



## Full wwPDB EM Validation Report ⓘ

Nov 17, 2024 – 01:00 am GMT

PDB ID : 9EOK  
EMDB ID : EMD-19862  
Title : Minus end of the vertebrate gamma-tubulin ring complex-capped microtubule  
Authors : Vermeulen, B.J.A.; Pfeffer, S.  
Deposited on : 2024-03-15  
Resolution : 23.00 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:

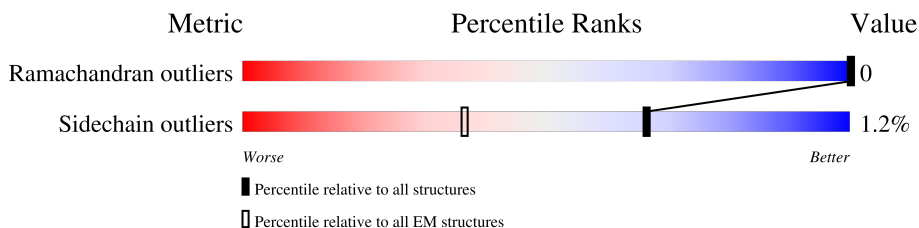
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 23.00 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	207382	16835
Sidechain outliers	206894	16415

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	450	58% 91% • •
1	C	450	24% 91% 5% •
1	D	450	20% 91% • •
1	E	450	40% 91% • •
1	G	450	17% 91% • •
1	H	450	18% 92% • •
1	I	450	15% 92% • •
1	J	450	10% 91% • •
1	K	450	14% 91% • •

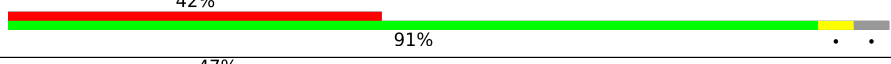
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Mol	Chain	Length	Quality of chain
1	L	450	20% 91%
1	M	450	16% 91%
1	N	450	14% 91%
1	O	450	6% 91%
1	P	450	12% 92%
1	c	450	22% 91%
1	d	450	19% 91%
1	e	450	18% 92%
1	f	450	21% 91%
1	g	450	22% 92%
1	h	450	16% 92%
1	i	450	34% 92%
1	j	450	38% 91%
1	k	450	62% 91%
2	B	445	36% 91%
2	F	445	72% 91%
2	Q	445	20% 91%
2	R	445	16% 91%
2	S	445	17% 91%
2	T	445	13% 91%
2	U	445	16% 91%
2	V	445	11% 91%
2	W	445	17% 91%
2	X	445	24% 91%
2	Y	445	22% 91%

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Mol	Chain	Length	Quality of chain
2	Z	445	
2	a	445	
2	b	445	
2	o	445	
2	p	445	
2	q	445	
2	r	445	
2	s	445	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 143457 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	430	3365	2127	574	641	23	0	0
1	C	430	3365	2127	574	641	23	0	0
1	D	430	3365	2127	574	641	23	0	0
1	E	430	3365	2127	574	641	23	0	0
1	G	430	3365	2127	574	641	23	0	0
1	H	430	3365	2127	574	641	23	0	0
1	I	430	3365	2127	574	641	23	0	0
1	J	430	3365	2127	574	641	23	0	0
1	K	430	3365	2127	574	641	23	0	0
1	L	430	3365	2127	574	641	23	0	0
1	M	430	3365	2127	574	641	23	0	0
1	N	430	3365	2127	574	641	23	0	0
1	O	430	3365	2127	574	641	23	0	0
1	P	430	3365	2127	574	641	23	0	0
1	c	430	3365	2127	574	641	23	0	0
1	d	430	3365	2127	574	641	23	0	0
1	e	430	3365	2127	574	641	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	g	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	h	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	i	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	j	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		
1	k	430	Total	C	N	O	S	0	0
			3365	2127	574	641	23		

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

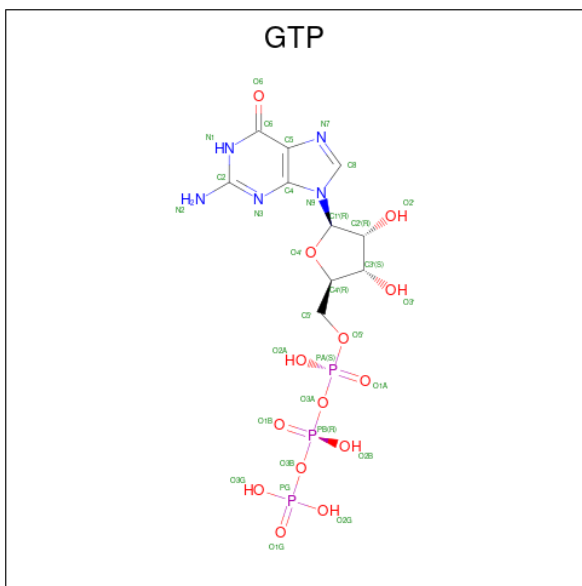
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	F	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	Q	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	R	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	S	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	T	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	U	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	V	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	W	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	X	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	Y	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	Z	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		
2	a	426	Total	C	N	O	S	0	0
			3347	2105	574	642	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	426	Total 3347	C 2105	N 574	O 642	S 26	0	0
2	o	426	Total 3347	C 2105	N 574	O 642	S 26	0	0
2	p	426	Total 3347	C 2105	N 574	O 642	S 26	0	0
2	q	426	Total 3347	C 2105	N 574	O 642	S 26	0	0
2	r	426	Total 3347	C 2105	N 574	O 642	S 26	0	0
2	s	426	Total 3347	C 2105	N 574	O 642	S 26	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total 32	C 10	N 5	O 14	P 3	0
3	C	1	Total 32	C 10	N 5	O 14	P 3	0
3	D	1	Total 32	C 10	N 5	O 14	P 3	0
3	E	1	Total 32	C 10	N 5	O 14	P 3	0
3	G	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
3	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	N	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	O	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	P	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	c	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	d	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	e	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	f	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	g	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	h	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	i	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	j	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	k	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

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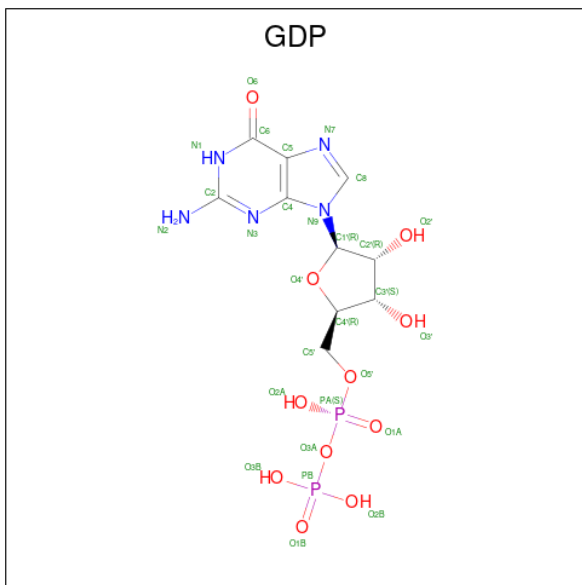
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	C	1	1	1	0
4	D	1	1	1	0
4	E	1	1	1	0
4	G	1	1	1	0
4	H	1	1	1	0
4	I	1	1	1	0
4	J	1	1	1	0
4	K	1	1	1	0
4	L	1	1	1	0
4	M	1	1	1	0
4	N	1	1	1	0
4	O	1	1	1	0
4	P	1	1	1	0
4	c	1	1	1	0
4	d	1	1	1	0
4	e	1	1	1	0
4	f	1	1	1	0
4	g	1	1	1	0
4	h	1	1	1	0
4	i	1	1	1	0
4	j	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
4	k	1	Total	Mg	0
			1	1	

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



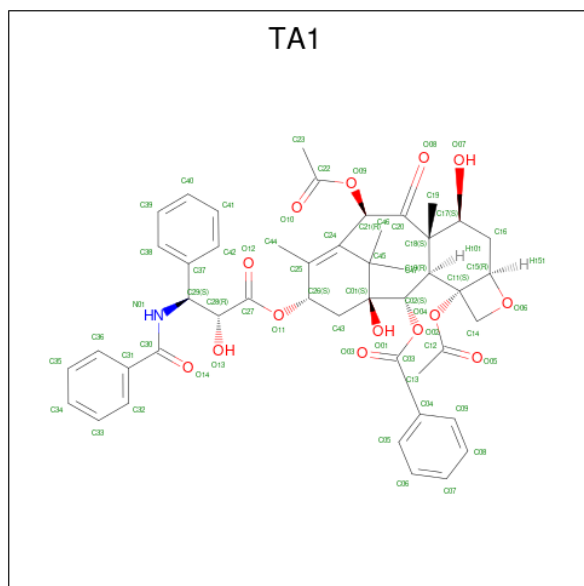
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	F	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	R	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	S	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	T	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	U	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	V	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	W	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	X	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
5	Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	Z	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	a	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	o	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	p	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	q	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	r	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	s	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 6 is TAXOL (three-letter code: TA1) (formula:  $C_{47}H_{51}NO_{14}$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	Total	C	N	O	0
			62	47	1	14	
6	F	1	Total	C	N	O	0
			62	47	1	14	

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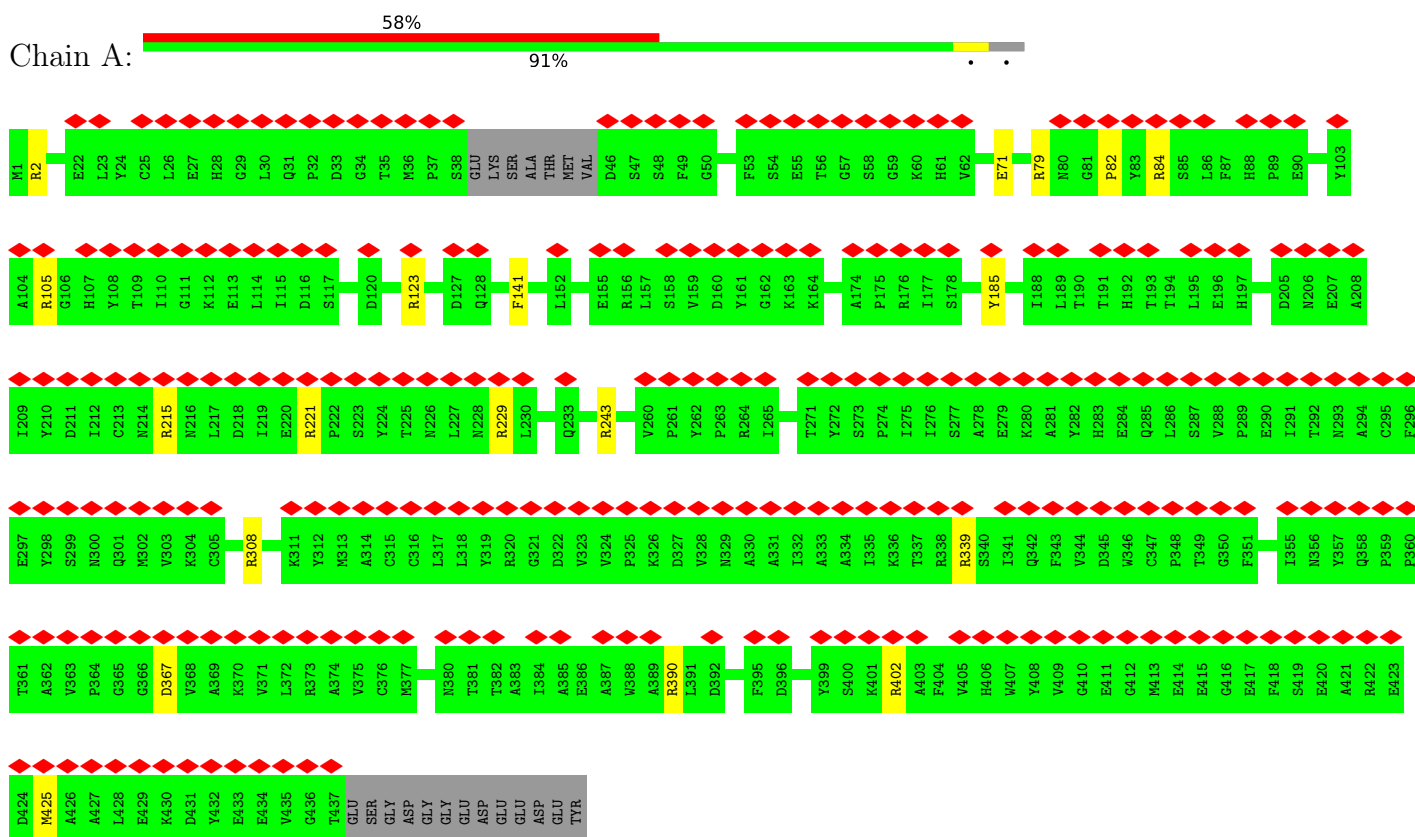
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	Q	1	Total 62	C 47	N 1	O 14	0
6	R	1	Total 62	C 47	N 1	O 14	0
6	S	1	Total 62	C 47	N 1	O 14	0
6	T	1	Total 62	C 47	N 1	O 14	0
6	U	1	Total 62	C 47	N 1	O 14	0
6	V	1	Total 62	C 47	N 1	O 14	0
6	W	1	Total 62	C 47	N 1	O 14	0
6	X	1	Total 62	C 47	N 1	O 14	0
6	Y	1	Total 62	C 47	N 1	O 14	0
6	Z	1	Total 62	C 47	N 1	O 14	0
6	a	1	Total 62	C 47	N 1	O 14	0
6	b	1	Total 62	C 47	N 1	O 14	0
6	o	1	Total 62	C 47	N 1	O 14	0
6	p	1	Total 62	C 47	N 1	O 14	0
6	q	1	Total 62	C 47	N 1	O 14	0
6	r	1	Total 62	C 47	N 1	O 14	0
6	s	1	Total 62	C 47	N 1	O 14	0

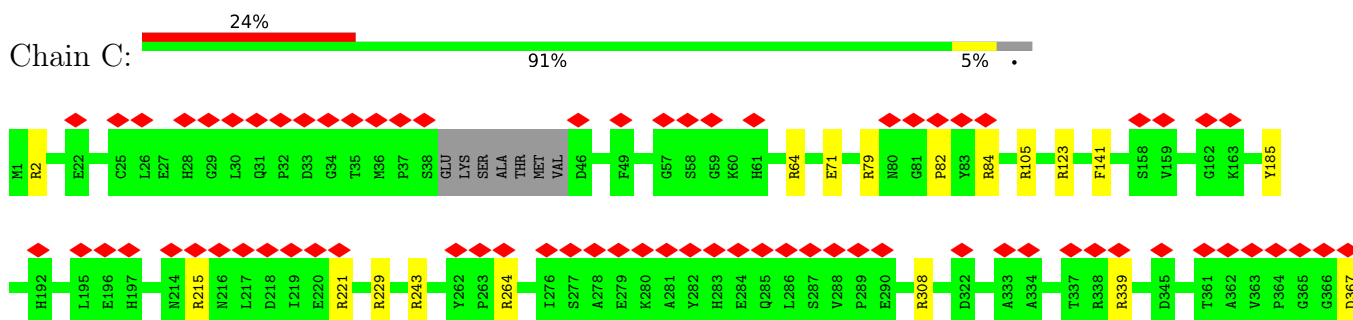
### 3 Residue-property plots [i](#)

