



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 02:27 AM EST

PDB ID : 7JU4
EMDB ID : EMD-22481
Title : Radial spoke 2 stalk, IDAc, and N-DRC attached with doublet microtubule
Authors : Gui, M.; Ma, M.; Sze-Tu, E.; Wang, X.; Koh, F.; Zhong, E.; Berger, B.; Davis, J.; Dutcher, S.; Zhang, R.; Brown, A.
Deposited on : 2020-08-19
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

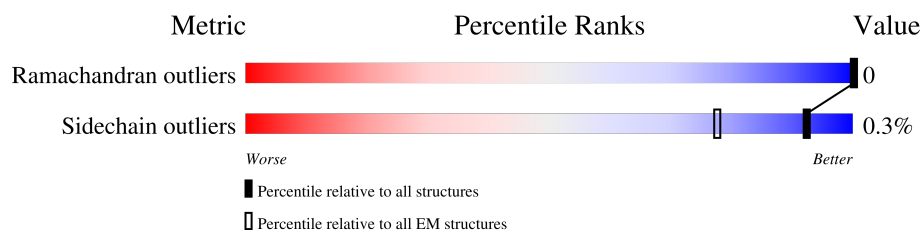
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY











The reported resolution of this entry is 3.40 Å.

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



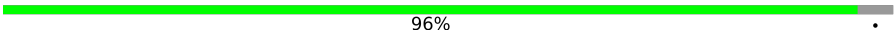
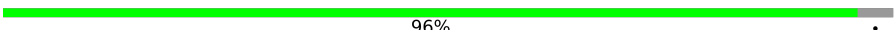
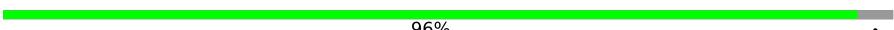
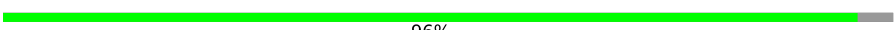
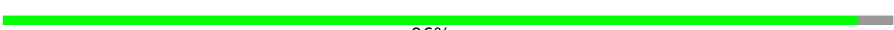





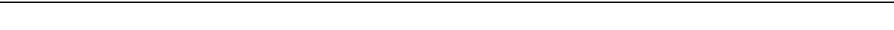

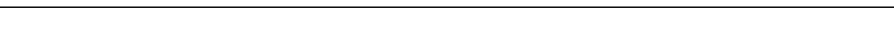
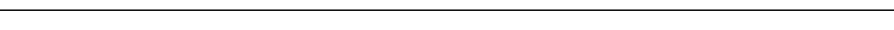
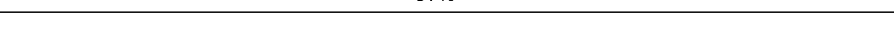
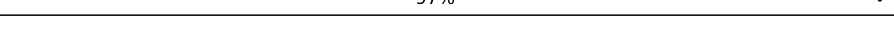
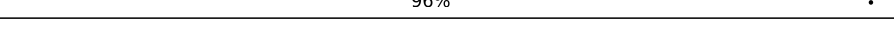
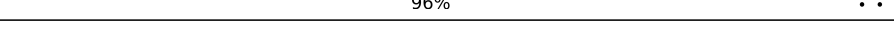
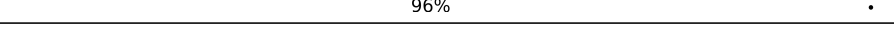
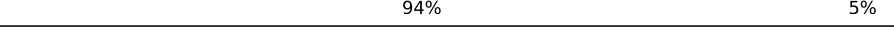
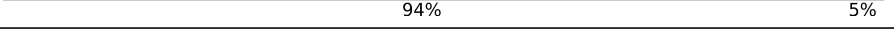
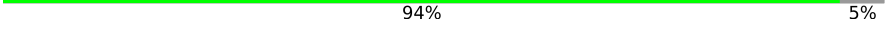
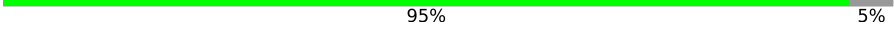


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	471	 37% 63%
1	4	471	 33% 67%
2	1	698	 24% 76%
3	2	573	 32% 68%
4	3	72	 100%
5	6	443	 96% .
5	8	443	 96% .
5	C	443	 96% .
5	G	443	 96% .
5	I	443	 96% .











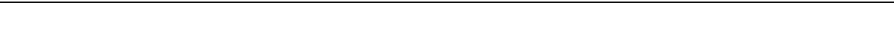

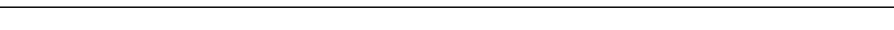
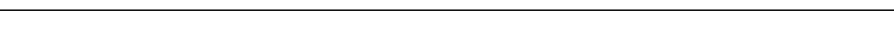

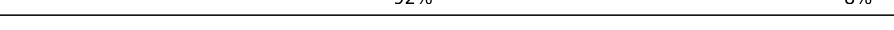

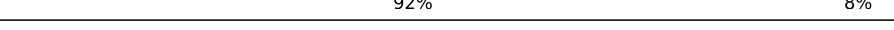

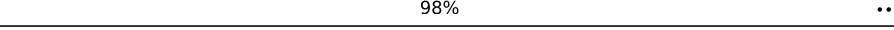



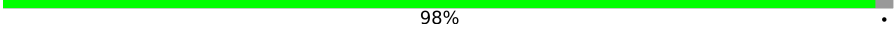

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Mol	Chain	Length	Quality of chain
5	K	443	 96% .
5	O	443	 96% .
5	Q	443	 96% .
5	S	443	 96% .
5	W	443	 96% .
5	Y	443	 96% .
5	i	443	 96% .
5	k	443	 96% .
5	y	443	 96% .
6	7	451	 94% . 5%
6	9	451	 94% 5%
6	D	451	 96% .
6	H	451	 96% .
6	J	451	 97% .
6	L	451	 97% .
6	P	451	 96% .
6	R	451	 96% . .
6	T	451	 96% .
6	X	451	 94% 5%
6	Z	451	 94% 5%
6	j	451	 94% 5%
6	t	451	 95% 5%
6	z	451	 94% 5%
7	A	925	 47% 53%
8	B	904	 48% 52%

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Mol	Chain	Length	Quality of chain
9	E	516	 17% 83%
9	F	516	 22% 77%
10	M	500	 9% 91%
10	N	500	 8% 92%
11	U	204	 24% 76%
11	V	204	 78% 22%
12	a	91	 92% 8%
12	b	91	 92% 8%
12	c	91	 92% 8%
12	d	91	 92% 8%
12	e	91	 92% 8%
12	f	91	 92% 8%
12	g	91	 92% 8%
12	h	91	 91% 8%
12	o	91	 92% 8%
12	p	91	 92% 8%
12	q	91	 92% 8%
12	r	91	 91% 8%
13	l	331	 98% ..
14	m	256	 80% 20%
15	n	378	 81% 19%
16	s	682	 26% 74%
17	u	377	 98% .
18	v	253	 60% 40%
18	w	253	 56% 43%

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Mol	Chain	Length	Quality of chain
19	x	1298	<div><div></div><div>17%</div><div>83%</div></div>

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 133504 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 Dynein regulatory complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	173	Total	C	N	O	S	0	0
			1364	858	235	270	1		
1	4	154	Total	C	N	O	S	0	0
			1246	788	214	243	1		

- Molecule 2 is a protein called Dynein regulatory complex protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	168	Total	C	N	O	S	0	0
			1431	896	265	267	3		

- Molecule 3 is a protein called Dynein regulatory complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	183	Total	C	N	O	S	0	0
			1497	933	281	279	4		

- Molecule 4 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	72	Total	C	N	O	0	0
			360	216	72	72		

- Molecule 5 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
5	8	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
5	C	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	I	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	K	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	O	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	Q	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	S	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	W	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	Y	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	i	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	k	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	y	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

- Molecule 6 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
6	9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
6	D	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	H	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	J	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	L	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	P	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	R	436	Total 3376	C 2136	N 575	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
6	X	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
6	Z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
6	j	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
6	t	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
6	z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 7 is a protein called Flagellar-associated protein 59.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	435	Total	C	N	O	S	0	0
			3535	2170	665	686	14		

- Molecule 8 is a protein called Flagellar-associated protein 172.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	435	Total	C	N	O	S	0	0
			3479	2134	655	674	16		

- Molecule 9 is a protein called Radial spoke protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	86	Total	C	N	O	S	0	0
			685	432	109	142	2		
9	F	117	Total	C	N	O	S	0	0
			931	583	150	195	3		

- Molecule 10 is a protein called Radial spoke protein 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	44	Total	C	N	O	0	0
			353	232	59	62		
10	N	40	Total	C	N	O	0	0
			316	208	53	55		

- Molecule 11 is a protein called Radial spoke protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	49	Total	C	N	O	S	0	0
			391	255	65	70	1		
11	V	160	Total	C	N	O		0	0
			891	544	172	175			

- Molecule 12 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	b	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	c	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	d	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	e	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	f	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	g	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	h	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	o	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	p	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	q	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	r	84	Total	C	N	O	S	0	0
			686	442	115	125	4		

- Molecule 13 is a protein called Radial spoke protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	l	327	Total	C	N	O	S	0	0
			2438	1529	434	465	10		

- Molecule 14 is a protein called FAP207.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	m	204	Total	C	N	O	S	0	0
			1639	1029	294	310	6		

- Molecule 15 is a protein called Radial spike protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	n	307	Total	C	N	O	S	0	0
			1516	902	307	307			

- Molecule 16 is a protein called FAP253.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	176	Total	C	N	O	S	0	0
			1465	924	265	273	3		

- Molecule 17 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	u	370	Total	C	N	O	S	0	0
			2880	1828	487	542	23		

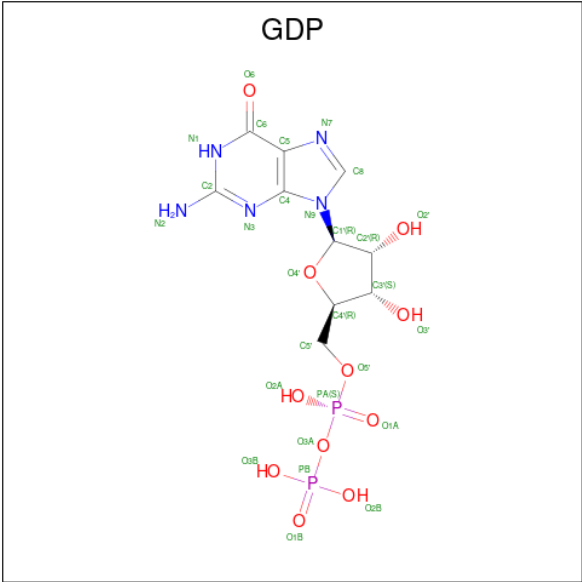
- Molecule 18 is a protein called 28 kDa inner dynein arm light chain, axonemal.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	v	152	Total	C	N	O	S	0	0
			1256	776	229	245	6		
18	w	143	Total	C	N	O	S	0	0
			1186	736	213	232	5		

- Molecule 19 is a protein called CFAP91 domain-containing protein.

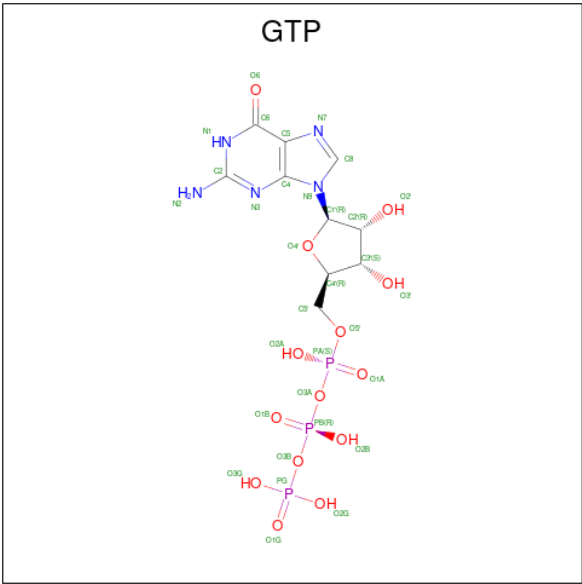
Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	224	Total	C	N	O	S	0	0
			1826	1135	343	343	5		

- Molecule 20 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
20	6	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	8	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	C	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	G	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	I	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	K	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	O	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	S	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	W	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	k	1	Total	C	N	O	P	0
			28	10	5	11	2	
20	y	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 21 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	9	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	P	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	R	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	T	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	X	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	j	1	Total	C	N	O	P	0
			32	10	5	14	3	

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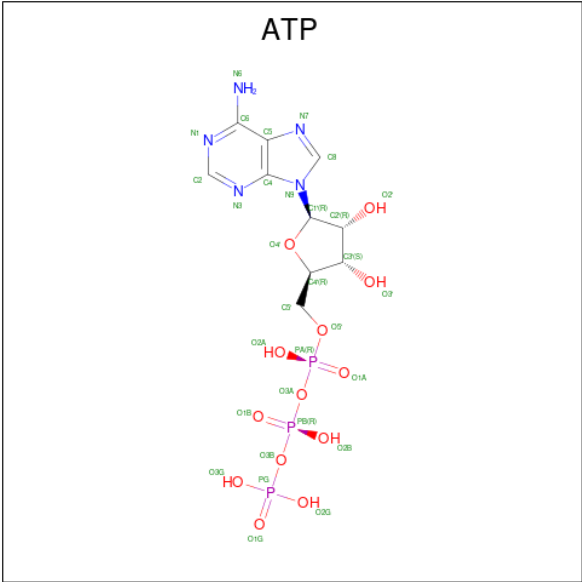
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Mol	Chain	Residues	Atoms					AltConf
21	y	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	z	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	7	1	Total	Mg	0
			1	1	
22	9	1	Total	Mg	0
			1	1	
22	D	1	Total	Mg	0
			1	1	
22	H	1	Total	Mg	0
			1	1	
22	J	1	Total	Mg	0
			1	1	
22	L	1	Total	Mg	0
			1	1	
22	P	1	Total	Mg	0
			1	1	
22	R	1	Total	Mg	0
			1	1	
22	T	1	Total	Mg	0
			1	1	
22	X	1	Total	Mg	0
			1	1	
22	Z	1	Total	Mg	0
			1	1	
22	j	1	Total	Mg	0
			1	1	
22	t	1	Total	Mg	0
			1	1	
22	z	1	Total	Mg	0
			1	1	

- Molecule 23 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



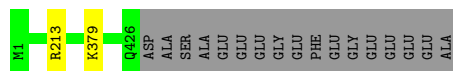
Mol	Chain	Residues	Atoms					AltConf
23	u	1	Total	C	N	O	P	0
			31	10	5	13	3	

Chain 3:  100%

There are no outlier residues recorded for this chain.

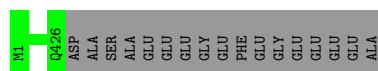
- Molecule 5: Tubulin beta

Chain 6:  96%



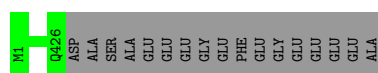
- Molecule 5: Tubulin beta

Chain 8:  96%



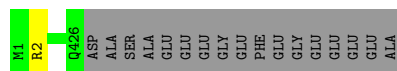
- Molecule 5: Tubulin beta

Chain C:  96%



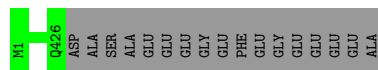
- Molecule 5: Tubulin beta

Chain G:  96%



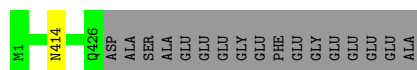
- Molecule 5: Tubulin beta

Chain I:  96%



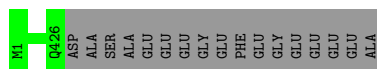
- Molecule 5: Tubulin beta

Chain K:  96%



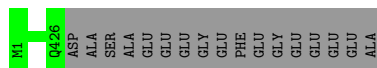
- Molecule 5: Tubulin beta

Chain O:  96%



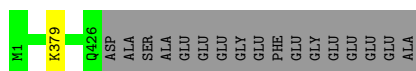
- Molecule 5: Tubulin beta

Chain Q: 96%



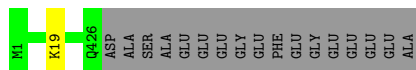
- Molecule 5: Tubulin beta

Chain S: 96%



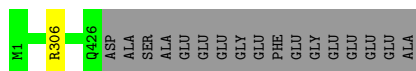
- Molecule 5: Tubulin beta

Chain W: 96%



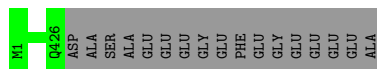
- Molecule 5: Tubulin beta

Chain Y: 96%



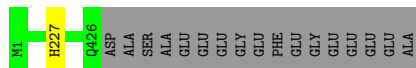
- Molecule 5: Tubulin beta

Chain i: 96%



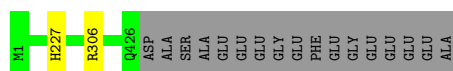
- Molecule 5: Tubulin beta

Chain k: 96%



- Molecule 5: Tubulin beta

Chain y: 96%



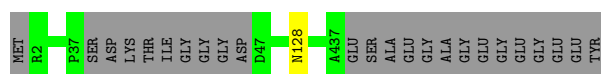
- Molecule 6: Tubulin alpha

Chain 7: 94% 5%



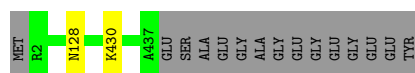
- Molecule 6: Tubulin alpha

Chain 9: 94% 5%



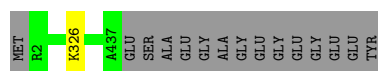
- Molecule 6: Tubulin alpha

Chain D: 96% .



