



## Full wwPDB EM Validation Report ⓘ

Jun 1, 2024 – 01:47 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

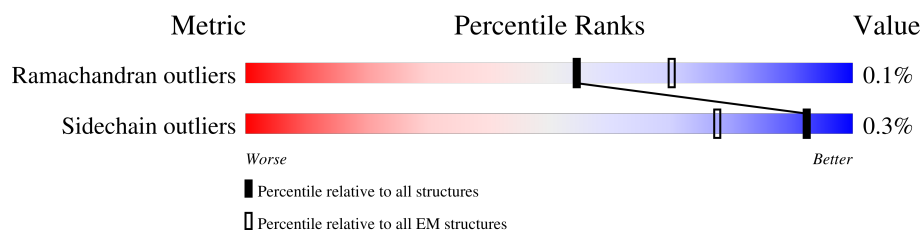
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  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

# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	222	<div> <div>44%</div> <div>72%</div> <div>28%</div> </div>
1	B	222	<div> <div>23%</div> <div>72%</div> <div>28%</div> </div>
1	C	222	<div> <div>13%</div> <div>71%</div> <div>29%</div> </div>
1	D	222	<div> <div>13%</div> <div>71%</div> <div>28%</div> </div>
1	E	222	<div> <div>9%</div> <div>72%</div> <div>28%</div> </div>
1	F	222	<div> <div>5%</div> <div>69%</div> <div>29%</div> </div>
1	G	222	<div> <div>8%</div> <div>72%</div> <div>28%</div> </div>
1	H	222	<div> <div>6%</div> <div>72%</div> <div>28%</div> </div>
1	I	222	<div> <div>7%</div> <div>72%</div> <div>28%</div> </div>

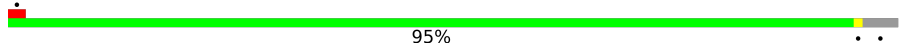
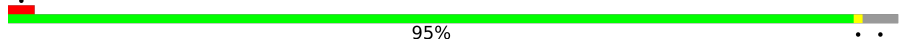
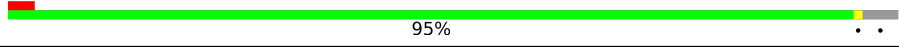
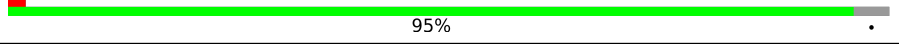
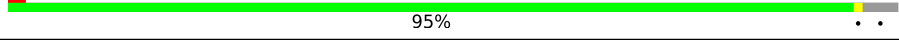
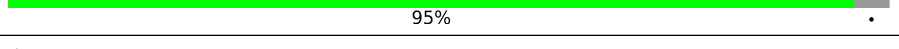
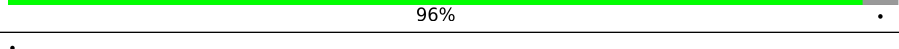
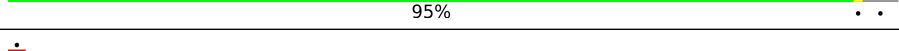
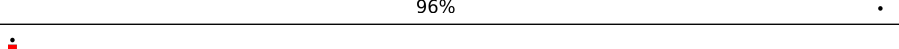
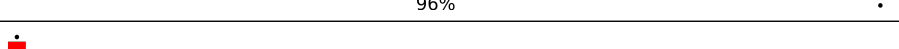
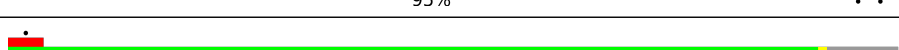
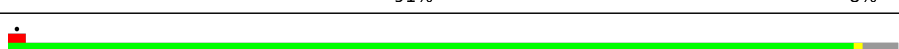
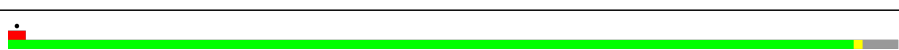
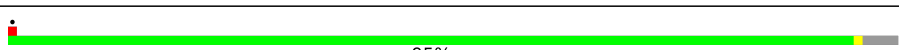
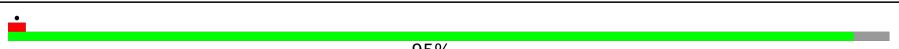

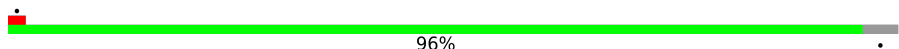
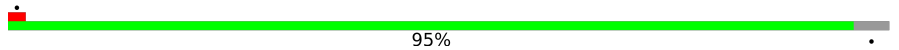
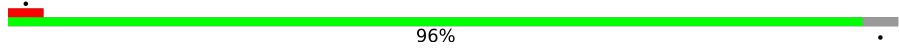
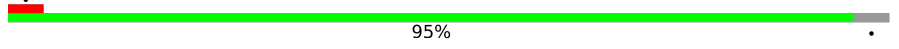
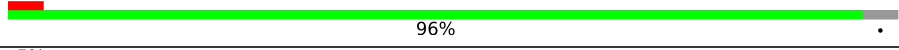
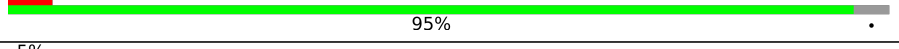
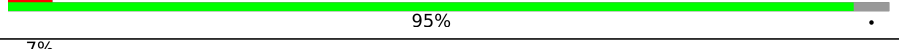
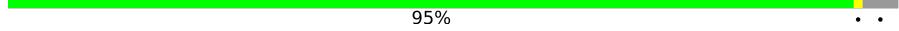

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Mol	Chain	Length	Quality of chain
1	J	222	7% 72% 28%
1	K	222	18% 72% 28%
1	L	222	41% 72% 28%
1	M	222	38% 72% 28%
1	N	222	13% 70% 30%
1	O	222	13% 72% 28%
1	P	222	11% 72% 28%
1	Q	222	10% 71% 29%
1	R	222	5% 72% 28%
1	S	222	6% 70% 30%
1	T	222	5% 72% 28%
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%

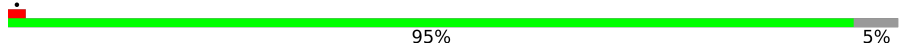
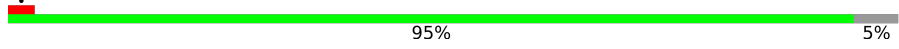
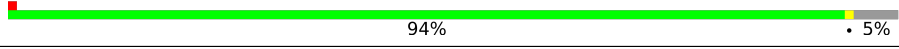
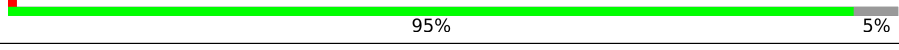
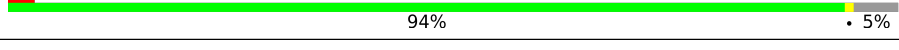
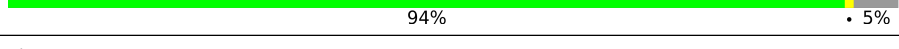
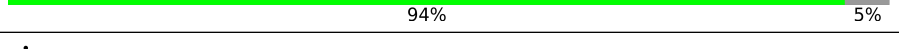
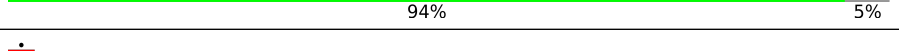
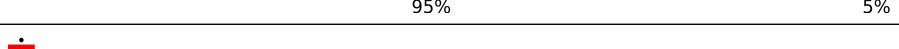
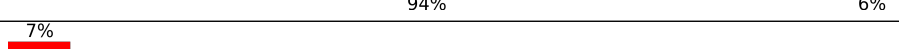
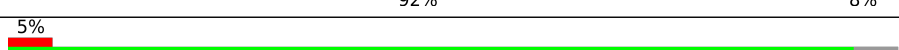
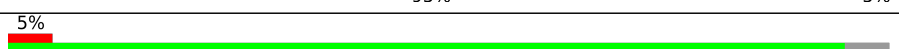
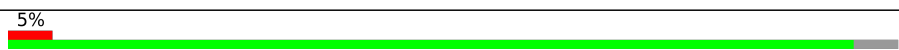
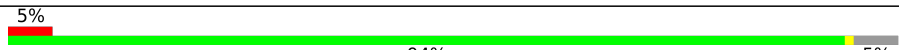
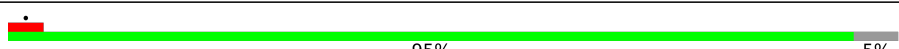
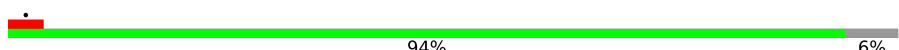
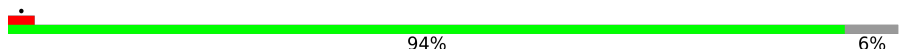
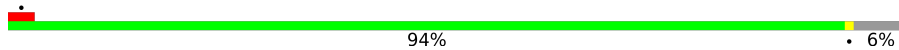
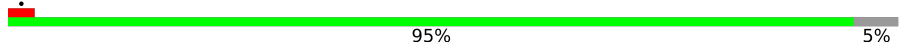
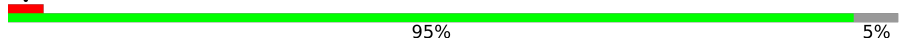
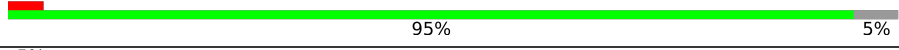
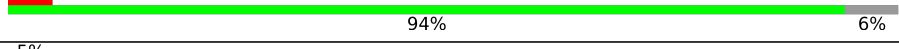
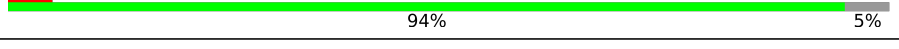


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Mol	Chain	Length	Quality of chain
2	IH	445	
2	JD	445	
2	JF	445	
2	KD	445	
2	KF	445	
2	KH	445	
2	LB	445	
2	LD	445	
2	LF	445	
2	MB	445	
2	MD	445	
2	MF	445	
3	AC	451	
3	AE	451	
3	BC	451	
3	BE	451	
3	BG	451	
3	CC	451	
3	CE	451	
3	CG	451	
3	DC	451	
3	DE	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	 92% 8% 7%
3	IE	451	 95% 5% 5%
3	IG	451	 94% 5% 5%
3	JC	451	 95% 5% 5%
3	JE	451	 94% 5% 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	 94% 6% 5%
3	MC	451	 94% 5% 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		0	0
			796	476	160	160			
1	B	160	Total	C	N	O		0	0
			796	476	160	160			
1	C	158	Total	C	N	O		0	0
			786	470	158	158			
1	D	160	Total	C	N	O	S	0	0
			1289	805	231	243	10		
1	E	160	Total	C	N	O	S	0	0
			1289	805	231	243	10		
1	F	157	Total	C	N	O	S	0	0
			1263	788	225	240	10		
1	G	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	H	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	I	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	J	159	Total	C	N	O		0	0
			791	473	159	159			
1	K	159	Total	C	N	O		0	0
			791	473	159	159			
1	L	159	Total	C	N	O		0	0
			791	473	159	159			
1	M	160	Total	C	N	O		0	0
			796	476	160	160			
1	N	156	Total	C	N	O		0	0
			776	464	156	156			
1	O	160	Total	C	N	O		0	0
			796	476	160	160			
1	P	160	Total	C	N	O	S	0	0
			1289	805	231	243	10		
1	Q	157	Total	C	N	O	S	0	0
			1263	788	225	240	10		

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

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

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

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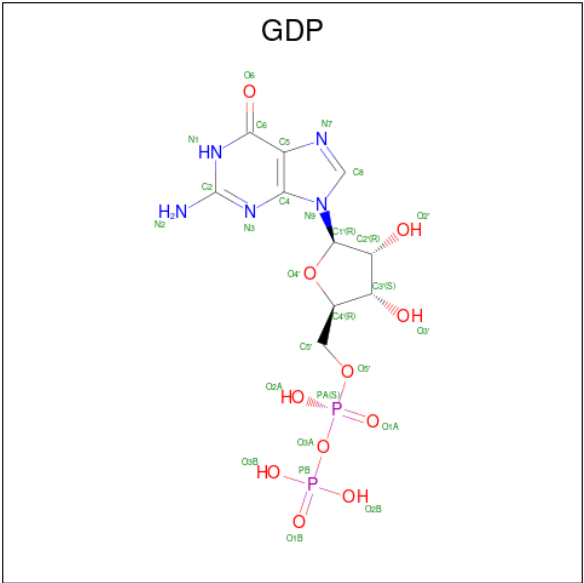
Mol	Chain	Residues	Atoms					AltConf	Trace
3	CC	430	Total 3369	C 2136	N 573	O 638	S 22	0	0
3	CE	431	Total 3377	C 2140	N 574	O 641	S 22	0	0
3	CG	429	Total 3363	C 2133	N 572	O 636	S 22	0	0
3	DC	428	Total 3357	C 2130	N 571	O 634	S 22	0	0
3	DE	428	Total 3357	C 2130	N 571	O 634	S 22	0	0
3	DG	429	Total 3363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

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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<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

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

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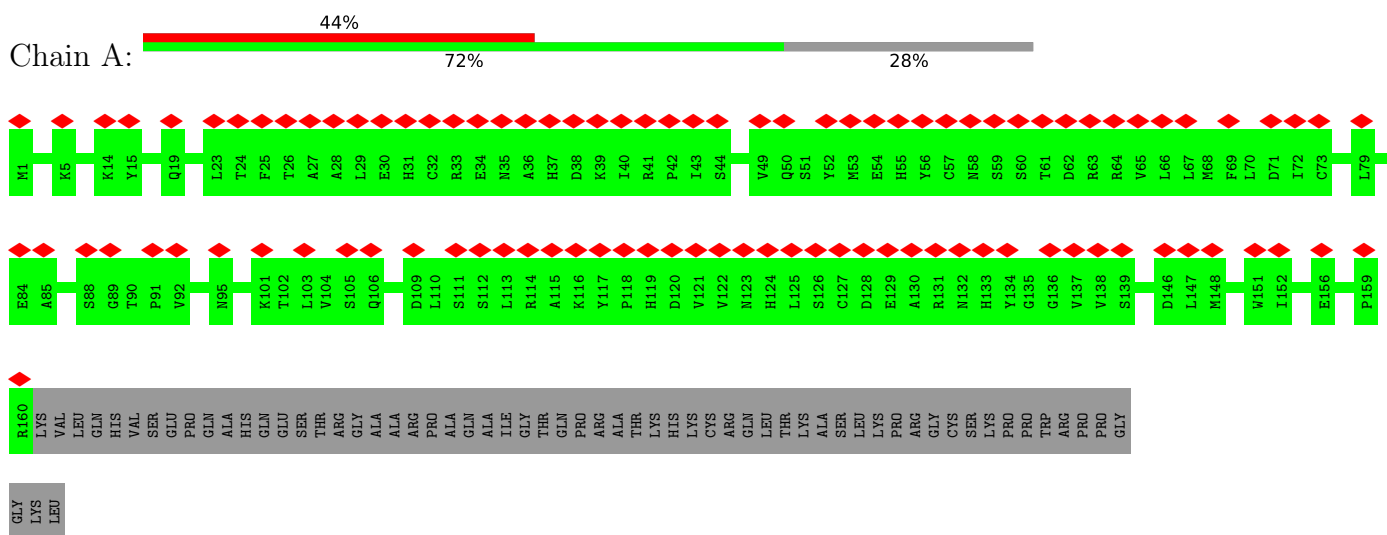
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	ME	1	1	1	0

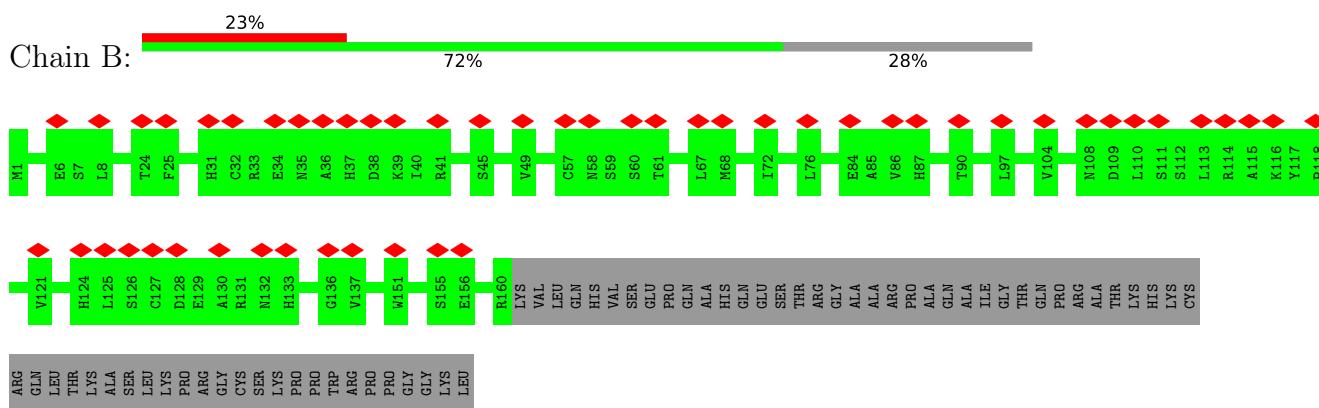
### 3 Residue-property plots

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.

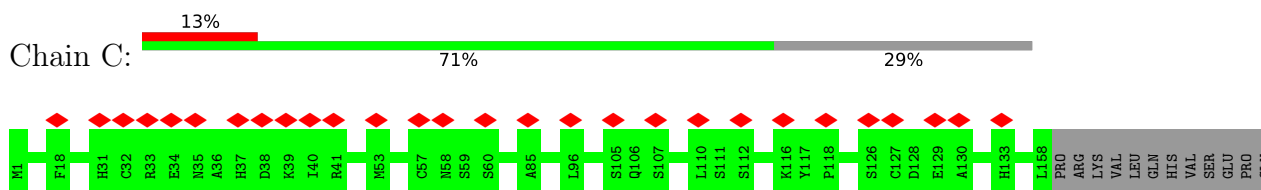
- Molecule 1: Sperm acrosome-associated protein 9



- Molecule 1: Sperm acrosome-associated protein 9



- Molecule 1: Sperm acrosome-associated protein 9



ALA HIS  
GLN GLN  
THR SER  
THR THR  
GLY ARG  
GLY  
ALA  
ALA  
ARG  
PRO  
PRO  
ALA  
ALA  
GLN  
GLN  
TLE  
TLE  
GLY  
THR  
THR  
GLN  
PRO  
ARG  
ALA  
ALA  
THR  
LYS  
LYS  
HIS  
LYS  
CYS  
ARG  
GLN  
LEU  
THR  
LYS  
LYS  
SER  
LEU  
LEU  
LYS  
PRO  
PRO  
ARG  
GLY  
CYS  
SER  
LYS  
PRO  
PRO  
TRP  
ARG  
PRO  
PRO  
GLY  
GLY  
LYS  
LEU

• Molecule 1: Sperm acrosome-associated protein 9

Chain D: 13% 71% 28%

H1 N2 E3 Q21 E30 R33 E34 N35 A36 H37 D38 K39 I40 R41 Y52 C57 N58 S59 R63 L67 E84 H87 S88 L110 A115 D120 A130 R131 N132 E156 K157 L158 P159 R160 LYS VAL LEU GLN HIS VAL SER GLU PRO GLN HIS

GLN  
GLU  
SER  
THR  
ARG  
GLY  
ALA  
ALA  
ARG  
PRO  
PRO  
ALA  
ALA  
GLN  
TLE  
TLE  
GLY  
THR  
GLN  
PRO  
PRO  
ARG  
ALA  
ALA  
THR  
LYS  
HIS  
LYS  
CYS  
ARG  
GLN  
LEU  
THR  
LYS  
SER  
LEU  
LYS  
PRO  
PRO  
ARG  
GLY  
CYS  
SER  
LYS  
PRO  
PRO  
TRP  
ARG  
PRO  
PRO  
GLY  
LYS  
LEU

• Molecule 1: Sperm acrosome-associated protein 9

Chain E: 9% 72% 28%

H1 L8 T24 H31 H37 D38 K39 I40 L43 Y52 H55 S60 T61 L79 A95 N95 L113 H119 R131 G136 K157 L158 P159 R160 LYS VAL LEU GLN HIS VAL SER GLU PRO GLN HIS

ARG  
PRO  
ALA  
GLN  
TLE  
GLY  
THR  
GLN  
GLN  
PRO  
ARG  
ALA  
ALA  
THR  
LYS  
HIS  
CYS  
ARG  
GLN  
LEU  
THR  
LYS  
ALA  
SER  
LEU  
LYS  
LYS  
PRO  
ARG  
GLY  
CYS  
SER  
LYS  
PRO  
TRP  
PRO  
PRO  
GLY  
LYS  
LEU

• Molecule 1: Sperm acrosome-associated protein 9

Chain F: 5% 69% 29%

H1 N2 C32 R33 H37 D38 K39 R41 Q48 L67 G89 S111 D120 N123 L147 K157 LEU PRO ARG LYS VAL LEU GLN HIS VAL SER GLU PRO GLN ALA HIS GLN GLU THR ARG GLY ALA ARG PRO GLN ALA TLE GLY THR GLN PRO

ARG  
ALA  
THR  
LYS  
HIS  
CYS  
ARG  
GLN  
LEU  
THR  
LYS  
LYS  
ALA  
SER  
LEU  
LYS  
PRO  
ARG  
GLY  
CYS  
SER  
PRO  
PRO  
TRP  
ARG  
PRO  
GLY  
LYS  
LEU

• Molecule 1: Sperm acrosome-associated protein 9

Chain G: 8% 72% 28%

H1 E12 A28 H31 H37 R41 H55 N58 D71 K73 A85 L97 H119 C127 R131 L147 H154 L158 P159 ARG LYS VAL LEU GLN HIS VAL SER GLU PRO GLN ALA HIS GLN GLU THR ARG GLY ALA ARG PRO GLN ALA TLE GLY THR GLN PRO

GLN  
ALA  
TLE  
GLY  
THR  
GLN  
PRO  
ARG  
ALA  
THR  
LYS  
HIS  
CYS  
ARG  
GLN  
LEU  
THR  
ALA  
SER  
LEU  
LYS  
LYS  
PRO  
ARG  
GLY  
CYS  
SER  
PRO  
PRO  
TRP  
ARG  
PRO  
PRO  
GLY  
LYS  
LEU


• Molecule 1: Sperm acrosome-associated protein 9

Chain H: 6% 72% 28%

H1 R9 A28 E34 H37 I40 C57 F83 E84 A85 L125 S126 C127 D128 E129 A130 E156 P159 ARG LYS VAL LEU GLN HIS VAL SER GLU PRO GLN ALA HIS GLU THR SER THR ARG GLY ALA ARG ALA ARG PRO GLN ALA TLE GLY THR GLN PRO ARG

ALA THR LYS HIS LYS CYS ARG GLN LEU THR LYS ALA SER LEU LYS PRO ARG GLY CYS SER LYS PRO THR ARG PRO PRO GLY GLY LYS LEU

• Molecule 1: Sperm acrosome-associated protein 9

Chain I:  7% 72% 28%

M1 E6 R33 E34 I40 Y52 N58 D62 D71 Q81 E84 A85 N94 N95 S111 L143 D146 P159 ARG LYS VAL LEU GLN HIS VAL SER GLU PRO GLN ALA ALA HIS GLN GLU THR ARG GLY ALA ARG PRO ALA ALA GLN ILE GLY

THR GLN PRO ARG ALA THR LYS HIS LYS CYS ARG GLN LEU THR LYS LYS SER LEU LYS PRO ARG GLY CYS SER LYS PRO THR ARG PRO PRO GLY GLY LYS LEU


• Molecule 1: Sperm acrosome-associated protein 9

Chain J:  7% 72% 28%

M1 A28 E34 D38 K39 I40 G47 N58 S59 S60 T61 T90 S111 M132 K149 E156 K157 L158 P159 ARG LYS VAL LEU GLN HIS VAL SER GLU PRO GLN ALA HIS GLN GLU THR ARG GLY ALA ARG PRO ALA ALA GLN ILE GLY PRO

ARG ALA THR LYS HIS LYS CYS ARG GLN LEU THR LYS ALA SER LEU LYS PRO ARG GLY CYS SER LYS PRO THR ARG PRO PRO GLY GLY LYS LEU

• Molecule 1: Sperm acrosome-associated protein 9

Chain K:  18% 72% 28%

M1 N2 E3 S10 K16 L17 Q21 T24 A28 H31 C32 R33 E34 D38 K39 I40 B41 G47 N58 S59 S60 T61 I67 S74 K78 L79 C80 A85 V86 T93 N94 T102 D109 L110 L113 R114 A115 K116 Y117 P118 H119 R131

M132 Y137 L143 K157 L158 P159 ARG LYS VAL LEU GLN HIS VAL SER GLU PRO GLN ALA HIS GLN GLU THR ARG GLY ALA ALA ARG PRO PRO GLN ILE GLY THR GLN PRO ARG ALA THR LYS HIS LYS CYS ARG GLN LEU THR LYS LYS ALA SER LEU PRO ARG GLY CYS

SER LYS PRO PRO TRP ARG PRO PRO GLY LYS LEU

• Molecule 1: Sperm acrosome-associated protein 9

Chain L:  41% 72% 28%

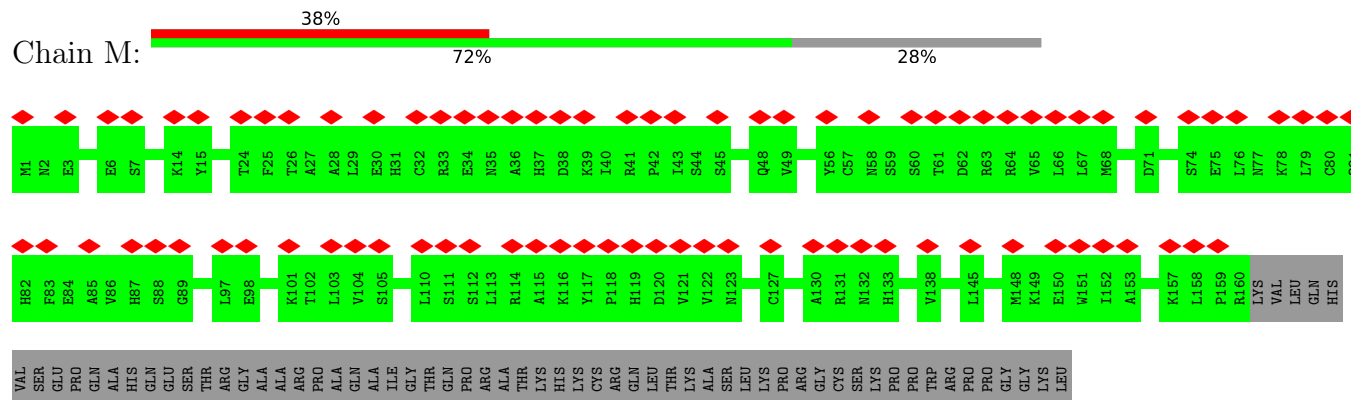
M1 N2 E3 V4 K5 E6 S7 L8 Y15 K16 L17 F18 Q19 Q20 Q21 Q22 Q23 T24 F25 T26 A27 A28 L29 E30 H31 C32 R33 E34 N35 A36 H37 D38 K39 I40 R41 P42 I43 I46 V49 E54 H55 N58 S59 S60 T61 D62 R63 R64 M68 F69 D71 I72 C73

C80 V86 H87 S88 G89 T90 P91 V92 T93 N94 K99 C100 K101 S107 N108 D109 L110 S111 S112 A113 L114 R114 A115 Y117 P118 H119 D120 V121 V122 N123 H124 L125 S126 C127 D128 E129 A130 R131 N132 H133 Y134 G136 L143 I144 L145 D146 W151 I152 A153 H154 S155 E156

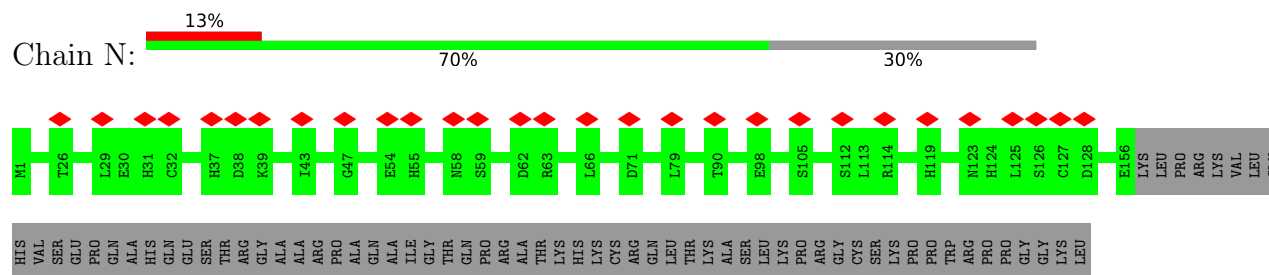
P159 ARG VAL LEU GLN HIS VAL SER GLU PRO GLN GLN ALA HIS GLN GLU THR ARG GLY ALA ARG PRO PRO GLN ILE GLY THR GLN PRO ARG ALA THR LYS HIS LYS CYS ARG GLN GLU LEU THR LYS LYS SER LEU LYS PRO ARG GLY CYS SER LYS PRO TRP PRO

GLY  
GLY  
LYS  
LEU

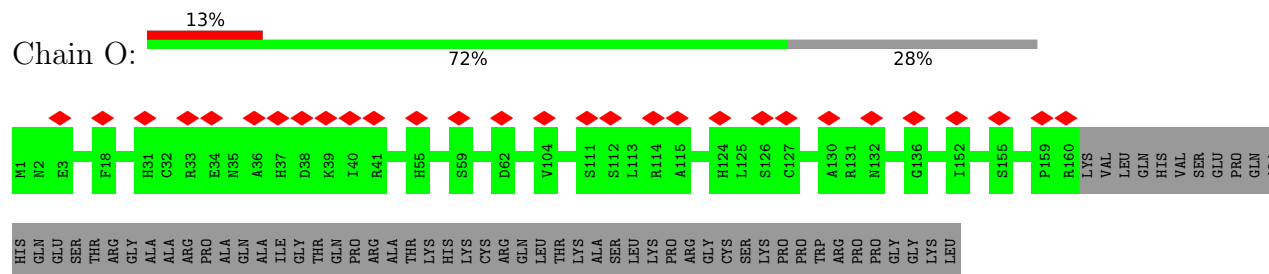
• Molecule 1: Sperm acrosome-associated protein 9



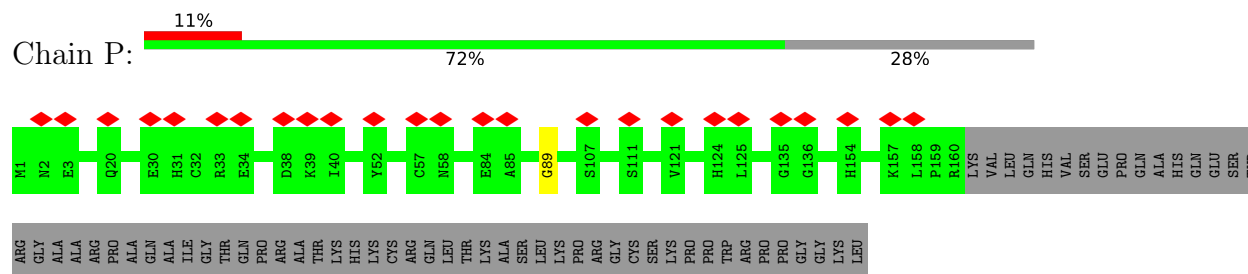
• Molecule 1: Sperm acrosome-associated protein 9



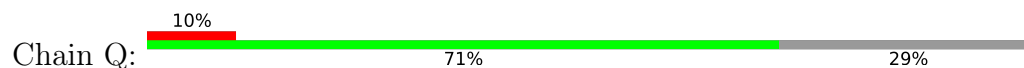
• Molecule 1: Sperm acrosome-associated protein 9

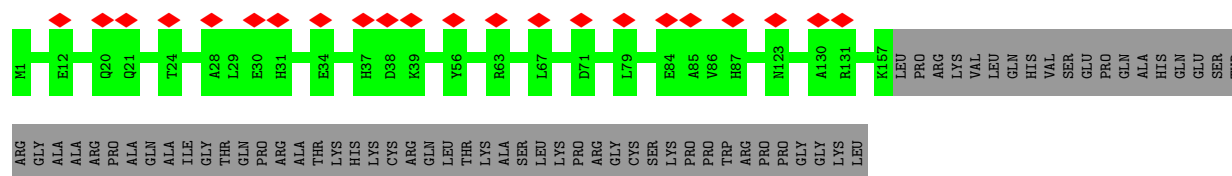


• Molecule 1: Sperm acrosome-associated protein 9

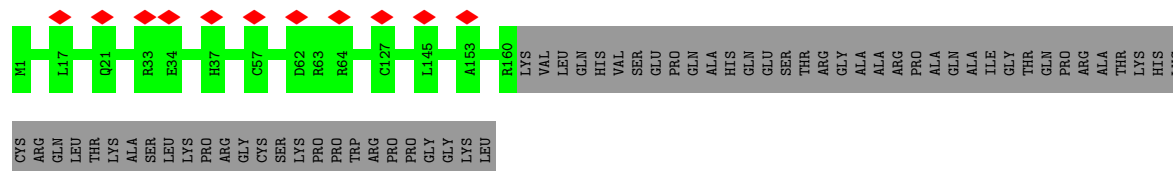
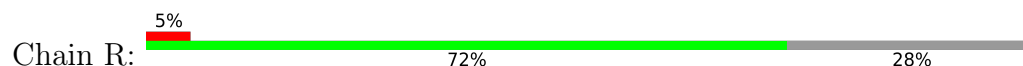


• Molecule 1: Sperm acrosome-associated protein 9

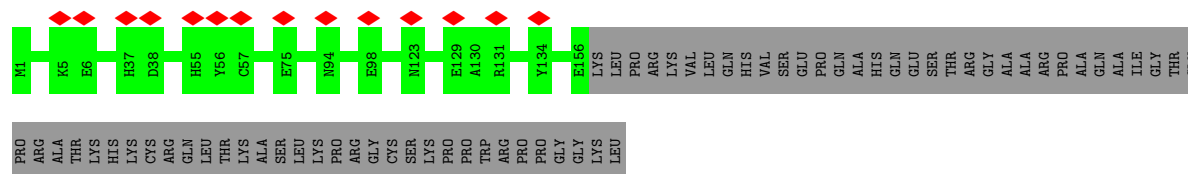




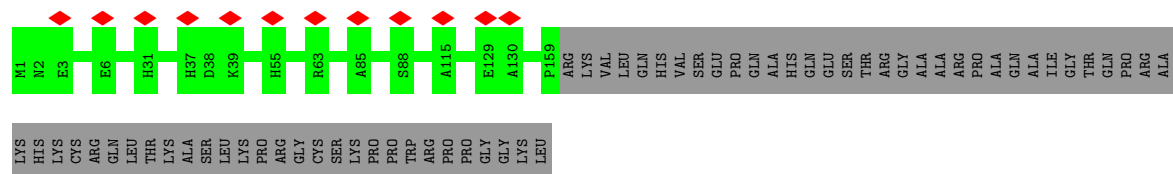
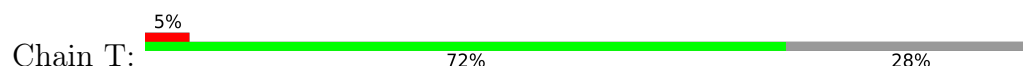
- Molecule 1: Sperm acrosome-associated protein 9



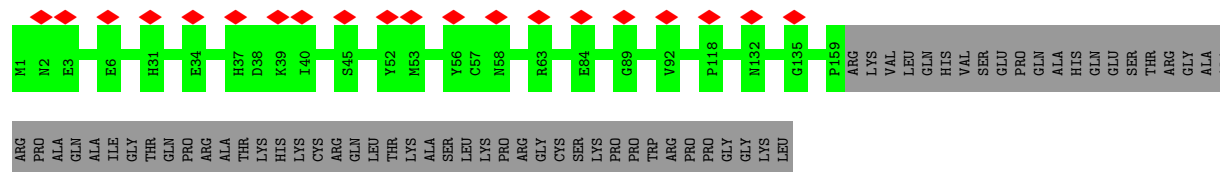
- Molecule 1: Sperm acrosome-associated protein 9



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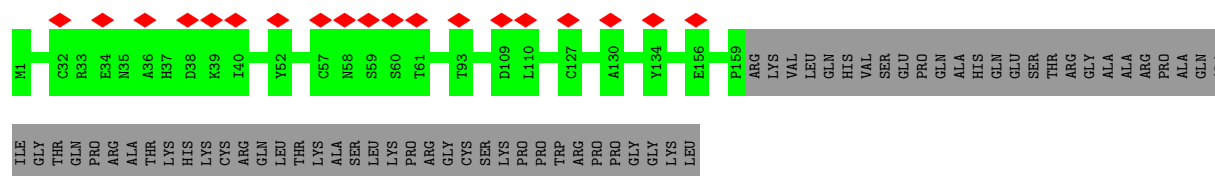
- Molecule 1: Sperm acrosome-associated protein 9



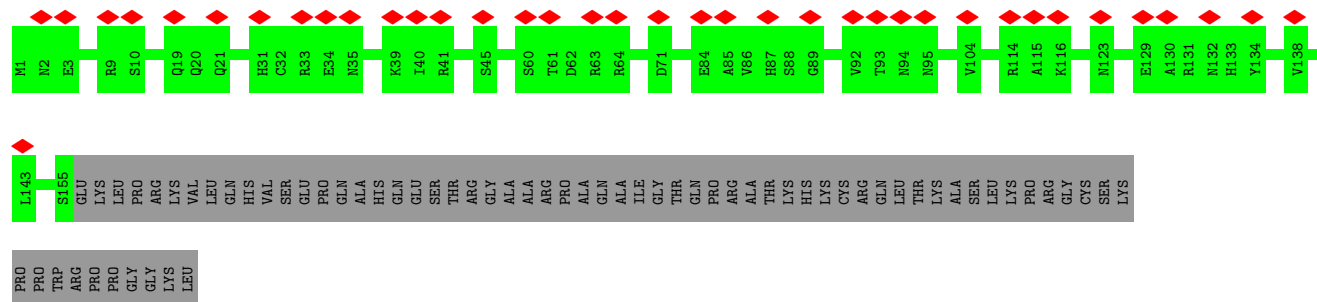
- Molecule 1: Sperm acrosome-associated protein 9



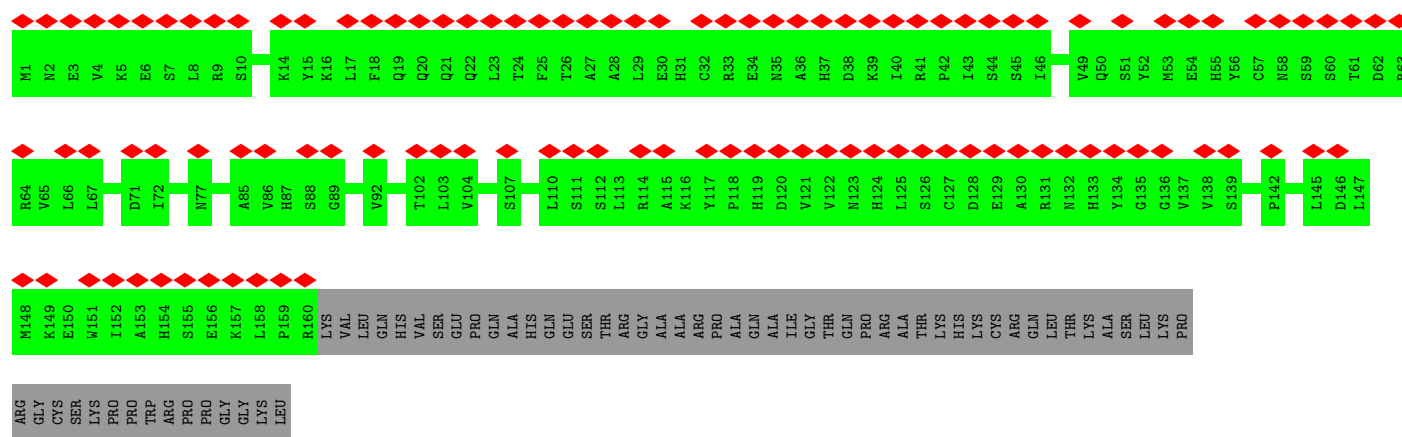




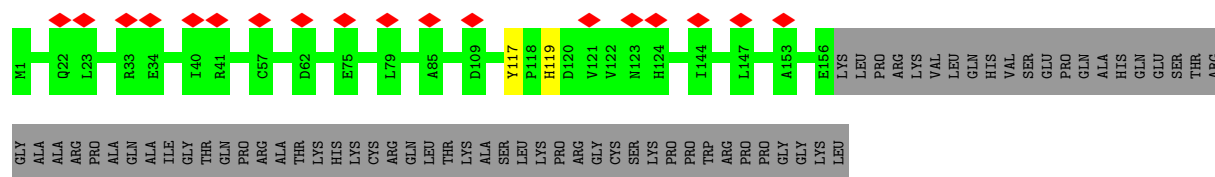
• Molecule 1: Sperm acrosome-associated protein 9



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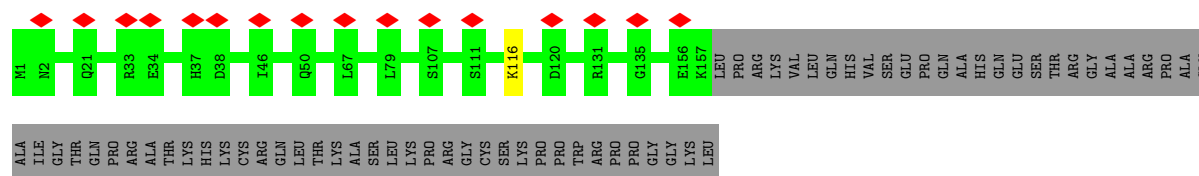


• Molecule 1: Sperm acrosome-associated protein 9



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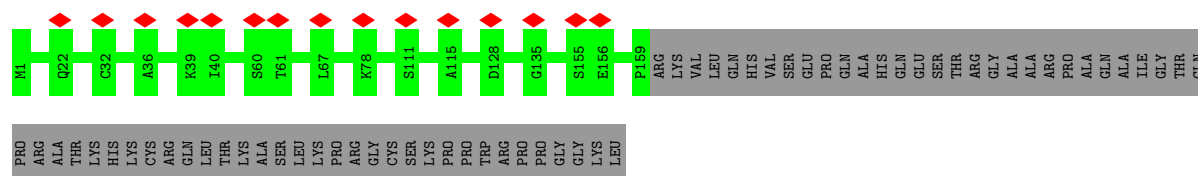


• Molecule 1: Sperm acrosome-associated protein 9

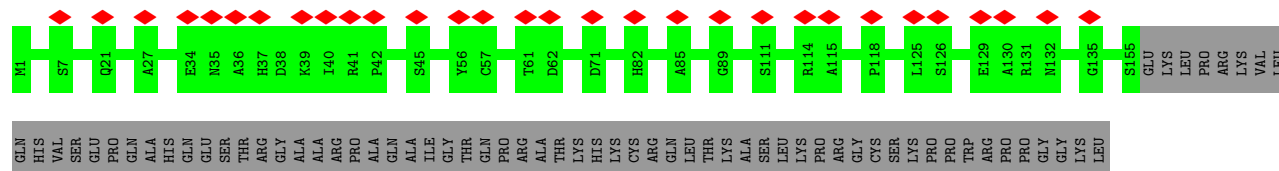


• Molecule 1: Sperm acrosome-associated protein 9

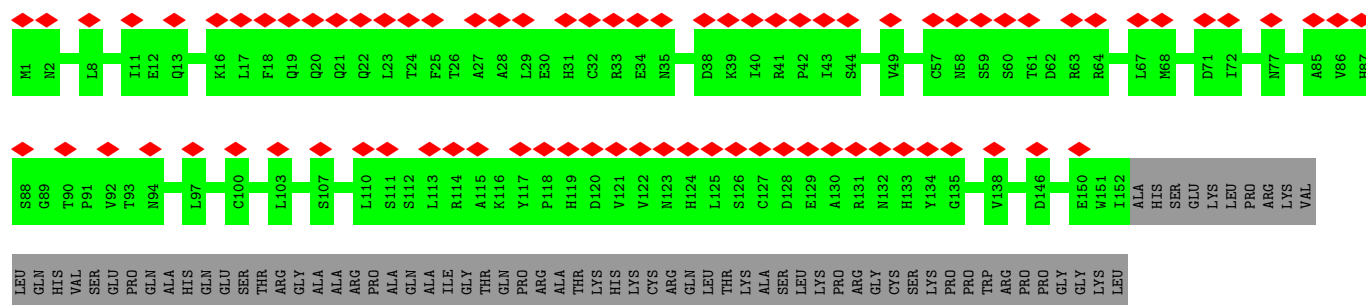




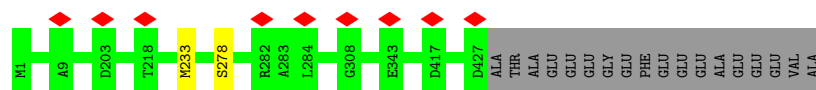
- Molecule 1: Sperm acrosome-associated protein 9



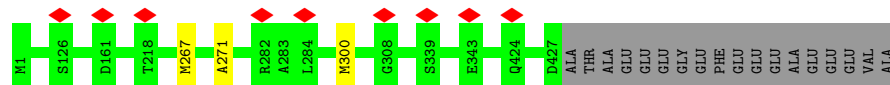
- Molecule 1: Sperm acrosome-associated protein 9



- Molecule 2: Tubulin beta-4B chain

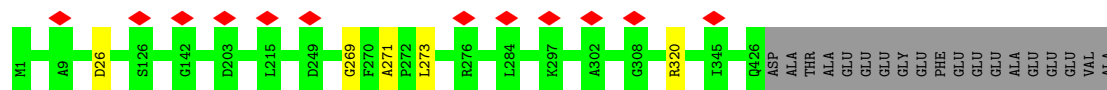


- Molecule 2: Tubulin beta-4B chain

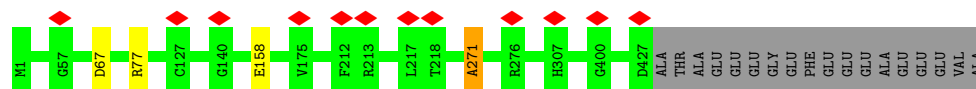


- Molecule 2: Tubulin beta-4B chain

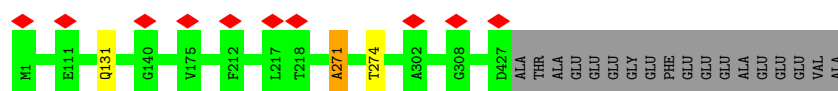




- Molecule 2: Tubulin beta-4B chain



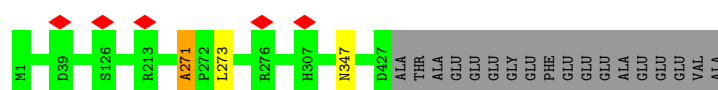
- Molecule 2: Tubulin beta-4B chain



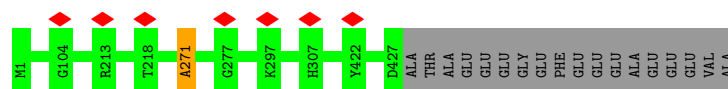
- Molecule 2: Tubulin beta-4B chain



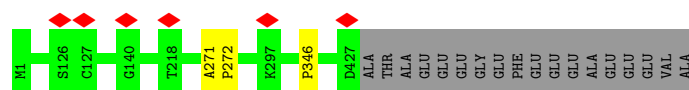
- Molecule 2: Tubulin beta-4B chain



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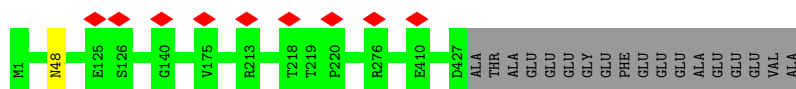


- Molecule 2: Tubulin beta-4B chain



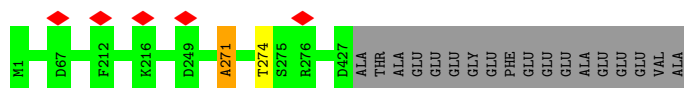
- Molecule 2: Tubulin beta-4B chain

Chain DB:  96%



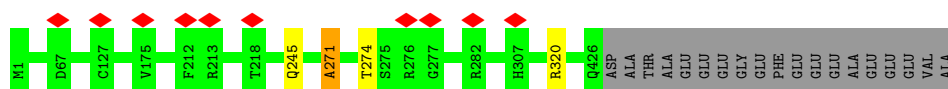
- Molecule 2: Tubulin beta-4B chain

Chain DD:  96%



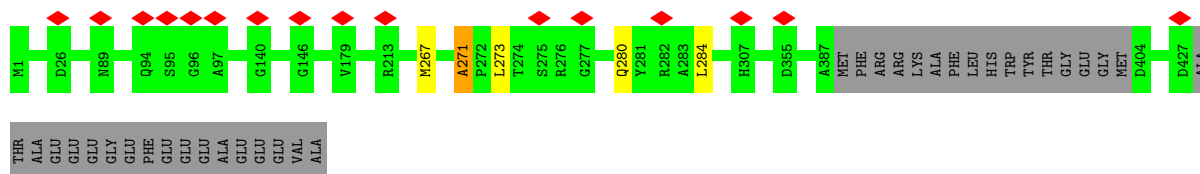
- Molecule 2: Tubulin beta-4B chain

Chain DF:  95%



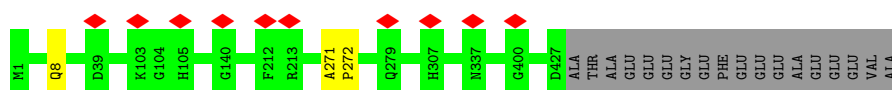
- Molecule 2: Tubulin beta-4B chain

Chain EB:  91% 8%



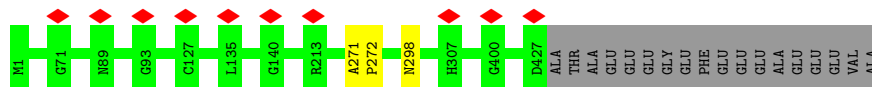
- Molecule 2: Tubulin beta-4B chain

Chain ED:  95%



- Molecule 2: Tubulin beta-4B chain

Chain EF:  95%



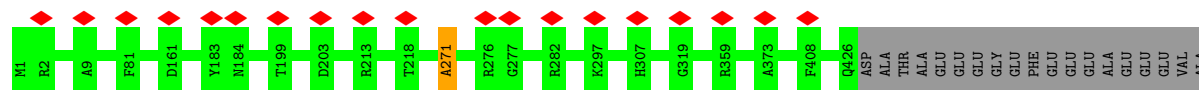
- Molecule 2: Tubulin beta-4B chain

Chain FD:  95%



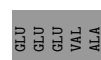
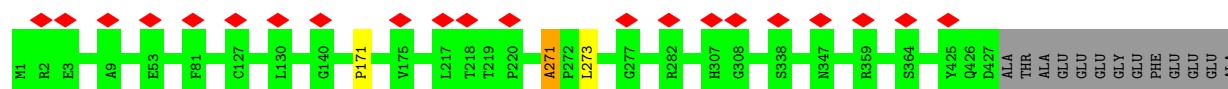
- Molecule 2: Tubulin beta-4B chain

Chain HF:  96%



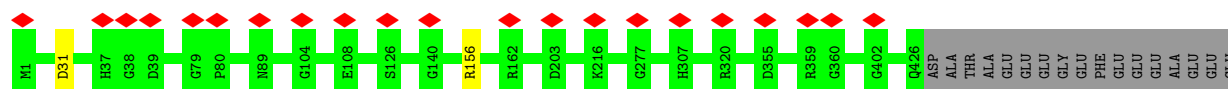
- Molecule 2: Tubulin beta-4B chain

Chain HH:  95%



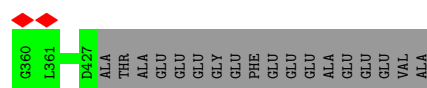
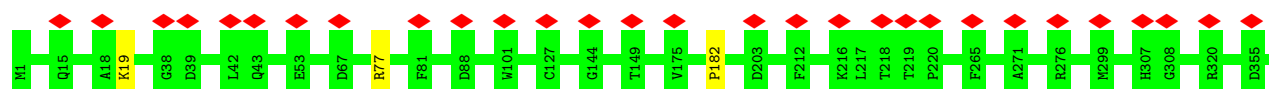
- Molecule 2: Tubulin beta-4B chain

Chain ID:  95%



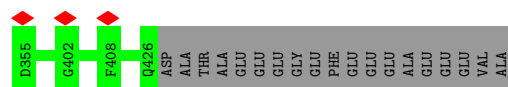
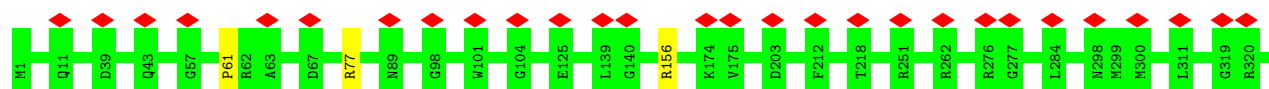
- Molecule 2: Tubulin beta-4B chain