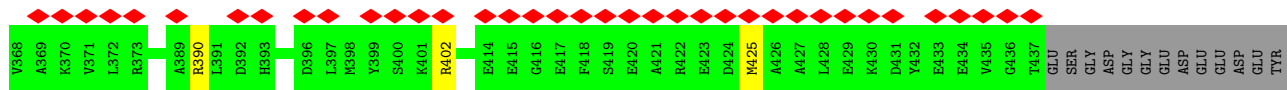
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Tubulin alpha chain

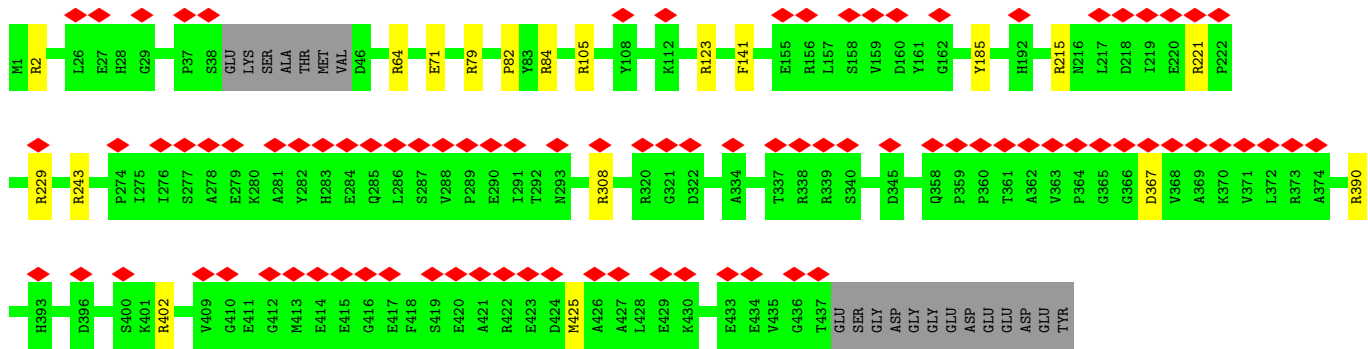
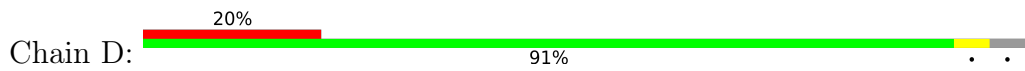


- Molecule 1: Tubulin alpha chain

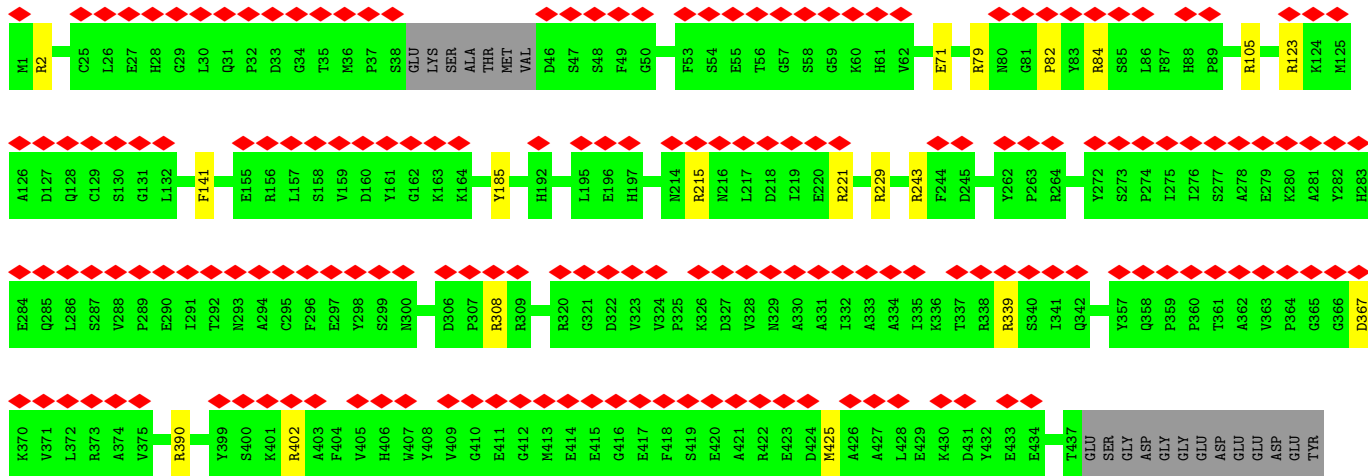
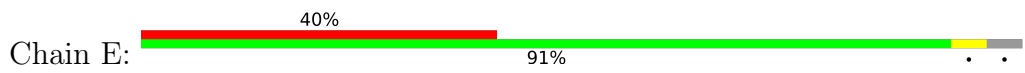




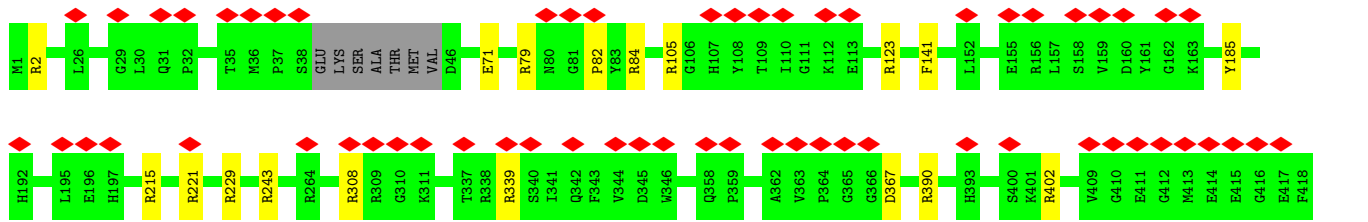
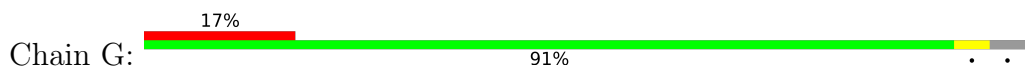
• Molecule 1: Tubulin alpha chain

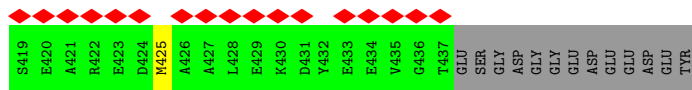


• Molecule 1: Tubulin alpha chain

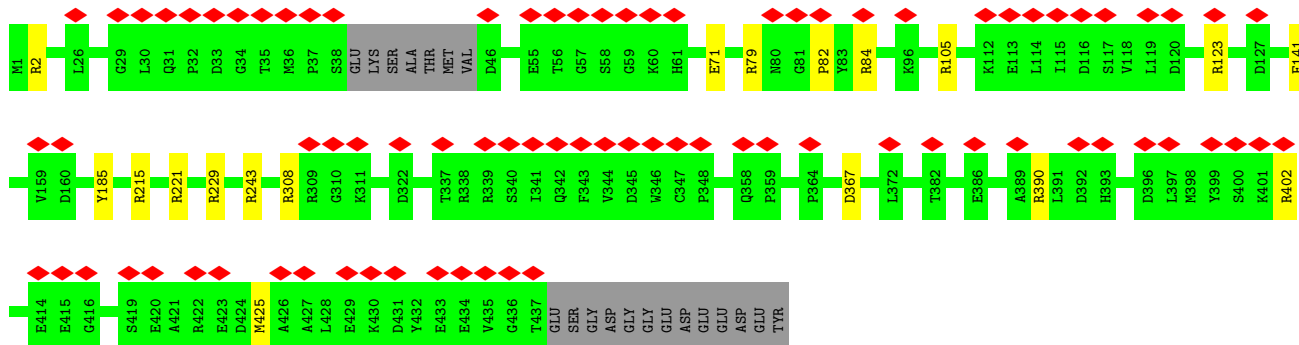
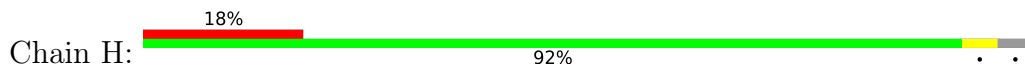


• Molecule 1: Tubulin alpha chain

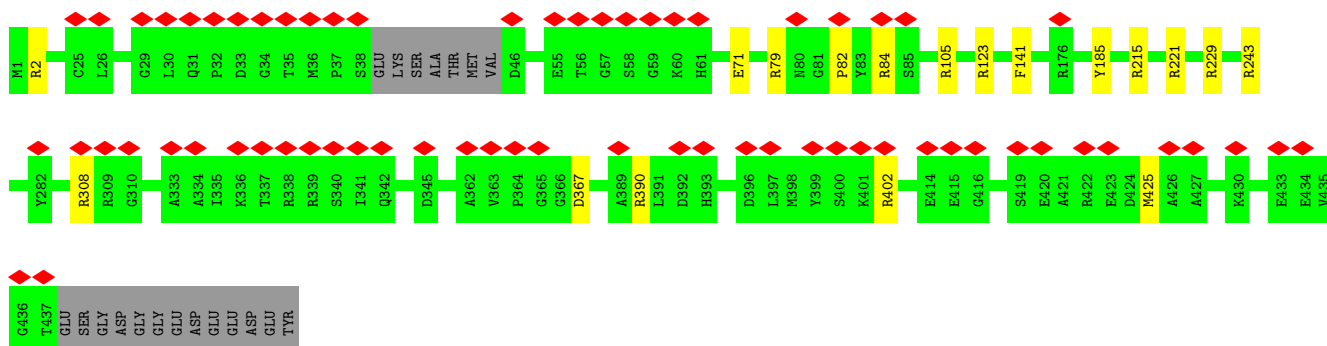
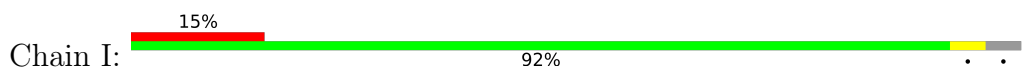




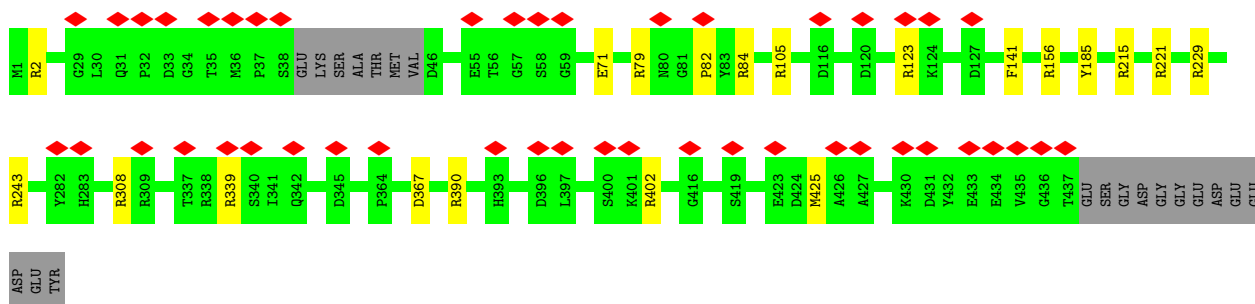
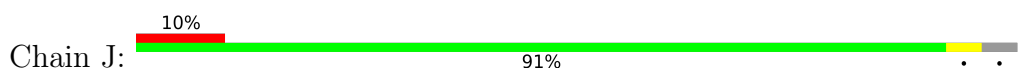
• Molecule 1: Tubulin alpha chain



• Molecule 1: Tubulin alpha chain

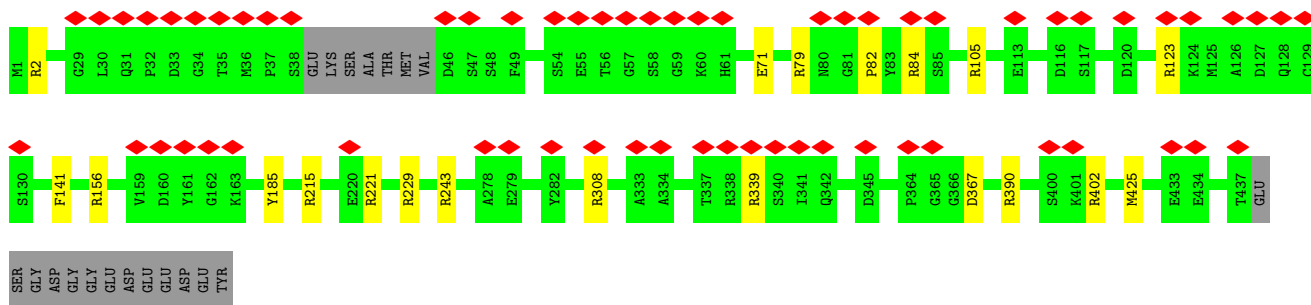


• Molecule 1: Tubulin alpha chain

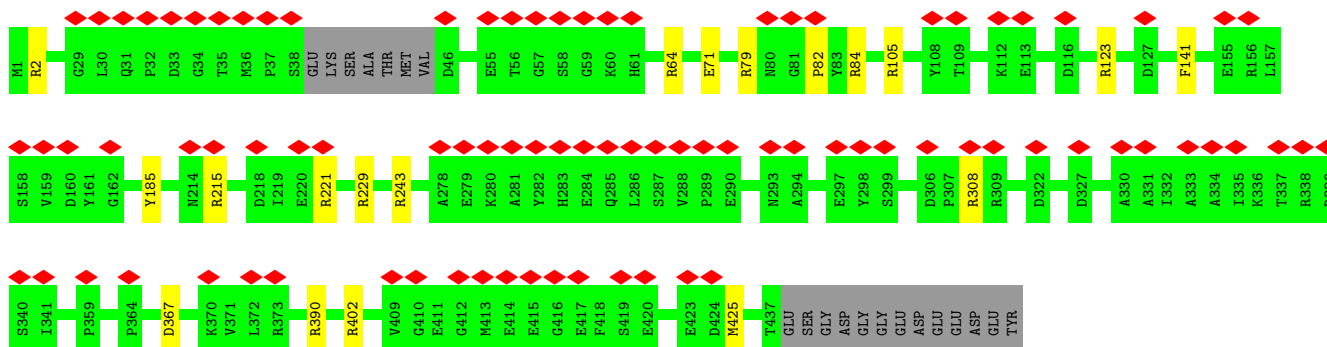
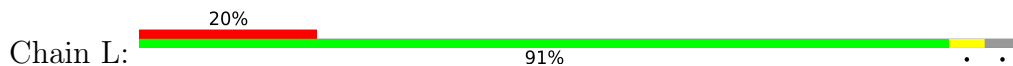