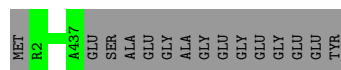
- Molecule 6: Tubulin alpha

Chain H: 96% .



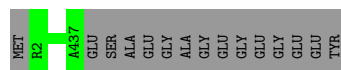
- Molecule 6: Tubulin alpha

Chain J: 97% .



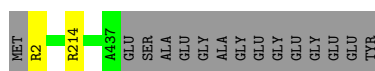
- Molecule 6: Tubulin alpha

Chain L: 97% .



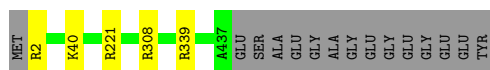
- Molecule 6: Tubulin alpha

Chain P: 96% .



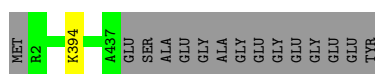
- Molecule 6: Tubulin alpha

Chain R: 96%



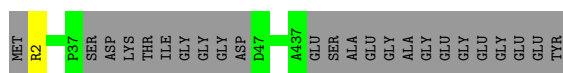
- Molecule 6: Tubulin alpha

Chain T: 96%



- Molecule 6: Tubulin alpha

Chain X: 94% 5%



- Molecule 6: Tubulin alpha

Chain Z: 94% 5%



- Molecule 6: Tubulin alpha

Chain j: 94% 5%



- Molecule 6: Tubulin alpha

Chain t: 95% 5%



- Molecule 6: Tubulin alpha

Chain z: 94% 5%

ILE	ASP	ILE	LEU	LEU	TYR	MET	ASP	LYS	GLY	ALA	ALA	ILE	THR	LYS	ASP	ALA	ALA	ILE	GLN	GLY	GLY	ARG	GLU	GLU	GLY	PRO	PRO	ALA	ALA	PRO	LEU	SER	GLY	VAL	GLU	PRO	ASP	ASP	VAL	VAL	GLU	VAL	VAL	VAL	LYS	LYS	ALA	ALA	ALA	ALA	GLU	GLU	GLY	THR	ASP	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 10: Radial spoke protein 7

Chain M:  9% 91%

[illegible]

- Molecule 10: Radial spoke protein 7

Chain N: 8% 92%


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

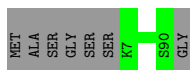
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain e:  92% 8%



- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain f:  92% 8%



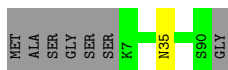
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain g:  92% 8%



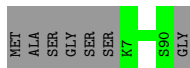
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain h:  91% 8%



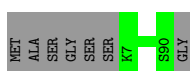
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain o:  92% 8%



- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain p:  92% 8%

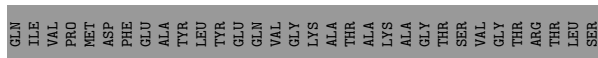


- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

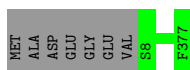
Chain q:  92% 8%



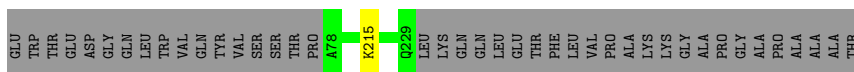
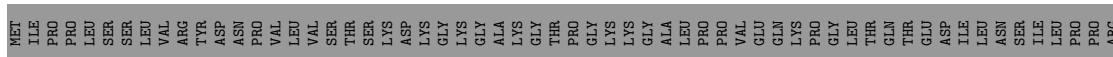
- [illegible]



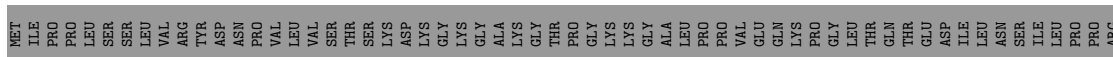
Chain u: 98%



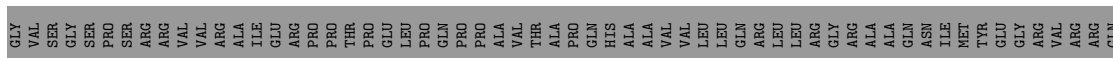
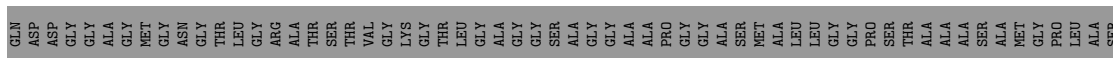
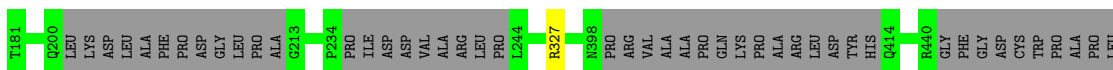
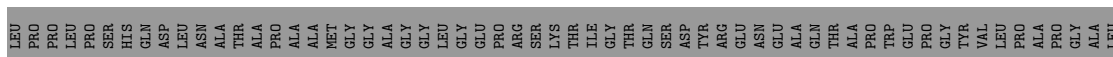
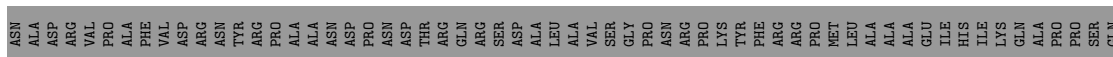
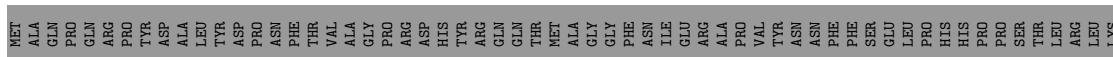
Chain v:  60% 40%



Chain w: 56% 43%



Chain x:  17% 83%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	202168	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 ($e^-/\text{\AA}^2$)	38.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, ATP, 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	0	0.28	0/1379	0.50	0/1860
1	4	0.27	0/1258	0.49	0/1690
2	1	0.27	0/1458	0.45	0/1962
3	2	0.33	0/1517	0.51	0/2038
5	6	0.28	0/3420	0.47	0/4628
5	8	0.29	0/3420	0.47	0/4628
5	C	0.28	0/3420	0.46	0/4628
5	G	0.29	0/3420	0.46	0/4628
5	I	0.29	0/3420	0.47	0/4628
5	K	0.32	0/3420	0.47	0/4628
5	O	0.30	0/3420	0.48	0/4628
5	Q	0.29	0/3420	0.47	0/4628
5	S	0.29	0/3420	0.47	0/4628
5	W	0.27	0/3420	0.46	0/4628
5	Y	0.28	0/3420	0.47	0/4628
5	i	0.28	0/3420	0.45	0/4628
5	k	0.29	0/3420	0.46	0/4628
5	y	0.29	0/3420	0.47	0/4628
6	7	0.29	0/3389	0.48	0/4595
6	9	0.28	0/3389	0.47	0/4595
6	D	0.30	0/3448	0.47	0/4675
6	H	0.30	0/3448	0.48	0/4675
6	J	0.29	0/3448	0.48	0/4675
6	L	0.31	0/3448	0.49	0/4675
6	P	0.29	0/3448	0.46	0/4675
6	R	0.29	0/3448	0.48	0/4675
6	T	0.28	0/3448	0.47	0/4675
6	X	0.29	0/3389	0.47	0/4595
6	Z	0.28	0/3389	0.46	0/4595
6	j	0.28	0/3389	0.48	0/4595
6	t	0.28	0/3389	0.49	0/4595
6	z	0.30	0/3389	0.49	0/4595

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	A	0.28	0/3562	0.42	0/4763
8	B	0.29	0/3499	0.46	0/4674
9	E	0.32	0/698	0.54	0/948
9	F	0.30	0/946	0.56	0/1287
10	M	0.33	0/363	0.48	0/491
10	N	0.29	0/325	0.46	0/439
11	U	0.29	0/399	0.48	0/543
11	V	0.27	0/891	0.43	0/1221
12	a	0.35	0/702	0.48	0/945
12	b	0.36	0/702	0.52	0/945
12	c	0.36	0/702	0.54	0/945
12	d	0.35	0/702	0.51	0/945
12	e	0.33	0/702	0.50	0/945
12	f	0.38	0/702	0.53	0/945
12	g	0.33	0/702	0.50	0/945
12	h	0.32	0/702	0.49	0/945
12	o	0.27	0/702	0.47	0/945
12	p	0.27	0/702	0.49	0/945
12	q	0.25	0/702	0.46	0/945
12	r	0.27	0/702	0.50	0/945
13	l	0.28	0/2469	0.54	0/3363
14	m	0.32	0/1688	0.54	0/2273
15	n	0.24	0/1515	0.39	0/2108
16	s	0.24	0/1487	0.41	0/2004
17	u	0.27	0/2942	0.48	0/3985
18	v	0.27	0/1267	0.48	0/1696
18	w	0.27	0/1196	0.42	0/1599
19	x	0.28	0/1847	0.43	0/2473
All	All	0.29	0/134869	0.47	0/182439

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles

5.3.1 Protein backbone

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	0	171/471 (36%)	166 (97%)	5 (3%)	0	100	100
1	4	150/471 (32%)	148 (99%)	2 (1%)	0	100	100
2	1	164/698 (24%)	157 (96%)	7 (4%)	0	100	100
3	2	179/573 (31%)	176 (98%)	3 (2%)	0	100	100
5	6	424/443 (96%)	398 (94%)	26 (6%)	0	100	100
5	8	424/443 (96%)	399 (94%)	25 (6%)	0	100	100
5	C	424/443 (96%)	410 (97%)	14 (3%)	0	100	100
5	G	424/443 (96%)	393 (93%)	31 (7%)	0	100	100
5	I	424/443 (96%)	398 (94%)	26 (6%)	0	100	100
5	K	424/443 (96%)	396 (93%)	28 (7%)	0	100	100
5	O	424/443 (96%)	401 (95%)	23 (5%)	0	100	100
5	Q	424/443 (96%)	396 (93%)	28 (7%)	0	100	100
5	S	424/443 (96%)	398 (94%)	26 (6%)	0	100	100
5	W	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
5	Y	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
5	i	424/443 (96%)	404 (95%)	20 (5%)	0	100	100
5	k	424/443 (96%)	398 (94%)	26 (6%)	0	100	100
5	y	424/443 (96%)	400 (94%)	24 (6%)	0	100	100
6	7	423/451 (94%)	396 (94%)	27 (6%)	0	100	100
6	9	423/451 (94%)	393 (93%)	30 (7%)	0	100	100
6	D	434/451 (96%)	413 (95%)	21 (5%)	0	100	100
6	H	434/451 (96%)	410 (94%)	24 (6%)	0	100	100
6	J	434/451 (96%)	402 (93%)	32 (7%)	0	100	100
6	L	434/451 (96%)	404 (93%)	30 (7%)	0	100	100
6	P	434/451 (96%)	405 (93%)	29 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	R	434/451 (96%)	410 (94%)	24 (6%)	0	100	100
6	T	434/451 (96%)	410 (94%)	24 (6%)	0	100	100
6	X	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
6	Z	423/451 (94%)	401 (95%)	22 (5%)	0	100	100
6	j	423/451 (94%)	402 (95%)	21 (5%)	0	100	100
6	t	423/451 (94%)	399 (94%)	24 (6%)	0	100	100
6	z	423/451 (94%)	398 (94%)	25 (6%)	0	100	100
7	A	429/925 (46%)	428 (100%)	1 (0%)	0	100	100
8	B	429/904 (48%)	428 (100%)	1 (0%)	0	100	100
9	E	84/516 (16%)	81 (96%)	3 (4%)	0	100	100
9	F	115/516 (22%)	105 (91%)	10 (9%)	0	100	100
10	M	42/500 (8%)	38 (90%)	4 (10%)	0	100	100
10	N	38/500 (8%)	33 (87%)	5 (13%)	0	100	100
11	U	47/204 (23%)	42 (89%)	5 (11%)	0	100	100
11	V	150/204 (74%)	133 (89%)	17 (11%)	0	100	100
12	a	82/91 (90%)	72 (88%)	10 (12%)	0	100	100
12	b	82/91 (90%)	76 (93%)	6 (7%)	0	100	100
12	c	82/91 (90%)	79 (96%)	3 (4%)	0	100	100
12	d	82/91 (90%)	76 (93%)	6 (7%)	0	100	100
12	e	82/91 (90%)	76 (93%)	6 (7%)	0	100	100
12	f	82/91 (90%)	75 (92%)	7 (8%)	0	100	100
12	g	82/91 (90%)	77 (94%)	5 (6%)	0	100	100
12	h	82/91 (90%)	79 (96%)	3 (4%)	0	100	100
12	o	82/91 (90%)	73 (89%)	9 (11%)	0	100	100
12	p	82/91 (90%)	73 (89%)	9 (11%)	0	100	100
12	q	82/91 (90%)	73 (89%)	9 (11%)	0	100	100
12	r	82/91 (90%)	78 (95%)	4 (5%)	0	100	100
13	l	325/331 (98%)	285 (88%)	40 (12%)	0	100	100
14	m	202/256 (79%)	174 (86%)	28 (14%)	0	100	100
15	n	305/378 (81%)	270 (88%)	35 (12%)	0	100	100
16	s	172/682 (25%)	160 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	u	368/377 (98%)	350 (95%)	18 (5%)	0	100	100
18	v	150/253 (59%)	144 (96%)	6 (4%)	0	100	100
18	w	139/253 (55%)	138 (99%)	1 (1%)	0	100	100
19	x	216/1298 (17%)	206 (95%)	10 (5%)	0	100	100
All	All	16794/23918 (70%)	15820 (94%)	974 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	0	146/418 (35%)	145 (99%)	1 (1%)	84	92
1	4	135/418 (32%)	135 (100%)	0	100	100
2	1	153/573 (27%)	153 (100%)	0	100	100
3	2	158/470 (34%)	156 (99%)	2 (1%)	69	84
5	6	367/379 (97%)	365 (100%)	2 (0%)	88	94
5	8	367/379 (97%)	367 (100%)	0	100	100
5	C	367/379 (97%)	367 (100%)	0	100	100
5	G	367/379 (97%)	366 (100%)	1 (0%)	92	97
5	I	367/379 (97%)	367 (100%)	0	100	100
5	K	367/379 (97%)	366 (100%)	1 (0%)	92	97
5	O	367/379 (97%)	367 (100%)	0	100	100
5	Q	367/379 (97%)	367 (100%)	0	100	100
5	S	367/379 (97%)	366 (100%)	1 (0%)	92	97
5	W	367/379 (97%)	366 (100%)	1 (0%)	92	97
5	Y	367/379 (97%)	366 (100%)	1 (0%)	92	97
5	i	367/379 (97%)	367 (100%)	0	100	100
5	k	367/379 (97%)	366 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	y	367/379 (97%)	365 (100%)	2 (0%)	88	94
6	7	359/374 (96%)	356 (99%)	3 (1%)	81	91
6	9	359/374 (96%)	358 (100%)	1 (0%)	92	97
6	D	365/374 (98%)	363 (100%)	2 (0%)	88	94
6	H	365/374 (98%)	364 (100%)	1 (0%)	92	97
6	J	365/374 (98%)	365 (100%)	0	100	100
6	L	365/374 (98%)	365 (100%)	0	100	100
6	P	365/374 (98%)	363 (100%)	2 (0%)	88	94
6	R	365/374 (98%)	360 (99%)	5 (1%)	67	83
6	T	365/374 (98%)	364 (100%)	1 (0%)	92	97
6	X	359/374 (96%)	358 (100%)	1 (0%)	92	97
6	Z	359/374 (96%)	358 (100%)	1 (0%)	92	97
6	j	359/374 (96%)	358 (100%)	1 (0%)	92	97
6	t	359/374 (96%)	359 (100%)	0	100	100
6	z	359/374 (96%)	358 (100%)	1 (0%)	92	97
7	A	368/766 (48%)	367 (100%)	1 (0%)	92	97
8	B	362/742 (49%)	361 (100%)	1 (0%)	92	97
9	E	76/406 (19%)	76 (100%)	0	100	100
9	F	102/406 (25%)	101 (99%)	1 (1%)	76	88
10	M	36/406 (9%)	36 (100%)	0	100	100
10	N	32/406 (8%)	32 (100%)	0	100	100
11	U	42/162 (26%)	42 (100%)	0	100	100
11	V	28/162 (17%)	28 (100%)	0	100	100
12	a	72/76 (95%)	72 (100%)	0	100	100
12	b	72/76 (95%)	72 (100%)	0	100	100
12	c	72/76 (95%)	72 (100%)	0	100	100
12	d	72/76 (95%)	72 (100%)	0	100	100
12	e	72/76 (95%)	72 (100%)	0	100	100
12	f	72/76 (95%)	72 (100%)	0	100	100
12	g	72/76 (95%)	72 (100%)	0	100	100
12	h	72/76 (95%)	71 (99%)	1 (1%)	67	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	o	72/76 (95%)	72 (100%)	0	100	100
12	p	72/76 (95%)	72 (100%)	0	100	100
12	q	72/76 (95%)	72 (100%)	0	100	100
12	r	72/76 (95%)	71 (99%)	1 (1%)	67	83
13	l	259/263 (98%)	256 (99%)	3 (1%)	71	85
14	m	159/197 (81%)	159 (100%)	0	100	100
16	s	162/553 (29%)	162 (100%)	0	100	100
17	u	313/318 (98%)	313 (100%)	0	100	100
18	v	134/218 (62%)	133 (99%)	1 (1%)	84	92
18	w	127/218 (58%)	126 (99%)	1 (1%)	81	91
19	x	191/884 (22%)	190 (100%)	1 (0%)	88	94
All	All	14053/19440 (72%)	14010 (100%)	43 (0%)	92	97

