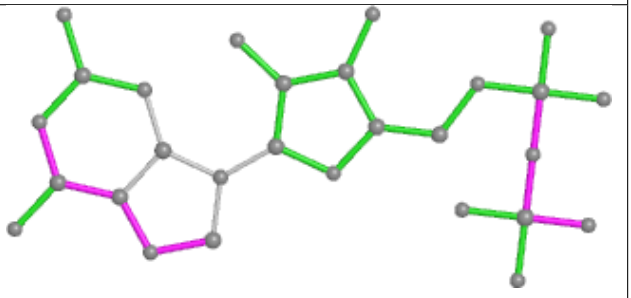

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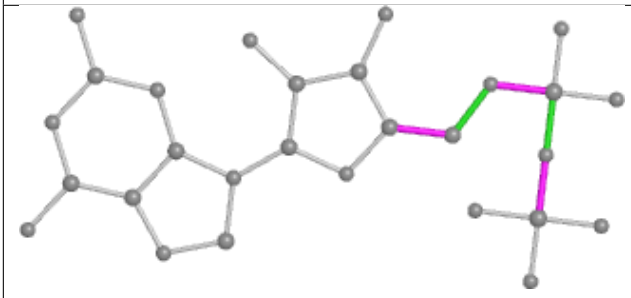

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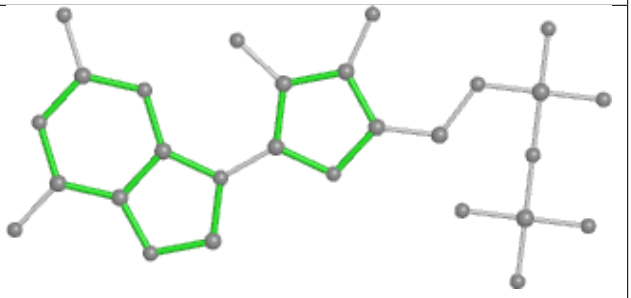

Rings

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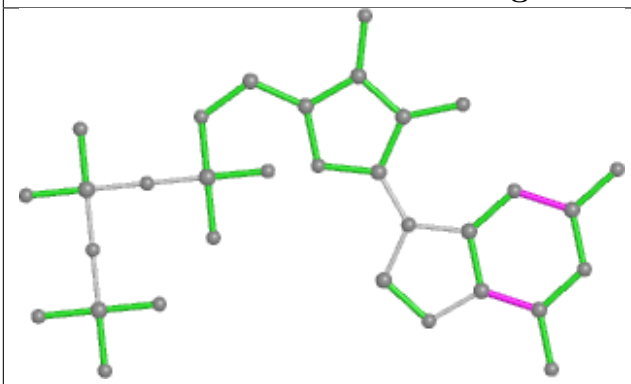

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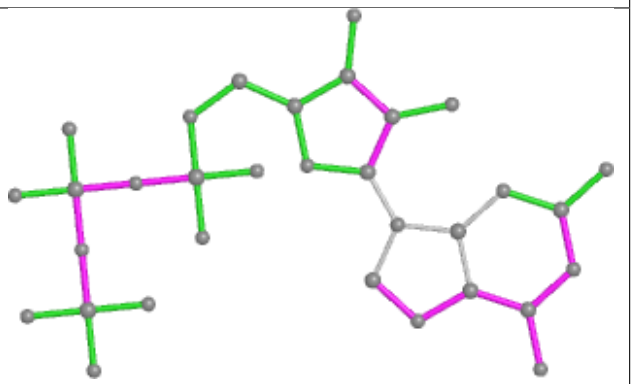

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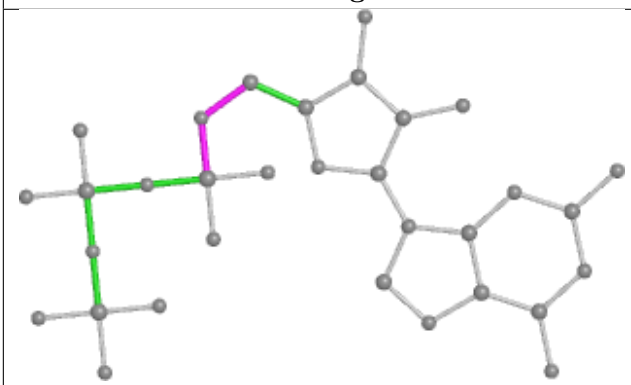

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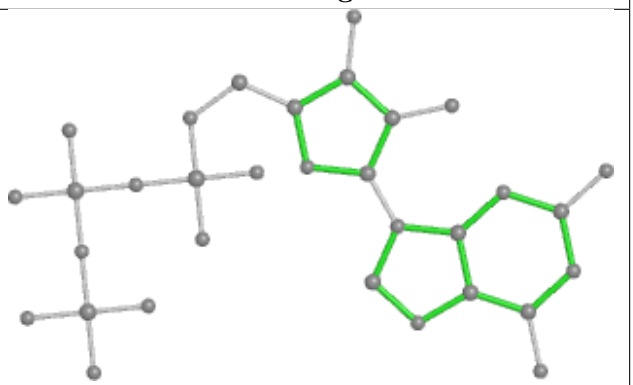
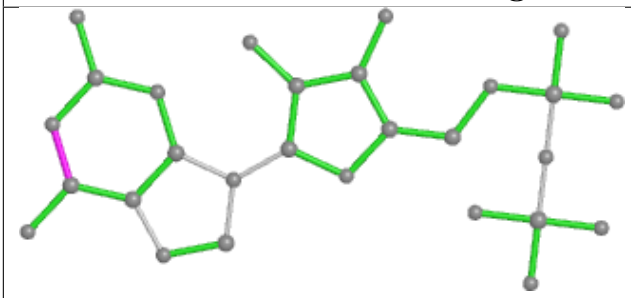


Rings

Ligand GDP BA 501



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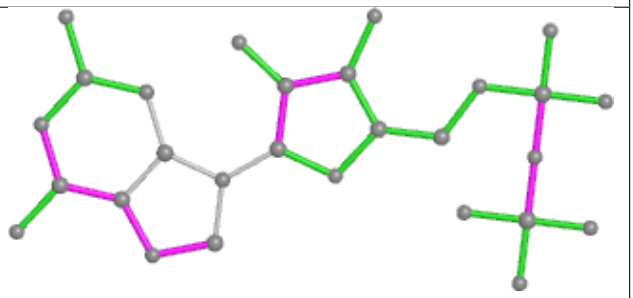

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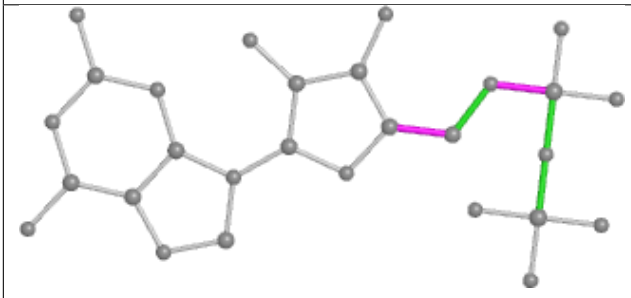

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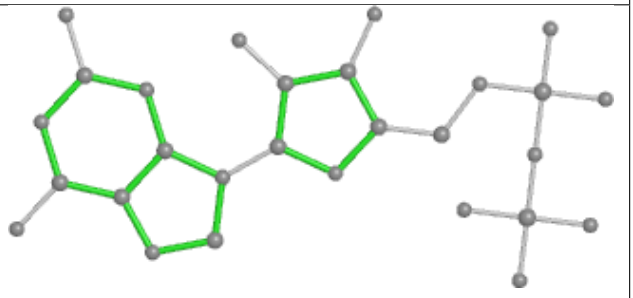

Rings

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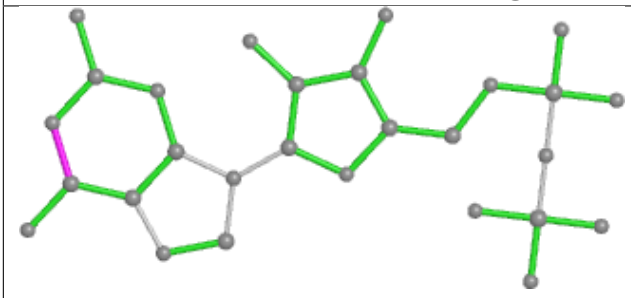

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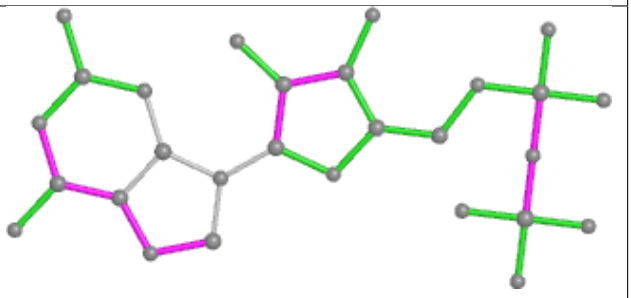

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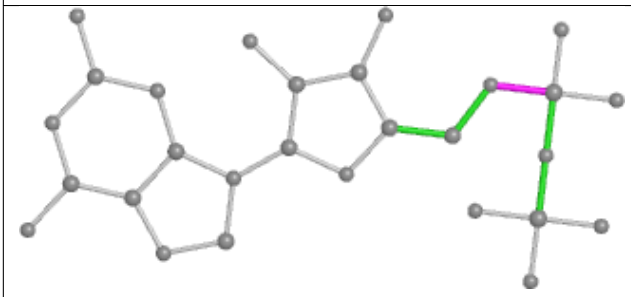

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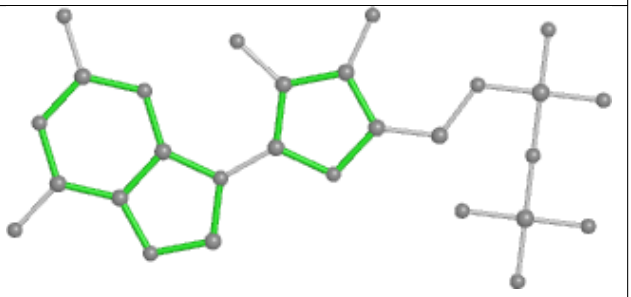
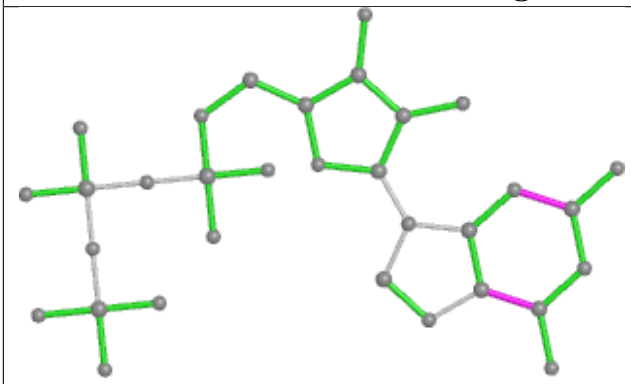


Rings

Ligand GTP FE 501



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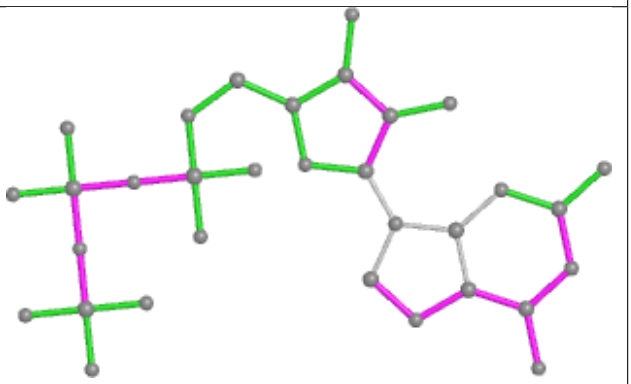

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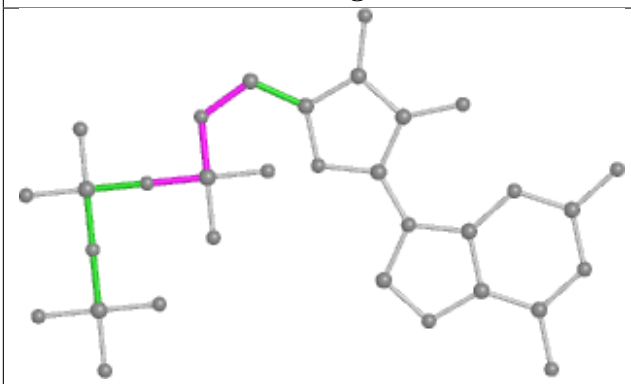
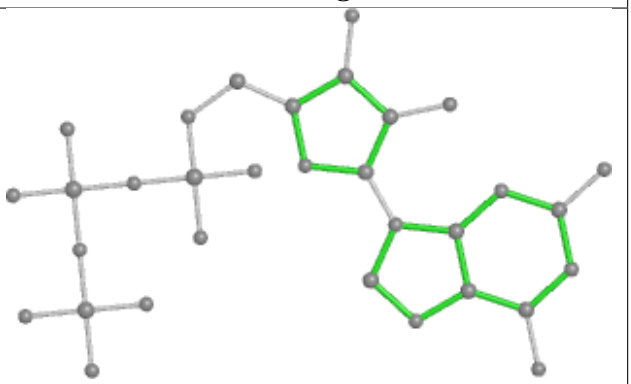
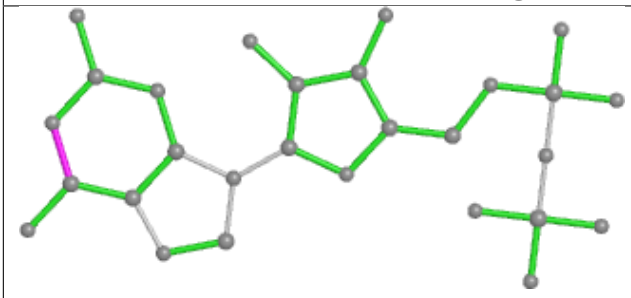


Torsions

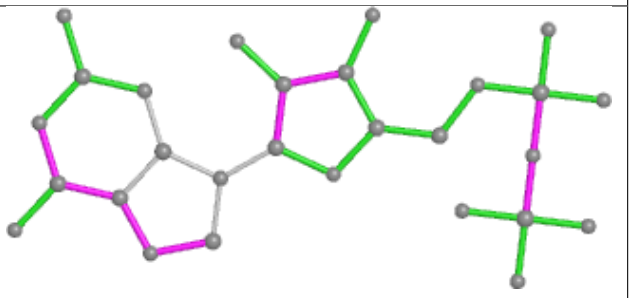


Rings

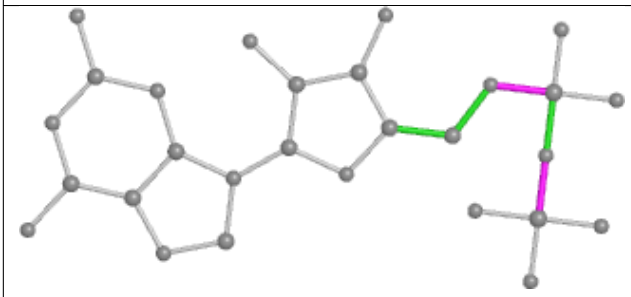
Ligand GDP EB 501



Bond lengths



Bond angles



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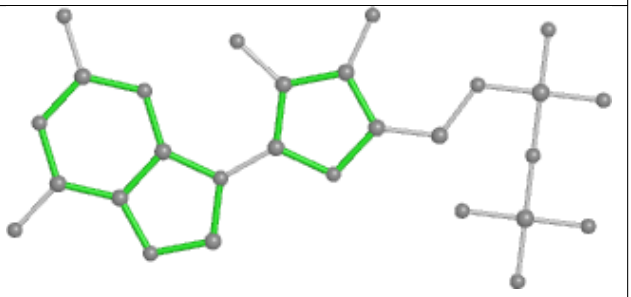
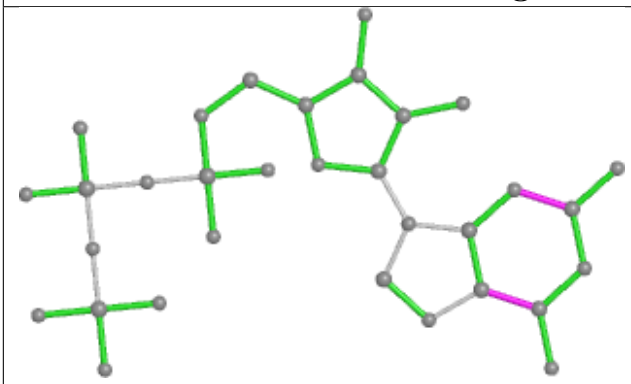


Rings

Ligand GTP LC 501



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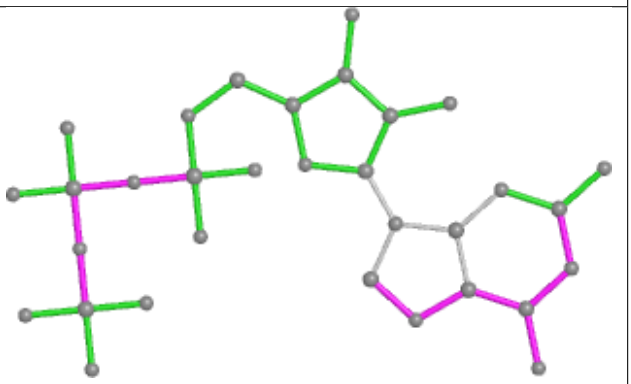

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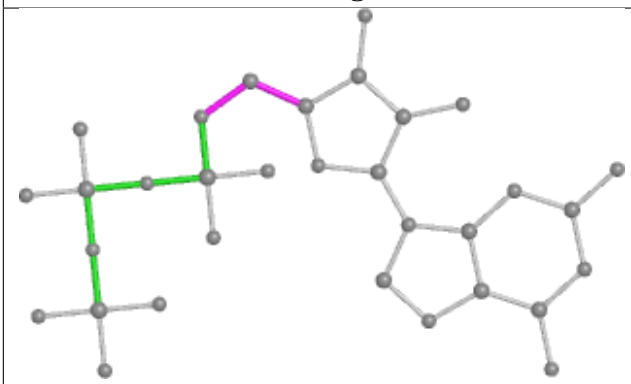

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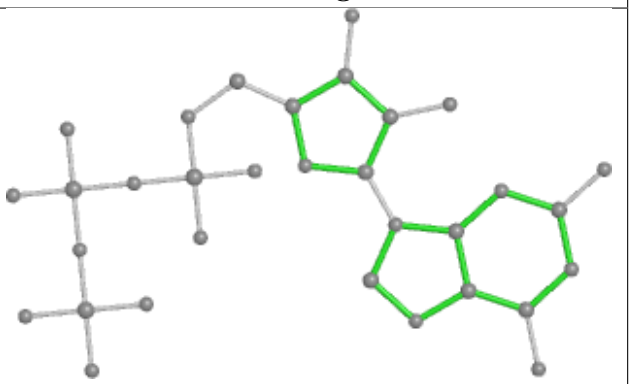
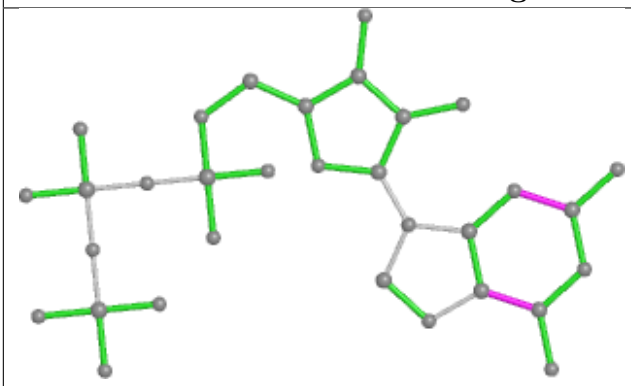


Rings

Ligand GTP AC 501



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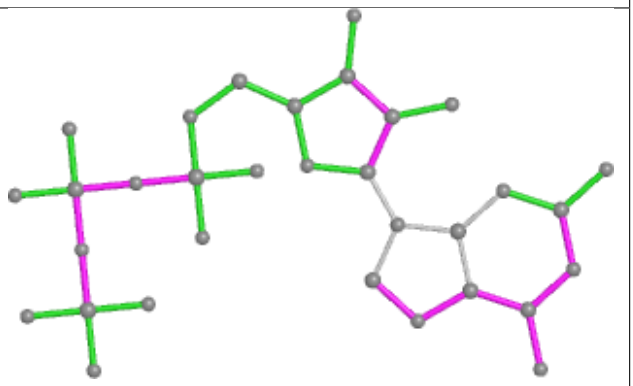
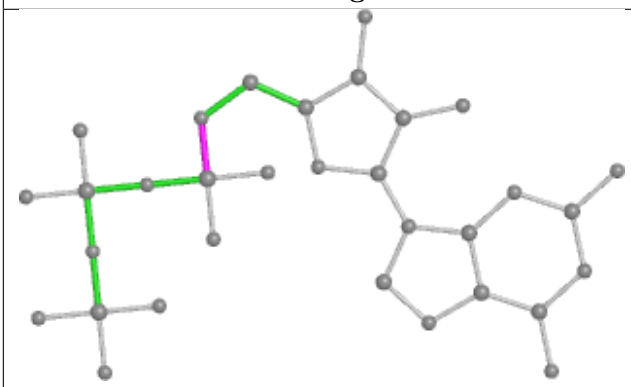


Bond angles



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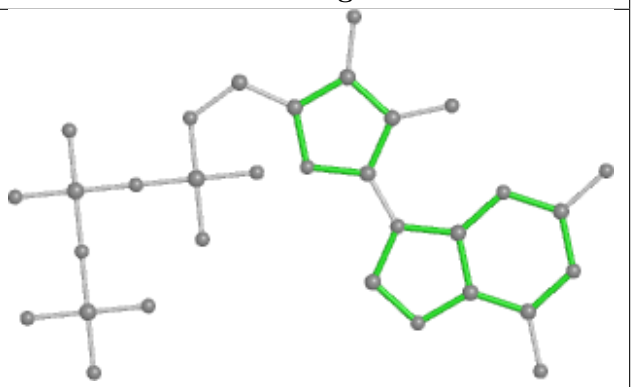
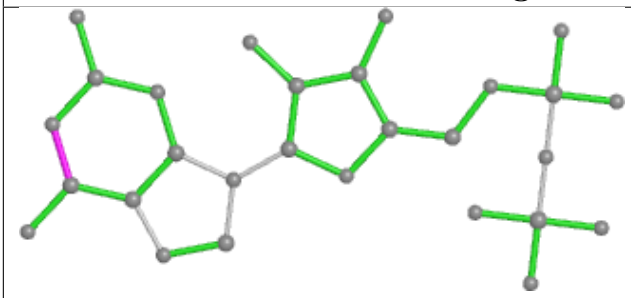


Rings

Ligand GDP LF 501



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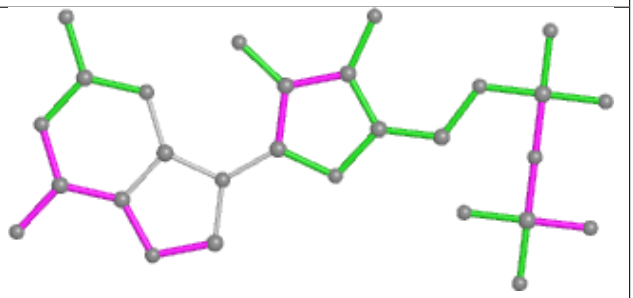

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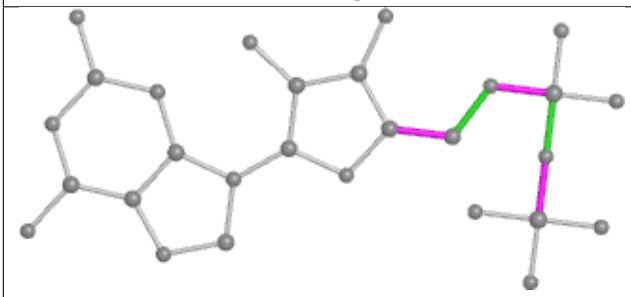

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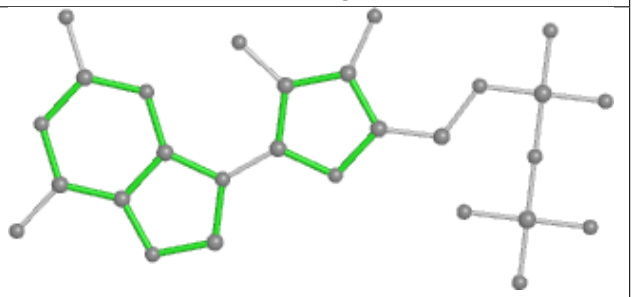