Chain IF:  95%

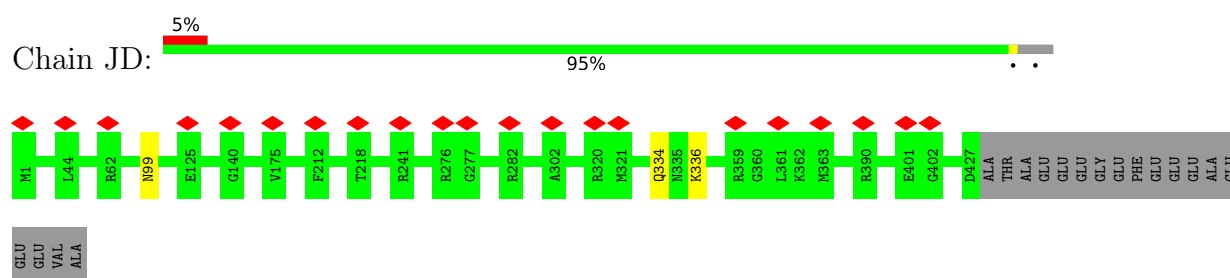


- Molecule 2: Tubulin beta-4B chain

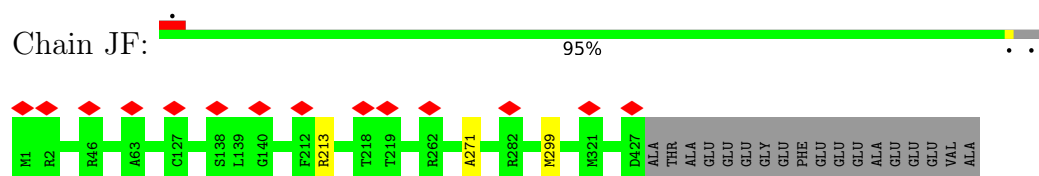
Chain IH:  95%



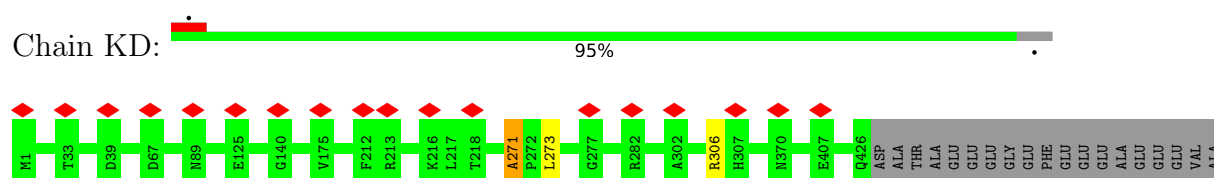
- Molecule 2: Tubulin beta-4B chain



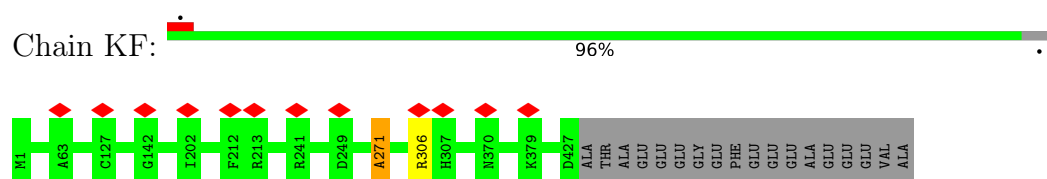
- Molecule 2: Tubulin beta-4B chain



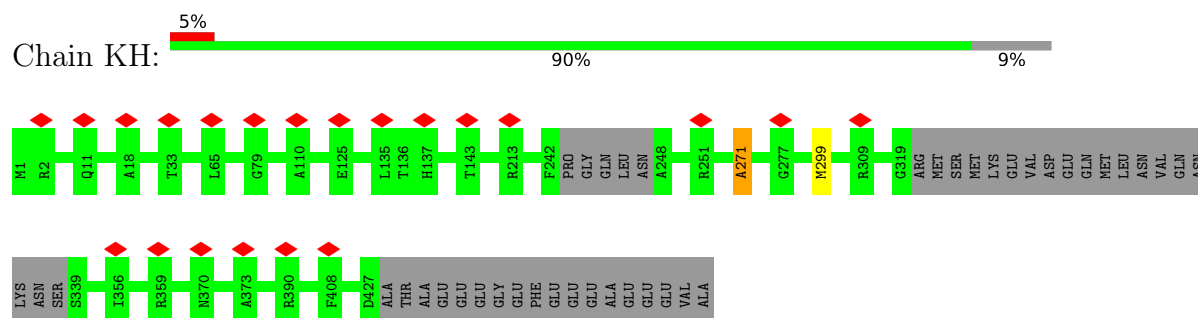
- Molecule 2: Tubulin beta-4B chain



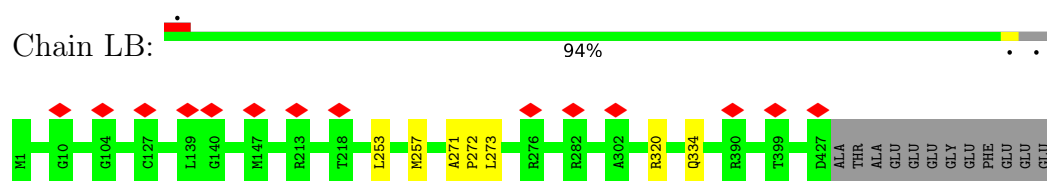
- Molecule 2: Tubulin beta-4B chain



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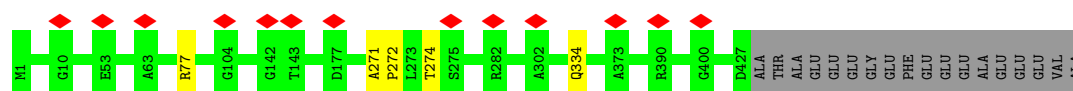
- Molecule 2: Tubulin beta-4B chain



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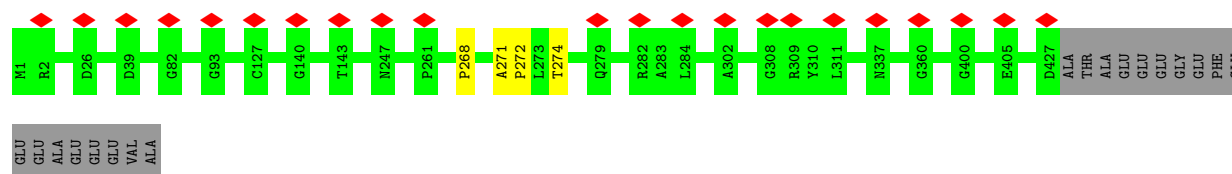


Chain LD:  95%



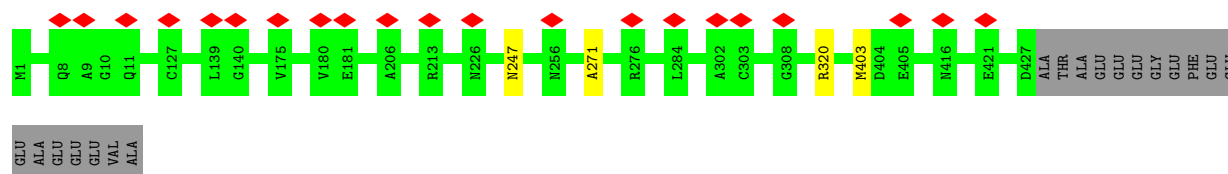
- Molecule 2: Tubulin beta-4B chain

Chain LF:  95%



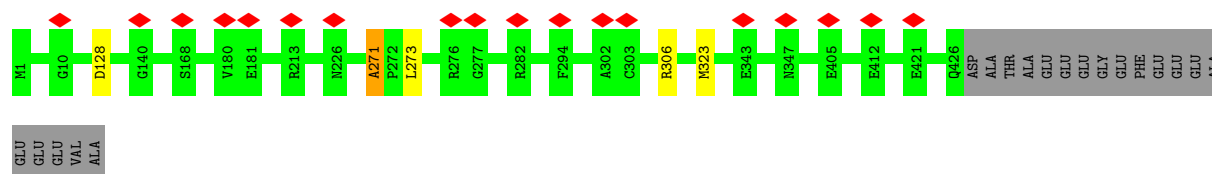
- Molecule 2: Tubulin beta-4B chain

Chain MB:  95%



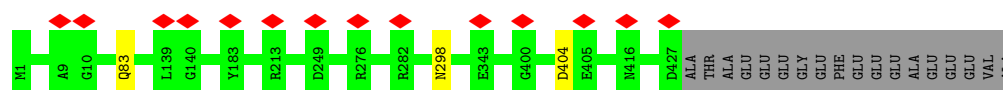
- Molecule 2: Tubulin beta-4B chain

Chain MD:  95%



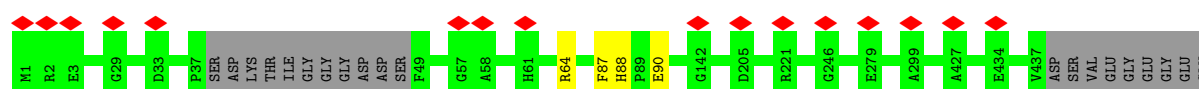
- Molecule 2: Tubulin beta-4B chain

Chain MF:  95%



- Molecule 3: Tubulin alpha-1A chain

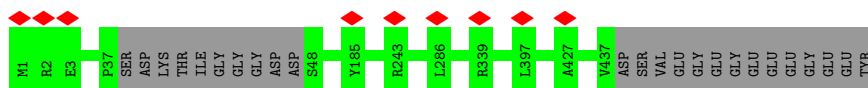
Chain AC:  94% 6%



GLU  
GLY  
GLU  
TYR

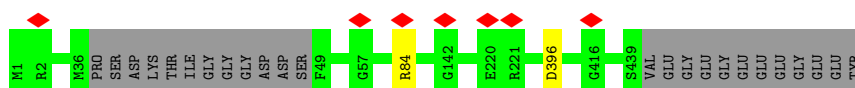
- Molecule 3: Tubulin alpha-1A chain

Chain AE:  95% 5%



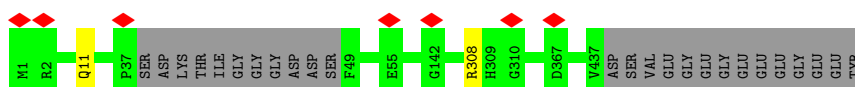
- Molecule 3: Tubulin alpha-1A chain

Chain BC:  94% 5%




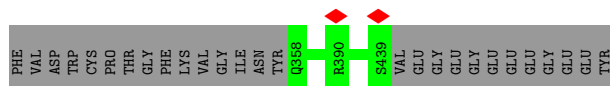
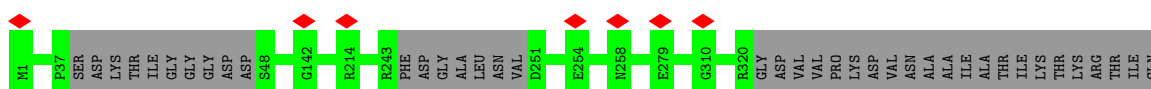
- Molecule 3: Tubulin alpha-1A chain

Chain BE:  94% 6%



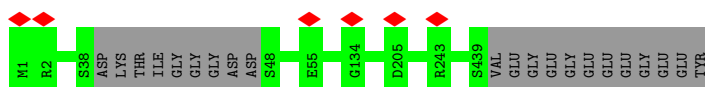
- Molecule 3: Tubulin alpha-1A chain

Chain BG:  85% 15%



- Molecule 3: Tubulin alpha-1A chain

Chain CC:  95% 5%



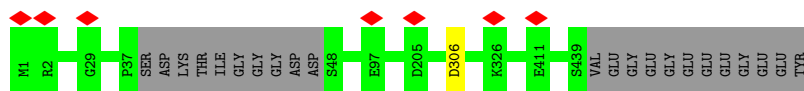
- Molecule 3: Tubulin alpha-1A chain

Chain CE:  95% .



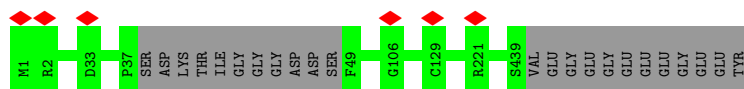
- Molecule 3: Tubulin alpha-1A chain

Chain CG: 95% 5%



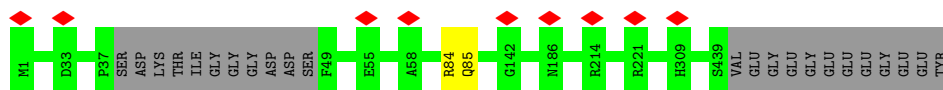
- Molecule 3: Tubulin alpha-1A chain

Chain DC: 95% 5%



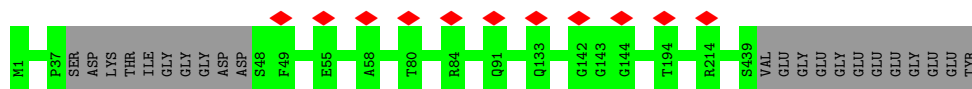
- Molecule 3: Tubulin alpha-1A chain

Chain DE: 94% 5%



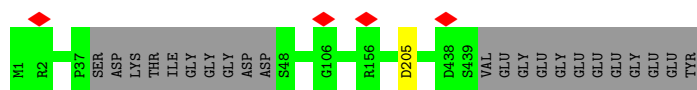
- Molecule 3: Tubulin alpha-1A chain

Chain DG: 95% 5%



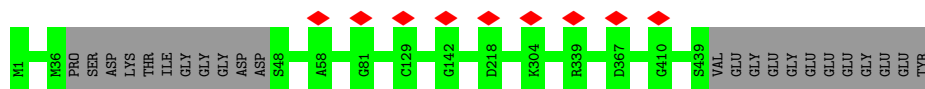
- Molecule 3: Tubulin alpha-1A chain

Chain EC: 95% 5%



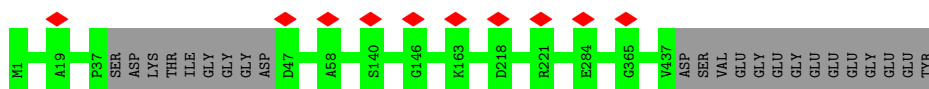
- Molecule 3: Tubulin alpha-1A chain

Chain EE: 95% 5%



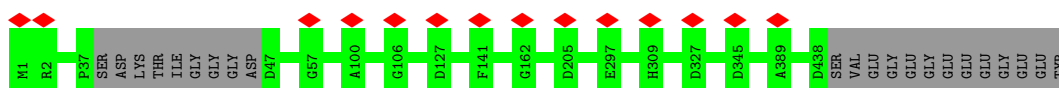
- Molecule 3: Tubulin alpha-1A chain

Chain EG:  95% 5%



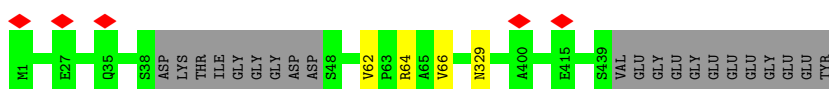
- Molecule 3: Tubulin alpha-1A chain

Chain FC:  95% 5%



- Molecule 3: Tubulin alpha-1A chain

Chain FE:  94% 5%



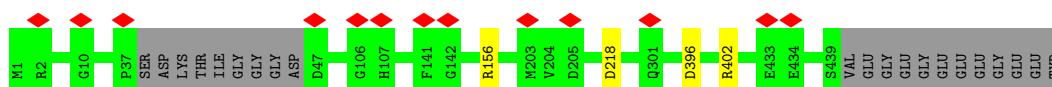
- Molecule 3: Tubulin alpha-1A chain

Chain FG:  95% 5%



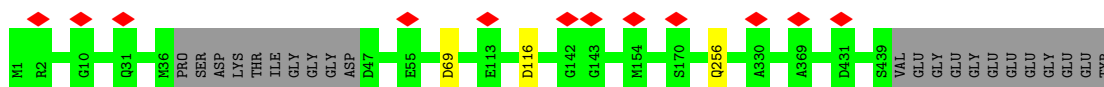
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Chain GC:  94% 5%



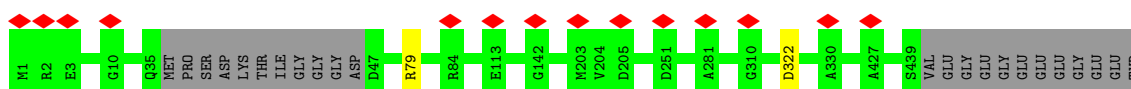
- Molecule 3: Tubulin alpha-1A chain

Chain GE:  94% 5%

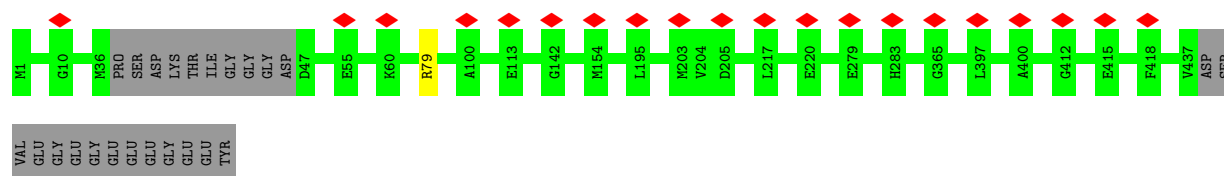


- Molecule 3: Tubulin alpha-1A chain

Chain GG:  94% 5%



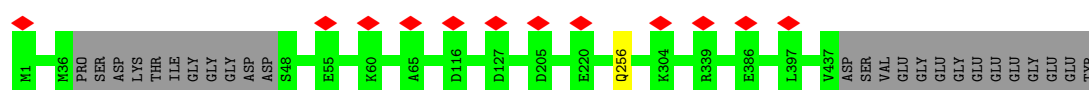
## • Molecule 3: Tubulin alpha-1A chain

Chain HC:  94% 5%

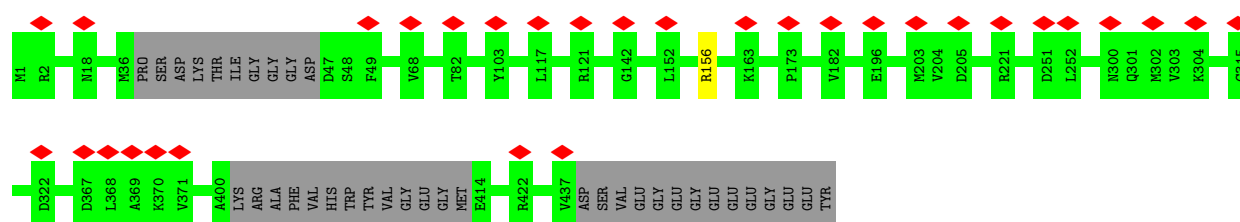
## • Molecule 3: Tubulin alpha-1A chain

Chain HE:  95% 5%

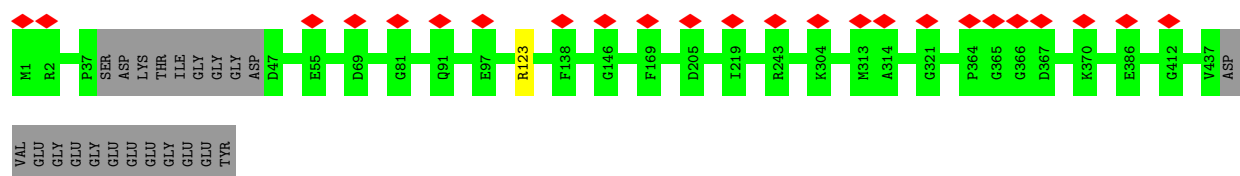
## • Molecule 3: Tubulin alpha-1A chain

Chain HG:  94% 6%

## • Molecule 3: Tubulin alpha-1A chain

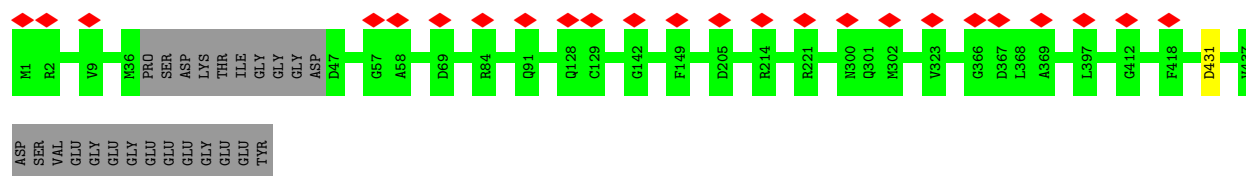
Chain IC:  7% 92% 8%

## • Molecule 3: Tubulin alpha-1A chain

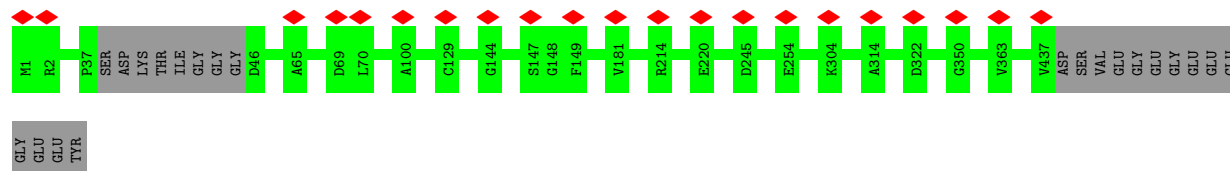
Chain IE:  5% 95% 5%

## • Molecule 3: Tubulin alpha-1A chain

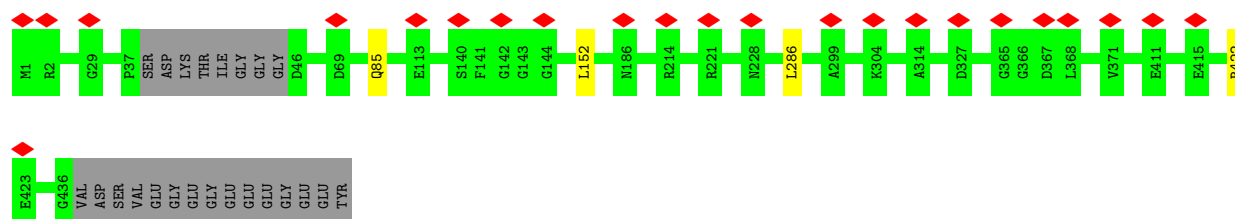
Chain IG:  5% 94% 5%



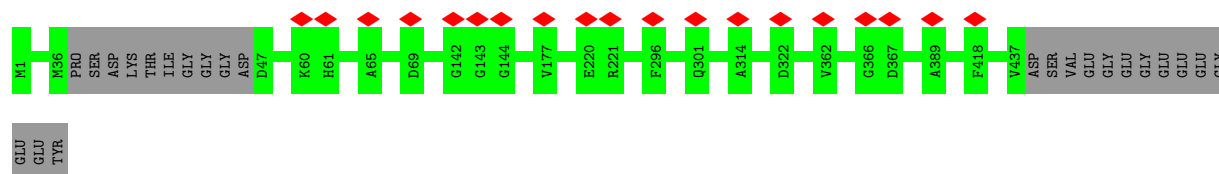
- Molecule 3: Tubulin alpha-1A chain



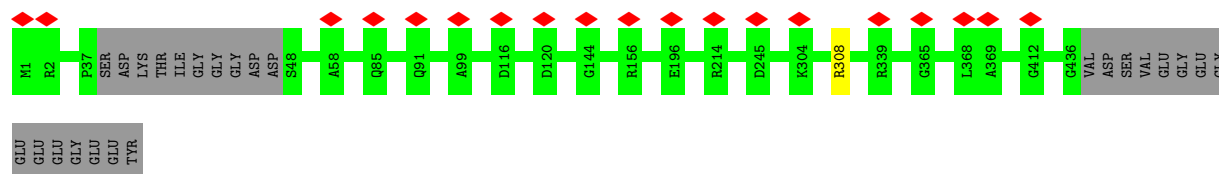
- Molecule 3: Tubulin alpha-1A chain



- Molecule 3: Tubulin alpha-1A chain

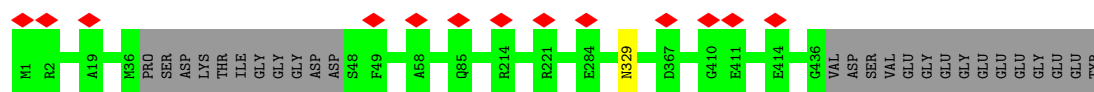


- Molecule 3: Tubulin alpha-1A chain



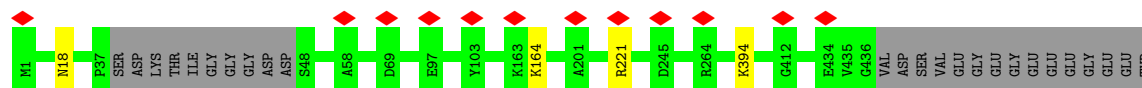
- Molecule 3: Tubulin alpha-1A chain





- Molecule 3: Tubulin alpha-1A chain

Chain KG: 94% 6%



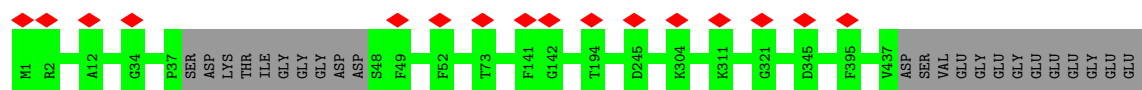
- Molecule 3: Tubulin alpha-1A chain

Chain LA: 95% 5%



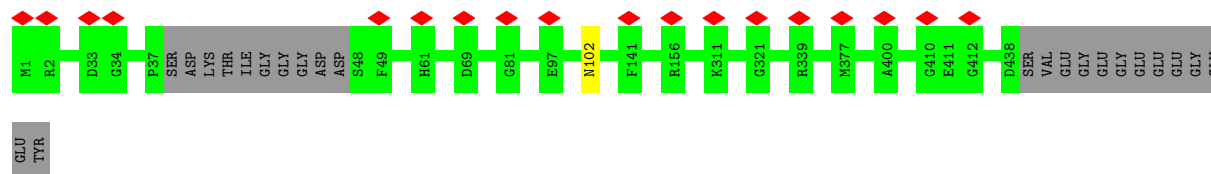
- Molecule 3: Tubulin alpha-1A chain

Chain LC: 95% 5%



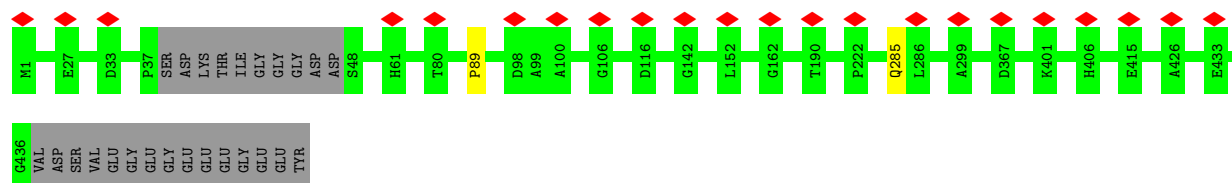
- Molecule 3: Tubulin alpha-1A chain

Chain LE: 95% 5%



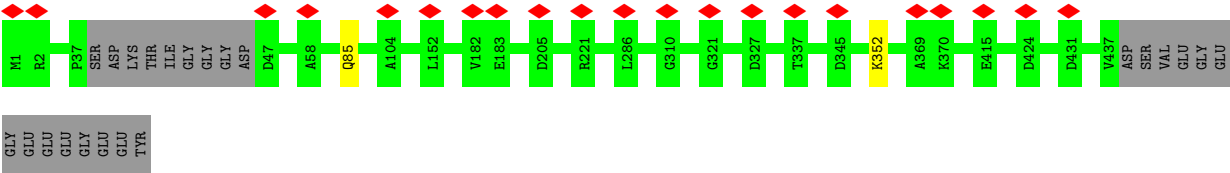
- Molecule 3: Tubulin alpha-1A chain

Chain MA: 94% 5% 6%

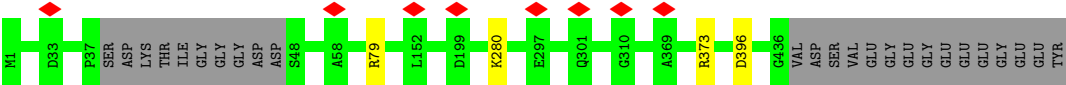


- Molecule 3: Tubulin alpha-1A chain

Chain MC: 94% 5% 5%



● Molecule 3: Tubulin alpha-1A chain





## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 [i](#)

### 5.1 Standard geometry [i](#)

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

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.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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(°)	Ideal(°)
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
2	BA	271	ALA	N-CA-C	7.05	130.04	111.00
2	JF	271	ALA	N-CA-C	7.04	130.02	111.00
2	ED	271	ALA	N-CA-C	7.03	129.98	111.00
2	KF	271	ALA	N-CA-C	6.97	129.82	111.00
2	EF	271	ALA	N-CA-C	6.97	129.81	111.00
2	DF	271	ALA	N-CA-C	6.96	129.79	111.00
3	GE	116	ASP	CB-CG-OD1	6.92	124.53	118.30
2	KD	271	ALA	N-CA-C	6.84	129.48	111.00
2	EB	271	ALA	N-CA-C	6.76	129.25	111.00
2	CB	271	ALA	N-CA-C	6.54	128.66	111.00
2	DD	271	ALA	N-CA-C	6.48	128.50	111.00
3	ME	396	ASP	CB-CG-OD1	6.43	124.09	118.30
2	AF	271	ALA	N-CA-C	6.40	128.28	111.00
2	LB	271	ALA	N-CA-C	6.37	128.21	111.00
2	MD	271	ALA	N-CA-C	6.33	128.09	111.00
2	BD	271	ALA	N-CA-C	6.31	128.04	111.00
2	HF	271	ALA	N-CA-C	6.29	127.99	111.00
2	BF	26	ASP	CB-CG-OD1	6.28	123.95	118.30
2	CF	271	ALA	N-CA-C	6.24	127.84	111.00
2	ID	31	ASP	CB-CG-OD2	6.21	123.89	118.30
2	MF	404	ASP	CB-CG-OD1	6.20	123.88	118.30
1	F	67	LEU	CA-CB-CG	6.14	129.43	115.30
2	FD	271	ALA	N-CA-C	6.14	127.58	111.00
3	GC	218	ASP	CB-CG-OD2	6.13	123.82	118.30
2	FF	203	ASP	CB-CG-OD1	6.11	123.80	118.30
3	CG	306	ASP	CB-CG-OD1	6.09	123.78	118.30
3	LA	120	ASP	CB-CG-OD1	6.06	123.75	118.30
2	CD	271	ALA	N-CA-C	6.00	127.21	111.00
2	CF	346	PRO	CA-N-CD	-5.95	103.17	111.50
2	AD	300	MET	CA-CB-CG	5.95	123.41	113.30
2	GD	271	ALA	N-CA-C	5.91	126.95	111.00
2	HD	271	ALA	N-CA-C	5.89	126.92	111.00
2	HH	271	ALA	N-CA-C	5.89	126.90	111.00
2	EB	267	MET	CA-CB-CG	5.82	123.19	113.30
3	JE	286	LEU	CA-CB-CG	5.80	128.63	115.30
2	GF	271	ALA	N-CA-C	5.76	126.55	111.00
1	P	89	GLY	C-N-CA	5.73	136.03	121.70
1	d	117	TYR	N-CA-C	5.72	126.44	111.00
3	GE	69	ASP	CB-CG-OD1	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	88	HIS	CB-CA-C	-5.68	99.04	110.40
2	LF	271	ALA	N-CA-C	5.61	126.14	111.00
2	AF	26	ASP	CB-CG-OD1	5.60	123.34	118.30
2	MD	128	ASP	CB-CG-OD2	5.58	123.32	118.30
2	FD	267	MET	CA-CB-CG	5.55	122.73	113.30
3	EC	205	ASP	CB-CG-OD1	5.54	123.29	118.30
1	i	109	ASP	CB-CG-OD1	5.50	123.25	118.30
1	i	143	LEU	CA-CB-CG	5.50	127.94	115.30
2	FD	268	PRO	N-CA-C	5.49	126.38	112.10
2	AD	271	ALA	N-CA-C	5.49	125.82	111.00
2	LB	257	MET	N-CA-C	5.43	125.65	111.00
3	MA	89	PRO	CA-N-CD	-5.37	103.98	111.50
2	BA	67	ASP	CB-CG-OD1	5.35	123.11	118.30
3	GC	396	ASP	CB-CG-OD1	5.31	123.08	118.30
2	FD	293	MET	CA-CB-CG	5.30	122.32	113.30
3	BC	396	ASP	CB-CG-OD1	5.30	123.07	118.30
2	IH	61	PRO	CA-N-CD	-5.27	104.12	111.50
2	HH	171	PRO	C-N-CA	5.25	134.81	121.70
2	AF	269	GLY	N-CA-C	-5.24	99.99	113.10
3	IG	431	ASP	CB-CG-OD1	5.24	123.02	118.30
2	AD	267	MET	CA-CB-CG	5.23	122.19	113.30
2	EB	284	LEU	CA-CB-CG	5.14	127.13	115.30
2	AB	233	MET	CB-CG-SD	5.14	127.83	112.40
3	JE	152	LEU	CA-CB-CG	5.03	126.87	115.30
2	LD	272	PRO	N-CA-C	-5.02	99.04	112.10

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
2	CD	271	ALA
2	EF	272	PRO
2	FD	271	ALA
2	KD	271	ALA
2	KF	271	ALA
2	LB	272	PRO
2	GD	271	ALA
2	MB	271	ALA
2	EB	271	ALA

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Mol	Chain	Res	Type
2	LF	272	PRO
2	BA	271	ALA
2	DF	271	ALA
2	FF	271	ALA
2	HD	271	ALA
2	KH	271	ALA
2	CF	272	PRO
2	DD	271	ALA
2	GF	271	ALA
2	HF	271	ALA
2	HH	271	ALA
2	BD	271	ALA
2	MD	271	ALA

### 5.3.2 Protein sidechains ⓘ

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
1	e	146/199 (73%)	145 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
2	IH	366/380 (96%)	364 (100%)	2 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
3	GG	361/378 (96%)	360 (100%)	1 (0%)	92	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	278	SER
3	AC	64	ARG
3	AC	87	PHE
3	AC	90	GLU
2	AF	273	LEU
2	AF	320	ARG
2	BA	77	ARG
3	BC	84	ARG
2	BD	131	GLN
2	BD	274	THR
3	BE	11	GLN
3	BE	308	ARG
2	BF	2	ARG

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Mol	Chain	Res	Type
2	BF	37	HIS
2	BF	336	LYS
2	CB	273	LEU
2	CB	347	ASN
3	CE	50	ASN
1	D	63	ARG
1	D	160	ARG
2	DB	48	ASN
2	DD	274	THR
3	DE	84	ARG
3	DE	85	GLN
2	DF	245	GLN
2	DF	274	THR
2	DF	320	ARG
1	E	119	HIS
2	EB	273	LEU
2	EB	280	GLN
2	ED	8	GLN
2	EF	298	ASN
1	F	41	ARG
1	F	48	GLN
2	FD	336	LYS
3	FE	62	VAL
3	FE	64	ARG
3	FE	66	VAL
3	FE	329	ASN
2	FF	336	LYS
3	FG	18	ASN
3	FG	221	ARG
2	FH	241	ARG
3	GC	156	ARG
3	GC	402	ARG
2	GD	247	ASN
3	GE	256	GLN
2	GF	274	THR
2	GF	276	ARG
3	GG	79	ARG
2	GH	251	ARG
3	HC	79	ARG
2	HD	274	THR
3	HG	256	GLN
2	HH	273	LEU

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Mol	Chain	Res	Type
3	IC	156	ARG
2	ID	156	ARG
3	IE	123	ARG
2	IF	19	LYS
2	IF	77	ARG
2	IH	77	ARG
2	IH	156	ARG
2	JD	99	ASN
2	JD	334	GLN
2	JD	336	LYS
3	JE	85	GLN
3	JE	422	ARG
2	JF	213	ARG
2	JF	299	MET
3	KC	308	ARG
2	KD	273	LEU
2	KD	306	ARG
3	KE	329	ASN
2	KF	306	ARG
3	KG	18	ASN
3	KG	164	LYS
3	KG	221	ARG
3	KG	394	LYS
2	KH	299	MET
2	LB	253	LEU
2	LB	273	LEU
2	LB	320	ARG
2	LB	334	GLN
2	LD	77	ARG
2	LD	274	THR
2	LD	334	GLN
3	LE	102	ASN
2	LF	274	THR
3	MA	285	GLN
2	MB	247	ASN
2	MB	320	ARG
2	MB	403	MET
3	MC	85	GLN
3	MC	352	LYS
2	MD	273	LEU
2	MD	306	ARG
2	MD	323	MET

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Mol	Chain	Res	Type
3	ME	79	ARG
3	ME	280	LYS
3	ME	373	ARG
2	MF	298	ASN
1	d	119	HIS
1	e	116	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
3	AC	101	ASN
2	AD	14	ASN
2	AD	105	HIS
2	AD	190	HIS
2	AD	298	ASN
2	AD	414	ASN
2	BA	131	GLN
3	BC	88	HIS
2	BD	8	GLN
2	BD	94	GLN
2	BD	99	ASN
3	BE	15	GLN
3	BE	61	HIS
3	BE	283	HIS
2	BF	348	ASN
2	BF	370	ASN
3	BG	139	HIS
2	CB	347	ASN
2	CD	348	ASN
2	CD	396	HIS
3	CG	85	GLN
3	CG	91	GLN
2	DB	14	ASN
3	DC	329	ASN
3	DE	85	GLN
3	DE	133	GLN
2	DF	298	ASN
2	EB	6	HIS
2	EB	134	GLN
3	EC	293	ASN
3	FC	329	ASN
2	FD	298	ASN

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Mol	Chain	Res	Type
3	FE	85	GLN
3	FG	11	GLN
3	FG	15	GLN
2	FH	292	GLN
1	G	22	GLN
2	GD	52	ASN
2	GD	131	GLN
2	GD	256	ASN
3	GE	18	ASN
2	GF	256	ASN
2	GF	298	ASN
2	GF	334	GLN
2	GH	292	GLN
3	HC	18	ASN
2	HD	335	ASN
2	HF	6	HIS
2	HF	256	ASN
2	HH	52	ASN
2	HH	329	GLN
3	IC	35	GLN
3	IC	293	ASN
2	ID	99	ASN
3	IE	342	GLN
2	IF	131	GLN
2	IF	256	ASN
2	IH	292	GLN
3	JC	91	GLN
3	JC	342	GLN
2	JD	226	ASN
3	JE	228	ASN
2	JF	14	ASN
2	JF	329	GLN
2	JF	334	GLN
3	JG	228	ASN
2	KD	99	ASN
2	KD	347	ASN
3	KE	258	ASN
2	KF	6	HIS
2	KF	165	ASN
2	KF	329	GLN
2	KH	94	GLN
3	LA	35	GLN

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Mol	Chain	Res	Type
3	LA	293	ASN
2	LD	329	GLN
2	LD	347	ASN
3	LE	102	ASN
3	MA	102	ASN
3	MA	380	ASN
2	MB	6	HIS
3	MC	406	HIS
1	U	108	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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	LB	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.23	4 (13%)
5	GTP	JE	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.58	6 (18%)
4	GDP	EF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	3 (10%)
4	GDP	MB	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.28	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GDP	GF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.40	5 (16%)
4	GDP	CB	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.25	4 (13%)
4	GDP	AF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	3 (10%)
5	GTP	EC	501	6	26,34,34	1.23	3 (11%)	32,54,54	1.68	6 (18%)
4	GDP	CF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
4	GDP	AB	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.36	4 (13%)
4	GDP	BF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.27	4 (13%)
4	GDP	DD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
4	GDP	HF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
5	GTP	CG	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.63	7 (21%)
4	GDP	AD	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.38	3 (10%)
5	GTP	IC	501	6	26,34,34	1.19	2 (7%)	32,54,54	1.57	7 (21%)
5	GTP	FC	501	6	26,34,34	1.19	2 (7%)	32,54,54	1.63	7 (21%)
4	GDP	HD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
4	GDP	KH	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.36	5 (16%)
5	GTP	HG	501	6	26,34,34	1.28	2 (7%)	32,54,54	1.66	7 (21%)
4	GDP	MF	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.34	4 (13%)
4	GDP	ID	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.22	4 (13%)
5	GTP	IE	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.58	7 (21%)
5	GTP	KC	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.50	7 (21%)
5	GTP	HE	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.60	7 (21%)
5	GTP	DE	501	6	26,34,34	1.20	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%)
5	GTP	KE	501	6	26,34,34	1.25	2 (7%)	32,54,54	1.56	6 (18%)
4	GDP	LF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.26	6 (20%)
5	GTP	CE	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.64	7 (21%)
4	GDP	CD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
5	GTP	AE	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.55	7 (21%)
5	GTP	JG	501	6	26,34,34	1.18	2 (7%)	32,54,54	1.55	6 (18%)
5	GTP	BG	501	6	26,34,34	1.19	1 (3%)	32,54,54	1.60	6 (18%)
5	GTP	FG	501	6	26,34,34	1.25	1 (3%)	32,54,54	1.59	6 (18%)
5	GTP	GC	501	6	26,34,34	1.24	2 (7%)	32,54,54	1.70	7 (21%)
5	GTP	JC	501	6	26,34,34	1.17	2 (7%)	32,54,54	1.58	7 (21%)
5	GTP	FE	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.61	7 (21%)
5	GTP	GE	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.67	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	DC	501	6	26,34,34	1.24	2 (7%)	32,54,54	1.61	6 (18%)
4	GDP	GH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
5	GTP	HC	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.56	7 (21%)
5	GTP	CC	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.45	6 (18%)
4	GDP	EB	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.30	4 (13%)
5	GTP	LE	501	6	26,34,34	1.23	2 (7%)	32,54,54	1.63	7 (21%)
4	GDP	FD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.27	4 (13%)
5	GTP	LC	501	6	26,34,34	1.22	2 (7%)	32,54,54	1.58	6 (18%)
5	GTP	ME	501	6	26,34,34	1.26	2 (7%)	32,54,54	1.67	8 (25%)
4	GDP	GD	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.32	4 (13%)
4	GDP	BA	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
4	GDP	DB	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.33	4 (13%)
4	GDP	IH	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.42	5 (16%)
4	GDP	JD	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
5	GTP	MA	501	6	26,34,34	1.23	2 (7%)	32,54,54	1.59	7 (21%)
5	GTP	MC	501	6	26,34,34	1.25	2 (7%)	32,54,54	1.54	6 (18%)
4	GDP	DF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	4 (13%)
4	GDP	BD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.29	4 (13%)
5	GTP	IG	501	6	26,34,34	1.19	2 (7%)	32,54,54	1.63	7 (21%)
4	GDP	ED	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
4	GDP	JF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.32	4 (13%)
4	GDP	IF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	4 (13%)
5	GTP	BC	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.51	7 (21%)
5	GTP	BE	501	6	26,34,34	1.23	2 (7%)	32,54,54	1.65	7 (21%)
5	GTP	KG	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.60	6 (18%)
4	GDP	MD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	4 (13%)
4	GDP	HH	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.41	4 (13%)
4	GDP	LD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	5 (16%)
4	GDP	KF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.19	3 (10%)
5	GTP	EE	501	6	26,34,34	1.25	2 (7%)	32,54,54	1.66	5 (15%)
5	GTP	DG	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.59	6 (18%)
5	GTP	GG	501	6	26,34,34	1.24	2 (7%)	32,54,54	1.74	7 (21%)
5	GTP	LA	501	6	26,34,34	1.17	2 (7%)	32,54,54	1.62	7 (21%)
5	GTP	AC	501	6	26,34,34	1.20	2 (7%)	32,54,54	1.72	7 (21%)
4	GDP	FH	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.38	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GDP	KD	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
4	GDP	FF	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.32	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	LB	501	-	-	4/12/32/32	0/3/3/3
5	GTP	JE	501	6	-	7/18/38/38	0/3/3/3
4	GDP	EF	501	-	-	2/12/32/32	0/3/3/3
4	GDP	MB	501	-	-	2/12/32/32	0/3/3/3
4	GDP	GF	501	-	-	3/12/32/32	0/3/3/3
4	GDP	CB	501	-	-	2/12/32/32	0/3/3/3
4	GDP	AF	501	-	-	5/12/32/32	0/3/3/3
5	GTP	EC	501	6	-	5/18/38/38	0/3/3/3
4	GDP	CF	501	-	-	1/12/32/32	0/3/3/3
4	GDP	AB	501	-	-	1/12/32/32	0/3/3/3
4	GDP	BF	501	-	-	2/12/32/32	0/3/3/3
4	GDP	DD	501	-	-	2/12/32/32	0/3/3/3
4	GDP	HF	501	-	-	3/12/32/32	0/3/3/3
5	GTP	CG	501	6	-	5/18/38/38	0/3/3/3
4	GDP	AD	501	-	-	4/12/32/32	0/3/3/3
5	GTP	IC	501	6	-	9/18/38/38	0/3/3/3
5	GTP	FC	501	6	-	4/18/38/38	0/3/3/3
4	GDP	HD	501	-	-	2/12/32/32	0/3/3/3
4	GDP	KH	501	-	-	3/12/32/32	0/3/3/3
5	GTP	HG	501	6	-	5/18/38/38	0/3/3/3
4	GDP	MF	501	-	-	2/12/32/32	0/3/3/3
4	GDP	ID	501	-	-	5/12/32/32	0/3/3/3
5	GTP	IE	501	6	-	8/18/38/38	0/3/3/3
5	GTP	KC	501	6	-	4/18/38/38	0/3/3/3
5	GTP	HE	501	6	-	7/18/38/38	0/3/3/3
5	GTP	DE	501	6	-	7/18/38/38	0/3/3/3
5	GTP	EG	501	6	-	5/18/38/38	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	LF	501	-	-	4/12/32/32	0/3/3/3
5	GTP	CE	501	6	-	5/18/38/38	0/3/3/3
4	GDP	CD	501	-	-	1/12/32/32	0/3/3/3
5	GTP	AE	501	6	-	2/18/38/38	0/3/3/3
5	GTP	JG	501	6	-	1/18/38/38	0/3/3/3
5	GTP	BG	501	6	-	6/18/38/38	0/3/3/3
5	GTP	FG	501	6	-	7/18/38/38	0/3/3/3
5	GTP	GC	501	6	-	6/18/38/38	0/3/3/3
5	GTP	JC	501	6	-	6/18/38/38	0/3/3/3
5	GTP	FE	501	6	-	5/18/38/38	0/3/3/3
5	GTP	GE	501	6	-	7/18/38/38	0/3/3/3
5	GTP	DC	501	6	-	7/18/38/38	0/3/3/3
4	GDP	GH	501	-	-	3/12/32/32	0/3/3/3
5	GTP	HC	501	6	-	7/18/38/38	0/3/3/3
5	GTP	CC	501	6	-	4/18/38/38	0/3/3/3
4	GDP	EB	501	-	-	3/12/32/32	0/3/3/3
5	GTP	LE	501	6	-	5/18/38/38	0/3/3/3
4	GDP	FD	501	-	-	1/12/32/32	0/3/3/3
5	GTP	LC	501	6	-	2/18/38/38	0/3/3/3
5	GTP	ME	501	6	-	5/18/38/38	0/3/3/3
4	GDP	GD	501	-	-	4/12/32/32	0/3/3/3
4	GDP	BA	501	-	-	3/12/32/32	0/3/3/3
4	GDP	DB	501	-	-	2/12/32/32	0/3/3/3
4	GDP	IH	501	-	-	1/12/32/32	0/3/3/3
4	GDP	JD	501	-	-	2/12/32/32	0/3/3/3
5	GTP	MA	501	6	-	1/18/38/38	0/3/3/3
5	GTP	MC	501	6	-	5/18/38/38	0/3/3/3
4	GDP	DF	501	-	-	1/12/32/32	0/3/3/3
4	GDP	BD	501	-	-	2/12/32/32	0/3/3/3
5	GTP	IG	501	6	-	2/18/38/38	0/3/3/3
4	GDP	ED	501	-	-	2/12/32/32	0/3/3/3
4	GDP	JF	501	-	-	4/12/32/32	0/3/3/3
4	GDP	IF	501	-	-	5/12/32/32	0/3/3/3
5	GTP	BC	501	6	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	BE	501	6	-	4/18/38/38	0/3/3/3
5	GTP	KG	501	6	-	5/18/38/38	0/3/3/3
4	GDP	MD	501	-	-	2/12/32/32	0/3/3/3
4	GDP	HH	501	-	-	2/12/32/32	0/3/3/3
4	GDP	LD	501	-	-	2/12/32/32	0/3/3/3
4	GDP	KF	501	-	-	1/12/32/32	0/3/3/3
5	GTP	EE	501	6	-	8/18/38/38	0/3/3/3
5	GTP	DG	501	6	-	6/18/38/38	0/3/3/3
5	GTP	GG	501	6	-	4/18/38/38	0/3/3/3
5	GTP	LA	501	6	-	6/18/38/38	0/3/3/3
5	GTP	AC	501	6	-	3/18/38/38	0/3/3/3
4	GDP	FH	501	-	-	3/12/32/32	0/3/3/3
4	GDP	KD	501	-	-	1/12/32/32	0/3/3/3
4	GDP	FF	501	-	-	2/12/32/32	0/3/3/3

All (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
5	KE	501	GTP	C5-C6	-4.51	1.38	1.47
5	BE	501	GTP	C5-C6	-4.51	1.38	1.47
5	MA	501	GTP	C5-C6	-4.46	1.38	1.47
5	HC	501	GTP	C5-C6	-4.45	1.38	1.47
5	GG	501	GTP	C5-C6	-4.43	1.38	1.47
5	FG	501	GTP	C5-C6	-4.43	1.38	1.47
5	LE	501	GTP	C5-C6	-4.39	1.38	1.47
5	IE	501	GTP	C5-C6	-4.39	1.38	1.47
5	LC	501	GTP	C5-C6	-4.37	1.38	1.47
5	IC	501	GTP	C5-C6	-4.37	1.38	1.47
5	CG	501	GTP	C5-C6	-4.35	1.38	1.47
5	CE	501	GTP	C5-C6	-4.34	1.38	1.47
5	BC	501	GTP	C5-C6	-4.31	1.38	1.47
5	DC	501	GTP	C5-C6	-4.31	1.38	1.47
5	EE	501	GTP	C5-C6	-4.31	1.38	1.47
5	HE	501	GTP	C5-C6	-4.30	1.38	1.47
5	AE	501	GTP	C5-C6	-4.30	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	FE	501	GTP	C5-C6	-4.29	1.38	1.47
5	KC	501	GTP	C5-C6	-4.29	1.38	1.47
5	BG	501	GTP	C5-C6	-4.26	1.38	1.47
5	GE	501	GTP	C5-C6	-4.26	1.38	1.47
5	KG	501	GTP	C5-C6	-4.25	1.38	1.47
5	EC	501	GTP	C5-C6	-4.24	1.38	1.47
5	AC	501	GTP	C5-C6	-4.22	1.38	1.47
5	DG	501	GTP	C5-C6	-4.22	1.38	1.47
5	JG	501	GTP	C5-C6	-4.21	1.38	1.47
5	FC	501	GTP	C5-C6	-4.20	1.38	1.47
5	CC	501	GTP	C5-C6	-4.19	1.38	1.47
5	IG	501	GTP	C5-C6	-4.19	1.38	1.47
5	DE	501	GTP	C5-C6	-4.18	1.38	1.47
5	JC	501	GTP	C5-C6	-4.17	1.38	1.47
5	LA	501	GTP	C5-C6	-4.04	1.39	1.47
5	JE	501	GTP	C5-C6	-4.02	1.39	1.47
4	MF	501	GDP	C6-N1	-3.01	1.33	1.37
4	LF	501	GDP	C6-N1	-2.89	1.33	1.37
4	AD	501	GDP	C6-N1	-2.86	1.33	1.37
4	KH	501	GDP	C6-N1	-2.85	1.33	1.37
4	JF	501	GDP	C6-N1	-2.82	1.33	1.37
4	GD	501	GDP	C6-N1	-2.80	1.33	1.37
4	EB	501	GDP	C6-N1	-2.79	1.33	1.37
4	MB	501	GDP	C6-N1	-2.79	1.33	1.37
4	BD	501	GDP	C6-N1	-2.78	1.33	1.37
4	LD	501	GDP	C6-N1	-2.78	1.33	1.37
4	FF	501	GDP	C6-N1	-2.76	1.33	1.37
4	GF	501	GDP	C6-N1	-2.75	1.33	1.37
4	DB	501	GDP	C6-N1	-2.75	1.33	1.37
4	MD	501	GDP	C6-N1	-2.75	1.33	1.37
4	GH	501	GDP	C6-N1	-2.74	1.33	1.37
4	BF	501	GDP	C6-N1	-2.74	1.33	1.37
4	BA	501	GDP	C6-N1	-2.74	1.33	1.37
4	AB	501	GDP	C6-N1	-2.74	1.33	1.37
4	LB	501	GDP	C6-N1	-2.71	1.33	1.37
4	KF	501	GDP	C6-N1	-2.70	1.33	1.37
4	FD	501	GDP	C6-N1	-2.69	1.33	1.37
4	EF	501	GDP	C6-N1	-2.68	1.33	1.37
4	ID	501	GDP	C6-N1	-2.66	1.33	1.37
4	FH	501	GDP	C6-N1	-2.64	1.33	1.37
4	HH	501	GDP	C6-N1	-2.64	1.33	1.37
4	JD	501	GDP	C6-N1	-2.63	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	CD	501	GDP	C6-N1	-2.63	1.34	1.37
4	DD	501	GDP	C6-N1	-2.61	1.34	1.37
4	DF	501	GDP	C6-N1	-2.60	1.34	1.37
4	KD	501	GDP	C6-N1	-2.56	1.34	1.37
4	HF	501	GDP	C6-N1	-2.53	1.34	1.37
4	CF	501	GDP	C6-N1	-2.52	1.34	1.37
4	IF	501	GDP	C6-N1	-2.51	1.34	1.37
4	CB	501	GDP	C6-N1	-2.51	1.34	1.37
4	ED	501	GDP	C6-N1	-2.50	1.34	1.37
4	HD	501	GDP	C6-N1	-2.49	1.34	1.37
4	IH	501	GDP	C6-N1	-2.49	1.34	1.37
4	AF	501	GDP	C6-N1	-2.47	1.34	1.37
5	AC	501	GTP	C2-N3	2.21	1.38	1.33
5	HE	501	GTP	C2-N3	2.21	1.38	1.33
5	DE	501	GTP	C2-N3	2.19	1.38	1.33
5	MC	501	GTP	C2-N3	2.18	1.38	1.33
5	FC	501	GTP	C2-N3	2.17	1.38	1.33
5	AE	501	GTP	C2-N3	2.16	1.38	1.33
5	JC	501	GTP	C2-N3	2.16	1.38	1.33
5	EG	501	GTP	C2-N3	2.16	1.38	1.33
5	KC	501	GTP	C2-N3	2.16	1.38	1.33
5	LE	501	GTP	C2-N3	2.15	1.38	1.33
5	IE	501	GTP	C2-N3	2.15	1.38	1.33
5	IG	501	GTP	C2-N3	2.15	1.38	1.33
5	DG	501	GTP	C2-N3	2.15	1.38	1.33
5	HC	501	GTP	C2-N3	2.14	1.38	1.33
5	CE	501	GTP	C2-N3	2.14	1.38	1.33
5	MA	501	GTP	C2-N3	2.14	1.38	1.33
5	KG	501	GTP	C2-N3	2.14	1.38	1.33
5	JE	501	GTP	C2-N3	2.14	1.38	1.33
5	GE	501	GTP	C2-N3	2.13	1.38	1.33
5	CG	501	GTP	C2-N3	2.13	1.38	1.33
5	FE	501	GTP	C2-N3	2.13	1.38	1.33
5	GG	501	GTP	C2-N3	2.12	1.38	1.33
5	EE	501	GTP	C2-N3	2.12	1.38	1.33
5	ME	501	GTP	C2-N3	2.12	1.38	1.33
5	HG	501	GTP	C2-N3	2.11	1.38	1.33
5	IC	501	GTP	C2-N3	2.10	1.38	1.33
5	BC	501	GTP	C2-N3	2.09	1.38	1.33
5	BE	501	GTP	C2-N3	2.08	1.38	1.33
5	CC	501	GTP	C2-N3	2.08	1.38	1.33
5	EC	501	GTP	C2-N3	2.08	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	GC	501	GTP	C2-N3	2.07	1.38	1.33
5	JG	501	GTP	C2-N3	2.07	1.38	1.33
5	LA	501	GTP	C2-N3	2.06	1.38	1.33
5	KE	501	GTP	C2-N3	2.06	1.38	1.33
5	LC	501	GTP	C2-N3	2.04	1.38	1.33
5	EC	501	GTP	C5-C4	-2.02	1.37	1.43
5	DC	501	GTP	C2-N3	2.01	1.38	1.33