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	Y	306	ARG
13	l	309	ARG
6	Z	308	ARG
5	k	227	HIS
18	v	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
6	T	176	GLN
6	z	11	GLN
12	d	70	HIS
5	y	414	ASN
6	t	258	ASN

5.3.3 RNA ⓘ

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 43 ligands modelled in this entry, 14 are monoatomic - leaving 29 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	$\# Z > 2$
23	ATP	u	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.49	5 (16%)
20	GDP	K	501	-	24,30,30	1.01	1 (4%)	30,47,47	1.22	2 (6%)
21	GTP	z	501	22	26,34,34	1.14	2 (7%)	32,54,54	1.61	8 (25%)
20	GDP	6	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.42	4 (13%)
21	GTP	J	501	22	26,34,34	1.17	2 (7%)	32,54,54	1.79	7 (21%)
20	GDP	i	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.44	4 (13%)
20	GDP	y	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
21	GTP	7	501	22	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
21	GTP	L	501	22	26,34,34	1.09	1 (3%)	32,54,54	1.55	6 (18%)
20	GDP	I	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.40	5 (16%)
20	GDP	C	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	5 (16%)
20	GDP	G	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
20	GDP	k	501	-	24,30,30	0.89	1 (4%)	30,47,47	1.50	6 (20%)
20	GDP	W	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.42	5 (16%)
21	GTP	y	501	22	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
20	GDP	Y	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
21	GTP	Z	501	22	26,34,34	1.18	2 (7%)	32,54,54	1.69	7 (21%)
21	GTP	R	501	22	26,34,34	1.21	2 (7%)	32,54,54	1.74	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	GDP	8	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.42	4 (13%)
21	GTP	D	501	22	26,34,34	1.20	2 (7%)	32,54,54	1.65	7 (21%)
21	GTP	9	501	22	26,34,34	1.17	2 (7%)	32,54,54	1.77	7 (21%)
20	GDP	Q	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.39	4 (13%)
20	GDP	S	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.39	4 (13%)
21	GTP	T	501	22	26,34,34	1.19	2 (7%)	32,54,54	1.70	7 (21%)
21	GTP	H	501	22	26,34,34	1.19	1 (3%)	32,54,54	1.59	8 (25%)
21	GTP	X	501	22	26,34,34	1.21	2 (7%)	32,54,54	1.69	7 (21%)
21	GTP	P	501	22	26,34,34	1.19	2 (7%)	32,54,54	1.52	7 (21%)
21	GTP	j	501	22	26,34,34	1.16	2 (7%)	32,54,54	1.67	7 (21%)
20	GDP	O	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.41	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
23	ATP	u	401	-	-	4/18/38/38	0/3/3/3
20	GDP	K	501	-	-	4/12/32/32	0/3/3/3
21	GTP	z	501	22	-	8/18/38/38	0/3/3/3
20	GDP	6	501	-	-	3/12/32/32	0/3/3/3
21	GTP	J	501	22	-	9/18/38/38	0/3/3/3
20	GDP	i	501	-	-	3/12/32/32	0/3/3/3
20	GDP	y	502	-	-	4/12/32/32	0/3/3/3
21	GTP	7	501	22	-	4/18/38/38	0/3/3/3
21	GTP	L	501	22	-	5/18/38/38	0/3/3/3
20	GDP	I	501	-	-	5/12/32/32	0/3/3/3
20	GDP	C	501	-	-	2/12/32/32	0/3/3/3
20	GDP	G	501	-	-	5/12/32/32	0/3/3/3
20	GDP	k	501	-	-	1/12/32/32	0/3/3/3
20	GDP	W	501	-	-	7/12/32/32	0/3/3/3
21	GTP	y	501	22	-	4/18/38/38	0/3/3/3
20	GDP	Y	501	-	-	1/12/32/32	0/3/3/3
21	GTP	Z	501	22	-	4/18/38/38	0/3/3/3
21	GTP	R	501	22	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GDP	8	501	-	-	4/12/32/32	0/3/3/3
21	GTP	D	501	22	-	6/18/38/38	0/3/3/3
21	GTP	9	501	22	-	6/18/38/38	0/3/3/3
20	GDP	Q	501	-	-	7/12/32/32	0/3/3/3
20	GDP	S	501	-	-	0/12/32/32	0/3/3/3
21	GTP	T	501	22	-	4/18/38/38	0/3/3/3
21	GTP	H	501	22	-	5/18/38/38	0/3/3/3
21	GTP	X	501	22	-	5/18/38/38	0/3/3/3
21	GTP	P	501	22	-	4/18/38/38	0/3/3/3
21	GTP	j	501	22	-	4/18/38/38	0/3/3/3
20	GDP	O	501	-	-	3/12/32/32	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	X	501	GTP	C5-C6	-4.33	1.38	1.47
21	D	501	GTP	C5-C6	-4.31	1.38	1.47
21	y	501	GTP	C5-C6	-4.28	1.38	1.47
21	P	501	GTP	C5-C6	-4.27	1.38	1.47
21	R	501	GTP	C5-C6	-4.25	1.38	1.47

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	501	GTP	PA-O3A-PB	-4.53	117.28	132.83
20	8	501	GDP	PA-O3A-PB	-4.53	117.29	132.83
21	R	501	GTP	PA-O3A-PB	-4.49	117.41	132.83
21	9	501	GTP	PA-O3A-PB	-4.46	117.52	132.83
20	6	501	GDP	PA-O3A-PB	-4.44	117.61	132.83

There are no chirality outliers.

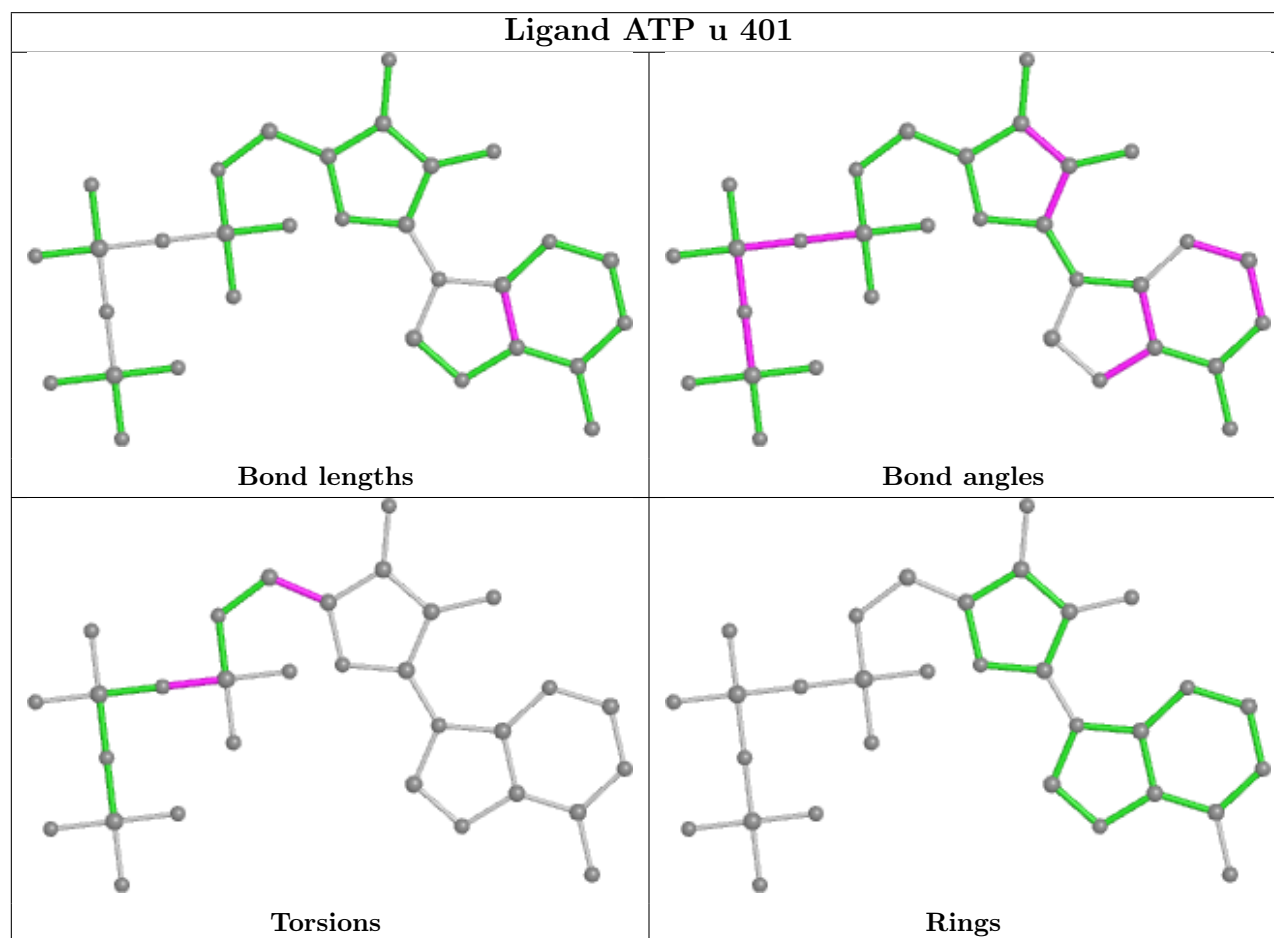
5 of 127 torsion outliers are listed below:

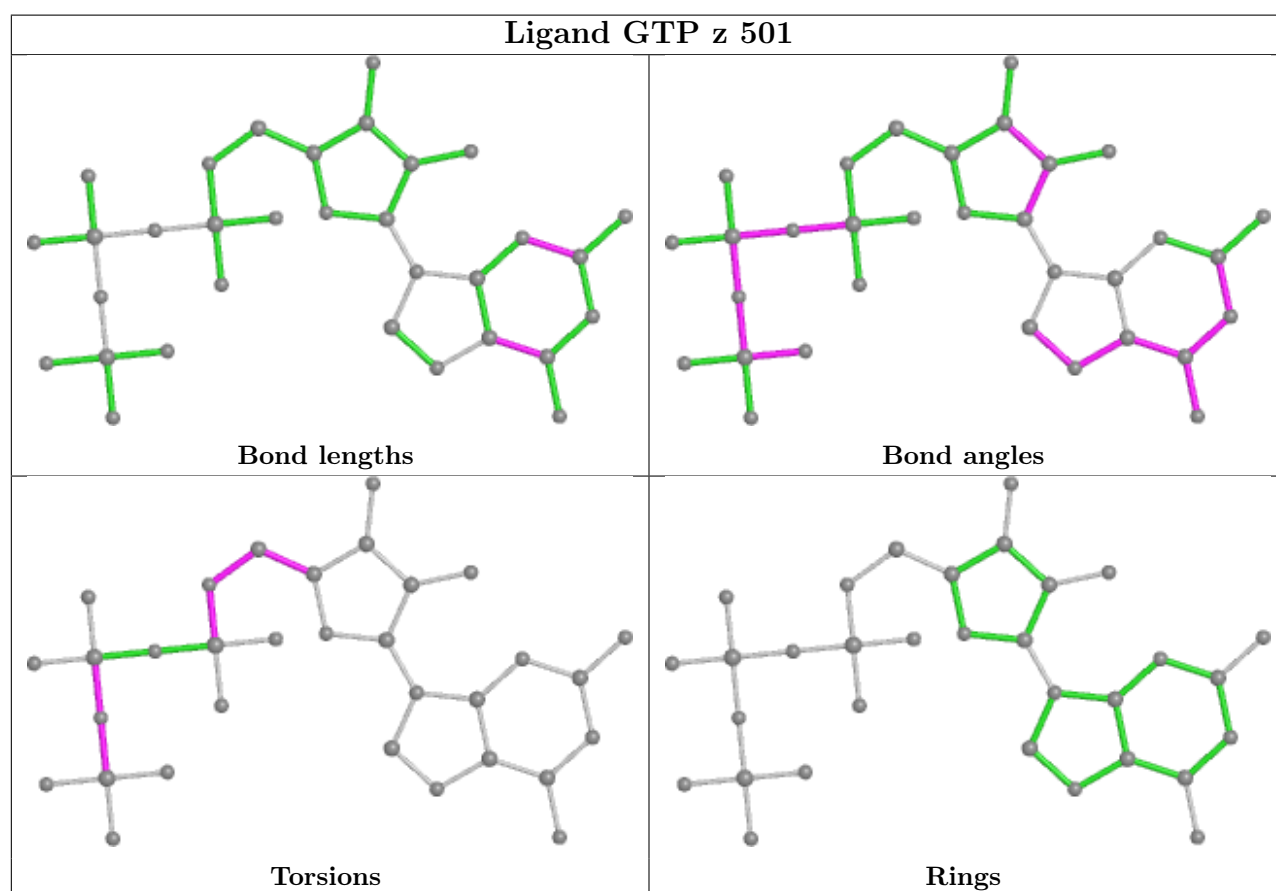
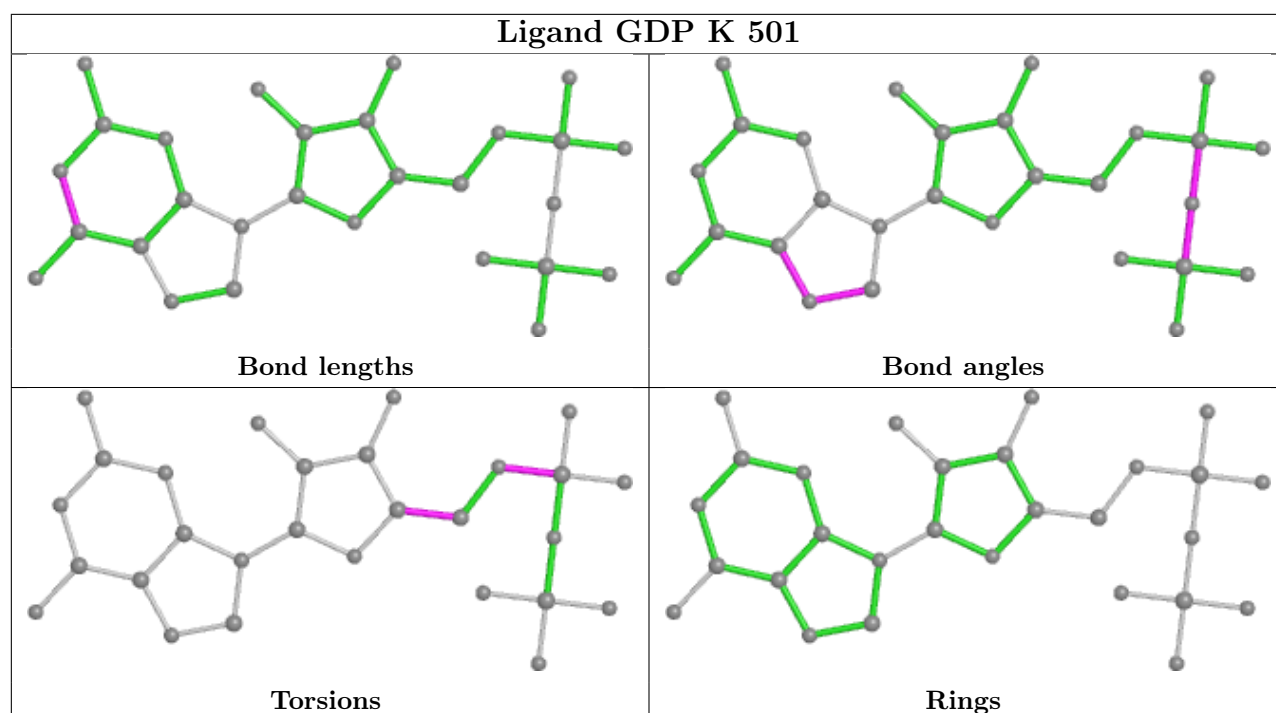
Mol	Chain	Res	Type	Atoms
20	6	501	GDP	C5'-O5'-PA-O2A
20	8	501	GDP	C5'-O5'-PA-O3A
20	8	501	GDP	C5'-O5'-PA-O1A
20	C	501	GDP	C5'-O5'-PA-O3A
20	C	501	GDP	C5'-O5'-PA-O1A