• Molecule 1: Tubulin alpha chain

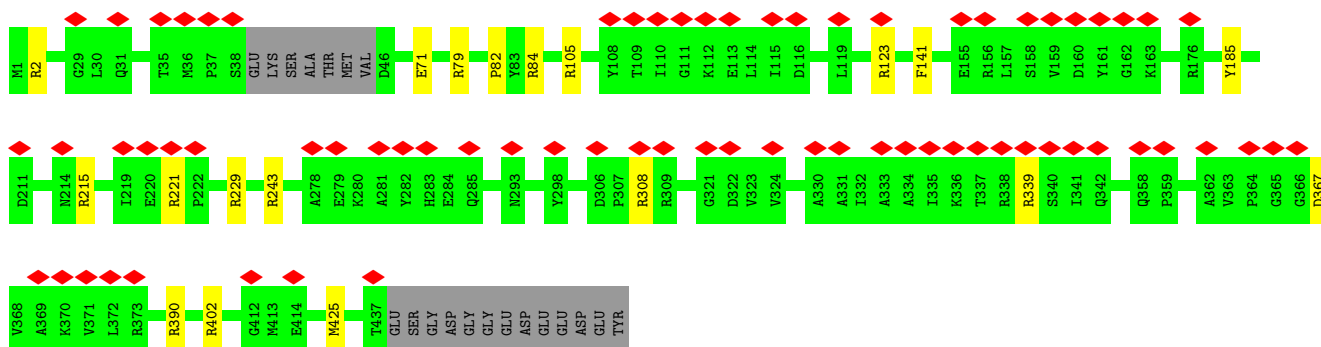




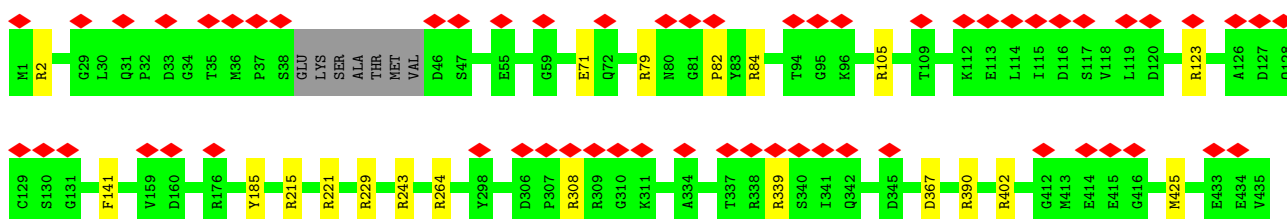
• Molecule 1: Tubulin alpha chain



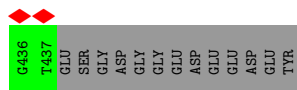
• Molecule 1: Tubulin alpha chain



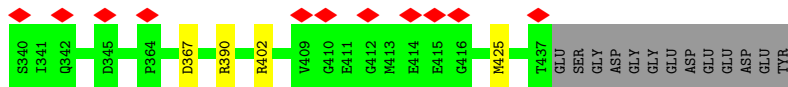
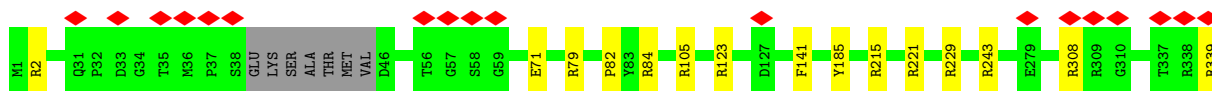
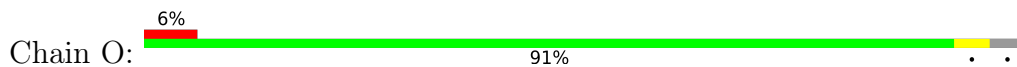
• Molecule 1: Tubulin alpha chain



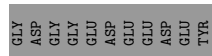
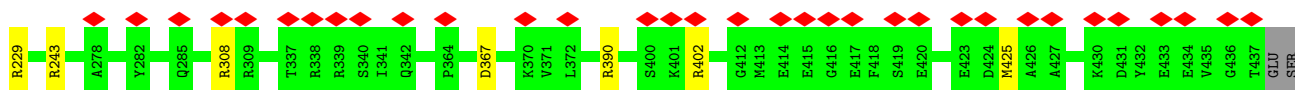
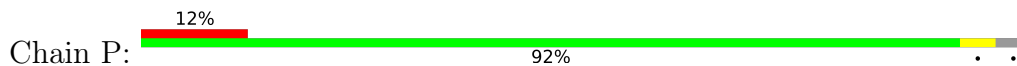




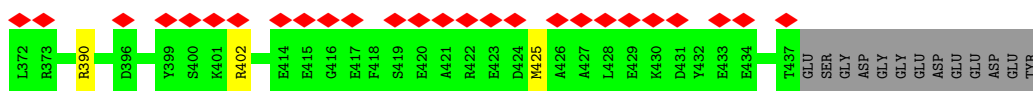
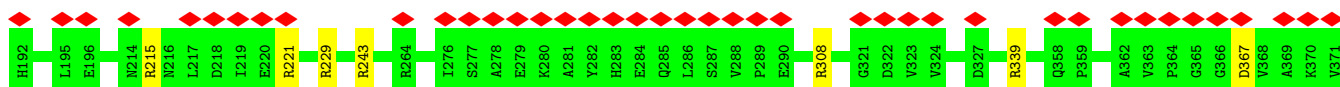
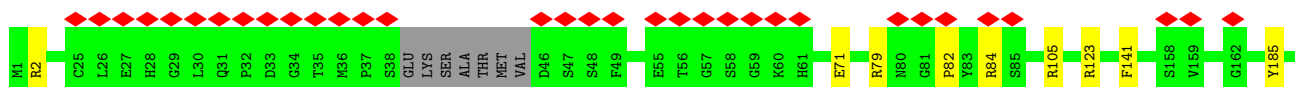
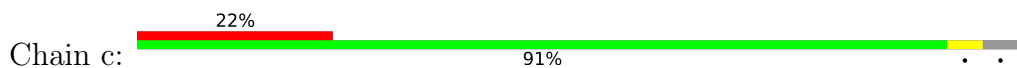
• Molecule 1: Tubulin alpha chain



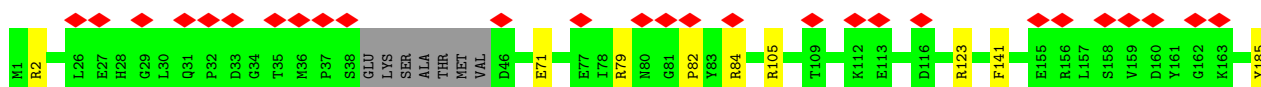
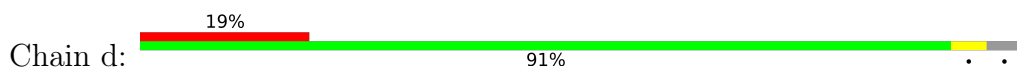
• Molecule 1: Tubulin alpha chain

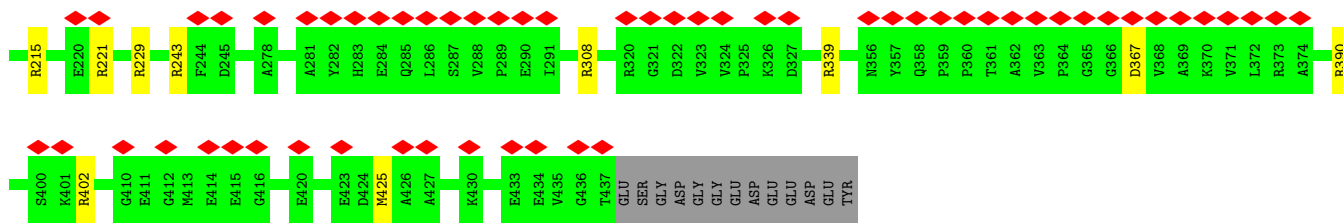


• Molecule 1: Tubulin alpha chain

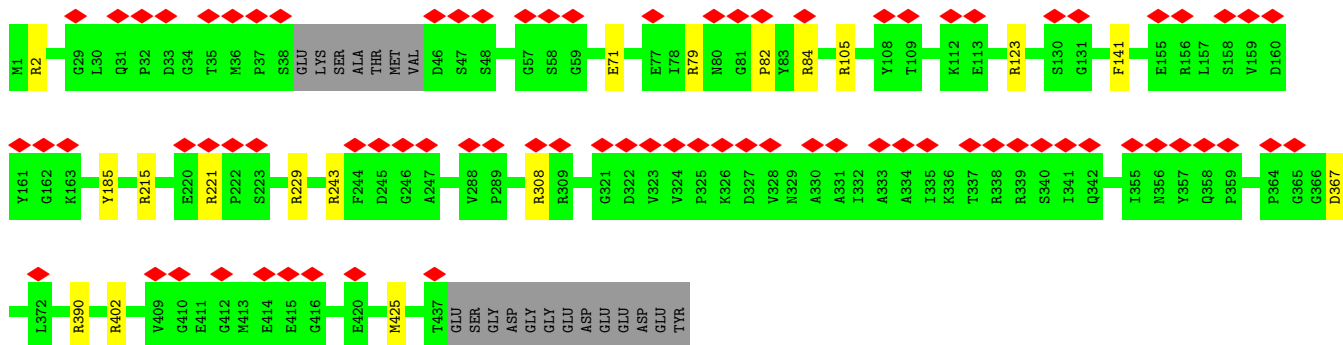
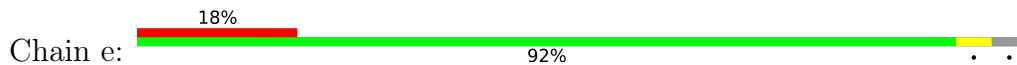


• Molecule 1: Tubulin alpha chain

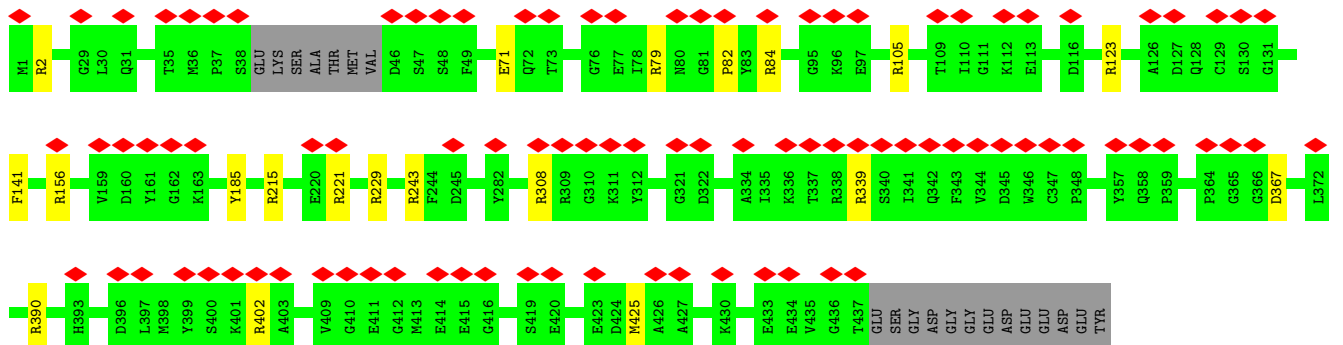
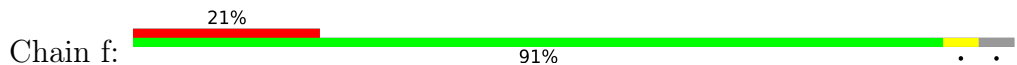




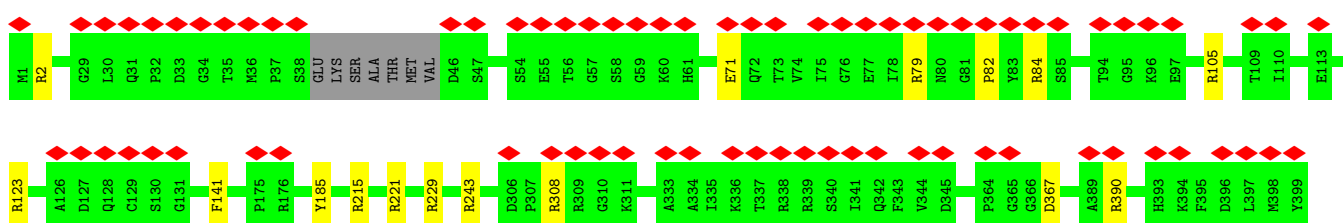
• Molecule 1: Tubulin alpha chain

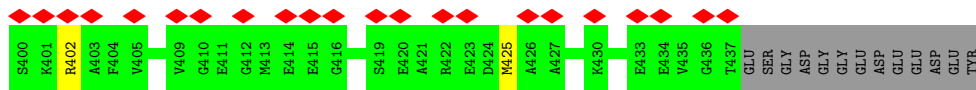


• Molecule 1: Tubulin alpha chain

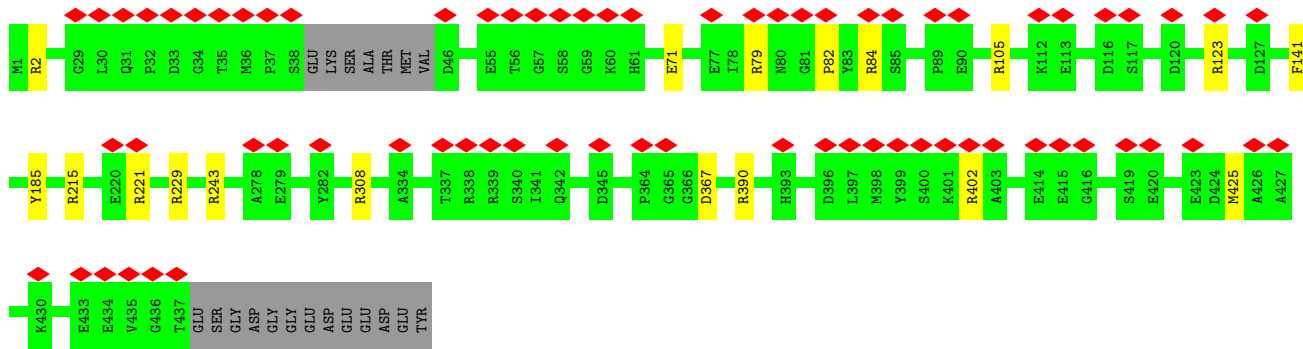
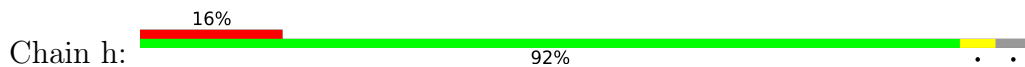