All (407) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	CG	501	GTP	PB-O3B-PG	-4.49	117.40	132.83
4	HF	501	GDP	PA-O3A-PB	-4.49	117.41	132.83
5	AC	501	GTP	PB-O3B-PG	-4.48	117.46	132.83
4	CD	501	GDP	PA-O3A-PB	-4.43	117.61	132.83
4	IH	501	GDP	PA-O3A-PB	-4.38	117.78	132.83
5	DE	501	GTP	PB-O3B-PG	-4.38	117.78	132.83
4	MD	501	GDP	PA-O3A-PB	-4.36	117.88	132.83
4	GD	501	GDP	PA-O3A-PB	-4.31	118.03	132.83
5	EE	501	GTP	PA-O3A-PB	-4.28	118.16	132.83
5	GC	501	GTP	PA-O3A-PB	-4.27	118.18	132.83
4	DF	501	GDP	PA-O3A-PB	-4.25	118.24	132.83
5	GG	501	GTP	PA-O3A-PB	-4.25	118.26	132.83
5	BE	501	GTP	PA-O3A-PB	-4.23	118.30	132.83
4	EF	501	GDP	PA-O3A-PB	-4.17	118.51	132.83
4	HD	501	GDP	PA-O3A-PB	-4.13	118.66	132.83
5	EG	501	GTP	PB-O3B-PG	-4.13	118.67	132.83
5	JG	501	GTP	PB-O3B-PG	-4.10	118.76	132.83
5	JE	501	GTP	PB-O3B-PG	-4.09	118.79	132.83
5	BG	501	GTP	PA-O3A-PB	-4.09	118.81	132.83
5	DC	501	GTP	PB-O3B-PG	-4.06	118.90	132.83
4	KD	501	GDP	PA-O3A-PB	-4.06	118.90	132.83
4	FH	501	GDP	PA-O3A-PB	-4.03	118.98	132.83
5	JC	501	GTP	PB-O3B-PG	-4.03	119.01	132.83
5	FG	501	GTP	PA-O3A-PB	-4.02	119.02	132.83
4	AD	501	GDP	PA-O3A-PB	-4.01	119.08	132.83
4	DD	501	GDP	PA-O3A-PB	-3.97	119.20	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	IE	501	GTP	PB-O3B-PG	-3.96	119.22	132.83
5	GC	501	GTP	PB-O3B-PG	-3.94	119.31	132.83
5	DC	501	GTP	PA-O3A-PB	-3.94	119.31	132.83
5	EG	501	GTP	PA-O3A-PB	-3.90	119.43	132.83
4	EB	501	GDP	PA-O3A-PB	-3.90	119.45	132.83
5	DG	501	GTP	PB-O3B-PG	-3.90	119.46	132.83
4	CF	501	GDP	PA-O3A-PB	-3.89	119.47	132.83
4	MF	501	GDP	PA-O3A-PB	-3.88	119.53	132.83
4	LD	501	GDP	PA-O3A-PB	-3.86	119.59	132.83
5	FC	501	GTP	PA-O3A-PB	-3.86	119.59	132.83
5	LA	501	GTP	PB-O3B-PG	-3.85	119.60	132.83
5	GE	501	GTP	PB-O3B-PG	-3.84	119.63	132.83
4	AF	501	GDP	PA-O3A-PB	-3.84	119.66	132.83
4	GH	501	GDP	PA-O3A-PB	-3.83	119.67	132.83
5	LE	501	GTP	PB-O3B-PG	-3.82	119.71	132.83
5	FG	501	GTP	PB-O3B-PG	-3.82	119.72	132.83
5	FC	501	GTP	PB-O3B-PG	-3.82	119.72	132.83
5	HE	501	GTP	PA-O3A-PB	-3.81	119.76	132.83
5	CE	501	GTP	PA-O3A-PB	-3.79	119.81	132.83
5	EE	501	GTP	PB-O3B-PG	-3.79	119.81	132.83
4	ED	501	GDP	PA-O3A-PB	-3.78	119.84	132.83
4	KH	501	GDP	PA-O3A-PB	-3.78	119.85	132.83
5	HG	501	GTP	PB-O3B-PG	-3.77	119.90	132.83
5	HG	501	GTP	PA-O3A-PB	-3.77	119.90	132.83
5	KG	501	GTP	PB-O3B-PG	-3.75	119.96	132.83
5	GE	501	GTP	PA-O3A-PB	-3.74	120.01	132.83
5	CE	501	GTP	PB-O3B-PG	-3.73	120.04	132.83
5	MC	501	GTP	PB-O3B-PG	-3.73	120.04	132.83
4	AB	501	GDP	PA-O3A-PB	-3.72	120.06	132.83
5	HE	501	GTP	PB-O3B-PG	-3.70	120.15	132.83
5	MA	501	GTP	PA-O3A-PB	-3.68	120.21	132.83
5	FE	501	GTP	PB-O3B-PG	-3.67	120.22	132.83
4	FF	501	GDP	PA-O3A-PB	-3.67	120.23	132.83
5	FE	501	GTP	PA-O3A-PB	-3.66	120.26	132.83
5	CG	501	GTP	PA-O3A-PB	-3.65	120.30	132.83
5	LC	501	GTP	PB-O3B-PG	-3.65	120.31	132.83
5	IC	501	GTP	PB-O3B-PG	-3.64	120.34	132.83
5	EC	501	GTP	PB-O3B-PG	-3.63	120.36	132.83
5	BG	501	GTP	PB-O3B-PG	-3.62	120.39	132.83
4	DB	501	GDP	PA-O3A-PB	-3.61	120.45	132.83
5	DG	501	GTP	PA-O3A-PB	-3.60	120.48	132.83
5	AE	501	GTP	PB-O3B-PG	-3.59	120.52	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	ME	501	GTP	PB-O3B-PG	-3.58	120.53	132.83
5	MA	501	GTP	PB-O3B-PG	-3.58	120.54	132.83
4	JD	501	GDP	C3'-C2'-C1'	3.58	106.37	100.98
5	BE	501	GTP	PB-O3B-PG	-3.57	120.59	132.83
5	IC	501	GTP	PA-O3A-PB	-3.54	120.67	132.83
5	KE	501	GTP	PB-O3B-PG	-3.54	120.69	132.83
5	GE	501	GTP	C5-C6-N1	3.53	120.19	113.95
5	HC	501	GTP	PB-O3B-PG	-3.51	120.77	132.83
5	ME	501	GTP	C5-C6-N1	3.50	120.12	113.95
5	AC	501	GTP	PA-O3A-PB	-3.49	120.84	132.83
5	KC	501	GTP	PB-O3B-PG	-3.49	120.85	132.83
5	EG	501	GTP	C5-C6-N1	3.48	120.09	113.95
5	ME	501	GTP	PA-O3A-PB	-3.48	120.90	132.83
5	CE	501	GTP	C5-C6-N1	3.46	120.06	113.95
5	LE	501	GTP	C5-C6-N1	3.44	120.03	113.95
5	KE	501	GTP	C5-C6-N1	3.43	120.02	113.95
4	IF	501	GDP	PA-O3A-PB	-3.43	121.06	132.83
4	BA	501	GDP	PA-O3A-PB	-3.43	121.07	132.83
5	AC	501	GTP	C5-C6-N1	3.42	119.99	113.95
5	EC	501	GTP	C5-C6-N1	3.41	119.97	113.95
5	GC	501	GTP	C5-C6-N1	3.39	119.93	113.95
5	MC	501	GTP	C5-C6-N1	3.39	119.93	113.95
4	AD	501	GDP	C3'-C2'-C1'	3.38	106.07	100.98
5	DE	501	GTP	PA-O3A-PB	-3.37	121.27	132.83
5	LA	501	GTP	C5-C6-N1	3.36	119.89	113.95
5	DG	501	GTP	C5-C6-N1	3.36	119.88	113.95
5	EE	501	GTP	C5-C6-N1	3.35	119.87	113.95
5	KC	501	GTP	C5-C6-N1	3.34	119.84	113.95
5	JG	501	GTP	C5-C6-N1	3.33	119.84	113.95
5	DE	501	GTP	C5-C6-N1	3.33	119.83	113.95
5	BE	501	GTP	C5-C6-N1	3.31	119.81	113.95
5	LC	501	GTP	C5-C6-N1	3.31	119.80	113.95
5	JE	501	GTP	C5-C6-N1	3.31	119.79	113.95
4	AB	501	GDP	C3'-C2'-C1'	3.31	105.96	100.98
5	GG	501	GTP	C5-C6-N1	3.31	119.79	113.95
5	JC	501	GTP	C5-C6-N1	3.31	119.79	113.95
5	LE	501	GTP	PA-O3A-PB	-3.29	121.52	132.83
4	LB	501	GDP	PA-O3A-PB	-3.28	121.57	132.83
4	CB	501	GDP	PA-O3A-PB	-3.28	121.58	132.83
5	FE	501	GTP	C5-C6-N1	3.27	119.73	113.95
5	HG	501	GTP	C5-C6-N1	3.27	119.73	113.95
5	LA	501	GTP	PA-O3A-PB	-3.27	121.61	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FG	501	GTP	C5-C6-N1	3.27	119.72	113.95
5	MA	501	GTP	C5-C6-N1	3.27	119.72	113.95
5	HC	501	GTP	C5-C6-N1	3.26	119.72	113.95
5	IG	501	GTP	C5-C6-N1	3.25	119.70	113.95
5	FC	501	GTP	C5-C6-N1	3.25	119.69	113.95
5	BC	501	GTP	C5-C6-N1	3.25	119.69	113.95
4	IH	501	GDP	C3'-C2'-C1'	3.24	105.86	100.98
4	GH	501	GDP	C3'-C2'-C1'	3.24	105.86	100.98
5	EC	501	GTP	C8-N7-C5	3.24	109.16	102.99
5	IE	501	GTP	C5-C6-N1	3.23	119.66	113.95
5	KG	501	GTP	C5-C6-N1	3.23	119.66	113.95
5	HE	501	GTP	C5-C6-N1	3.22	119.64	113.95
5	IC	501	GTP	C5-C6-N1	3.22	119.63	113.95
5	CC	501	GTP	C5-C6-N1	3.22	119.63	113.95
5	KE	501	GTP	PA-O3A-PB	-3.21	121.81	132.83
5	DC	501	GTP	C5-C6-N1	3.21	119.61	113.95
5	BC	501	GTP	PA-O3A-PB	-3.21	121.83	132.83
5	CG	501	GTP	C5-C6-N1	3.20	119.60	113.95
5	HC	501	GTP	PA-O3A-PB	-3.20	121.86	132.83
5	JE	501	GTP	C8-N7-C5	3.19	109.08	102.99
5	BG	501	GTP	C5-C6-N1	3.19	119.58	113.95
4	MF	501	GDP	C3'-C2'-C1'	3.18	105.76	100.98
4	BD	501	GDP	PA-O3A-PB	-3.17	121.94	132.83
5	AE	501	GTP	C5-C6-N1	3.17	119.55	113.95
5	IE	501	GTP	PA-O3A-PB	-3.17	121.95	132.83
5	LA	501	GTP	C2-N1-C6	-3.16	119.28	125.10
5	JC	501	GTP	C8-N7-C5	3.14	108.98	102.99
5	MC	501	GTP	C8-N7-C5	3.13	108.96	102.99
4	JF	501	GDP	C3'-C2'-C1'	3.12	105.68	100.98
5	HG	501	GTP	C3'-C2'-C1'	3.12	105.68	100.98
5	EG	501	GTP	C3'-C2'-C1'	3.12	105.67	100.98
5	CG	501	GTP	C8-N7-C5	3.11	108.91	102.99
5	FC	501	GTP	C8-N7-C5	3.10	108.89	102.99
4	JD	501	GDP	PA-O3A-PB	-3.09	122.24	132.83
5	CE	501	GTP	C8-N7-C5	3.07	108.84	102.99
5	CC	501	GTP	PB-O3B-PG	-3.07	122.30	132.83
4	FH	501	GDP	C3'-C2'-C1'	3.06	105.59	100.98
5	KC	501	GTP	C8-N7-C5	3.06	108.82	102.99
5	CE	501	GTP	C2-N1-C6	-3.06	119.46	125.10
5	KG	501	GTP	C8-N7-C5	3.06	108.82	102.99
5	ME	501	GTP	C8-N7-C5	3.06	108.81	102.99
5	AC	501	GTP	C2-N1-C6	-3.05	119.49	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	EE	501	GTP	C8-N7-C5	3.05	108.79	102.99
5	LC	501	GTP	C2-N1-C6	-3.04	119.49	125.10
5	LA	501	GTP	C8-N7-C5	3.04	108.78	102.99
5	EG	501	GTP	C2-N1-C6	-3.04	119.51	125.10
5	IG	501	GTP	C8-N7-C5	3.03	108.76	102.99
5	ME	501	GTP	C2-N1-C6	-3.03	119.52	125.10
4	DB	501	GDP	C3'-C2'-C1'	3.03	105.53	100.98
4	HF	501	GDP	C3'-C2'-C1'	3.02	105.53	100.98
5	BC	501	GTP	C8-N7-C5	3.02	108.73	102.99
5	BE	501	GTP	C2-N1-C6	-3.01	119.55	125.10
5	JG	501	GTP	C8-N7-C5	3.01	108.73	102.99
5	MA	501	GTP	C8-N7-C5	3.01	108.73	102.99
5	GE	501	GTP	C8-N7-C5	3.01	108.73	102.99
5	FE	501	GTP	C8-N7-C5	3.01	108.72	102.99
5	GG	501	GTP	C8-N7-C5	3.01	108.72	102.99
5	AC	501	GTP	C3'-C2'-C1'	3.00	105.50	100.98
5	LE	501	GTP	C2-N1-C6	-3.00	119.57	125.10
5	EE	501	GTP	C2-N1-C6	-3.00	119.58	125.10
5	DE	501	GTP	C8-N7-C5	3.00	108.70	102.99
5	DG	501	GTP	C8-N7-C5	2.99	108.69	102.99
5	JG	501	GTP	C2-N1-C6	-2.98	119.61	125.10
5	DC	501	GTP	C8-N7-C5	2.98	108.66	102.99
5	MC	501	GTP	C2-N1-C6	-2.97	119.62	125.10
5	GG	501	GTP	C2-N1-C6	-2.97	119.62	125.10
5	KE	501	GTP	C8-N7-C5	2.97	108.65	102.99
4	BD	501	GDP	C3'-C2'-C1'	2.97	105.45	100.98
5	BE	501	GTP	C8-N7-C5	2.96	108.64	102.99
5	GC	501	GTP	C2-N1-C6	-2.96	119.64	125.10
5	LE	501	GTP	C8-N7-C5	2.96	108.63	102.99
5	CC	501	GTP	C8-N7-C5	2.95	108.61	102.99
5	AC	501	GTP	C8-N7-C5	2.95	108.61	102.99
5	IC	501	GTP	C8-N7-C5	2.95	108.60	102.99
5	LC	501	GTP	PA-O3A-PB	-2.94	122.72	132.83
5	BC	501	GTP	C2-N1-C6	-2.94	119.68	125.10
5	EC	501	GTP	C2-N1-C6	-2.94	119.68	125.10
4	AF	501	GDP	C3'-C2'-C1'	2.94	105.40	100.98
5	DG	501	GTP	C2-N1-C6	-2.94	119.69	125.10
5	LC	501	GTP	C8-N7-C5	2.94	108.58	102.99
4	FD	501	GDP	PA-O3A-PB	-2.93	122.76	132.83
5	DE	501	GTP	C2-N1-C6	-2.93	119.70	125.10
5	JC	501	GTP	PA-O3A-PB	-2.93	122.78	132.83
4	BF	501	GDP	C3'-C2'-C1'	2.92	105.38	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FE	501	GTP	C2-N1-C6	-2.92	119.72	125.10
5	HE	501	GTP	C8-N7-C5	2.92	108.55	102.99
5	IG	501	GTP	C2-N1-C6	-2.91	119.73	125.10
5	FC	501	GTP	C2-N1-C6	-2.91	119.74	125.10
5	HC	501	GTP	C2-N1-C6	-2.91	119.74	125.10
5	FG	501	GTP	C8-N7-C5	2.91	108.53	102.99
5	KG	501	GTP	PA-O3A-PB	-2.91	122.86	132.83
5	KG	501	GTP	C2-N1-C6	-2.90	119.76	125.10
5	IC	501	GTP	C3'-C2'-C1'	2.90	105.34	100.98
5	KE	501	GTP	C2-N1-C6	-2.89	119.77	125.10
4	JF	501	GDP	PA-O3A-PB	-2.89	122.91	132.83
4	MB	501	GDP	C3'-C2'-C1'	2.89	105.33	100.98
5	JC	501	GTP	C2-N1-C6	-2.89	119.78	125.10
5	IC	501	GTP	C2-N1-C6	-2.89	119.78	125.10
5	CG	501	GTP	C2-N1-C6	-2.89	119.78	125.10
5	GC	501	GTP	C8-N7-C5	2.88	108.48	102.99
5	BG	501	GTP	C8-N7-C5	2.88	108.48	102.99
5	HE	501	GTP	C2-N1-C6	-2.88	119.79	125.10
5	BG	501	GTP	C2-N1-C6	-2.88	119.80	125.10
4	BF	501	GDP	PA-O3A-PB	-2.87	122.99	132.83
5	EG	501	GTP	C8-N7-C5	2.86	108.44	102.99
5	BC	501	GTP	PB-O3B-PG	-2.86	123.01	132.83
5	KC	501	GTP	C2-N1-C6	-2.86	119.84	125.10
5	JE	501	GTP	PA-O3A-PB	-2.86	123.02	132.83
5	HG	501	GTP	C8-N7-C5	2.85	108.43	102.99
5	AE	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
5	CC	501	GTP	C2-N1-C6	-2.85	119.86	125.10
4	HH	501	GDP	C3'-C2'-C1'	2.84	105.26	100.98
5	AE	501	GTP	C8-N7-C5	2.84	108.40	102.99
5	FG	501	GTP	C2-N1-C6	-2.84	119.87	125.10
5	MA	501	GTP	C2-N1-C6	-2.83	119.88	125.10
4	IF	501	GDP	C3'-C2'-C1'	2.83	105.24	100.98
5	FE	501	GTP	C3'-C2'-C1'	2.83	105.24	100.98
5	GC	501	GTP	C3'-C2'-C1'	2.83	105.23	100.98
5	GE	501	GTP	C2-N1-C6	-2.82	119.91	125.10
5	GE	501	GTP	C3'-C2'-C1'	2.82	105.22	100.98
5	JE	501	GTP	C2-N1-C6	-2.81	119.92	125.10
5	IE	501	GTP	C2-N1-C6	-2.81	119.92	125.10
5	HG	501	GTP	C2-N1-C6	-2.81	119.92	125.10
4	BA	501	GDP	C3'-C2'-C1'	2.81	105.21	100.98
5	DC	501	GTP	C2-N1-C6	-2.79	119.96	125.10
5	JE	501	GTP	C3'-C2'-C1'	2.78	105.17	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	HC	501	GTP	C3'-C2'-C1'	2.77	105.15	100.98
5	CC	501	GTP	PA-O3A-PB	-2.77	123.33	132.83
4	HD	501	GDP	C3'-C2'-C1'	2.75	105.12	100.98
5	IE	501	GTP	C3'-C2'-C1'	2.75	105.12	100.98
5	AE	501	GTP	C2-N1-C6	-2.74	120.05	125.10
5	KC	501	GTP	C3'-C2'-C1'	2.74	105.10	100.98
5	BG	501	GTP	C3'-C2'-C1'	2.73	105.09	100.98
5	ME	501	GTP	C3'-C2'-C1'	2.73	105.09	100.98
5	AE	501	GTP	PA-O3A-PB	-2.72	123.48	132.83
5	HC	501	GTP	C8-N7-C5	2.72	108.17	102.99
4	DD	501	GDP	C3'-C2'-C1'	2.72	105.07	100.98
4	FD	501	GDP	C3'-C2'-C1'	2.72	105.07	100.98
5	BE	501	GTP	C3'-C2'-C1'	2.71	105.06	100.98
5	JG	501	GTP	C3'-C2'-C1'	2.71	105.06	100.98
4	FF	501	GDP	C3'-C2'-C1'	2.69	105.03	100.98
5	BC	501	GTP	C3'-C2'-C1'	2.69	105.02	100.98
5	IE	501	GTP	C8-N7-C5	2.68	108.09	102.99
4	GF	501	GDP	C3'-C2'-C1'	2.66	104.98	100.98
5	IG	501	GTP	PA-O3A-PB	-2.66	123.70	132.83
4	CB	501	GDP	C3'-C2'-C1'	2.65	104.97	100.98
5	GG	501	GTP	C3'-C2'-C1'	2.64	104.96	100.98
5	KG	501	GTP	C3'-C2'-C1'	2.63	104.94	100.98
5	JC	501	GTP	C3'-C2'-C1'	2.62	104.92	100.98
5	MA	501	GTP	C3'-C2'-C1'	2.61	104.91	100.98
5	EG	501	GTP	O6-C6-C5	-2.61	119.28	124.37
4	ID	501	GDP	O3B-PB-O3A	2.60	113.35	104.64
5	IG	501	GTP	C3'-C2'-C1'	2.60	104.89	100.98
5	LE	501	GTP	C3'-C2'-C1'	2.60	104.89	100.98
5	LA	501	GTP	C3'-C2'-C1'	2.60	104.89	100.98
4	MB	501	GDP	PA-O3A-PB	-2.58	123.97	132.83
4	ED	501	GDP	C5-C6-N1	2.58	118.50	113.95
4	KH	501	GDP	C3'-C2'-C1'	2.58	104.86	100.98
4	LD	501	GDP	C3'-C2'-C1'	2.54	104.80	100.98
5	FC	501	GTP	C3'-C2'-C1'	2.53	104.79	100.98
4	LF	501	GDP	C5-C6-N1	2.51	118.39	113.95
5	CE	501	GTP	C3'-C2'-C1'	2.50	104.74	100.98
4	LD	501	GDP	C5-C6-N1	2.50	118.36	113.95
5	MC	501	GTP	C3'-C2'-C1'	2.49	104.72	100.98
4	ID	501	GDP	C8-N7-C5	2.48	107.72	102.99
4	ED	501	GDP	C8-N7-C5	2.48	107.72	102.99
4	DF	501	GDP	C3'-C2'-C1'	2.48	104.71	100.98
5	HE	501	GTP	C3'-C2'-C1'	2.47	104.70	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	HC	501	GTP	O6-C6-C5	-2.46	119.57	124.37
4	KD	501	GDP	C8-N7-C5	2.45	107.65	102.99
5	IE	501	GTP	O6-C6-C5	-2.44	119.61	124.37
4	GH	501	GDP	C5-C6-N1	2.43	118.25	113.95
5	MC	501	GTP	O6-C6-C5	-2.43	119.62	124.37
4	IH	501	GDP	C5-C6-N1	2.42	118.22	113.95
4	DB	501	GDP	C5-C6-N1	2.40	118.20	113.95
5	BE	501	GTP	O6-C6-C5	-2.40	119.68	124.37
4	AD	501	GDP	C5-C6-N1	2.40	118.20	113.95
4	GD	501	GDP	C3'-C2'-C1'	2.40	104.59	100.98
4	JD	501	GDP	C5-C6-N1	2.40	118.19	113.95
4	KF	501	GDP	C5-C6-N1	2.40	118.19	113.95
4	GF	501	GDP	C5-C6-N1	2.39	118.18	113.95
4	FF	501	GDP	C8-N7-C5	2.39	107.54	102.99
4	EF	501	GDP	C5-C6-N1	2.38	118.16	113.95
4	FF	501	GDP	C5-C6-N1	2.38	118.16	113.95
4	MF	501	GDP	C5-C6-N1	2.38	118.16	113.95
5	CG	501	GTP	C3'-C2'-C1'	2.38	104.56	100.98
4	JF	501	GDP	C5-C6-N1	2.38	118.15	113.95
4	MD	501	GDP	C5-C6-N1	2.38	118.15	113.95
4	JF	501	GDP	C8-N7-C5	2.37	107.50	102.99
4	AB	501	GDP	C5-C6-N1	2.37	118.14	113.95
4	KF	501	GDP	PA-O3A-PB	-2.37	124.70	132.83
4	LF	501	GDP	C3'-C2'-C1'	2.36	104.54	100.98
5	DE	501	GTP	C3'-C2'-C1'	2.36	104.54	100.98
5	ME	501	GTP	O6-C6-C5	-2.36	119.75	124.37
4	EB	501	GDP	C8-N7-C5	2.36	107.49	102.99
4	EB	501	GDP	C3'-C2'-C1'	2.36	104.53	100.98
4	FH	501	GDP	C5-C6-N1	2.35	118.11	113.95
5	GG	501	GTP	O6-C6-C5	-2.35	119.78	124.37
4	CF	501	GDP	C3'-C2'-C1'	2.35	104.52	100.98
5	HG	501	GTP	O6-C6-C5	-2.35	119.79	124.37
4	EB	501	GDP	C5-C6-N1	2.34	118.09	113.95
4	LB	501	GDP	C8-N7-C5	2.34	107.45	102.99
4	CB	501	GDP	C8-N7-C5	2.34	107.45	102.99
4	FD	501	GDP	C5-C6-N1	2.34	118.08	113.95
4	KF	501	GDP	C8-N7-C5	2.33	107.44	102.99
4	MB	501	GDP	C8-N7-C5	2.33	107.44	102.99
4	MB	501	GDP	C5-C6-N1	2.33	118.07	113.95
5	CE	501	GTP	O6-C6-C5	-2.33	119.83	124.37
4	DF	501	GDP	C5-C6-N1	2.33	118.06	113.95
4	LD	501	GDP	C8-N7-C5	2.32	107.42	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	HD	501	GDP	C5-C6-N1	2.32	118.05	113.95
4	LF	501	GDP	O6-C6-C5	-2.32	119.85	124.37
5	IG	501	GTP	O6-C6-C5	-2.32	119.85	124.37
4	FD	501	GDP	C8-N7-C5	2.32	107.40	102.99
4	DD	501	GDP	C5-C6-N1	2.31	118.04	113.95
4	MD	501	GDP	C3'-C2'-C1'	2.31	104.46	100.98
4	KD	501	GDP	C5-C6-N1	2.31	118.03	113.95
4	HF	501	GDP	C8-N7-C5	2.31	107.39	102.99
4	BA	501	GDP	C8-N7-C5	2.31	107.39	102.99
5	GC	501	GTP	O6-C6-C5	-2.31	119.87	124.37
4	BA	501	GDP	C5-C6-N1	2.30	118.02	113.95
4	CD	501	GDP	C5-C6-N1	2.30	118.02	113.95
4	DF	501	GDP	C8-N7-C5	2.30	107.38	102.99
4	HH	501	GDP	C5-C6-N1	2.30	118.01	113.95
4	KH	501	GDP	C5-C6-N1	2.30	118.01	113.95
4	BD	501	GDP	C5-C6-N1	2.30	118.00	113.95
5	LC	501	GTP	O6-C6-C5	-2.29	119.89	124.37
4	IF	501	GDP	C8-N7-C5	2.29	107.36	102.99
4	ID	501	GDP	PA-O3A-PB	-2.29	124.96	132.83
5	KE	501	GTP	O6-C6-C5	-2.29	119.89	124.37
4	CF	501	GDP	C5-C6-N1	2.29	118.00	113.95
4	ID	501	GDP	C5-C6-N1	2.29	117.99	113.95
4	CB	501	GDP	C5-C6-N1	2.28	117.98	113.95
4	GD	501	GDP	C8-N7-C5	2.28	107.33	102.99
4	LB	501	GDP	C5-C6-N1	2.28	117.97	113.95
4	CD	501	GDP	C8-N7-C5	2.27	107.32	102.99
4	MD	501	GDP	C8-N7-C5	2.27	107.31	102.99
4	DD	501	GDP	C8-N7-C5	2.27	107.31	102.99
4	FH	501	GDP	C8-N7-C5	2.26	107.30	102.99
4	AB	501	GDP	C8-N7-C5	2.26	107.30	102.99
4	GF	501	GDP	C8-N7-C5	2.26	107.30	102.99
4	MF	501	GDP	C8-N7-C5	2.26	107.29	102.99
4	DB	501	GDP	C8-N7-C5	2.24	107.27	102.99
4	KD	501	GDP	C3'-C2'-C1'	2.24	104.36	100.98
5	LE	501	GTP	O6-C6-C5	-2.24	119.99	124.37
4	HD	501	GDP	C8-N7-C5	2.24	107.26	102.99
4	EF	501	GDP	C8-N7-C5	2.24	107.26	102.99
4	IF	501	GDP	C5-C6-N1	2.24	117.90	113.95
4	BF	501	GDP	C5-C6-N1	2.24	117.90	113.95
4	GD	501	GDP	C5-C6-N1	2.22	117.87	113.95
4	HF	501	GDP	C5-C6-N1	2.22	117.87	113.95
4	BD	501	GDP	C8-N7-C5	2.21	107.21	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	IH	501	GDP	C8-N7-C5	2.21	107.21	102.99
4	LF	501	GDP	PA-O3A-PB	-2.21	125.23	132.83
5	FG	501	GTP	O6-C6-C5	-2.21	120.05	124.37
5	EC	501	GTP	C3'-C2'-C1'	2.21	104.31	100.98
4	GH	501	GDP	C8-N7-C5	2.21	107.20	102.99
5	BC	501	GTP	O6-C6-C5	-2.20	120.07	124.37
4	BF	501	GDP	C8-N7-C5	2.20	107.18	102.99
4	CD	501	GDP	C3'-C2'-C1'	2.19	104.27	100.98
4	KH	501	GDP	C8-N7-C5	2.18	107.15	102.99
4	CF	501	GDP	C8-N7-C5	2.18	107.14	102.99
5	FE	501	GTP	O6-C6-C5	-2.18	120.12	124.37
5	DC	501	GTP	O6-C6-C5	-2.18	120.12	124.37
4	JD	501	GDP	C8-N7-C5	2.17	107.13	102.99
5	KC	501	GTP	O6-C6-C5	-2.17	120.12	124.37
4	LB	501	GDP	C3'-C2'-C1'	2.17	104.25	100.98
5	DE	501	GTP	O6-C6-C5	-2.16	120.16	124.37
5	AC	501	GTP	O6-C6-C5	-2.16	120.16	124.37
5	MA	501	GTP	O6-C6-C5	-2.15	120.18	124.37
5	ME	501	GTP	C2'-C3'-C4'	2.14	106.80	102.64
4	HH	501	GDP	C8-N7-C5	2.14	107.06	102.99
5	FC	501	GTP	O6-C6-C5	-2.13	120.21	124.37
4	LF	501	GDP	C8-N7-C5	2.13	107.04	102.99
5	CC	501	GTP	O6-C6-C5	-2.12	120.23	124.37
4	AF	501	GDP	C2'-C3'-C4'	2.12	106.76	102.64
5	LA	501	GTP	O6-C6-C5	-2.11	120.25	124.37
5	IC	501	GTP	O6-C6-C5	-2.10	120.27	124.37
5	AE	501	GTP	O6-C6-C5	-2.09	120.28	124.37
5	DG	501	GTP	O6-C6-C5	-2.09	120.29	124.37
5	HE	501	GTP	O6-C6-C5	-2.07	120.33	124.37
4	ED	501	GDP	C3'-C2'-C1'	2.05	104.07	100.98
5	JC	501	GTP	O6-C6-C5	-2.05	120.36	124.37
4	IH	501	GDP	O6-C6-C5	-2.05	120.37	124.37
5	CG	501	GTP	O6-C6-C5	-2.05	120.38	124.37
5	KC	501	GTP	PA-O3A-PB	-2.05	125.81	132.83
5	JG	501	GTP	O6-C6-C5	-2.04	120.38	124.37
4	LF	501	GDP	O3B-PB-O3A	2.04	111.48	104.64
4	GF	501	GDP	O6-C6-C5	-2.04	120.39	124.37
4	MB	501	GDP	O3B-PB-O3A	2.02	111.41	104.64
4	LD	501	GDP	O6-C6-C5	-2.01	120.44	124.37
4	KH	501	GDP	C2'-C3'-C4'	2.00	106.54	102.64

There are no chirality outliers.

All (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'
4	AF	501	GDP	C3'-C4'-C5'-O5'
4	BA	501	GDP	C5'-O5'-PA-O1A
4	BD	501	GDP	C5'-O5'-PA-O1A
4	BF	501	GDP	C5'-O5'-PA-O1A
4	CB	501	GDP	PA-O3A-PB-O2B
4	CD	501	GDP	C5'-O5'-PA-O1A
4	CF	501	GDP	C5'-O5'-PA-O1A
4	DB	501	GDP	C5'-O5'-PA-O3A
4	DB	501	GDP	C5'-O5'-PA-O1A
4	EB	501	GDP	C5'-O5'-PA-O1A
4	EF	501	GDP	C5'-O5'-PA-O3A
4	EF	501	GDP	C5'-O5'-PA-O1A
4	FF	501	GDP	C5'-O5'-PA-O3A
4	FF	501	GDP	C5'-O5'-PA-O1A
4	FH	501	GDP	C5'-O5'-PA-O3A
4	FH	501	GDP	C5'-O5'-PA-O2A
4	GD	501	GDP	C5'-O5'-PA-O1A
4	GF	501	GDP	C5'-O5'-PA-O3A
4	GF	501	GDP	C5'-O5'-PA-O1A
4	GH	501	GDP	C5'-O5'-PA-O1A
4	GH	501	GDP	C5'-O5'-PA-O2A
4	HD	501	GDP	C5'-O5'-PA-O3A
4	HD	501	GDP	C5'-O5'-PA-O1A
4	HF	501	GDP	C5'-O5'-PA-O1A
4	HH	501	GDP	C5'-O5'-PA-O1A
4	ID	501	GDP	C5'-O5'-PA-O1A
4	IF	501	GDP	C5'-O5'-PA-O3A
4	JD	501	GDP	C5'-O5'-PA-O1A
4	JF	501	GDP	C5'-O5'-PA-O3A
4	JF	501	GDP	C5'-O5'-PA-O1A
4	KH	501	GDP	C5'-O5'-PA-O1A
4	LB	501	GDP	C5'-O5'-PA-O3A
4	LB	501	GDP	C5'-O5'-PA-O1A
4	LD	501	GDP	PA-O3A-PB-O2B
4	LD	501	GDP	PA-O3A-PB-O3B
4	MB	501	GDP	C5'-O5'-PA-O3A
4	MB	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	MD	501	GDP	C5'-O5'-PA-O3A
4	MD	501	GDP	C5'-O5'-PA-O1A
4	MF	501	GDP	C5'-O5'-PA-O3A
4	MF	501	GDP	C5'-O5'-PA-O1A
5	AC	501	GTP	C5'-O5'-PA-O1A
5	AE	501	GTP	PB-O3A-PA-O5'
5	BE	501	GTP	C5'-O5'-PA-O1A
5	BG	501	GTP	C5'-O5'-PA-O1A
5	BG	501	GTP	C5'-O5'-PA-O2A
5	CC	501	GTP	C5'-O5'-PA-O3A
5	CC	501	GTP	C5'-O5'-PA-O1A
5	CE	501	GTP	C5'-O5'-PA-O1A
5	CE	501	GTP	C5'-O5'-PA-O2A
5	CG	501	GTP	C5'-O5'-PA-O1A
5	CG	501	GTP	C5'-O5'-PA-O2A
5	DC	501	GTP	C5'-O5'-PA-O1A
5	DE	501	GTP	C5'-O5'-PA-O1A
5	DE	501	GTP	C5'-O5'-PA-O2A
5	DG	501	GTP	C5'-O5'-PA-O1A
5	DG	501	GTP	C5'-O5'-PA-O2A
5	EC	501	GTP	C3'-C4'-C5'-O5'
5	EG	501	GTP	O4'-C4'-C5'-O5'
5	EG	501	GTP	C3'-C4'-C5'-O5'
5	FC	501	GTP	C5'-O5'-PA-O1A
5	FC	501	GTP	C5'-O5'-PA-O2A
5	FE	501	GTP	C5'-O5'-PA-O1A
5	FG	501	GTP	C5'-O5'-PA-O1A
5	GC	501	GTP	C5'-O5'-PA-O1A
5	GE	501	GTP	PB-O3B-PG-O3G
5	HC	501	GTP	C5'-O5'-PA-O1A
5	HC	501	GTP	C5'-O5'-PA-O2A
5	HE	501	GTP	C5'-O5'-PA-O1A
5	HE	501	GTP	C5'-O5'-PA-O2A
5	HG	501	GTP	C5'-O5'-PA-O1A
5	IC	501	GTP	C5'-O5'-PA-O1A
5	IC	501	GTP	C5'-O5'-PA-O2A
5	IE	501	GTP	C5'-O5'-PA-O1A
5	IE	501	GTP	C3'-C4'-C5'-O5'
5	JC	501	GTP	C5'-O5'-PA-O1A
5	JE	501	GTP	C5'-O5'-PA-O1A
5	KG	501	GTP	C5'-O5'-PA-O3A
5	KG	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	LA	501	GTP	C5'-O5'-PA-O1A
5	LA	501	GTP	C5'-O5'-PA-O2A
5	LE	501	GTP	C5'-O5'-PA-O1A
5	LE	501	GTP	C5'-O5'-PA-O2A
5	MC	501	GTP	C5'-O5'-PA-O3A
5	ME	501	GTP	C5'-O5'-PA-O1A
5	ME	501	GTP	C5'-O5'-PA-O2A
4	GD	501	GDP	C3'-C4'-C5'-O5'
5	EC	501	GTP	O4'-C4'-C5'-O5'
5	EE	501	GTP	C3'-C4'-C5'-O5'
5	GE	501	GTP	C3'-C4'-C5'-O5'
5	IE	501	GTP	O4'-C4'-C5'-O5'
5	IG	501	GTP	C3'-C4'-C5'-O5'
4	GD	501	GDP	O4'-C4'-C5'-O5'
5	GE	501	GTP	O4'-C4'-C5'-O5'
5	IG	501	GTP	O4'-C4'-C5'-O5'
4	AD	501	GDP	C3'-C4'-C5'-O5'
4	IF	501	GDP	C3'-C4'-C5'-O5'
5	CC	501	GTP	C3'-C4'-C5'-O5'
5	FG	501	GTP	C3'-C4'-C5'-O5'
4	AD	501	GDP	O4'-C4'-C5'-O5'
4	ID	501	GDP	C3'-C4'-C5'-O5'
4	LF	501	GDP	C3'-C4'-C5'-O5'
5	CC	501	GTP	O4'-C4'-C5'-O5'
5	DC	501	GTP	C3'-C4'-C5'-O5'
5	EE	501	GTP	O4'-C4'-C5'-O5'
5	MC	501	GTP	C4'-C5'-O5'-PA
4	DD	501	GDP	PA-O3A-PB-O1B
4	EB	501	GDP	PA-O3A-PB-O1B
4	ID	501	GDP	PA-O3A-PB-O1B
4	LF	501	GDP	PA-O3A-PB-O1B
5	DG	501	GTP	PB-O3A-PA-O1A
5	FE	501	GTP	PB-O3A-PA-O1A
5	ME	501	GTP	PB-O3A-PA-O1A
5	BC	501	GTP	C3'-C4'-C5'-O5'
5	KG	501	GTP	PA-O3A-PB-O3B
5	DE	501	GTP	C4'-C5'-O5'-PA
5	FC	501	GTP	C4'-C5'-O5'-PA
5	HC	501	GTP	C4'-C5'-O5'-PA
5	JC	501	GTP	C4'-C5'-O5'-PA
5	KC	501	GTP	C4'-C5'-O5'-PA
5	LC	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
5	IC	501	GTP	PB-O3A-PA-O5'
4	IF	501	GDP	O4'-C4'-C5'-O5'
5	FG	501	GTP	O4'-C4'-C5'-O5'
5	IC	501	GTP	PB-O3B-PG-O1G
5	GE	501	GTP	PB-O3B-PG-O2G
4	BD	501	GDP	C5'-O5'-PA-O3A
4	GD	501	GDP	C5'-O5'-PA-O3A
4	HF	501	GDP	C5'-O5'-PA-O3A
4	HH	501	GDP	C5'-O5'-PA-O3A
5	AC	501	GTP	C5'-O5'-PA-O3A
5	BE	501	GTP	C5'-O5'-PA-O3A
5	DC	501	GTP	C5'-O5'-PA-O3A
5	EE	501	GTP	C5'-O5'-PA-O3A
5	FC	501	GTP	C5'-O5'-PA-O3A
5	FG	501	GTP	C5'-O5'-PA-O3A
5	GC	501	GTP	C5'-O5'-PA-O3A
5	HE	501	GTP	C5'-O5'-PA-O3A
5	HG	501	GTP	C5'-O5'-PA-O3A
5	IE	501	GTP	C5'-O5'-PA-O3A
5	JC	501	GTP	C5'-O5'-PA-O3A
5	JE	501	GTP	C5'-O5'-PA-O3A
4	ID	501	GDP	O4'-C4'-C5'-O5'
4	LB	501	GDP	C3'-C4'-C5'-O5'
4	LF	501	GDP	O4'-C4'-C5'-O5'
5	DC	501	GTP	O4'-C4'-C5'-O5'
5	GC	501	GTP	C3'-C4'-C5'-O5'
5	GG	501	GTP	C3'-C4'-C5'-O5'
4	JF	501	GDP	PB-O3A-PA-O2A
5	CE	501	GTP	PB-O3A-PA-O2A
5	DC	501	GTP	PB-O3A-PA-O1A
5	EC	501	GTP	PB-O3A-PA-O2A
5	GG	501	GTP	PB-O3A-PA-O2A
5	HE	501	GTP	PA-O3A-PB-O2B
5	HG	501	GTP	PB-O3A-PA-O1A
5	JE	501	GTP	PB-O3A-PA-O2A
5	KE	501	GTP	PB-O3A-PA-O1A
5	MC	501	GTP	PB-O3A-PA-O2A
5	CE	501	GTP	C4'-C5'-O5'-PA
5	CG	501	GTP	C4'-C5'-O5'-PA
5	DG	501	GTP	C4'-C5'-O5'-PA
5	EE	501	GTP	C4'-C5'-O5'-PA
5	HE	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
5	JE	501	GTP	C4'-C5'-O5'-PA
4	AF	501	GDP	C5'-O5'-PA-O1A
4	FH	501	GDP	C5'-O5'-PA-O1A
4	IF	501	GDP	C5'-O5'-PA-O1A
5	AC	501	GTP	C5'-O5'-PA-O2A
5	BE	501	GTP	C5'-O5'-PA-O2A
5	DC	501	GTP	C5'-O5'-PA-O2A
5	EE	501	GTP	C5'-O5'-PA-O2A
5	FE	501	GTP	C5'-O5'-PA-O2A
5	FG	501	GTP	C5'-O5'-PA-O2A
5	GC	501	GTP	C5'-O5'-PA-O2A
5	GE	501	GTP	C5'-O5'-PA-O2A
5	HG	501	GTP	C5'-O5'-PA-O2A
5	IE	501	GTP	C5'-O5'-PA-O2A
5	JC	501	GTP	C5'-O5'-PA-O2A
5	JE	501	GTP	C5'-O5'-PA-O2A
5	MC	501	GTP	C5'-O5'-PA-O2A
5	DE	501	GTP	C3'-C4'-C5'-O5'
5	IE	501	GTP	C4'-C5'-O5'-PA
5	JG	501	GTP	C4'-C5'-O5'-PA
4	ED	501	GDP	C3'-C4'-C5'-O5'
5	BC	501	GTP	O4'-C4'-C5'-O5'
5	HE	501	GTP	C3'-C4'-C5'-O5'
5	EC	501	GTP	C4'-C5'-O5'-PA
5	FG	501	GTP	C4'-C5'-O5'-PA
5	GG	501	GTP	O4'-C4'-C5'-O5'
5	BG	501	GTP	PB-O3A-PA-O2A
5	EG	501	GTP	PB-O3A-PA-O1A
5	HC	501	GTP	PA-O3A-PB-O2B
5	IE	501	GTP	PA-O3A-PB-O2B
5	JC	501	GTP	PA-O3A-PB-O2B
5	KC	501	GTP	PB-O3A-PA-O2A
5	LA	501	GTP	PB-O3A-PA-O2A
5	LE	501	GTP	PB-O3A-PA-O2A
5	MC	501	GTP	PA-O3A-PB-O2B
5	BC	501	GTP	C4'-C5'-O5'-PA
5	BE	501	GTP	C4'-C5'-O5'-PA
5	DC	501	GTP	C4'-C5'-O5'-PA
5	FE	501	GTP	C4'-C5'-O5'-PA
5	GC	501	GTP	C4'-C5'-O5'-PA
4	BA	501	GDP	C3'-C4'-C5'-O5'
5	KE	501	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	BG	501	GTP	C4'-C5'-O5'-PA
5	LA	501	GTP	C4'-C5'-O5'-PA
4	DF	501	GDP	C3'-C4'-C5'-O5'
4	BF	501	GDP	PA-O3A-PB-O1B
5	EG	501	GTP	C4'-C5'-O5'-PA
5	ME	501	GTP	C4'-C5'-O5'-PA
5	EE	501	GTP	PB-O3A-PA-O1A
5	EE	501	GTP	PB-O3A-PA-O2A
5	EG	501	GTP	PB-O3A-PA-O2A
5	FG	501	GTP	PB-O3A-PA-O1A
5	IC	501	GTP	PB-O3A-PA-O1A
5	KC	501	GTP	PA-O3A-PB-O1B
5	KE	501	GTP	PB-O3A-PA-O2A
4	LB	501	GDP	O4'-C4'-C5'-O5'
5	GC	501	GTP	O4'-C4'-C5'-O5'
4	GF	501	GDP	C3'-C4'-C5'-O5'
4	HF	501	GDP	C3'-C4'-C5'-O5'
4	JF	501	GDP	C3'-C4'-C5'-O5'
5	DE	501	GTP	O4'-C4'-C5'-O5'
5	HC	501	GTP	C3'-C4'-C5'-O5'
5	LC	501	GTP	C3'-C4'-C5'-O5'
4	KH	501	GDP	C3'-C4'-C5'-O5'
4	EB	501	GDP	PA-O3A-PB-O2B
5	IC	501	GTP	PB-O3B-PG-O2G
5	IC	501	GTP	PB-O3B-PG-O3G
4	AD	501	GDP	C5'-O5'-PA-O3A
4	BA	501	GDP	C5'-O5'-PA-O3A
4	GH	501	GDP	C5'-O5'-PA-O3A
4	ID	501	GDP	C5'-O5'-PA-O3A
4	KH	501	GDP	C5'-O5'-PA-O3A
5	AE	501	GTP	C5'-O5'-PA-O3A
5	BG	501	GTP	C5'-O5'-PA-O3A
5	CE	501	GTP	C5'-O5'-PA-O3A
5	CG	501	GTP	C5'-O5'-PA-O3A
5	DE	501	GTP	C5'-O5'-PA-O3A
5	DG	501	GTP	C5'-O5'-PA-O3A
5	FE	501	GTP	C5'-O5'-PA-O3A
5	GE	501	GTP	C5'-O5'-PA-O3A
5	HC	501	GTP	C5'-O5'-PA-O3A
5	IC	501	GTP	C5'-O5'-PA-O3A
5	LA	501	GTP	C5'-O5'-PA-O3A
5	LE	501	GTP	C5'-O5'-PA-O3A

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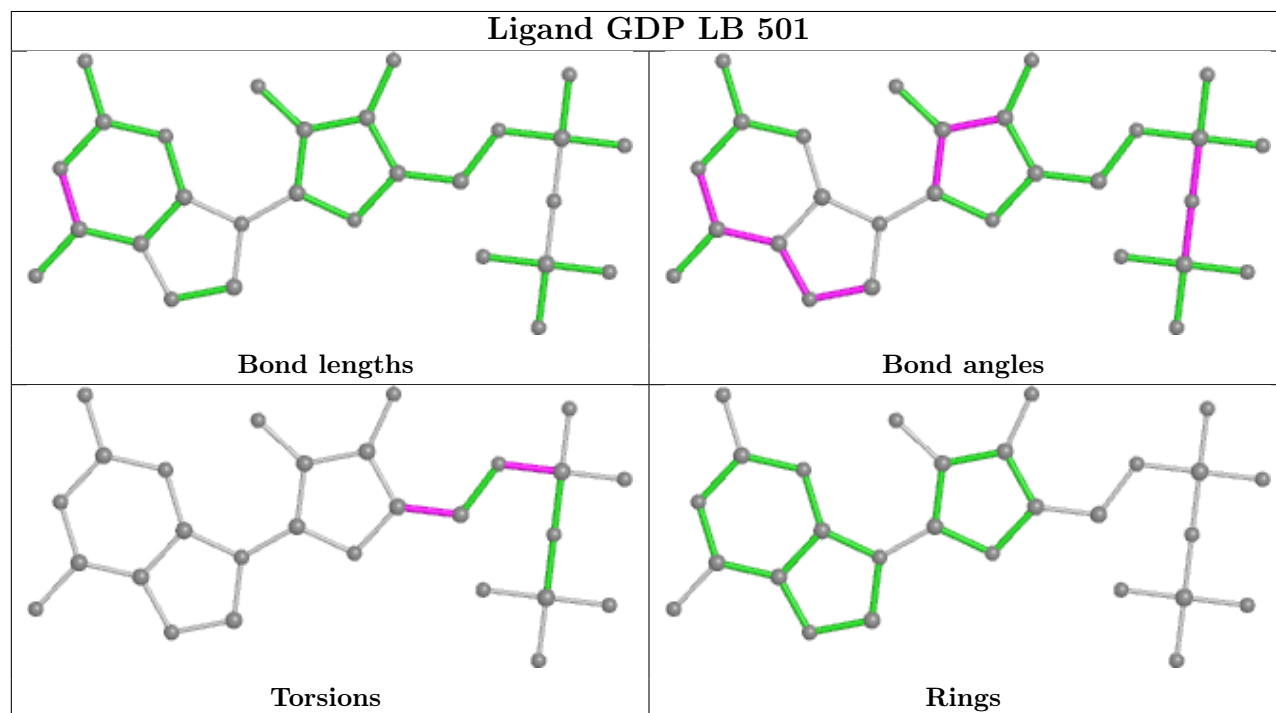
Mol	Chain	Res	Type	Atoms
5	ME	501	GTP	C5'-O5'-PA-O3A
5	HG	501	GTP	C4'-C5'-O5'-PA
5	IC	501	GTP	C4'-C5'-O5'-PA
4	JD	501	GDP	PB-O3A-PA-O2A
5	BG	501	GTP	PB-O3A-PA-O1A
5	CG	501	GTP	PB-O3A-PA-O2A
5	DE	501	GTP	PA-O3A-PB-O2B
5	DG	501	GTP	PB-O3A-PA-O2A
5	EC	501	GTP	PB-O3A-PA-O1A
5	GE	501	GTP	PA-O3A-PB-O2B
5	GG	501	GTP	PB-O3A-PA-O1A
5	HC	501	GTP	PA-O3A-PB-O1B
5	IE	501	GTP	PA-O3A-PB-O1B
5	JC	501	GTP	PA-O3A-PB-O1B
5	JE	501	GTP	PB-O3A-PA-O1A
5	KC	501	GTP	PA-O3A-PB-O2B
5	KG	501	GTP	PG-O3B-PB-O1B
5	KG	501	GTP	PA-O3A-PB-O2B
5	LA	501	GTP	PB-O3A-PA-O1A
4	DD	501	GDP	C5'-O5'-PA-O1A
4	ED	501	GDP	C5'-O5'-PA-O1A
4	FD	501	GDP	C5'-O5'-PA-O1A
4	IF	501	GDP	C5'-O5'-PA-O2A
4	IH	501	GDP	C5'-O5'-PA-O1A
4	KD	501	GDP	C5'-O5'-PA-O1A
4	KF	501	GDP	C5'-O5'-PA-O1A
4	LF	501	GDP	C5'-O5'-PA-O1A
5	EE	501	GTP	C5'-O5'-PA-O1A
5	MA	501	GTP	C5'-O5'-PA-O2A
5	HE	501	GTP	O4'-C4'-C5'-O5'
5	JE	501	GTP	C3'-C4'-C5'-O5'
5	KE	501	GTP	O4'-C4'-C5'-O5'
4	CB	501	GDP	PA-O3A-PB-O1B
5	LE	501	GTP	C4'-C5'-O5'-PA

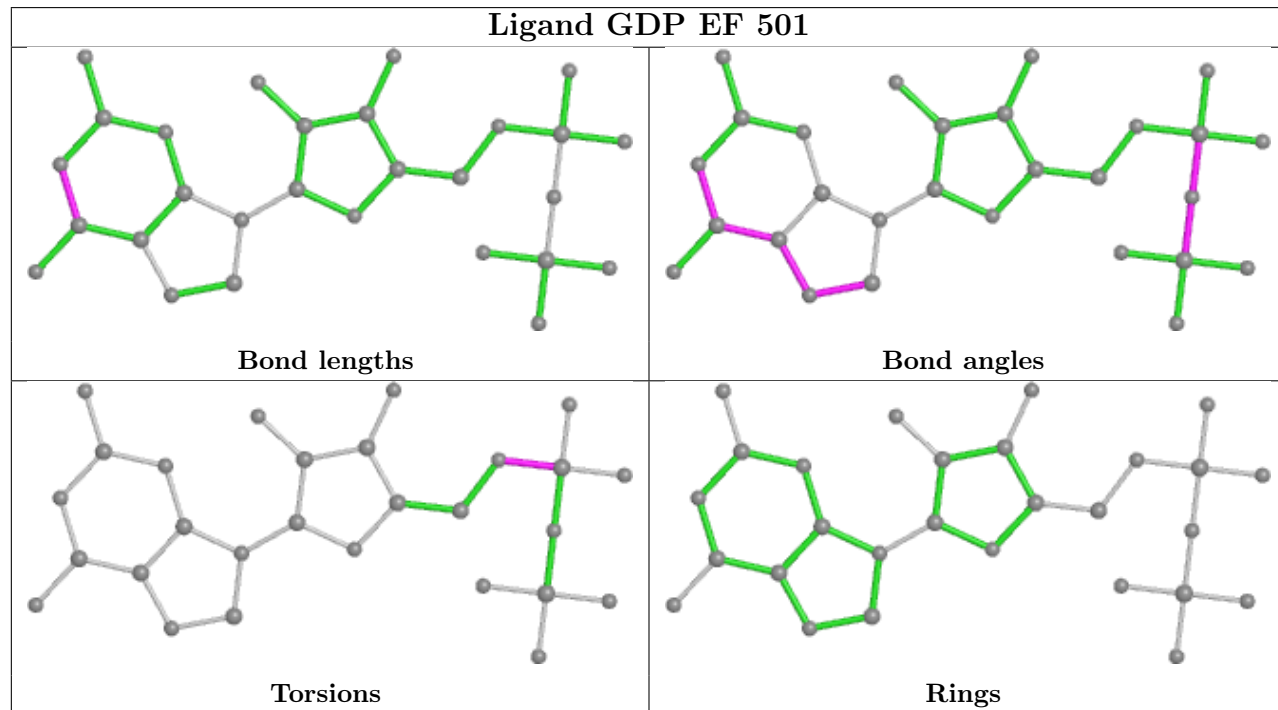
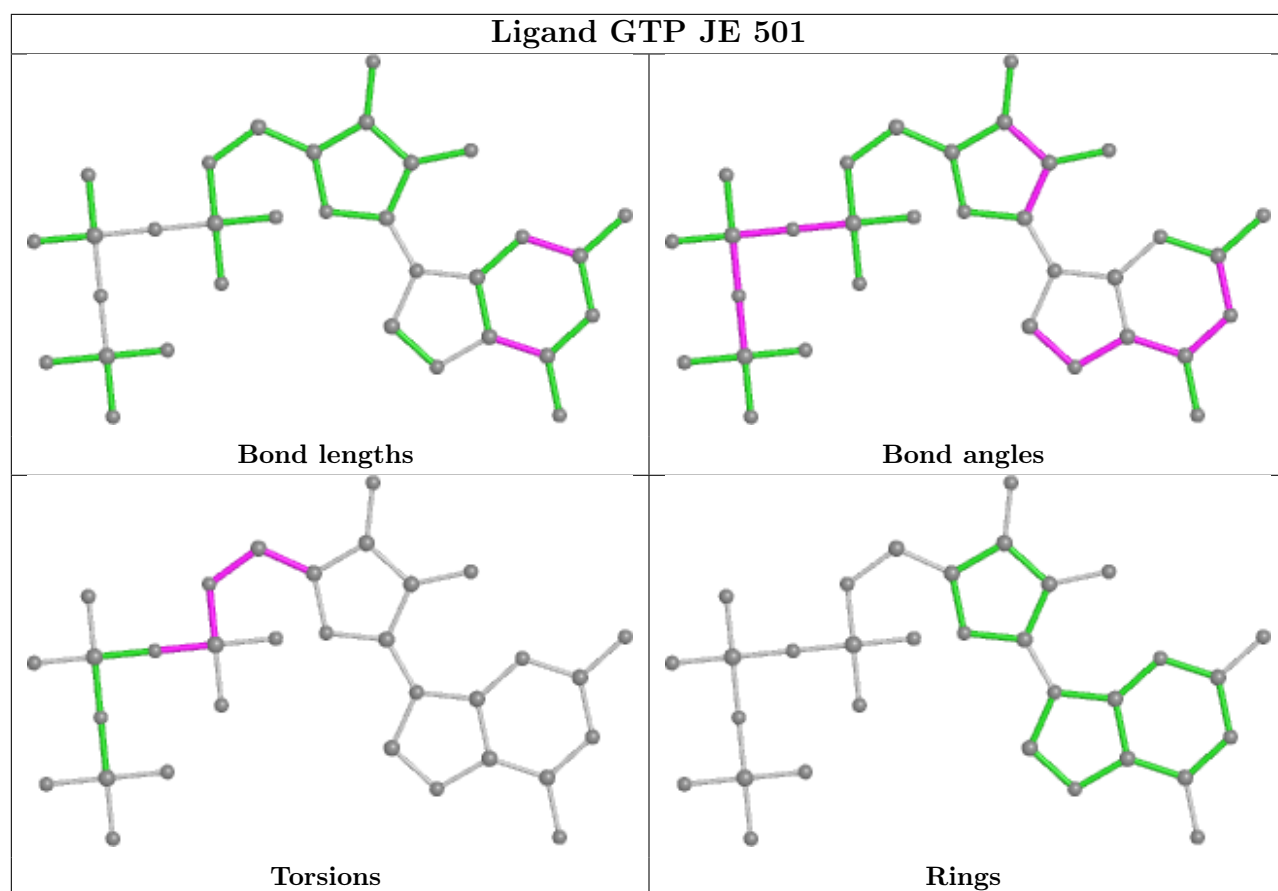
There are no ring outliers.