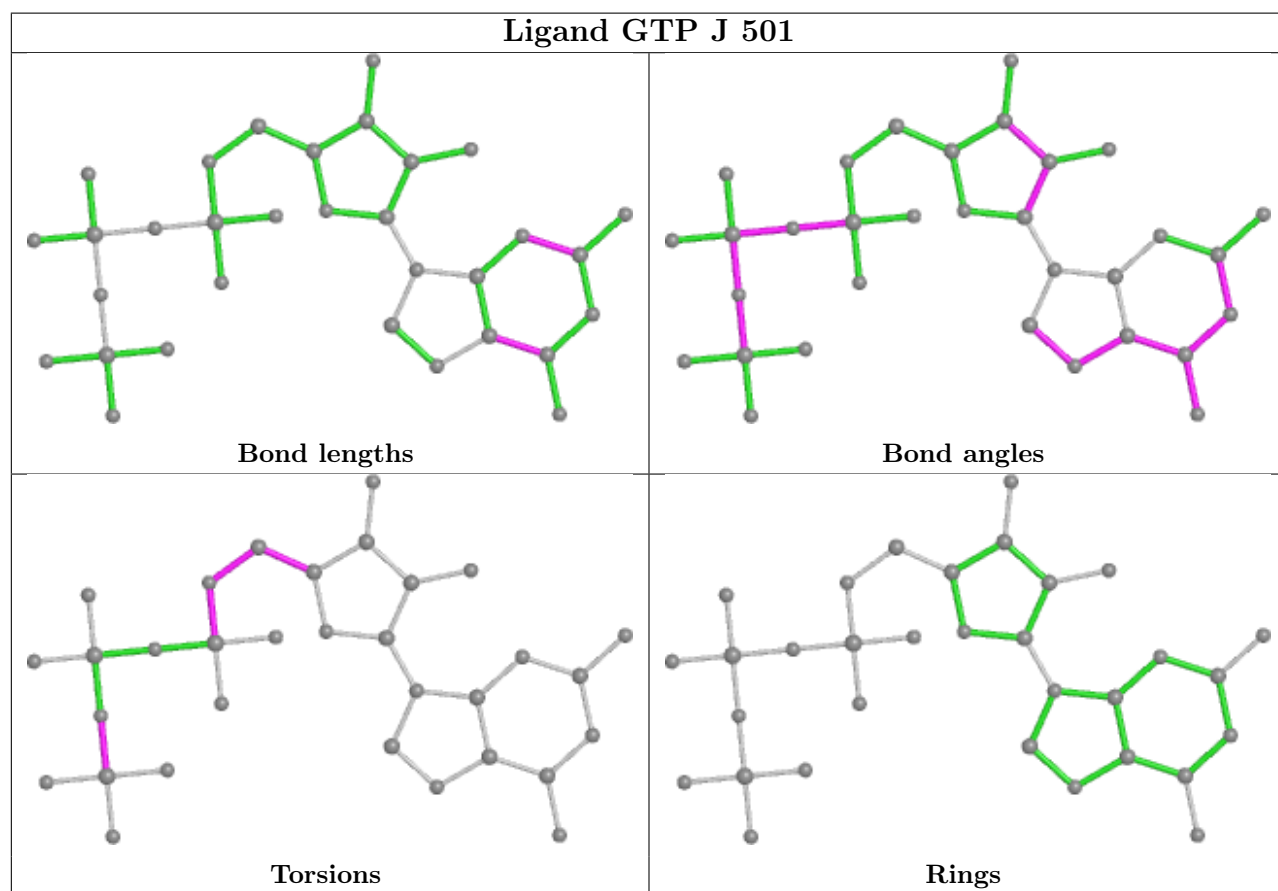
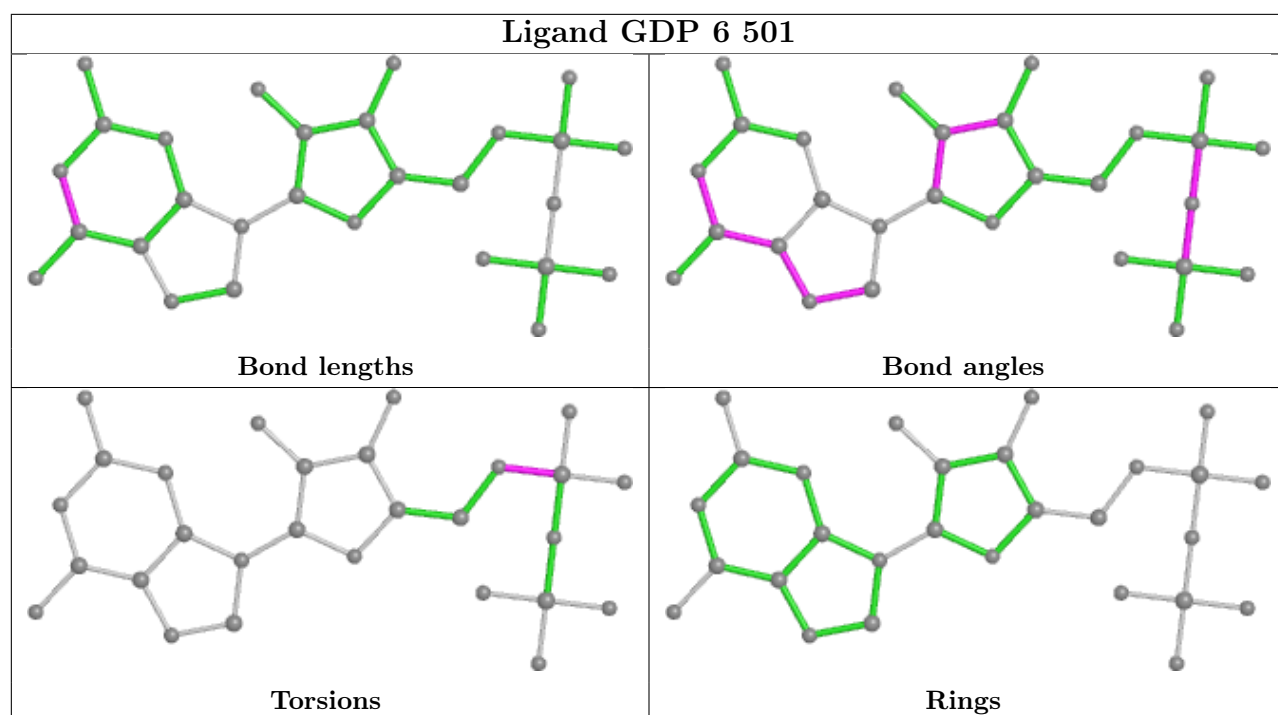
There are no ring outliers.

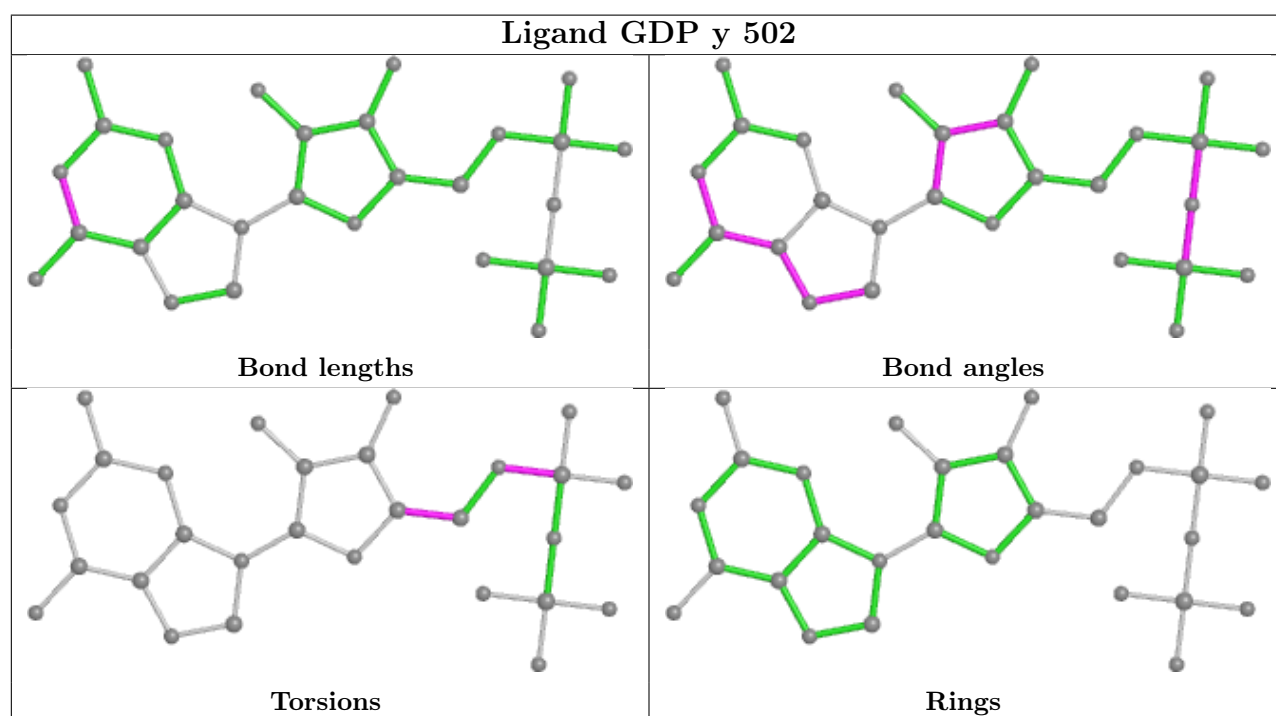
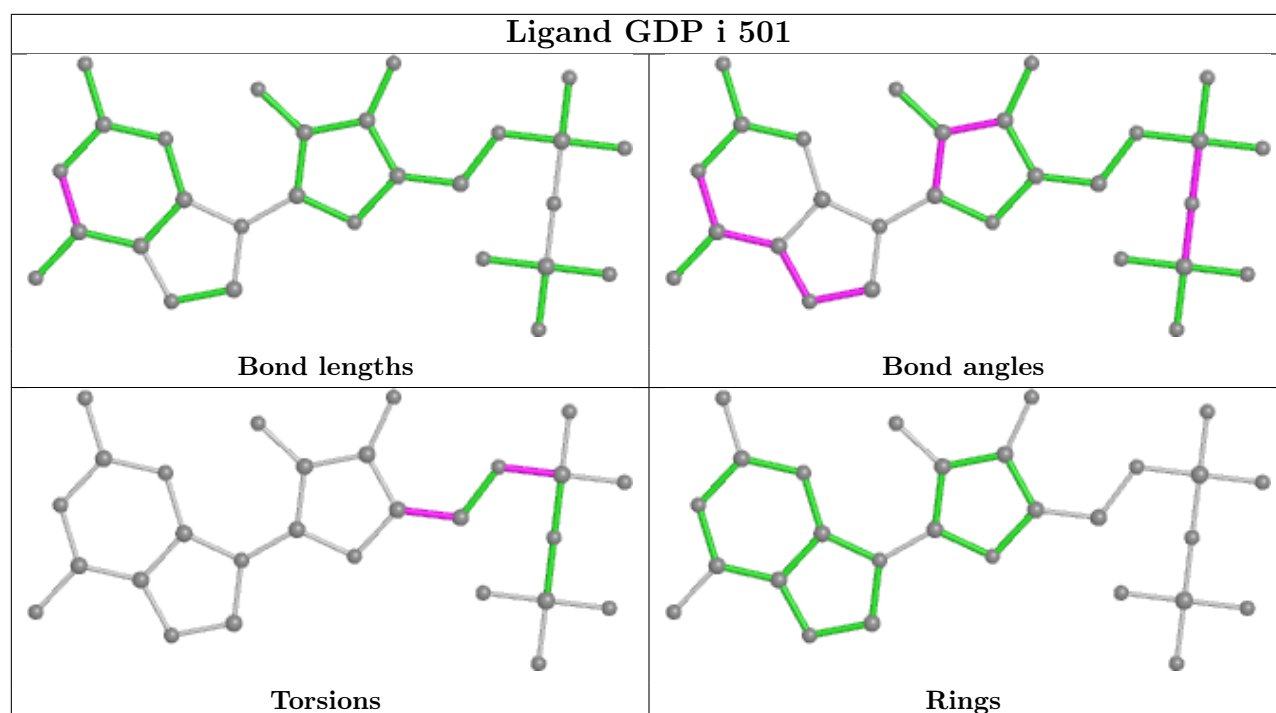
No monomer is involved in short contacts.

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.