• Molecule 1: Tubulin alpha chain

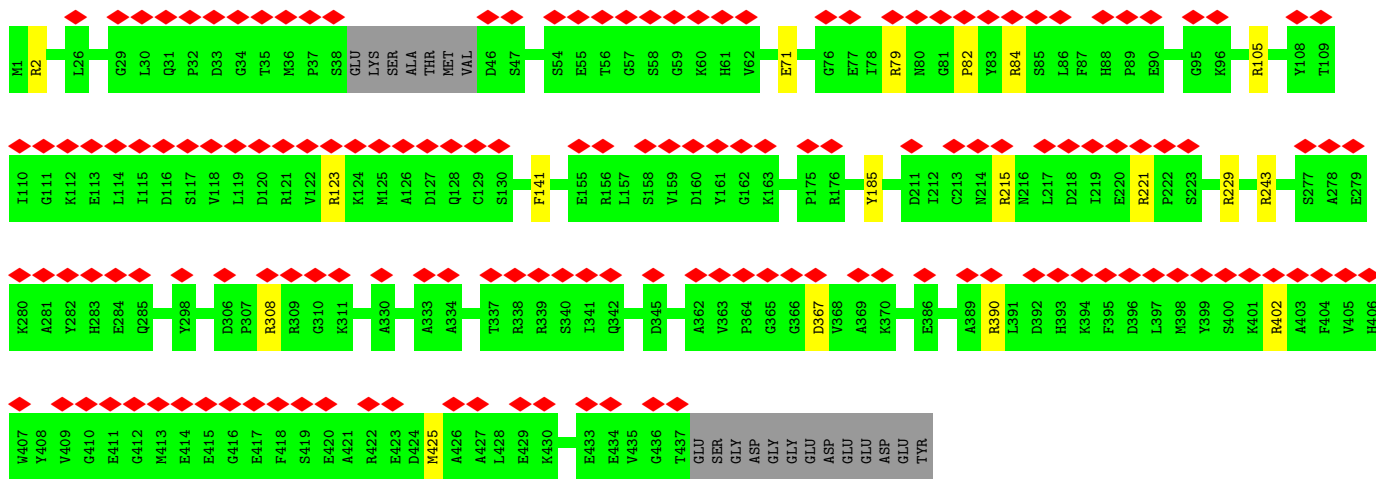
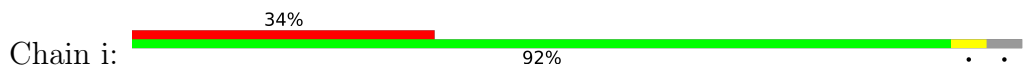




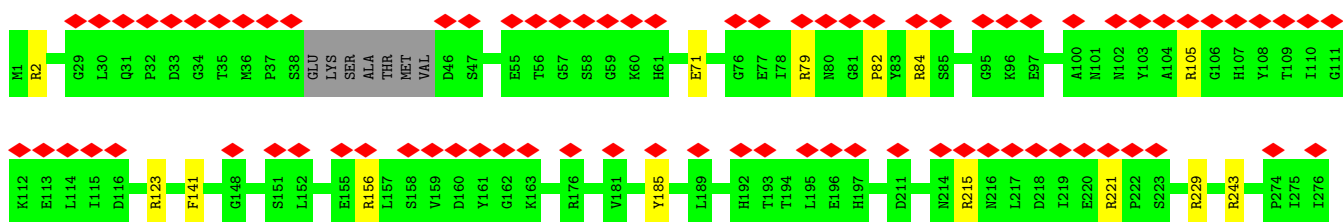
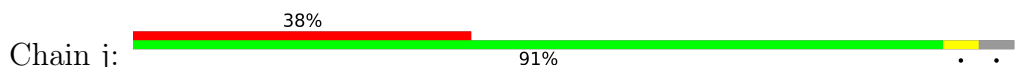
• Molecule 1: Tubulin alpha chain

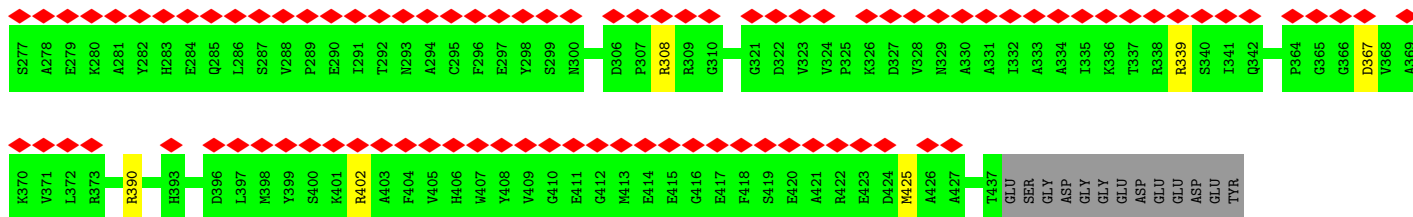


• Molecule 1: Tubulin alpha chain

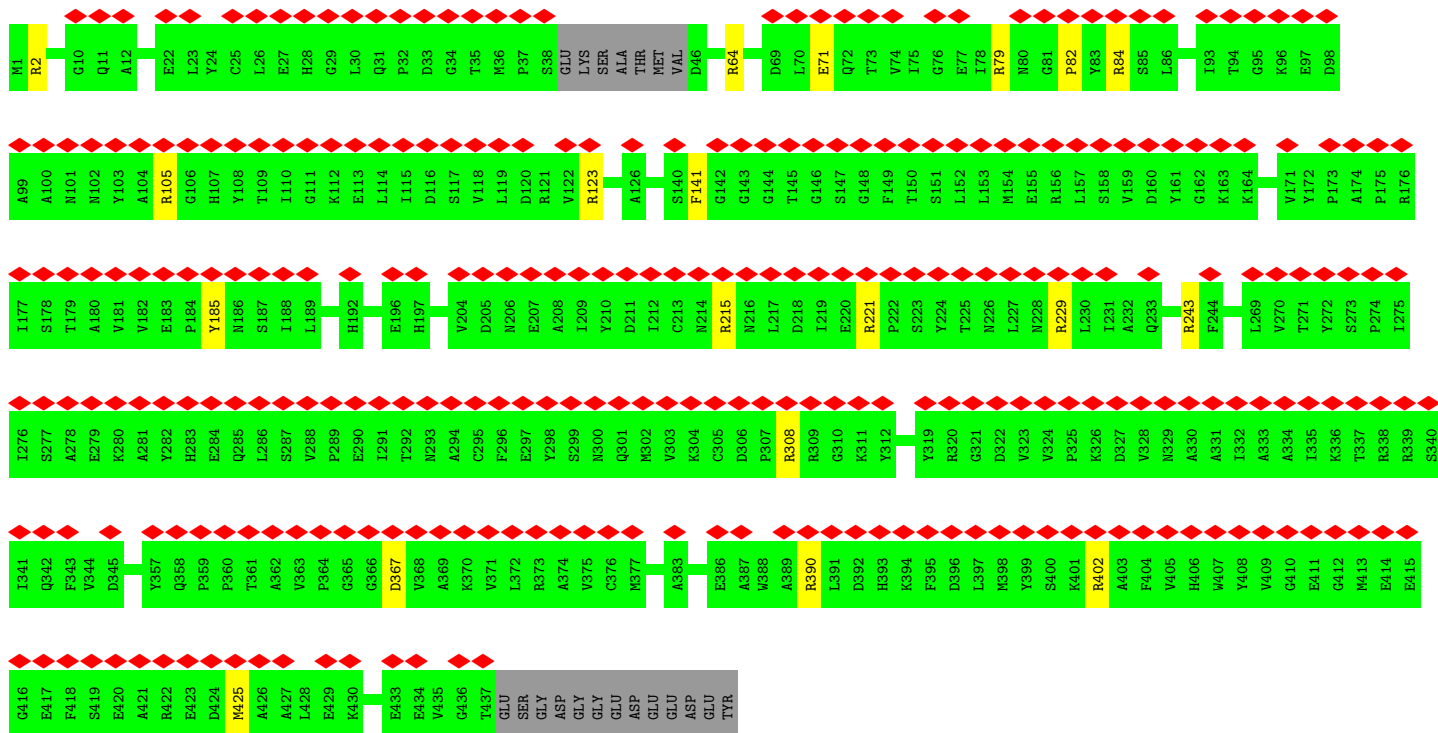
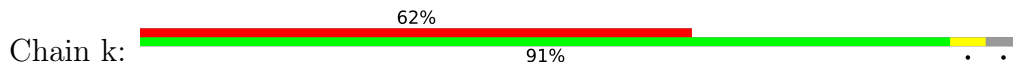


• Molecule 1: Tubulin alpha chain

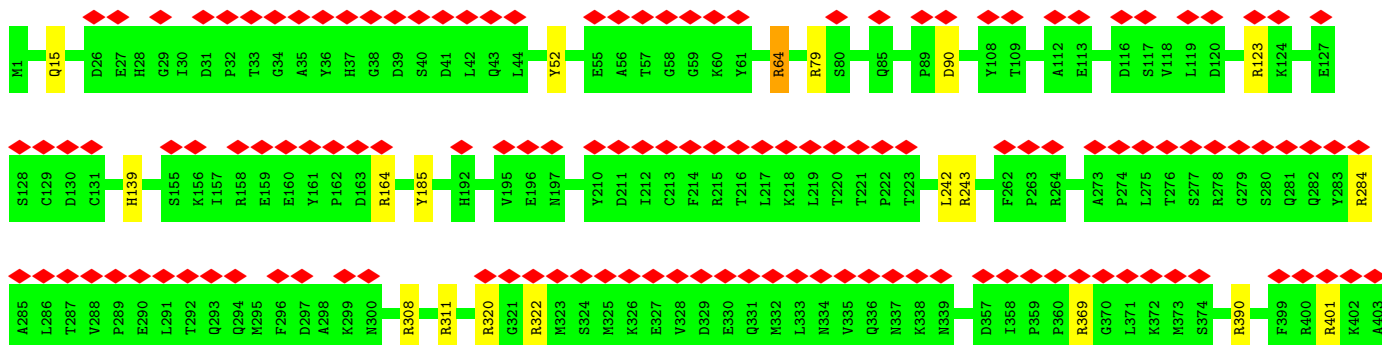
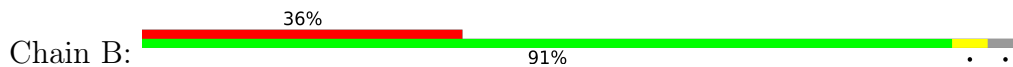