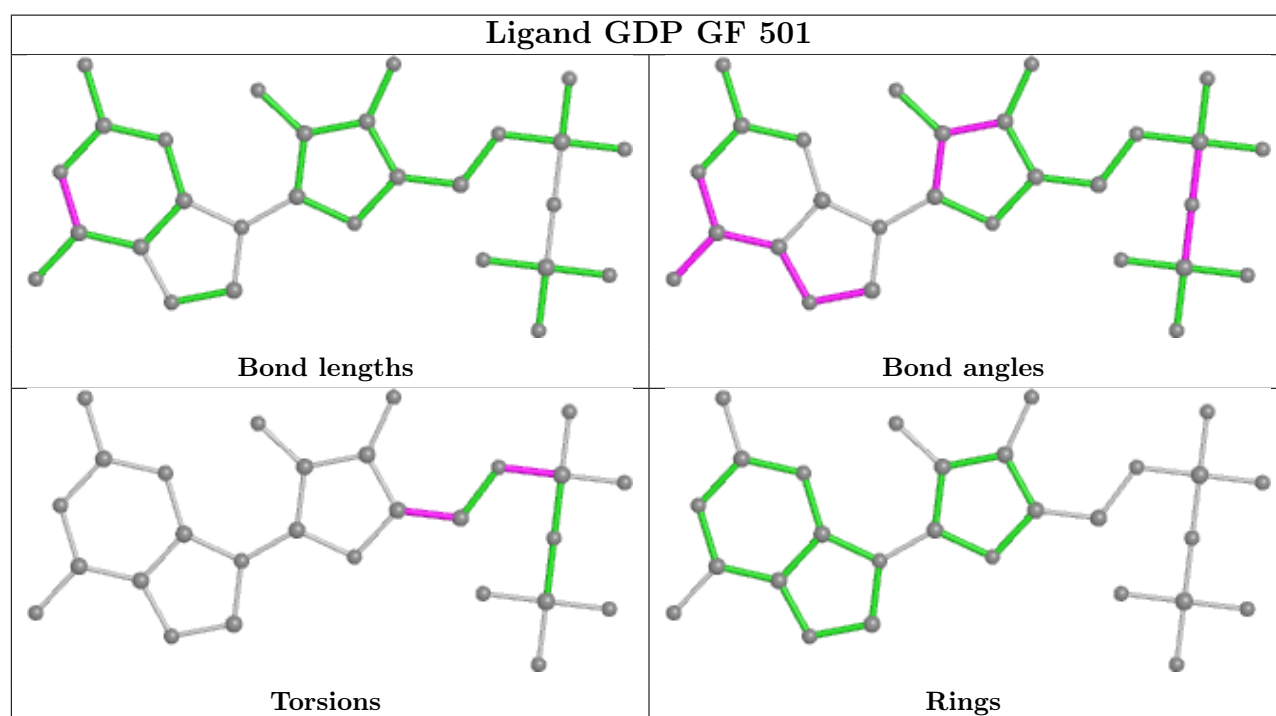
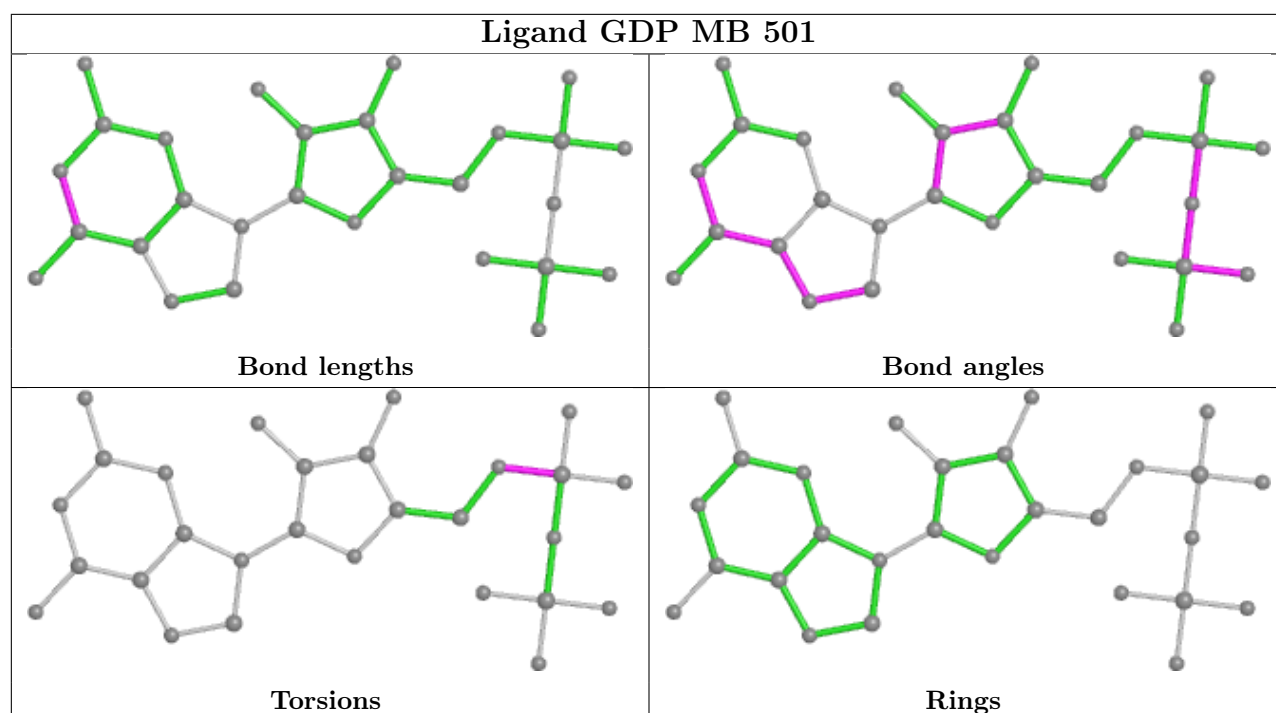
No monomer is involved in short contacts.

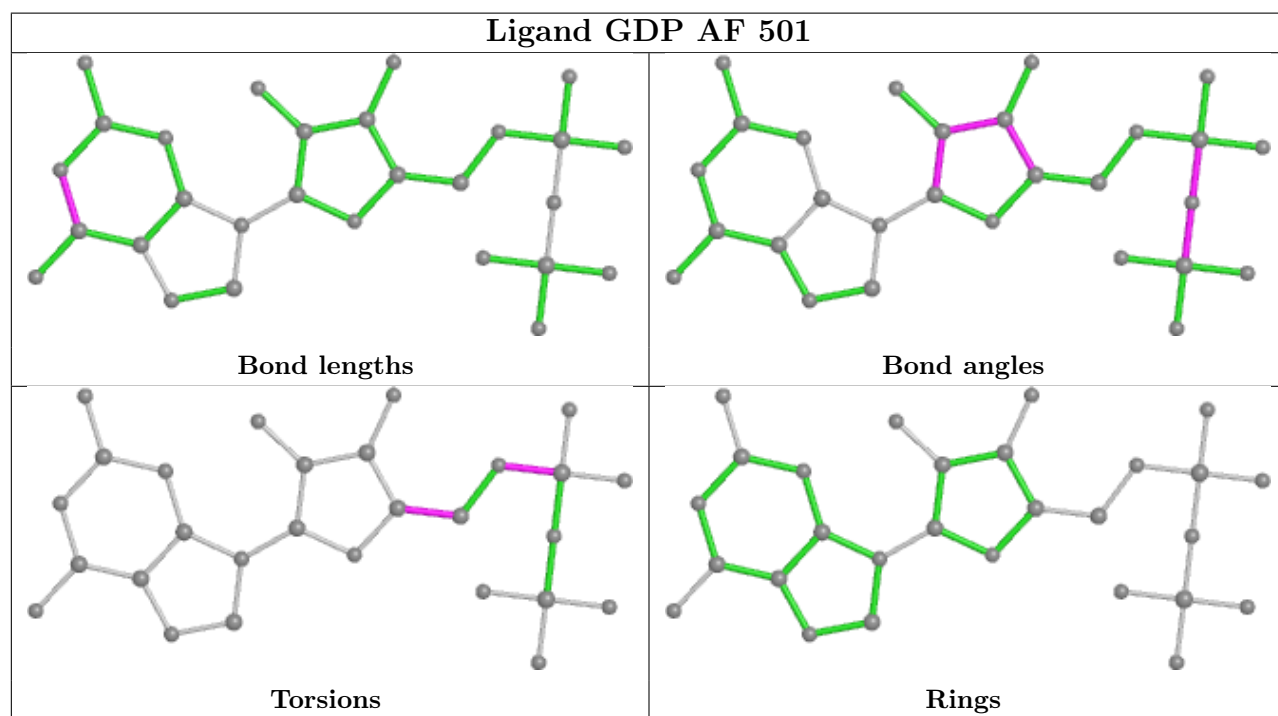
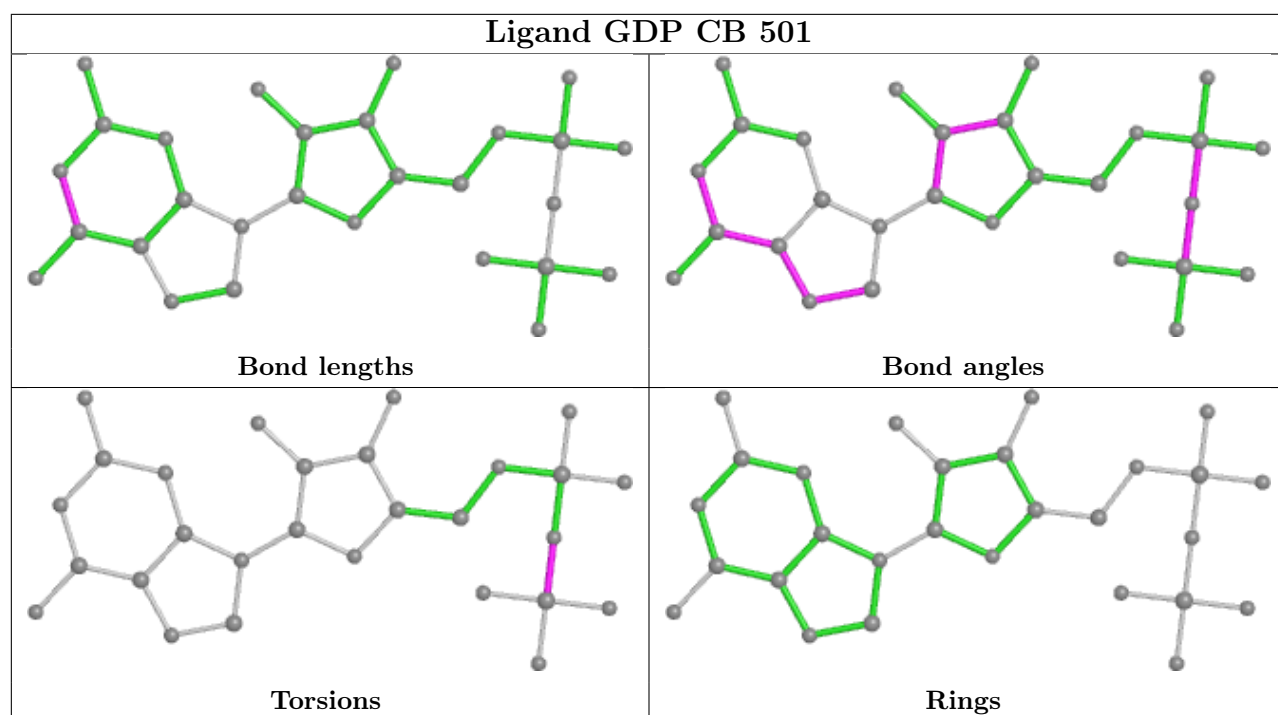
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

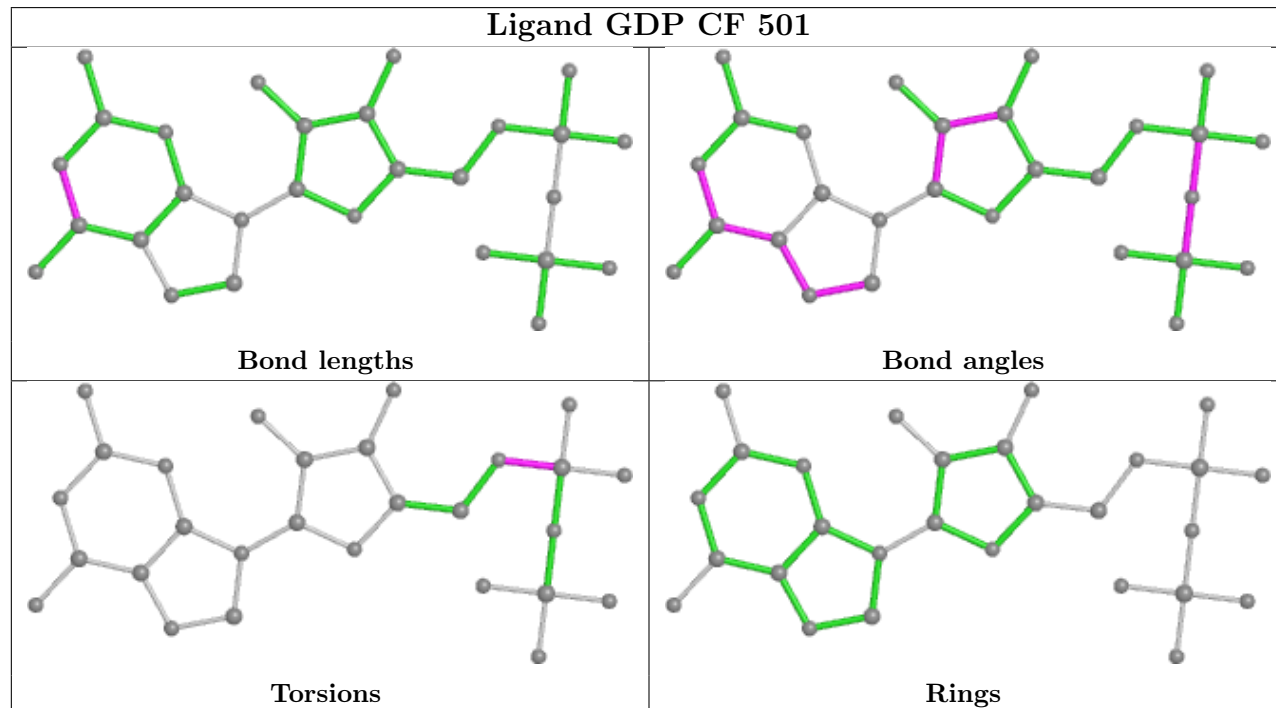
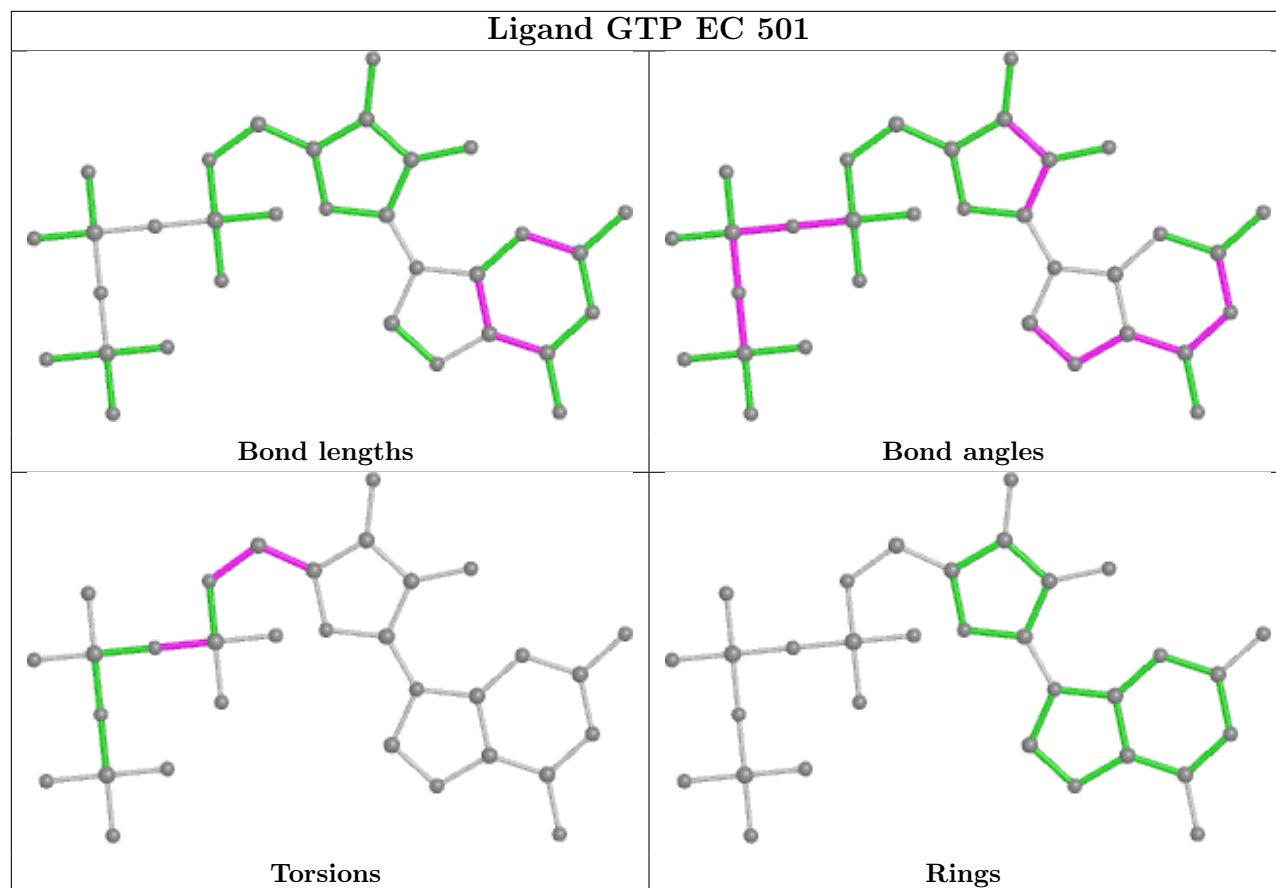
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



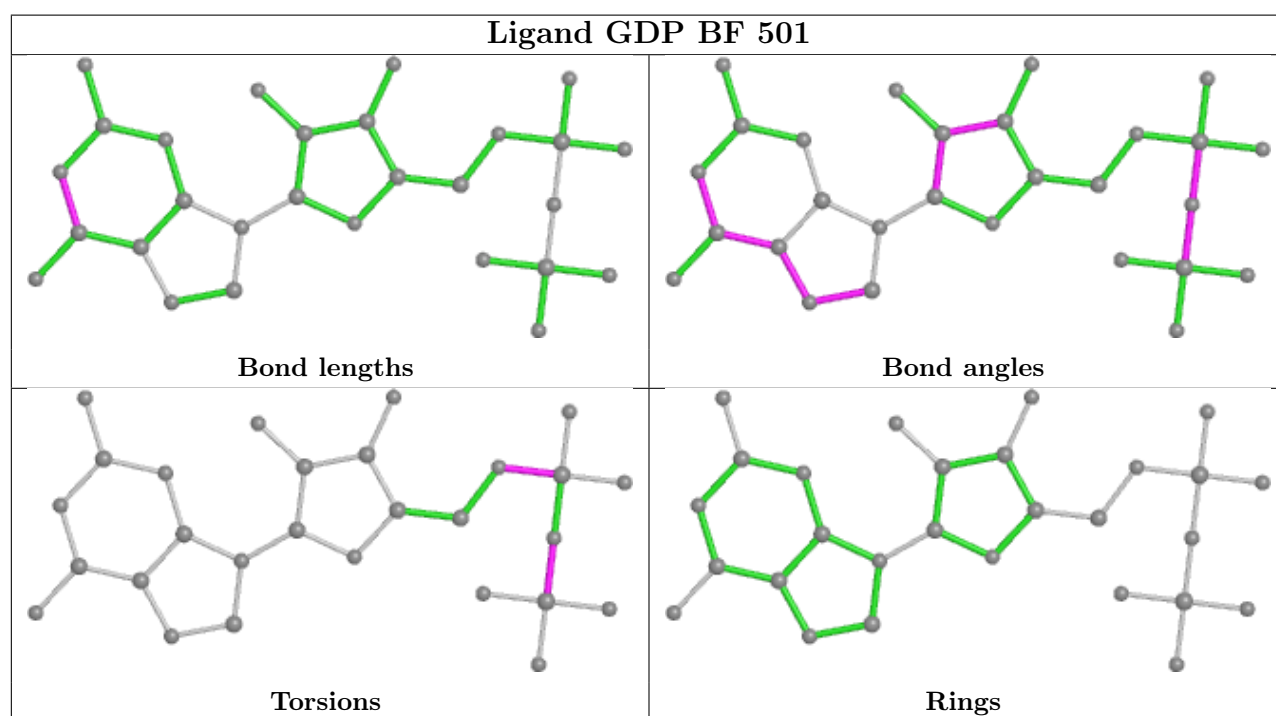
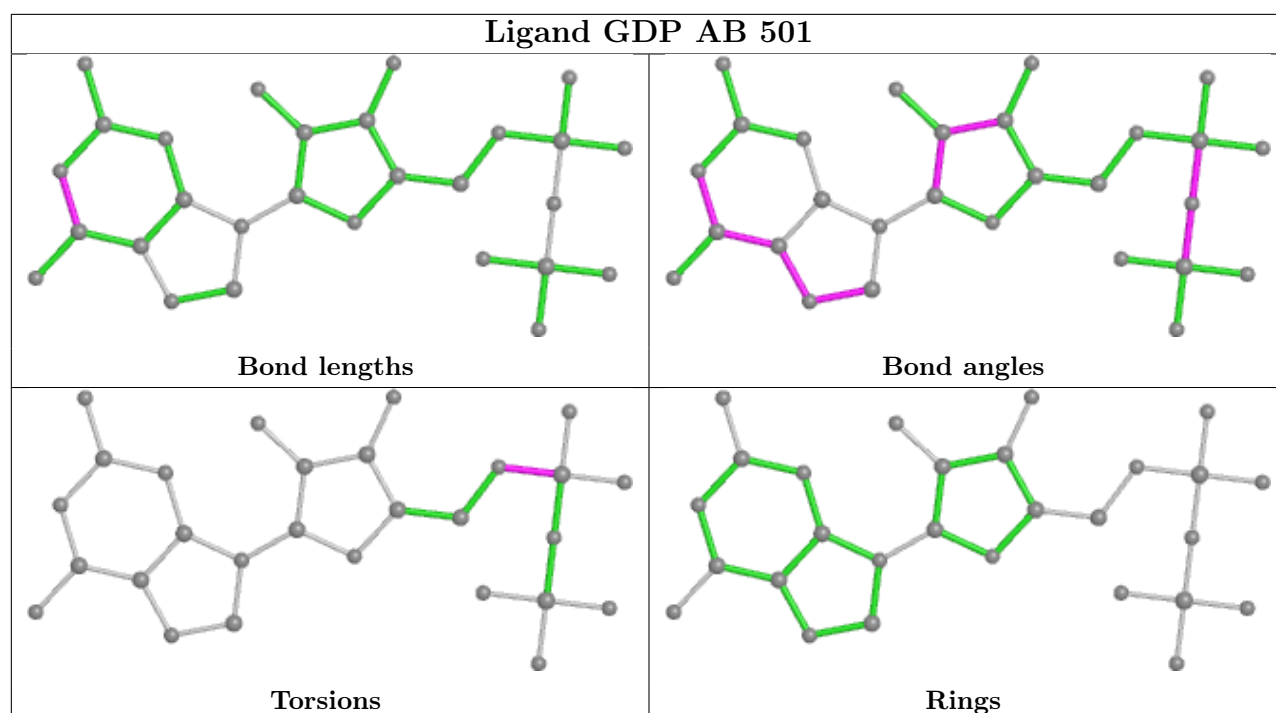


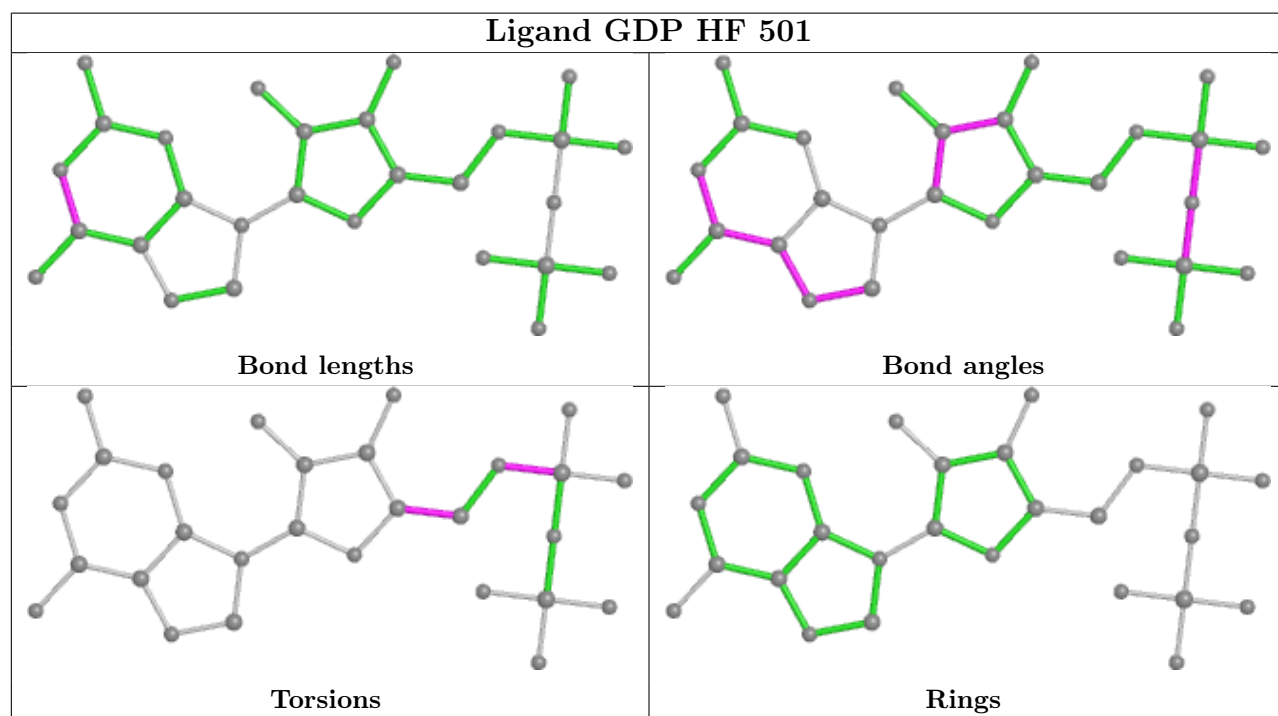
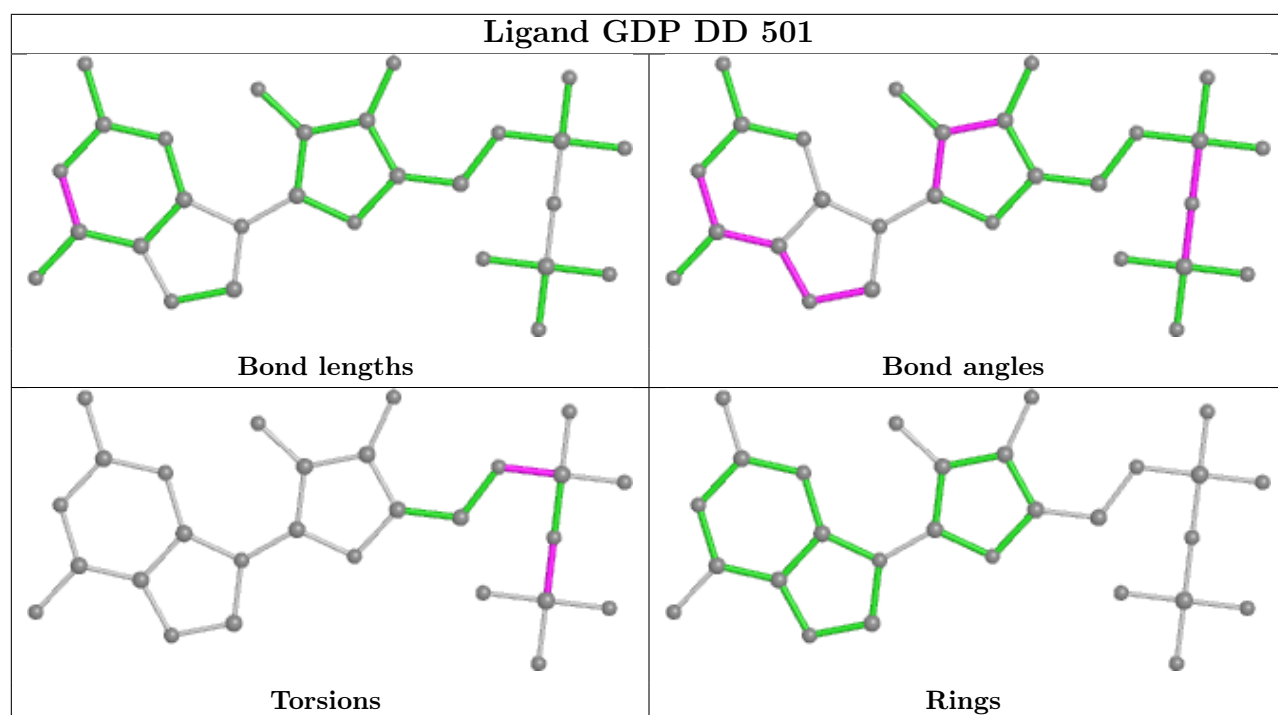


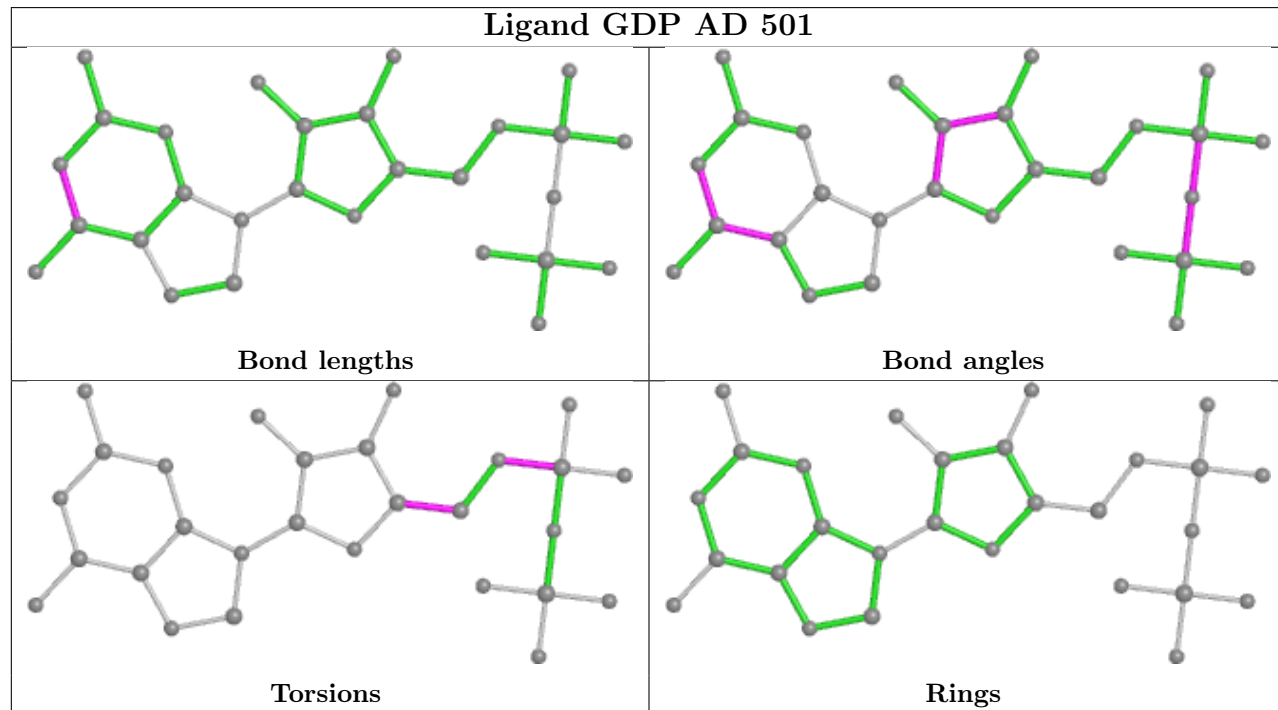
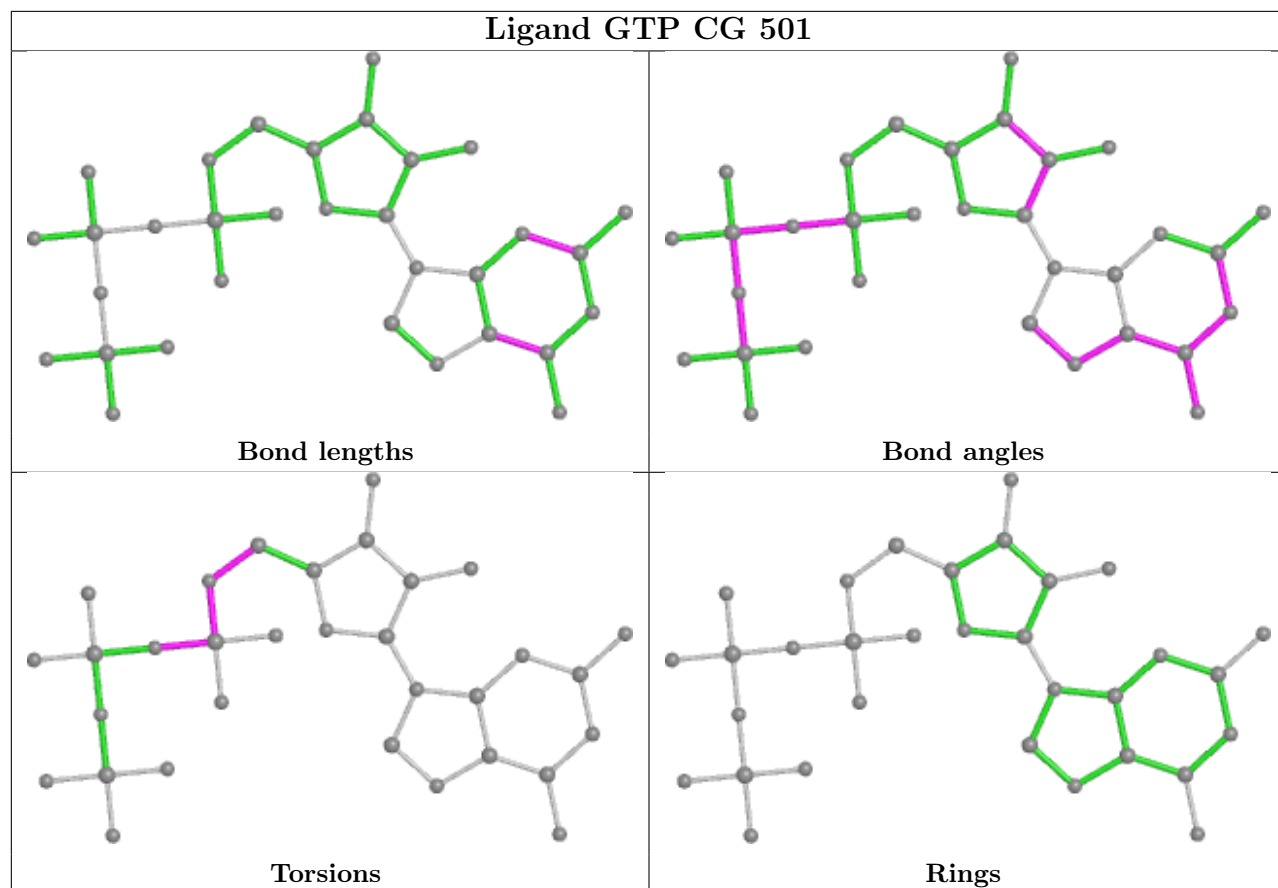


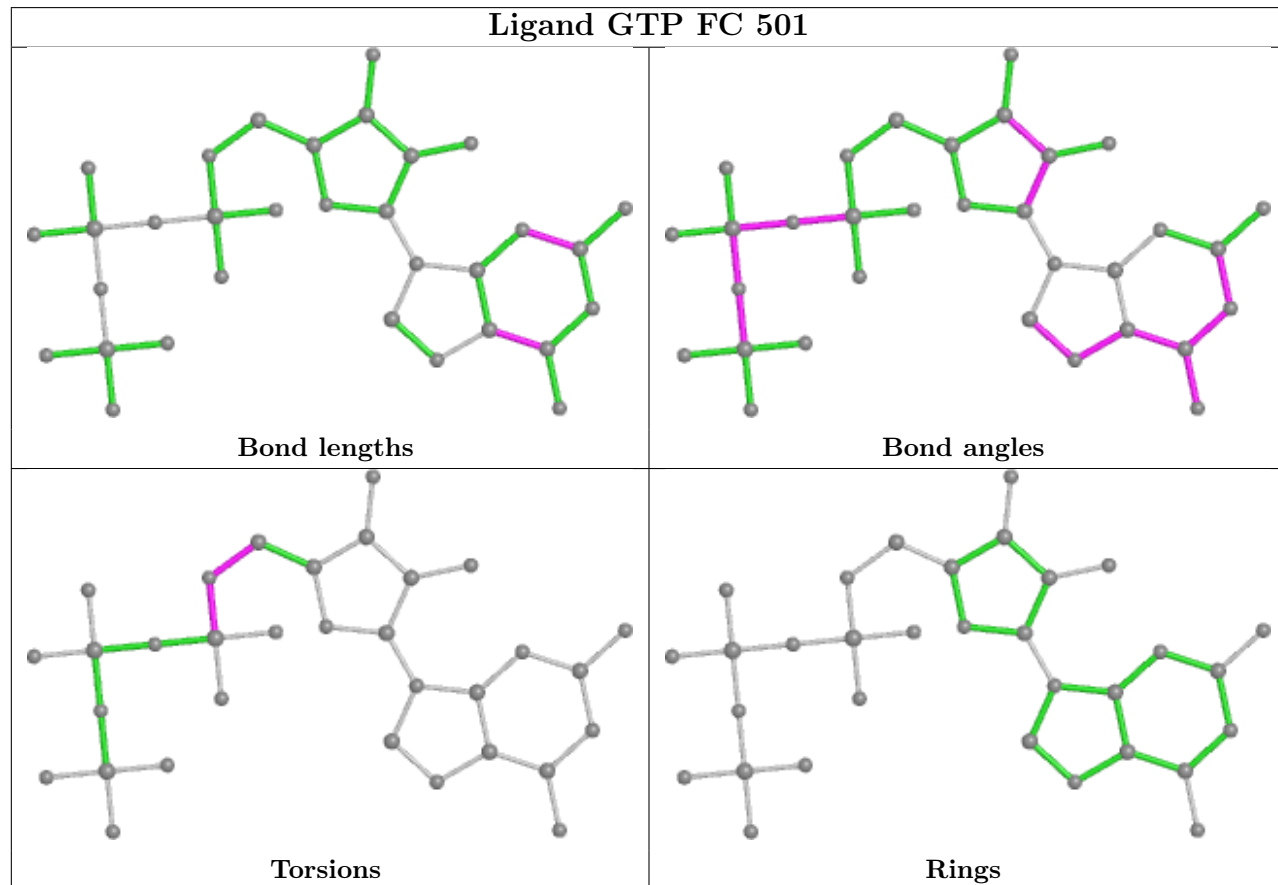
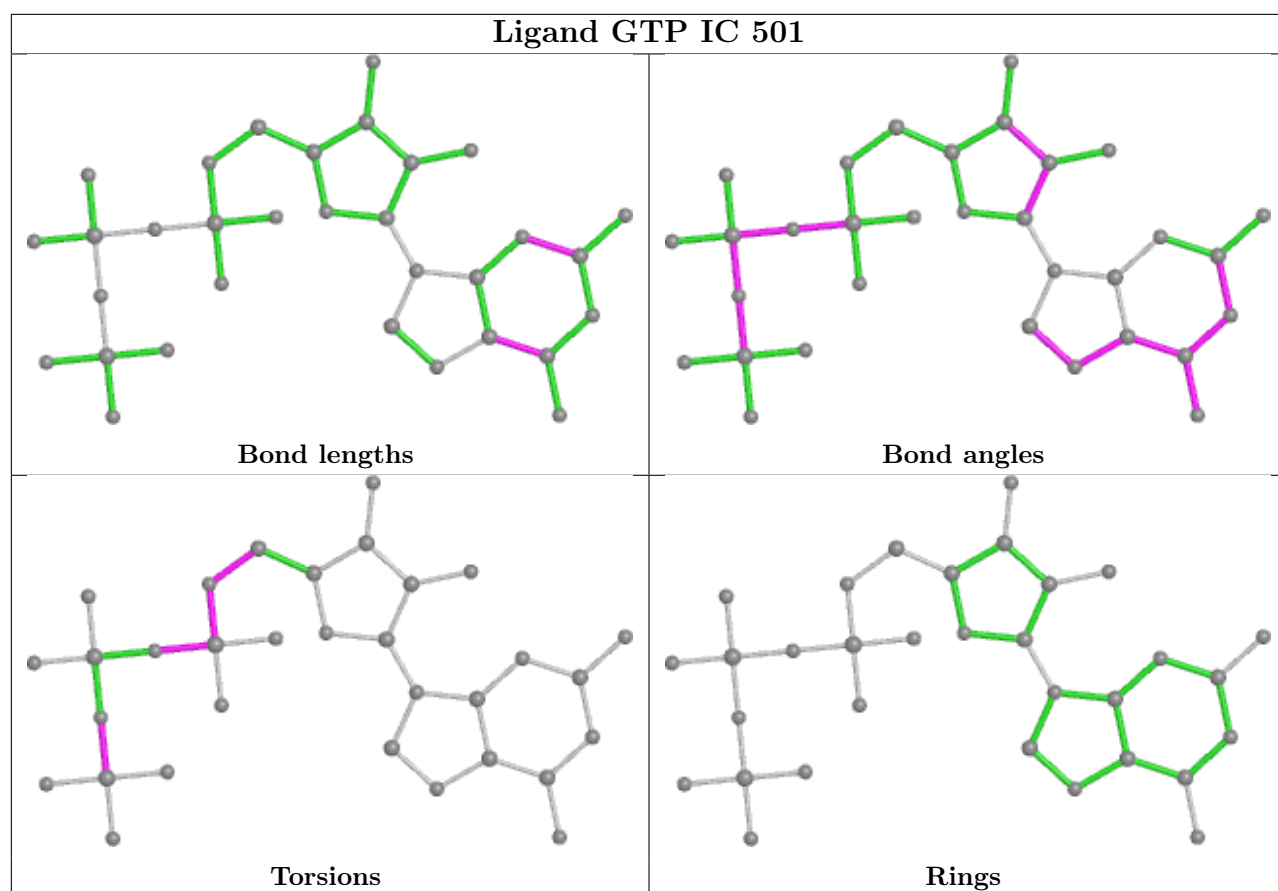


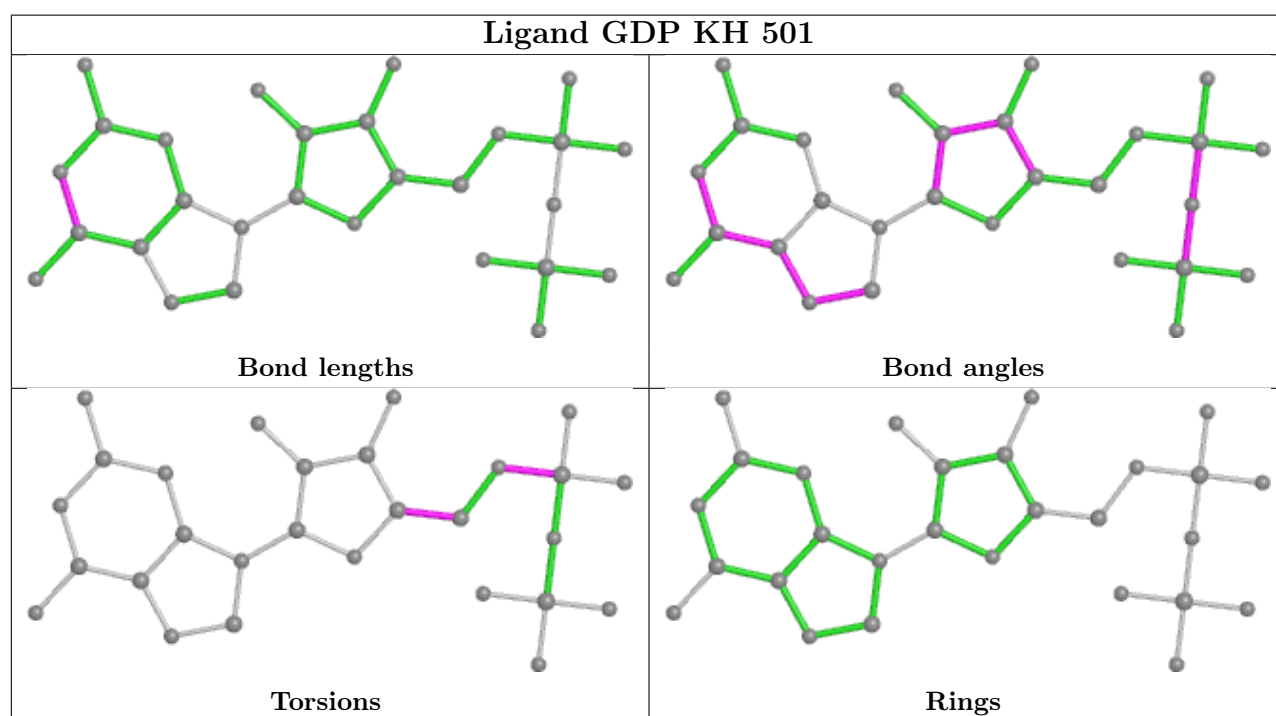
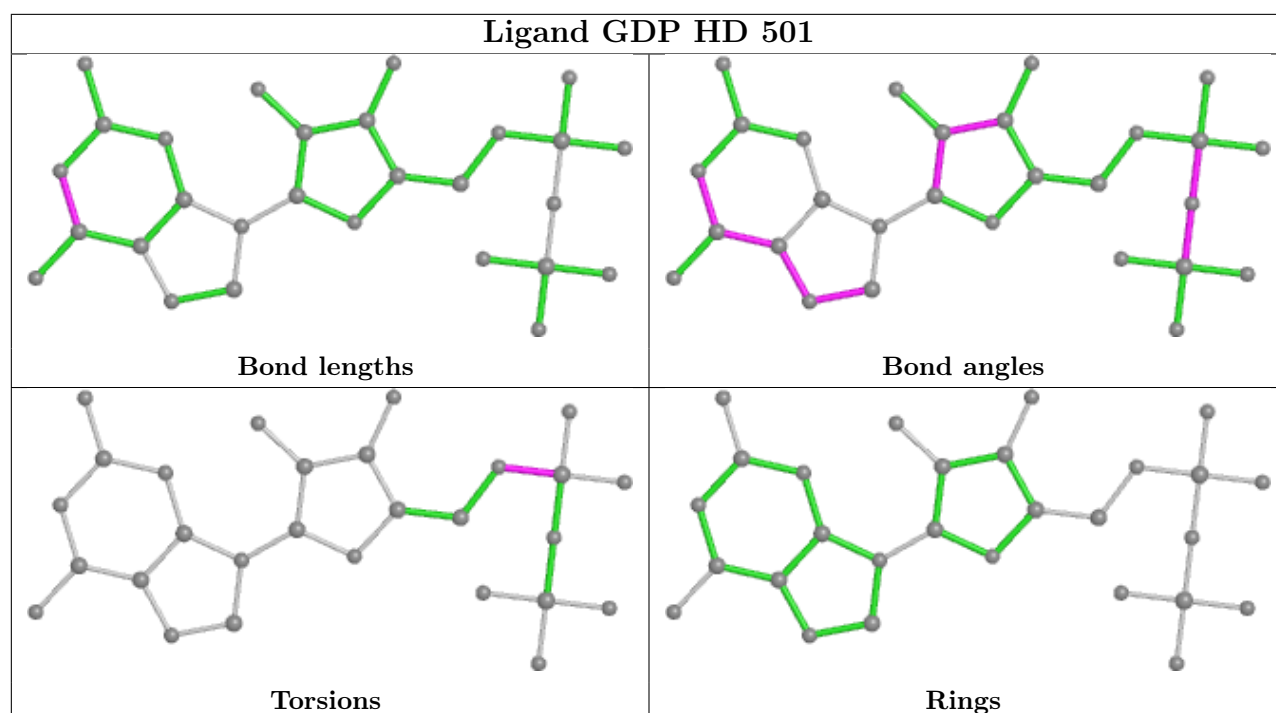