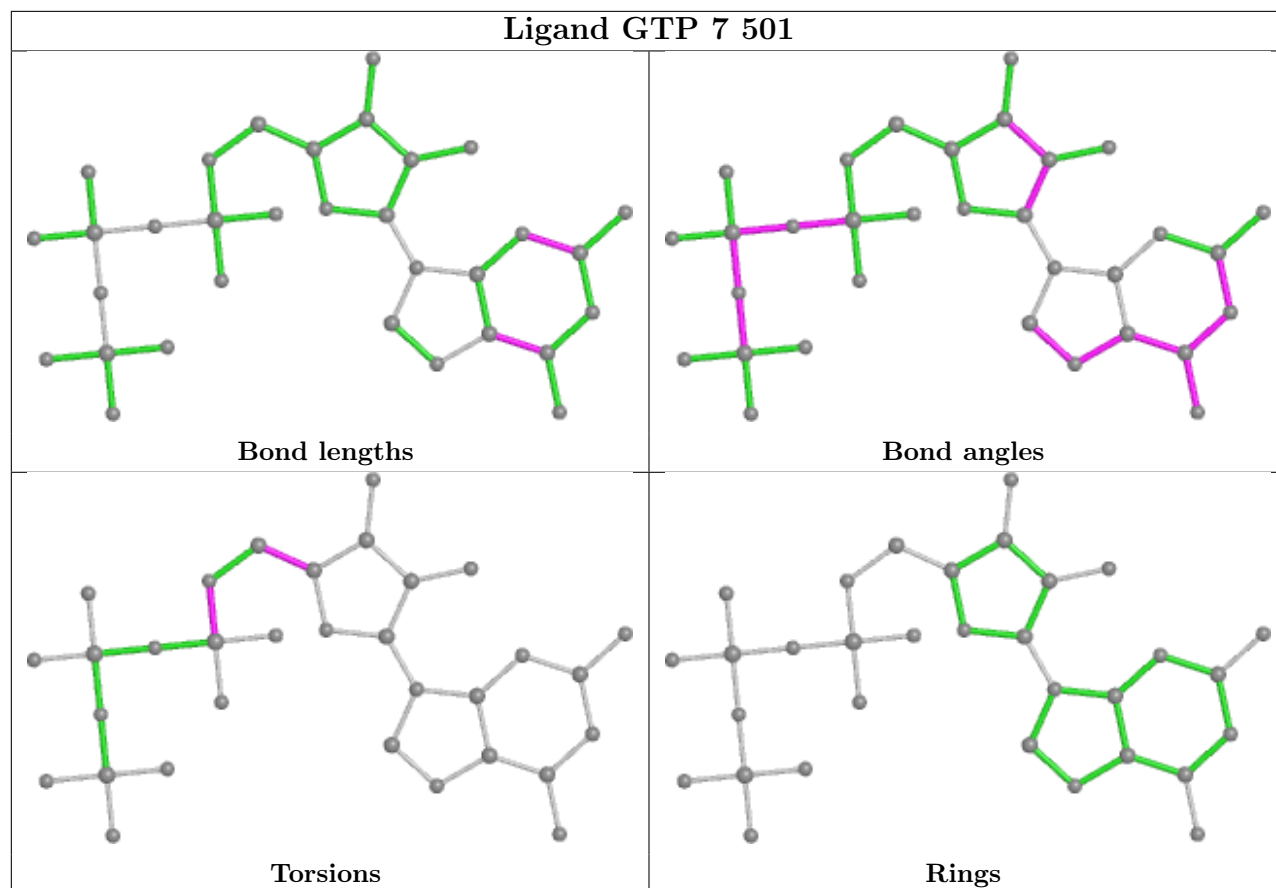




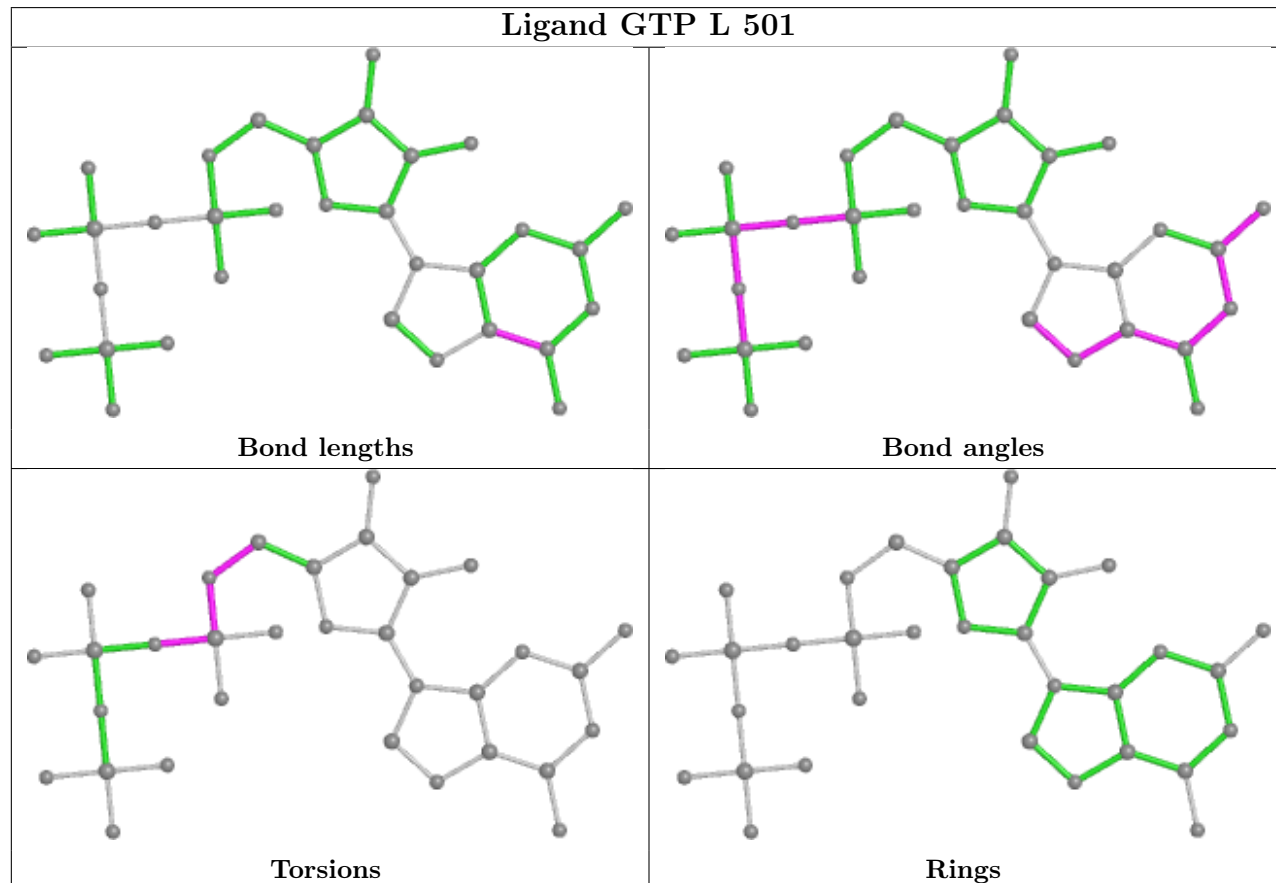


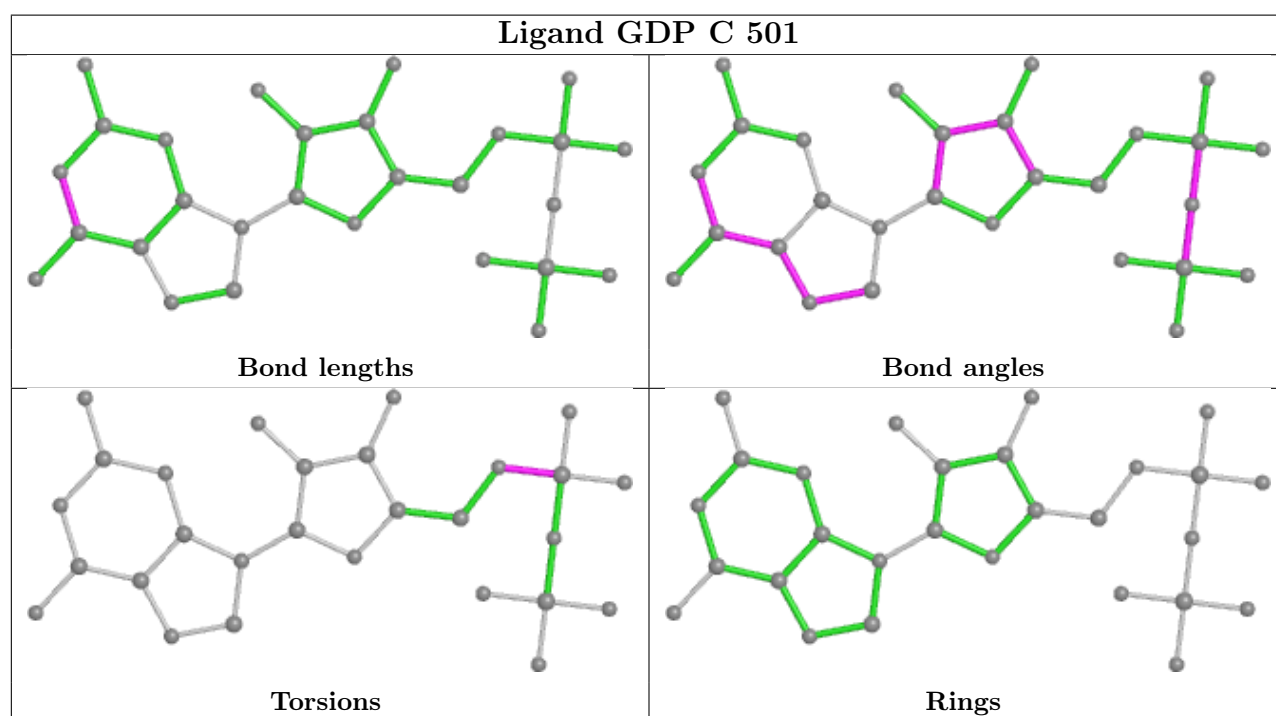
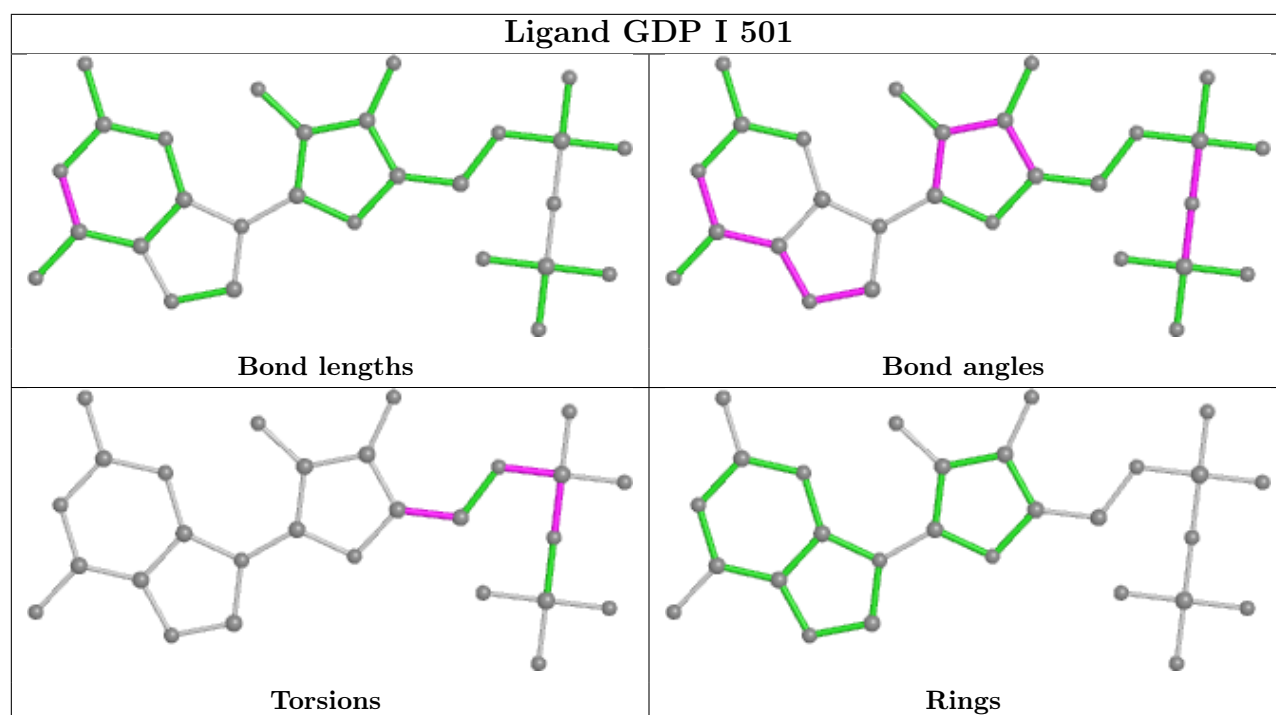


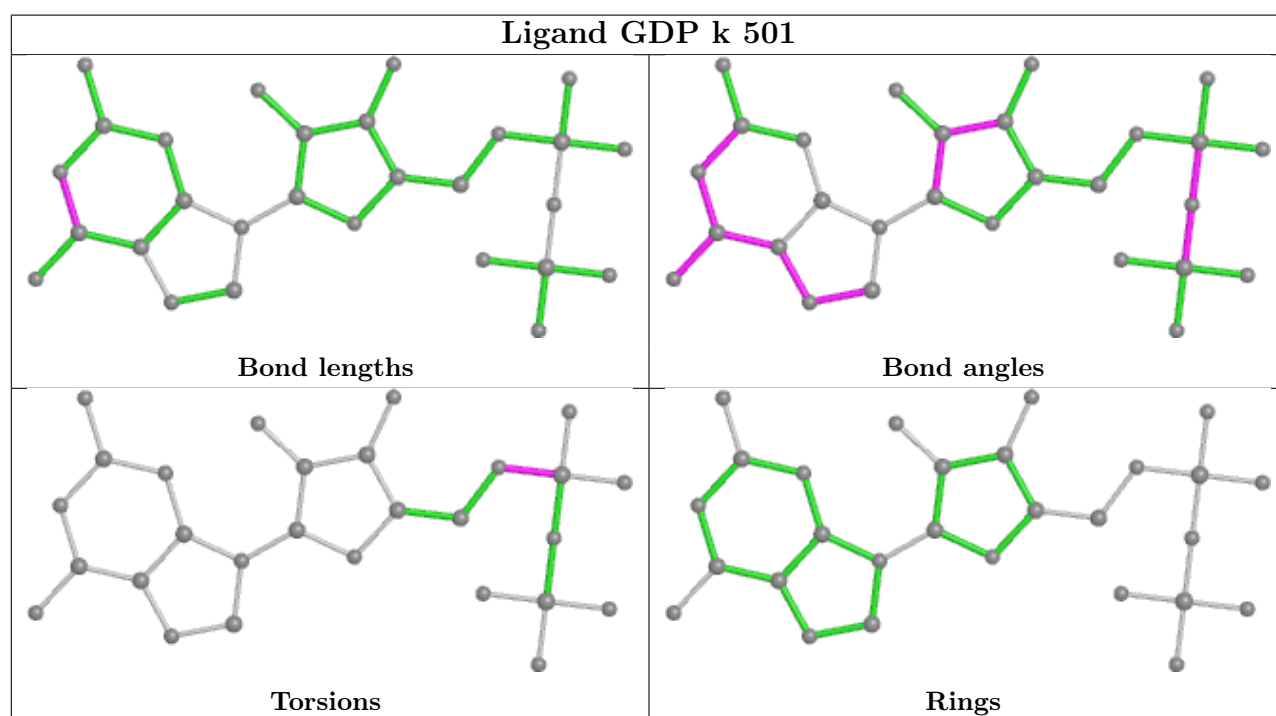
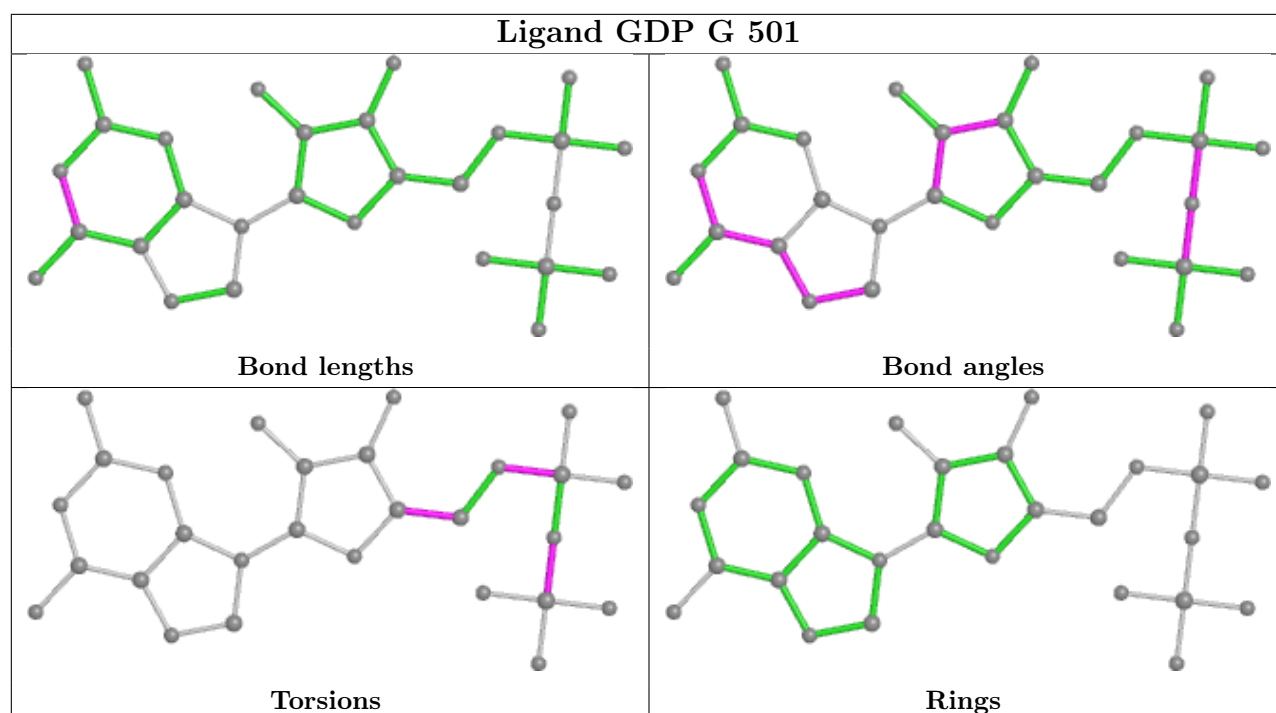
Ligand GTP 7 501