Rings

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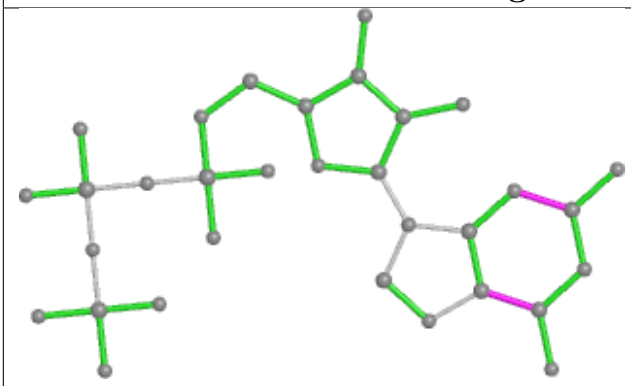

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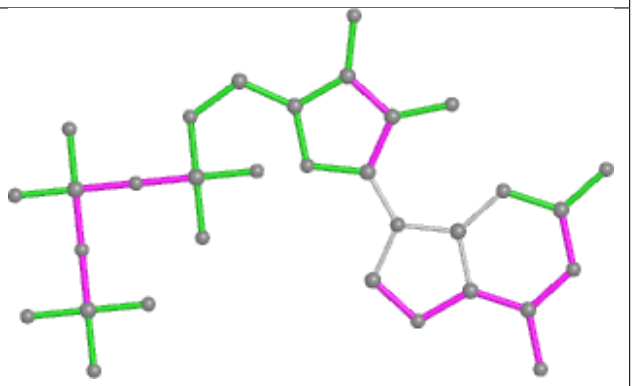

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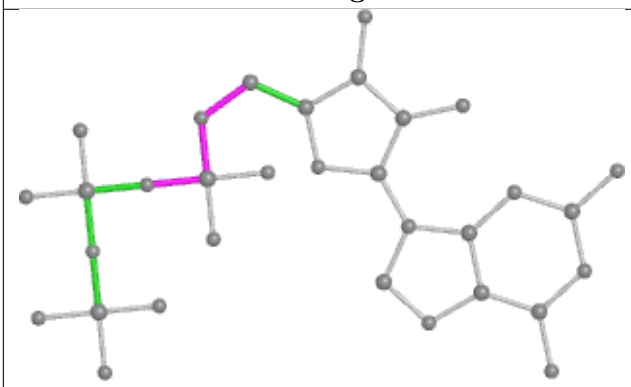

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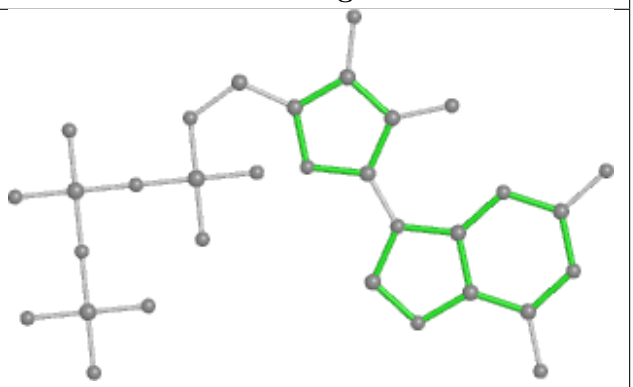

Rings

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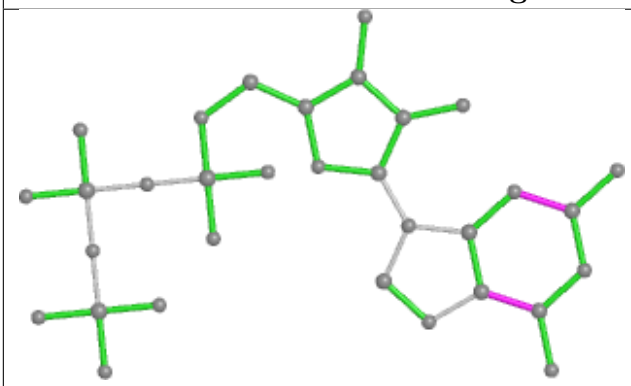

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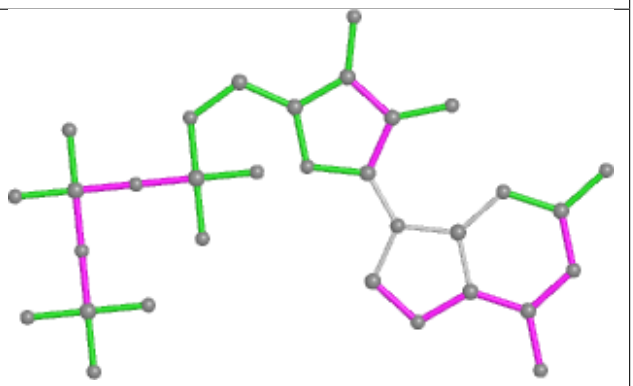

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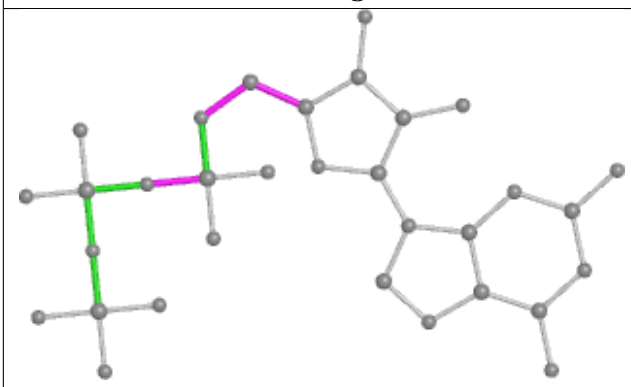

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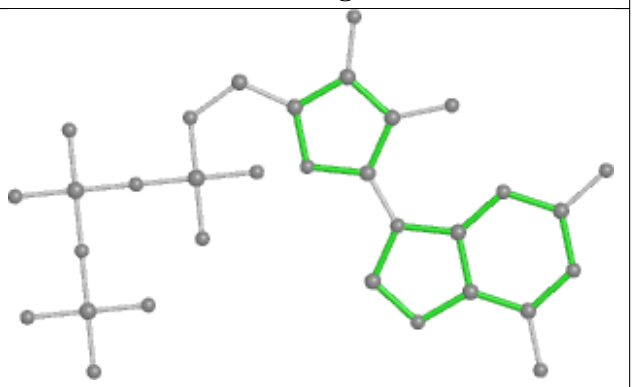

Rings

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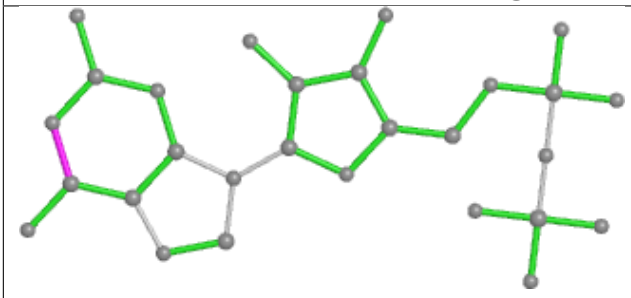

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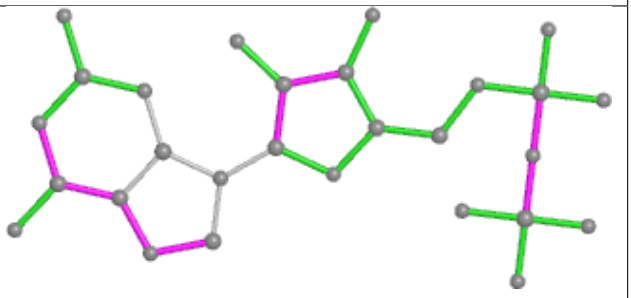

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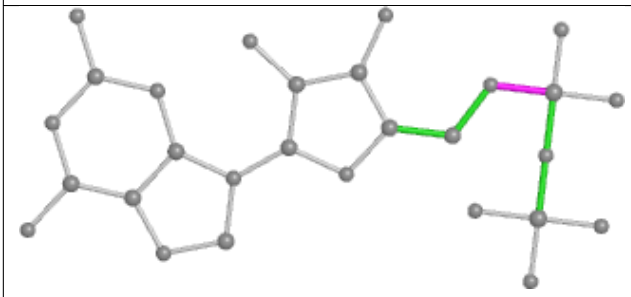

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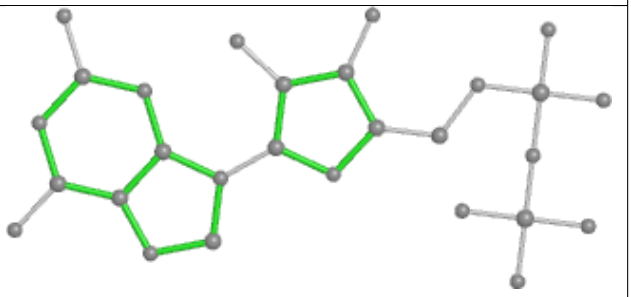
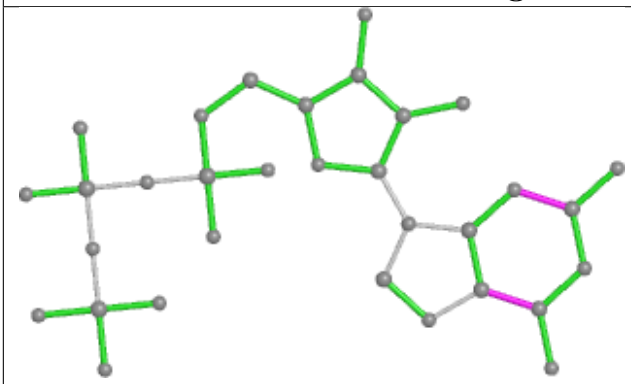


Rings

Ligand GTP GG 501



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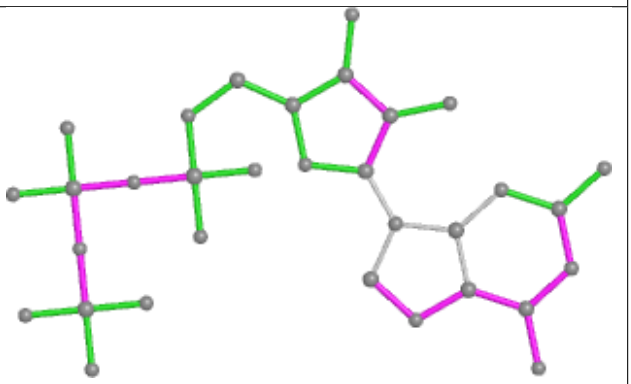

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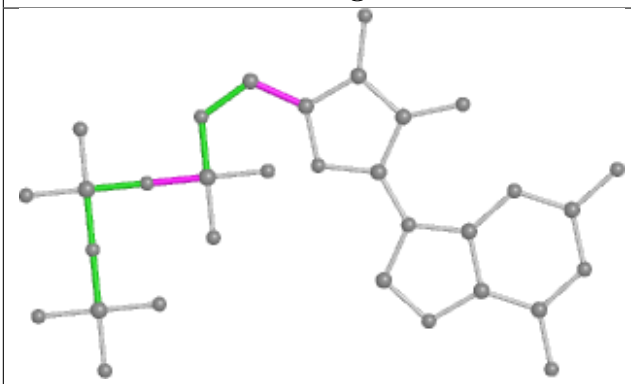

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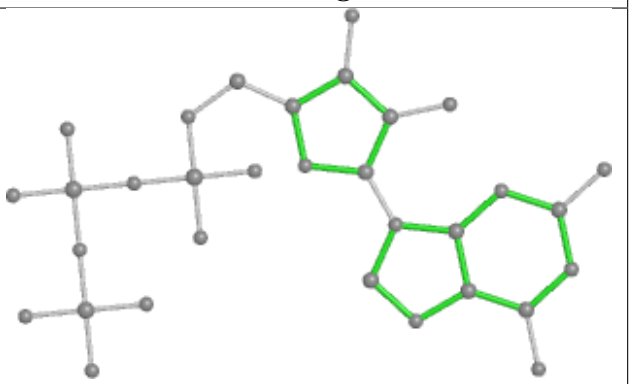
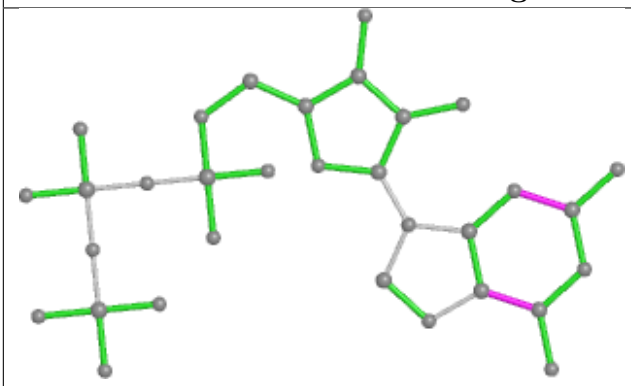


Rings

Ligand GTP KE 501



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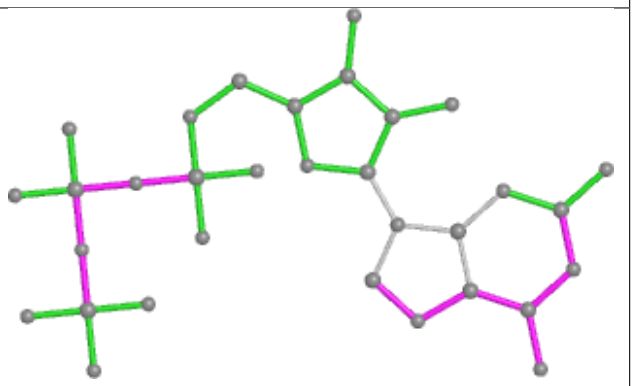

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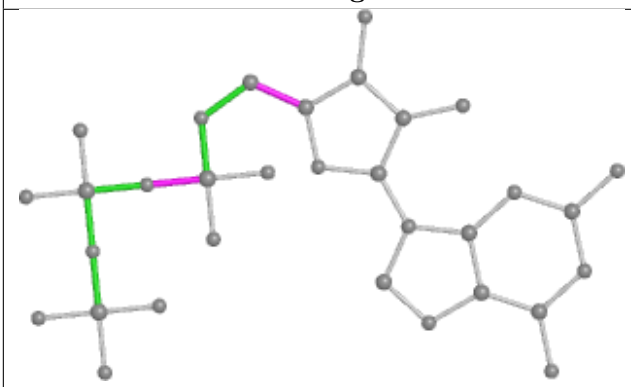

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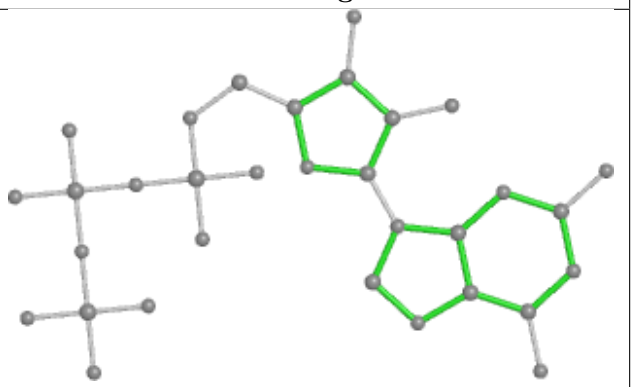
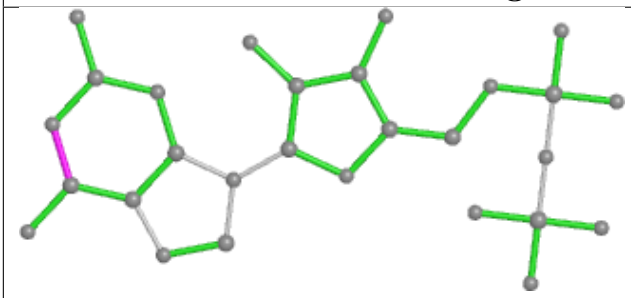


Rings

Ligand GDP MF 501



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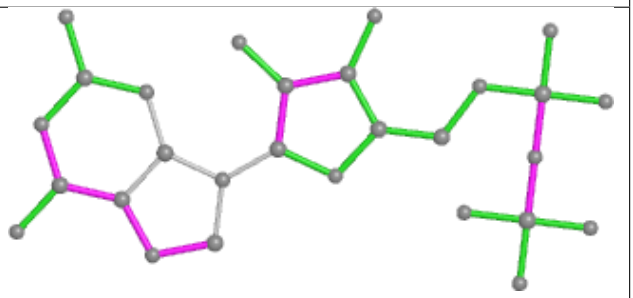

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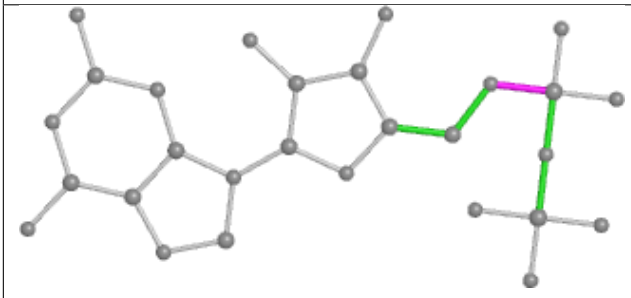

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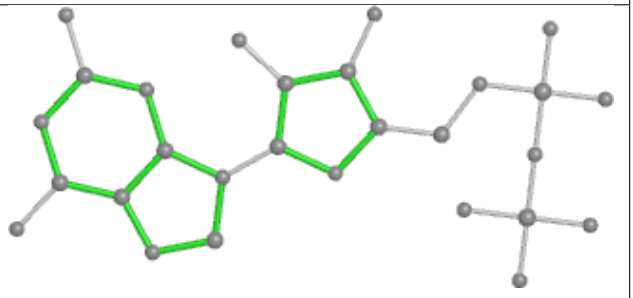
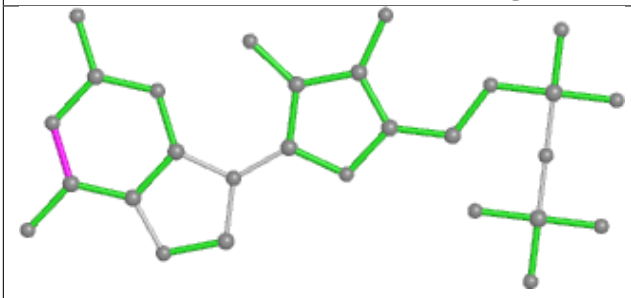


Rings

Ligand GDP DD 501



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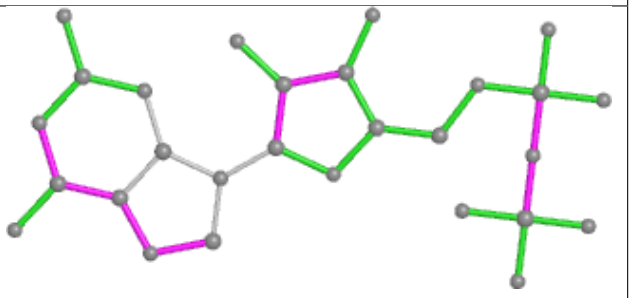

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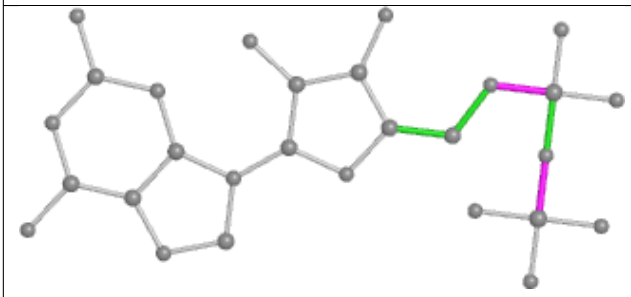

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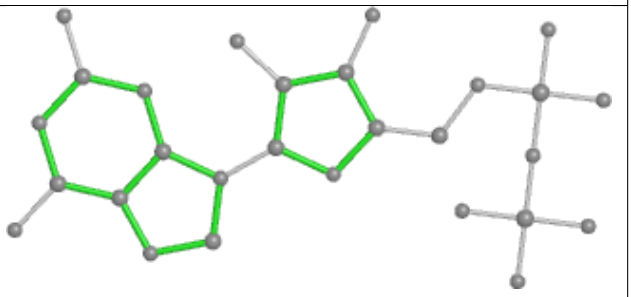
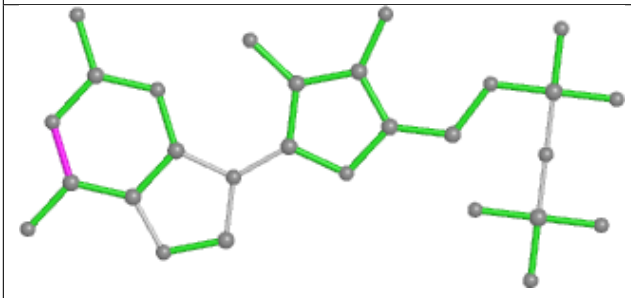


Rings

Ligand GDP BF 501



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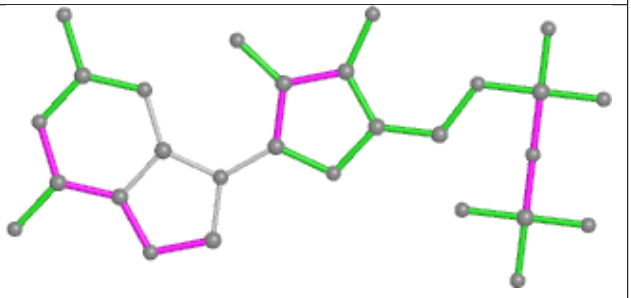

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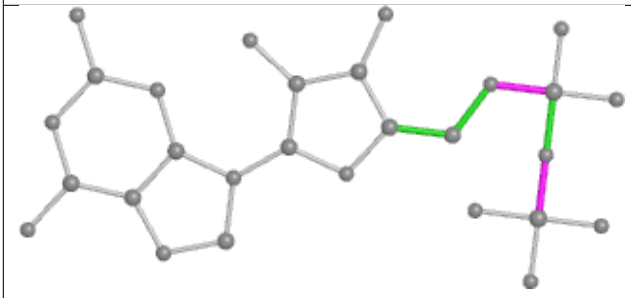

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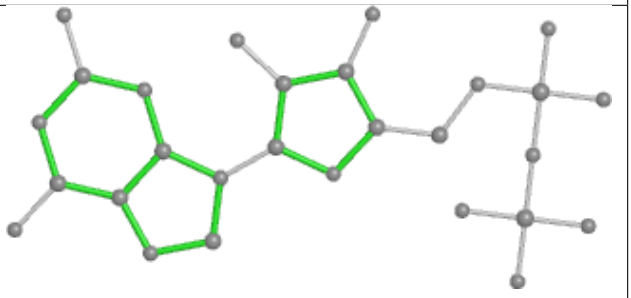
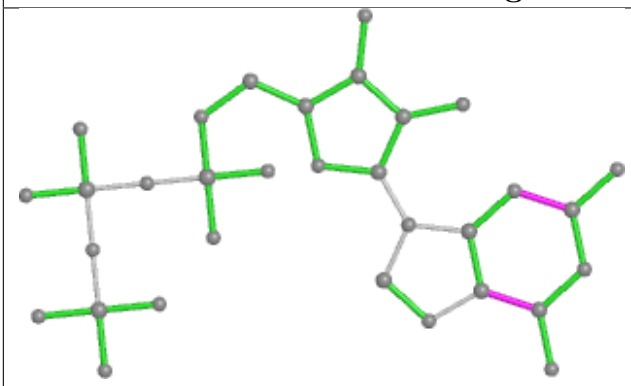


Rings

Ligand GTP MA 501



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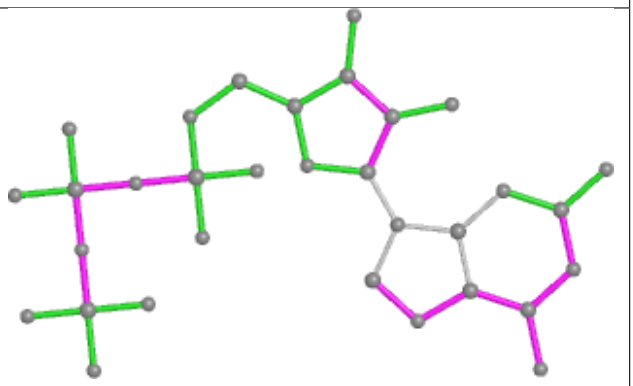
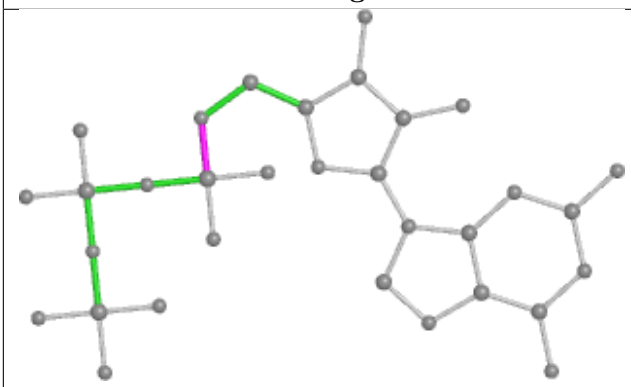