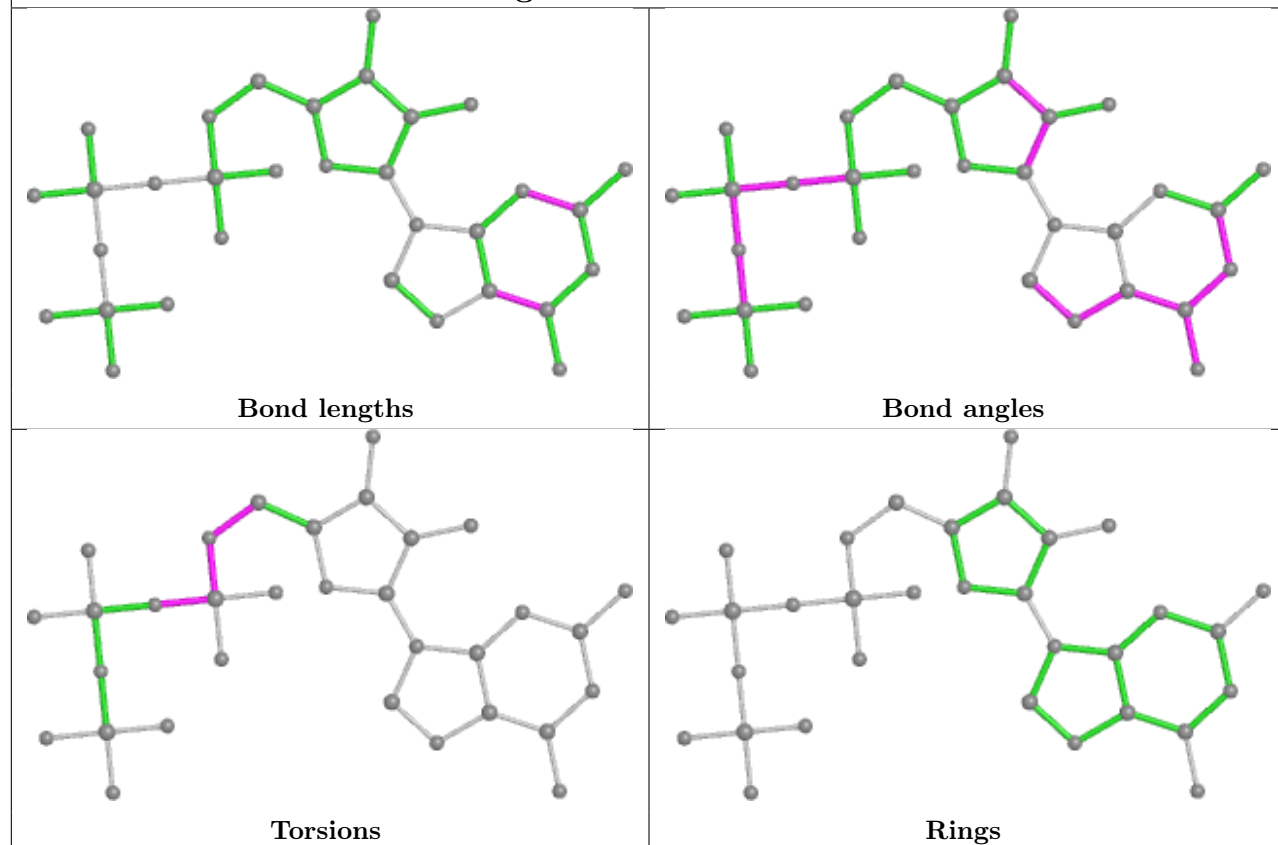




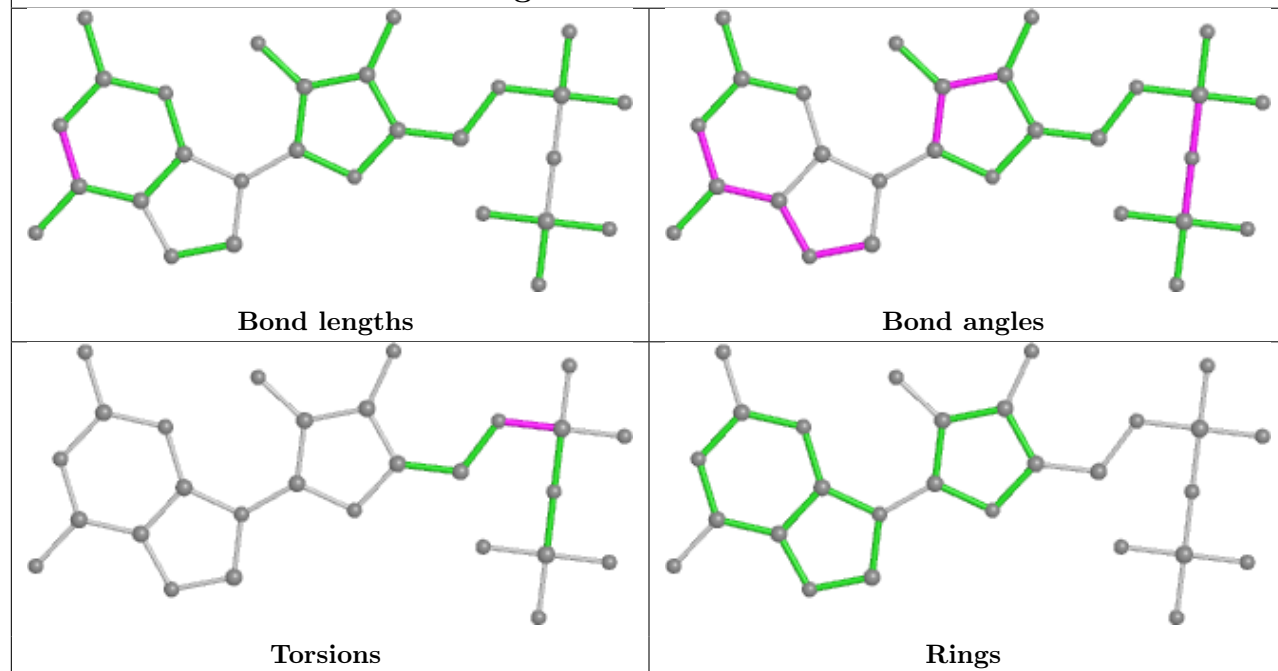


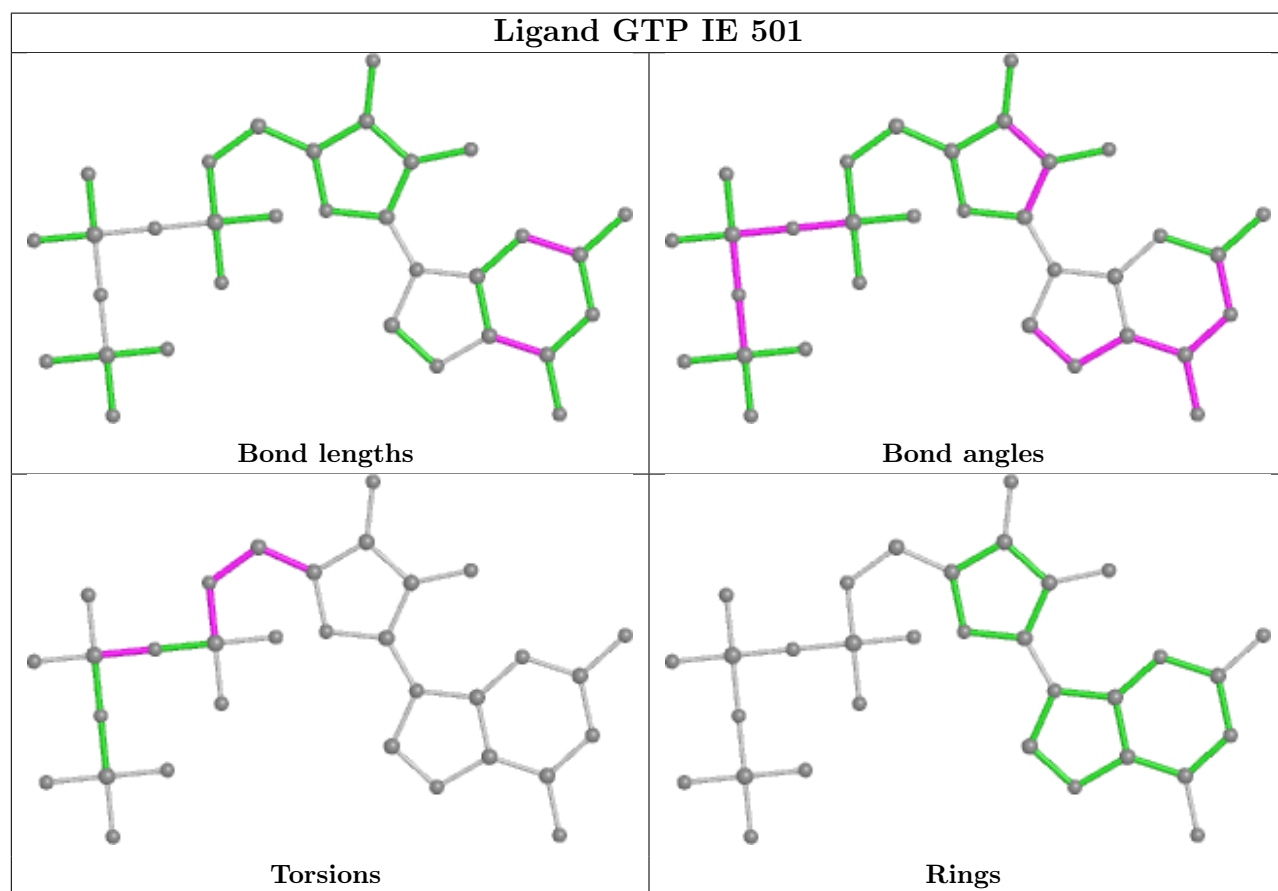
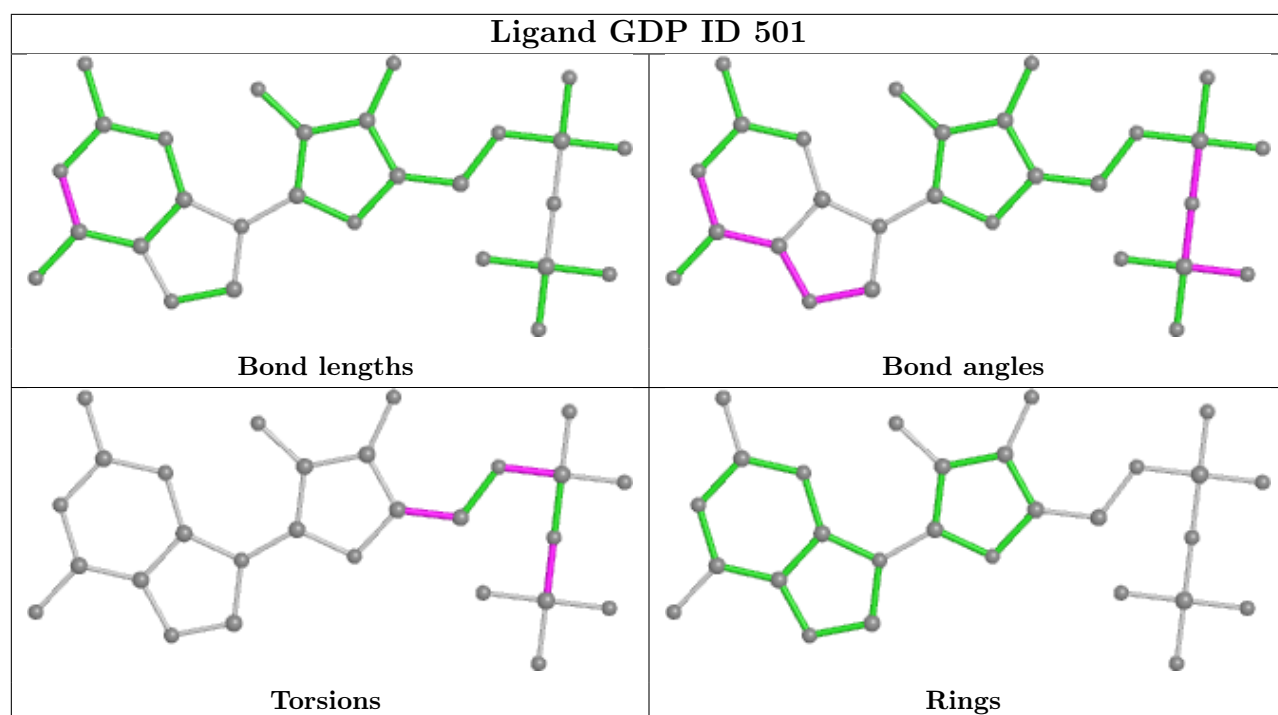


## Ligand GTP HG 501

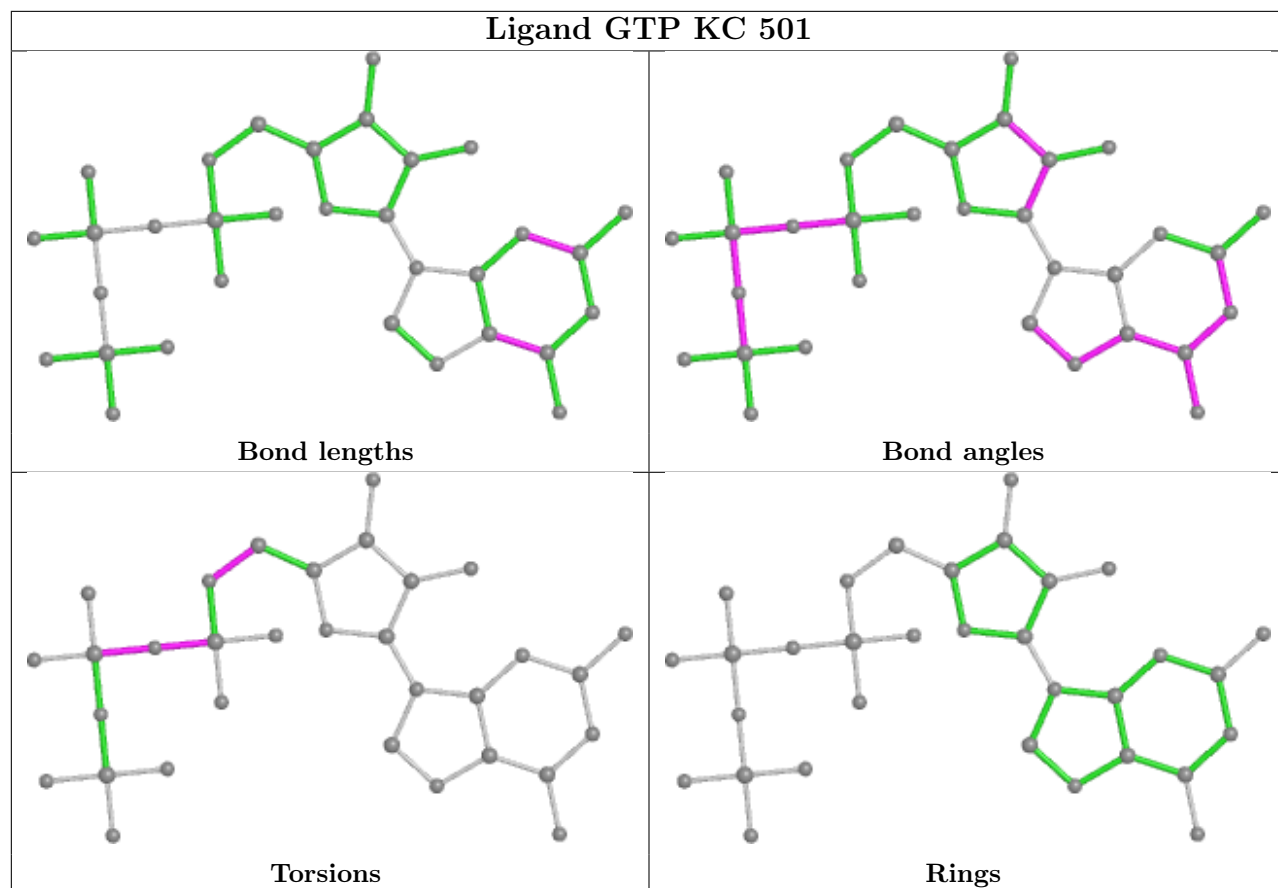


## Ligand GDP MF 501

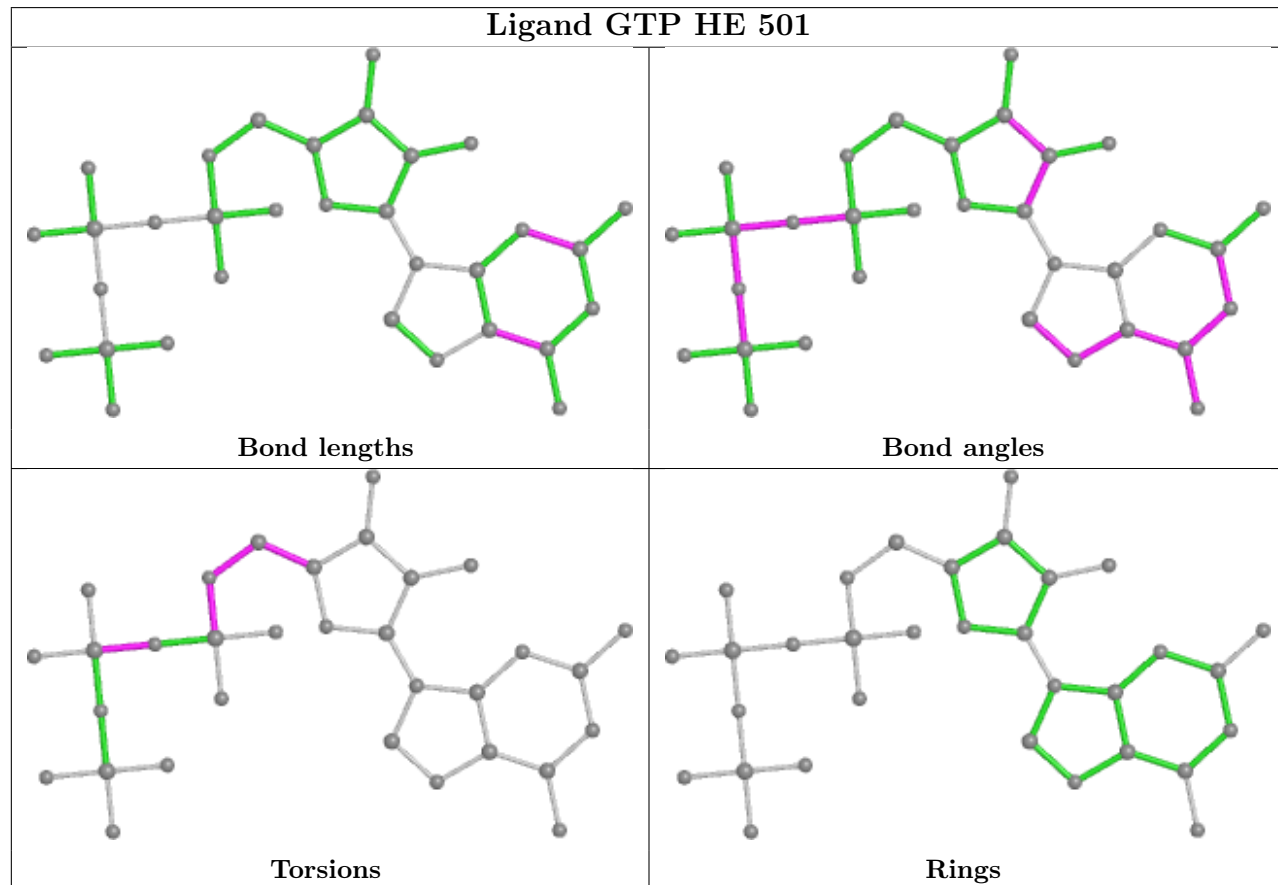




## Ligand GTP KC 501

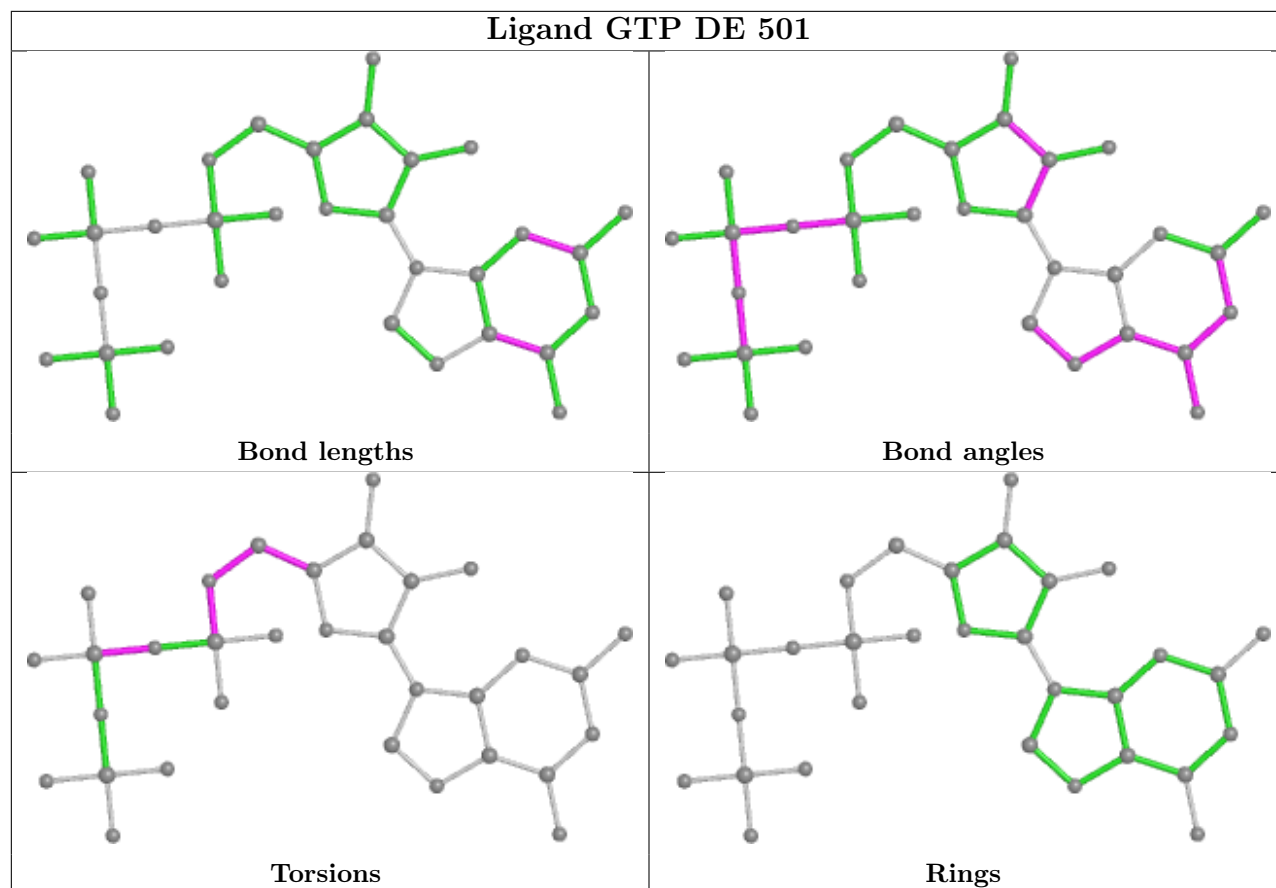


## Ligand GTP HE 501

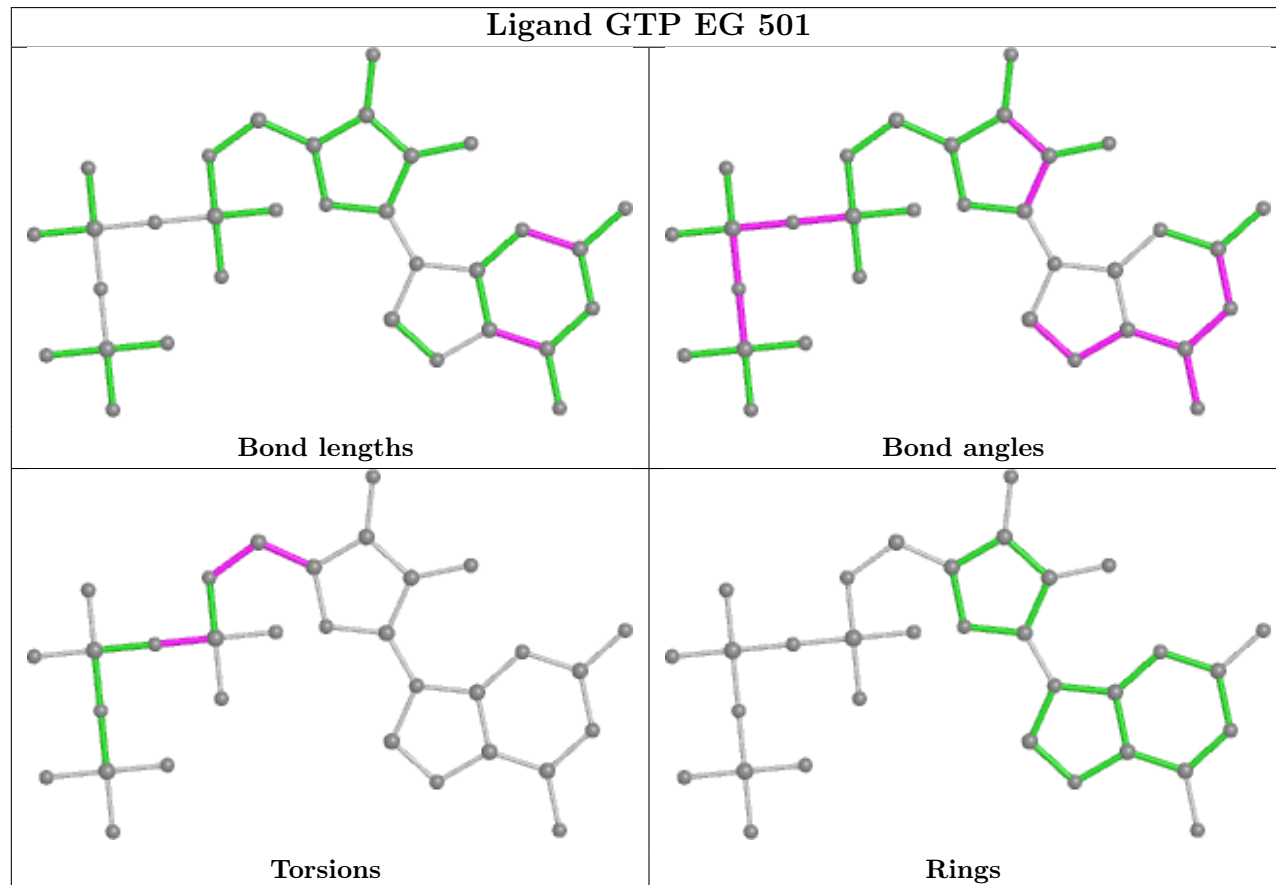


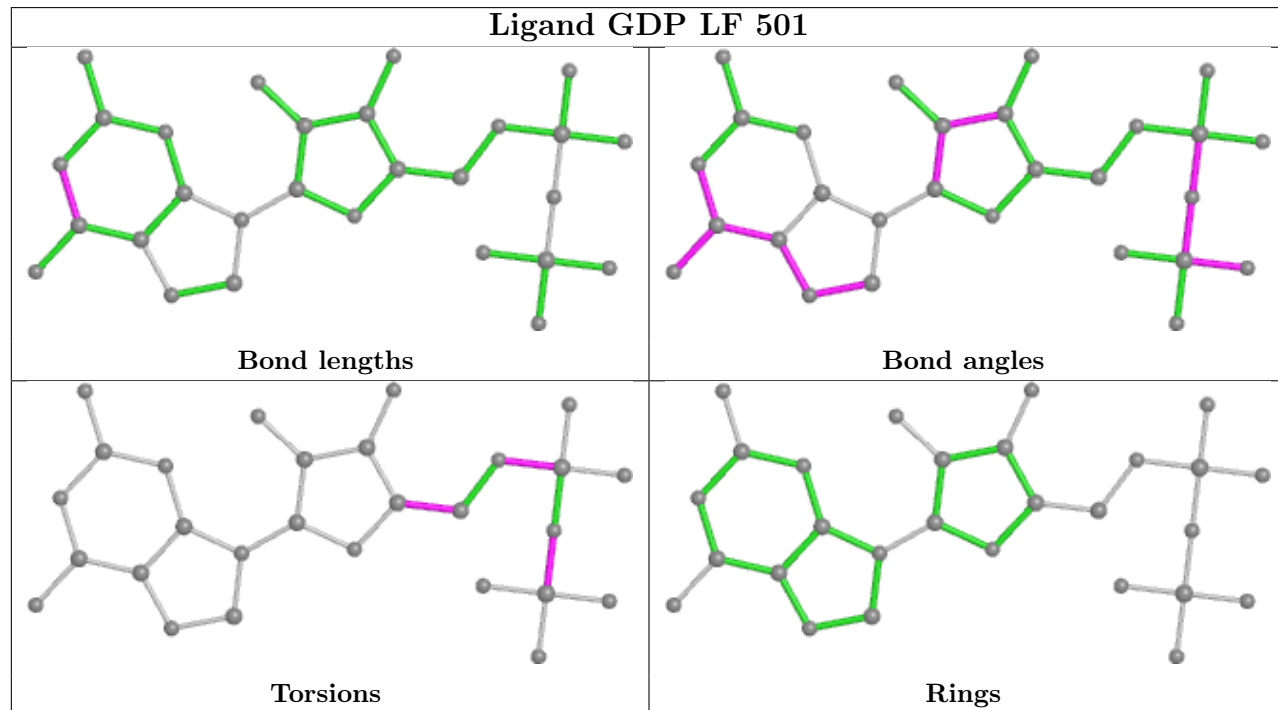
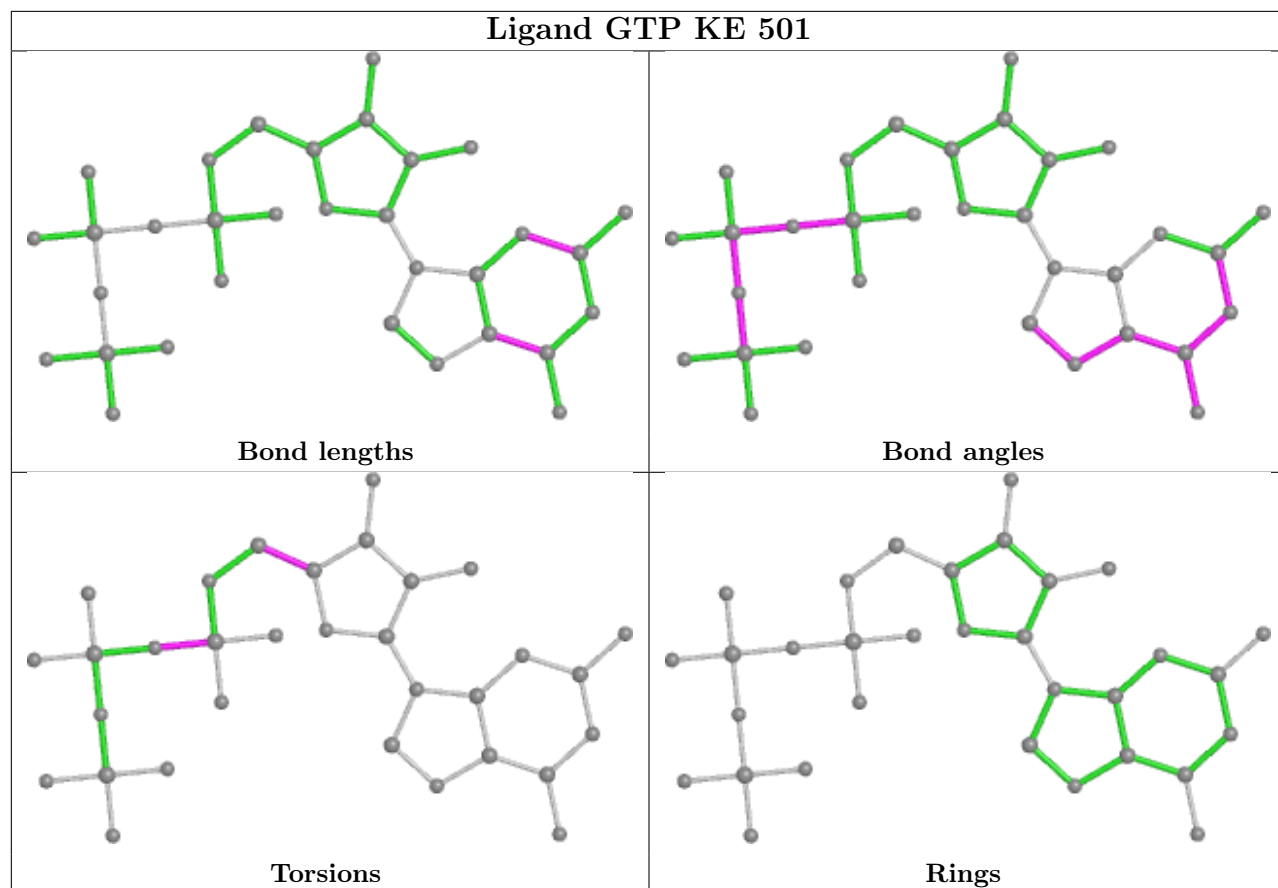


## Ligand GTP DE 501

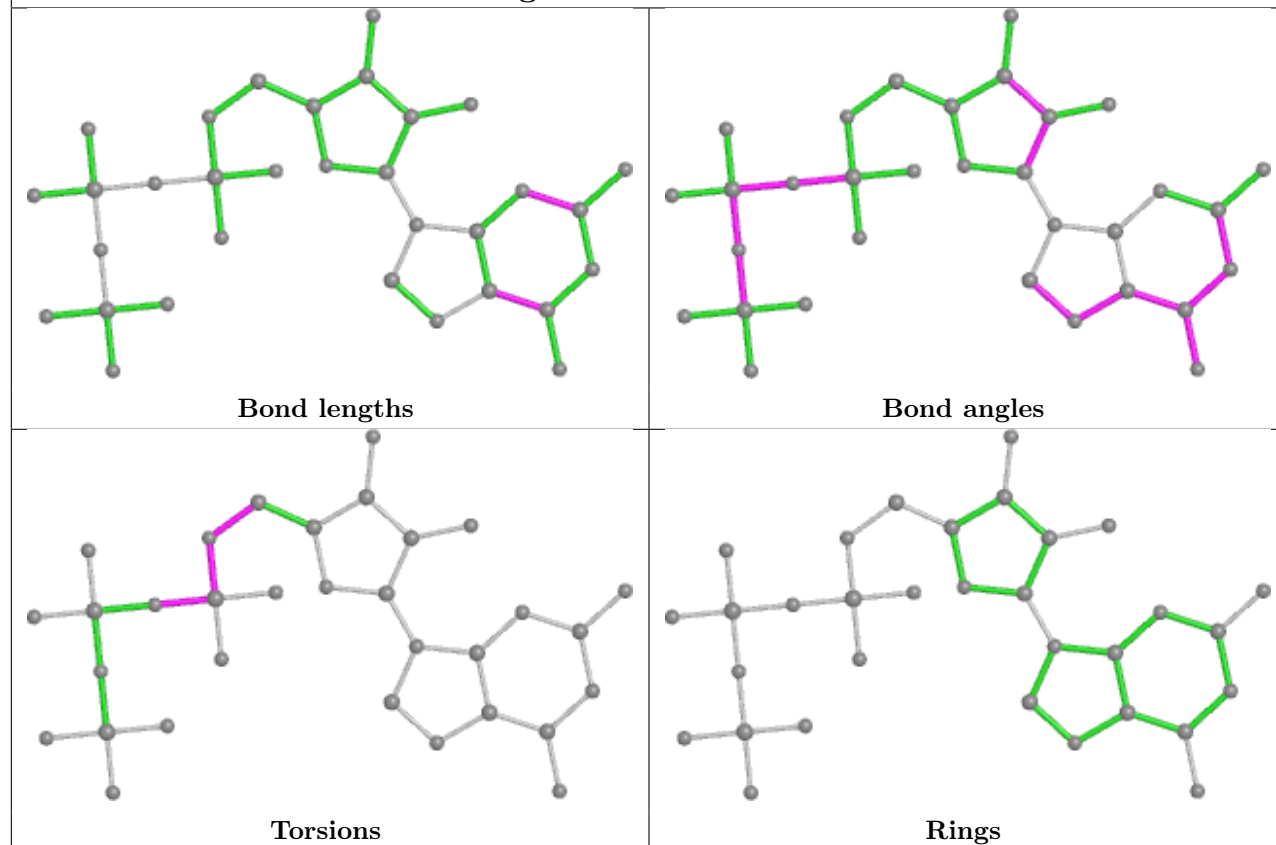


## Ligand GTP EG 501

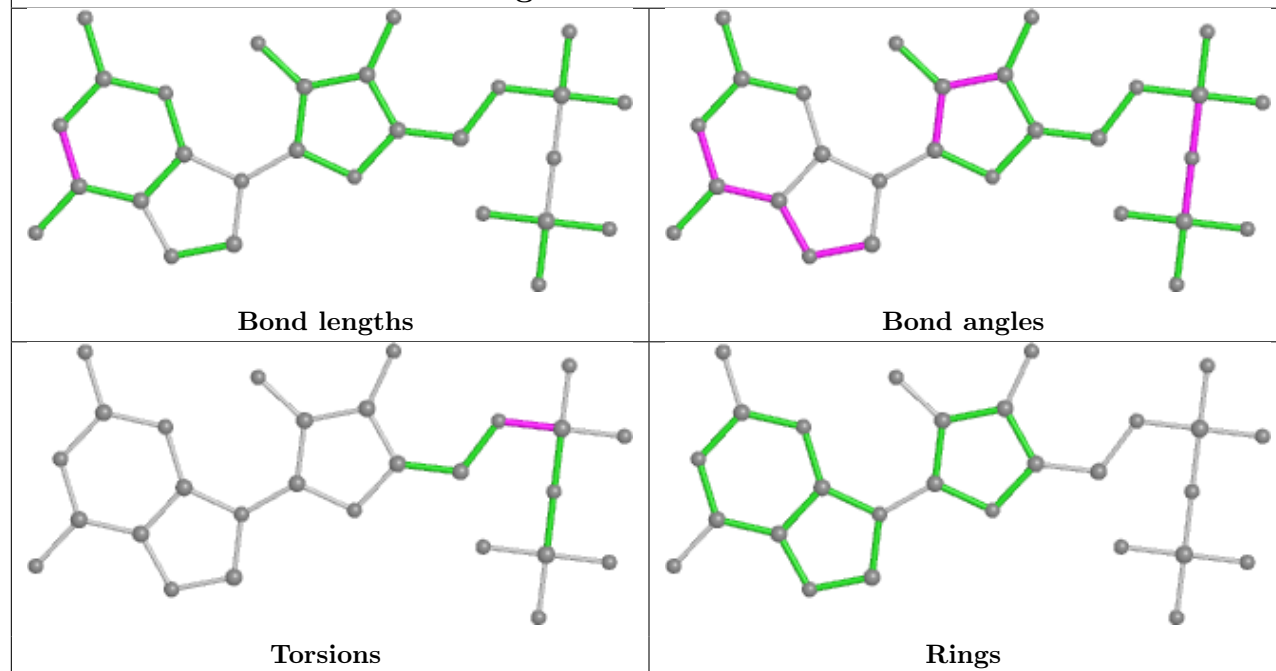




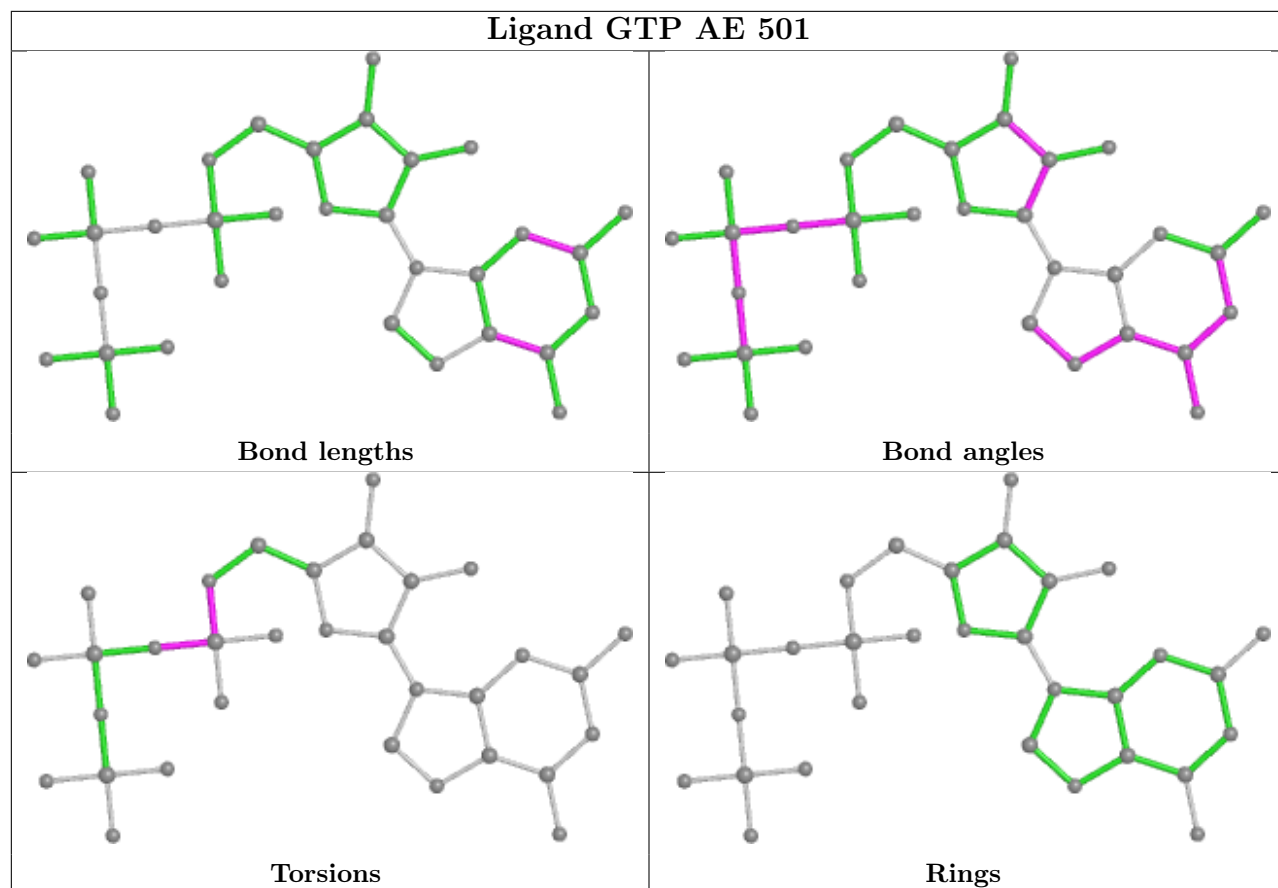
## Ligand GTP CE 501



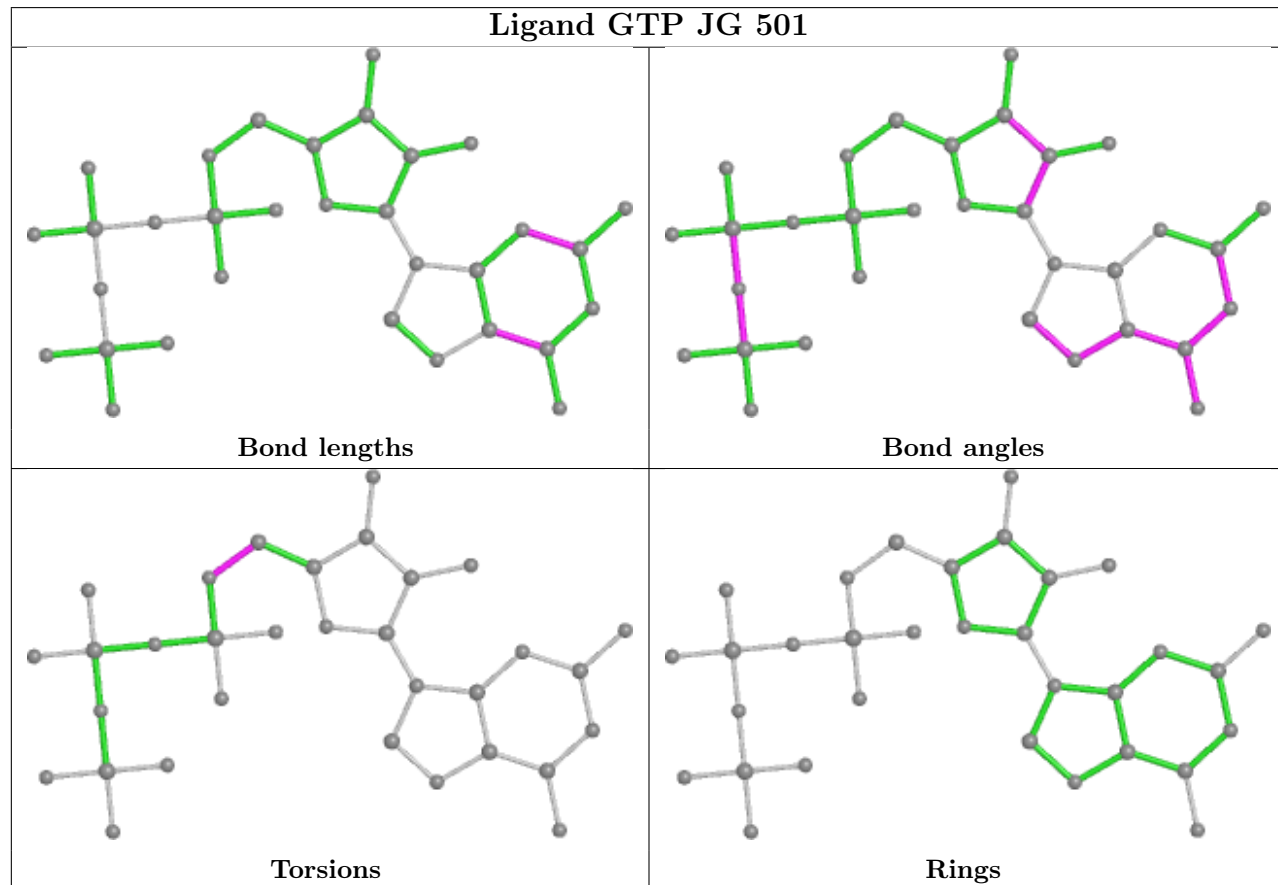
## Ligand GDP CD 501



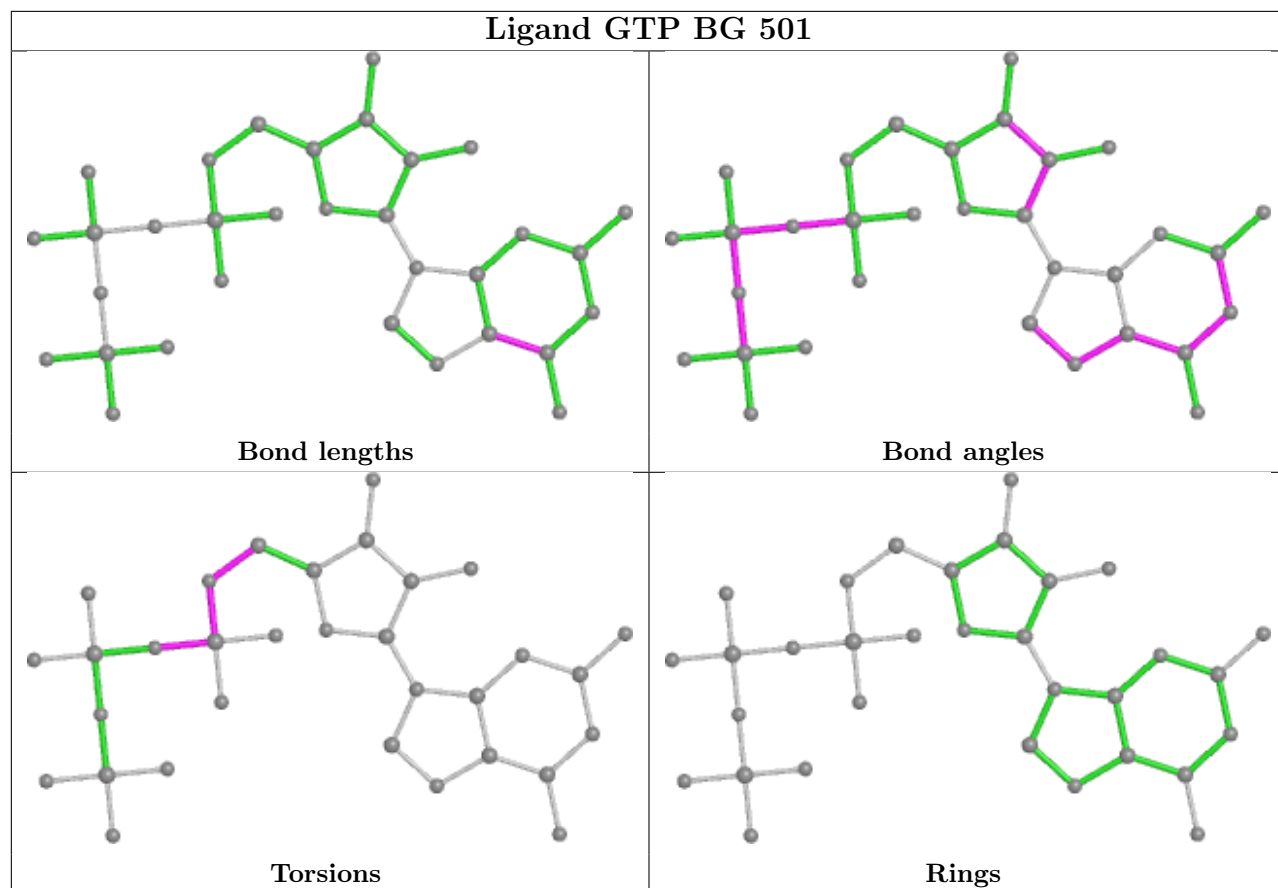
## Ligand GTP AE 501



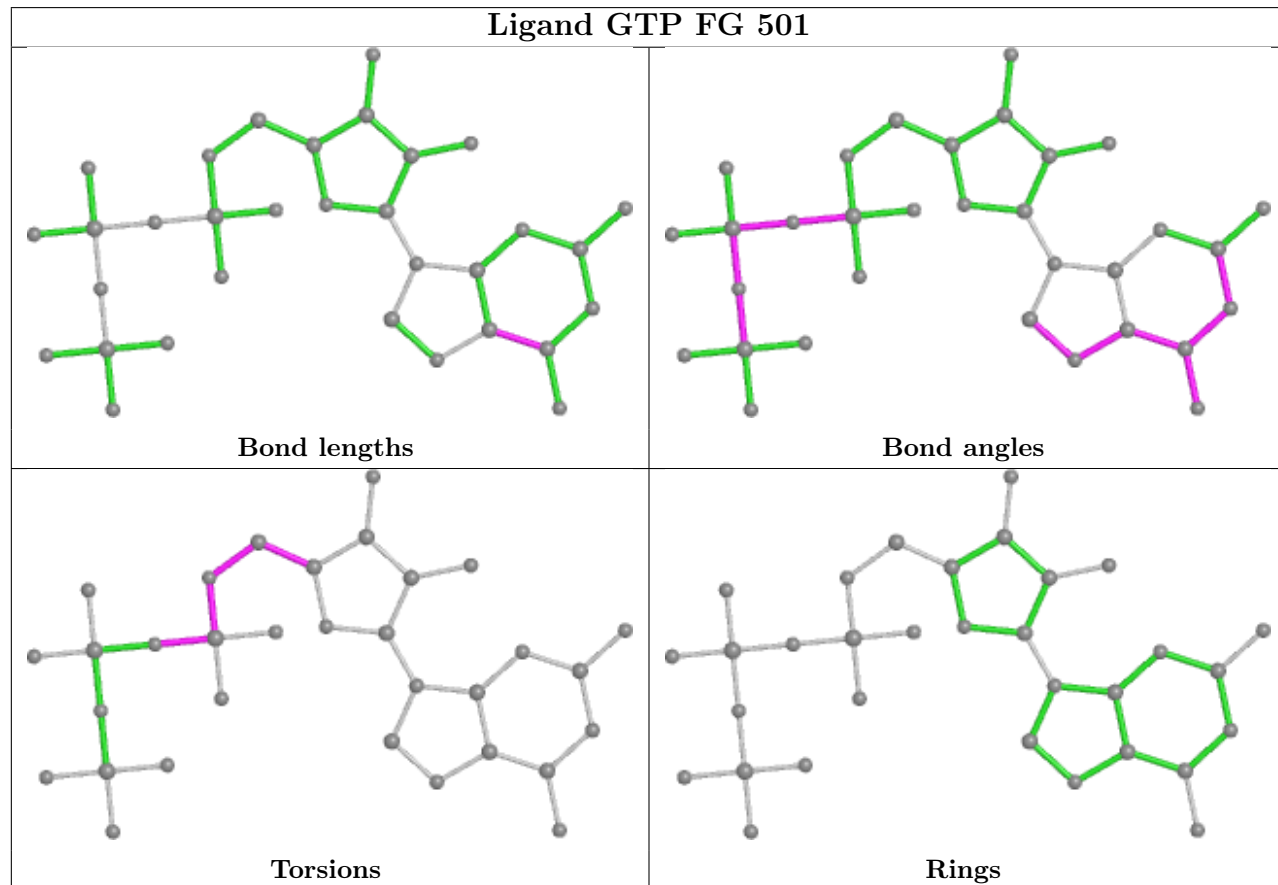
## Ligand GTP JG 501



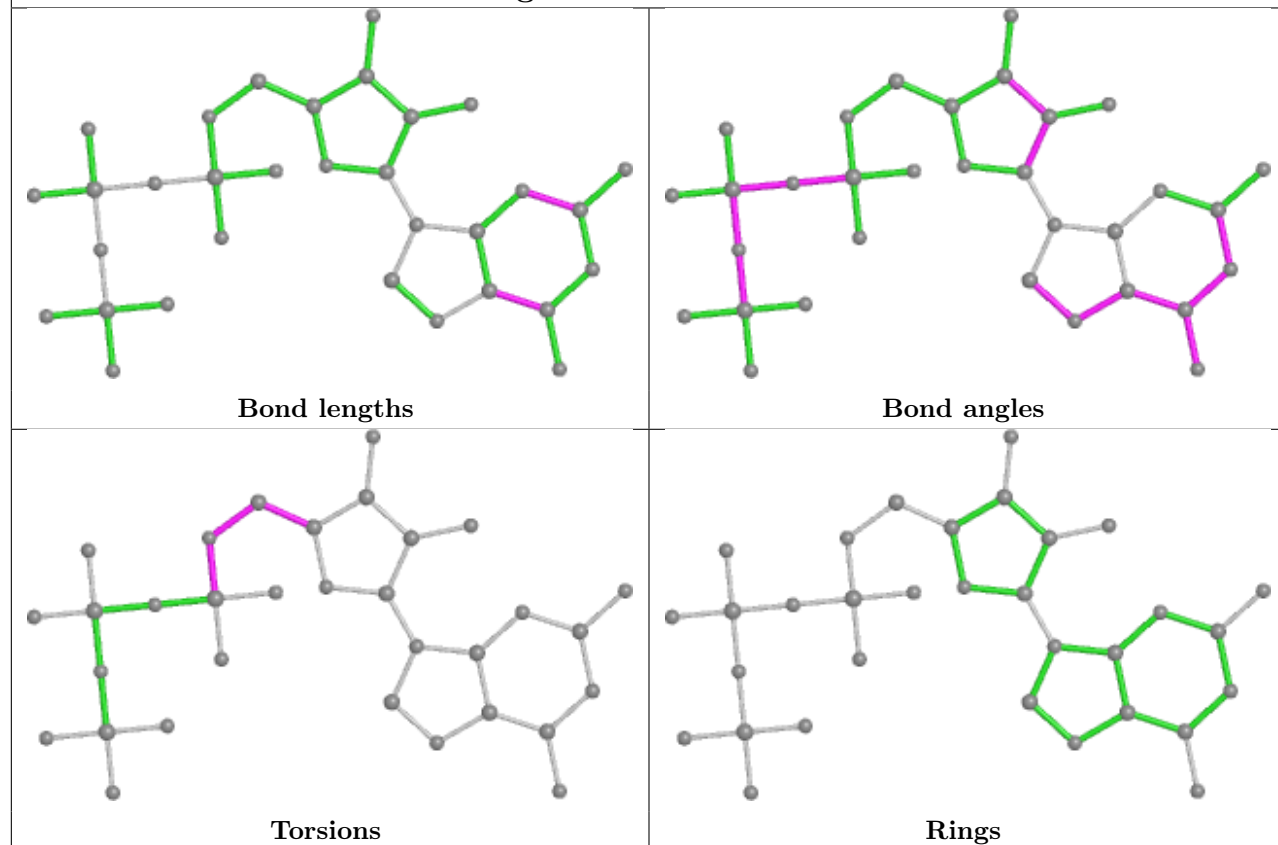
## Ligand GTP BG 501



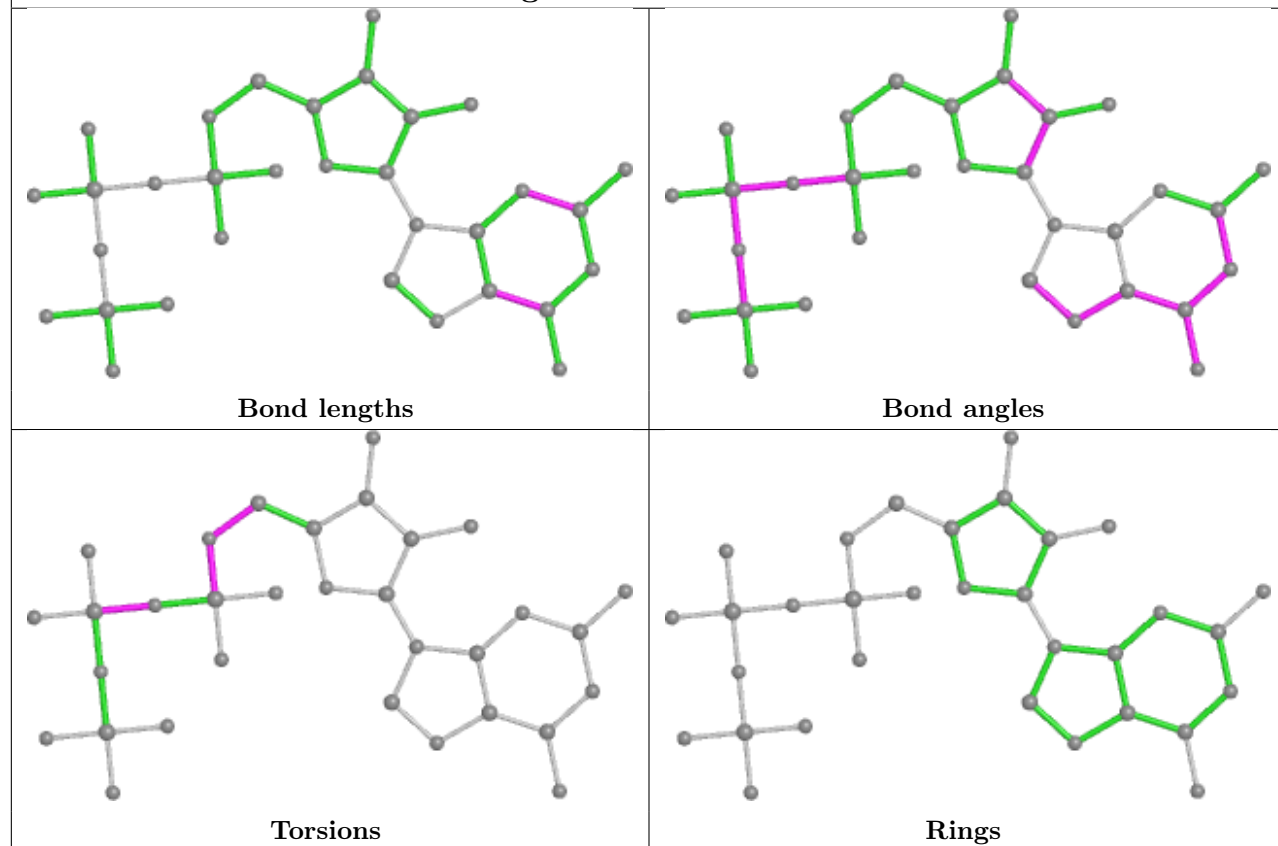
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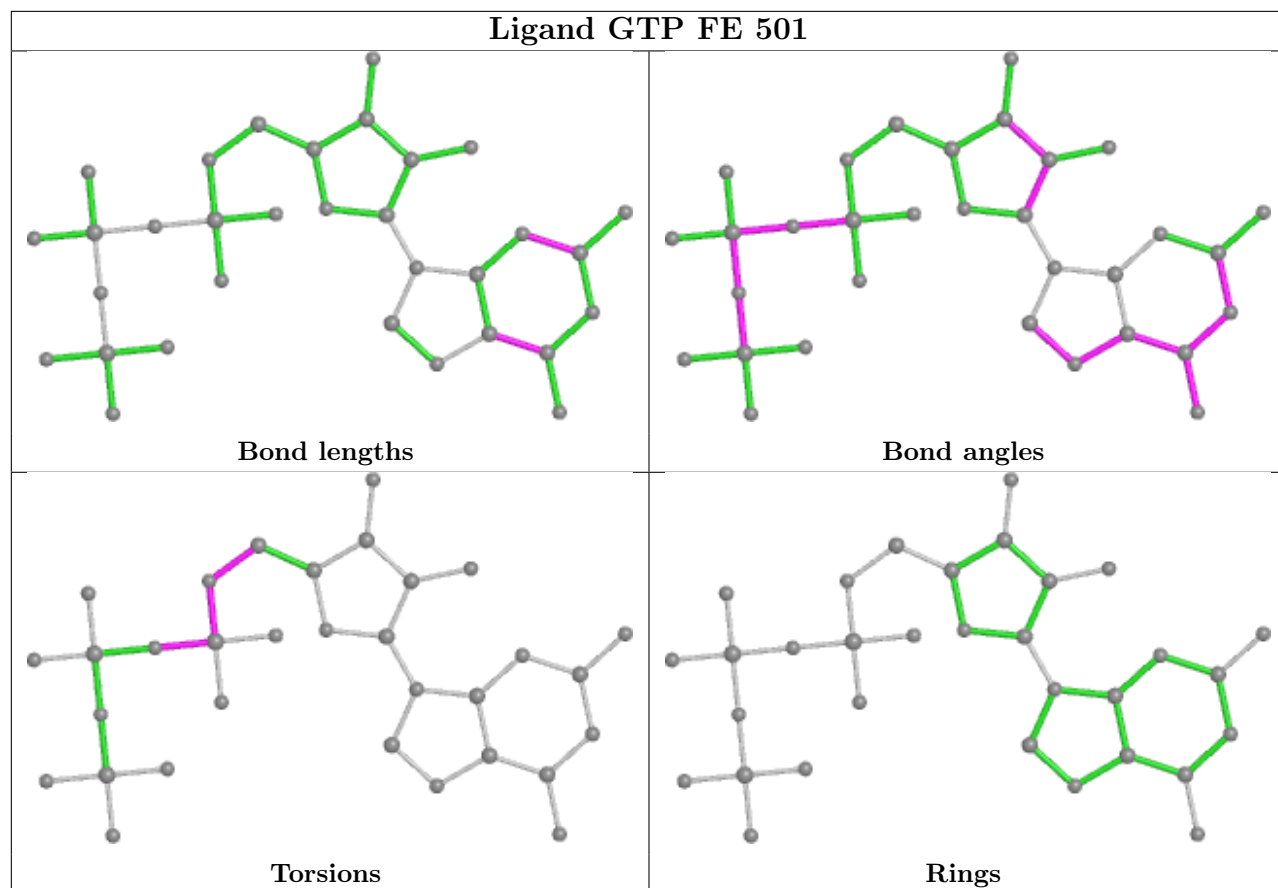
## Ligand GTP GC 501