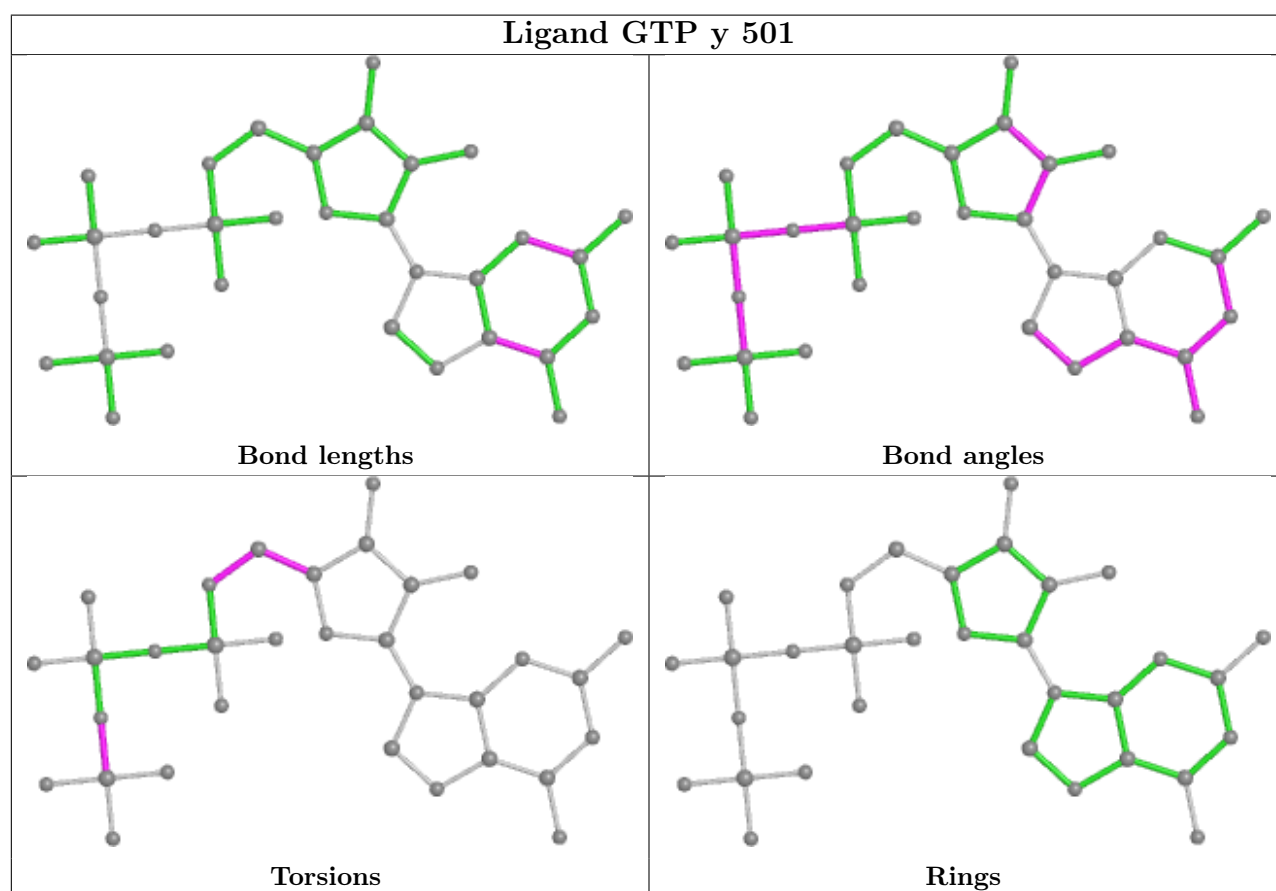
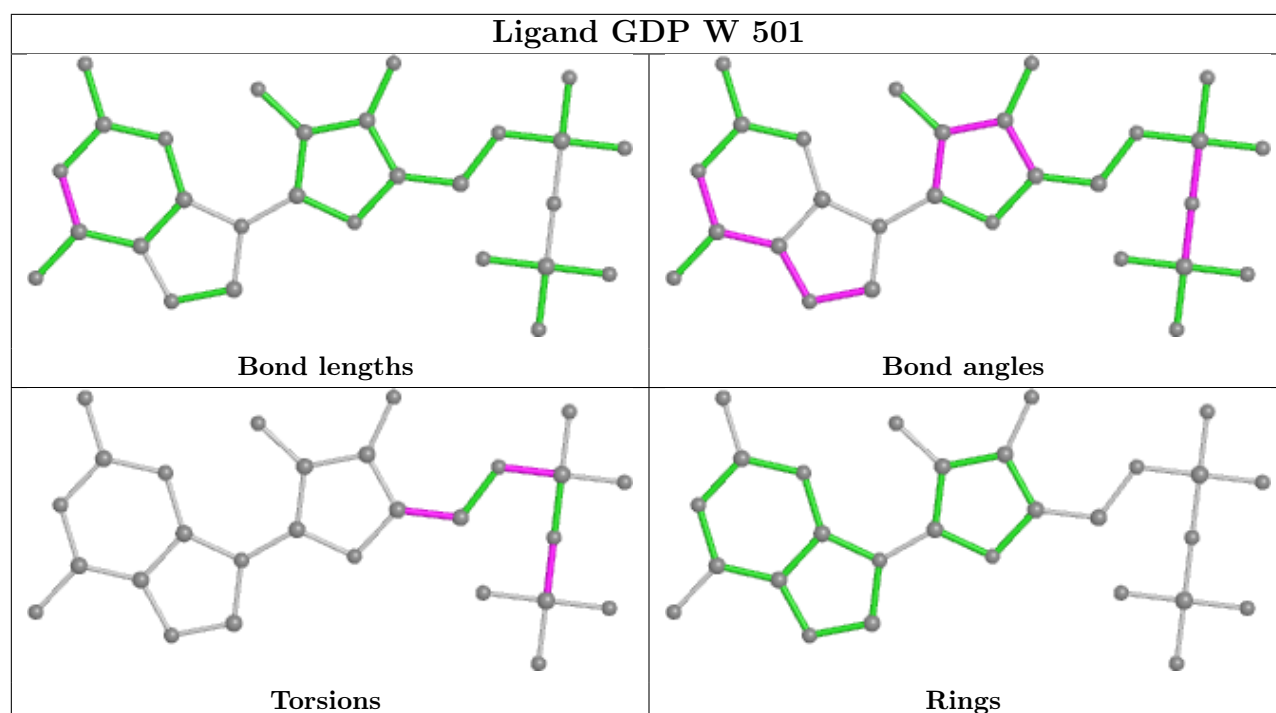


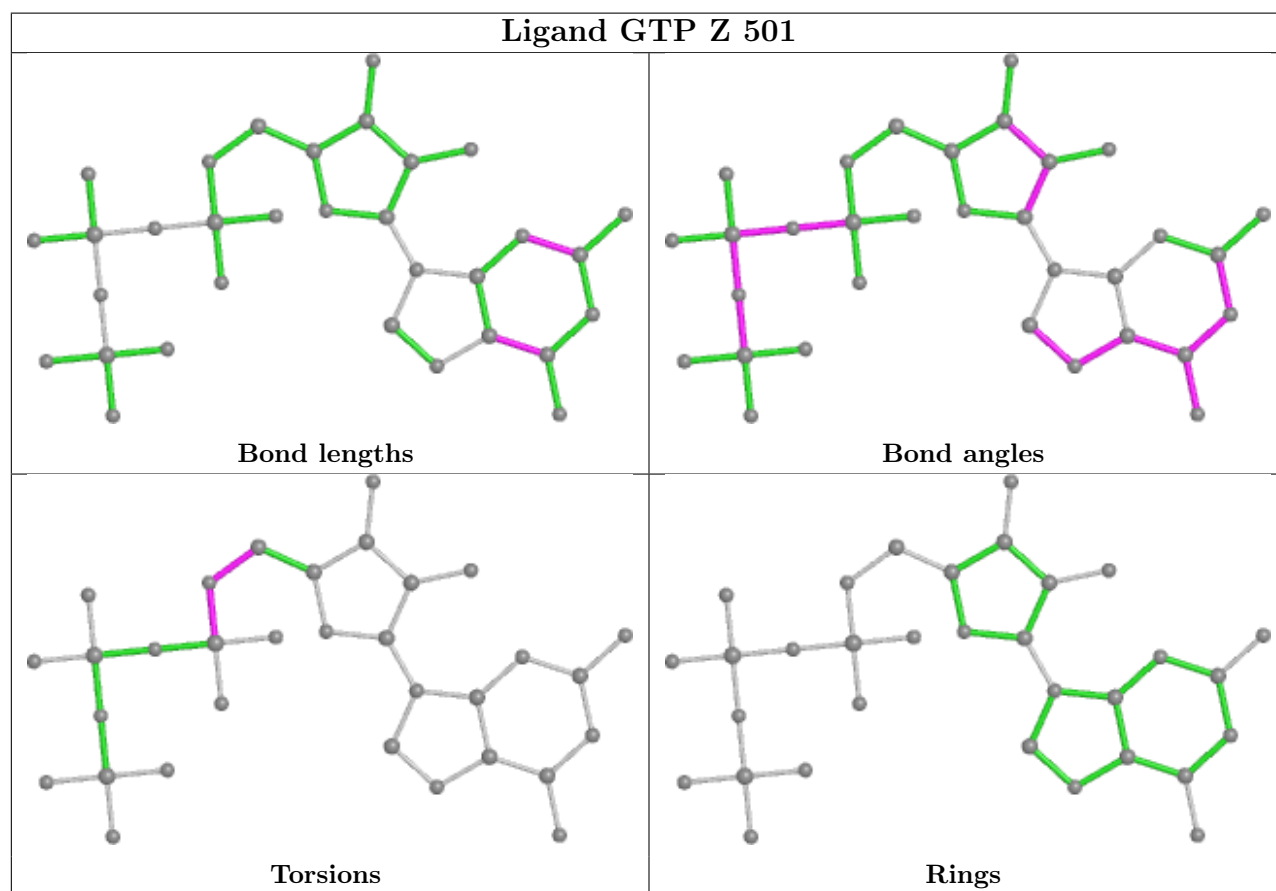
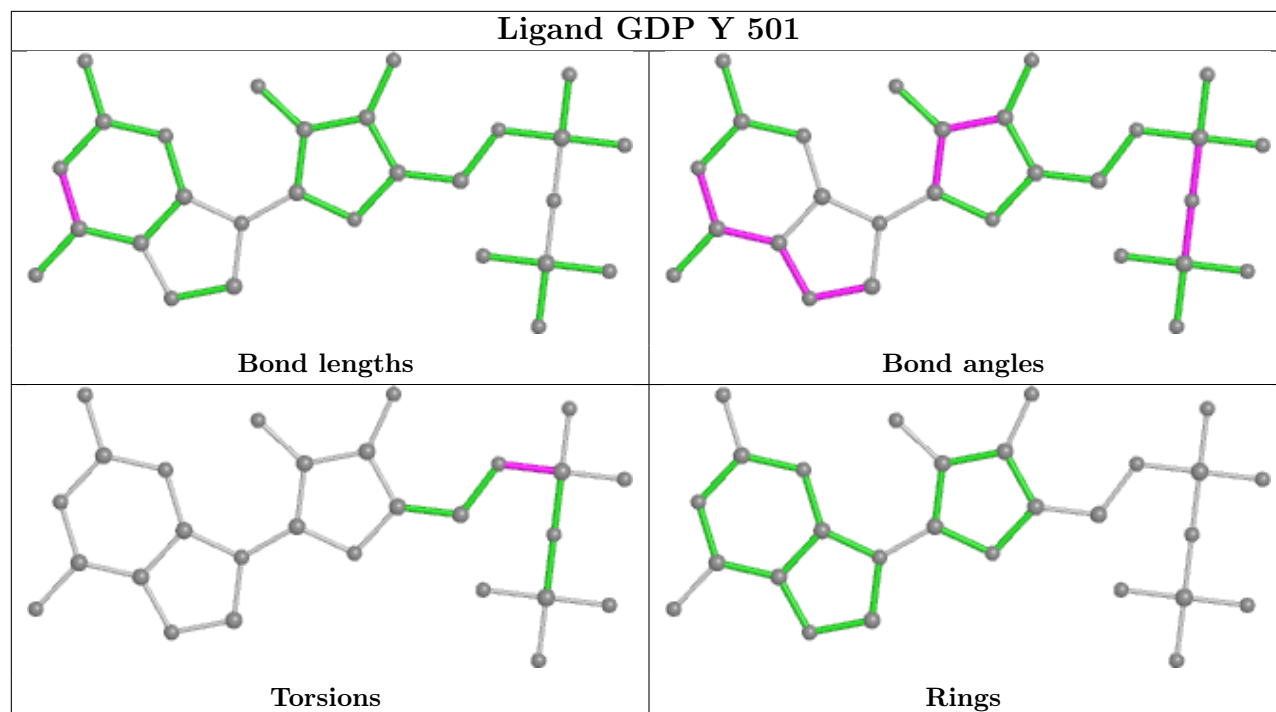
Ligand GTP L 501

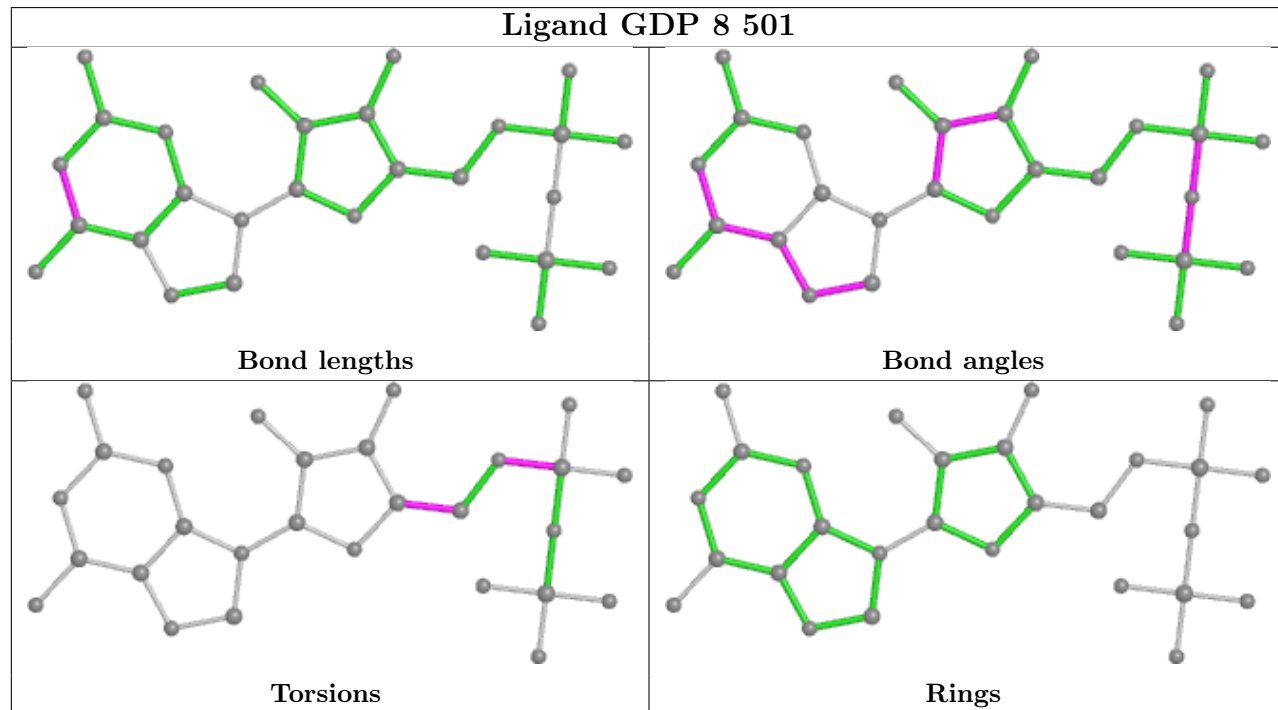
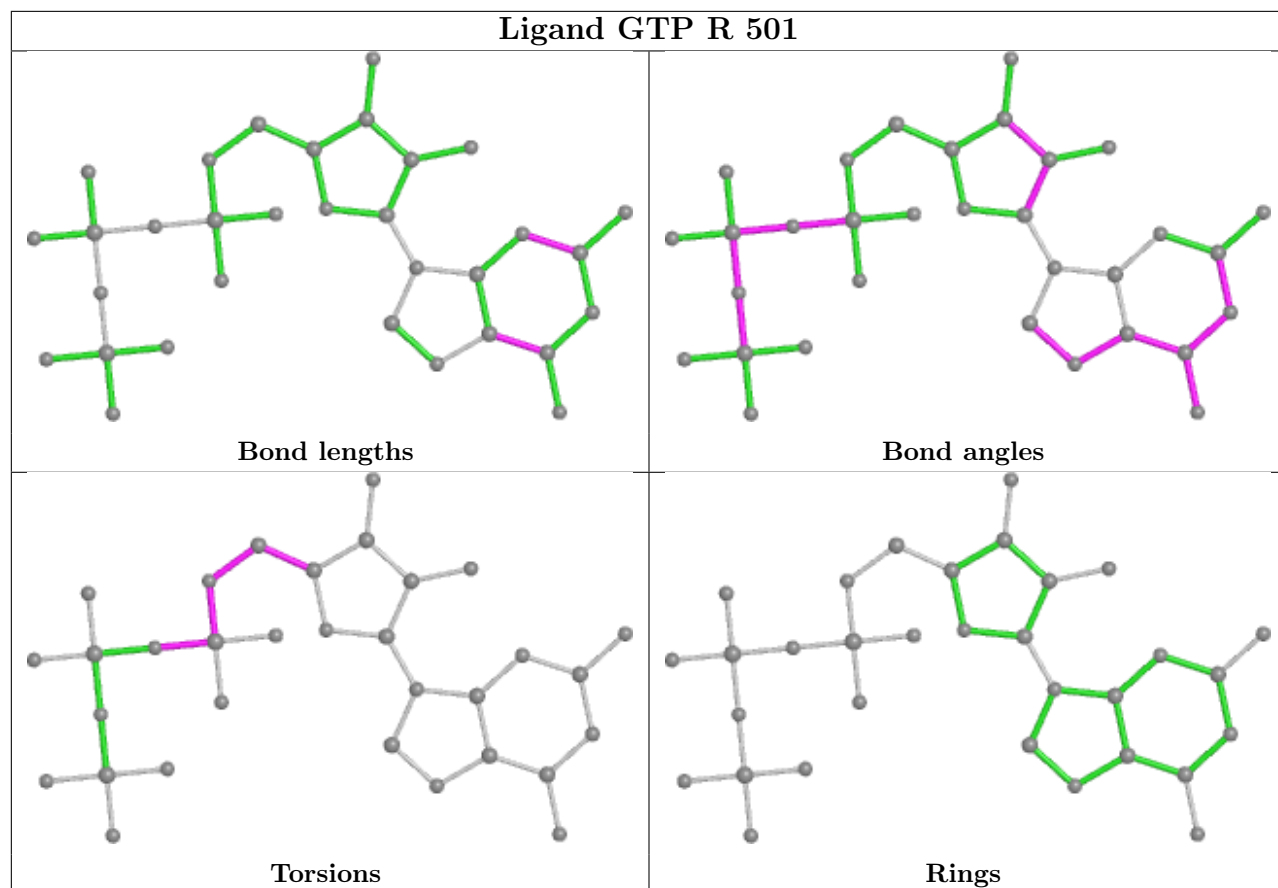