Bond angles



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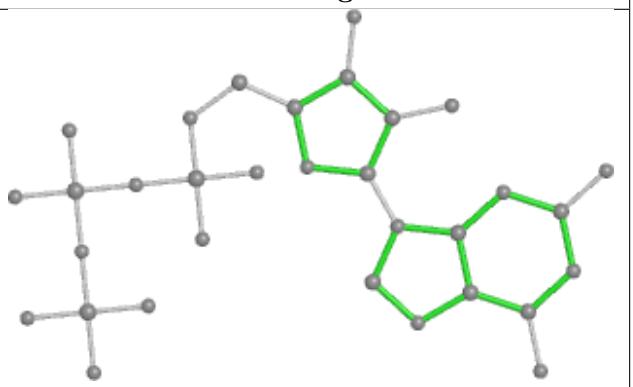
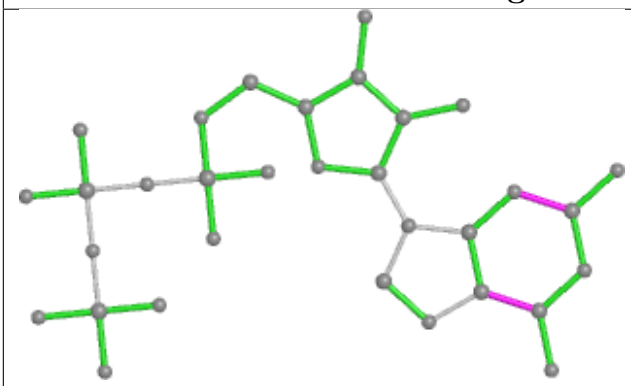


Rings

Ligand GTP DG 501



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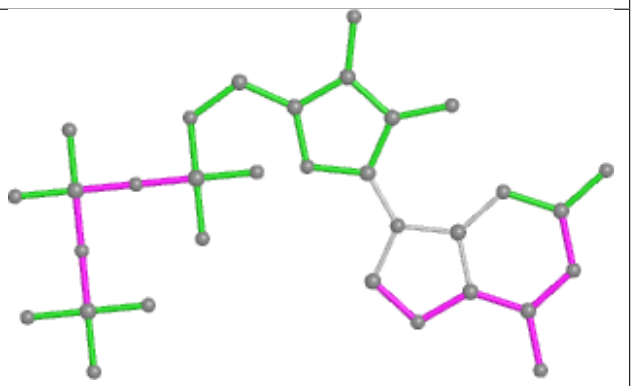
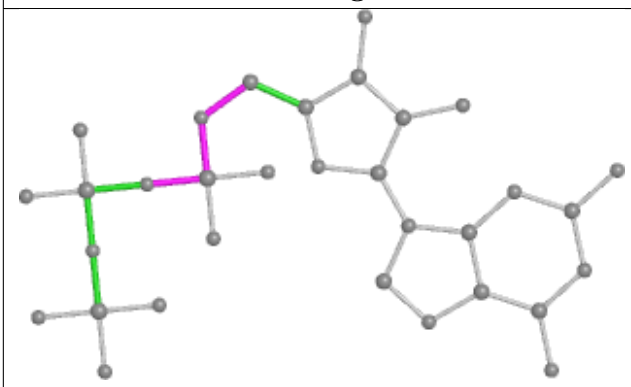


Bond angles



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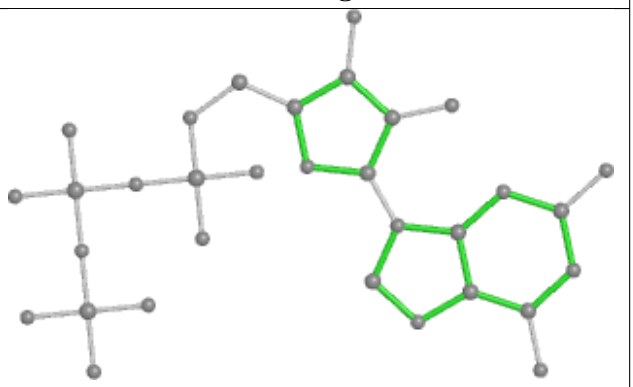
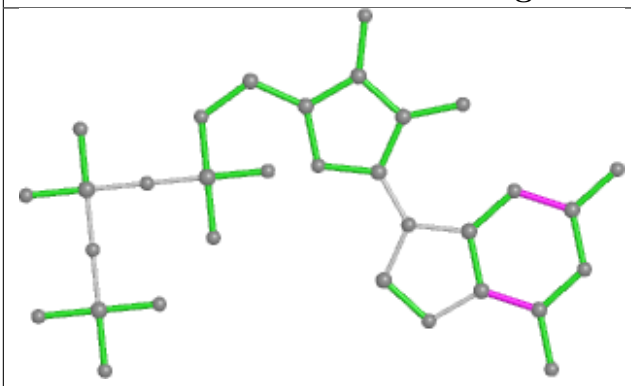
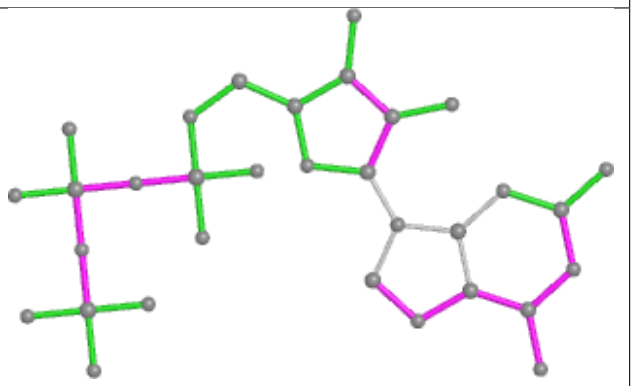


Rings

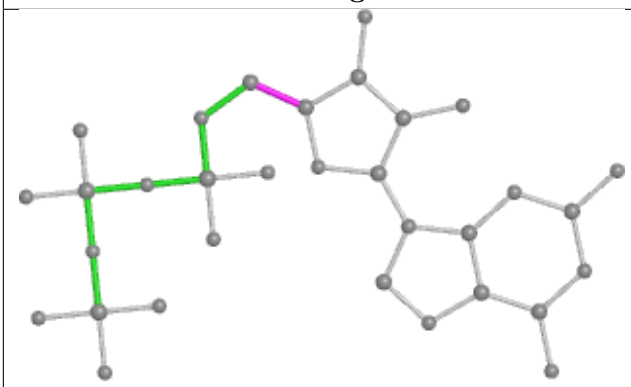
Ligand GTP IG 501



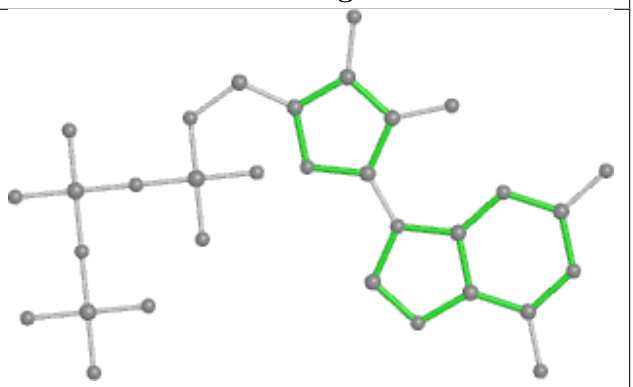
Bond lengths



Bond angles

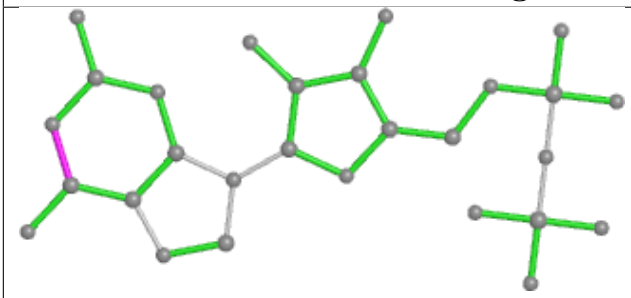


Torsions



Rings

Ligand GDP LB 501



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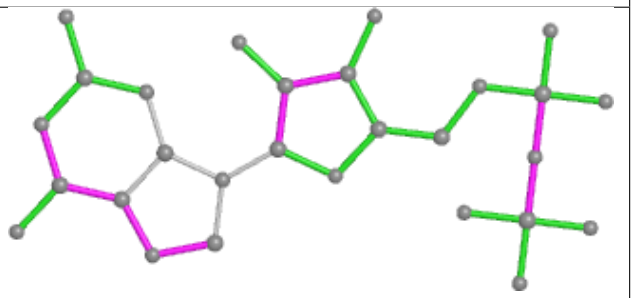

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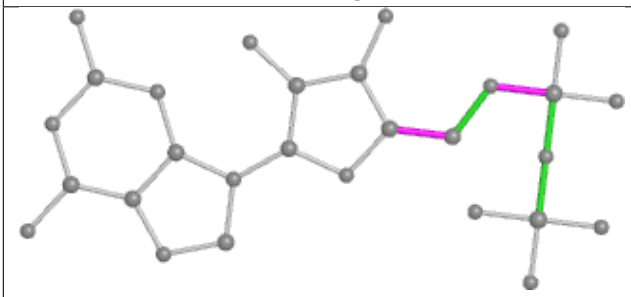

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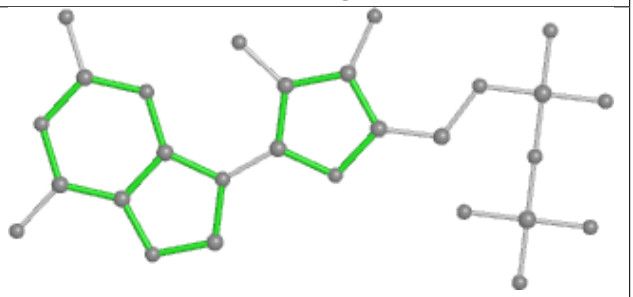
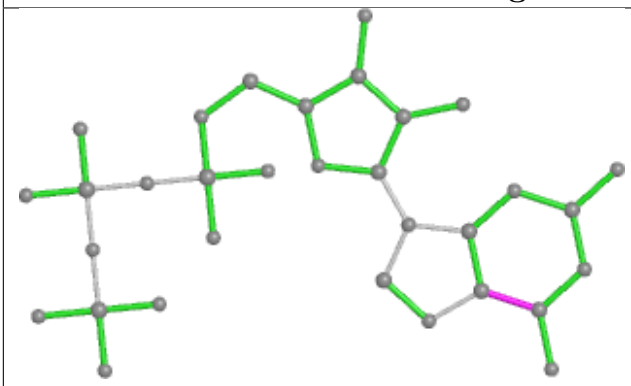


Rings

Ligand GTP BG 501



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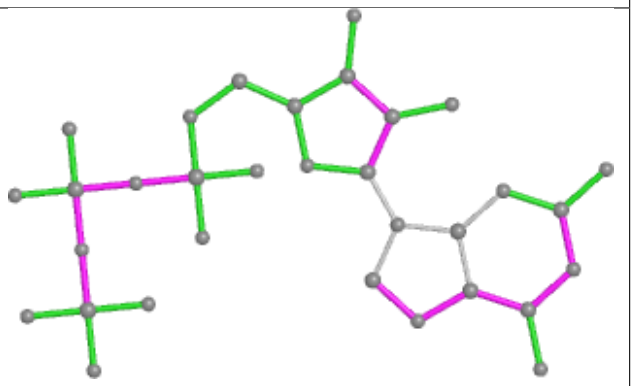

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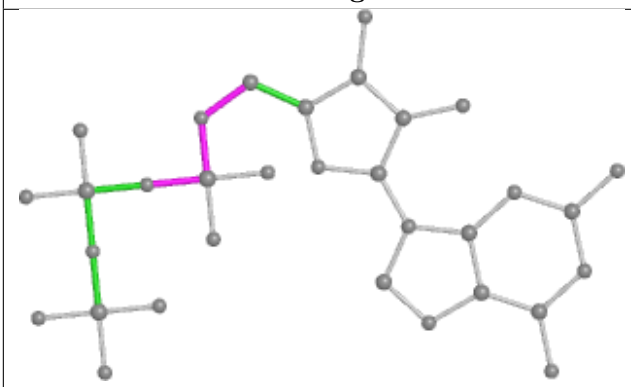

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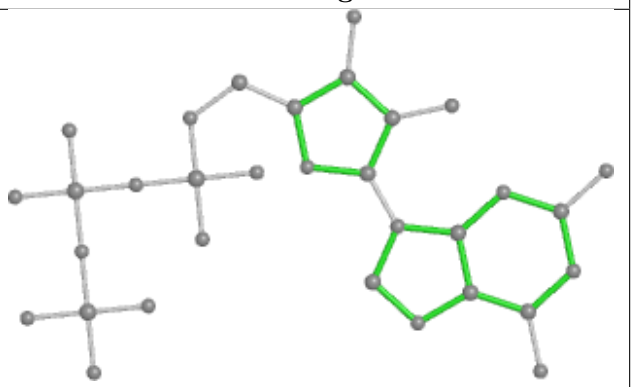
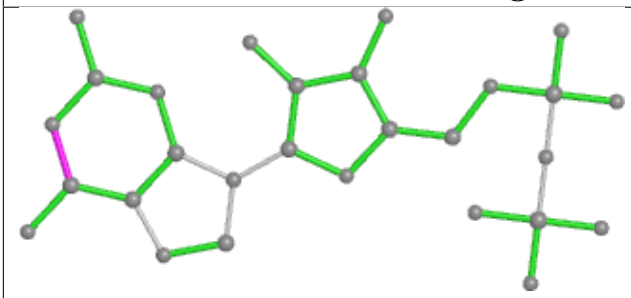


Rings

Ligand GDP KF 501



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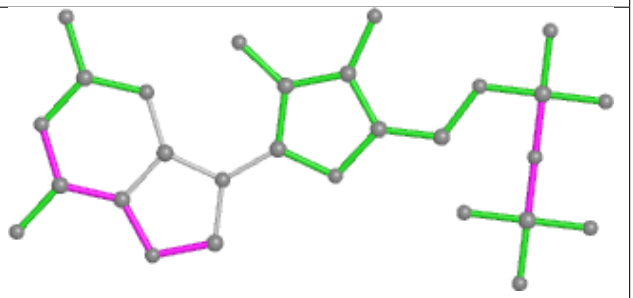

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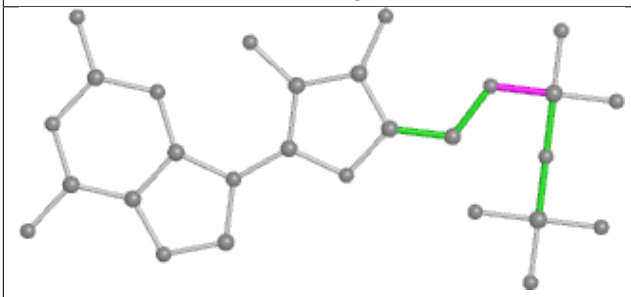

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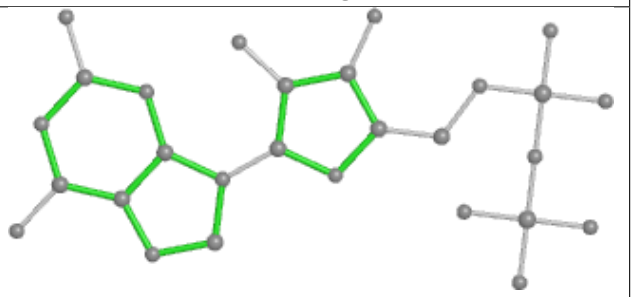
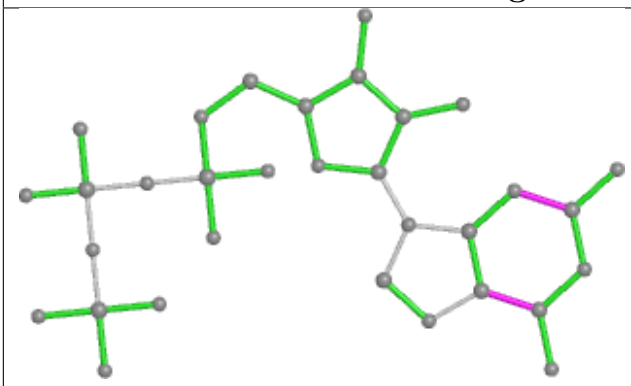


Rings

Ligand GTP HC 501



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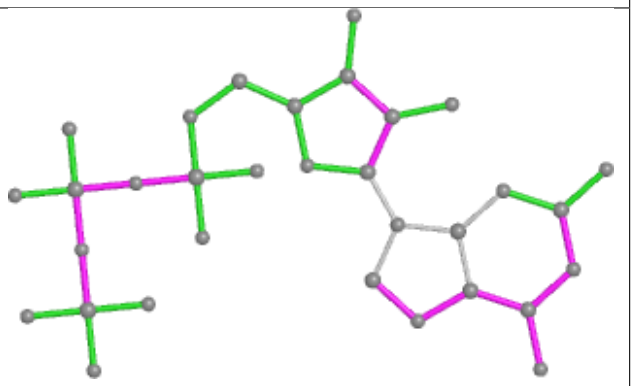

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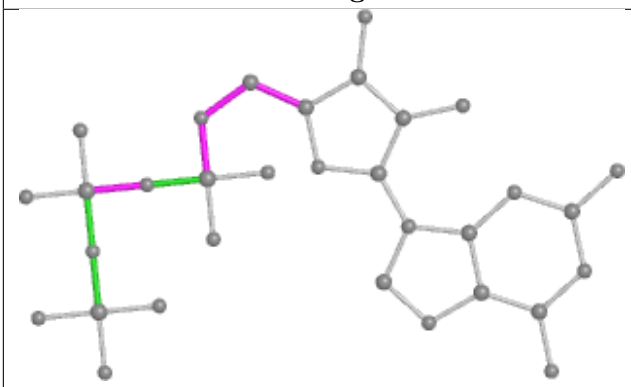

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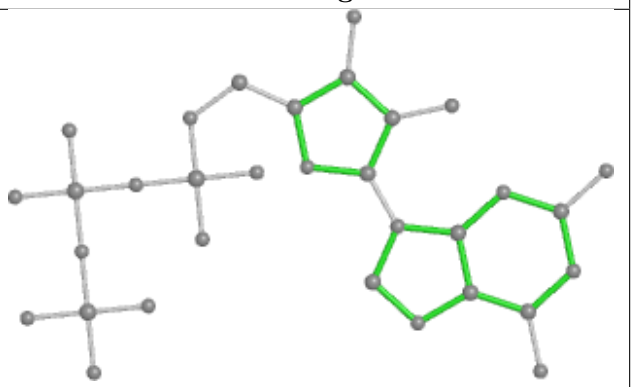
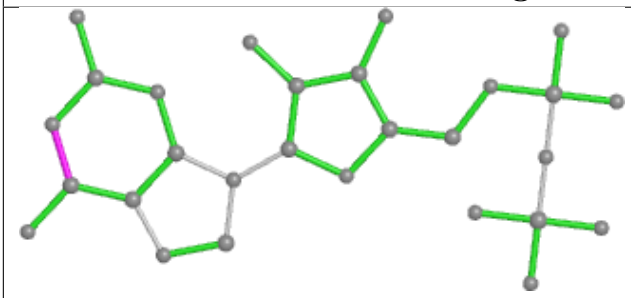


Rings

Ligand GDP FF 501



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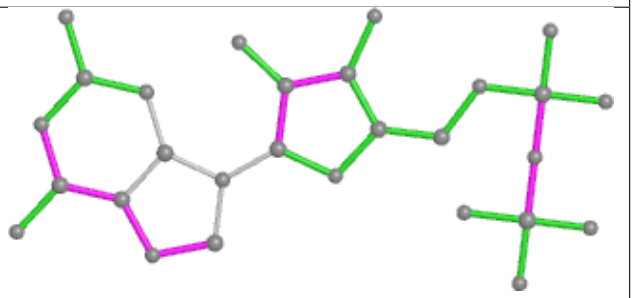

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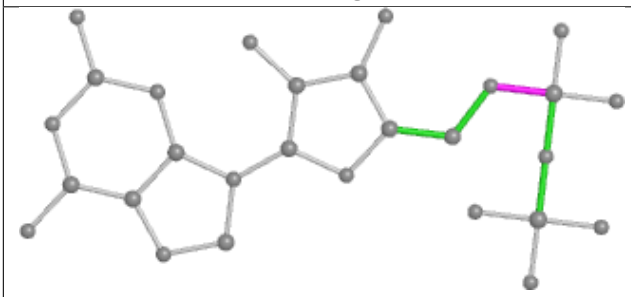

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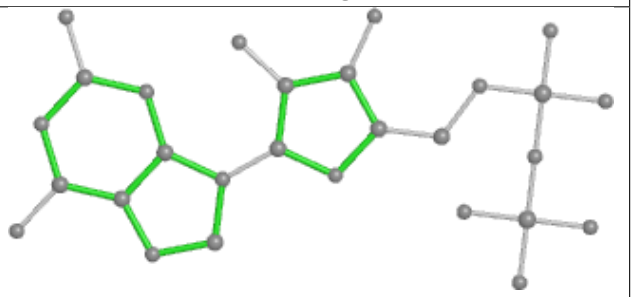
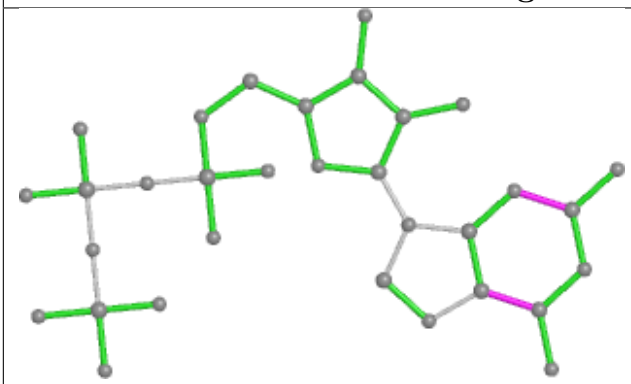


Rings

Ligand GTP IE 501



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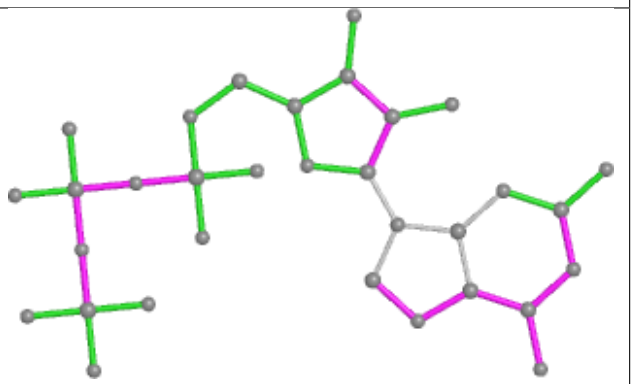

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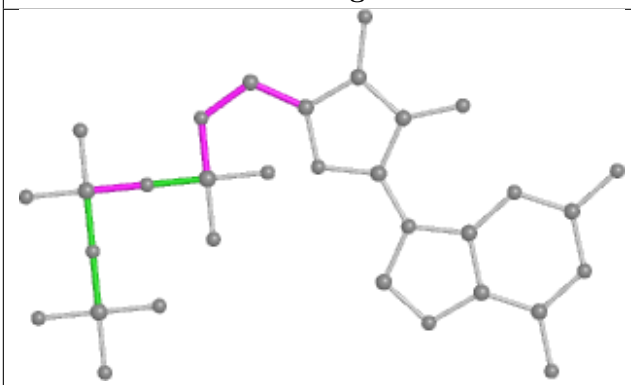

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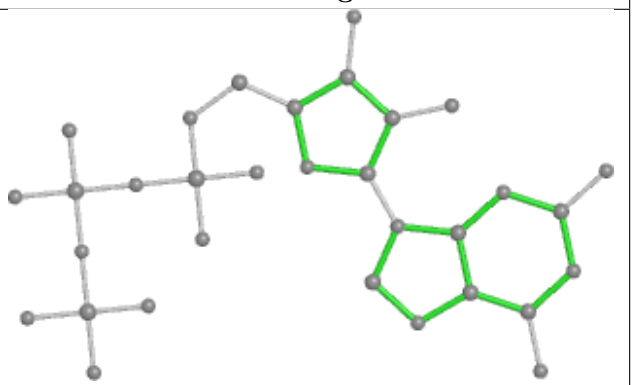
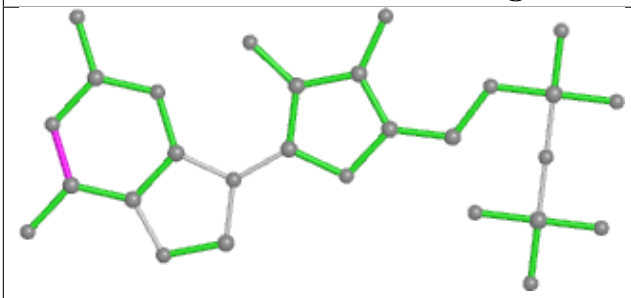