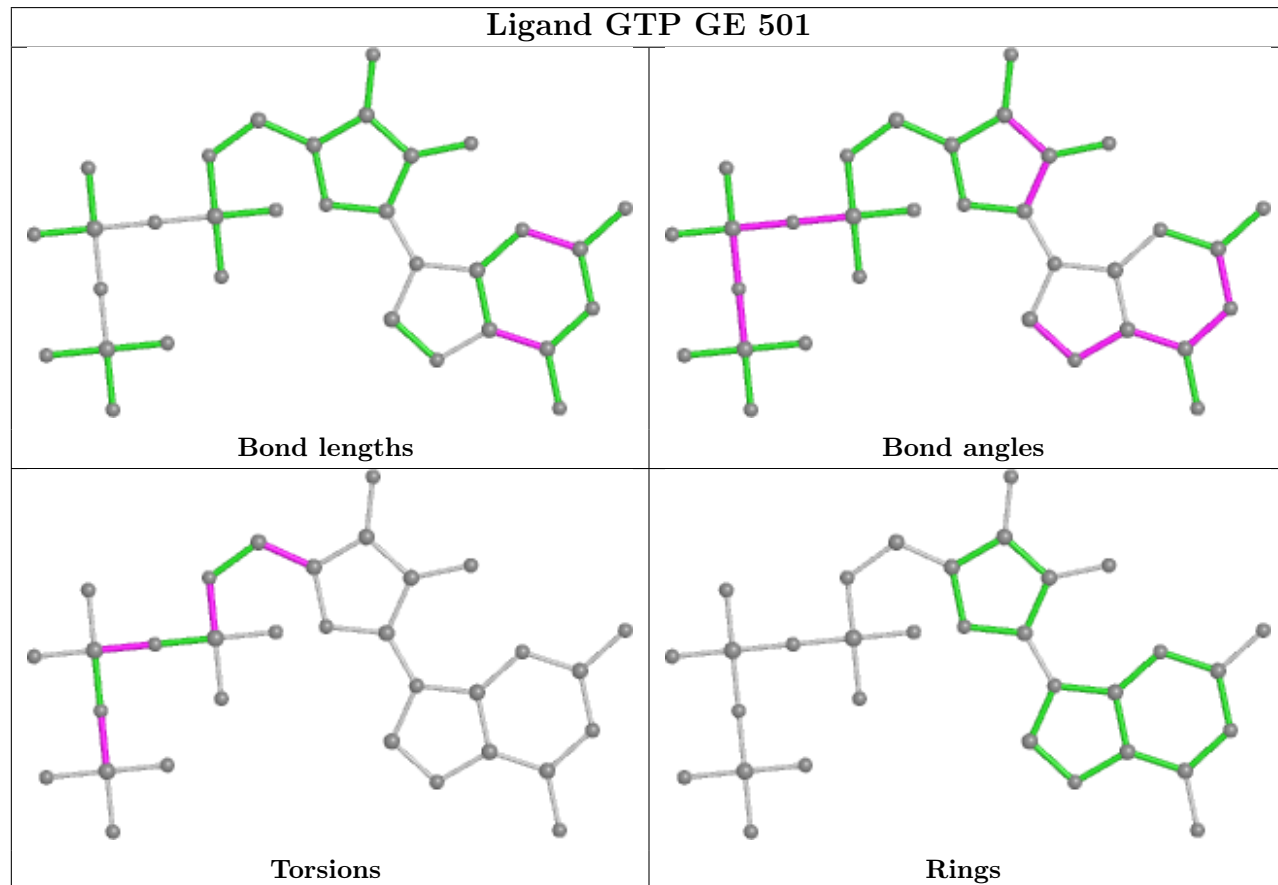
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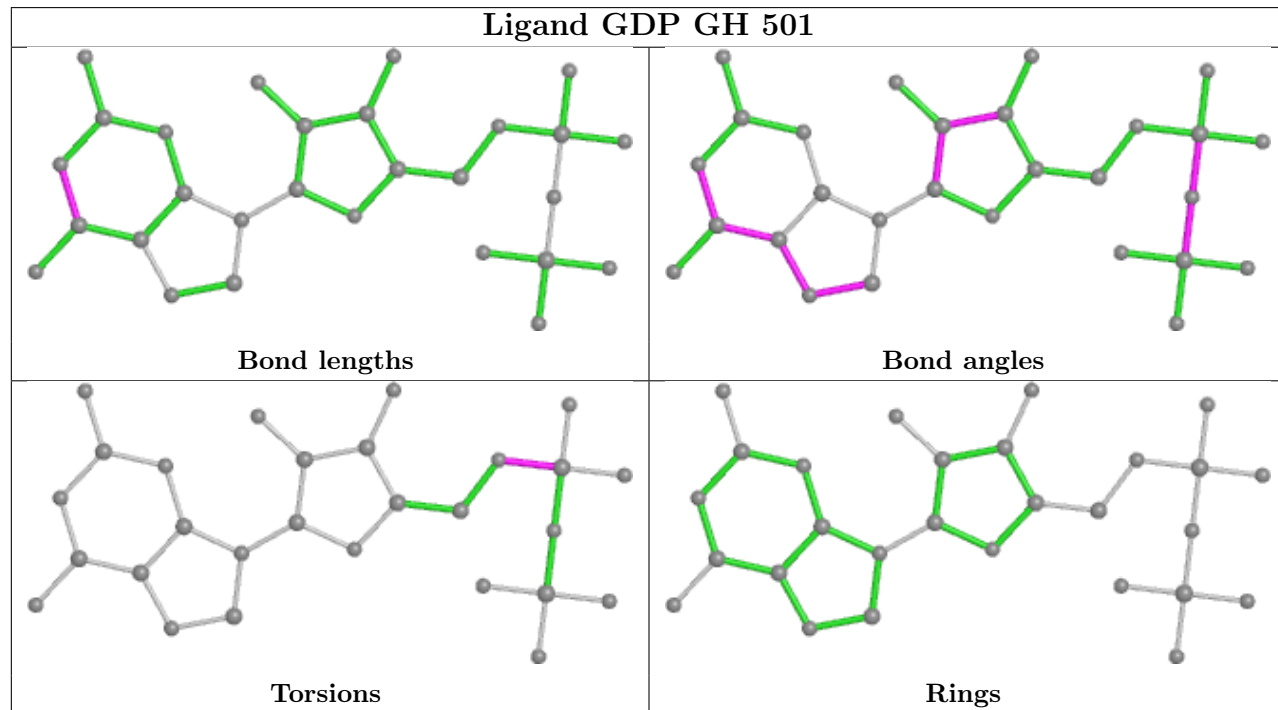
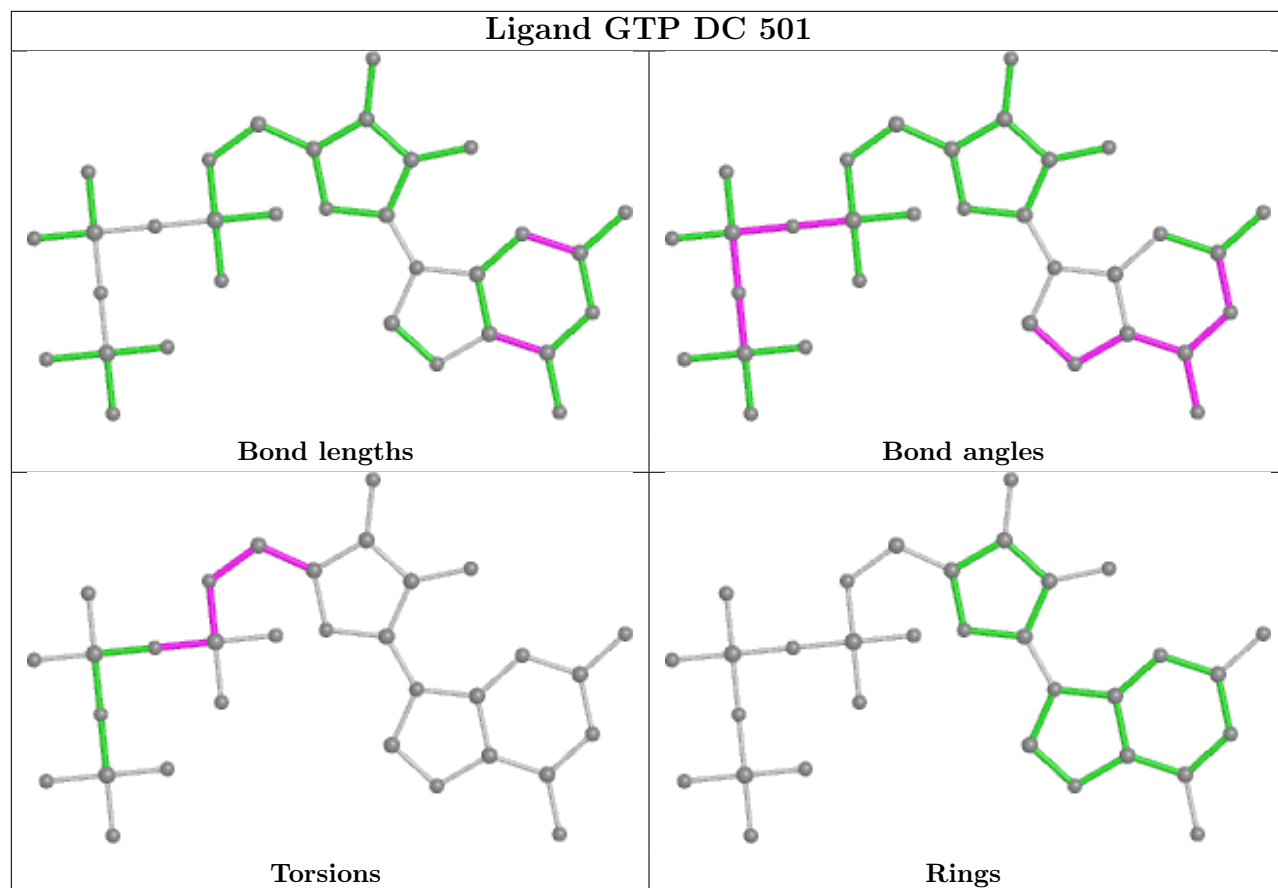


## Ligand GTP FE 501



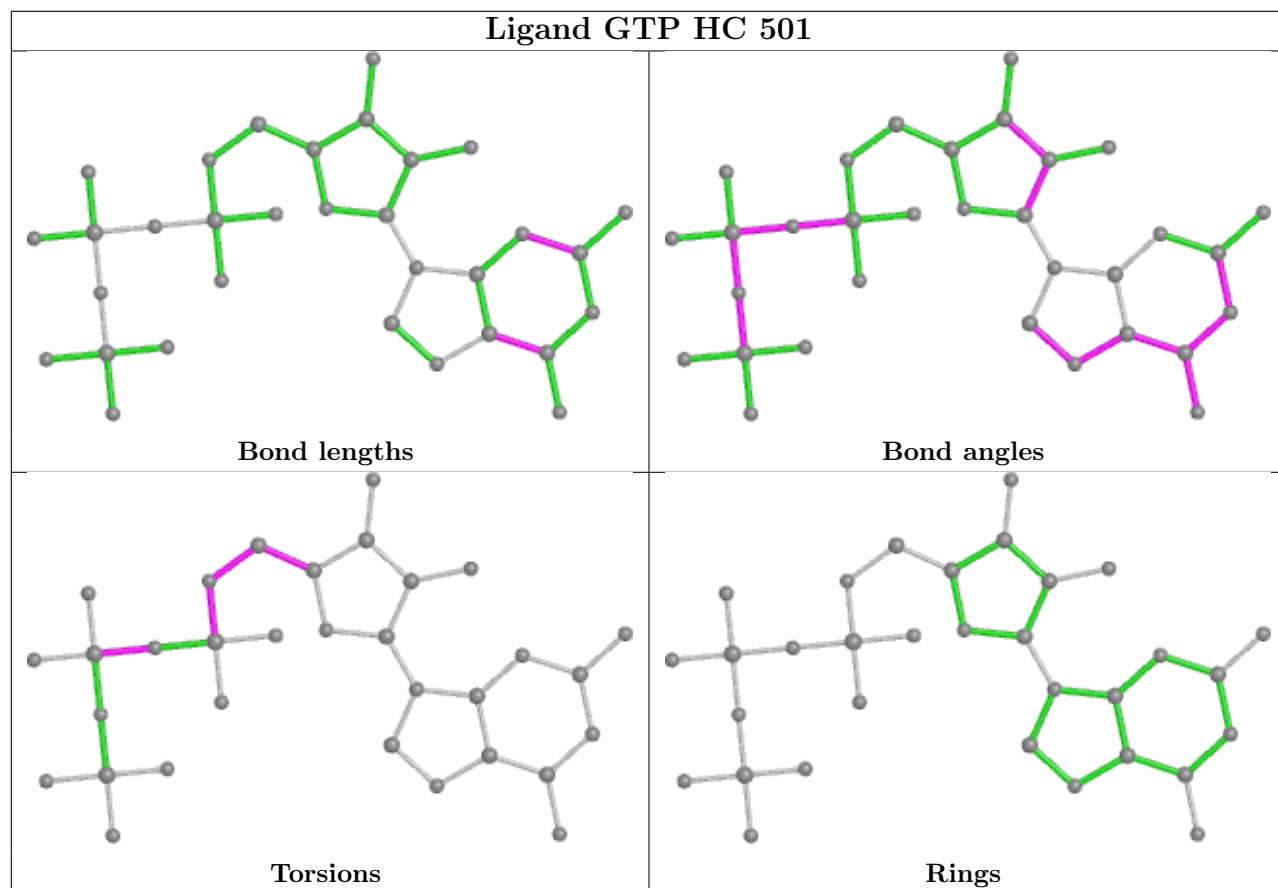
## Ligand GTP GE 501



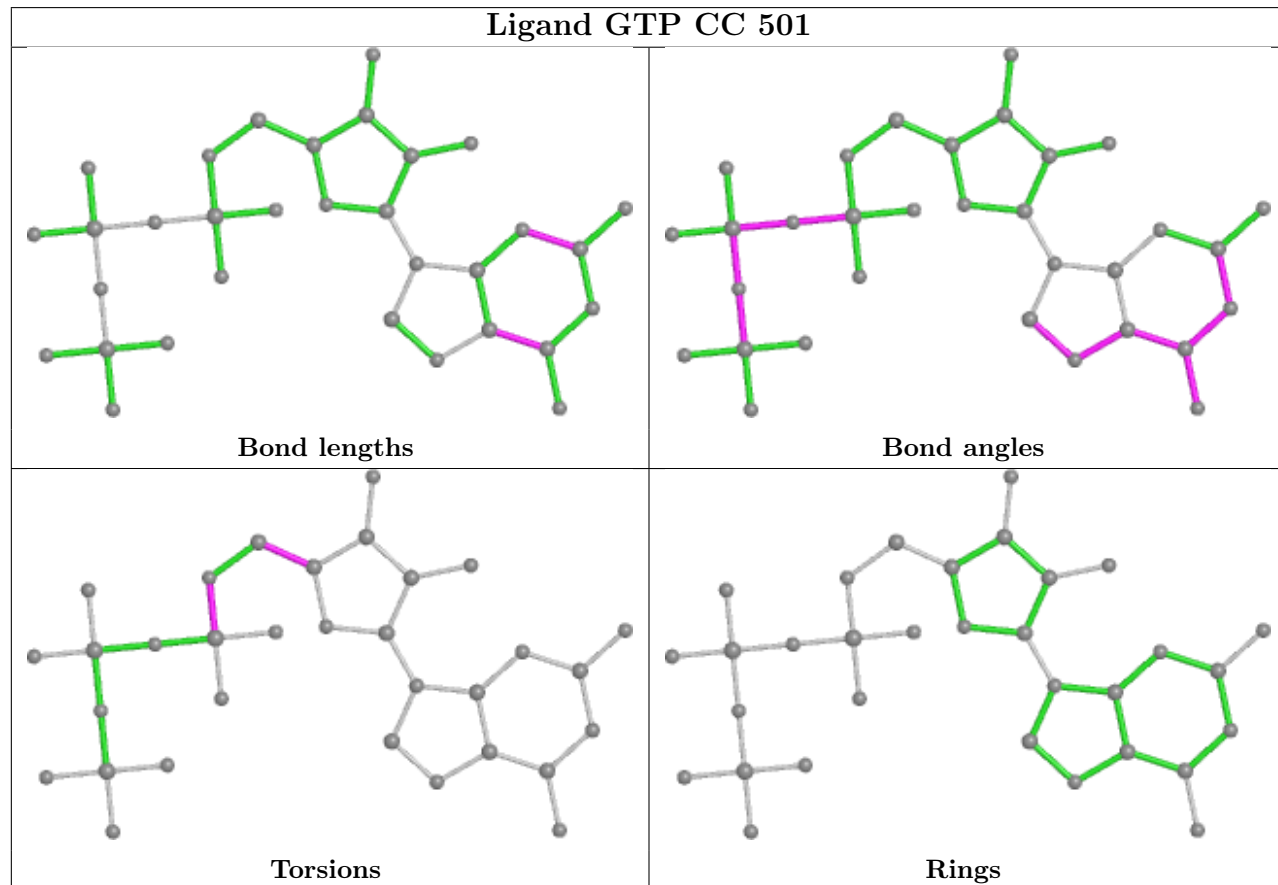


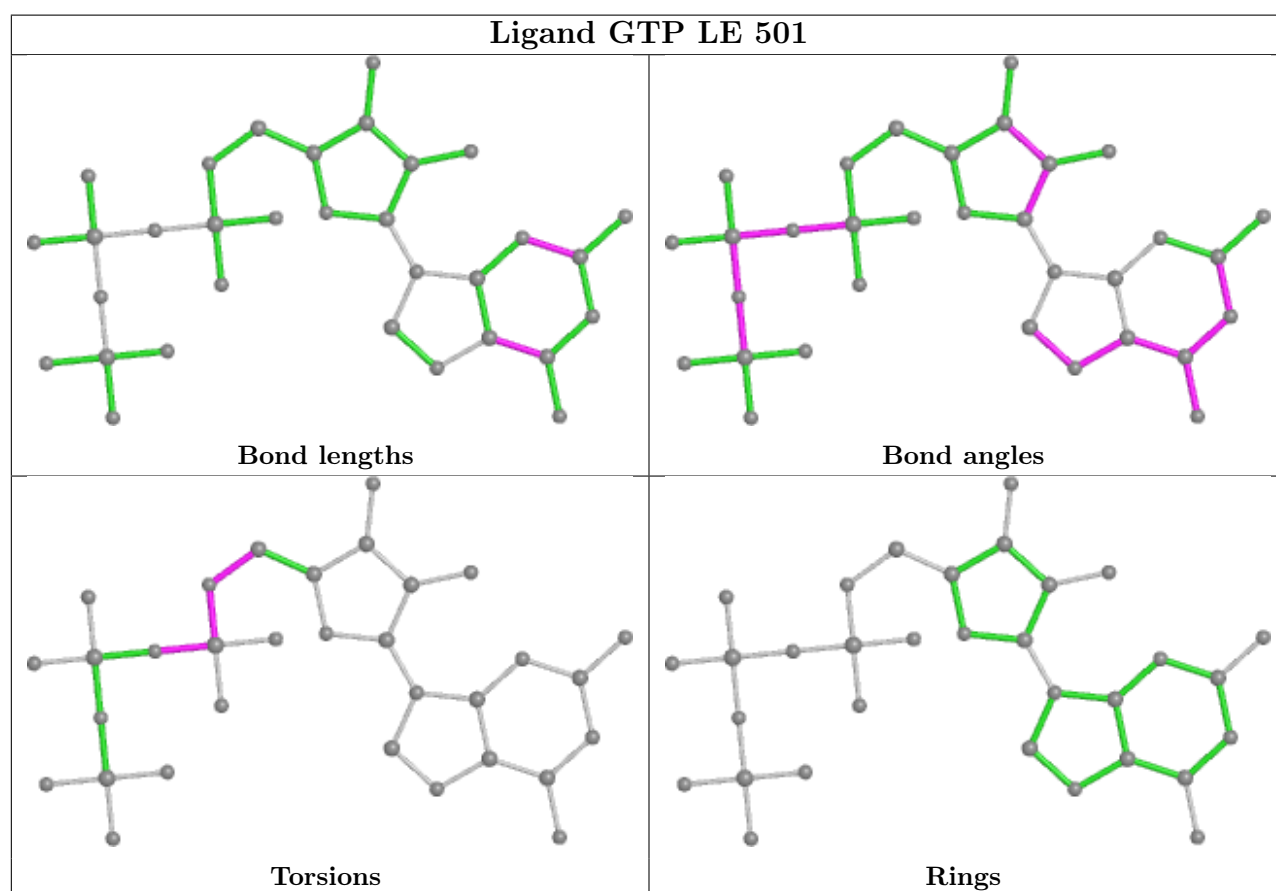
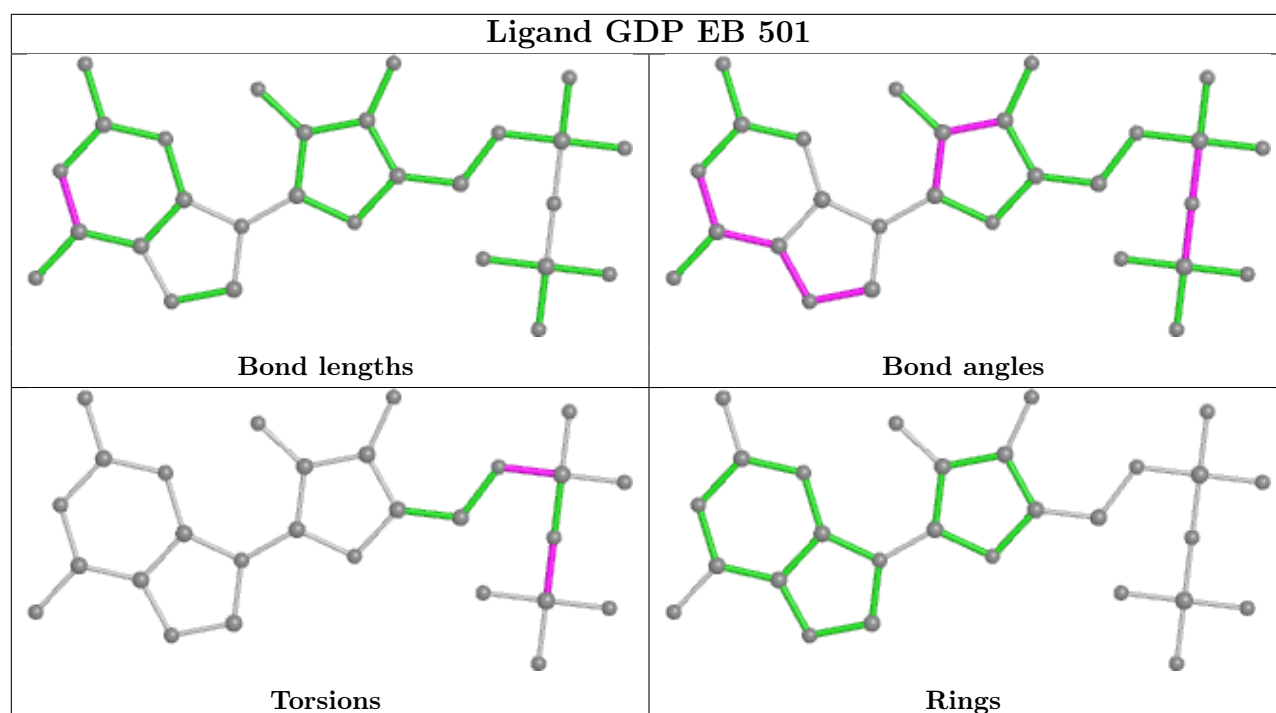


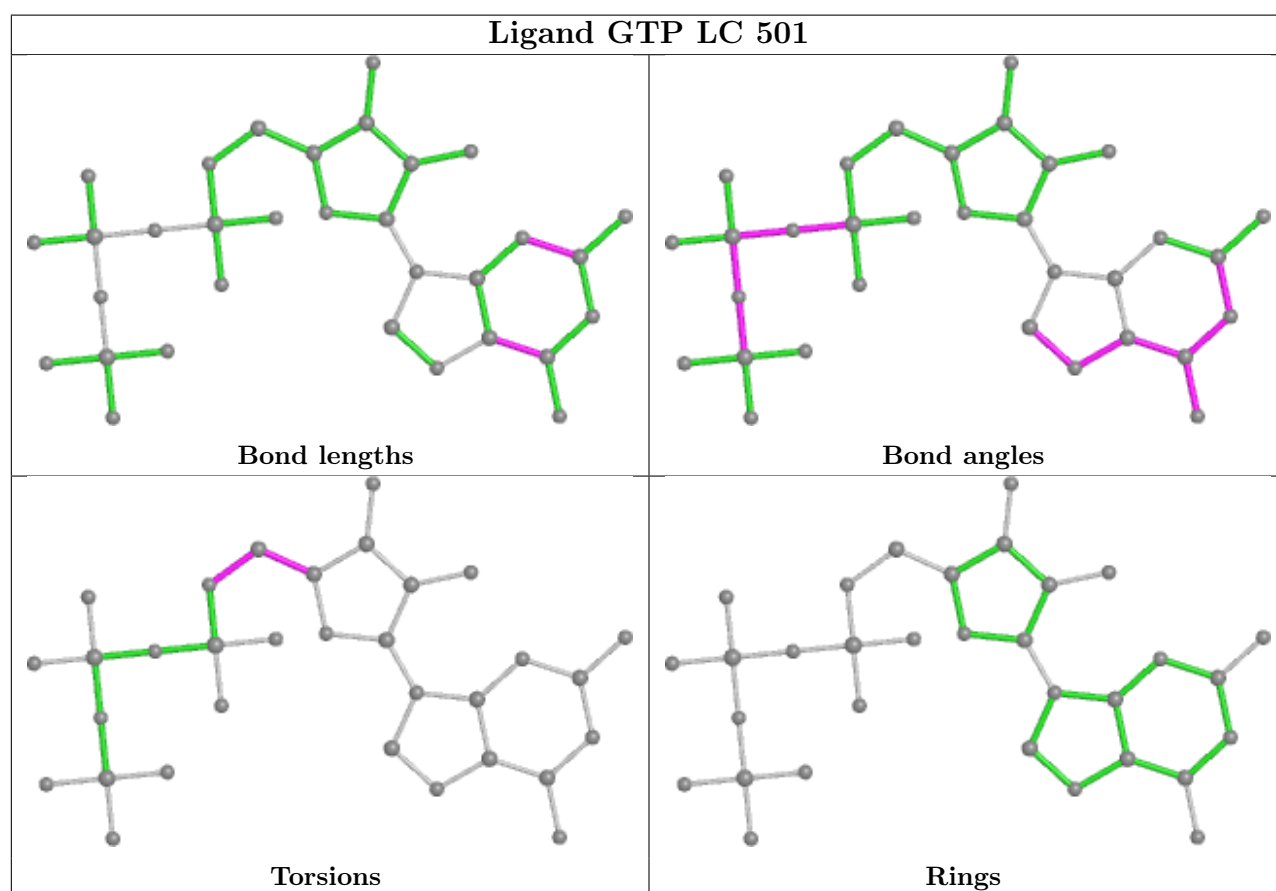
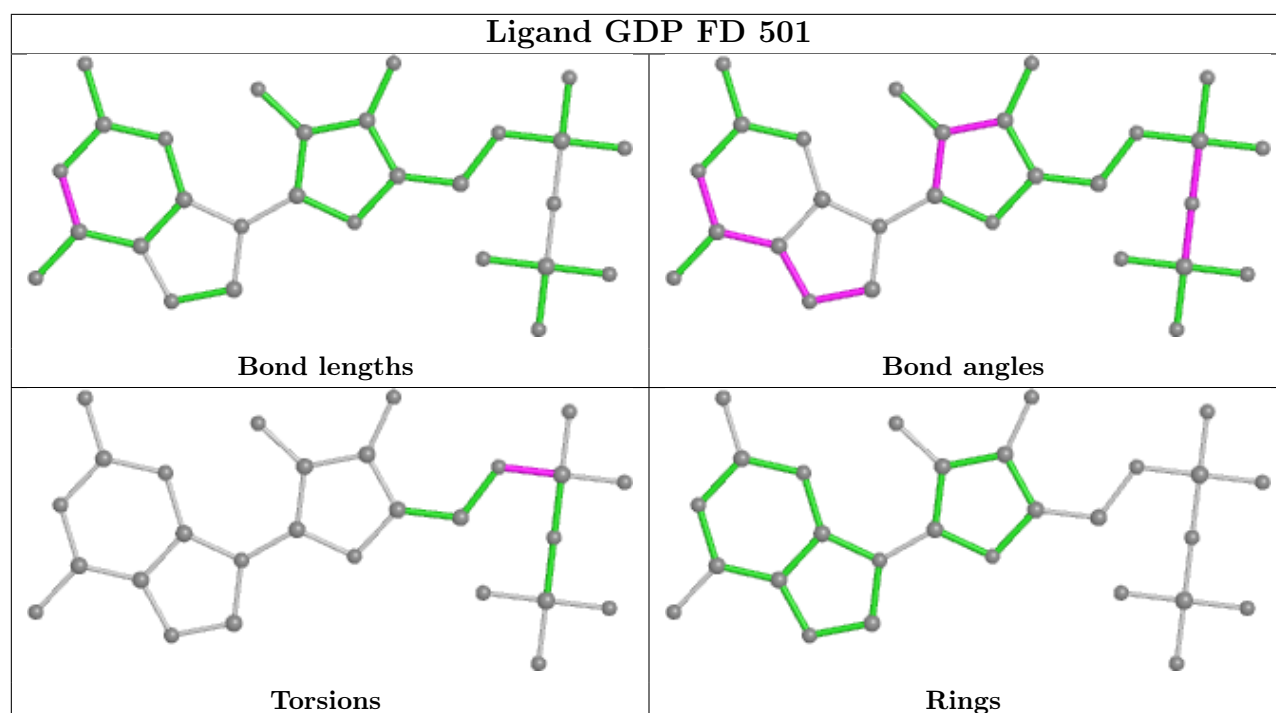
## Ligand GTP HC 501



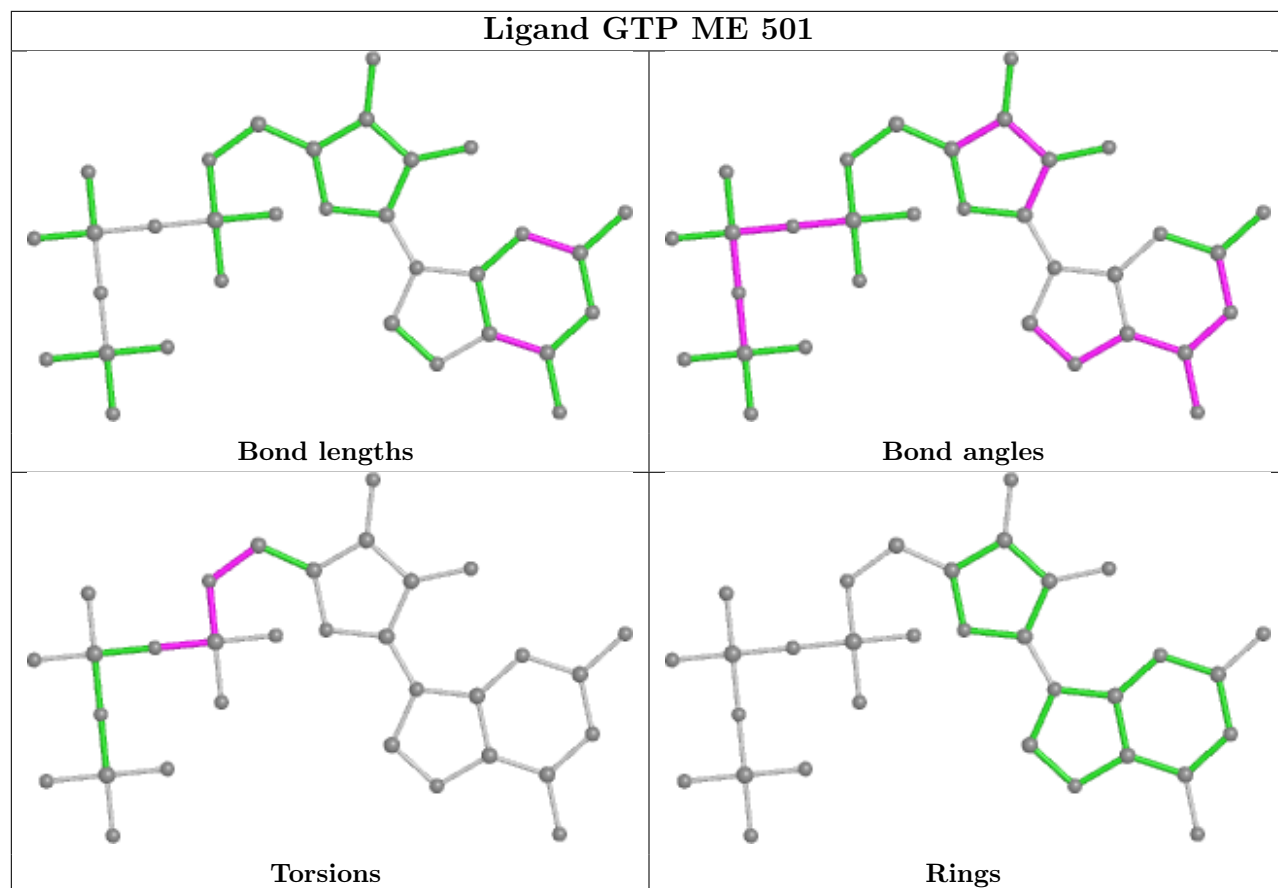
## Ligand GTP CC 501



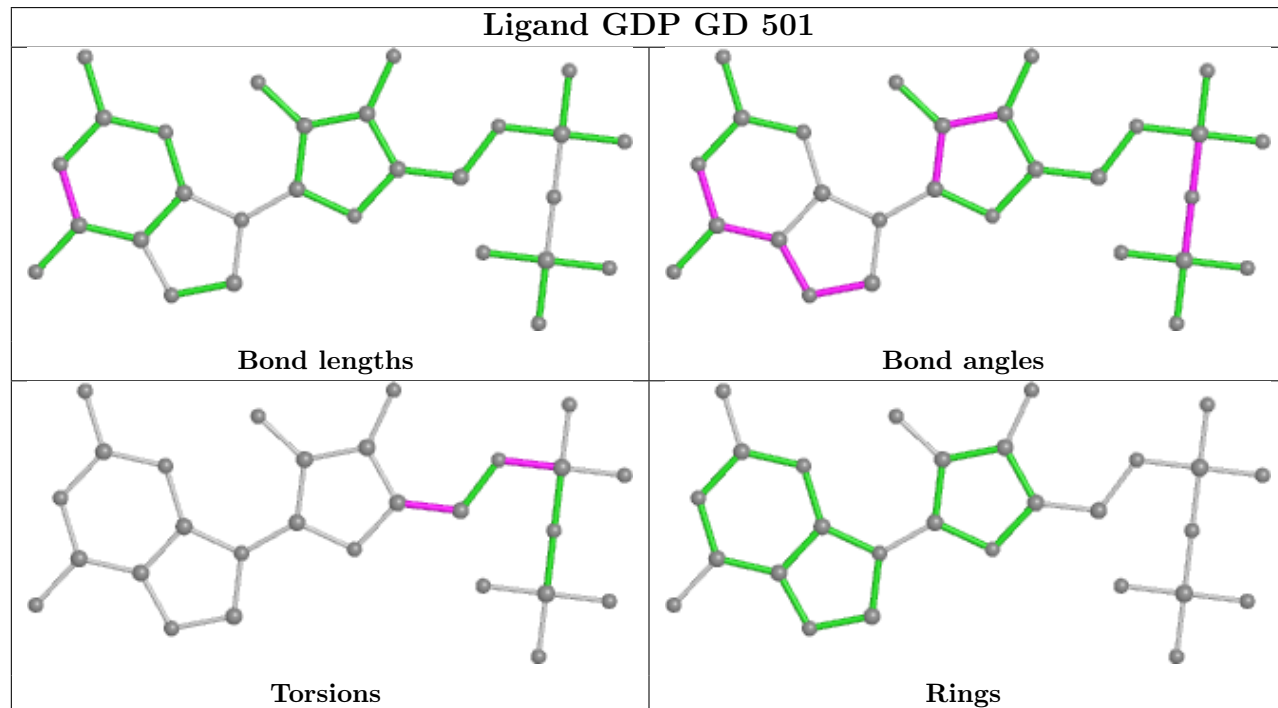




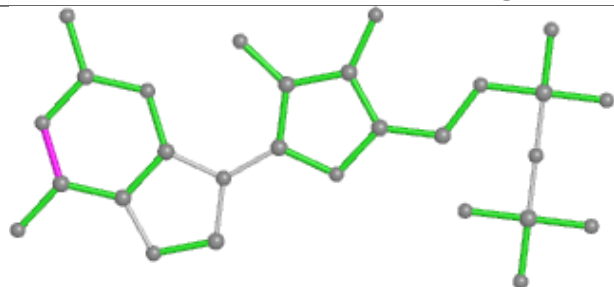
## Ligand GTP ME 501



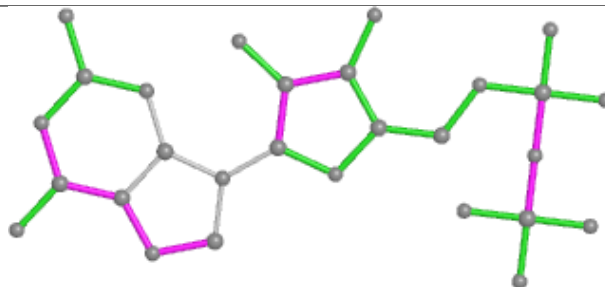
## Ligand GDP GD 501



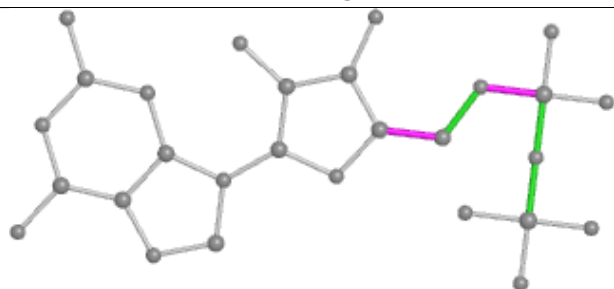
## Ligand GDP BA 501



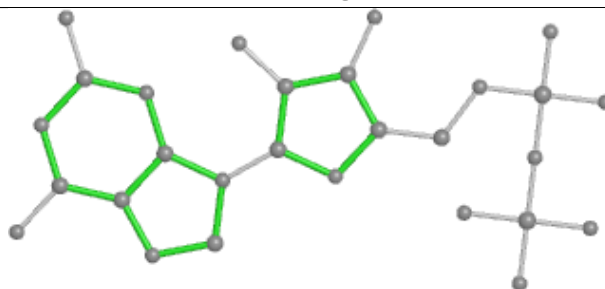
Bond lengths



Bond angles

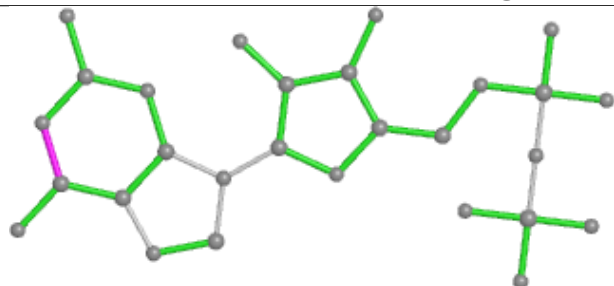


Torsions

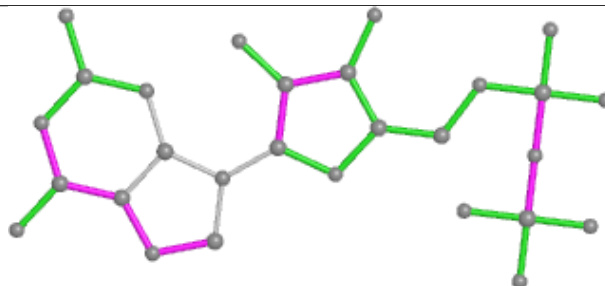


Rings

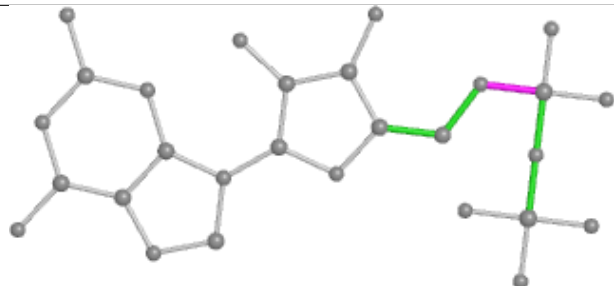
## Ligand GDP DB 501



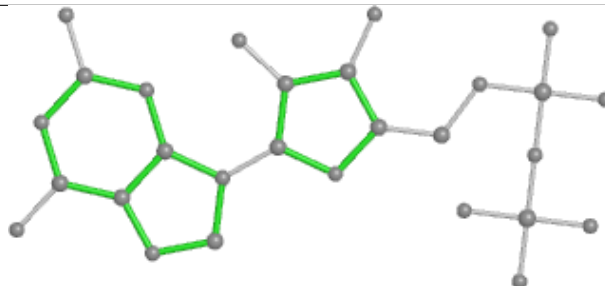
Bond lengths



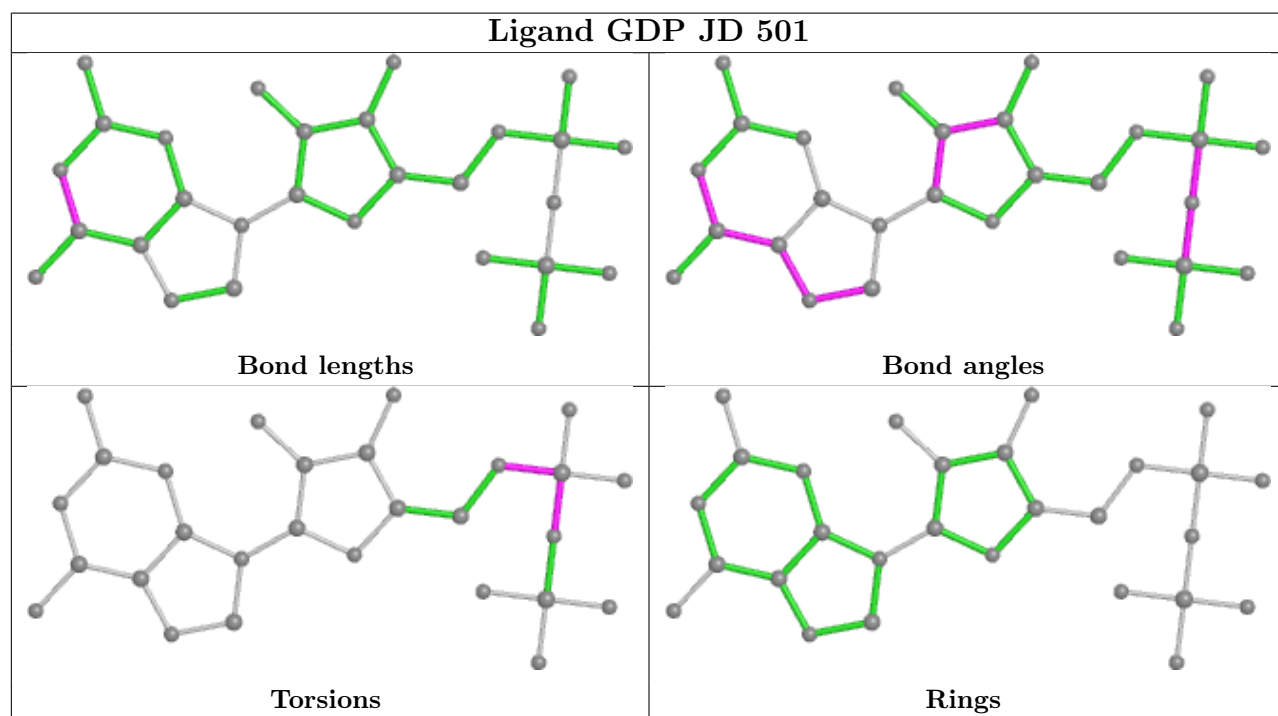
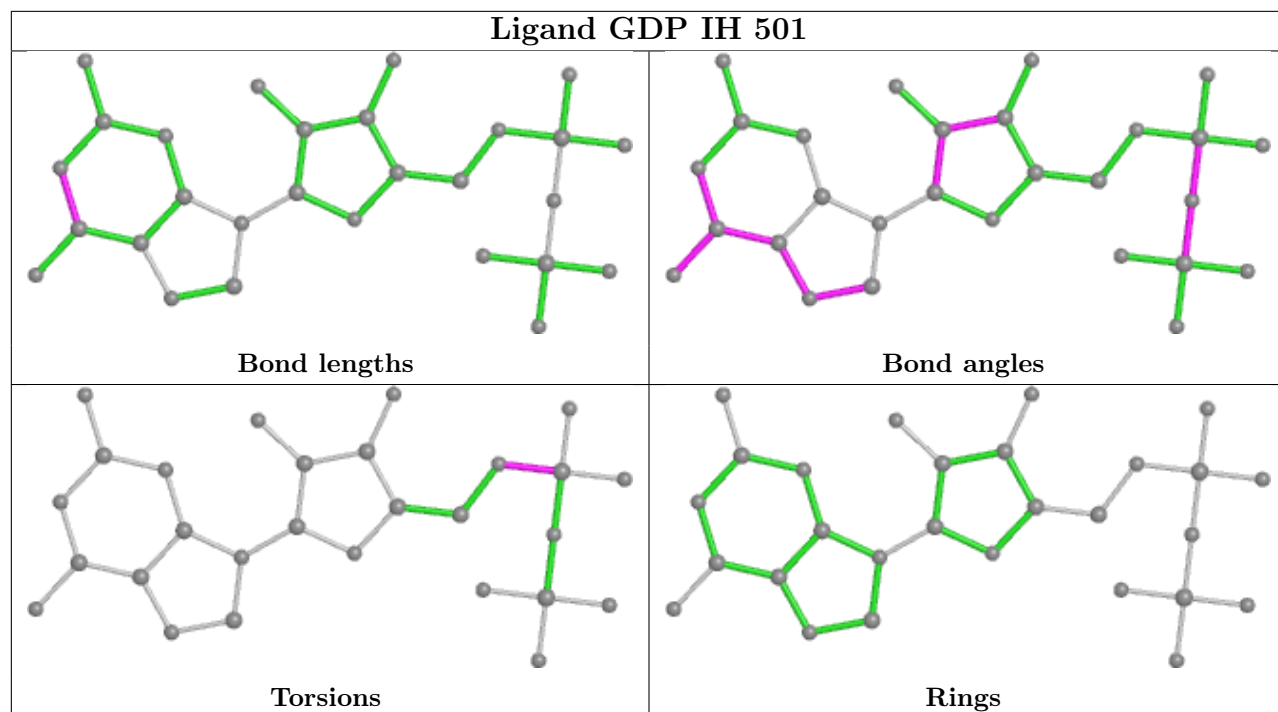
Bond angles