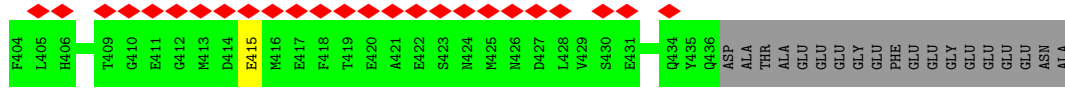


• Molecule 1: Tubulin alpha chain



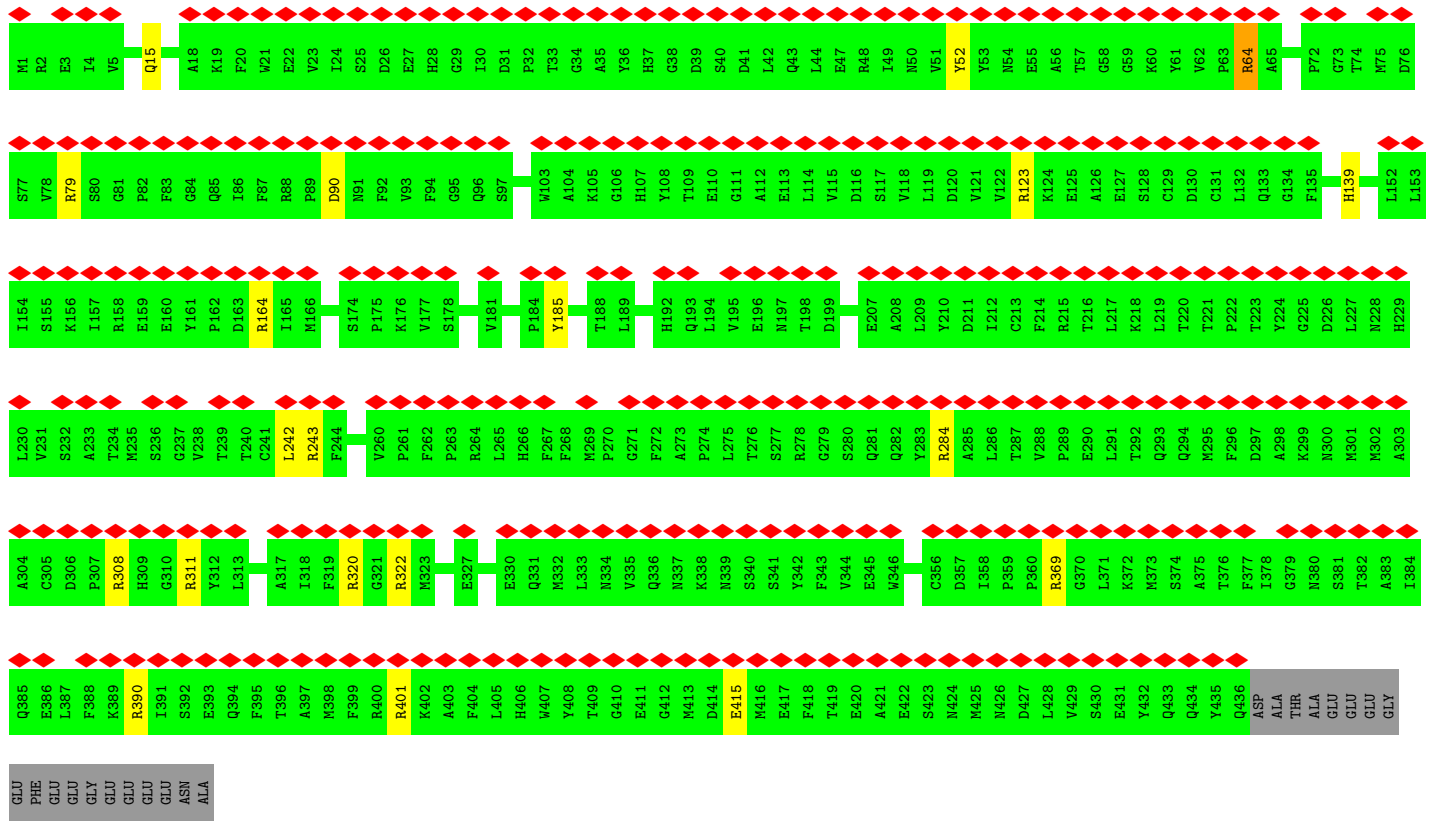
• Molecule 2: Tubulin beta-4 chain





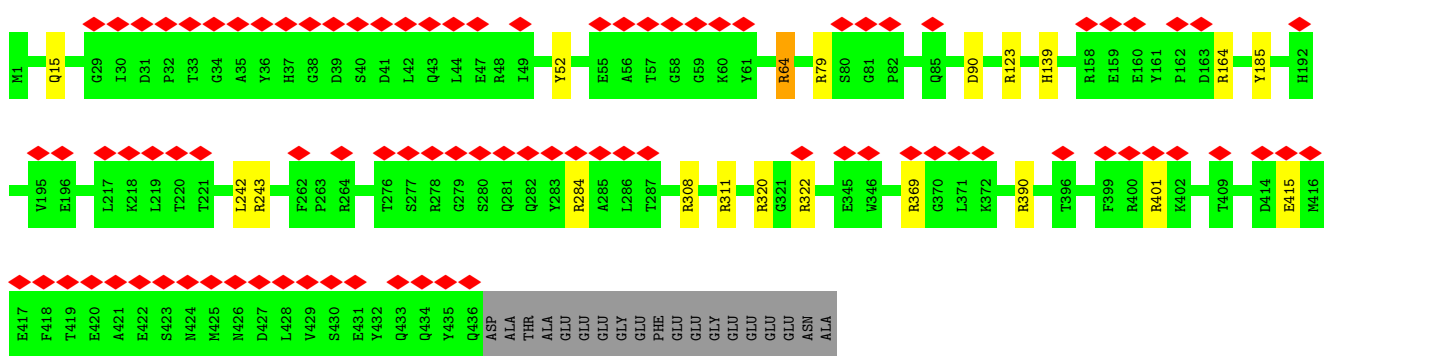
• Molecule 2: Tubulin beta-4 chain

Chain F:



• Molecule 2: Tubulin beta-4 chain

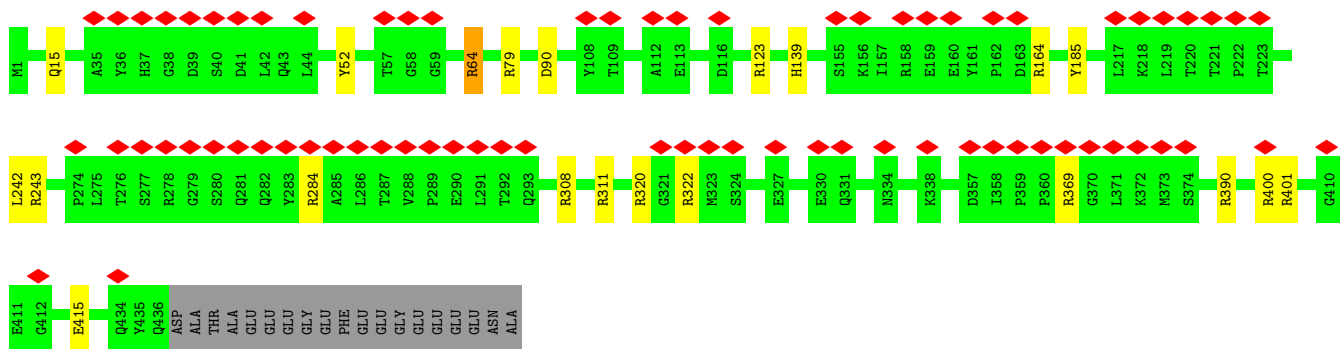
Chain Q:



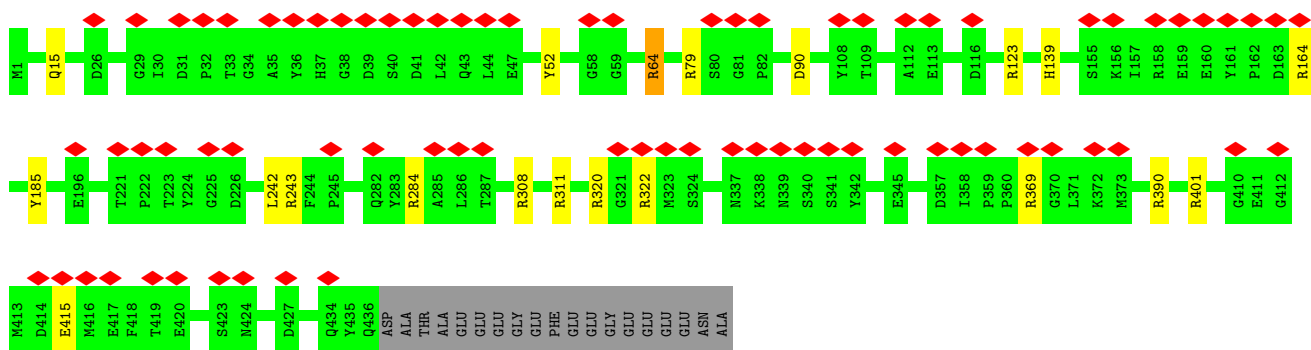
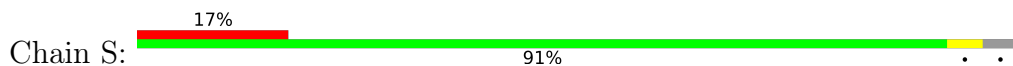
• Molecule 2: Tubulin beta-4 chain

Chain R:

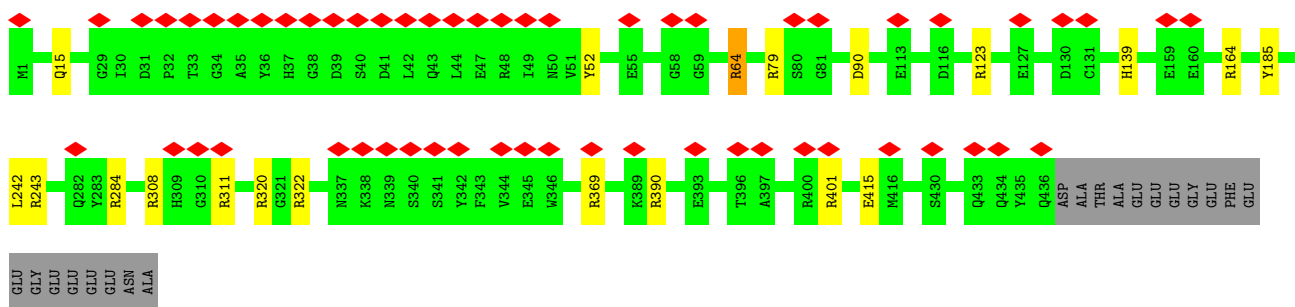
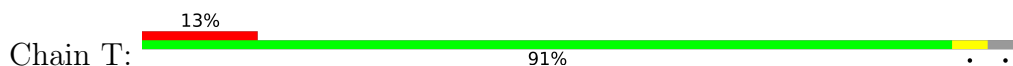




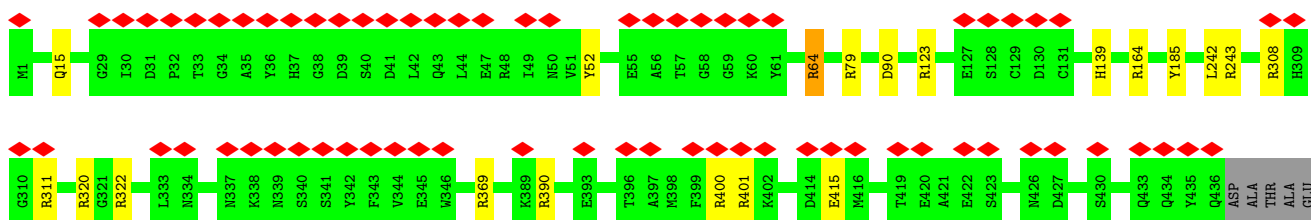
• Molecule 2: Tubulin beta-4 chain



• Molecule 2: Tubulin beta-4 chain

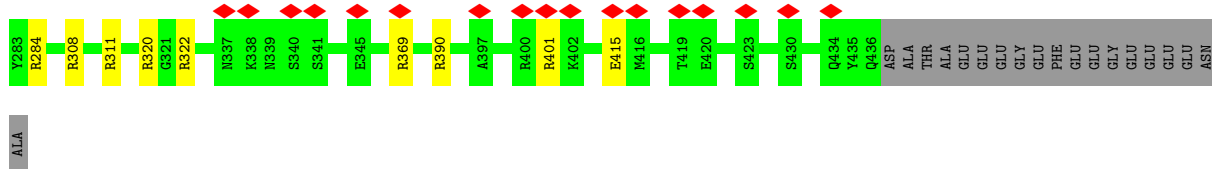
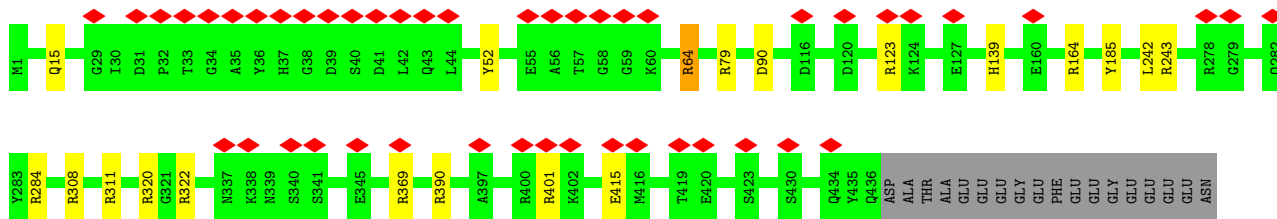
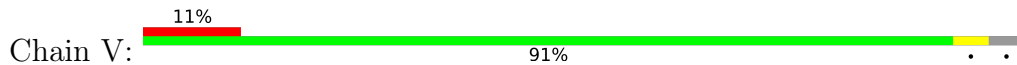


• Molecule 2: Tubulin beta-4 chain



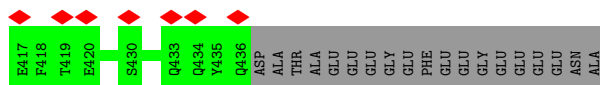
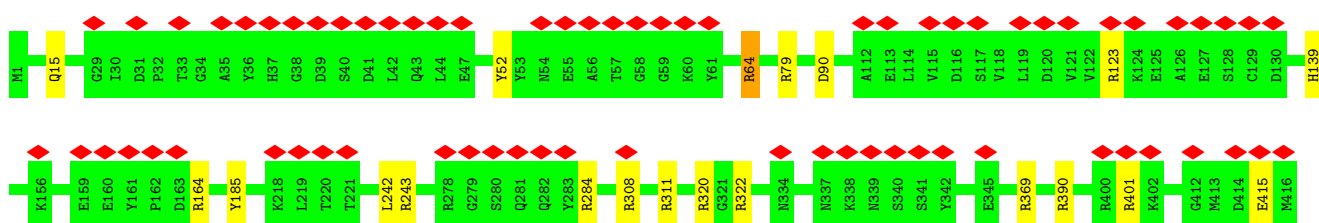
GLU  
GLU  
GLY  
GLY  
PHE  
GLU  
GLU  
GLU  
GLY  
GLY  
GLU  
GLU  
GLU  
ASN  
ALA

• Molecule 2: Tubulin beta-4 chain

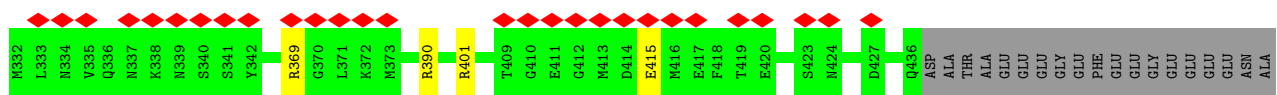
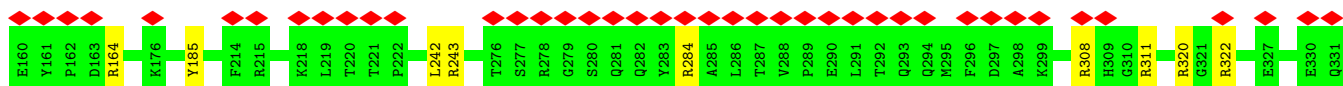
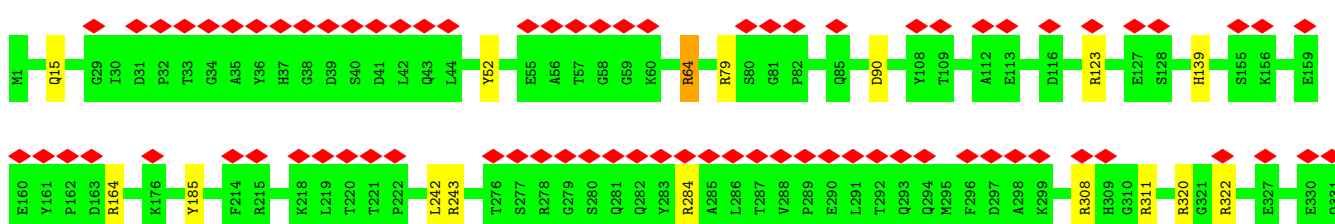