Rings

Ligand GDP AD 501



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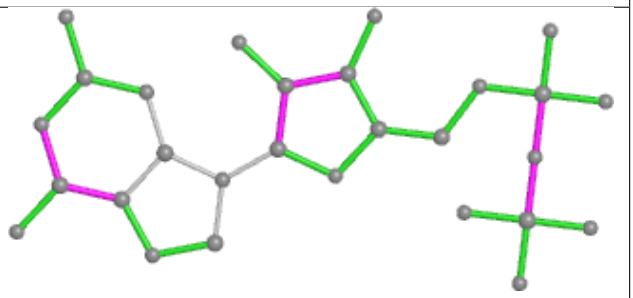

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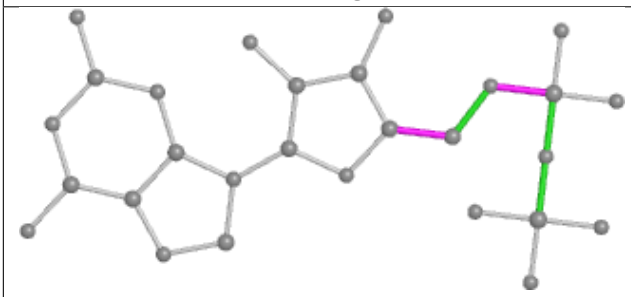

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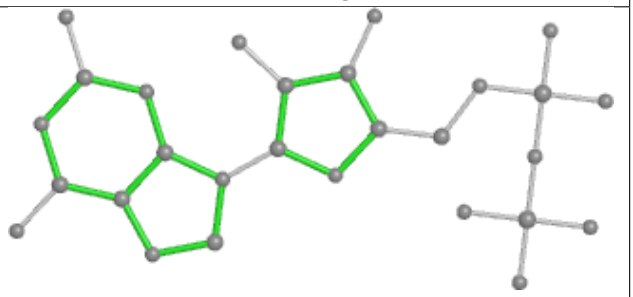
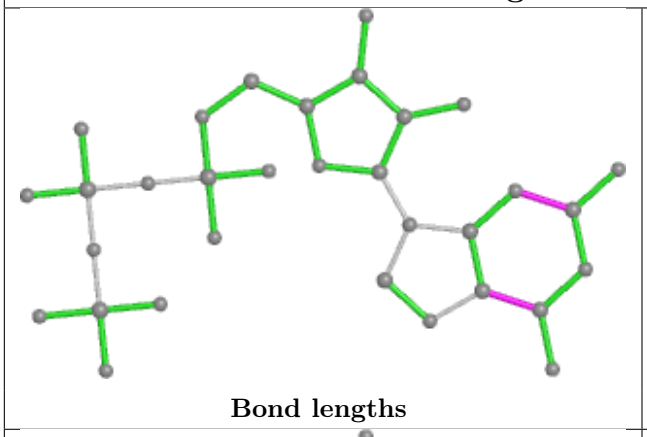


Rings

Ligand GTP MC 501



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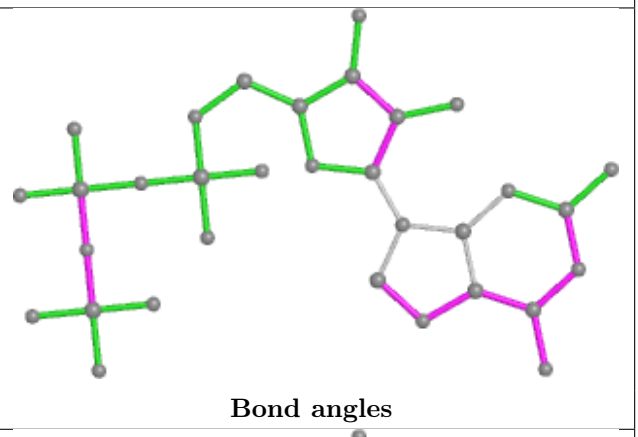

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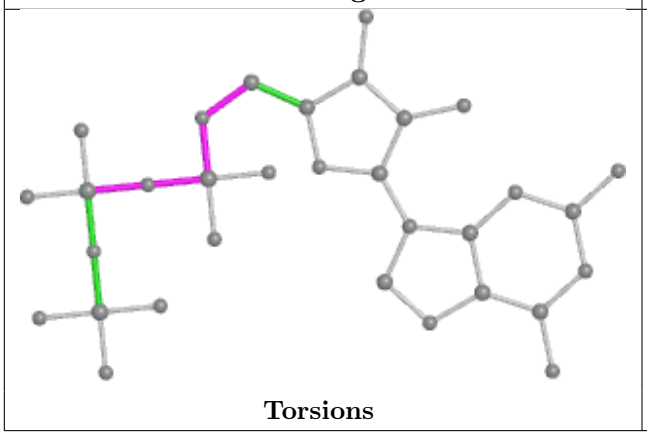

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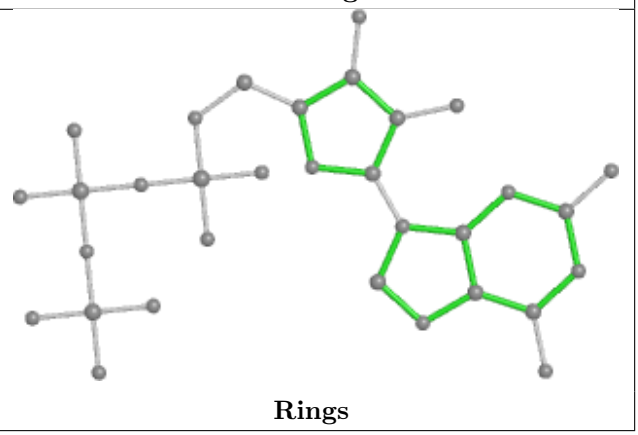
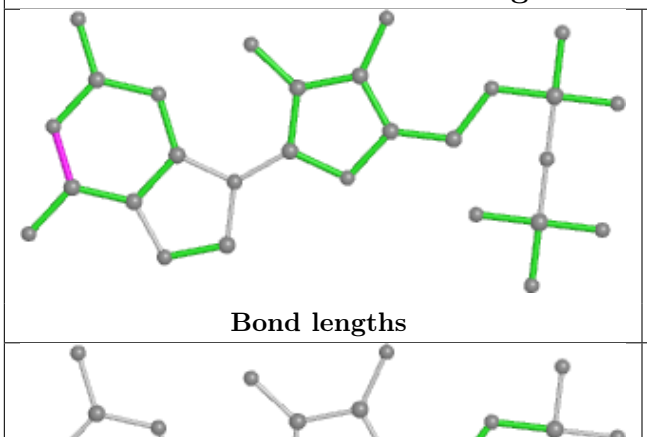


Rings

Ligand GDP LD 501



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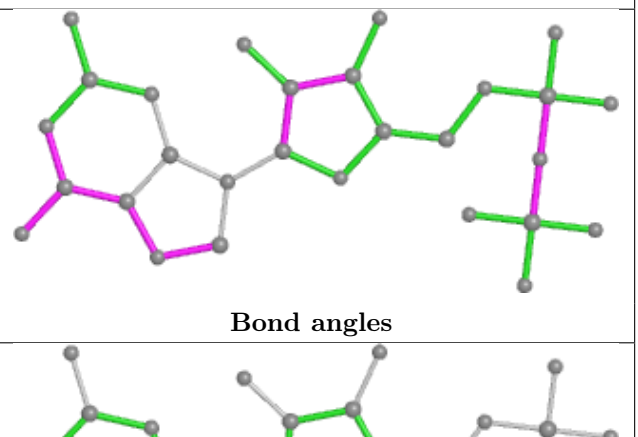

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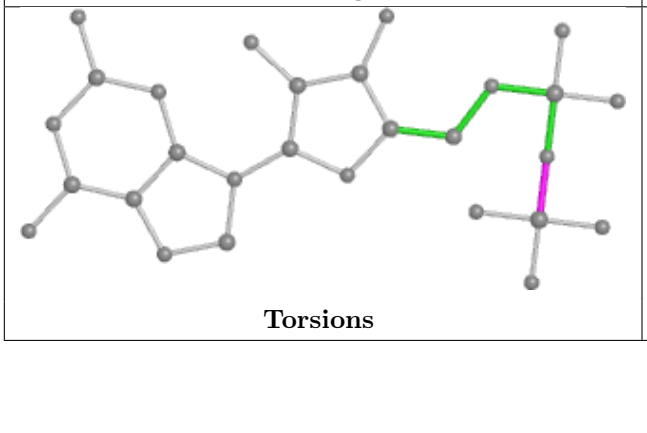

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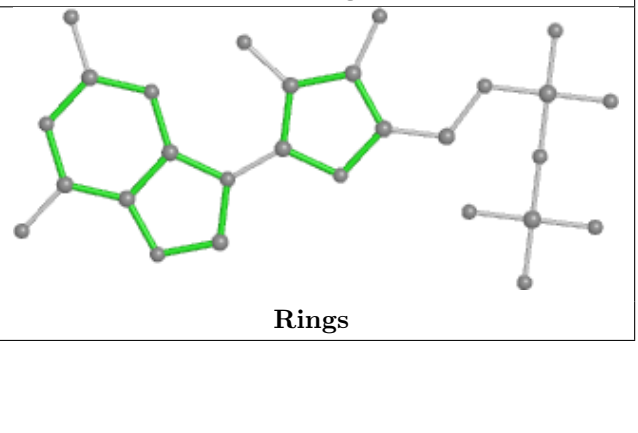
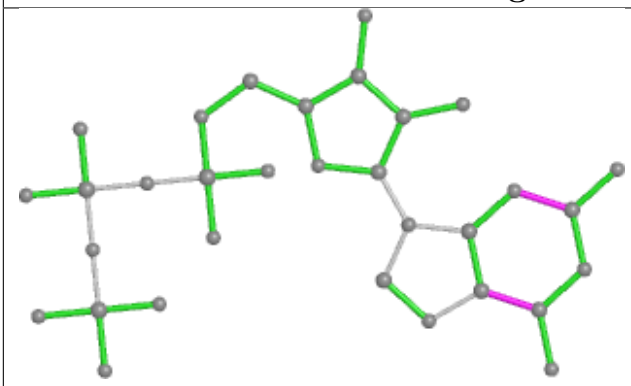


Rings

Ligand GTP GC 501



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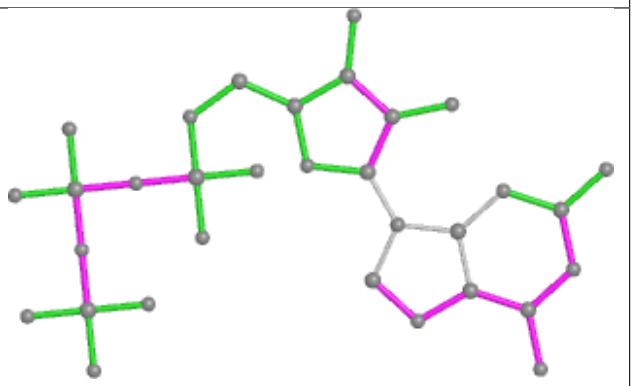

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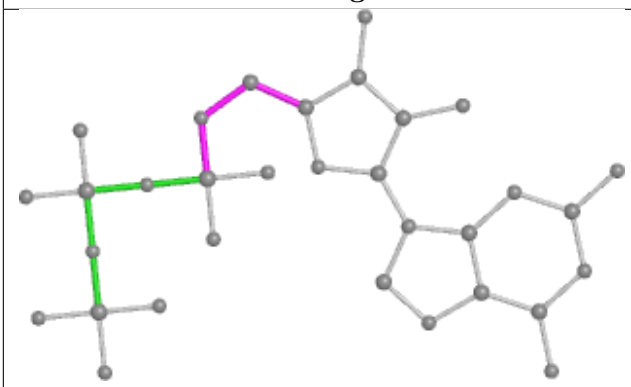

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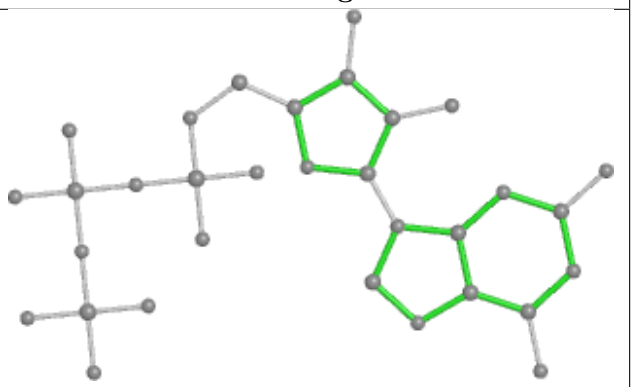

Rings

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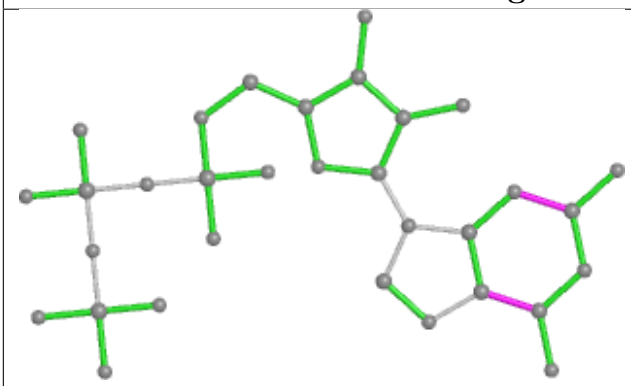

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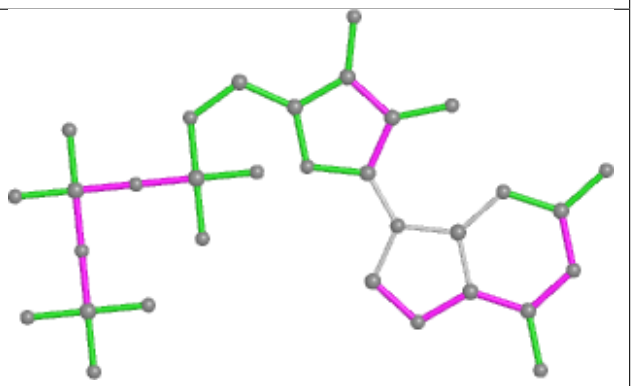

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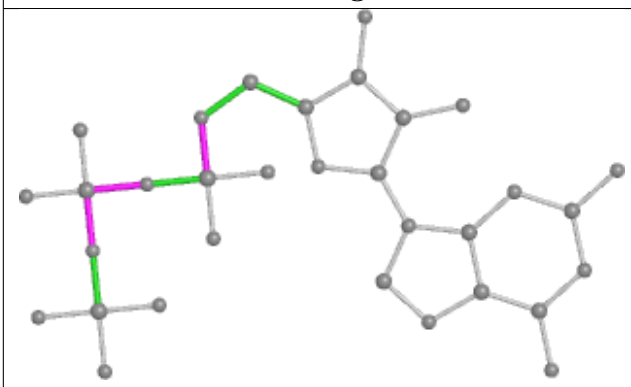

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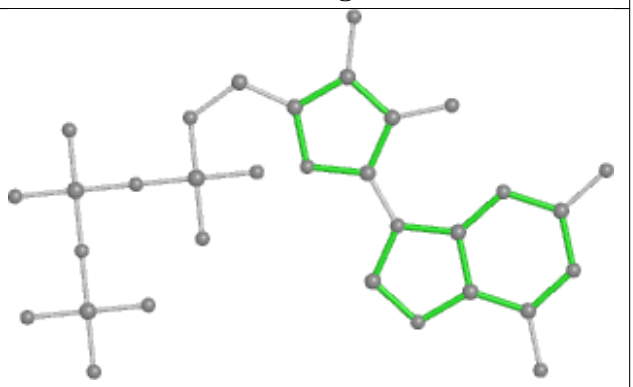
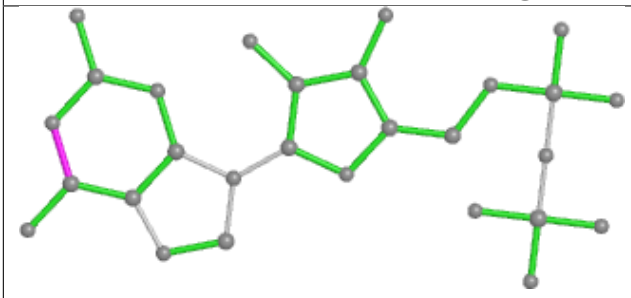


Rings

Ligand GDP IF 501



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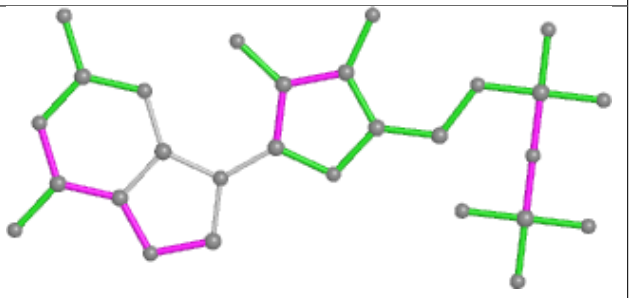

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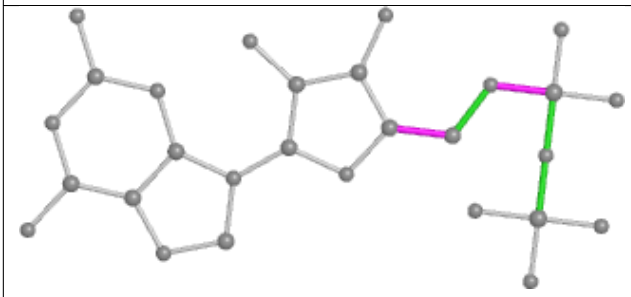

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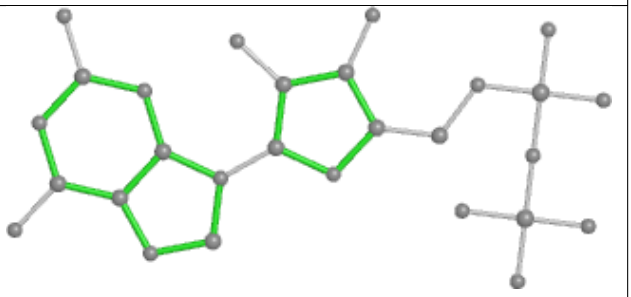
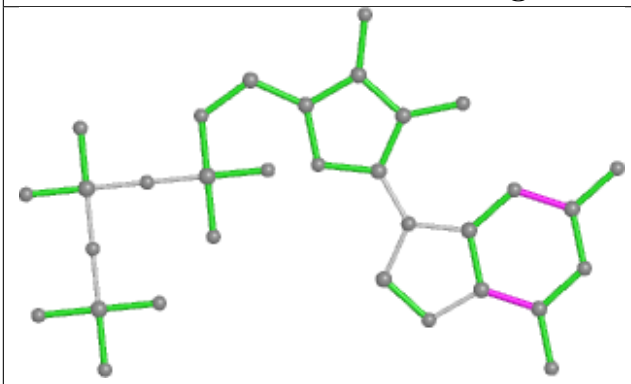


Rings

Ligand GTP GE 501



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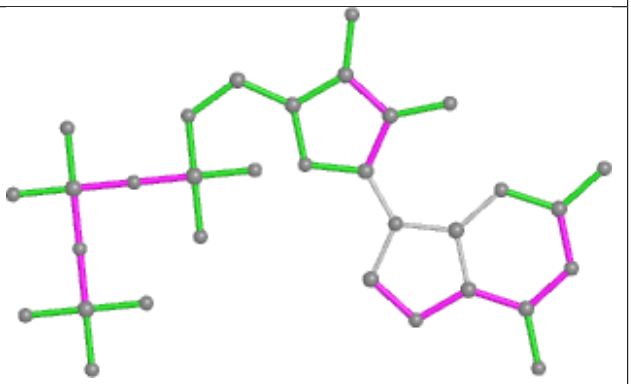
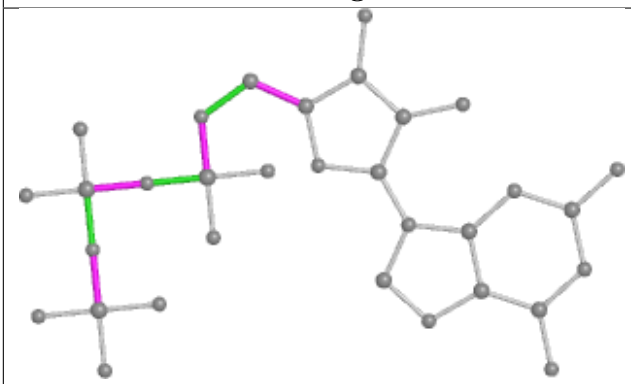


Bond angles



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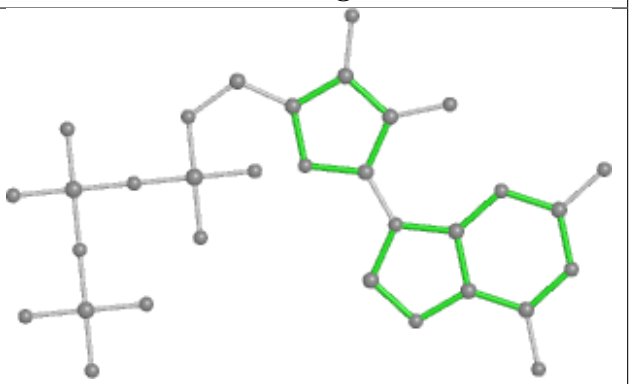
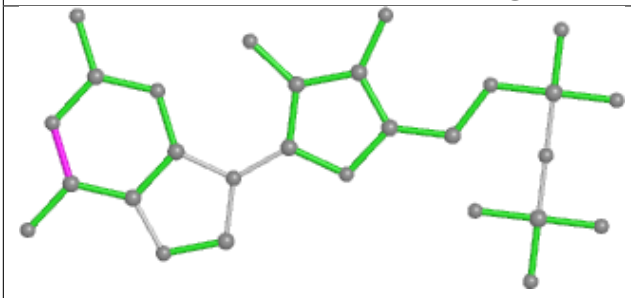
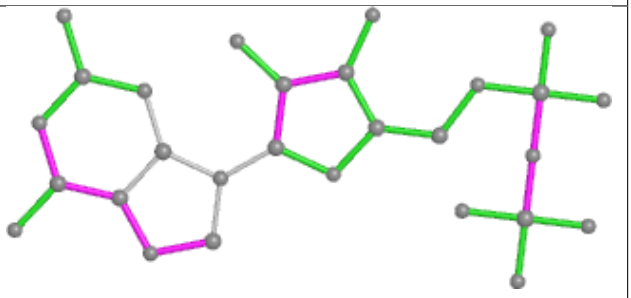
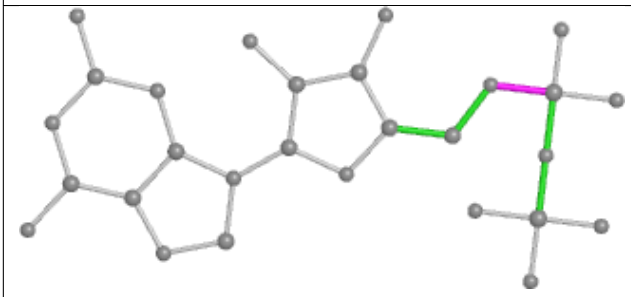
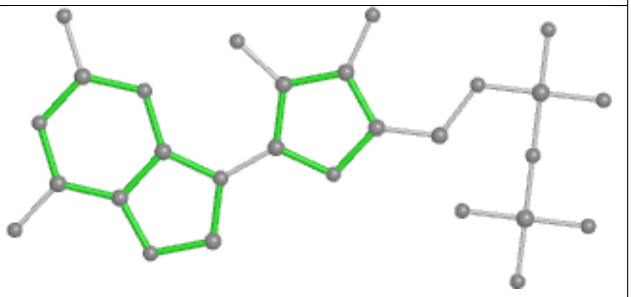
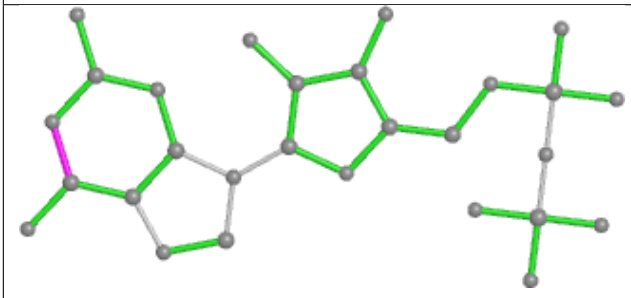
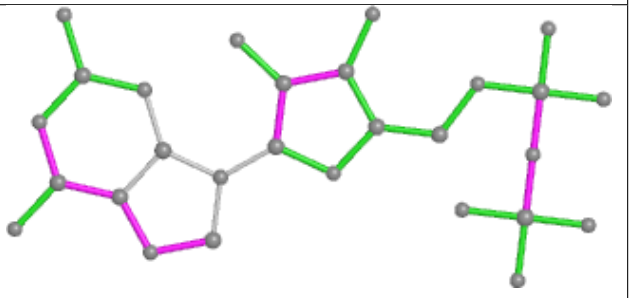