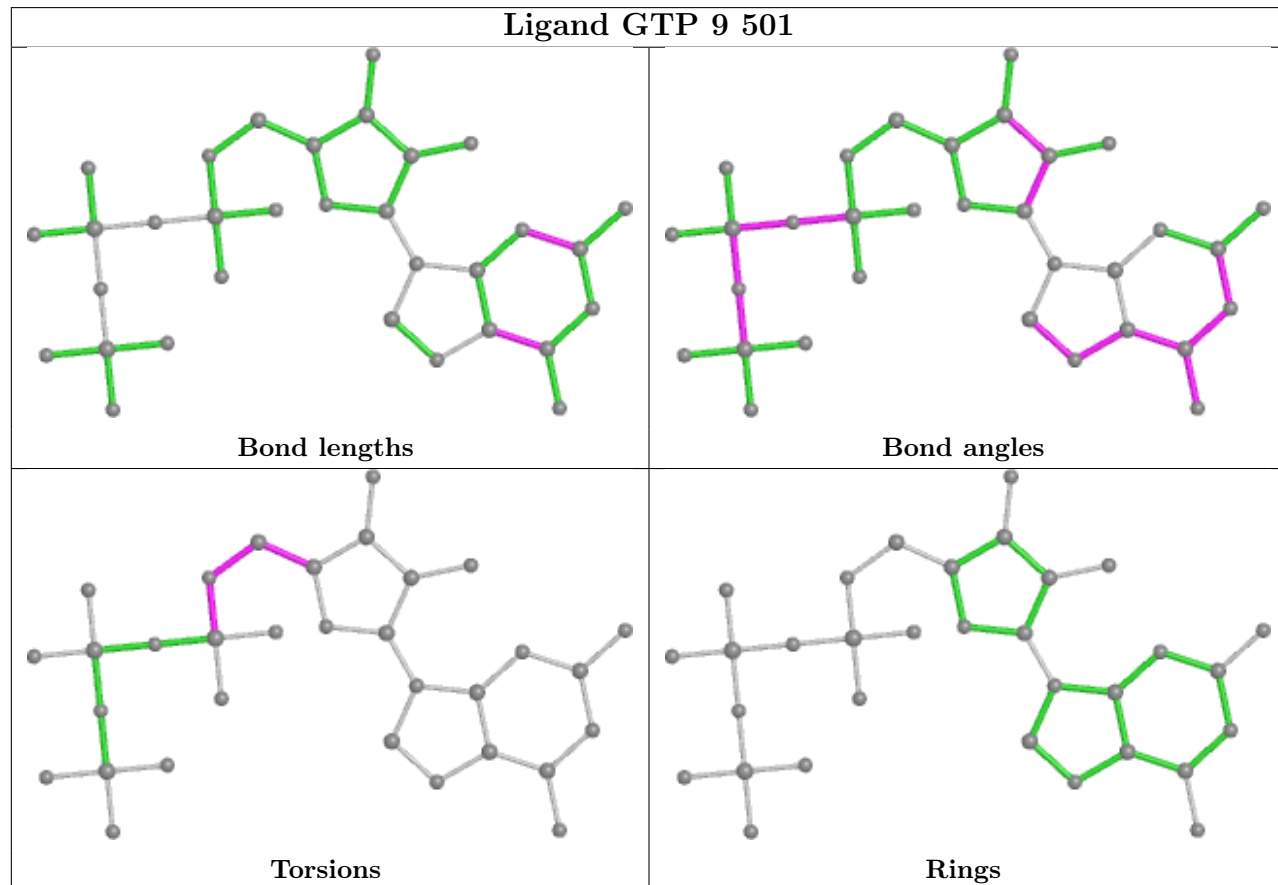
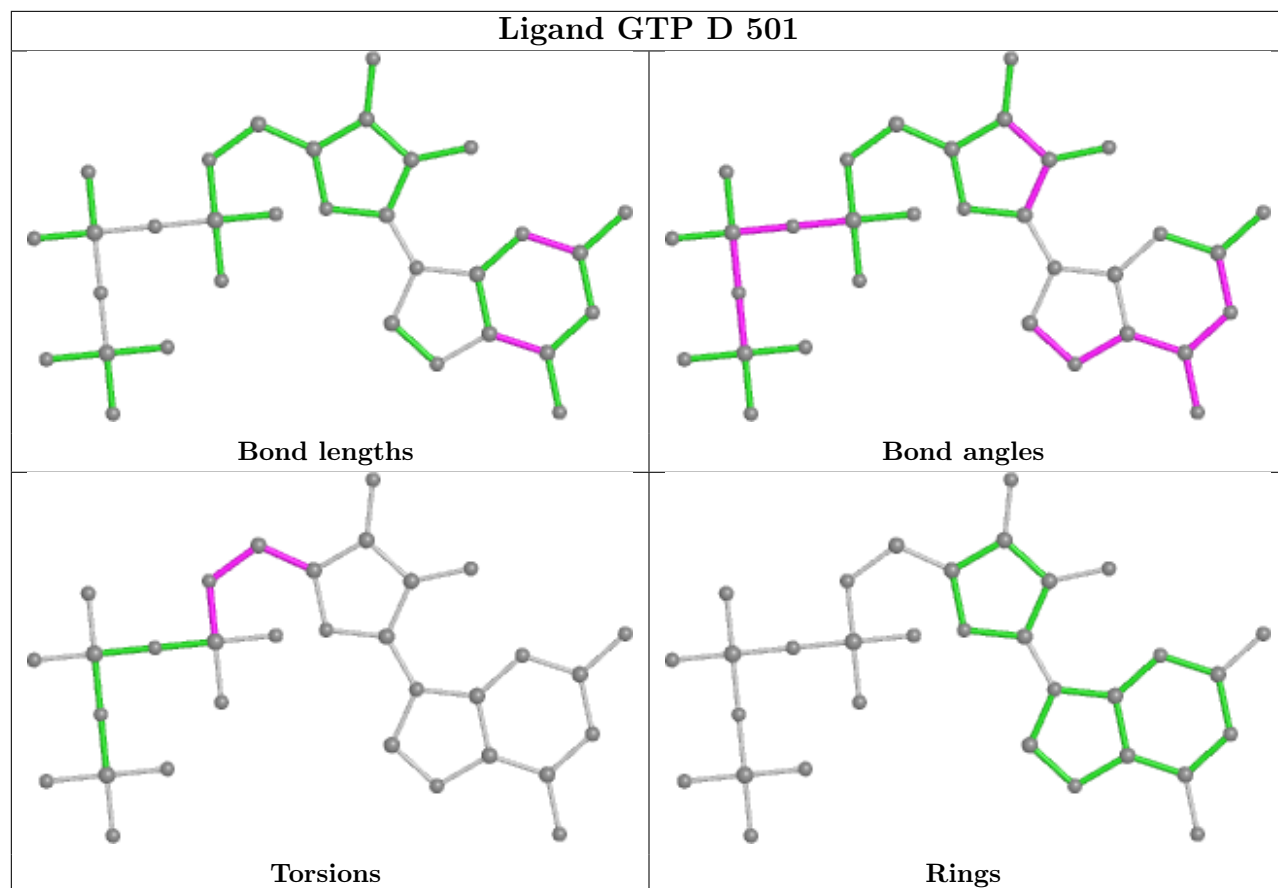


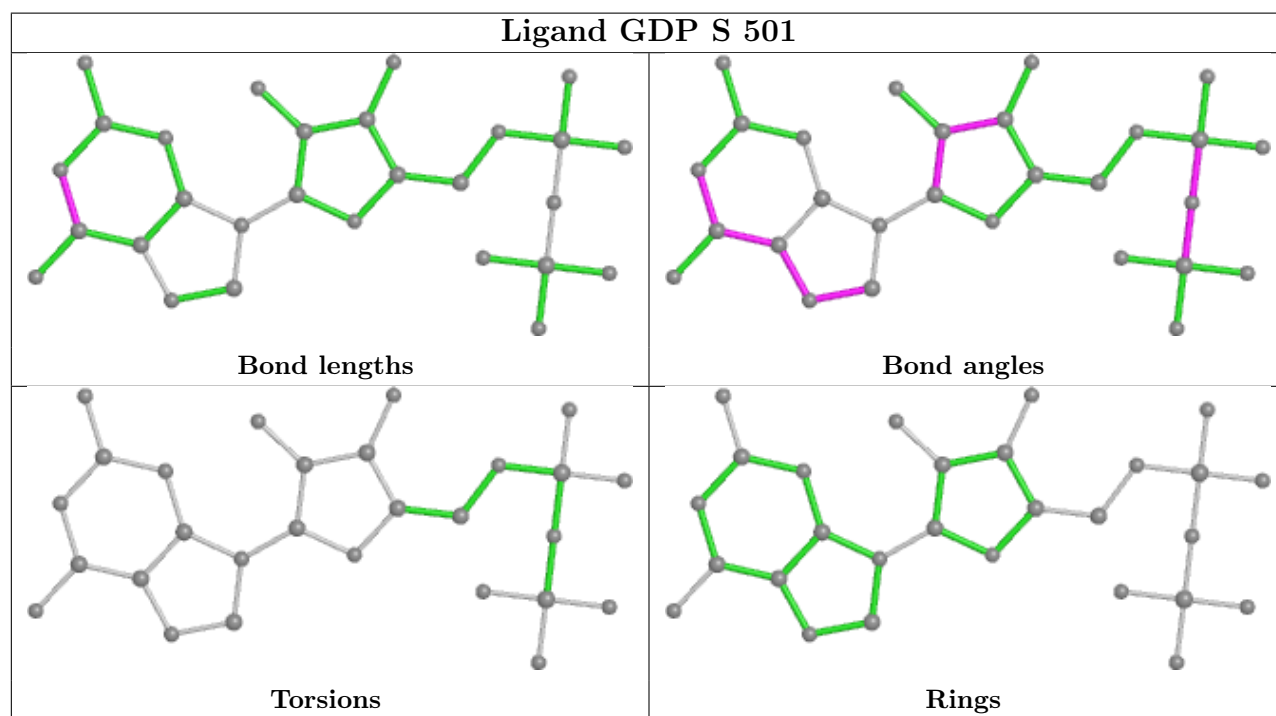
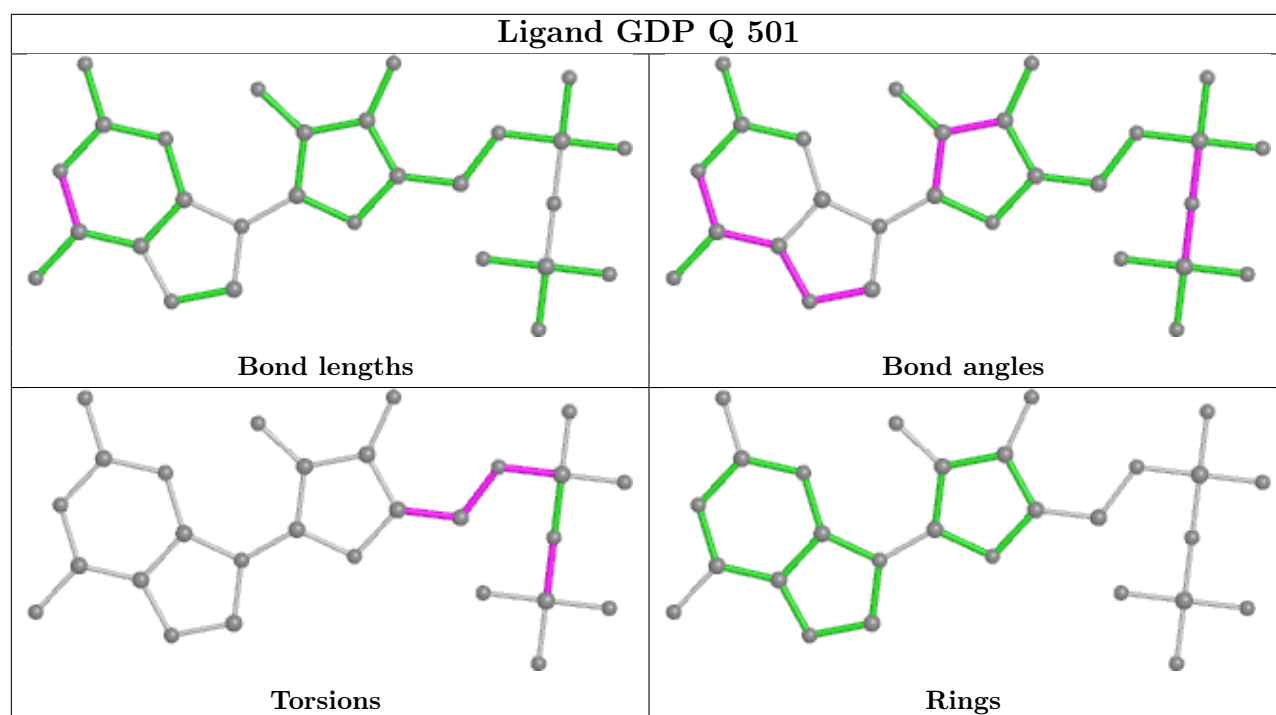