ALA

• Molecule 2: Tubulin beta-4 chain

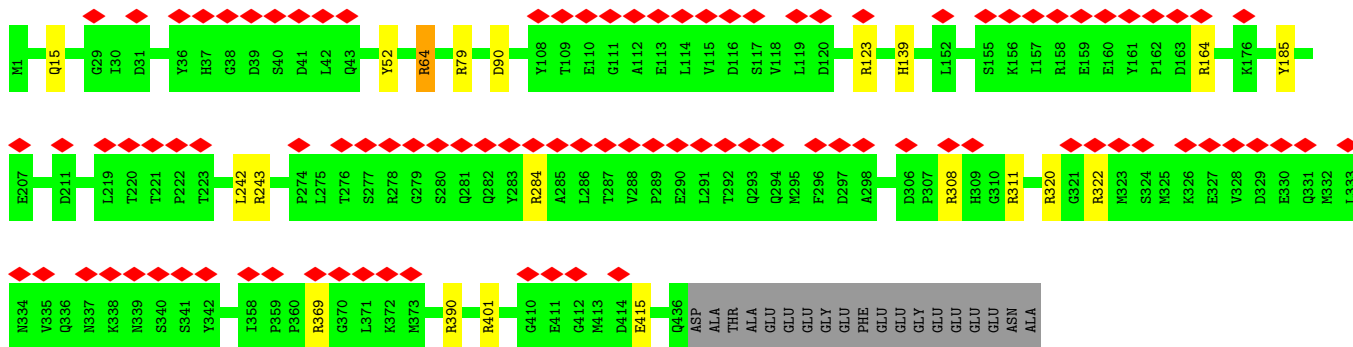


• Molecule 2: Tubulin beta-4 chain

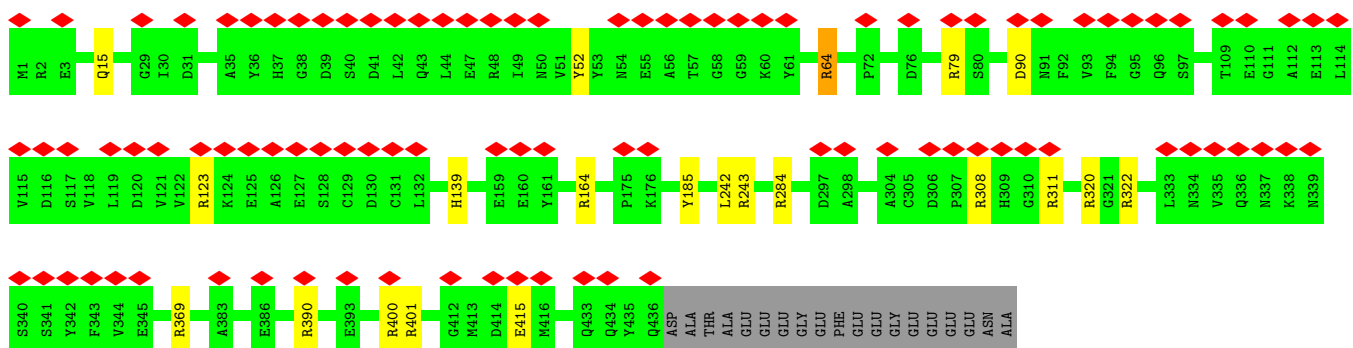
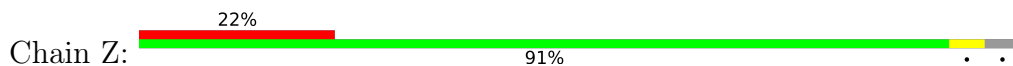


• Molecule 2: Tubulin beta-4 chain

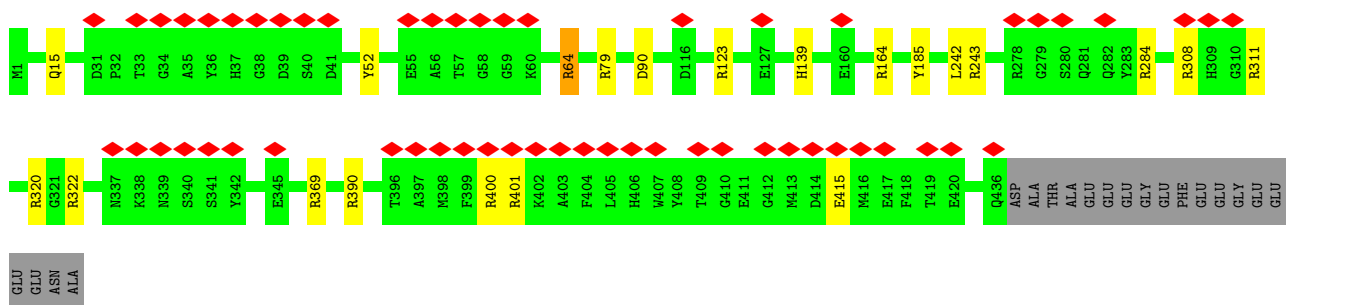
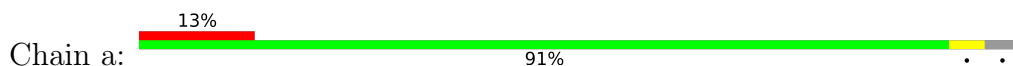




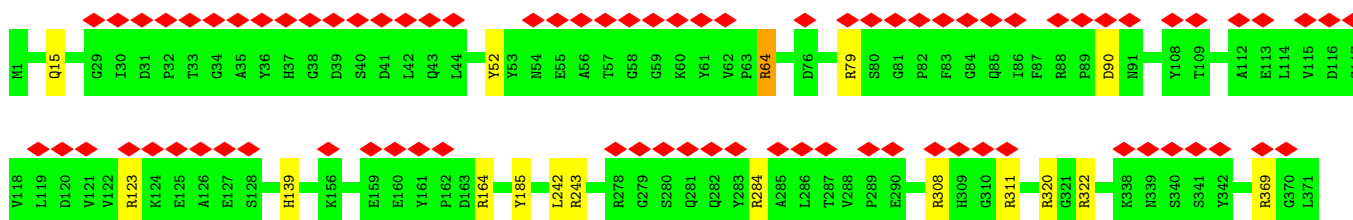
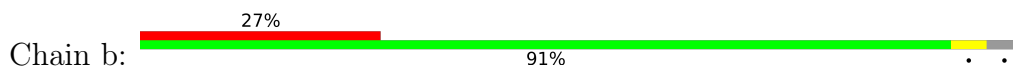
• Molecule 2: Tubulin beta-4 chain



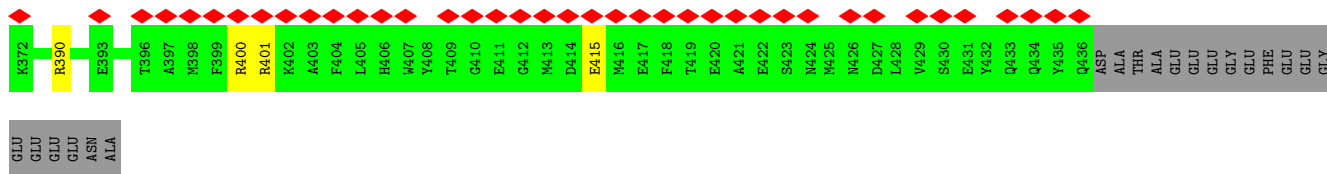
• Molecule 2: Tubulin beta-4 chain



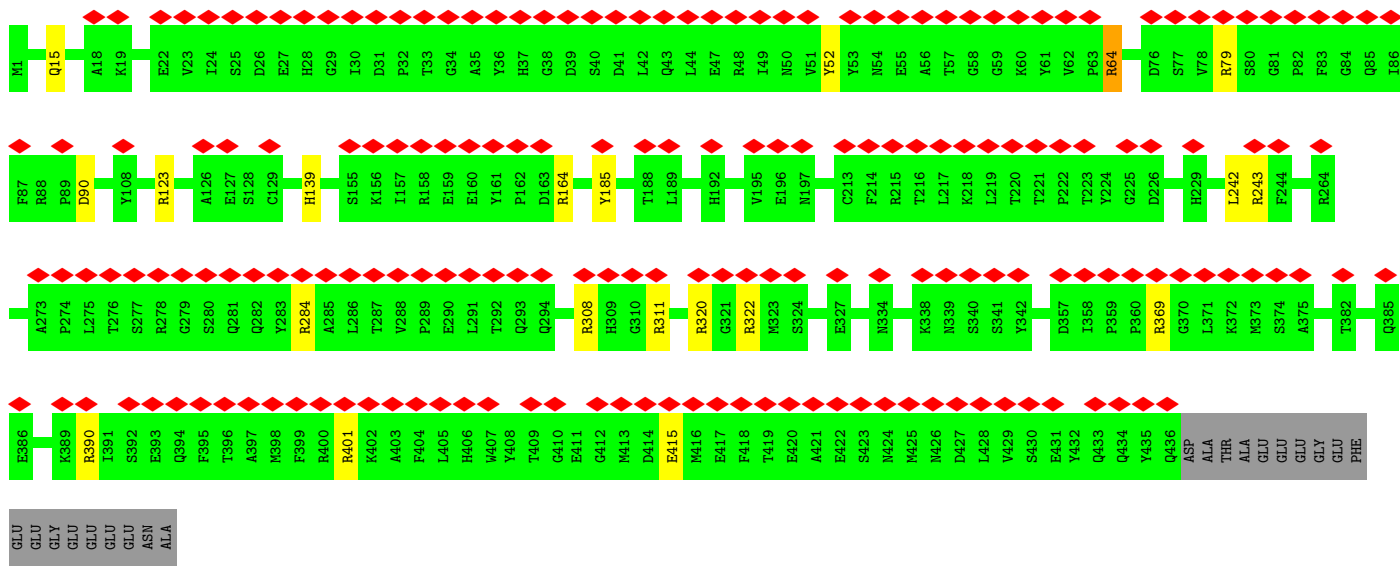
• Molecule 2: Tubulin beta-4 chain



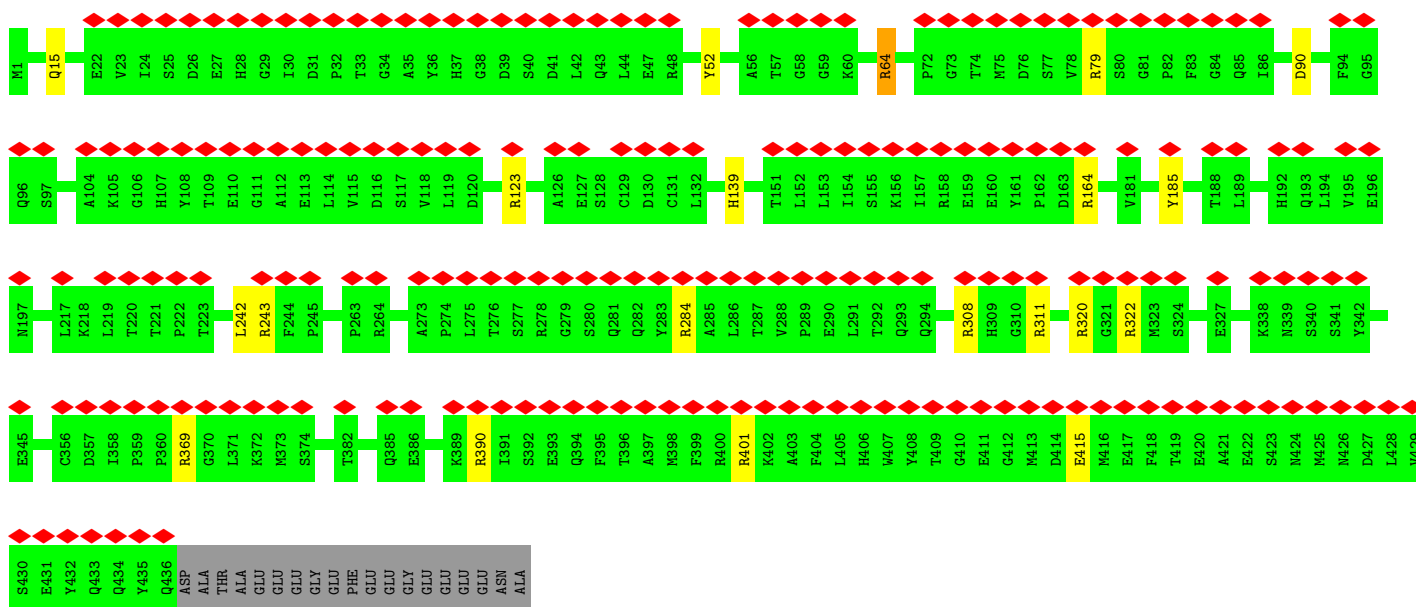
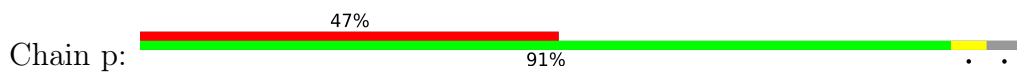