Rings

Ligand GDP GH 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP HF 501	
	
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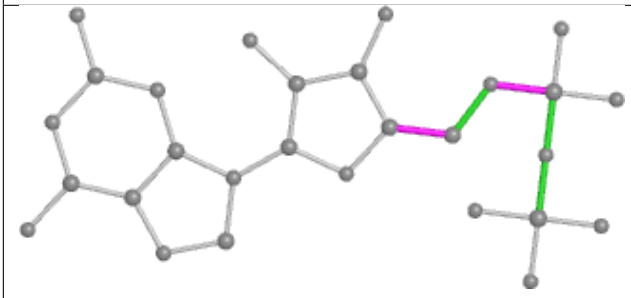
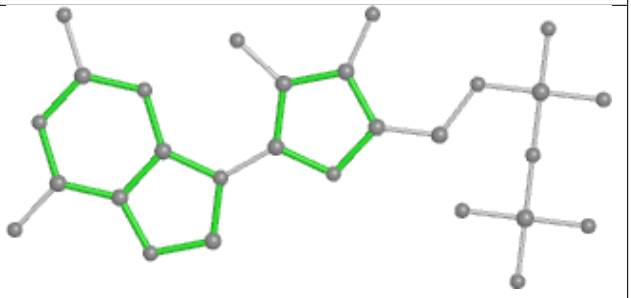
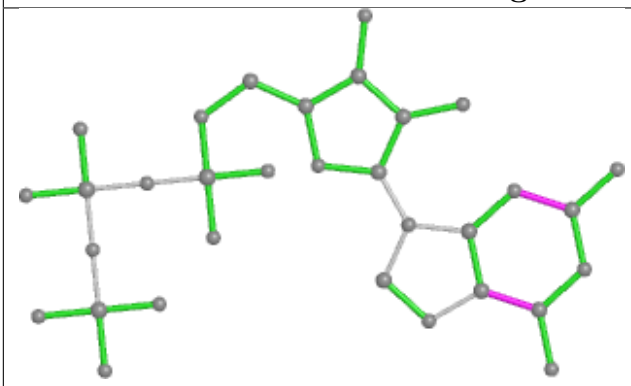
	
Torsions	Rings

Ligand GTP DE 501



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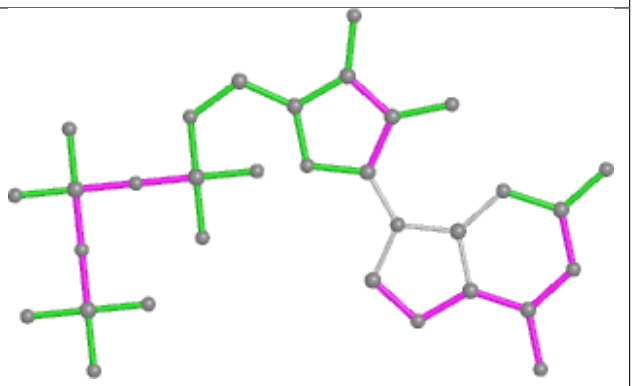

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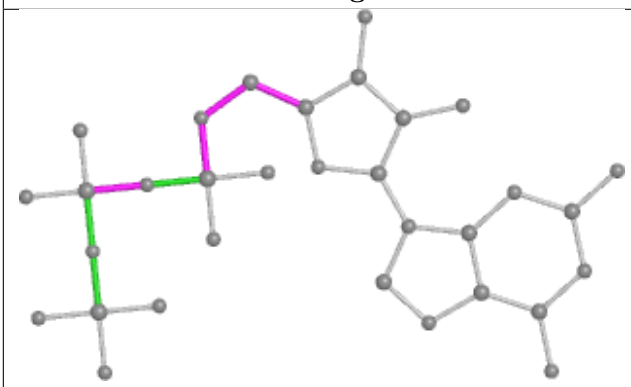

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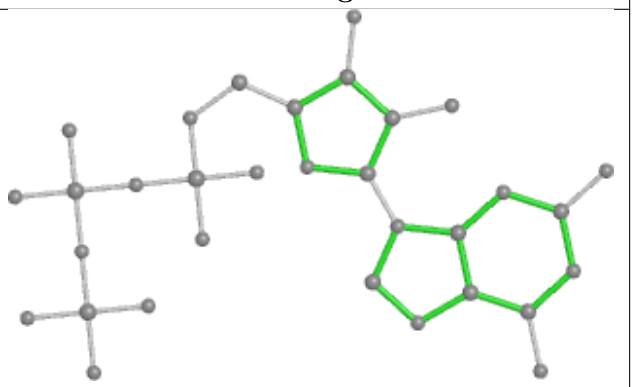

Rings

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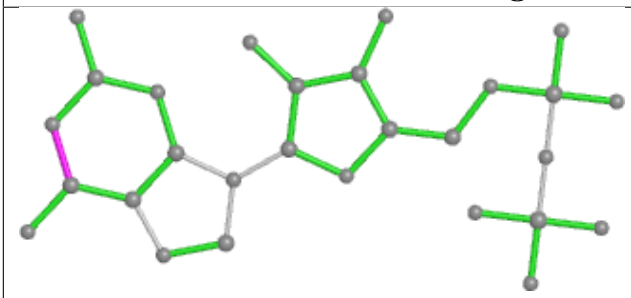

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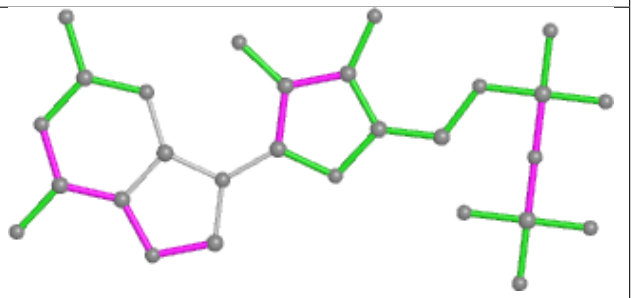

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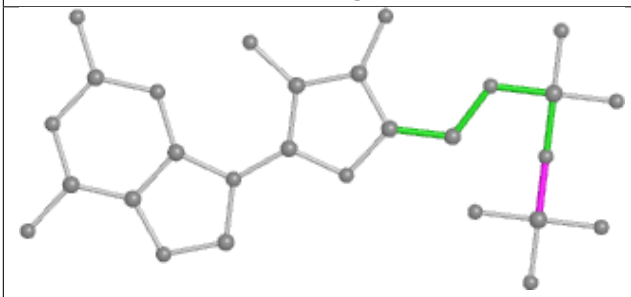

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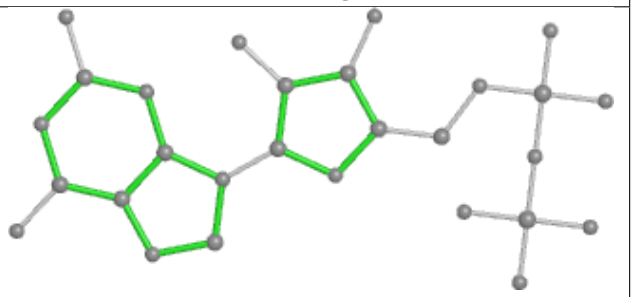

Rings

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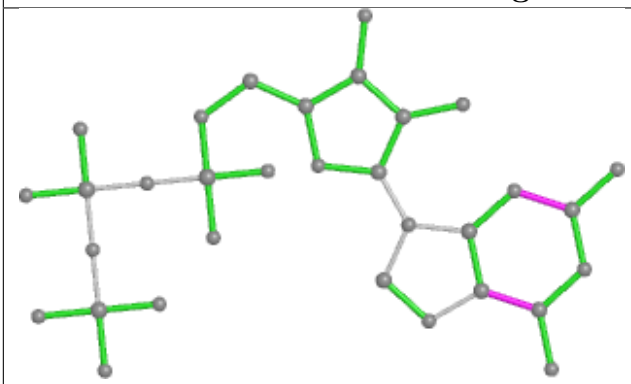

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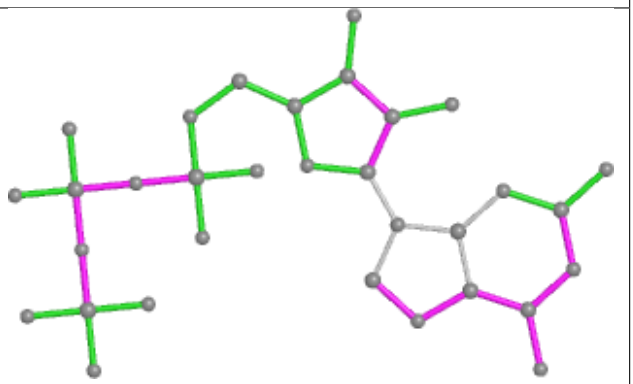

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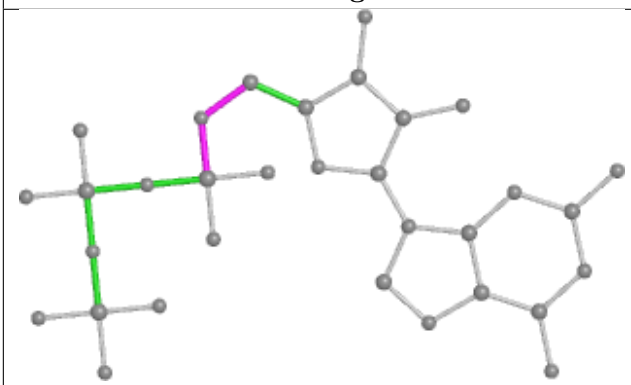

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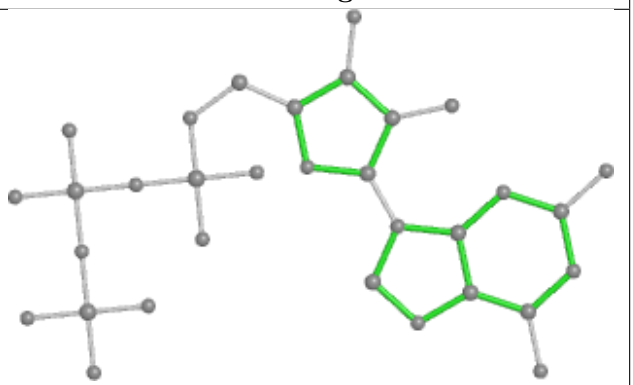

Rings

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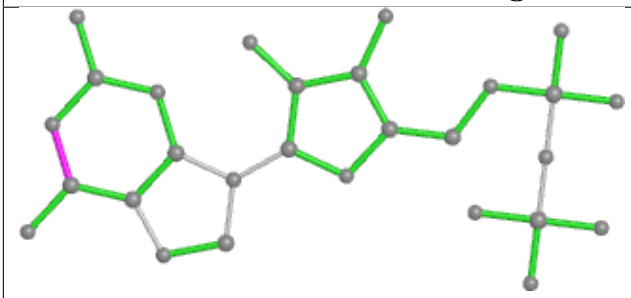

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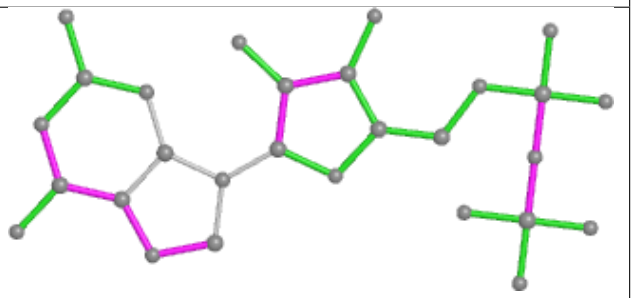

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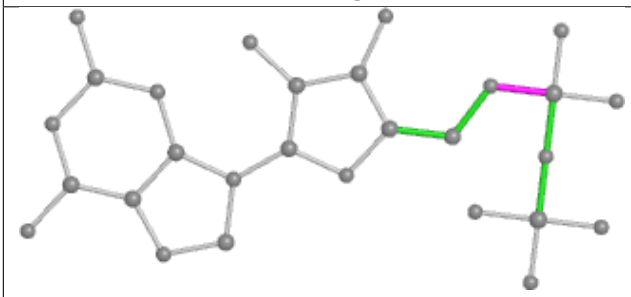

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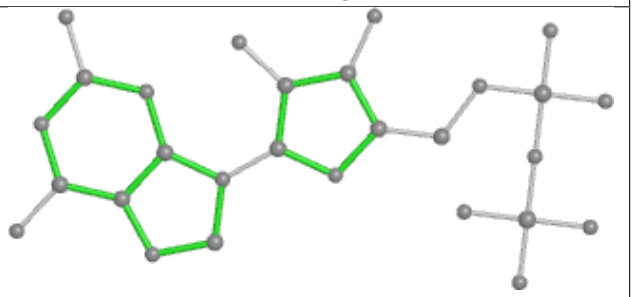

Rings

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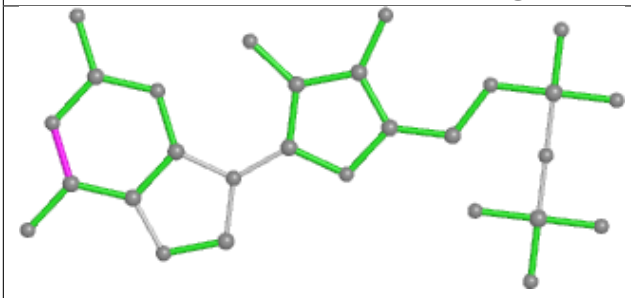

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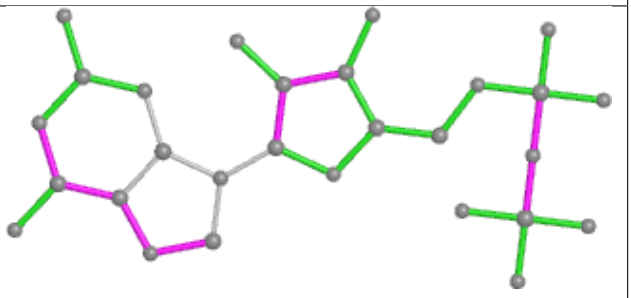

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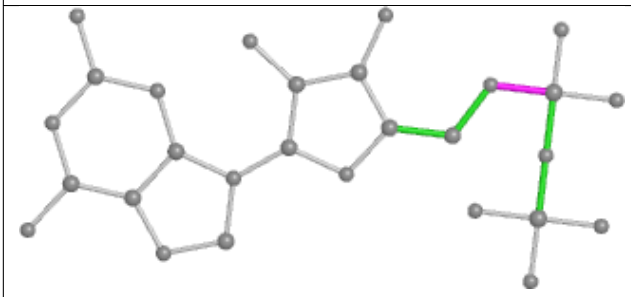

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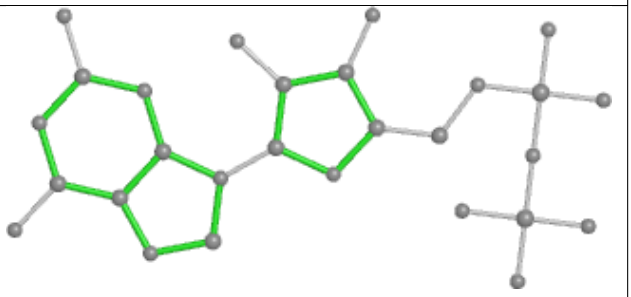
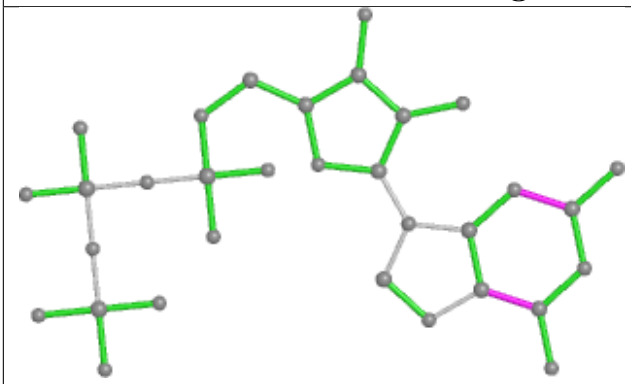


Rings

Ligand GTP BC 501



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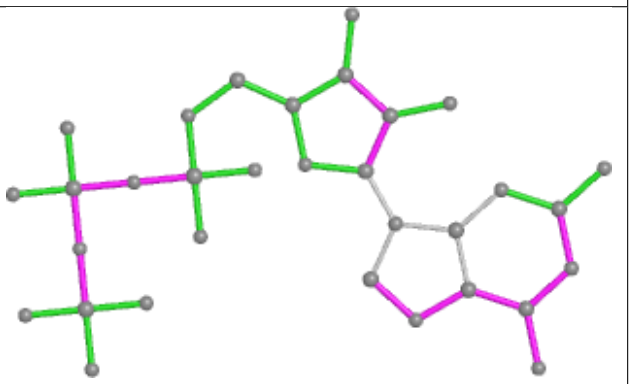

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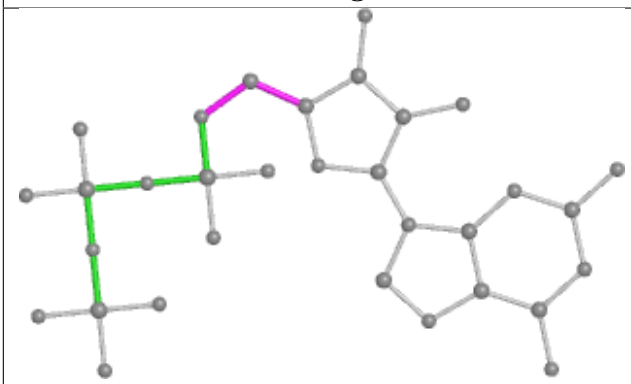

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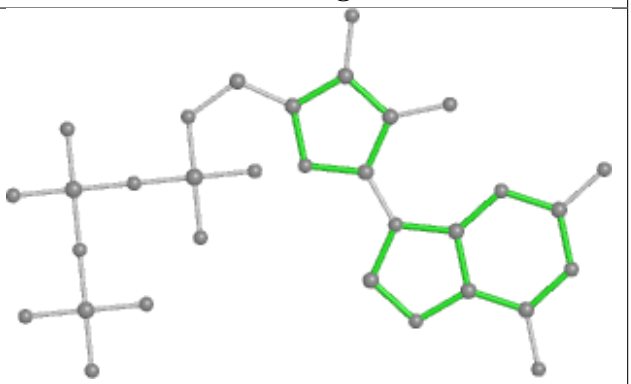

Rings

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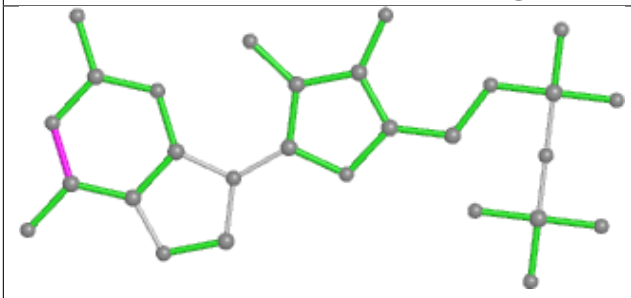

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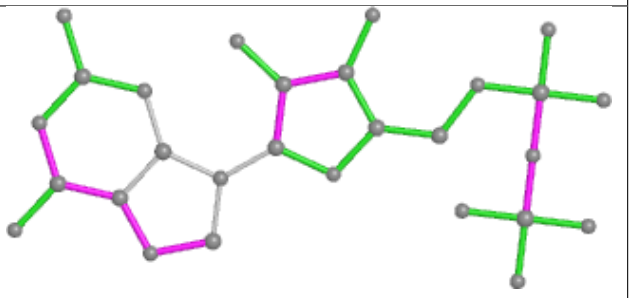

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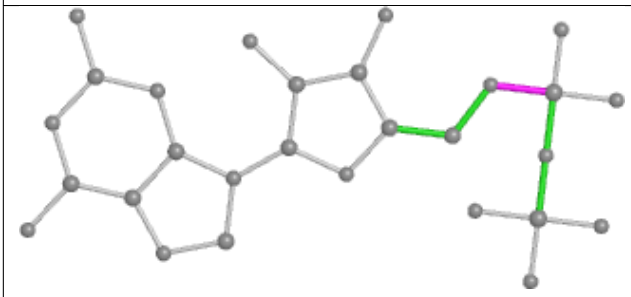

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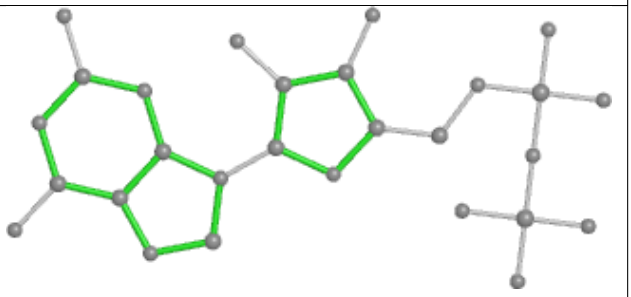

Rings

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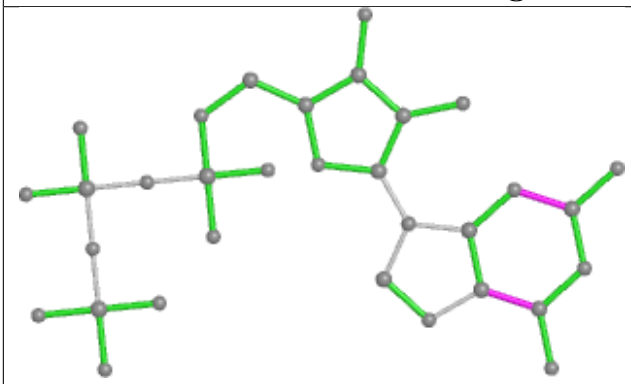

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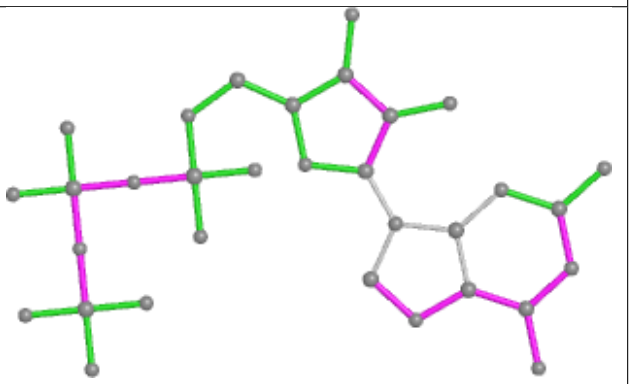

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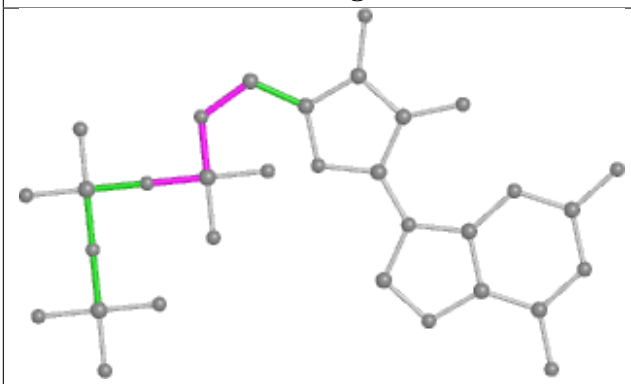

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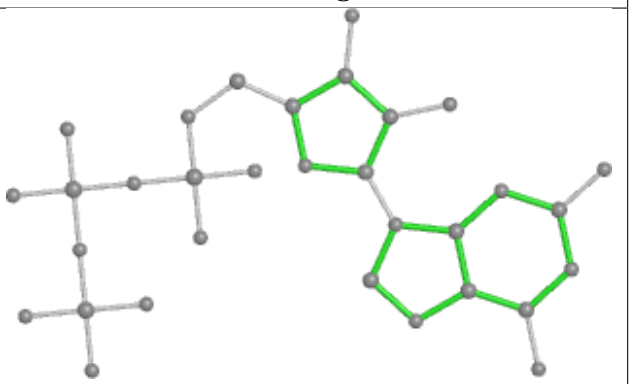

Rings

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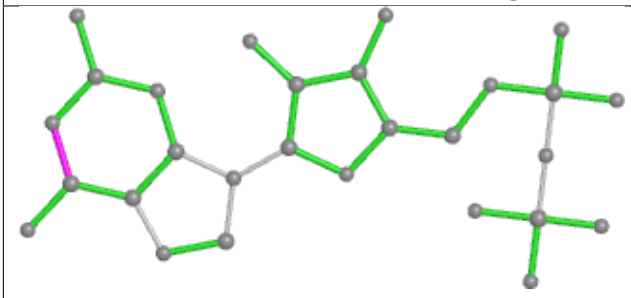