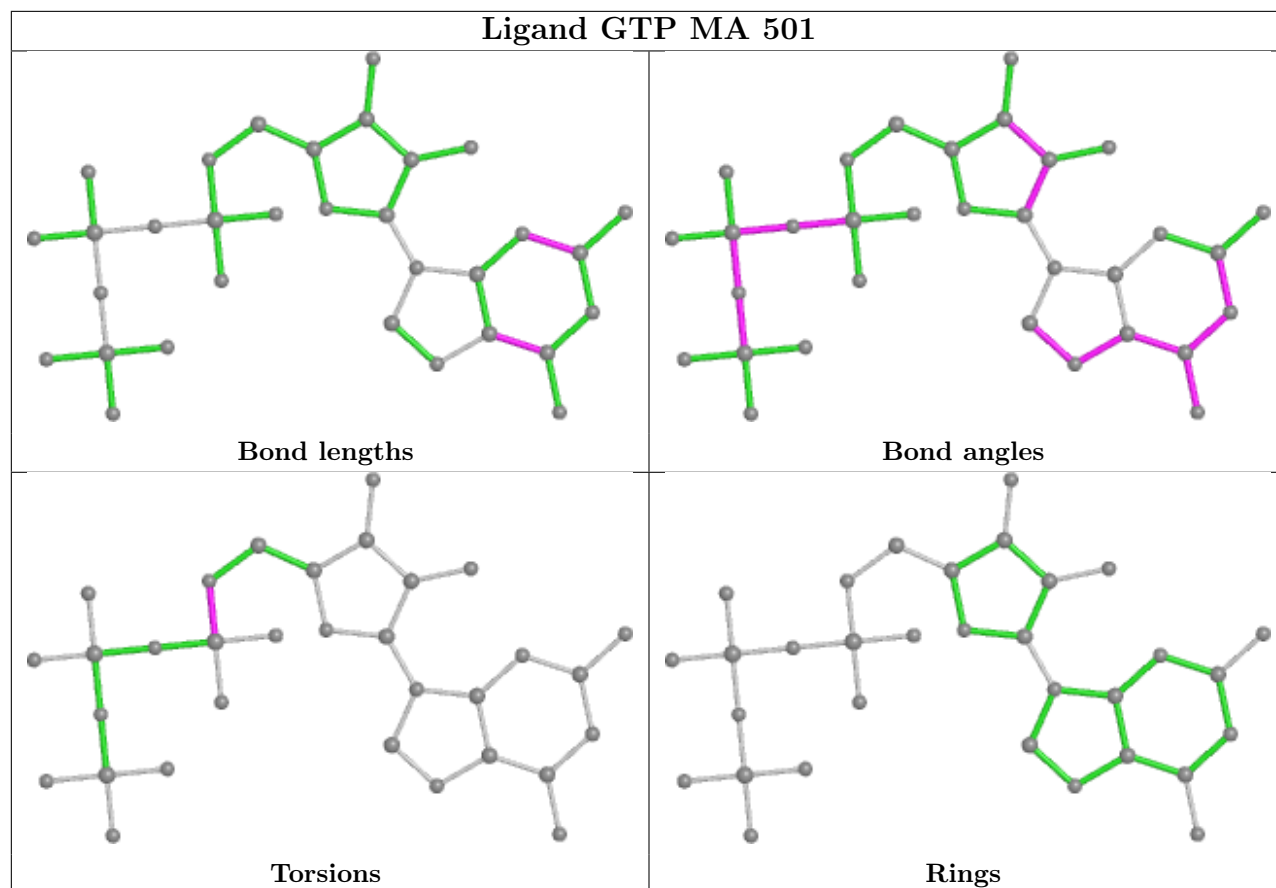
Torsions



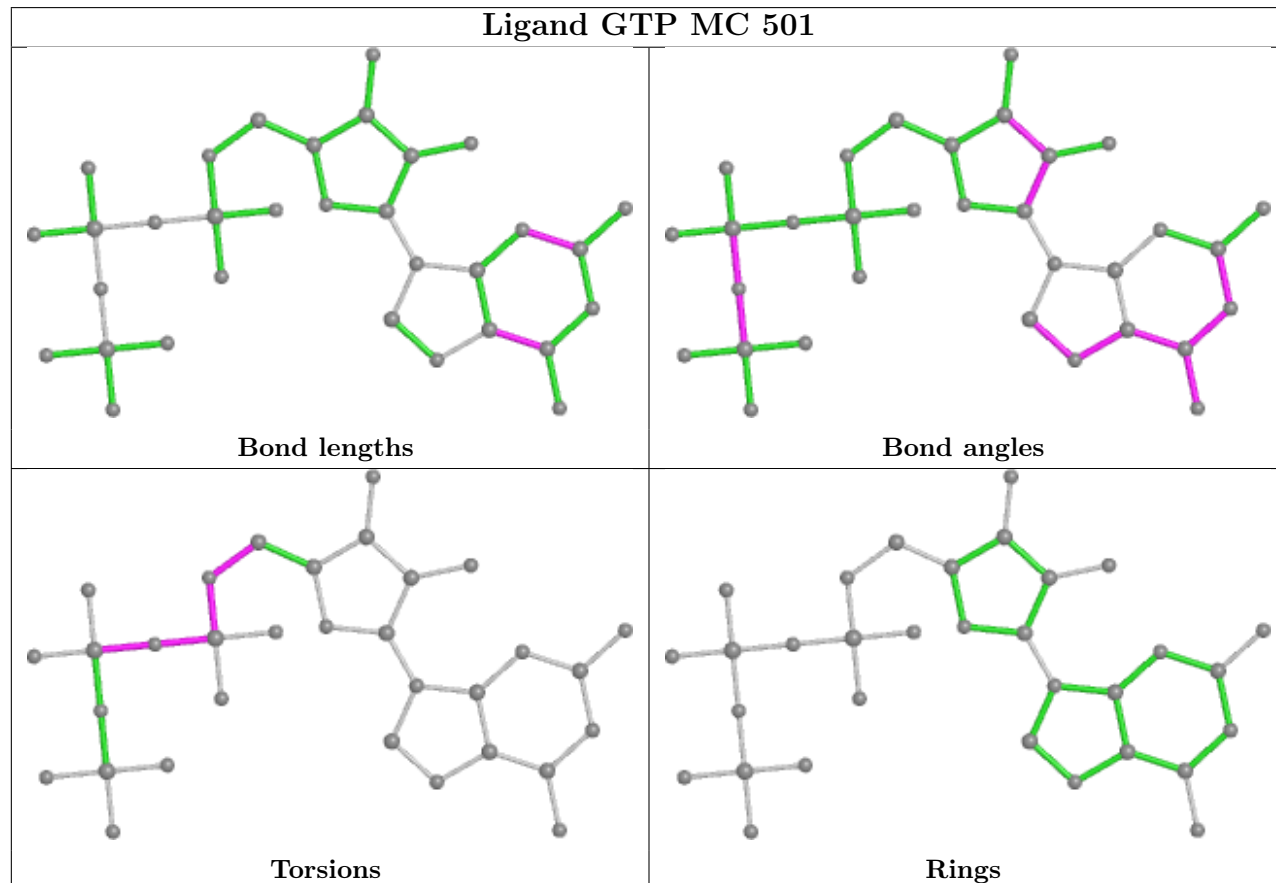
Rings

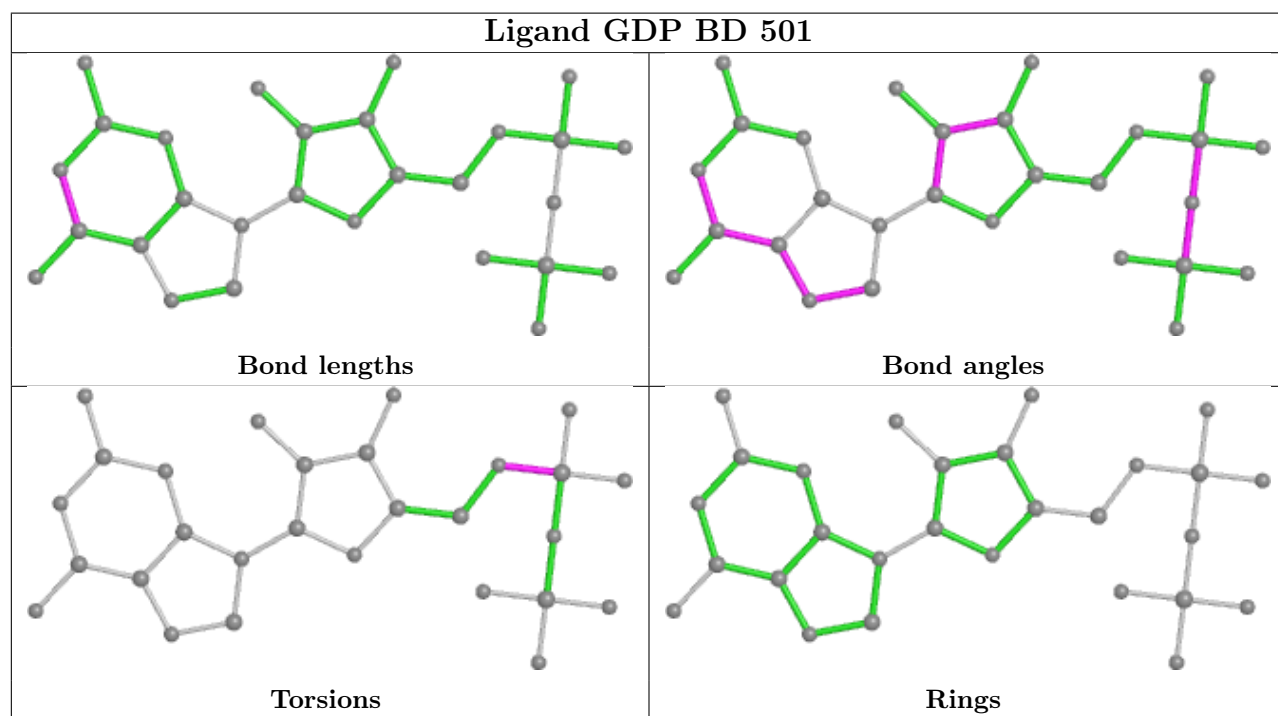
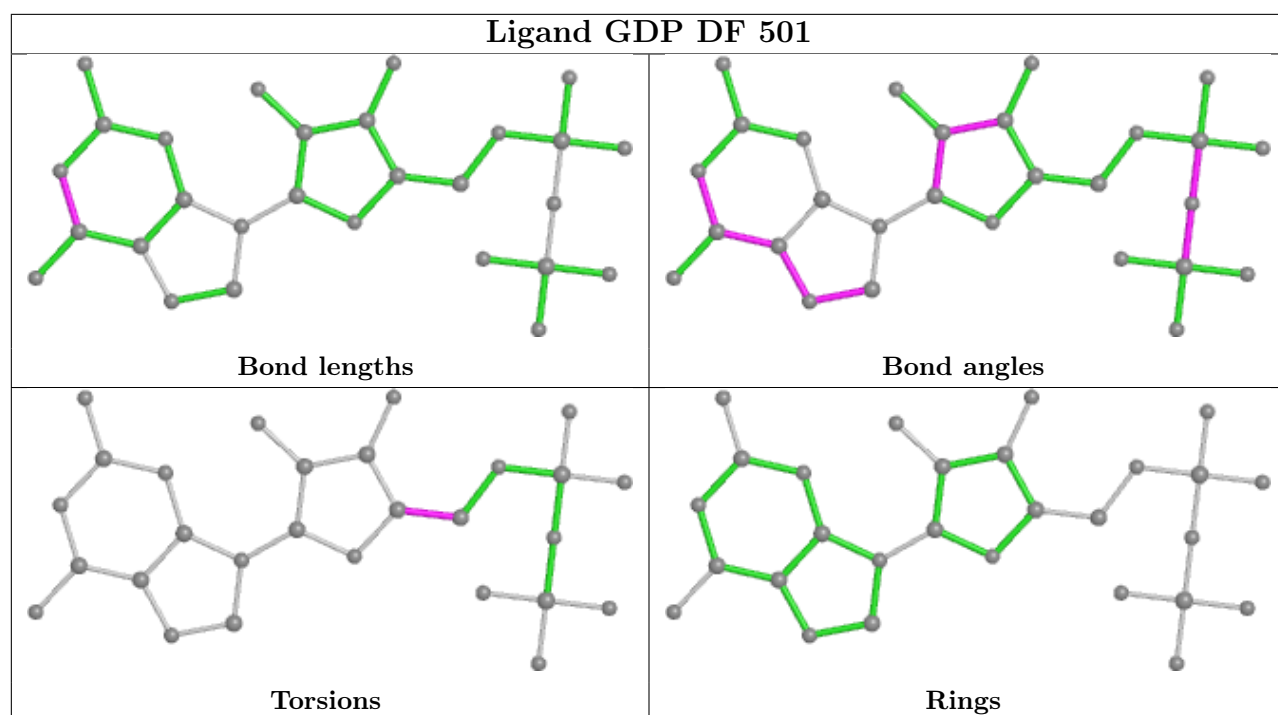


## Ligand GTP MA 501

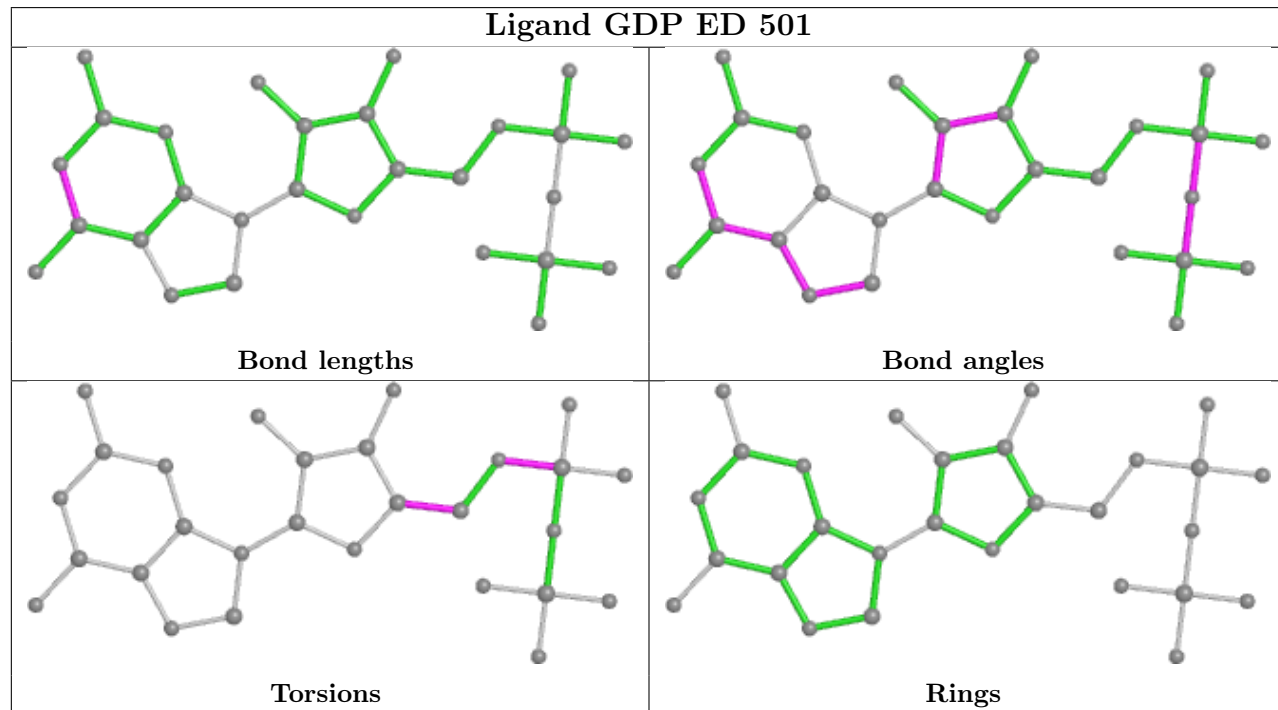
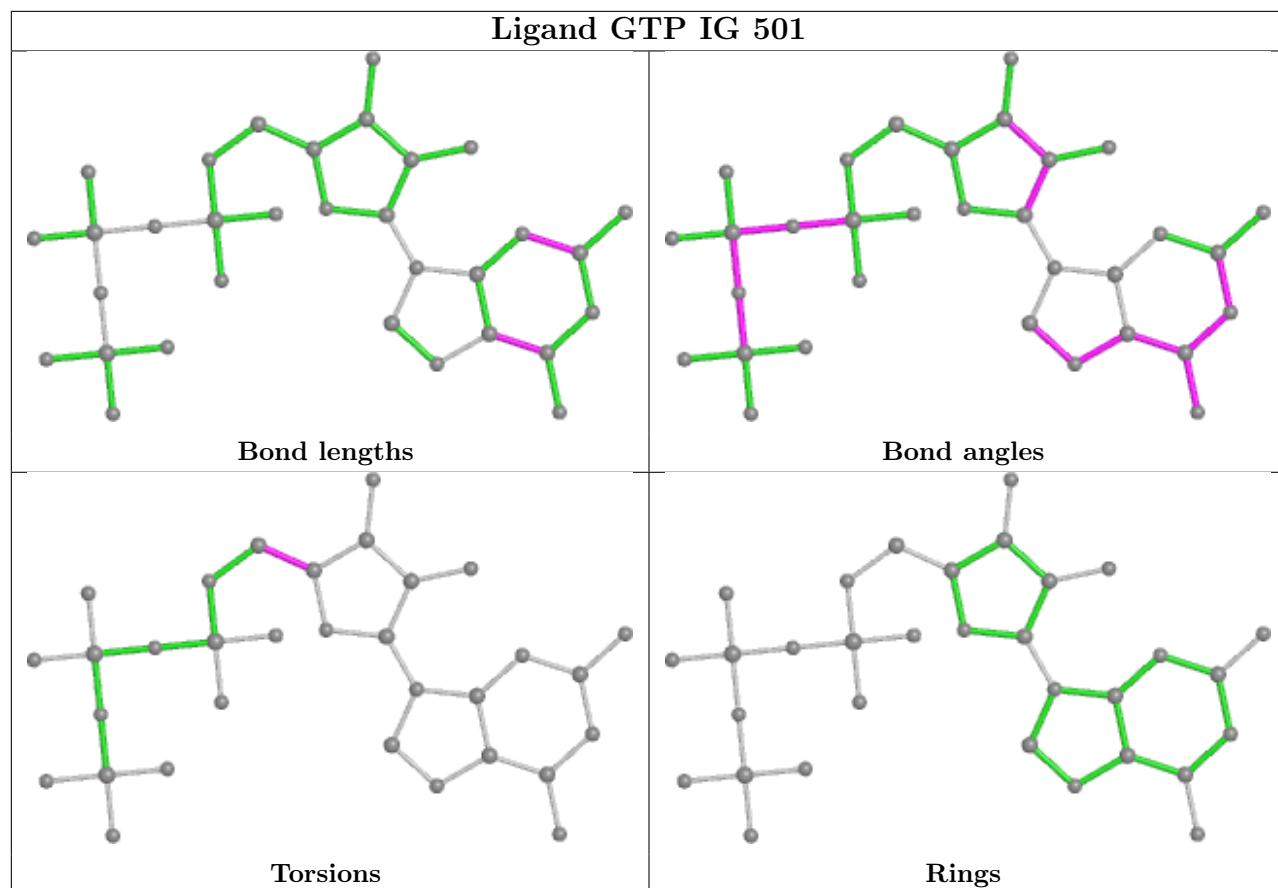


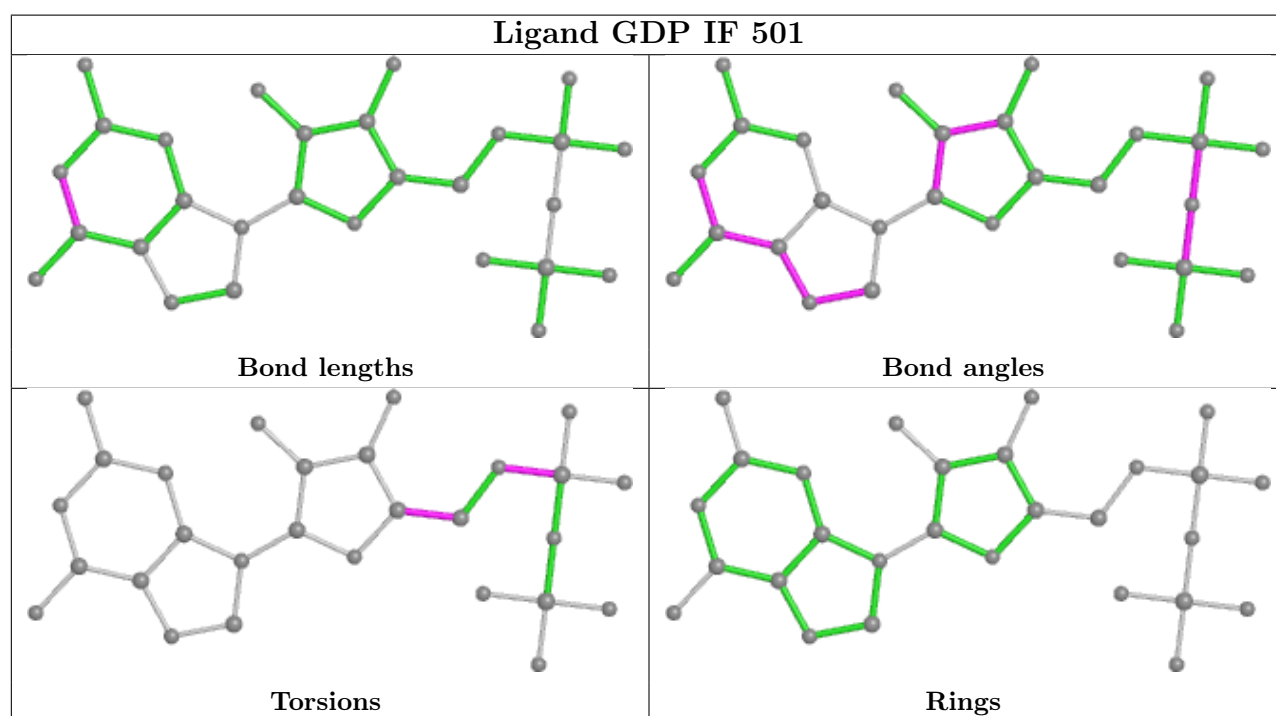
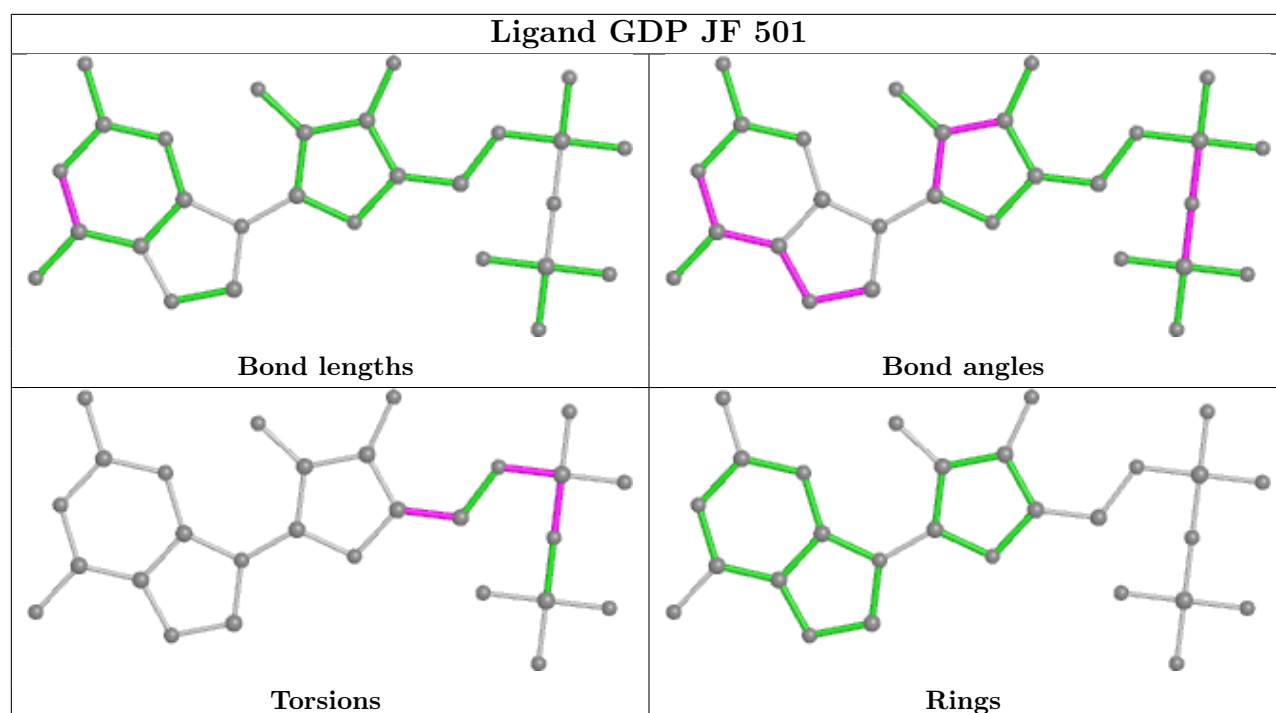
## Ligand GTP MC 501