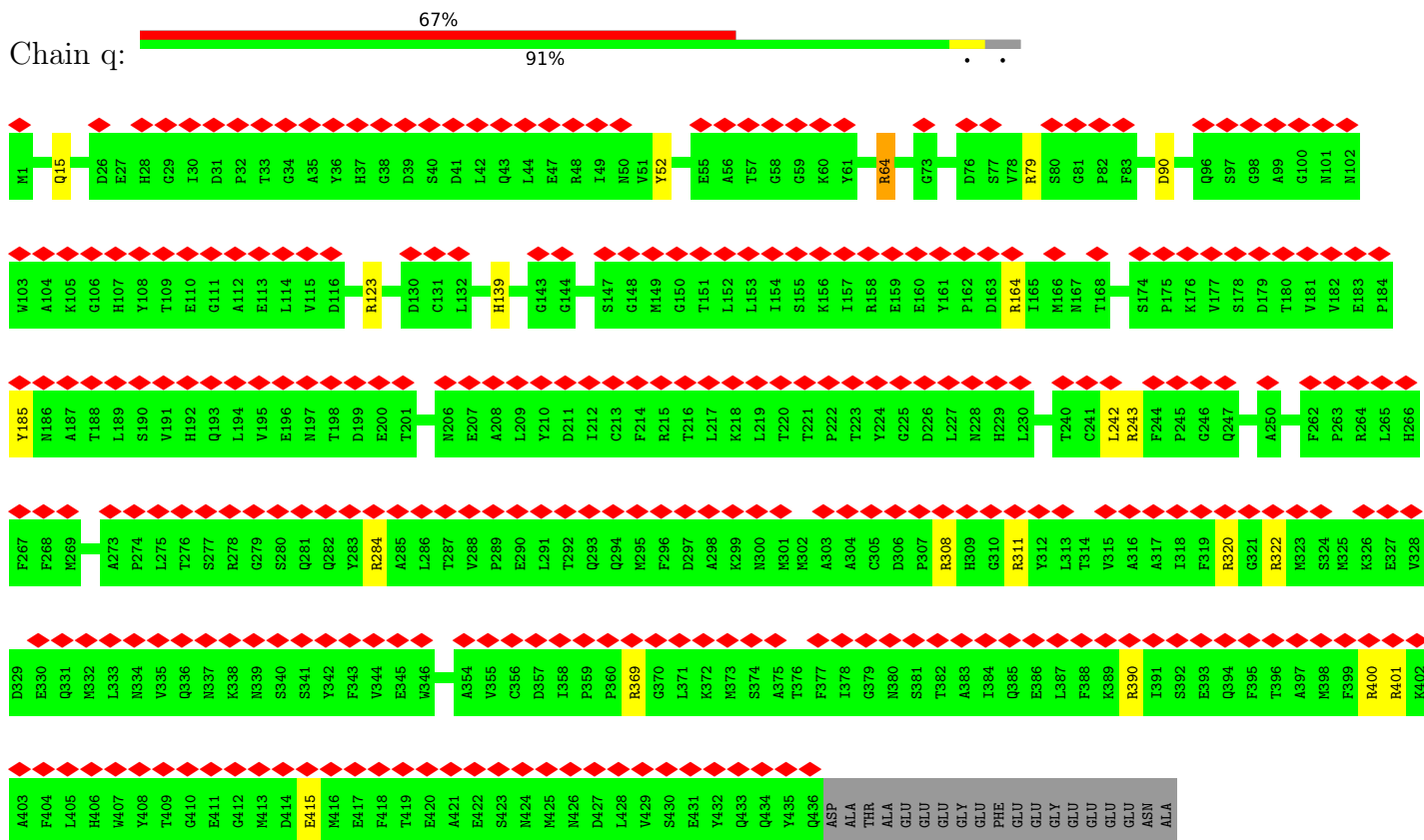
• Molecule 2: Tubulin beta-4 chain



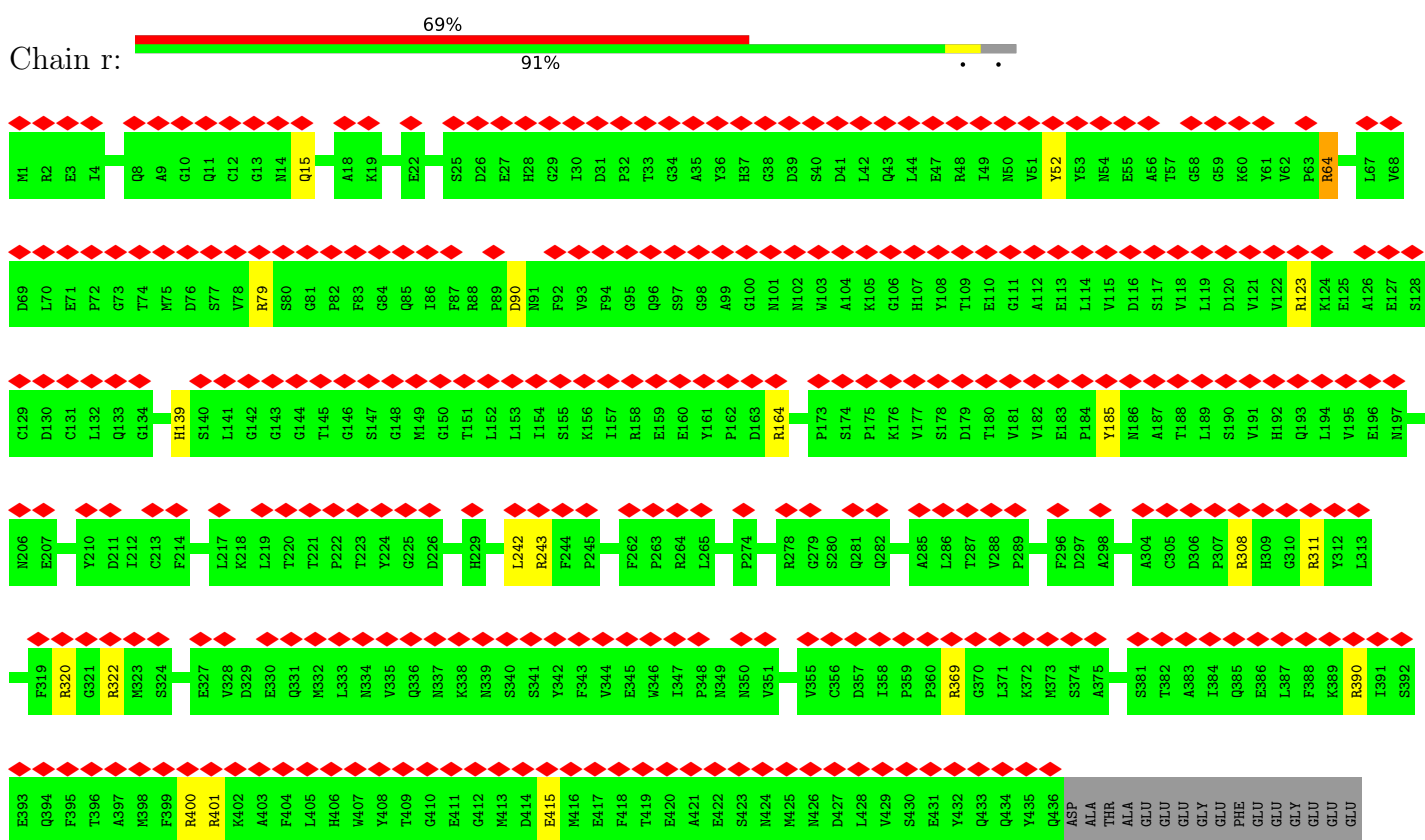
• Molecule 2: Tubulin beta-4 chain



• Molecule 2: Tubulin beta-4 chain

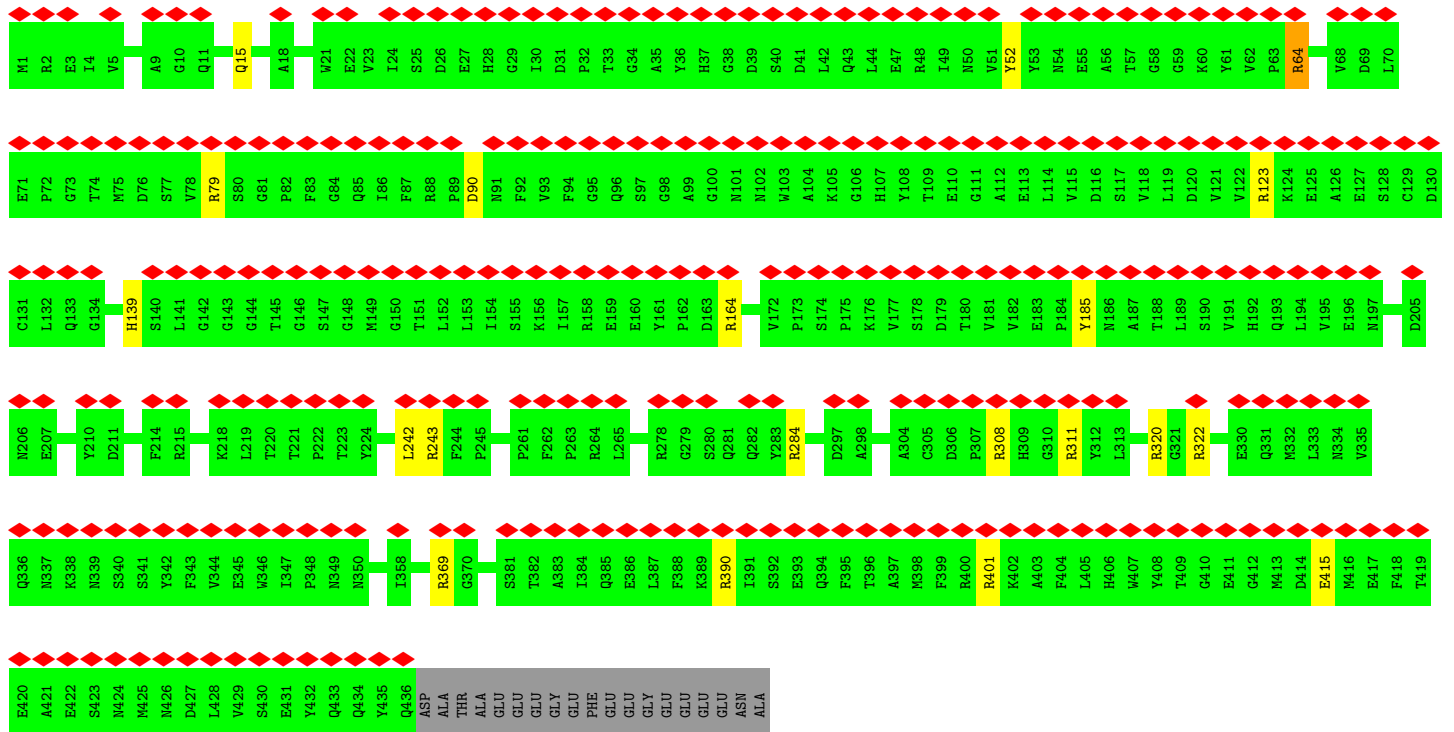
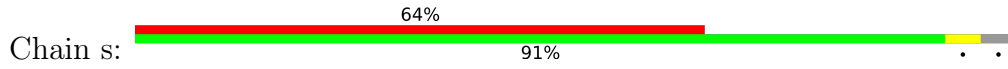


• Molecule 2: Tubulin beta-4 chain



GLU  
ASN  
ALA

• Molecule 2: Tubulin beta-4 chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8497	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 ( $e^-/\text{\AA}^2$ )	43	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	33000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0157	Depositor
Map size (Å)	513.024, 513.024, 513.024	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.004, 2.004, 2.004	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: GTP, GDP, TA1, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.66	0/3442	1.05	15/4667 (0.3%)
1	C	0.66	0/3442	1.05	17/4667 (0.4%)
1	D	0.66	0/3442	1.05	15/4667 (0.3%)
1	E	0.66	0/3442	1.05	15/4667 (0.3%)
1	G	0.66	0/3442	1.05	15/4667 (0.3%)
1	H	0.66	0/3442	1.05	14/4667 (0.3%)
1	I	0.66	0/3442	1.05	14/4667 (0.3%)
1	J	0.66	0/3442	1.05	16/4667 (0.3%)
1	K	0.66	0/3442	1.05	16/4667 (0.3%)
1	L	0.66	0/3442	1.05	15/4667 (0.3%)
1	M	0.66	0/3442	1.05	15/4667 (0.3%)
1	N	0.66	0/3442	1.05	16/4667 (0.3%)
1	O	0.66	0/3442	1.05	15/4667 (0.3%)
1	P	0.66	0/3442	1.05	14/4667 (0.3%)
1	c	0.66	0/3442	1.05	15/4667 (0.3%)
1	d	0.66	0/3442	1.05	15/4667 (0.3%)
1	e	0.66	0/3442	1.05	14/4667 (0.3%)
1	f	0.66	0/3442	1.05	16/4667 (0.3%)
1	g	0.66	0/3442	1.05	14/4667 (0.3%)
1	h	0.66	0/3442	1.05	14/4667 (0.3%)
1	i	0.66	0/3442	1.05	14/4667 (0.3%)
1	j	0.66	0/3442	1.05	16/4667 (0.3%)
1	k	0.66	0/3442	1.05	15/4667 (0.3%)
2	B	0.65	0/3422	1.05	16/4636 (0.3%)
2	F	0.65	0/3422	1.05	16/4636 (0.3%)
2	Q	0.65	0/3422	1.05	16/4636 (0.3%)
2	R	0.65	0/3422	1.05	17/4636 (0.4%)
2	S	0.65	0/3422	1.05	16/4636 (0.3%)
2	T	0.65	0/3422	1.05	16/4636 (0.3%)
2	U	0.65	0/3422	1.05	16/4636 (0.3%)
2	V	0.65	0/3422	1.05	16/4636 (0.3%)
2	W	0.65	0/3422	1.05	16/4636 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	X	0.65	0/3422	1.05	16/4636 (0.3%)
2	Y	0.65	0/3422	1.05	16/4636 (0.3%)
2	Z	0.65	0/3422	1.05	17/4636 (0.4%)
2	a	0.65	0/3422	1.05	17/4636 (0.4%)
2	b	0.65	0/3422	1.05	17/4636 (0.4%)
2	o	0.65	0/3422	1.05	16/4636 (0.3%)
2	p	0.65	0/3422	1.05	16/4636 (0.3%)
2	q	0.65	0/3422	1.05	17/4636 (0.4%)
2	r	0.65	0/3422	1.05	16/4636 (0.3%)
2	s	0.65	0/3422	1.05	16/4636 (0.3%)
All	All	0.65	0/144184	1.05	654/195425 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	F	0	2
2	Q	0	2
2	R	0	2
2	S	0	2
2	T	0	2
2	U	0	2
2	V	0	2
2	W	0	2
2	X	0	2
2	Y	0	2
2	Z	0	2
2	a	0	2
2	b	0	2
2	o	0	2
2	p	0	2
2	q	0	2
2	r	0	2
2	s	0	2
All	All	0	38

There are no bond length outliers.