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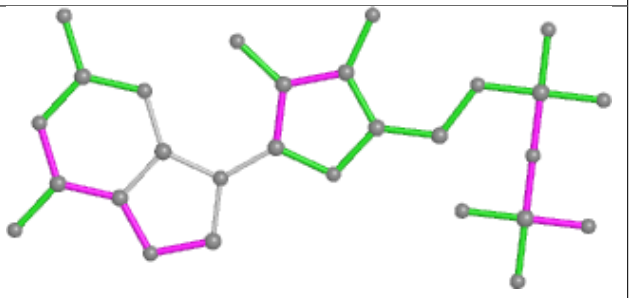

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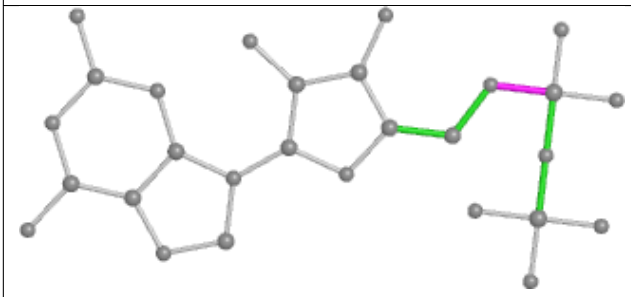

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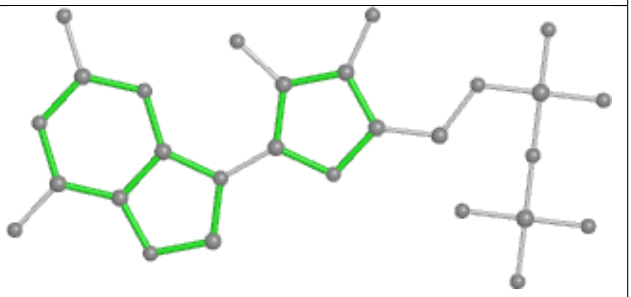

Rings

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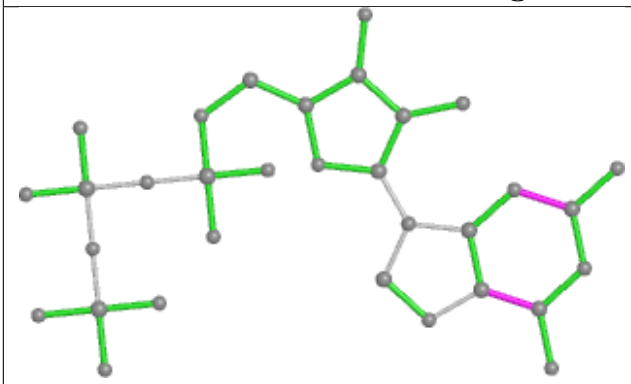

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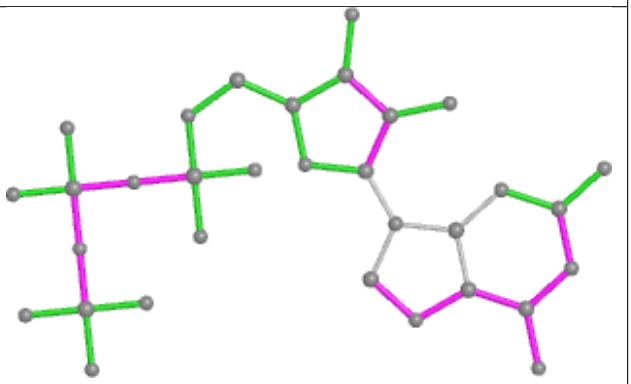

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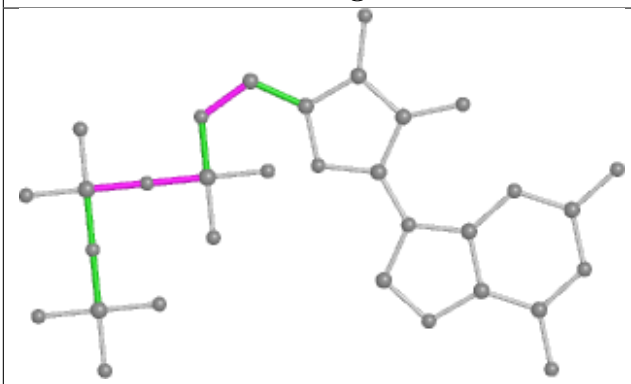

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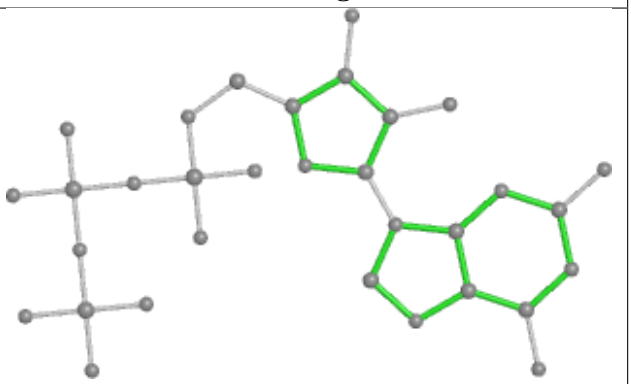
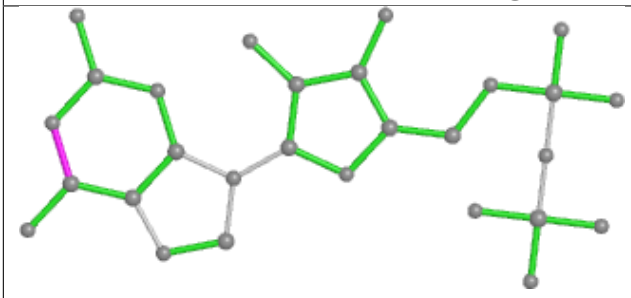


Rings

Ligand GDP KH 501



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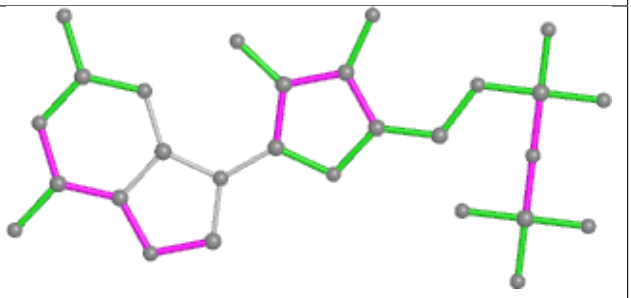

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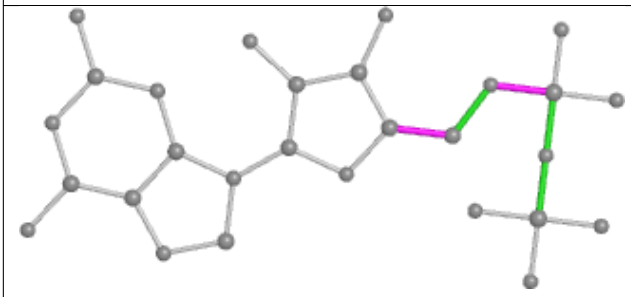

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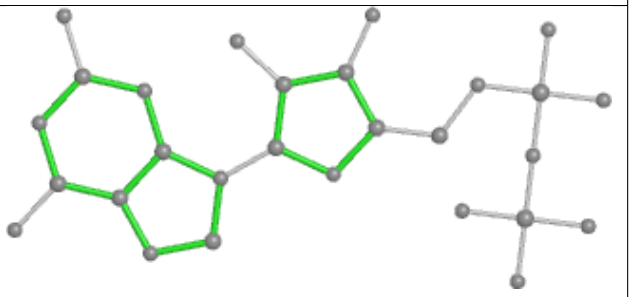
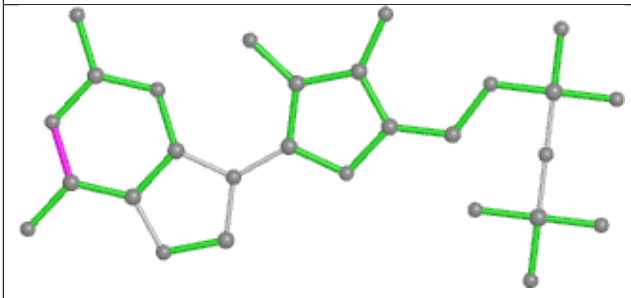


Rings

Ligand GDP IH 501



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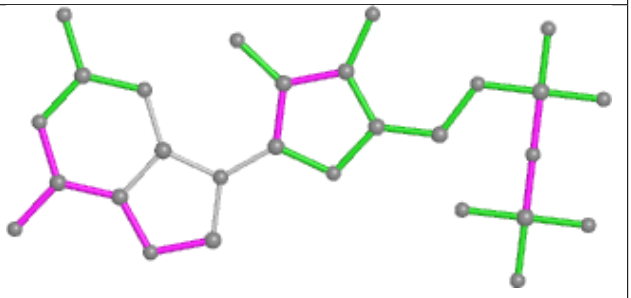

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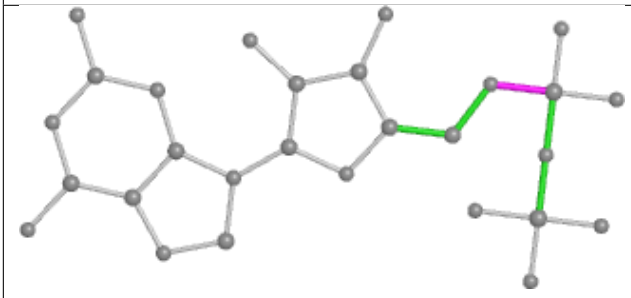

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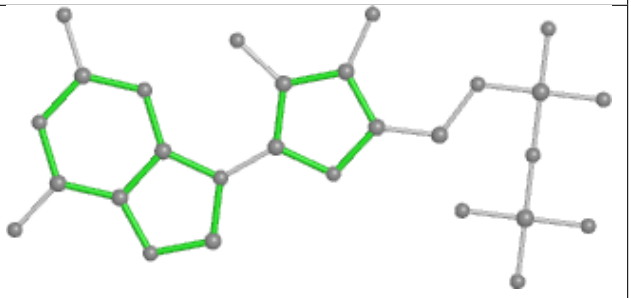
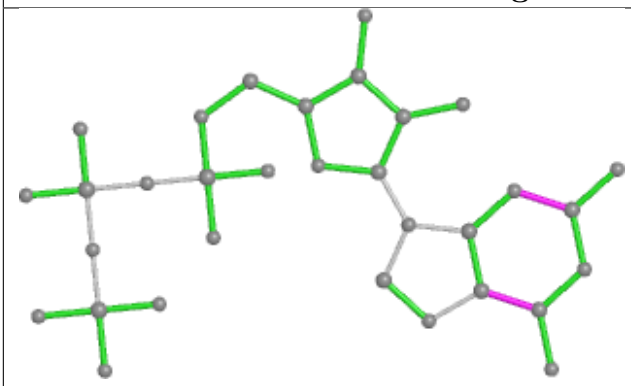


Rings

Ligand GTP LA 501



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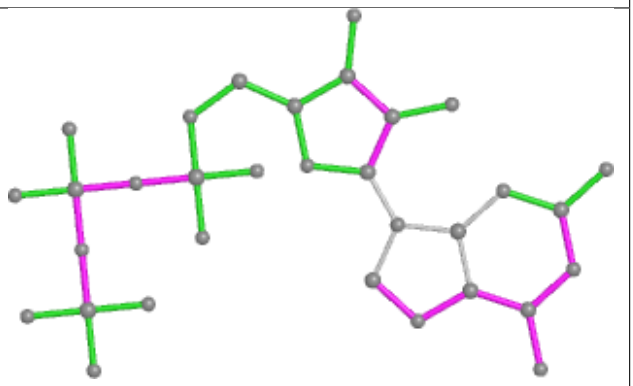
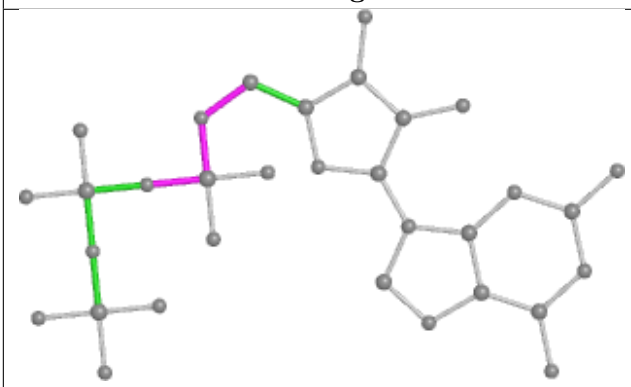
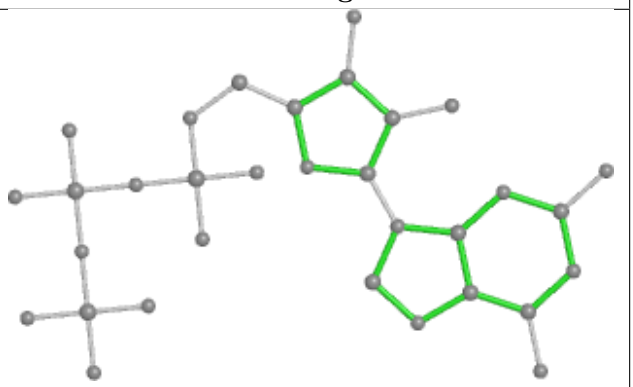