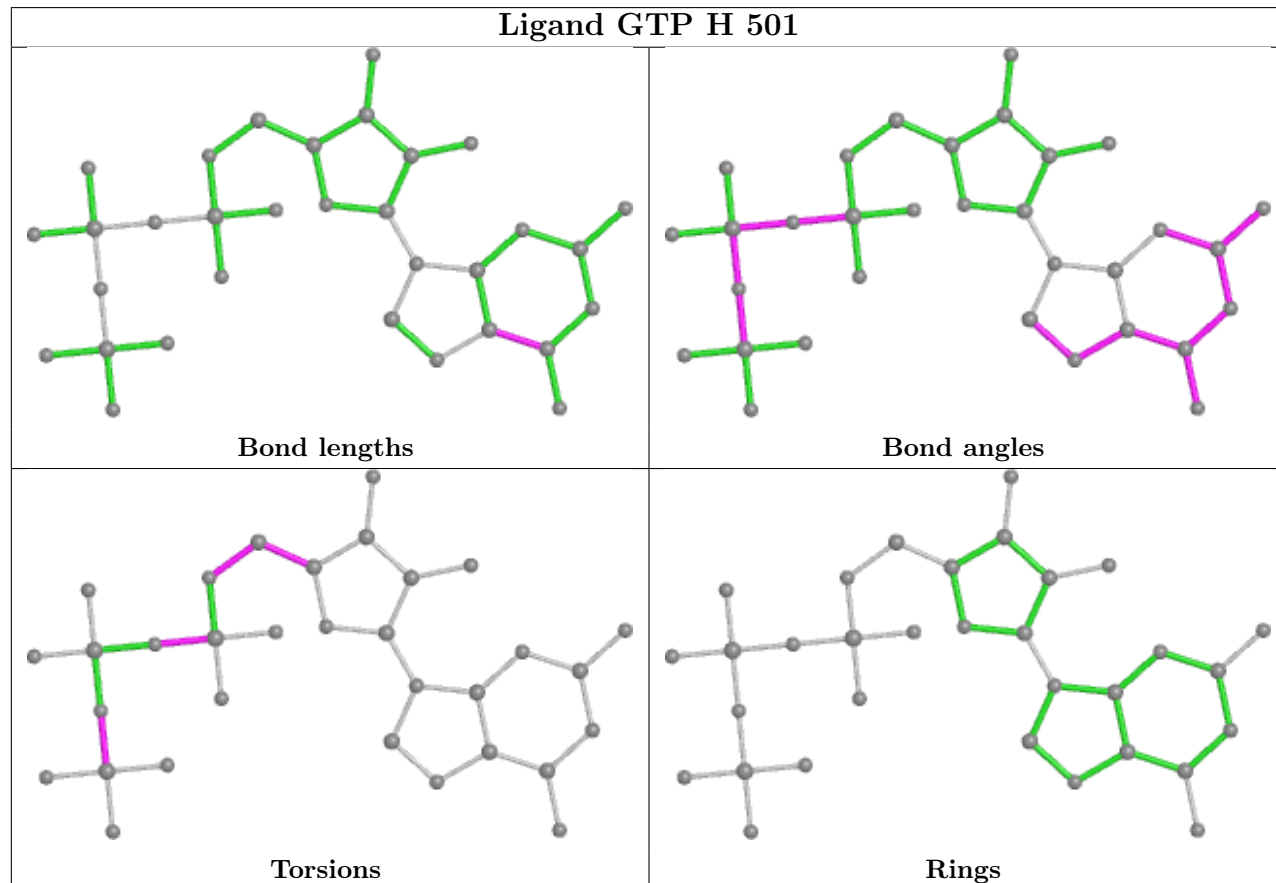
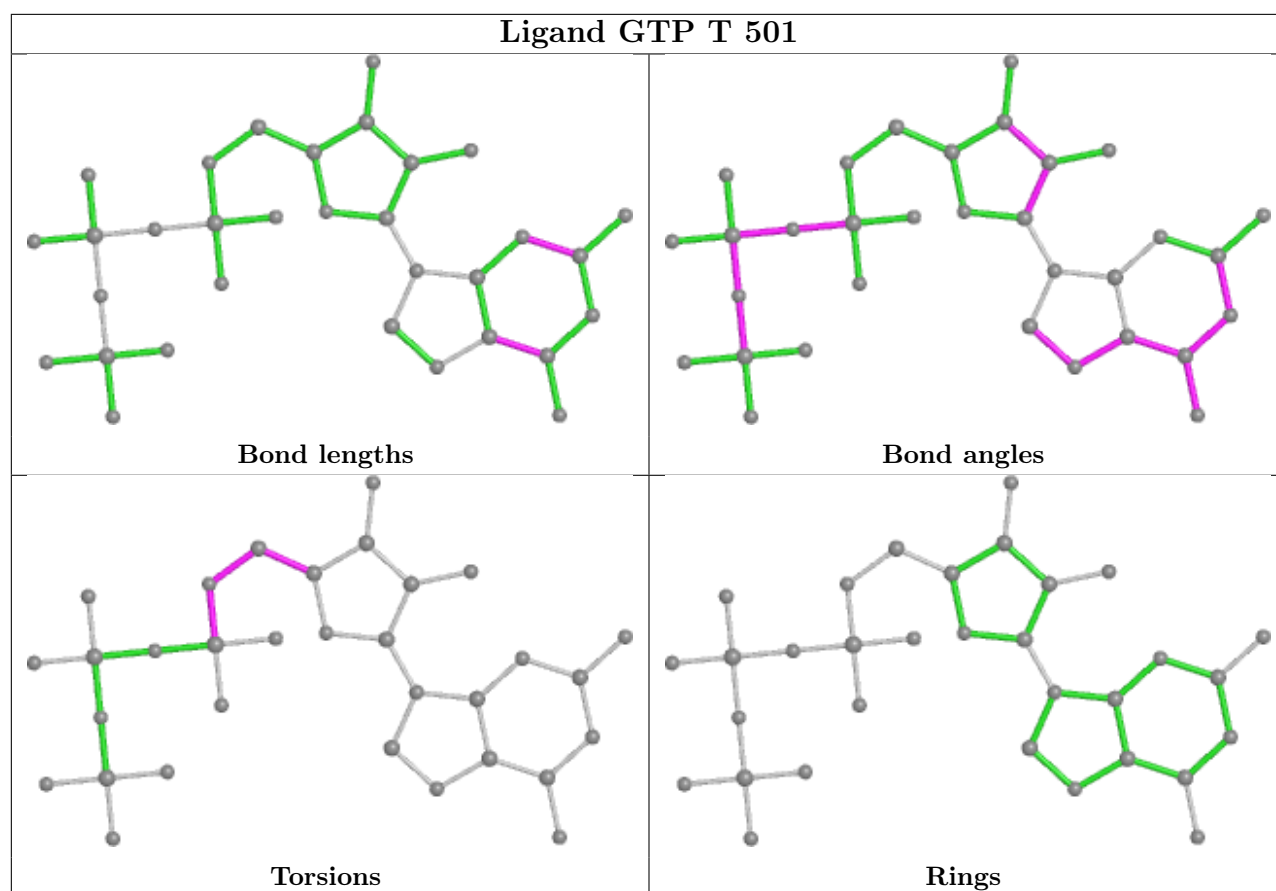


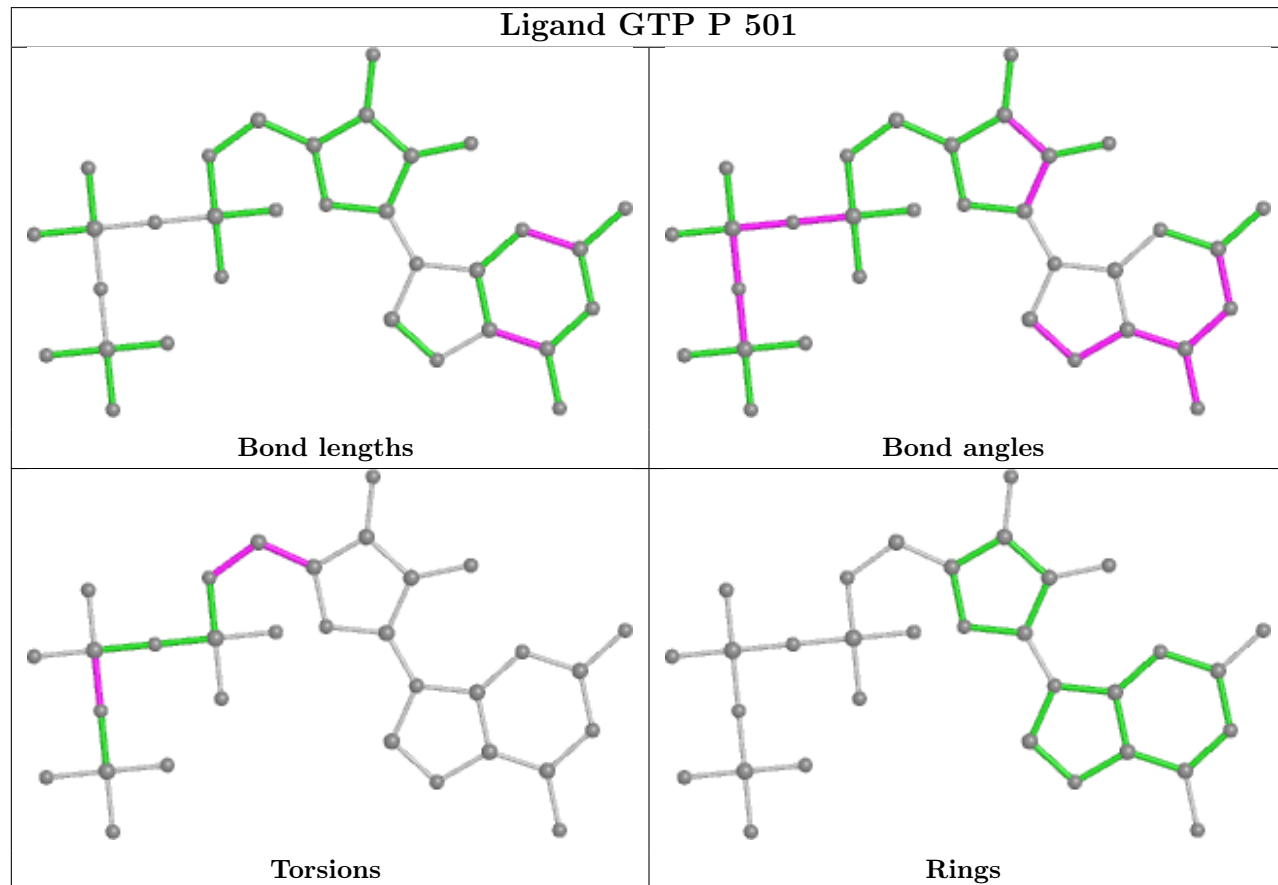
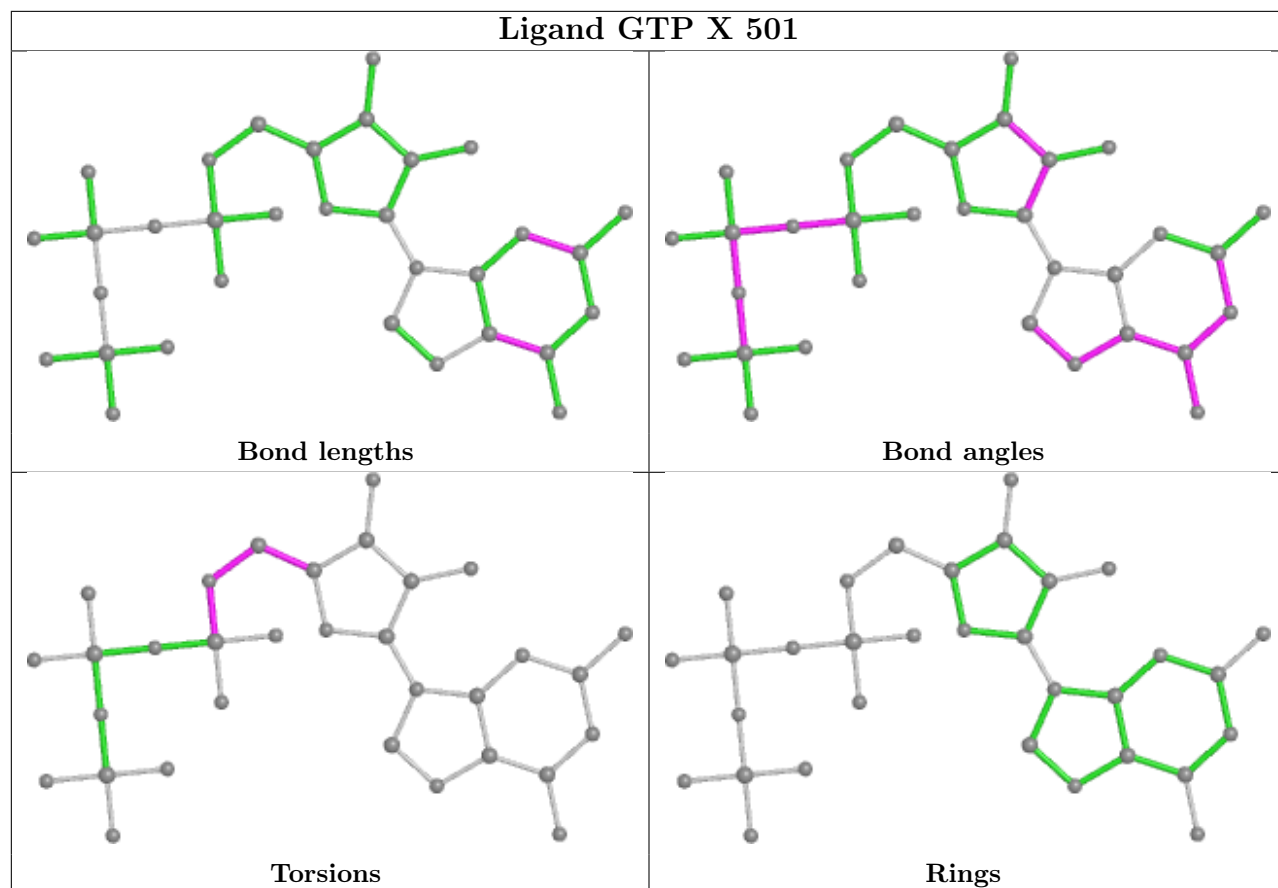


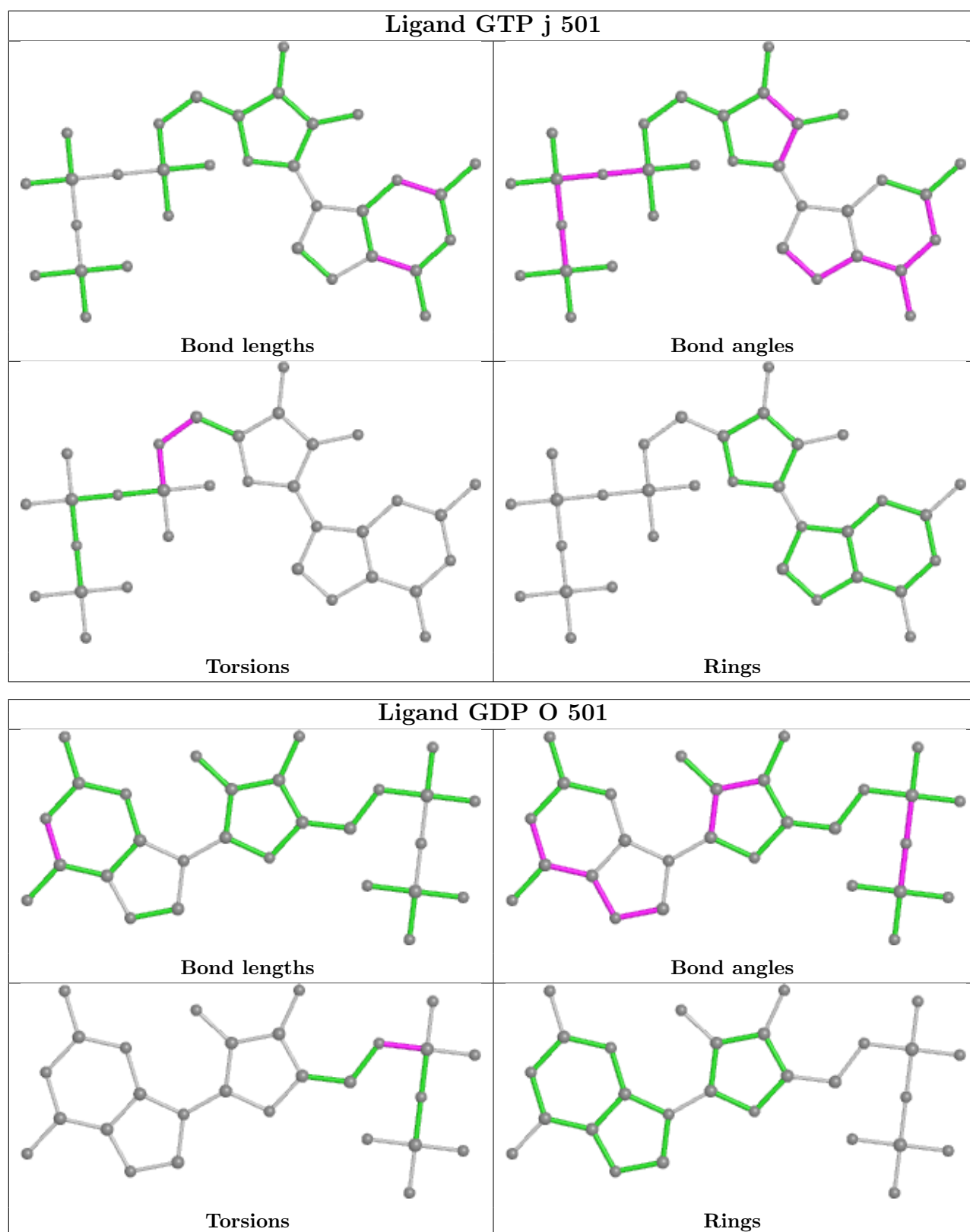












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22481. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.