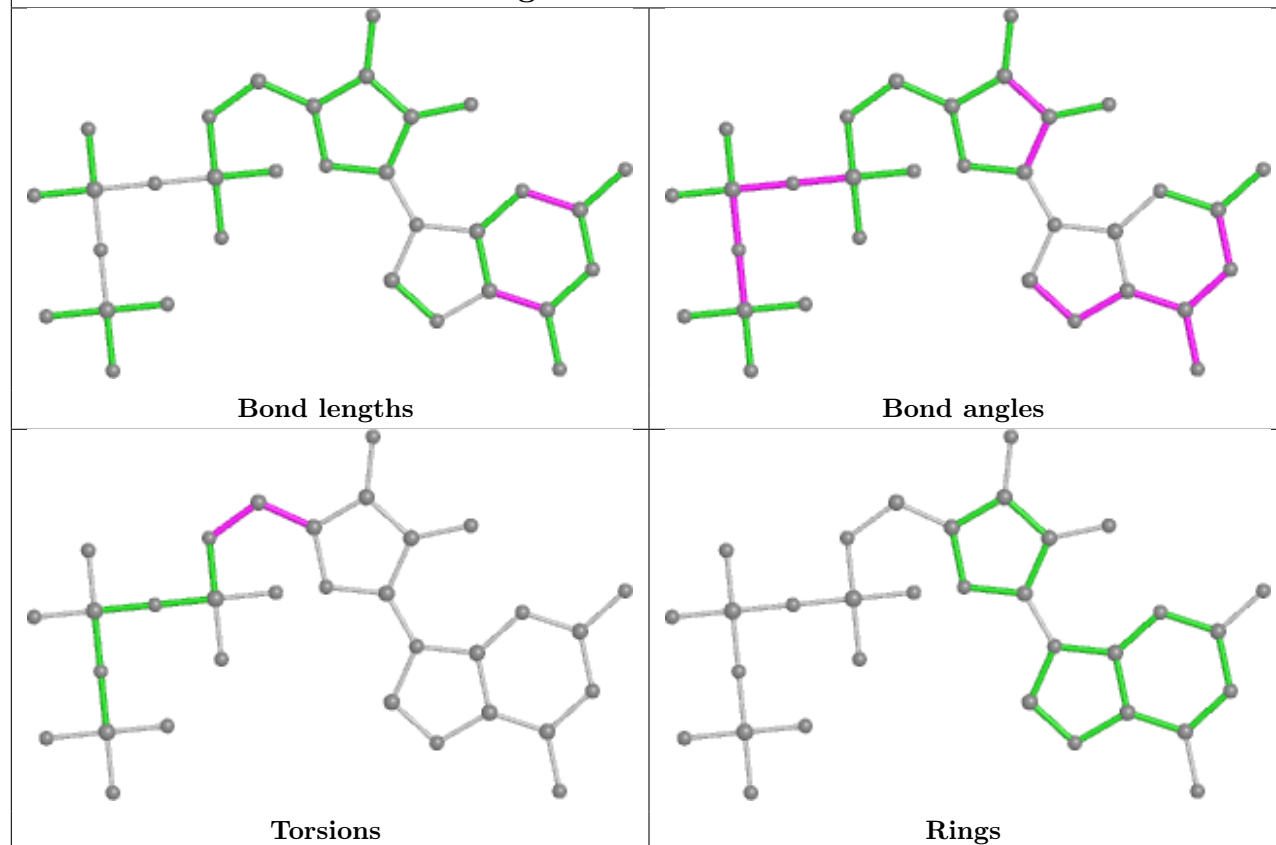




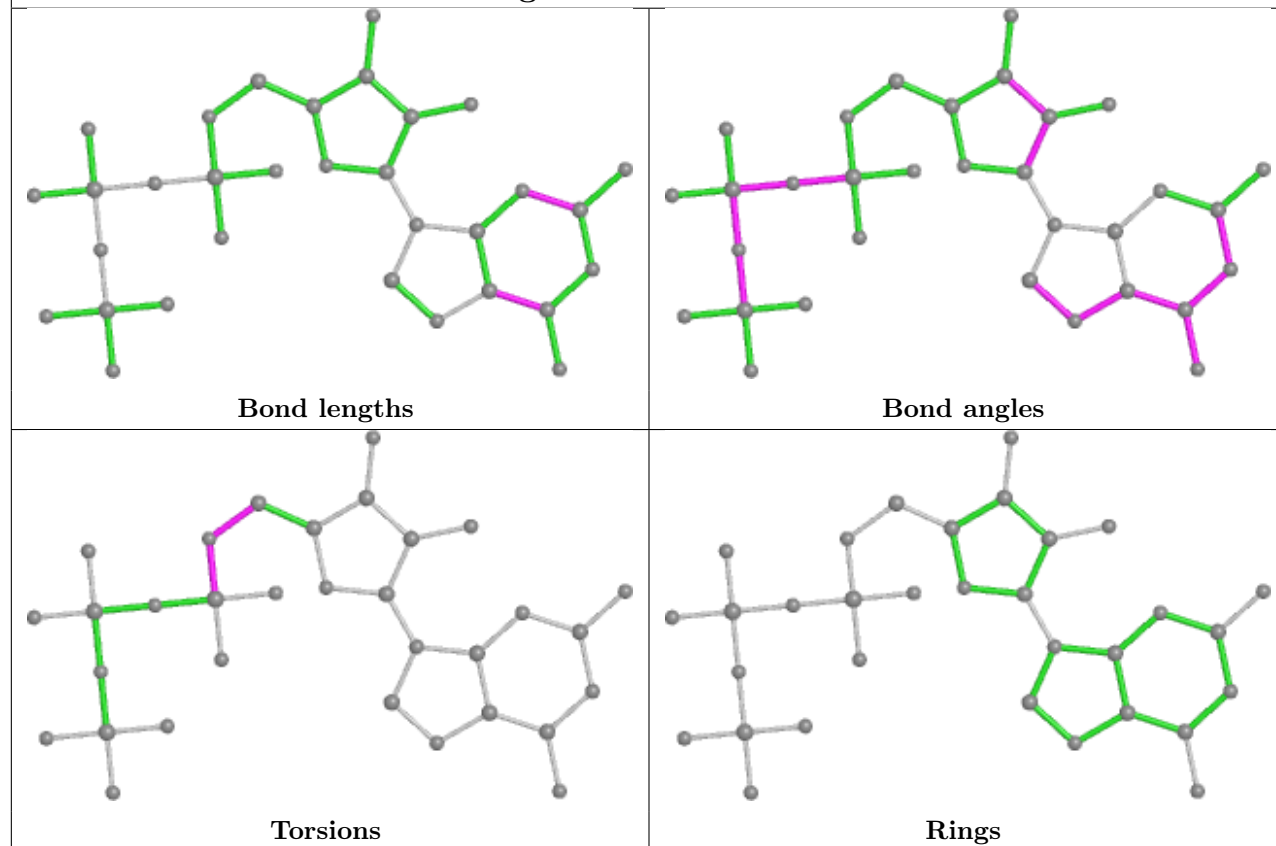




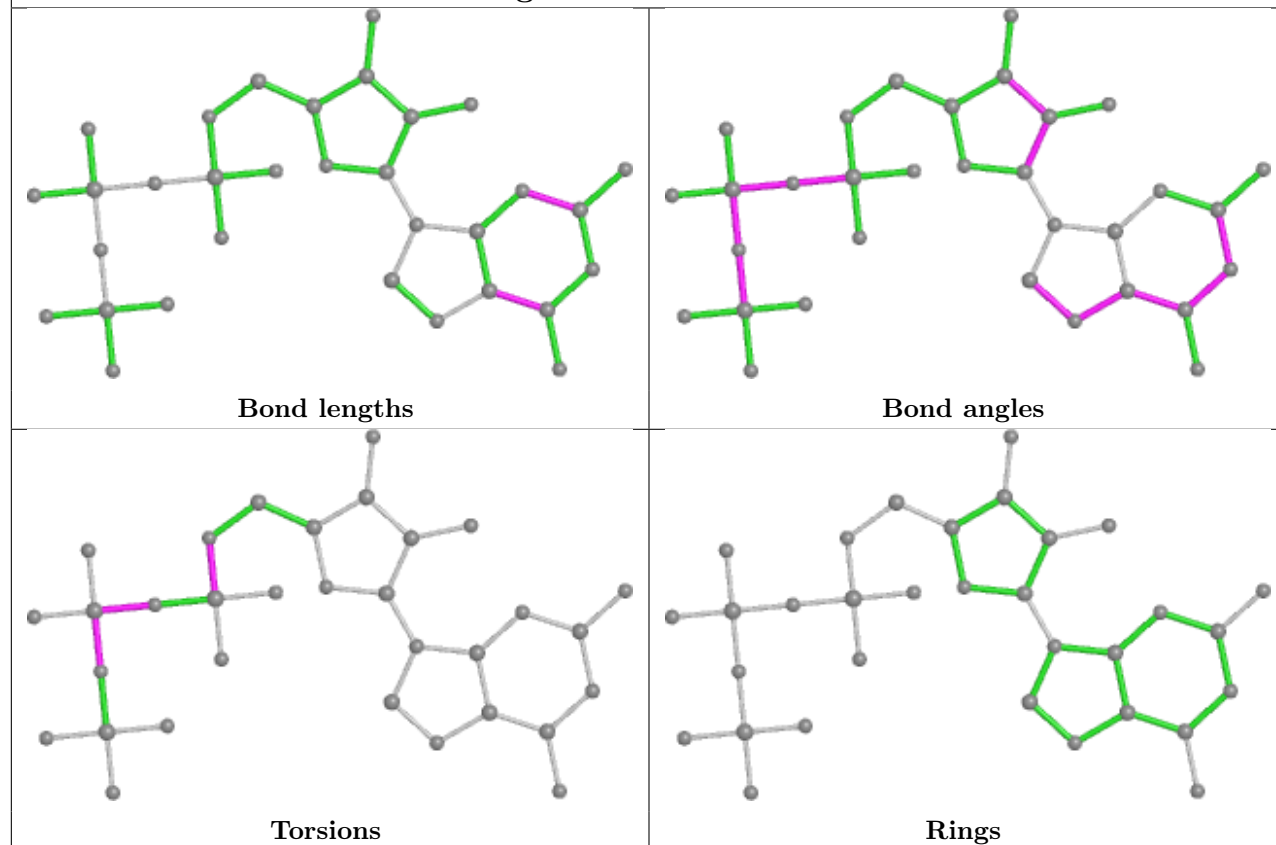
## Ligand GTP BC 501



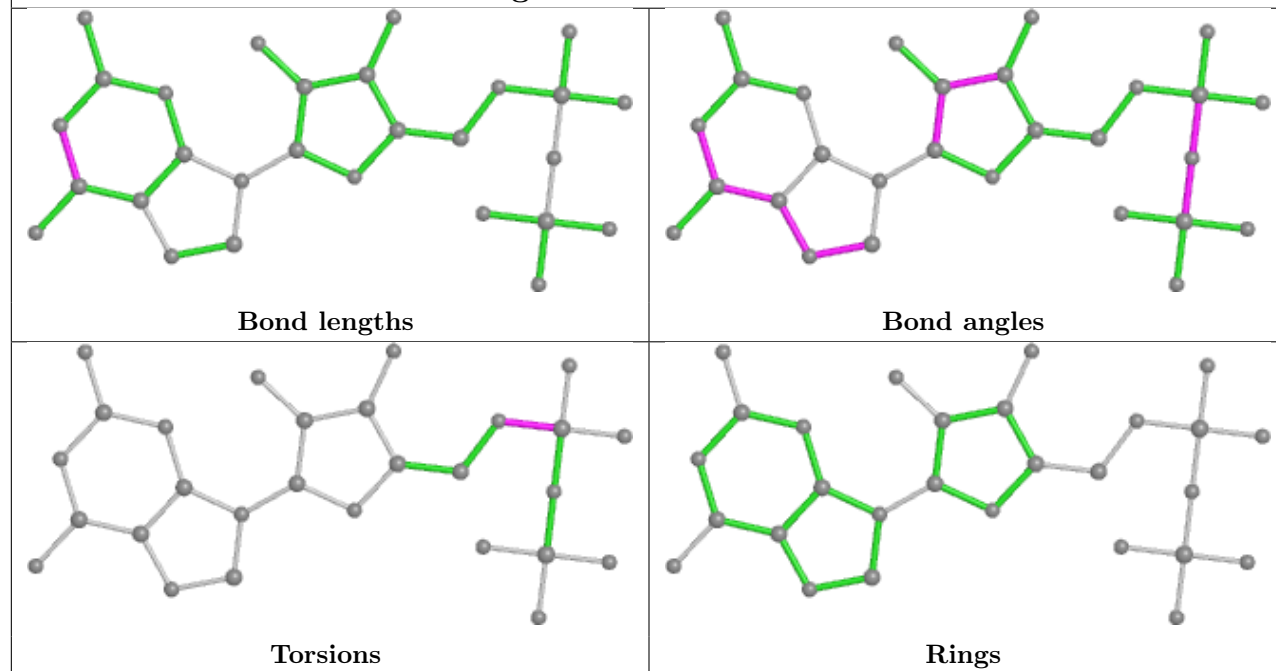
## Ligand GTP BE 501



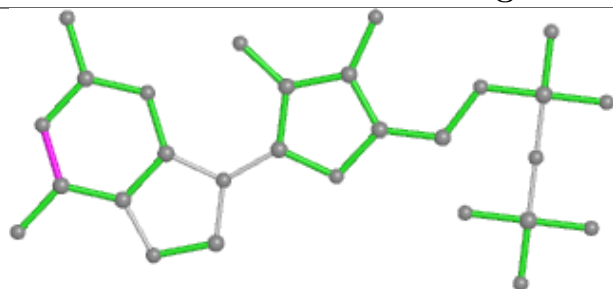
## Ligand GTP KG 501



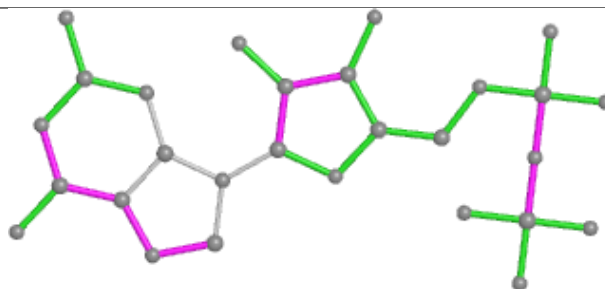
## Ligand GDP MD 501



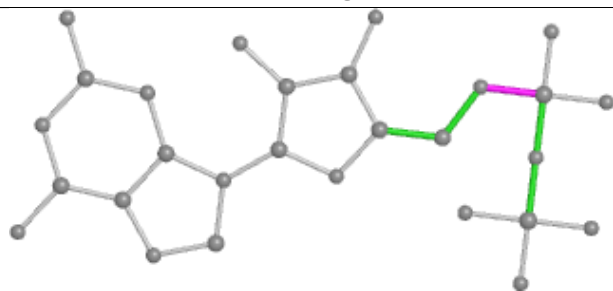
## Ligand GDP HH 501



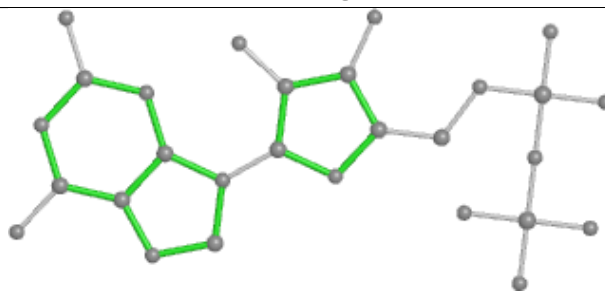
Bond lengths



Bond angles

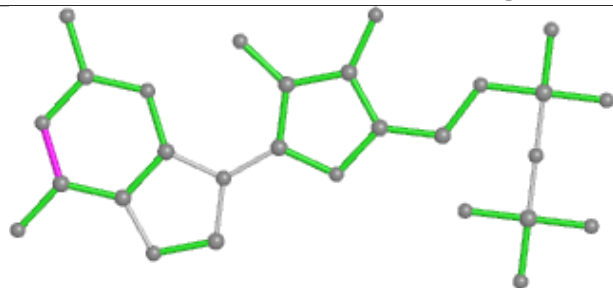


Torsions

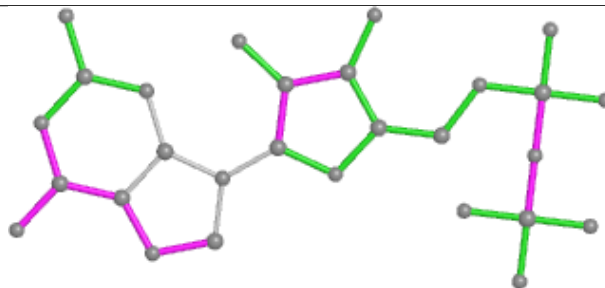


Rings

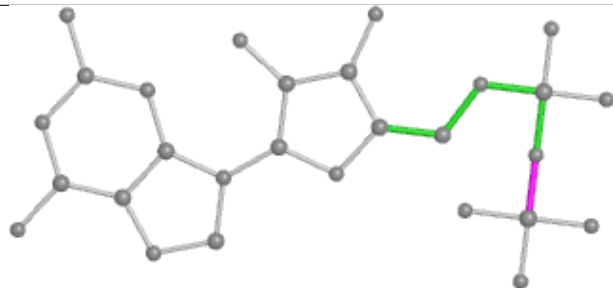
## Ligand GDP LD 501



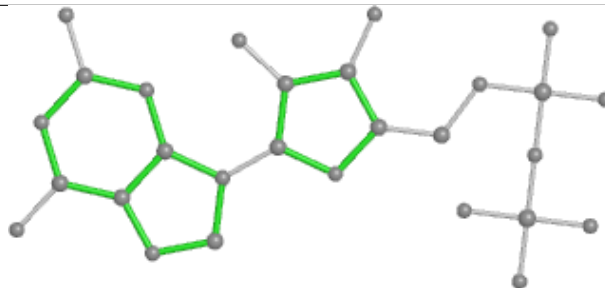
Bond lengths



Bond angles

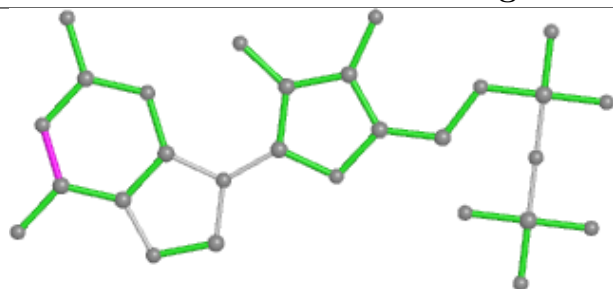


Torsions

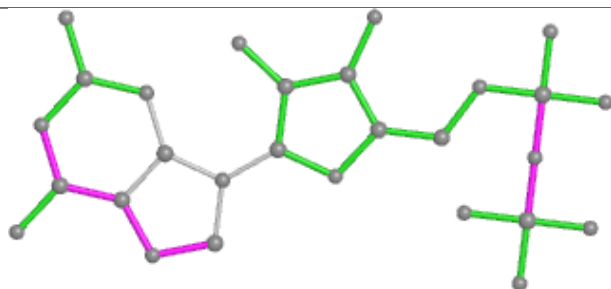


Rings

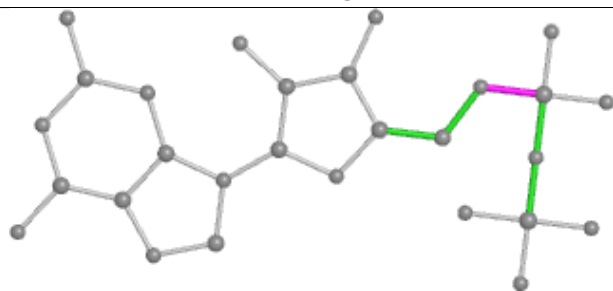
## Ligand GDP KF 501



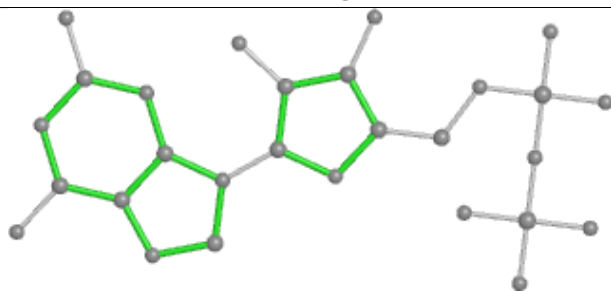
Bond lengths



Bond angles

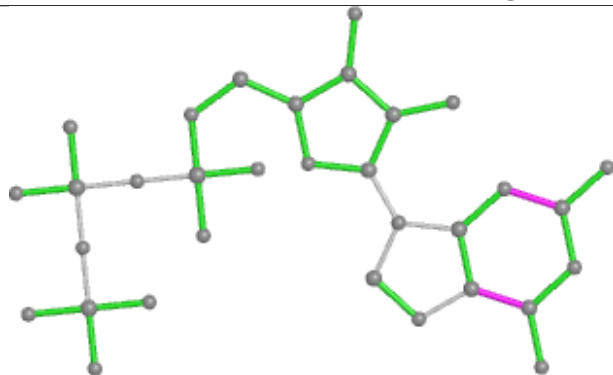


Torsions

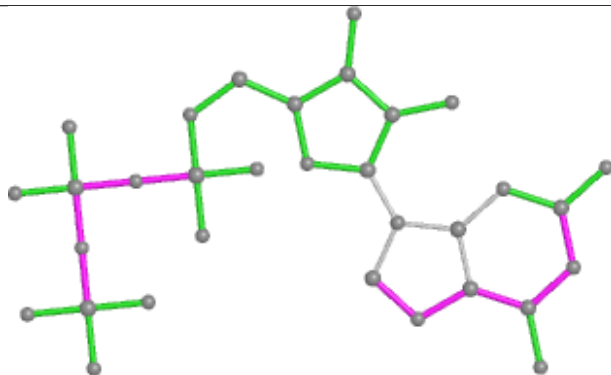


Rings

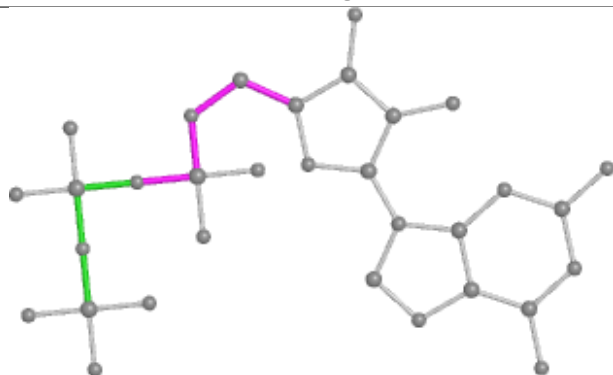
## Ligand GTP EE 501



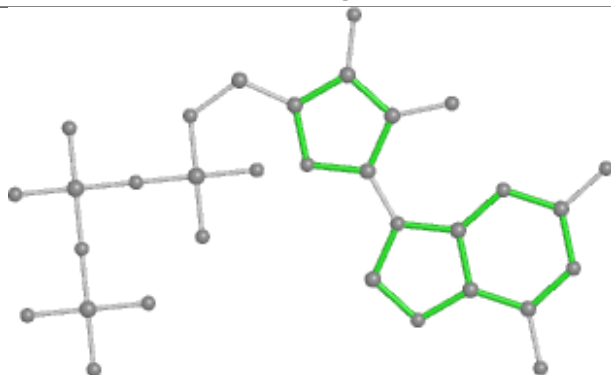
Bond lengths



Bond angles

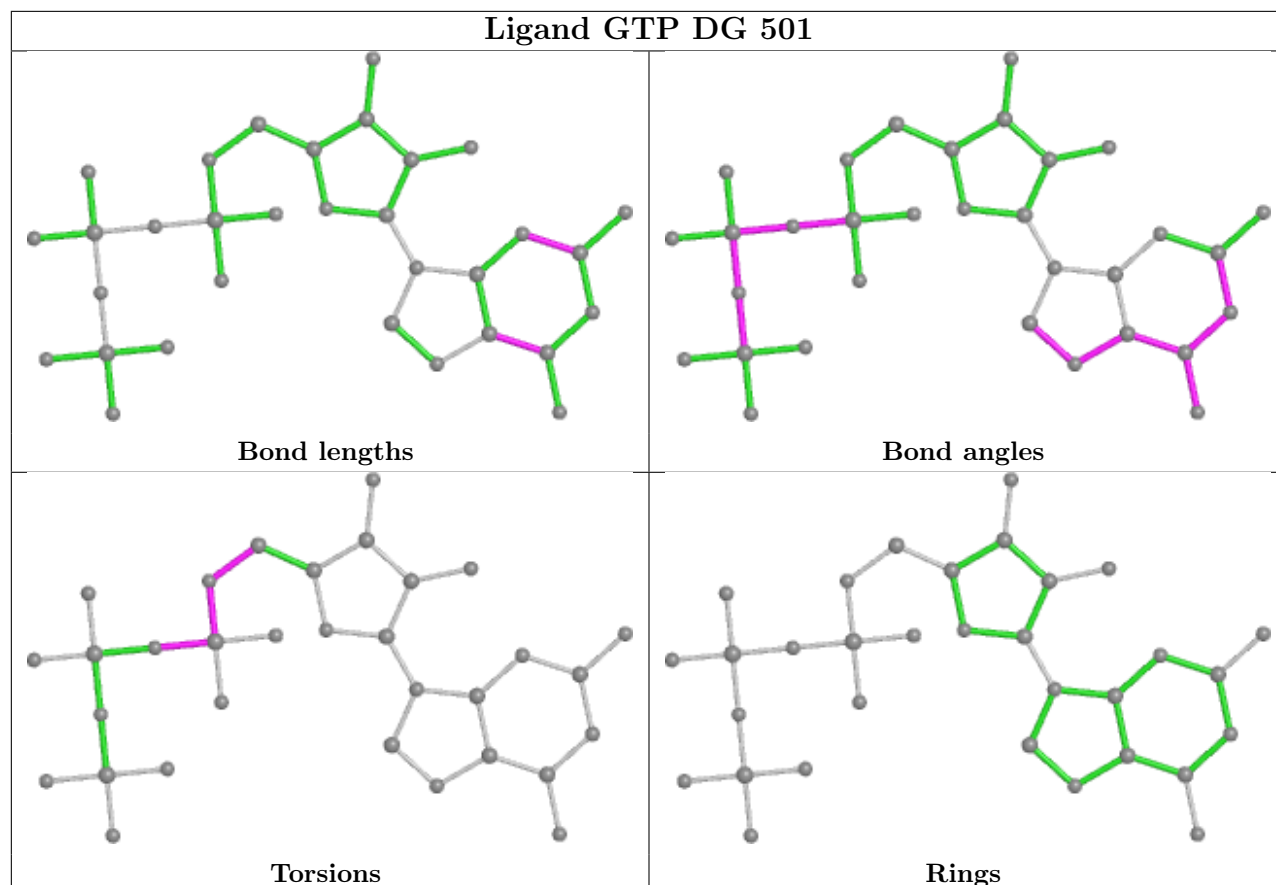


Torsions

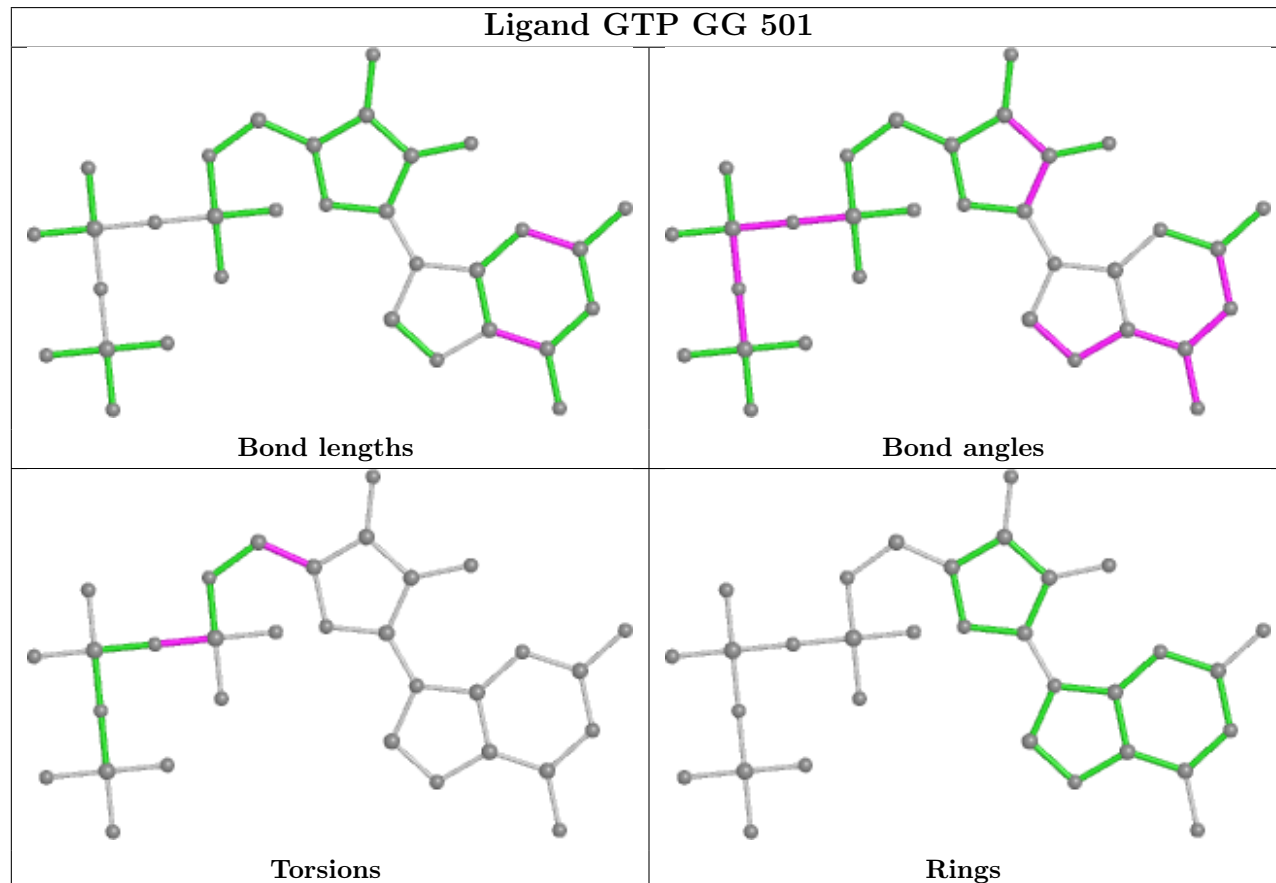


Rings

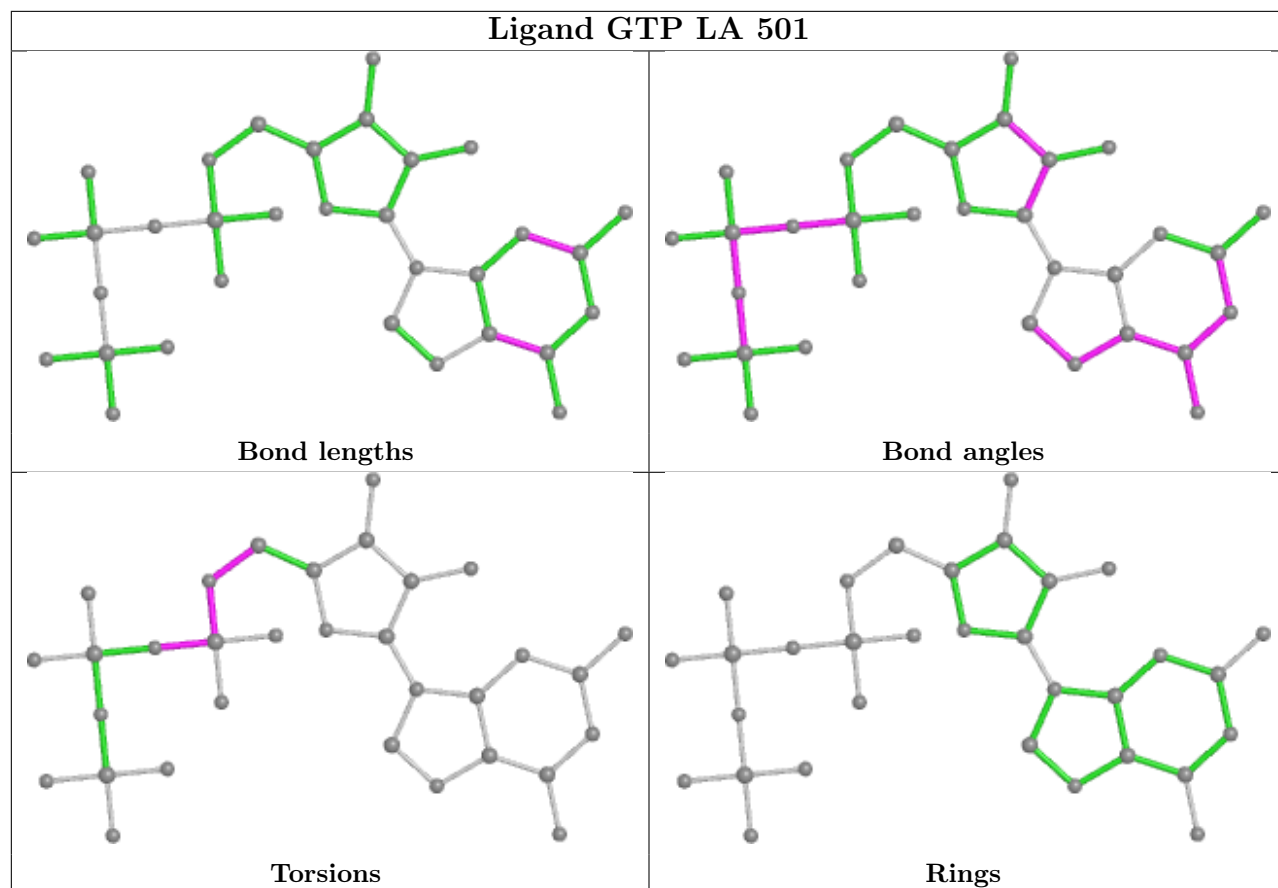
## Ligand GTP DG 501



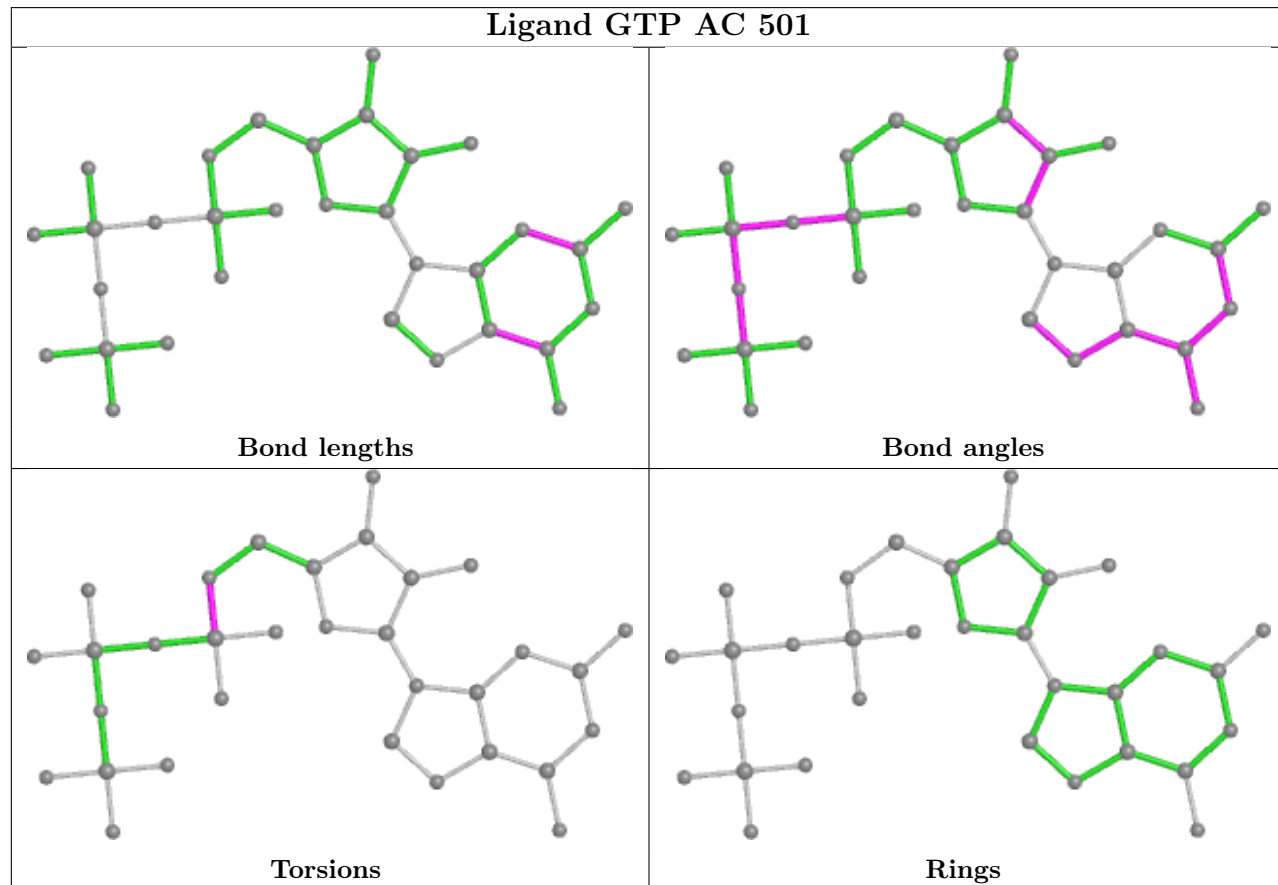
## Ligand GTP GG 501



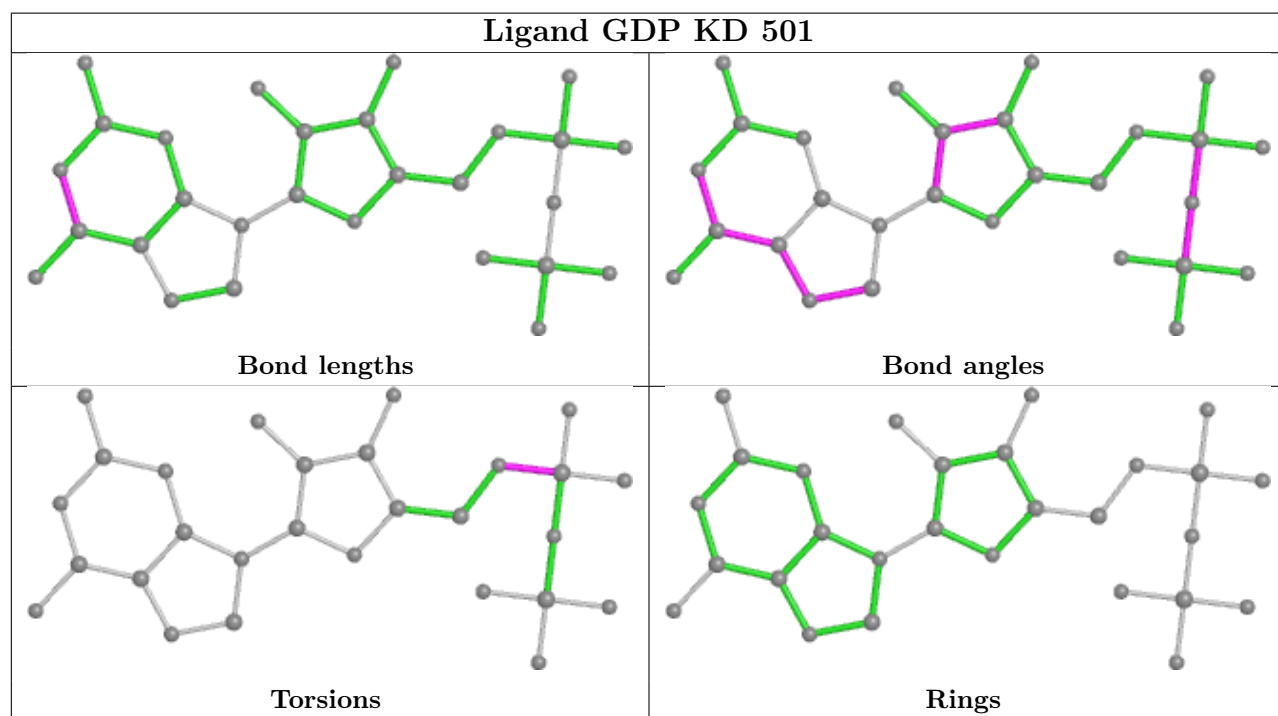
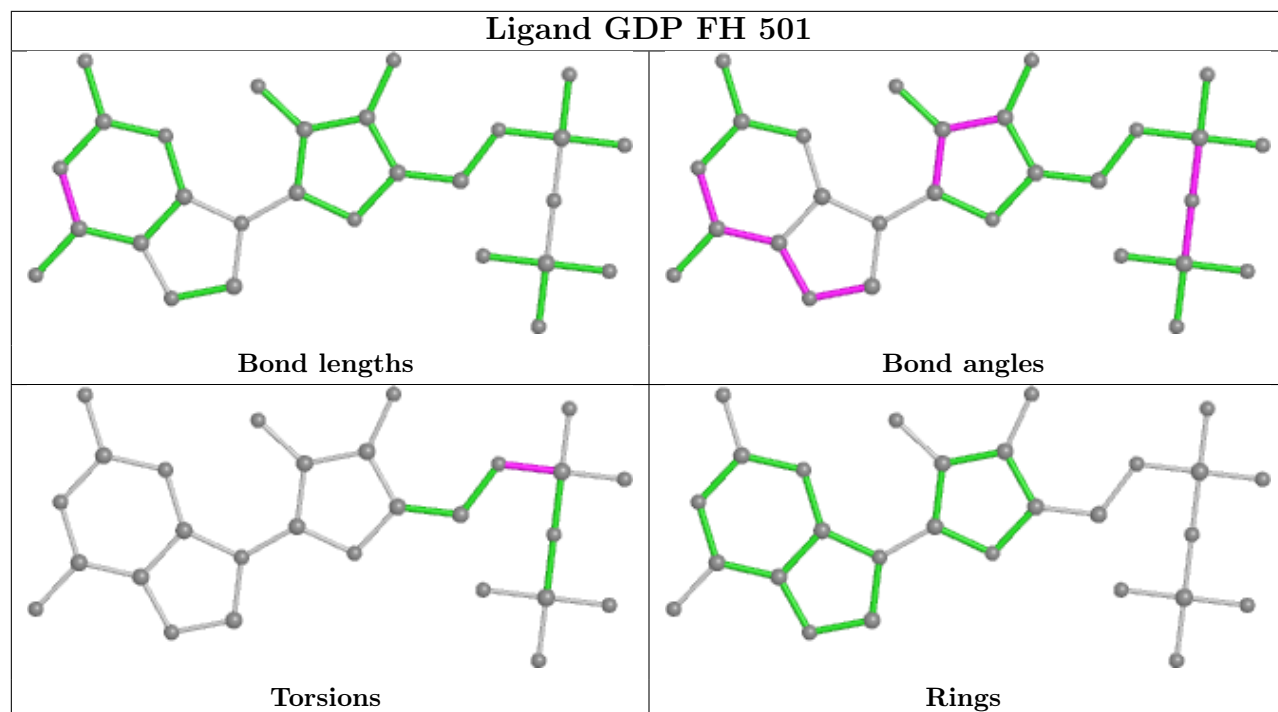
## Ligand GTP LA 501

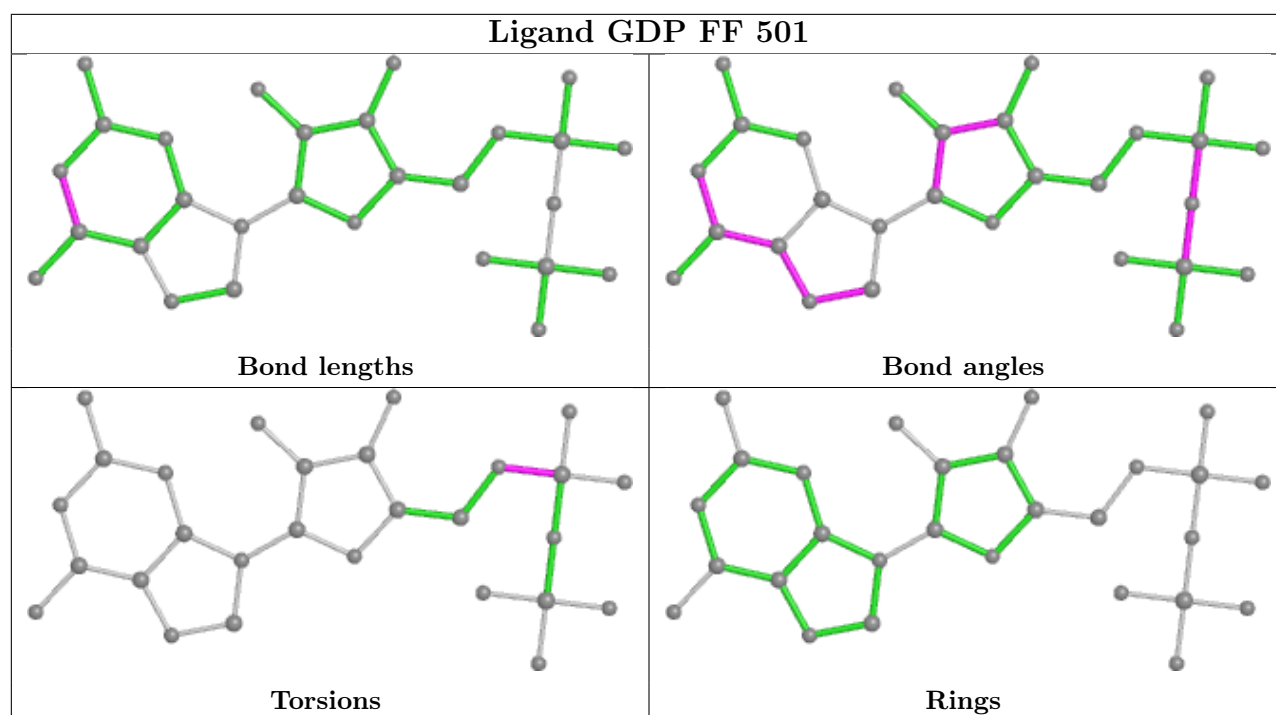


## Ligand GTP AC 501









## 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.

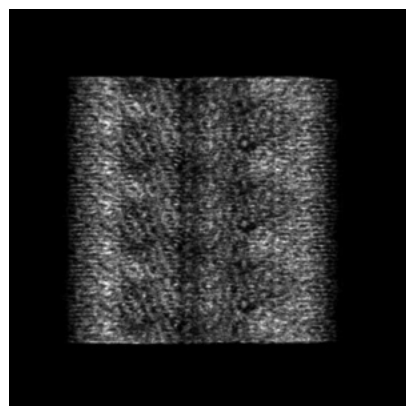
## 6 Map visualisation [i](#)

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.

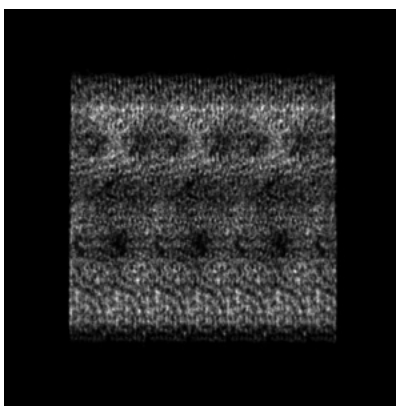
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

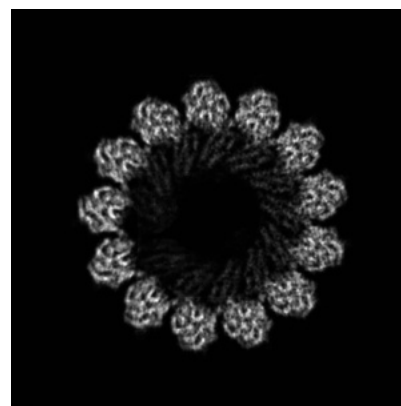
#### 6.1.1 Primary map



X

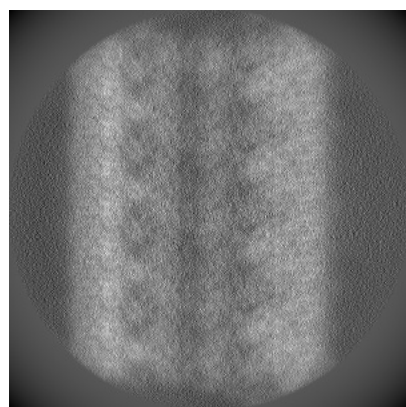


Y

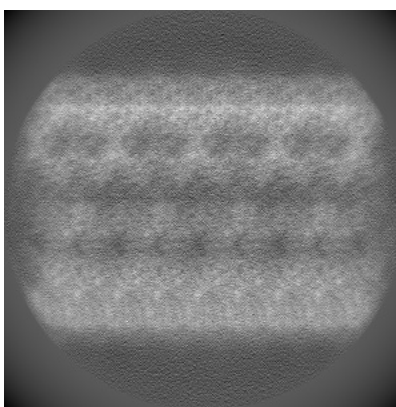


Z

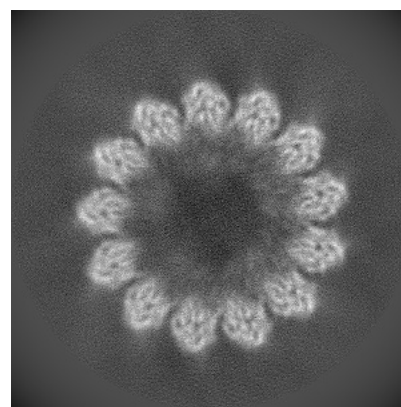
#### 6.1.2 Raw map



X



Y

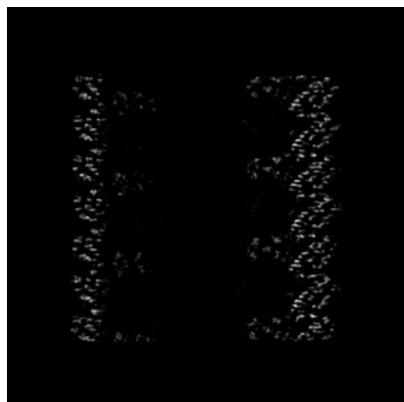


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 240

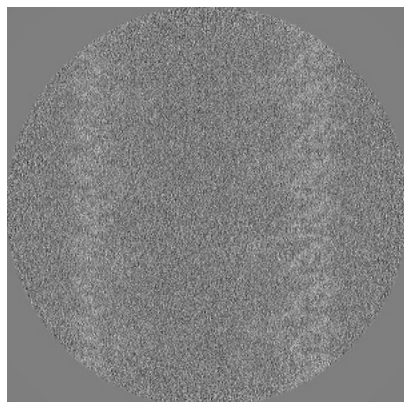


Y Index: 240

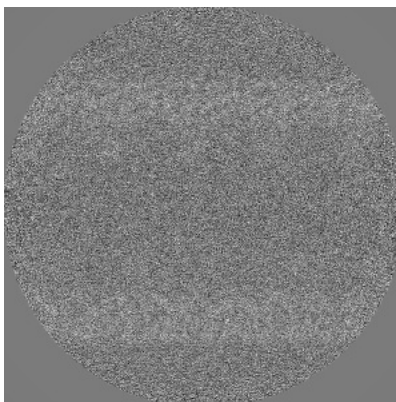


Z Index: 240

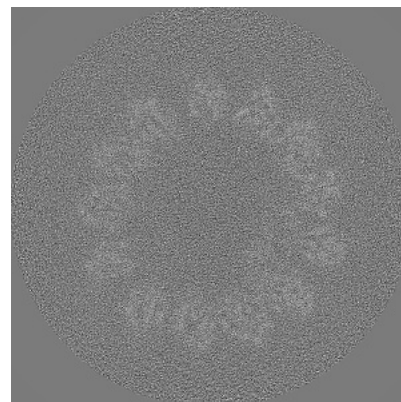
### 6.2.2 Raw map



X Index: 240



Y Index: 240

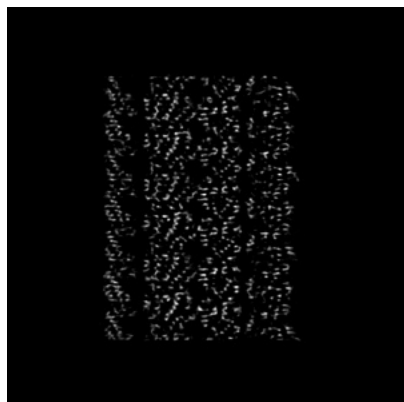


Z Index: 240

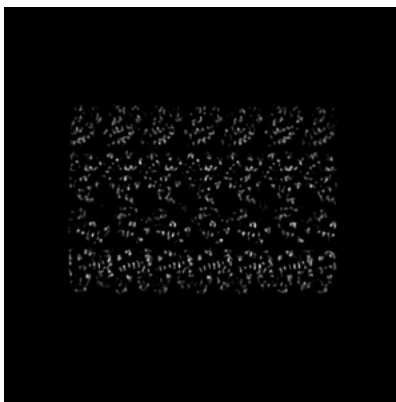
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 359

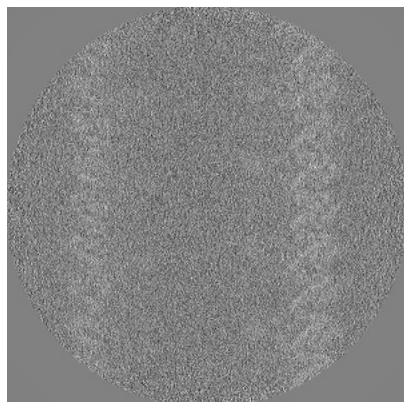


Y Index: 118

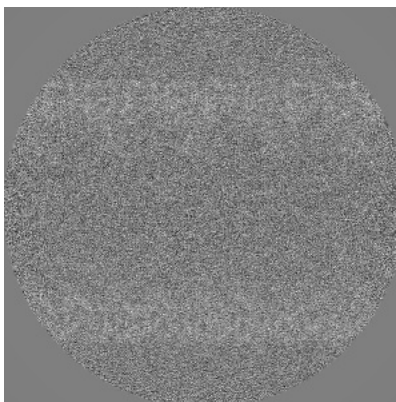


Z Index: 160

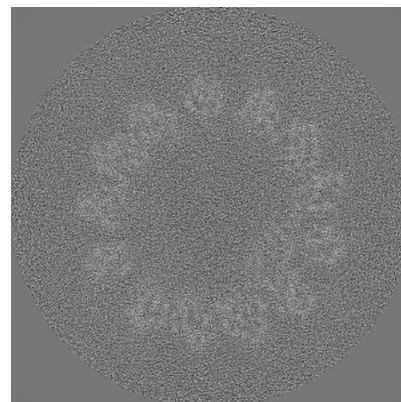
### 6.3.2 Raw map



X Index: 238



Y Index: 239



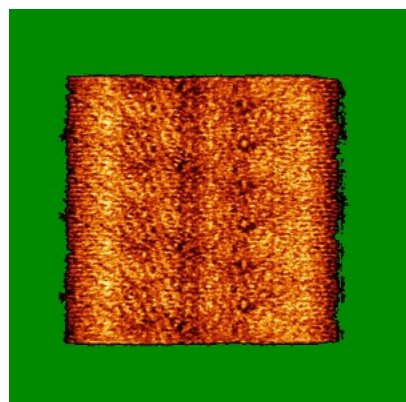
Z Index: 244

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

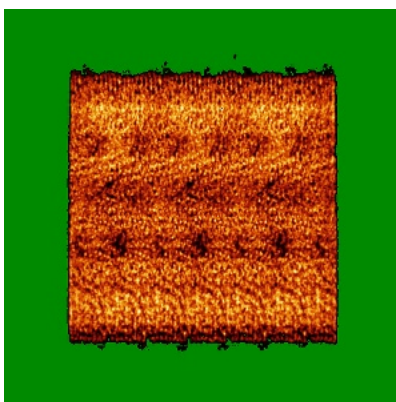


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

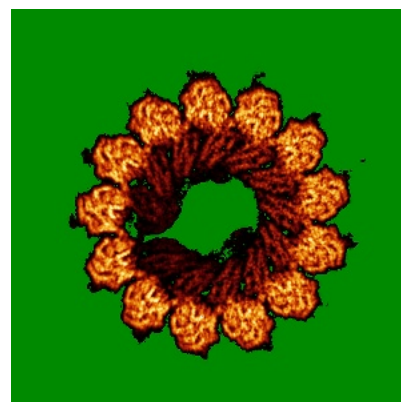
### 6.4.1 Primary map



X

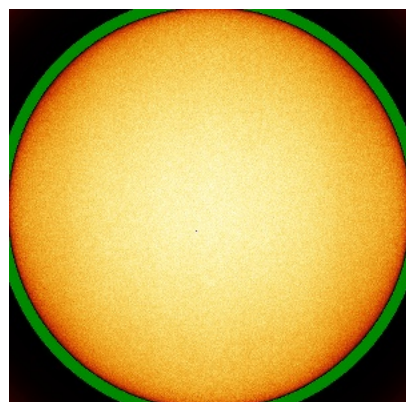


Y

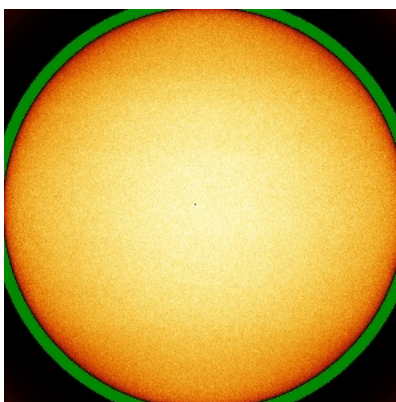


Z

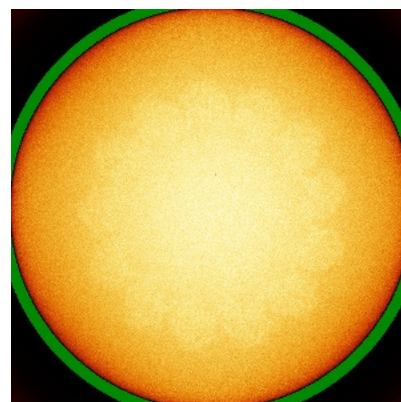
### 6.4.2 Raw map



X



Y

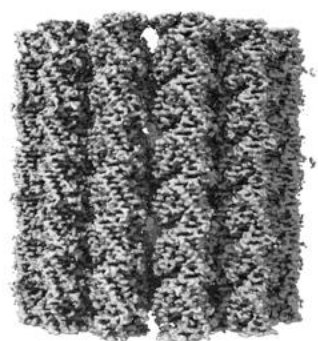


Z

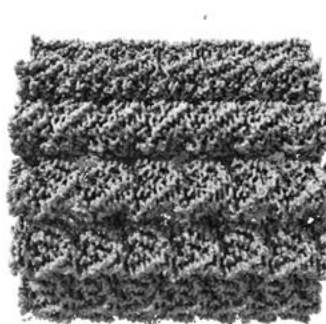
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



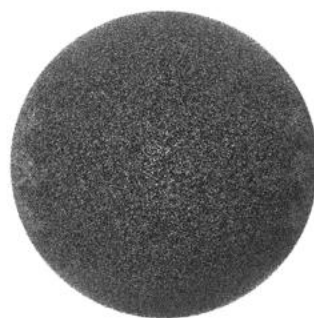
Z

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

### 6.5.2 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.

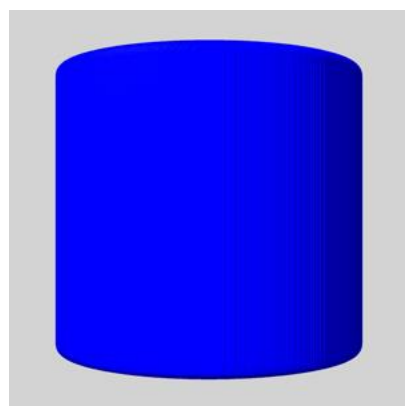
## 6.6 Mask visualisation [i](#)

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

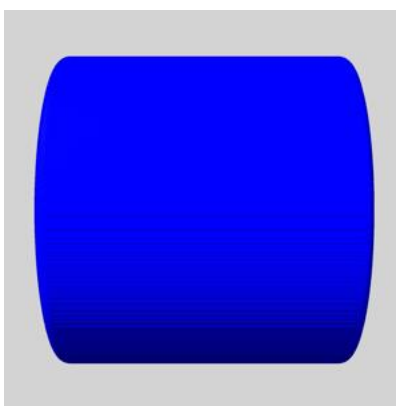
A mask typically either:

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

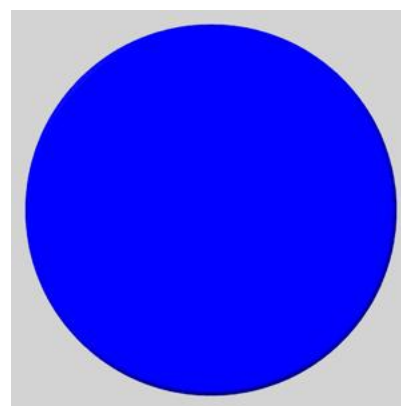
### 6.6.1 emd\_26611\_msk\_1.map [i](#)



X



Y



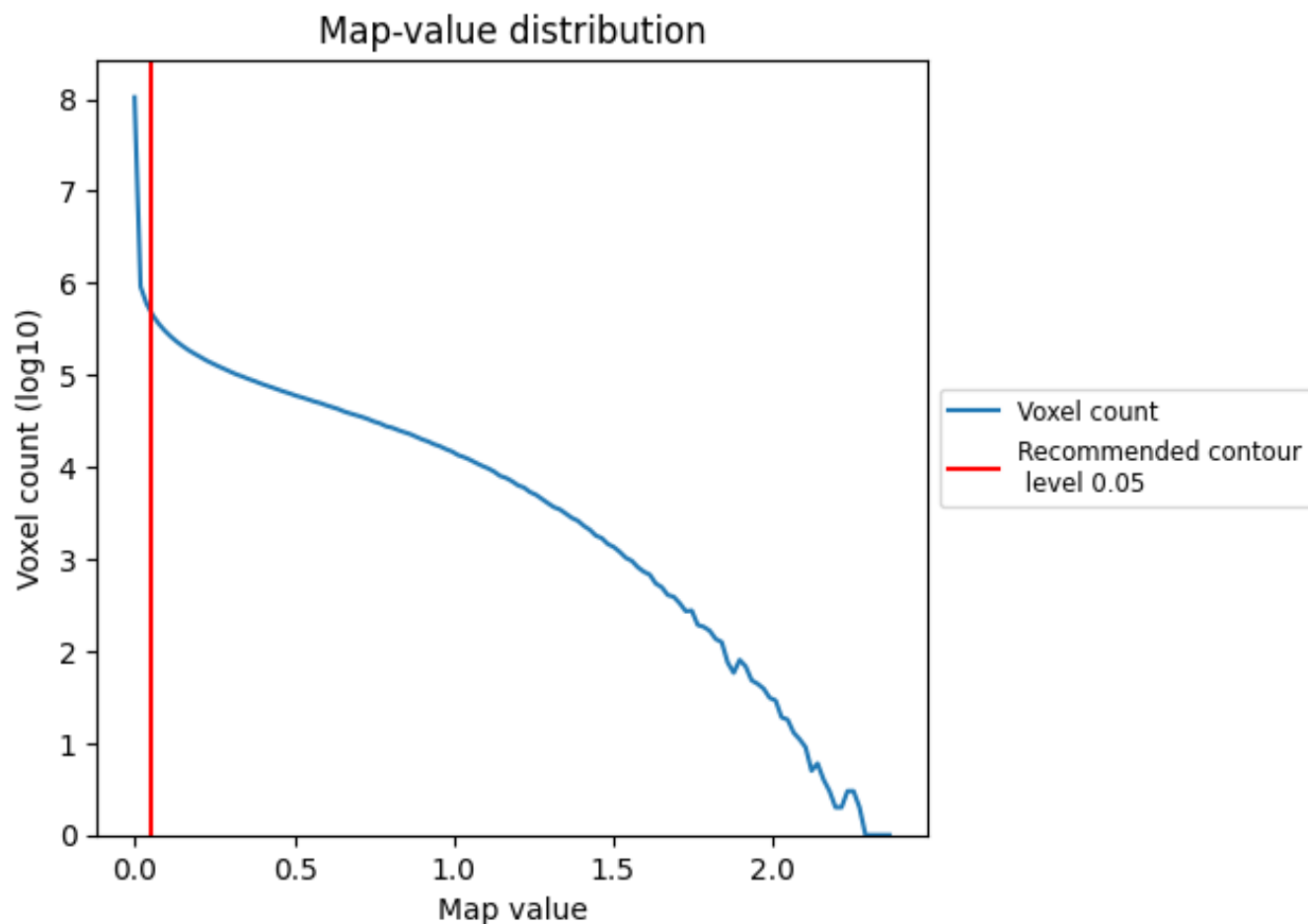
Z



## 7 Map analysis [i](#)

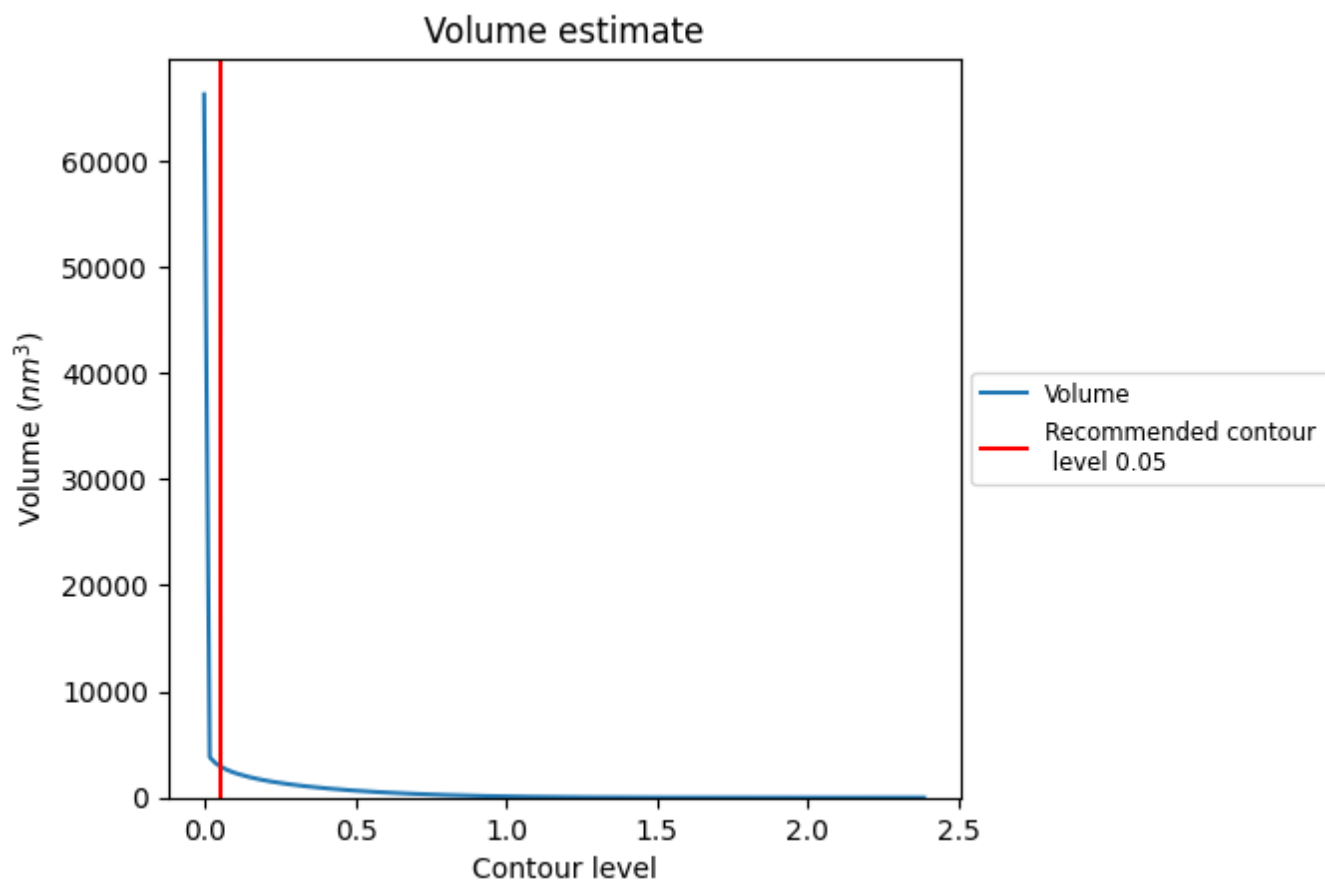
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

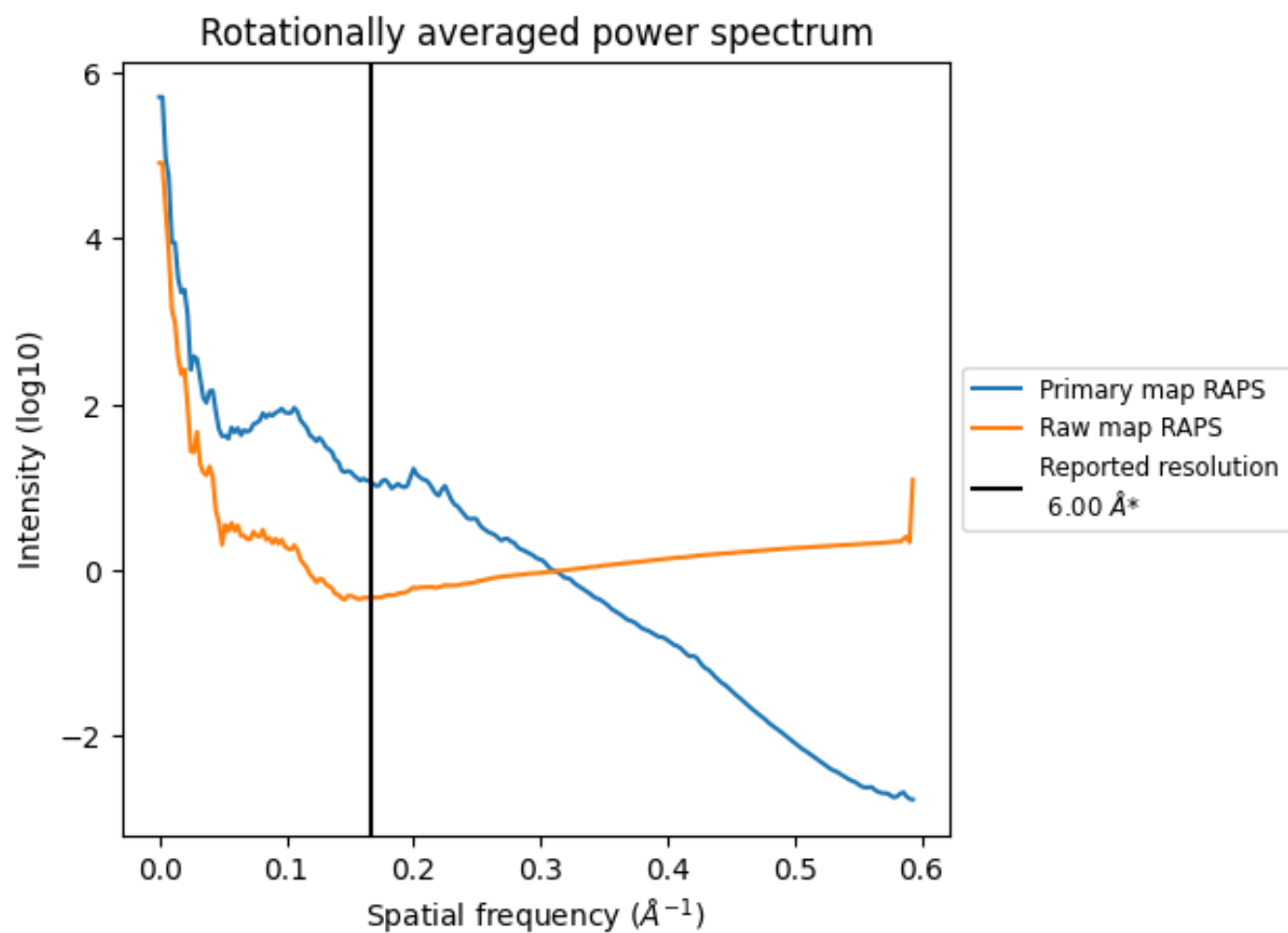
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2981  $\text{nm}^3$ ; 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 ⓘ

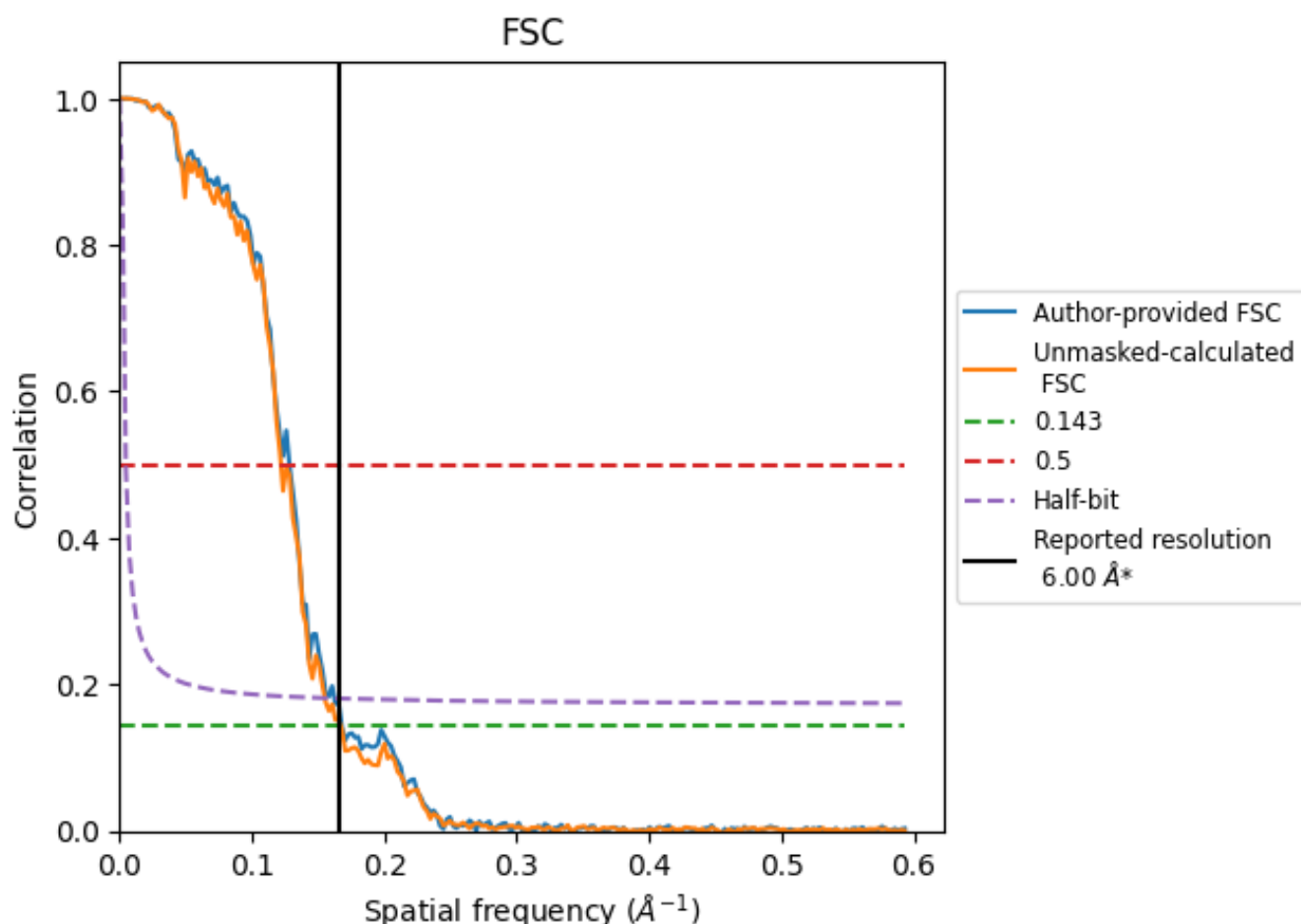


\*Reported resolution corresponds to spatial frequency of 0.167 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.167 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

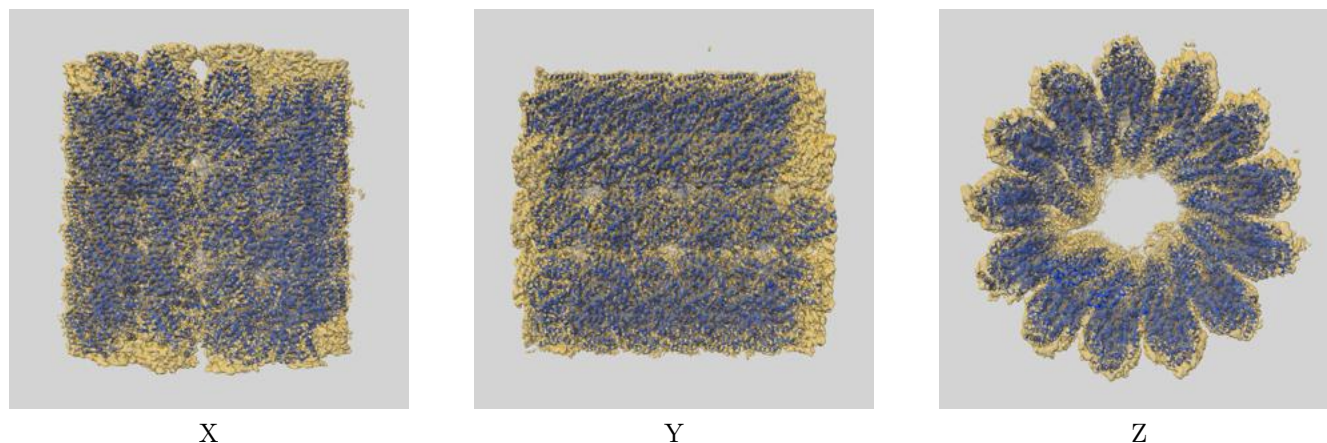
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	5.96	7.79	6.16
Unmasked-calculated*	5.98	8.20	6.45

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

## 9 Map-model fit [i](#)

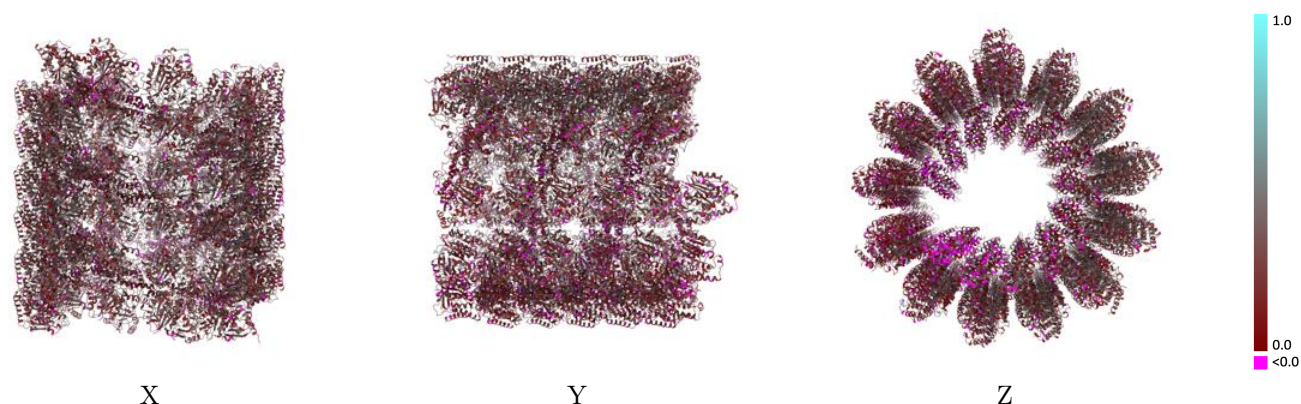
This section contains information regarding the fit between EMDB map EMD-26611 and PDB model 7UN1. Per-residue inclusion information can be found in section [3](#) on page [20](#).

### 9.1 Map-model overlay [i](#)



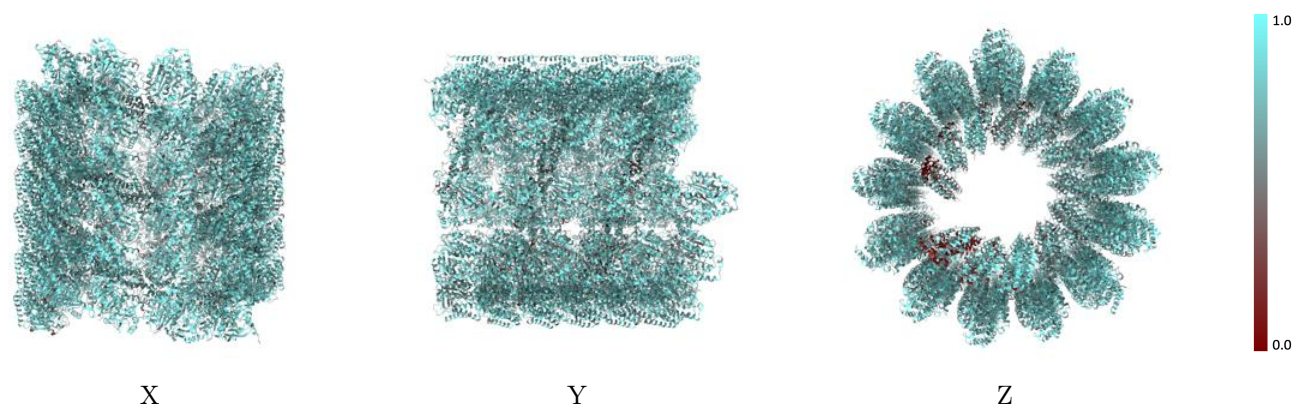
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



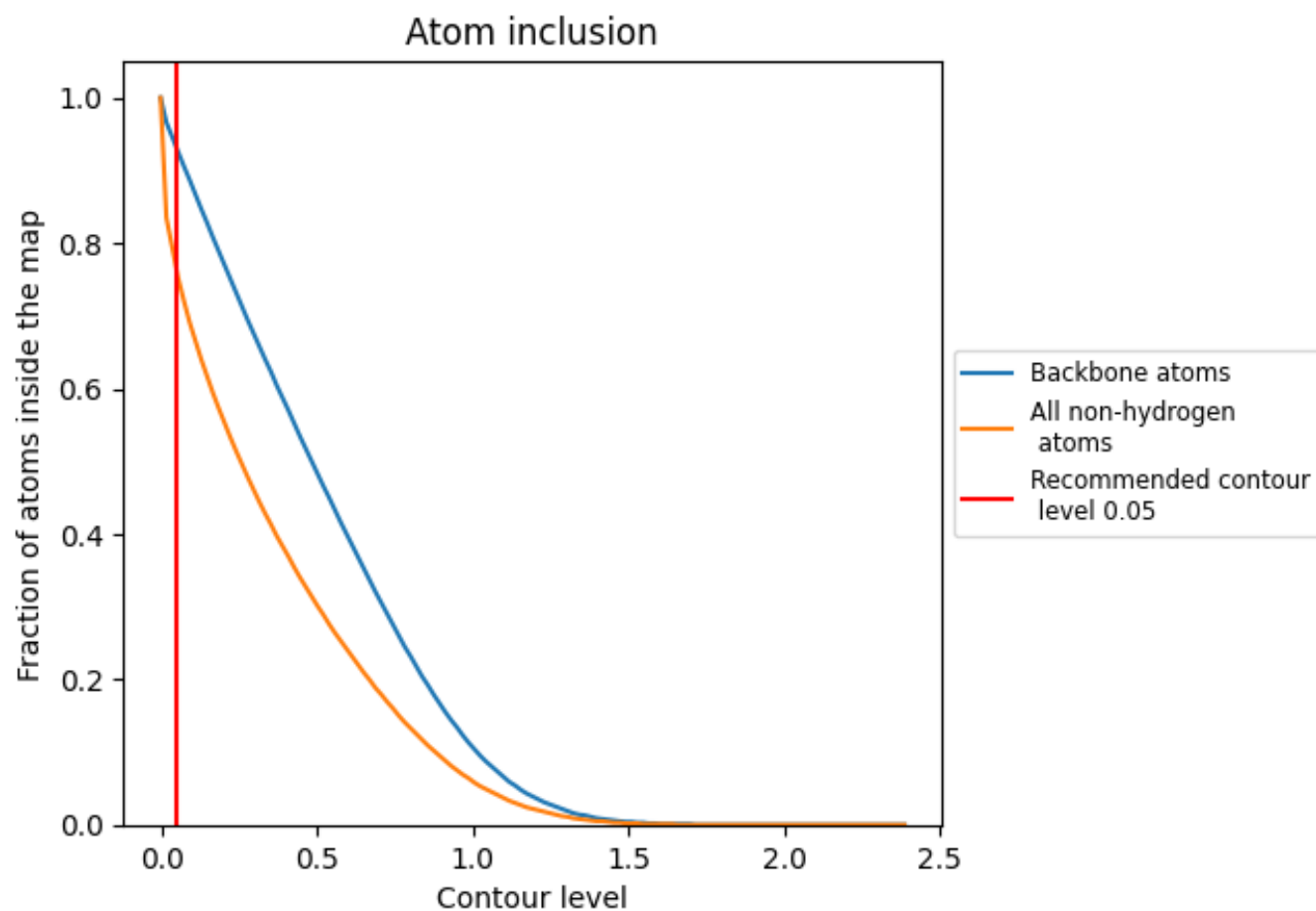
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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	 0.7610	 0.2540
A	 0.4030	 0.0620
AB	 0.7900	 0.2920
AC	 0.7980	 0.2980
AD	 0.8030	 0.3010
AE	 0.8030	 0.2950
AF	 0.7810	 0.2790
B	 0.6180	 0.1090
BA	 0.7960	 0.3010
BC	 0.8140	 0.3250
BD	 0.8060	 0.3210
BE	 0.8090	 0.3180
BF	 0.8070	 0.3040
BG	 0.7870	 0.2760
C	 0.7700	 0.1700
CB	 0.7920	 0.3000
CC	 0.8180	 0.3250
CD	 0.7990	 0.3240
CE	 0.8150	 0.3330
CF	 0.8010	 0.3120
CG	 0.7970	 0.3020
D	 0.6090	 0.1440
DB	 0.7840	 0.2810
DC	 0.8020	 0.3180
DD	 0.8080	 0.3220
DE	 0.7980	 0.3180
DF	 0.8080	 0.3130
DG	 0.7930	 0.2890
E	 0.6830	 0.1840
EB	 0.7800	 0.2850
EC	 0.7860	 0.3030
ED	 0.8070	 0.3020
EE	 0.8040	 0.3100
EF	 0.7930	 0.2920
EG	 0.7870	 0.2900





































































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Chain	Atom inclusion	Q-score
F	 0.7160	 0.1960
FC	 0.7820	 0.2870
FD	 0.7820	 0.2930
FE	 0.8000	 0.3050
FF	 0.7900	 0.2960
FG	 0.7940	 0.2880
FH	 0.7500	 0.2570
G	 0.7000	 0.2100
GC	 0.7600	 0.2560
GD	 0.7670	 0.2730
GE	 0.7760	 0.2790
GF	 0.7600	 0.2650
GG	 0.7640	 0.2570
GH	 0.7440	 0.2370
H	 0.6760	 0.1900
HC	 0.7510	 0.2230
HD	 0.7590	 0.2430
HE	 0.7670	 0.2500
HF	 0.7590	 0.2420
HG	 0.7760	 0.2490
HH	 0.7470	 0.2160
I	 0.6540	 0.1660
IC	 0.7220	 0.1860
ID	 0.7280	 0.1950
IE	 0.7350	 0.2120
IF	 0.7330	 0.2030
IG	 0.7470	 0.2110
IH	 0.7270	 0.1840
J	 0.8230	 0.2300
JC	 0.7320	 0.1860
JD	 0.7470	 0.2110
JE	 0.7420	 0.2020
JF	 0.7450	 0.2140
JG	 0.7370	 0.1920
K	 0.6880	 0.1610
KC	 0.7550	 0.2210
KD	 0.7590	 0.2250
KE	 0.7550	 0.2450
KF	 0.7590	 0.2210
KG	 0.7630	 0.2290
KH	 0.7380	 0.2000
L	 0.4310	 0.0510

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Chain	Atom inclusion	Q-score
LA	 0.7560	 0.2360
LB	 0.7760	 0.2510
LC	 0.7670	 0.2550
LD	 0.7730	 0.2640
LE	 0.7520	 0.2410
LF	 0.7540	 0.2280
M	 0.4850	 0.0630
MA	 0.7590	 0.2560
MB	 0.7670	 0.2620
MC	 0.7710	 0.2690
MD	 0.7700	 0.2630
ME	 0.7740	 0.2700
MF	 0.7720	 0.2510
N	 0.7290	 0.1880
O	 0.7510	 0.2030
P	 0.6070	 0.1340
Q	 0.6900	 0.1970
R	 0.6950	 0.1950
S	 0.7120	 0.2180
T	 0.6900	 0.1780
U	 0.6640	 0.1820
V	 0.8100	 0.2280
W	 0.7030	 0.1940
X	 0.3390	 0.0160
d	 0.6440	 0.1400
e	 0.6860	 0.1880
f	 0.7090	 0.2040
g	 0.6940	 0.2040
h	 0.6950	 0.1950
i	 0.6700	 0.1830
j	 0.8240	 0.2460
k	 0.7020	 0.1810
l	 0.4420	 0.0520