Bond angles

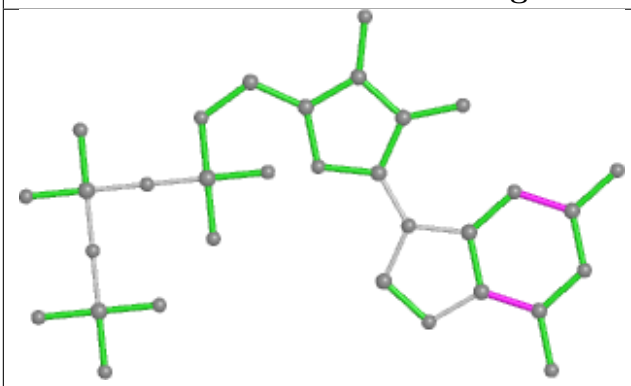


Torsions

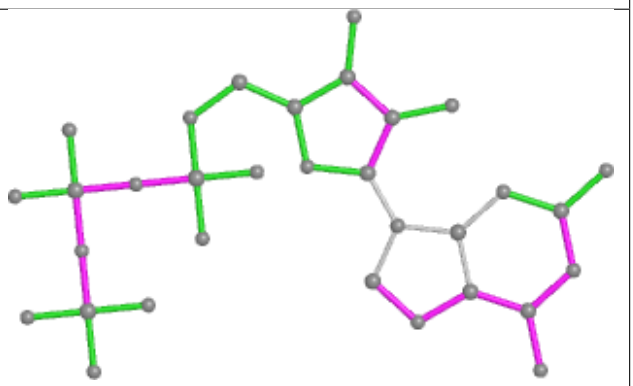


Rings

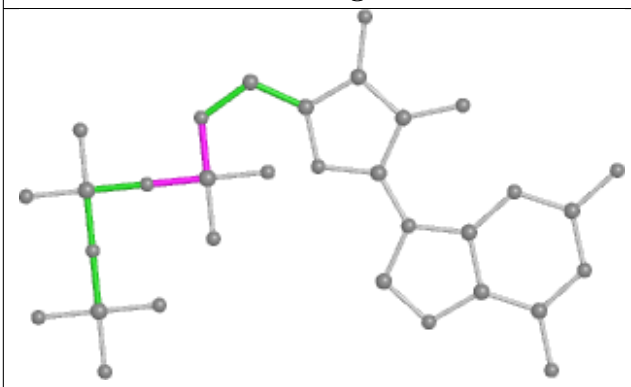
Ligand GTP AE 501



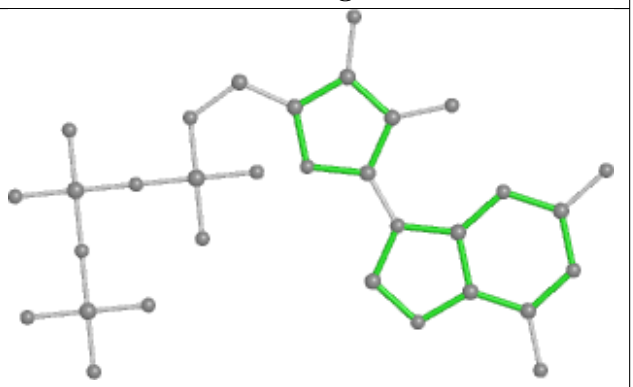
Bond lengths



Bond angles

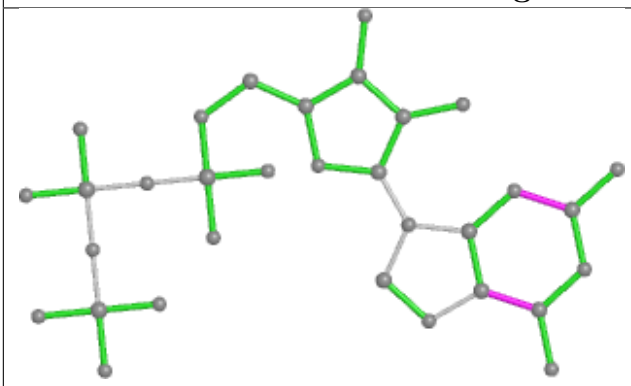


Torsions

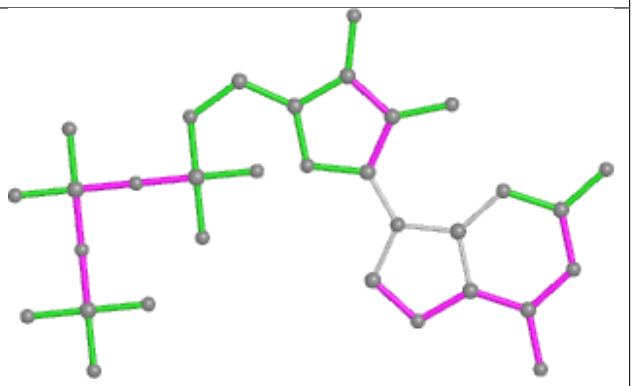


Rings

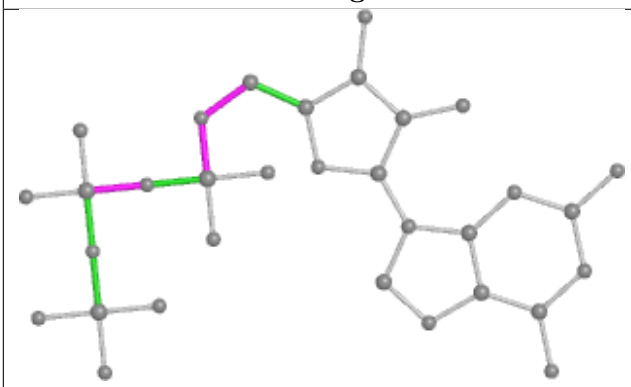
Ligand GTP JC 501



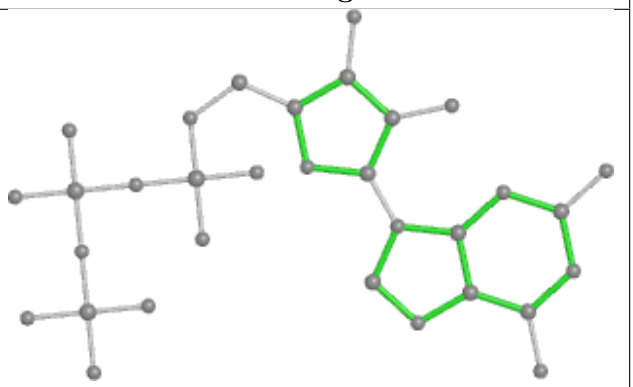
Bond lengths



Bond angles

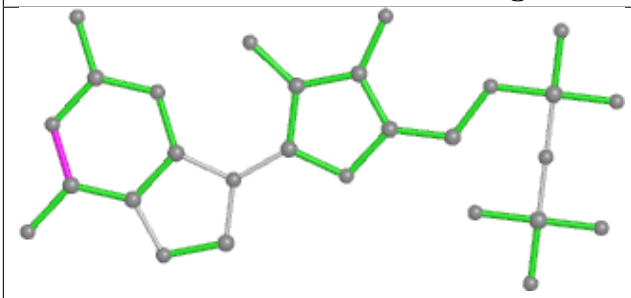


Torsions

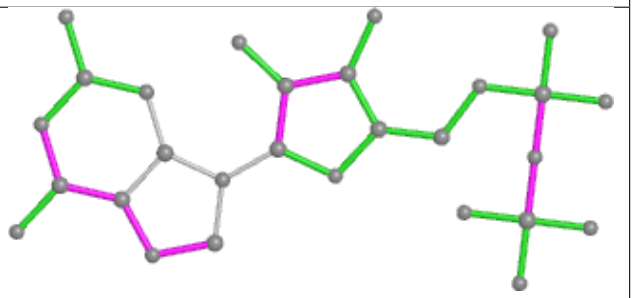


Rings

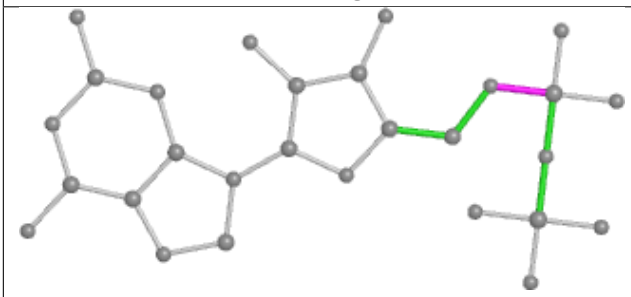
Ligand GDP FH 501



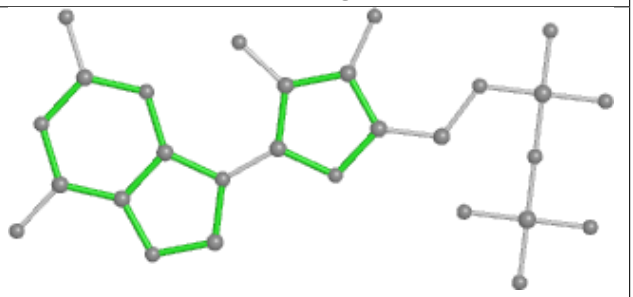
Bond lengths



Bond angles

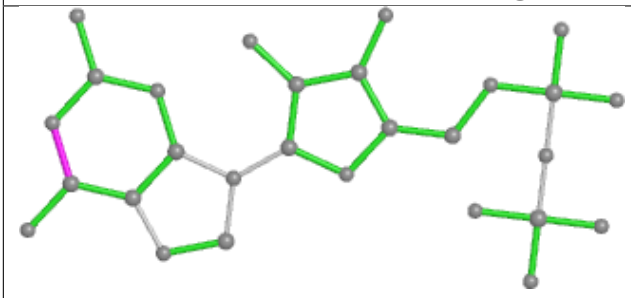


Torsions

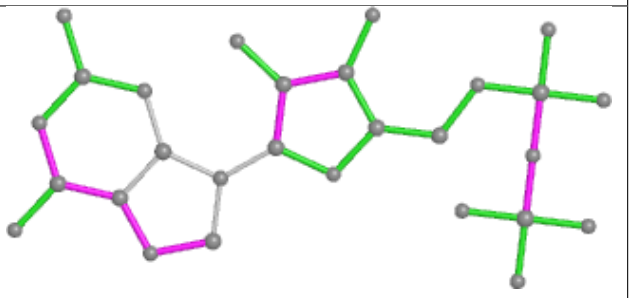


Rings

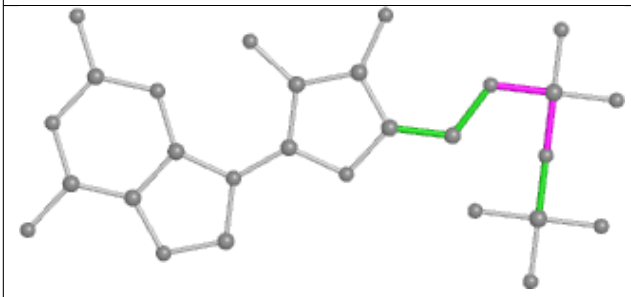
Ligand GDP JD 501



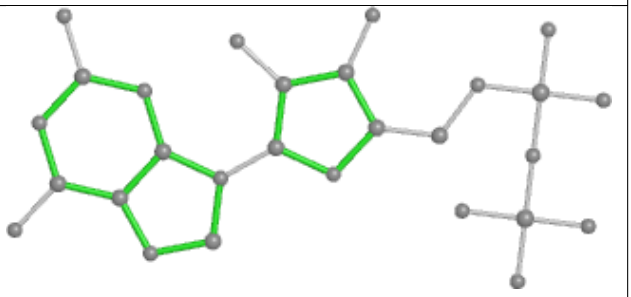
Bond lengths



Bond angles

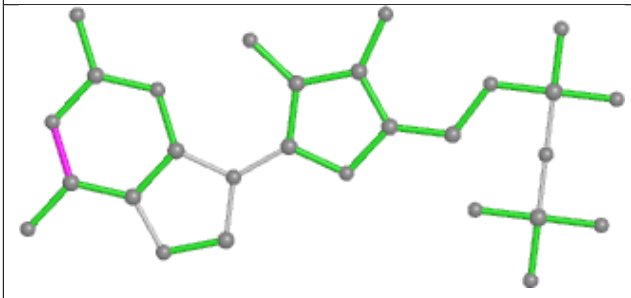


Torsions

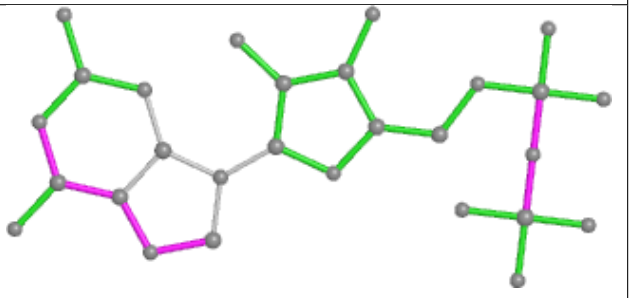


Rings

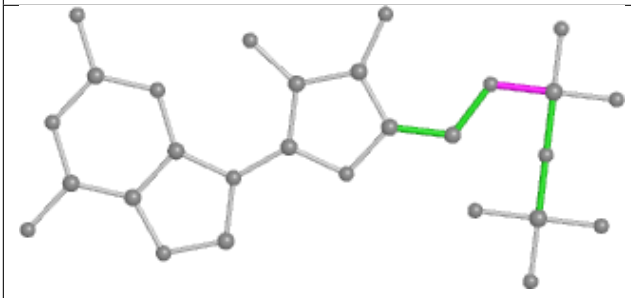
Ligand GDP EF 501



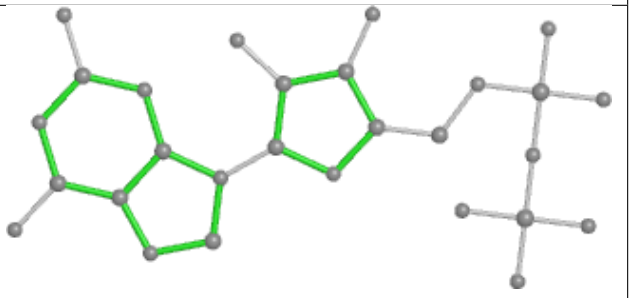
Bond lengths



Bond angles

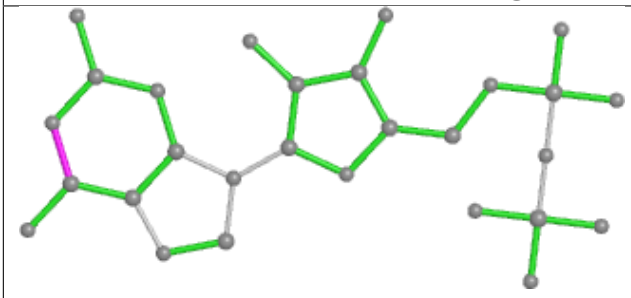


Torsions

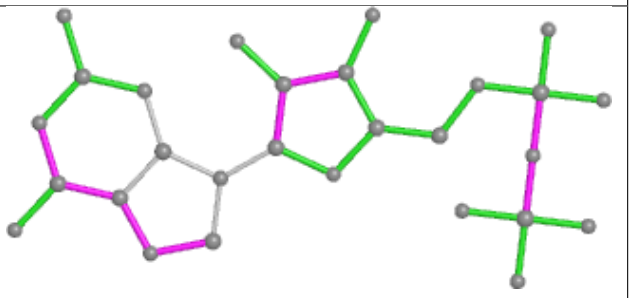


Rings

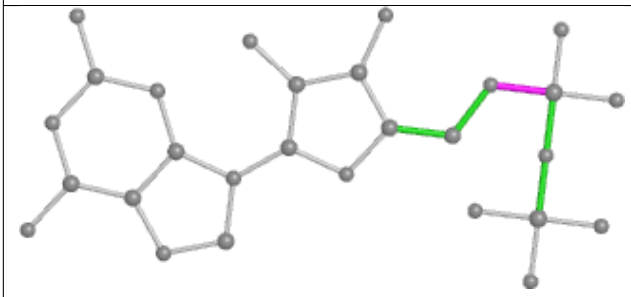
Ligand GDP AB 501



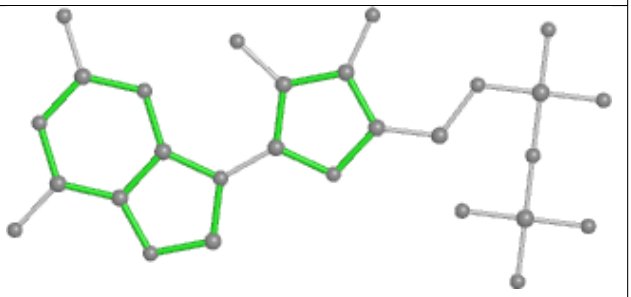
Bond lengths



Bond angles

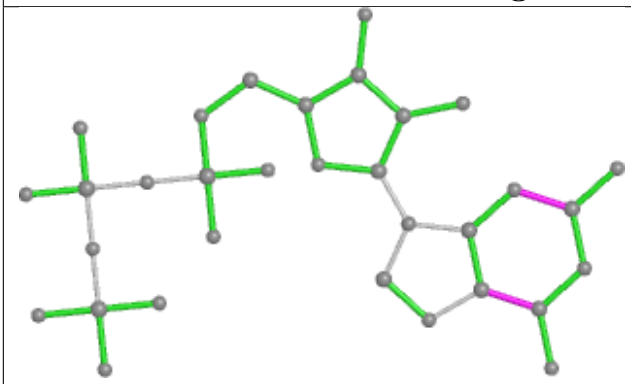


Torsions

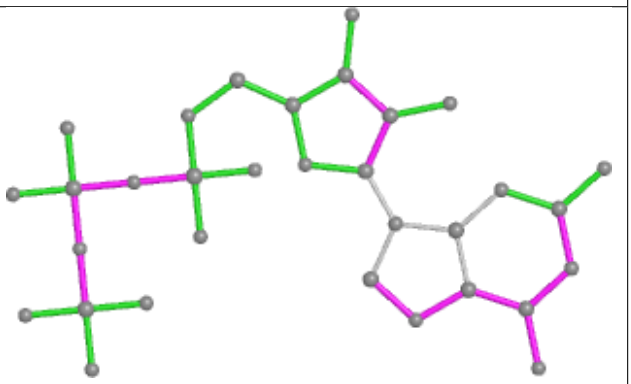


Rings

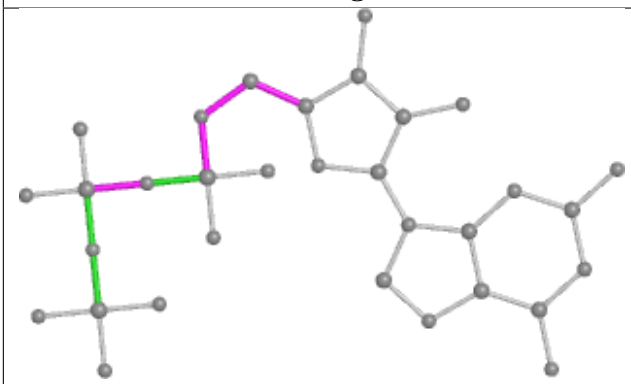
Ligand GTP HE 501



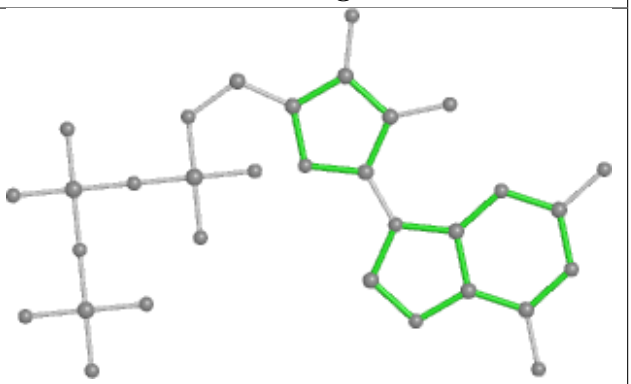
Bond lengths



Bond angles

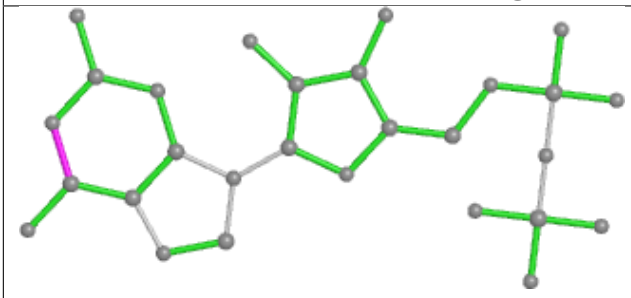


Torsions

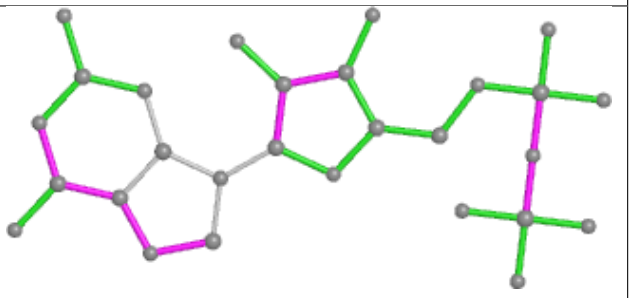


Rings

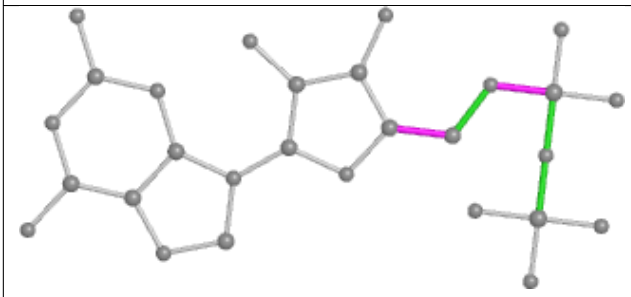
Ligand GDP ED 501



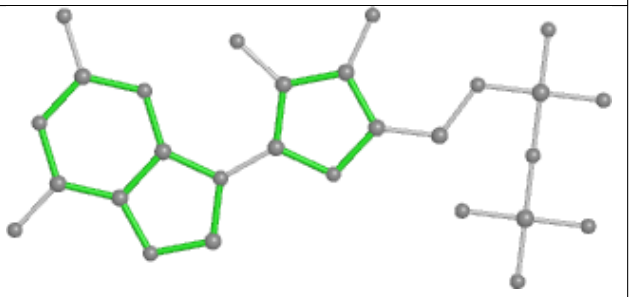
Bond lengths



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.

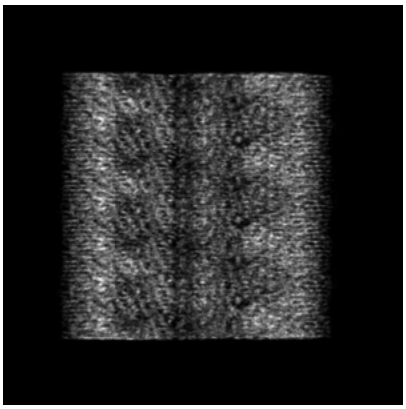
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26611. These allow visual inspection of the internal detail of the map and identification of artifacts.

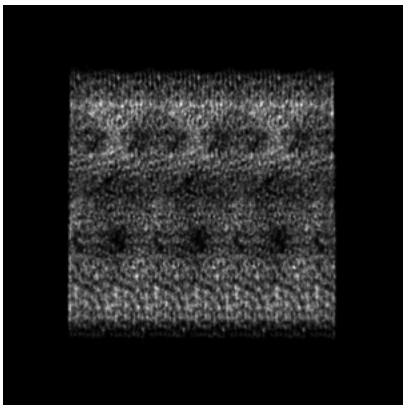
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

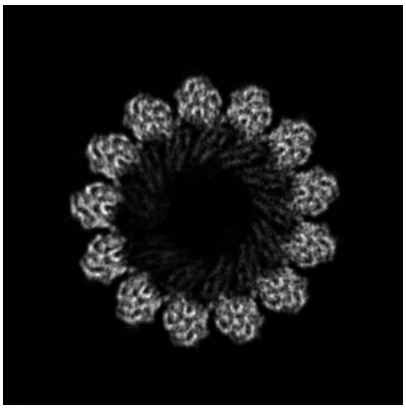
6.1.1 Primary map



X

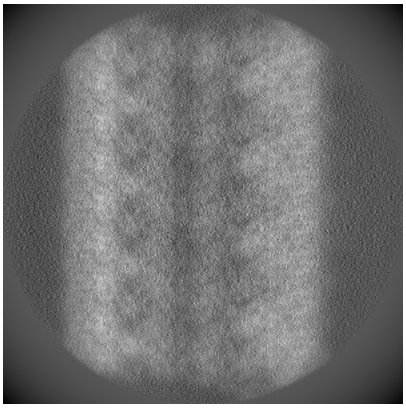


Y

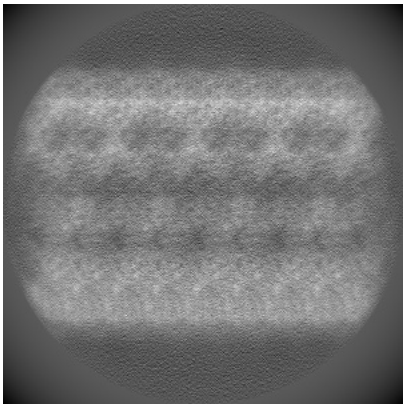


Z

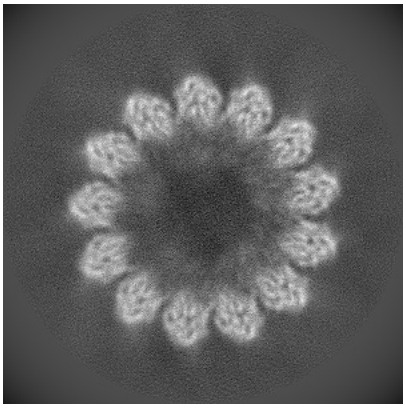
6.1.2 Raw map



X



Y



Z

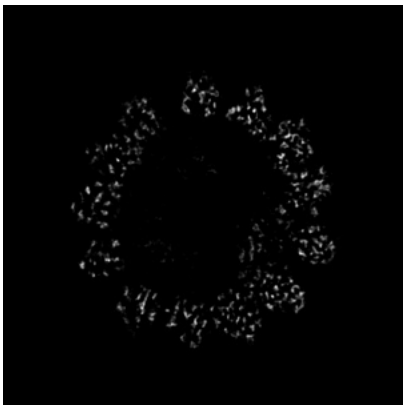
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

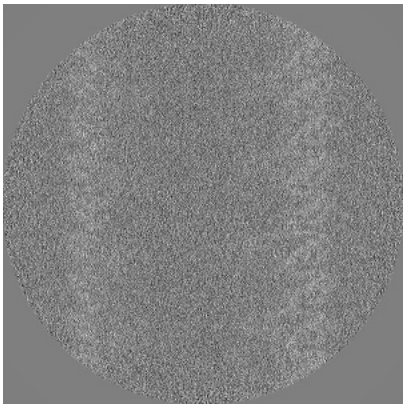
X Index: 240

Y Index: 240

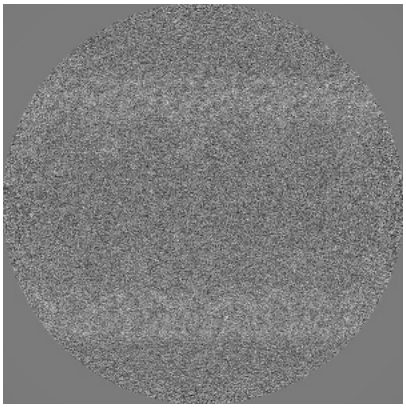


Z Index: 240

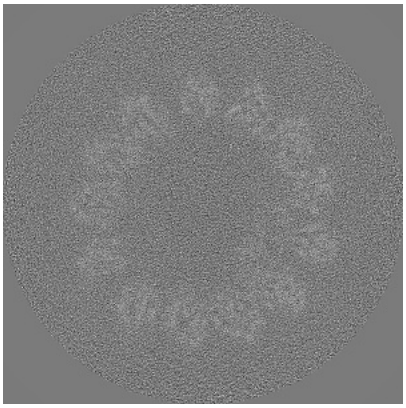
6.2.2 Raw map



X Index: 240



Y Index: 240



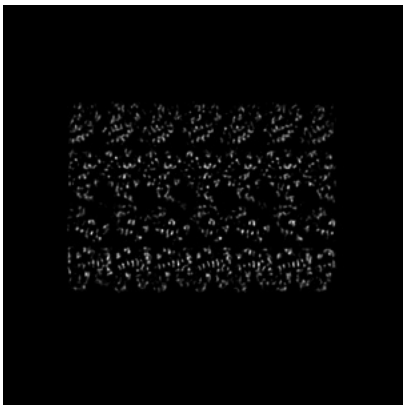
Z Index: 240

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

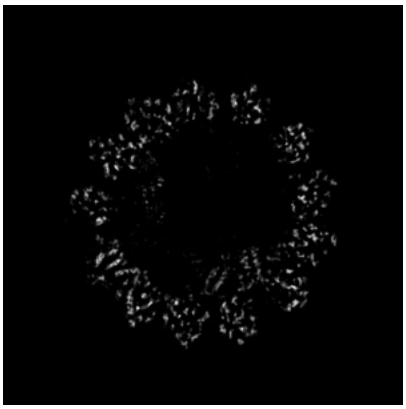
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 359

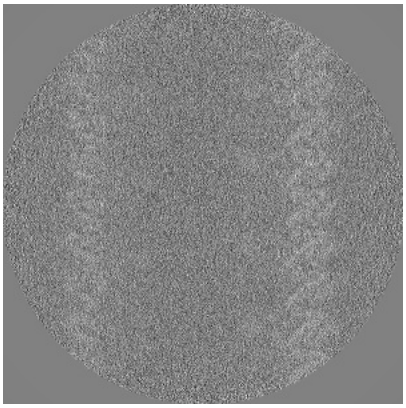


Y Index: 118

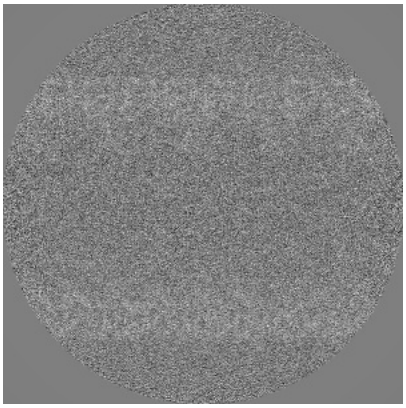


Z Index: 160

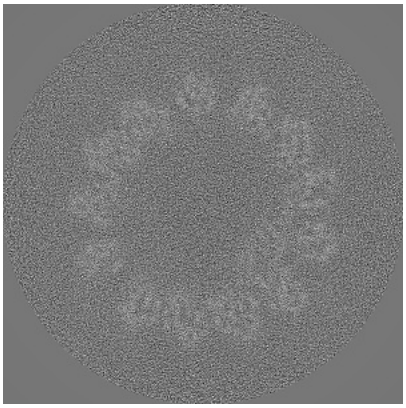
6.3.2 Raw map



X Index: 238



Y Index: 239

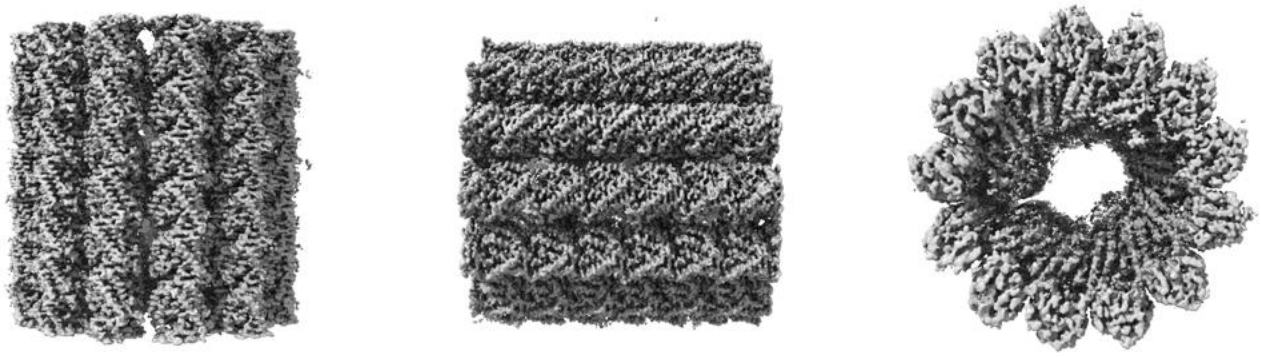


Z Index: 244

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

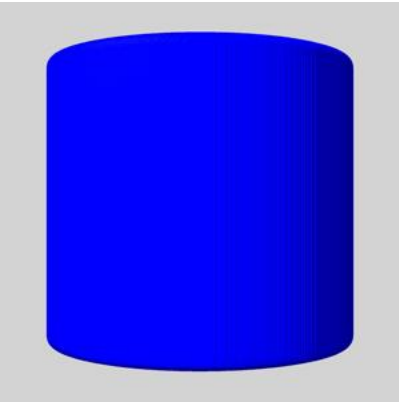
6.5 Mask visualisation (i)

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

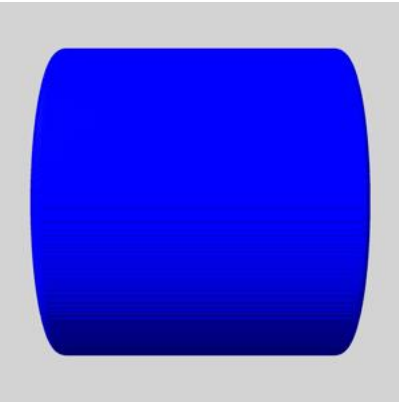
A mask typically either:

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

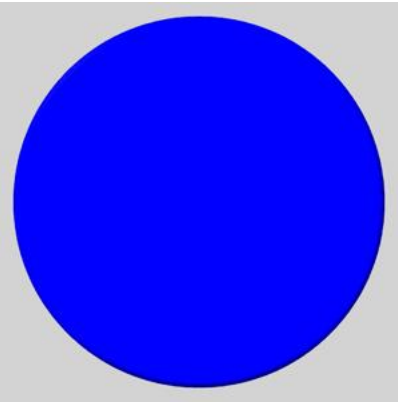
6.5.1 emd_26611_msk_1.map (i)



X



Y

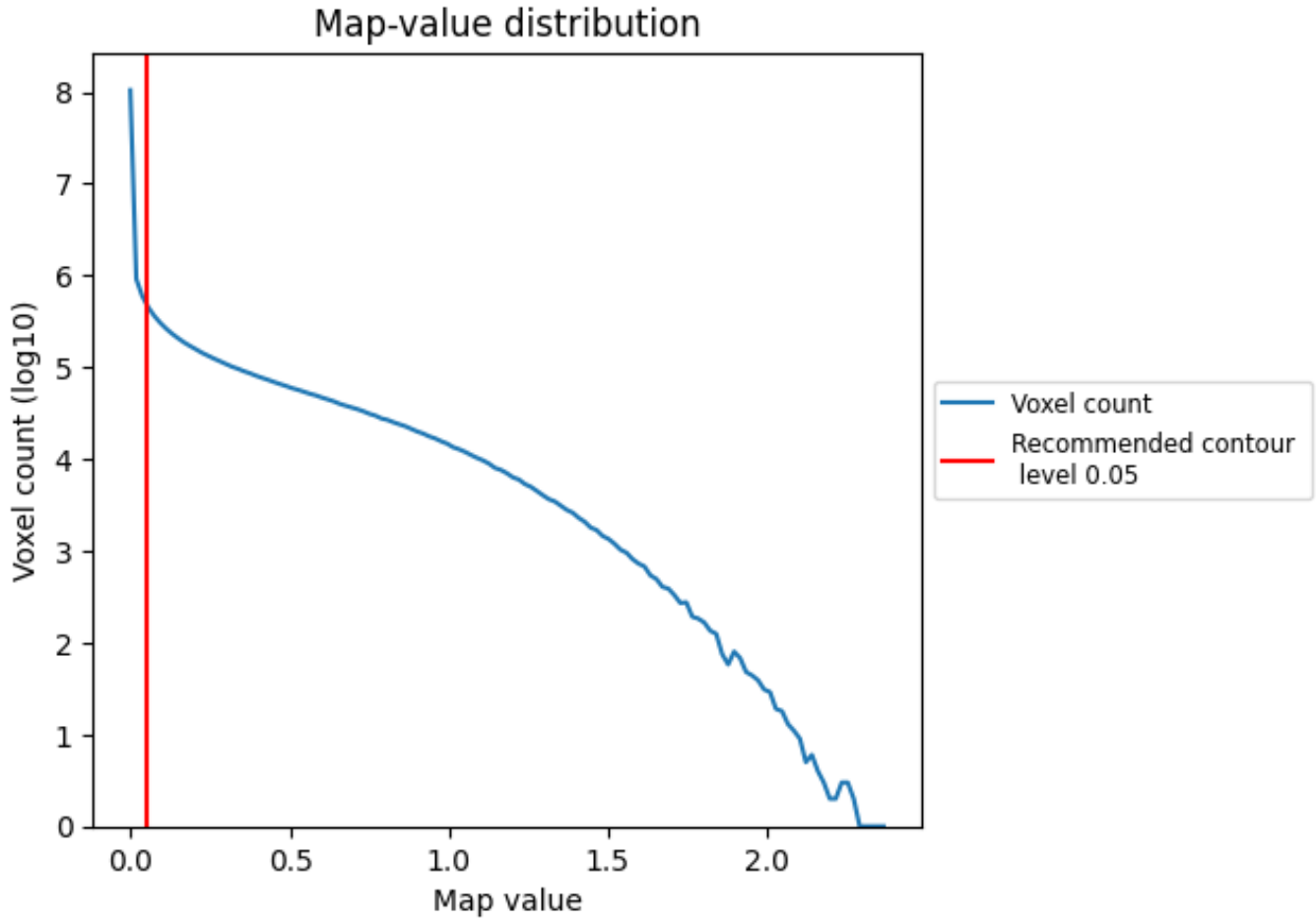


Z

7 Map analysis

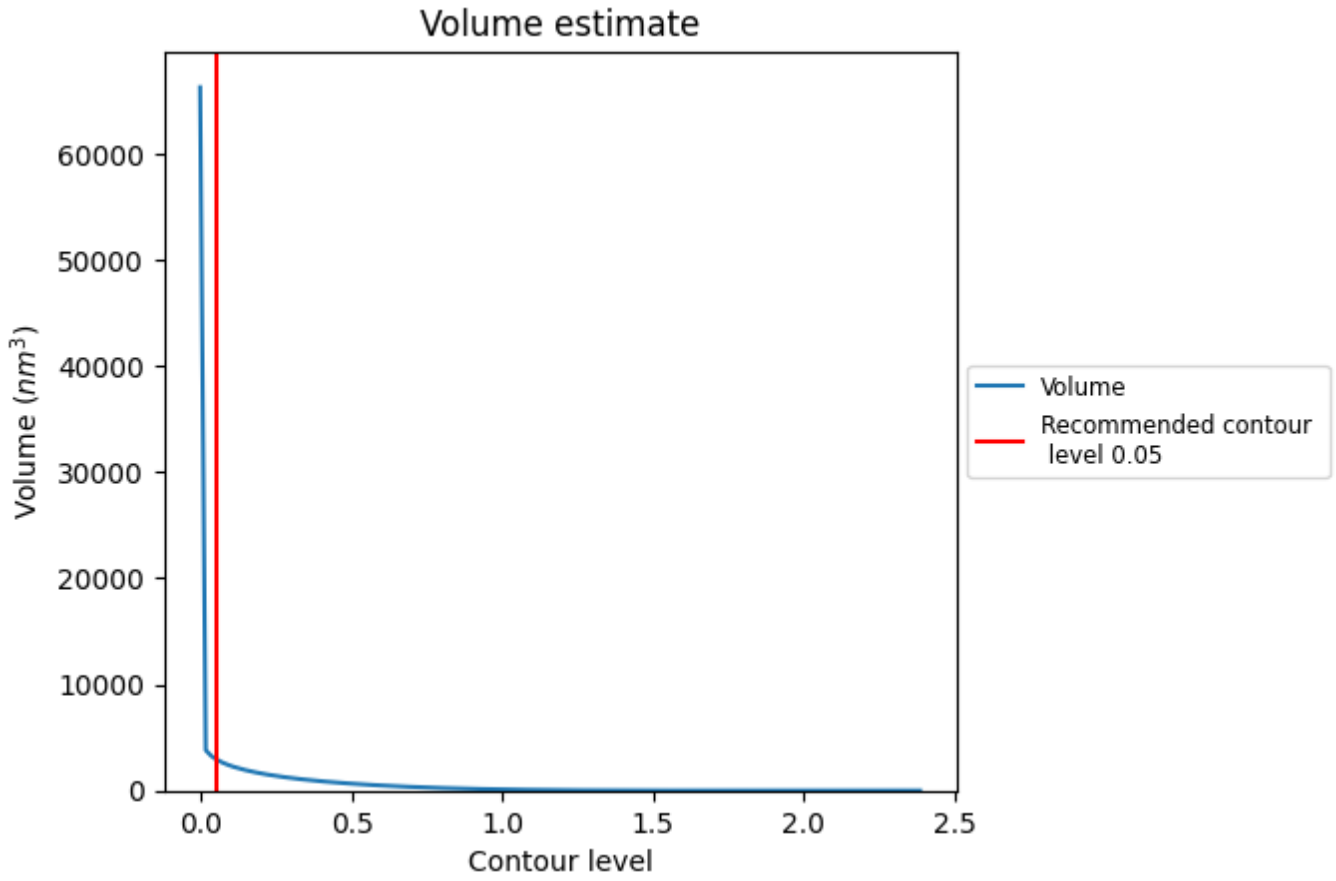
This section contains the results of statistical analysis of the map.

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.

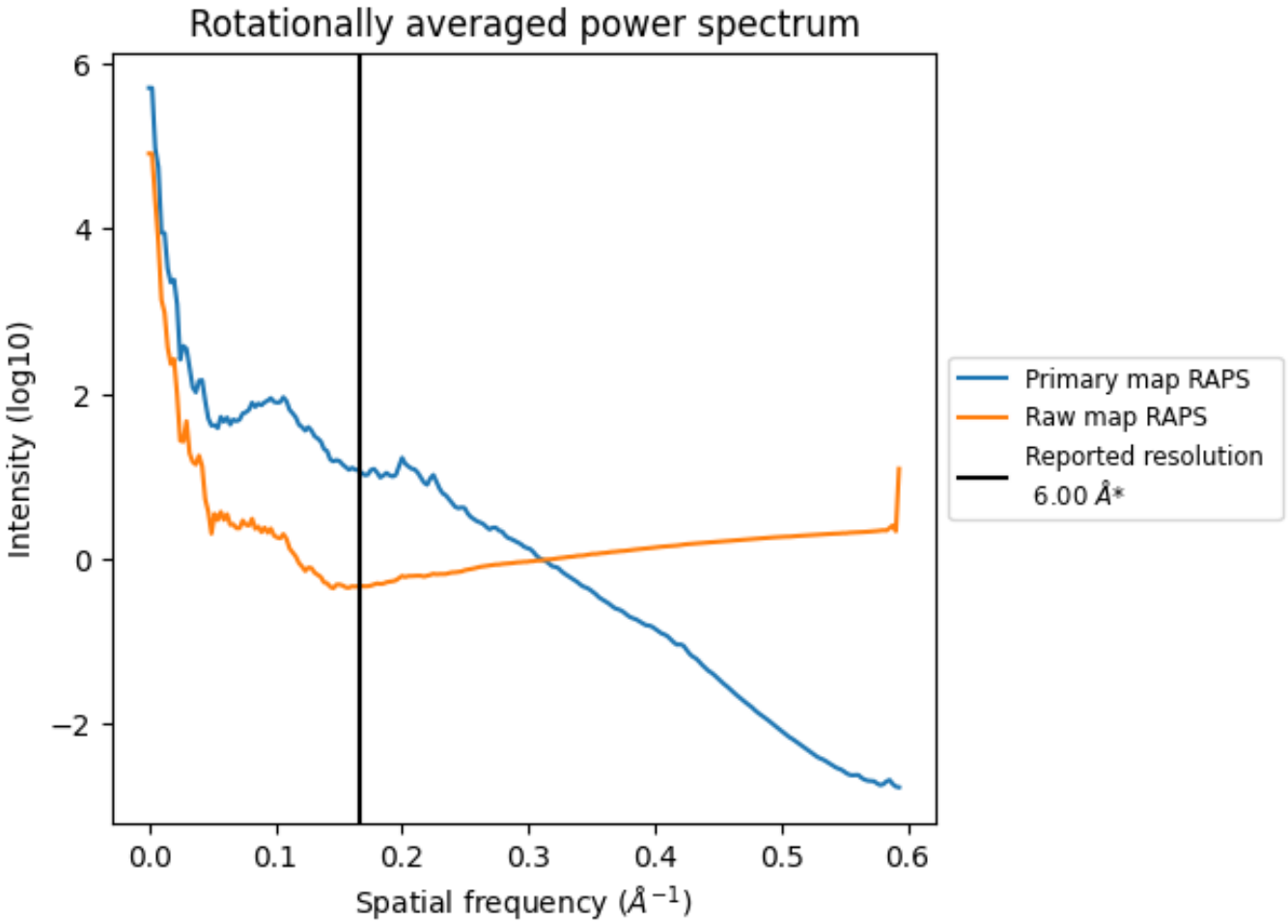
7.2 Volume estimate



The volume at the recommended contour level is 2981 nm^3; this corresponds to an approximate mass of 2692 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)

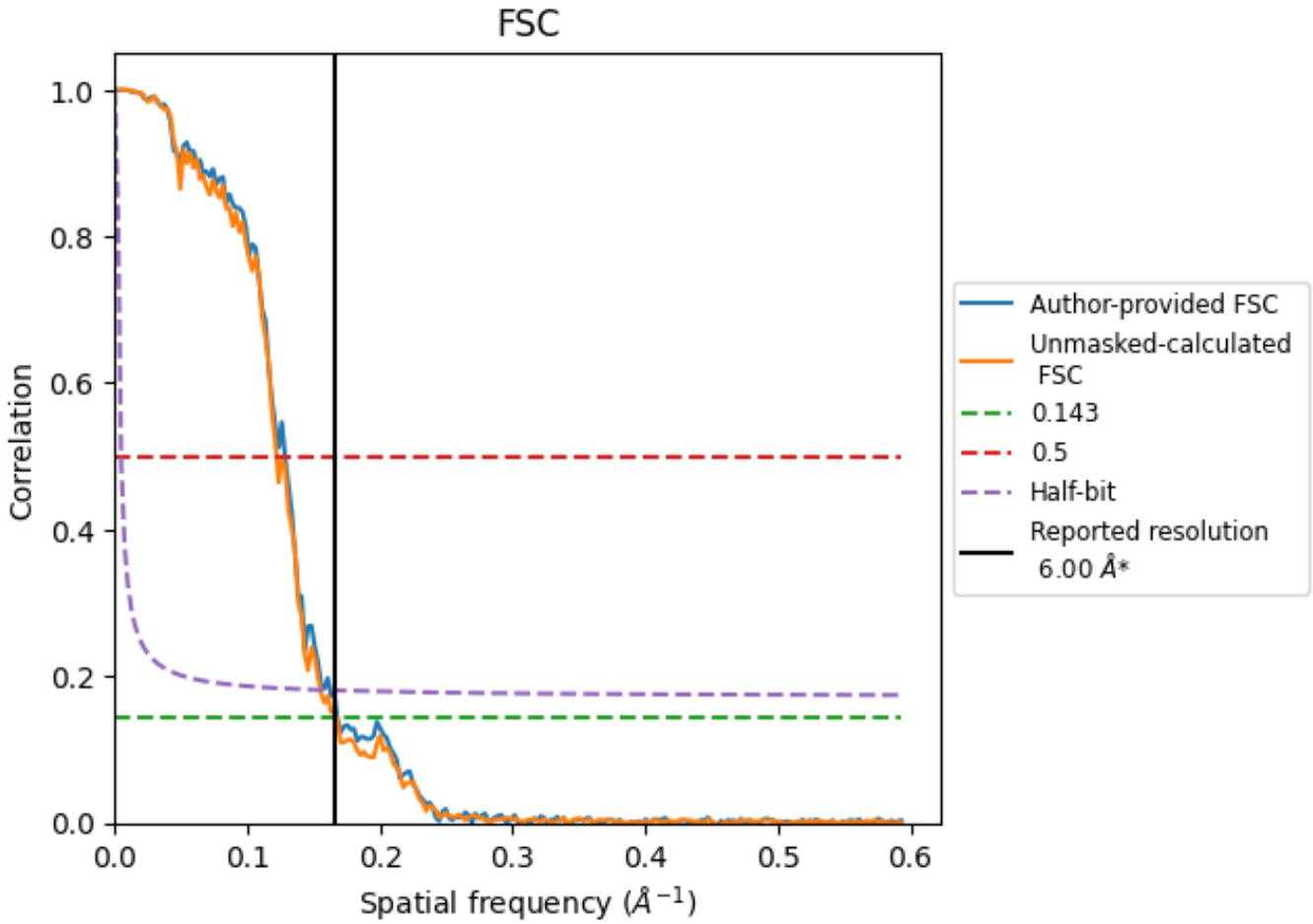


*Reported resolution corresponds to spatial frequency of 0.167 Å^{-1}

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 0.167 Å^{-1}

8.2 Resolution estimates (i)

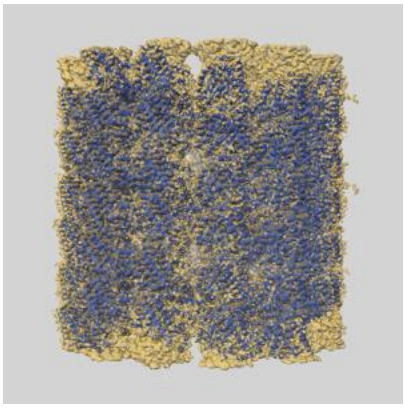
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	5.96	7.79	6.16
Unmasked-calculated*	5.98	8.20	6.45

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

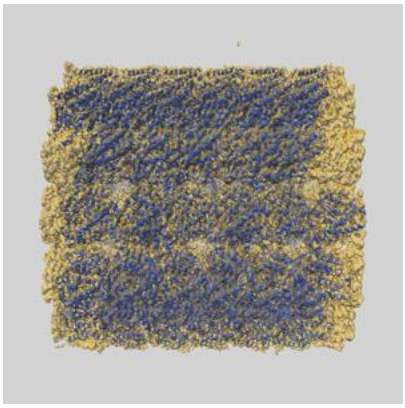
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26611 and PDB model 7UN1. Per-residue inclusion information can be found in section 3 on page 20.

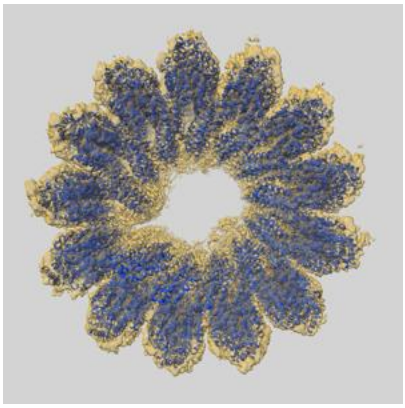
9.1 Map-model overlay



X



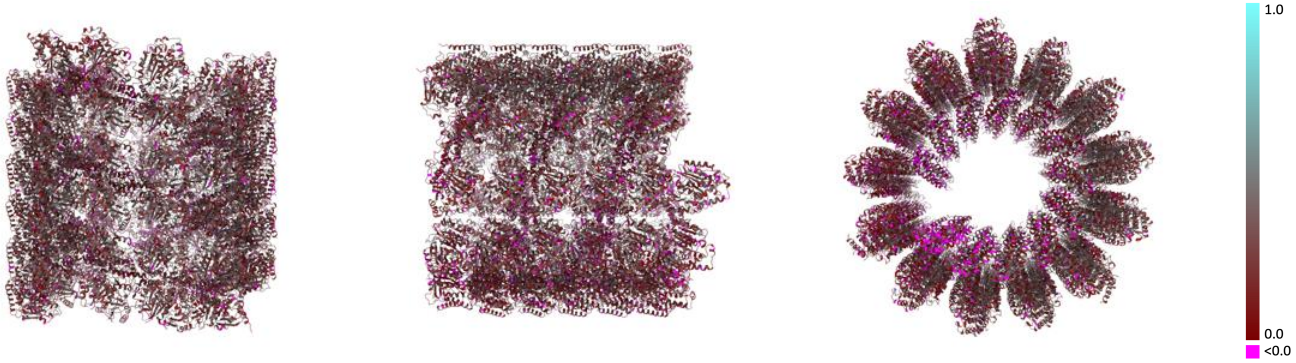
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

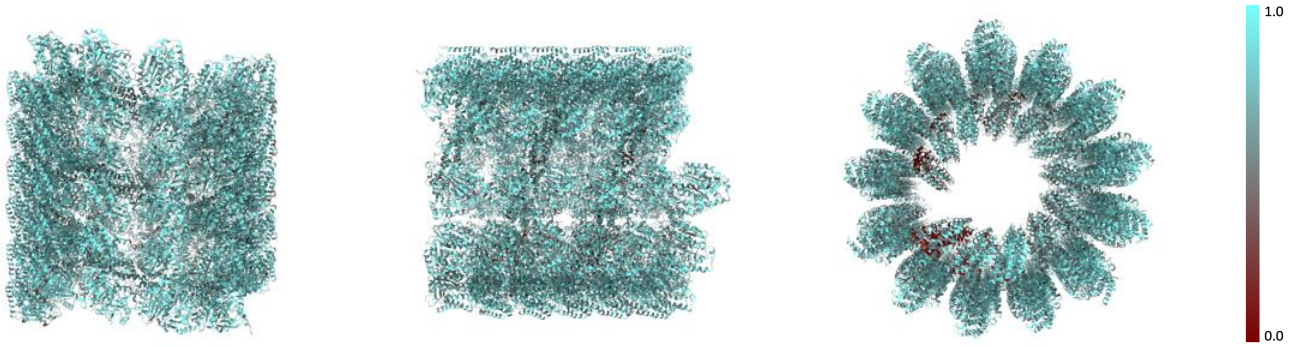
9.2 Q-score mapped to coordinate model (i)



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.

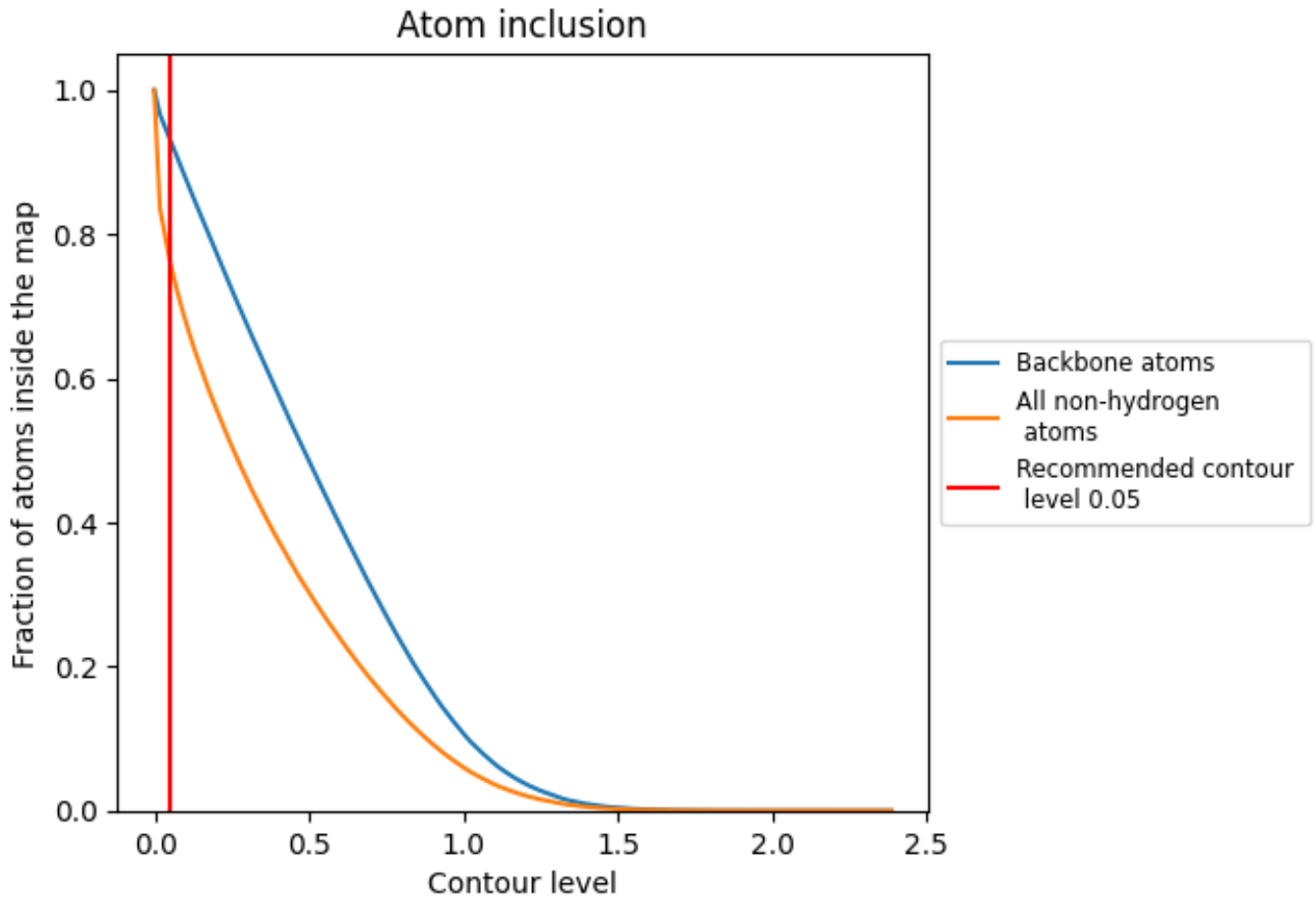
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 76% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7606	0.2540
A	0.4033	0.0620
AB	0.7898	0.2920
AC	0.7980	0.2980
AD	0.8033	0.3010
AE	0.8026	0.2950
AF	0.7814	0.2790
B	0.6181	0.1090
BA	0.7958	0.3010
BC	0.8138	0.3250
BD	0.8057	0.3210
BE	0.8089	0.3180
BF	0.8072	0.3040
BG	0.7873	0.2760
C	0.7697	0.1700
CB	0.7916	0.3000
CC	0.8176	0.3250
CD	0.7991	0.3240
CE	0.8153	0.3330
CF	0.8009	0.3120
CG	0.7968	0.3020
D	0.6085	0.1440
DB	0.7843	0.2810
DC	0.8025	0.3180
DD	0.8081	0.3220
DE	0.7983	0.3180
DF	0.8080	0.3130
DG	0.7935	0.2890
E	0.6835	0.1840
EB	0.7798	0.2850
EC	0.7863	0.3030
ED	0.8069	0.3020
EE	0.8039	0.3100
EF	0.7934	0.2920
EG	0.7871	0.2900

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Chain	Atom inclusion	Q-score
F	0.7160	0.1960
FC	0.7822	0.2870
FD	0.7825	0.2930
FE	0.7999	0.3050
FF	0.7904	0.2960
FG	0.7944	0.2880
FH	0.7497	0.2570
G	0.7003	0.2100
GC	0.7599	0.2560
GD	0.7672	0.2730
GE	0.7762	0.2790
GF	0.7605	0.2650
GG	0.7645	0.2570
GH	0.7440	0.2370
H	0.6757	0.1900
HC	0.7514	0.2230
HD	0.7594	0.2430
HE	0.7670	0.2500
HF	0.7588	0.2420
HG	0.7765	0.2490
HH	0.7473	0.2160
I	0.6542	0.1660
IC	0.7223	0.1860
ID	0.7277	0.1950
IE	0.7354	0.2120
IF	0.7331	0.2030
IG	0.7469	0.2110
IH	0.7271	0.1840
J	0.8230	0.2300
JC	0.7316	0.1860
JD	0.7467	0.2110
JE	0.7415	0.2020
JF	0.7446	0.2140
JG	0.7367	0.1920
K	0.6877	0.1610
KC	0.7554	0.2210
KD	0.7594	0.2250
KE	0.7548	0.2450
KF	0.7590	0.2210
KG	0.7626	0.2290
KH	0.7378	0.2000
L	0.4311	0.0510

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Chain	Atom inclusion	Q-score
LA	0.7565	0.2360
LB	0.7759	0.2510
LC	0.7673	0.2550
LD	0.7732	0.2640
LE	0.7523	0.2410
LF	0.7542	0.2280
M	0.4849	0.0630
MA	0.7590	0.2560
MB	0.7675	0.2620
MC	0.7706	0.2690
MD	0.7699	0.2630
ME	0.7744	0.2700
MF	0.7717	0.2510
N	0.7294	0.1880
O	0.7513	0.2030
P	0.6069	0.1340
Q	0.6895	0.1970
R	0.6953	0.1950
S	0.7123	0.2180
T	0.6900	0.1780
U	0.6645	0.1820
V	0.8104	0.2280
W	0.7030	0.1940
X	0.3392	0.0160
d	0.6442	0.1400
e	0.6862	0.1880
f	0.7088	0.2040
g	0.6940	0.2040
h	0.6945	0.1950
i	0.6701	0.1830
j	0.8243	0.2460
k	0.7017	0.1810
l	0.4418	0.0520