All (654) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	82	PRO	CA-N-CD	-9.54	98.14	111.50
1	G	82	PRO	CA-N-CD	-9.53	98.15	111.50
1	d	82	PRO	CA-N-CD	-9.53	98.16	111.50
1	C	82	PRO	CA-N-CD	-9.52	98.17	111.50
1	A	82	PRO	CA-N-CD	-9.52	98.18	111.50
1	H	82	PRO	CA-N-CD	-9.51	98.18	111.50
1	K	82	PRO	CA-N-CD	-9.51	98.18	111.50
1	M	82	PRO	CA-N-CD	-9.51	98.18	111.50
1	g	82	PRO	CA-N-CD	-9.51	98.18	111.50
1	e	82	PRO	CA-N-CD	-9.51	98.19	111.50
1	k	82	PRO	CA-N-CD	-9.51	98.19	111.50
1	h	82	PRO	CA-N-CD	-9.51	98.19	111.50
1	j	82	PRO	CA-N-CD	-9.51	98.19	111.50
1	L	82	PRO	CA-N-CD	-9.51	98.19	111.50
1	E	82	PRO	CA-N-CD	-9.50	98.19	111.50
1	P	82	PRO	CA-N-CD	-9.50	98.19	111.50
1	D	82	PRO	CA-N-CD	-9.50	98.20	111.50
1	i	82	PRO	CA-N-CD	-9.50	98.20	111.50
1	f	82	PRO	CA-N-CD	-9.50	98.20	111.50
1	I	82	PRO	CA-N-CD	-9.50	98.20	111.50
1	O	82	PRO	CA-N-CD	-9.49	98.22	111.50
1	c	82	PRO	CA-N-CD	-9.48	98.22	111.50
1	N	82	PRO	CA-N-CD	-9.47	98.24	111.50
2	o	64	ARG	NE-CZ-NH1	9.27	124.94	120.30
2	b	64	ARG	NE-CZ-NH1	9.27	124.93	120.30
2	Y	64	ARG	NE-CZ-NH1	9.24	124.92	120.30
2	a	64	ARG	NE-CZ-NH1	9.21	124.91	120.30
2	S	64	ARG	NE-CZ-NH1	9.19	124.90	120.30
2	Z	64	ARG	NE-CZ-NH1	9.19	124.89	120.30
2	q	64	ARG	NE-CZ-NH1	9.17	124.88	120.30
2	r	64	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	W	64	ARG	NE-CZ-NH1	9.15	124.88	120.30
2	B	64	ARG	NE-CZ-NH1	9.15	124.87	120.30
2	T	64	ARG	NE-CZ-NH1	9.14	124.87	120.30
2	s	64	ARG	NE-CZ-NH1	9.13	124.86	120.30
2	U	64	ARG	NE-CZ-NH1	9.11	124.86	120.30
2	V	64	ARG	NE-CZ-NH1	9.10	124.85	120.30
2	Q	64	ARG	NE-CZ-NH1	9.09	124.85	120.30
2	F	64	ARG	NE-CZ-NH1	9.09	124.84	120.30
2	X	64	ARG	NE-CZ-NH1	9.07	124.83	120.30
2	p	64	ARG	NE-CZ-NH1	9.06	124.83	120.30
2	R	64	ARG	NE-CZ-NH1	9.05	124.83	120.30
2	Y	164	ARG	NE-CZ-NH1	8.45	124.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	164	ARG	NE-CZ-NH1	8.37	124.48	120.30
2	o	164	ARG	NE-CZ-NH1	8.37	124.48	120.30
2	V	164	ARG	NE-CZ-NH1	8.34	124.47	120.30
2	W	164	ARG	NE-CZ-NH1	8.34	124.47	120.30
2	q	164	ARG	NE-CZ-NH1	8.34	124.47	120.30
2	Q	164	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	s	164	ARG	NE-CZ-NH1	8.30	124.45	120.30
2	Z	164	ARG	NE-CZ-NH1	8.30	124.45	120.30
2	r	164	ARG	NE-CZ-NH1	8.30	124.45	120.30
2	B	164	ARG	NE-CZ-NH1	8.29	124.45	120.30
2	T	164	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	R	164	ARG	NE-CZ-NH1	8.27	124.44	120.30
2	X	164	ARG	NE-CZ-NH1	8.27	124.44	120.30
2	a	164	ARG	NE-CZ-NH1	8.27	124.44	120.30
2	p	164	ARG	NE-CZ-NH1	8.27	124.43	120.30
2	b	164	ARG	NE-CZ-NH1	8.25	124.42	120.30
2	F	164	ARG	NE-CZ-NH1	8.21	124.41	120.30
2	S	164	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	h	243	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	f	243	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	b	320	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	j	243	ARG	NE-CZ-NH1	7.75	124.17	120.30
2	T	320	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	L	243	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	P	243	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	e	243	ARG	NE-CZ-NH1	7.72	124.16	120.30
2	W	320	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	D	243	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	Q	320	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	M	243	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	243	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	J	243	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	E	243	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	o	320	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	G	243	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	K	243	ARG	NE-CZ-NH1	7.67	124.14	120.30
2	Z	320	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	g	243	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	I	243	ARG	NE-CZ-NH1	7.67	124.14	120.30
2	q	320	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	V	320	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	i	215	ARG	NE-CZ-NH2	7.66	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	320	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	a	320	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	d	243	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	c	243	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	C	243	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	O	243	ARG	NE-CZ-NH1	7.64	124.12	120.30
2	U	320	ARG	NE-CZ-NH1	7.64	124.12	120.30
2	r	320	ARG	NE-CZ-NH1	7.64	124.12	120.30
2	R	320	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	i	243	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	k	243	ARG	NE-CZ-NH1	7.63	124.12	120.30
2	F	320	ARG	NE-CZ-NH1	7.63	124.11	120.30
2	S	320	ARG	NE-CZ-NH1	7.62	124.11	120.30
2	Y	320	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	L	215	ARG	NE-CZ-NH2	7.61	124.11	120.30
2	p	320	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	N	243	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	s	320	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	X	320	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	g	215	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	K	215	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	P	215	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	c	215	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	H	243	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	M	215	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	h	215	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	O	215	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	I	215	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	A	215	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	e	215	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	G	215	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	E	215	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	f	215	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	H	215	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	N	215	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	C	215	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	k	215	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	J	215	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	j	215	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	D	215	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	d	215	ARG	NE-CZ-NH2	7.39	124.00	120.30
2	W	243	ARG	NE-CZ-NH1	7.21	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	243	ARG	NE-CZ-NH1	7.15	123.87	120.30
2	Y	243	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	X	243	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	i	390	ARG	NE-CZ-NH1	7.10	123.85	120.30
2	r	243	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	E	390	ARG	NE-CZ-NH1	7.09	123.84	120.30
2	p	243	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	S	243	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	C	390	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	q	243	ARG	NE-CZ-NH1	7.05	123.83	120.30
2	B	243	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	k	390	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	r	311	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	G	390	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	T	311	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	U	243	ARG	NE-CZ-NH1	7.03	123.82	120.30
2	F	243	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	V	243	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	g	390	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	c	390	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	p	311	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	b	243	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	b	311	ARG	NE-CZ-NH1	7.01	123.81	120.30
2	s	243	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	Z	243	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	390	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	P	390	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	h	390	ARG	NE-CZ-NH1	6.99	123.80	120.30
2	a	243	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	j	390	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	q	311	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	K	390	ARG	NE-CZ-NH1	6.97	123.78	120.30
2	T	401	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	f	390	ARG	NE-CZ-NH1	6.97	123.78	120.30
2	R	311	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	D	390	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	L	390	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	R	401	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	W	311	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	J	390	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	Q	401	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	T	243	ARG	NE-CZ-NH1	6.96	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	311	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	X	311	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	I	390	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	S	311	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	e	390	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	o	243	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	q	401	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	V	311	ARG	NE-CZ-NH1	6.95	123.77	120.30
2	R	243	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	H	390	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	B	311	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	a	311	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	N	390	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	s	401	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	F	311	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	Q	311	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	Y	401	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	s	311	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	O	390	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	a	401	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	M	390	ARG	NE-CZ-NH1	6.89	123.75	120.30
2	B	401	ARG	NE-CZ-NH1	6.89	123.74	120.30
2	o	311	ARG	NE-CZ-NH1	6.89	123.74	120.30
2	F	401	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	Z	311	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	Z	401	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	U	401	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	b	401	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	o	401	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	r	401	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	S	401	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	d	390	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	Y	311	ARG	NE-CZ-NH1	6.83	123.71	120.30
2	X	401	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	p	401	ARG	NE-CZ-NH1	6.79	123.70	120.30
2	V	401	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	W	401	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	e	402	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	J	402	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	H	402	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	f	402	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	i	402	ARG	NE-CZ-NH1	6.23	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	402	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	G	402	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	K	402	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	L	402	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	g	402	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	402	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	h	402	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	402	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	D	402	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	N	402	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	E	402	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	j	402	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	O	402	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	c	402	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	I	402	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	k	402	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	I	105	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	d	402	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	M	105	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	S	369	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	N	105	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	M	402	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	I	185	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	c	105	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	H	105	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	K	105	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	h	105	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	P	105	ARG	NE-CZ-NH1	6.01	123.31	120.30
2	s	369	ARG	NE-CZ-NH2	6.01	123.30	120.30
1	E	105	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	k	105	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	i	105	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	105	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	r	369	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	g	105	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	k	308	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	p	369	ARG	NE-CZ-NH2	5.96	123.28	120.30
2	X	369	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	K	308	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	f	185	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	G	185	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	O	105	ARG	NE-CZ-NH1	5.95	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	369	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	h	308	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	R	369	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	j	308	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	i	185	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	e	105	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	N	185	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	L	308	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	f	105	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	B	369	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	C	105	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	j	185	TYR	CB-CG-CD2	-5.92	117.45	121.00
2	F	369	ARG	NE-CZ-NH2	5.92	123.26	120.30
2	U	369	ARG	NE-CZ-NH2	5.92	123.26	120.30
2	b	369	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	D	105	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	q	369	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	J	308	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	Q	369	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	G	105	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	P	185	TYR	CB-CG-CD2	-5.91	117.46	121.00
1	L	105	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	a	369	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	C	185	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	e	308	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	k	185	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	J	105	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	o	369	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	g	185	TYR	CB-CG-CD2	-5.89	117.46	121.00
1	A	185	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	d	185	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	H	185	TYR	CB-CG-CD2	-5.89	117.47	121.00
2	Z	369	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	J	185	TYR	CB-CG-CD2	-5.88	117.47	121.00
2	V	369	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	M	185	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	O	185	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	i	308	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	H	308	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	h	185	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	c	308	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	308	ARG	NE-CZ-NH1	5.87	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	308	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	T	369	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	c	185	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	D	308	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	185	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	e	185	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	A	308	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	E	308	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	j	105	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	E	185	TYR	CB-CG-CD2	-5.86	117.49	121.00
2	Y	369	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	d	105	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	e	229	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	P	308	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	O	308	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	M	308	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	G	308	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	M	229	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	M	79	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	g	308	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	L	185	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	P	79	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	J	229	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	c	229	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	j	79	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	d	308	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	K	185	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	K	229	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	N	308	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	O	229	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	229	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	G	79	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	H	79	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	N	229	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	O	79	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	c	79	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	s	123	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	229	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	h	79	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	I	308	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	k	79	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	P	229	ARG	NE-CZ-NH1	5.75	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	g	229	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	I	229	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	o	123	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	G	229	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	j	229	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	H	229	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	i	229	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	k	229	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	79	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	V	123	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	79	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	79	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	E	229	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	O	2	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	Y	123	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	c	2	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	S	123	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	N	79	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	e	79	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	I	79	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	L	229	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	C	2	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	E	79	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	a	123	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	d	229	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	f	229	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	h	229	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	K	79	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	J	79	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	F	123	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	r	123	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	W	123	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	f	79	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	g	79	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	E	2	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	i	79	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	q	123	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	L	79	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	k	2	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	h	2	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	i	2	ARG	NE-CZ-NH1	5.64	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	2	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	P	2	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	B	123	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	Q	123	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	2	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	K	2	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	d	79	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	e	2	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	X	123	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	G	2	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	f	2	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	b	123	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	h	123	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	U	123	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	123	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	d	2	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	M	2	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	I	2	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	J	2	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	L	123	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	T	123	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	I	123	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	H	2	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	e	123	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	N	2	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	Z	123	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	d	123	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	2	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	g	2	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	L	2	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	p	123	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	c	123	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	J	123	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	E	123	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	g	123	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	123	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	N	123	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	k	123	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	123	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	P	123	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	R	123	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	j	123	ARG	NE-CZ-NH1	5.49	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	123	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	K	123	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	W	185	TYR	CB-CG-CD2	-5.46	117.72	121.00
2	o	185	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	H	123	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	s	185	TYR	CB-CG-CD2	-5.46	117.72	121.00
2	S	185	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	O	123	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	i	123	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	G	123	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	f	221	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	p	185	TYR	CB-CG-CD2	-5.43	117.74	121.00
2	T	185	TYR	CB-CG-CD2	-5.42	117.75	121.00
2	T	322	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	U	185	TYR	CB-CG-CD2	-5.42	117.75	121.00
2	b	185	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	E	221	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	Z	185	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	P	84	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	M	123	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	R	185	TYR	CB-CG-CD2	-5.41	117.76	121.00
2	B	185	TYR	CB-CG-CD2	-5.40	117.76	121.00
2	Q	185	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	g	221	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	q	185	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	G	84	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	V	185	TYR	CB-CG-CD2	-5.39	117.76	121.00
2	a	322	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	e	221	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	W	322	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	C	221	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	F	185	TYR	CB-CG-CD2	-5.38	117.78	121.00
1	I	84	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	Y	185	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	F	322	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	I	221	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	i	221	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	L	221	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	R	322	ARG	NE-CZ-NH2	5.36	122.98	120.30
2	r	185	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	d	221	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	X	322	ARG	NE-CZ-NH2	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	322	ARG	NE-CZ-NH2	5.35	122.97	120.30
2	b	322	ARG	NE-CZ-NH2	5.35	122.97	120.30
2	a	185	TYR	CB-CG-CD2	-5.34	117.80	121.00
2	X	185	TYR	CB-CG-CD2	-5.33	117.80	121.00
2	a	308	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	o	64	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	K	221	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	s	79	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	N	84	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	S	64	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	S	243	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
2	Y	322	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	q	322	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	S	322	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	P	221	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	221	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	B	322	ARG	NE-CZ-NH2	5.31	122.96	120.30
2	S	308	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	h	221	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	W	243	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
2	Y	243	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
2	b	64	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	U	243	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
2	X	243	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	D	221	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	U	322	ARG	NE-CZ-NH2	5.30	122.95	120.30
2	F	243	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	M	84	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	V	243	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
2	a	243	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	k	221	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	q	64	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	G	221	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	Q	243	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	H	221	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	Y	79	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	j	84	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	q	243	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
2	T	243	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
2	b	243	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	c	221	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	Y	64	ARG	NE-CZ-NH2	-5.29	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	84	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	o	243	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	J	221	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	Z	243	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
2	a	64	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	r	64	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	B	243	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	M	221	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	W	308	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	s	322	ARG	NE-CZ-NH2	5.28	122.94	120.30
2	V	322	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	O	84	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	T	79	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	X	308	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	e	84	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	84	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	W	64	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	Q	322	ARG	NE-CZ-NH2	5.26	122.93	120.30
2	R	243	ARG	NH1-CZ-NH2	-5.26	113.62	119.40
2	o	322	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	C	84	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	F	79	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	k	84	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	U	308	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	p	243	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
2	s	243	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	N	221	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	Z	64	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	H	84	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	U	390	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	j	221	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	p	79	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	r	243	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
1	i	84	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	L	84	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	J	84	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	s	390	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	p	308	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	K	84	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	p	322	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	s	64	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	B	308	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	221	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	Y	308	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	o	308	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	B	64	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	r	322	ARG	NE-CZ-NH2	5.21	122.91	120.30
2	b	308	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	S	390	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	T	390	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	V	79	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	f	84	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	g	84	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	R	390	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	T	308	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	Z	308	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	c	84	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	h	84	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	E	84	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	Q	64	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	B	79	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	Z	79	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	T	64	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	V	308	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	84	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	R	64	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	W	284	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	b	284	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	F	308	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	Q	284	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	R	308	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	R	79	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	Q	308	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	a	79	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	b	79	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	o	79	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	U	64	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	Z	390	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	p	64	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	F	64	ARG	NE-CZ-NH2	-5.15	117.72	120.30
2	s	308	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	F	284	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	W	79	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	X	284	ARG	NE-CZ-NH1	5.15	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	79	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	X	64	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	V	390	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	Q	390	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	U	79	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	p	390	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	q	79	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	r	308	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	S	79	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	r	79	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	X	79	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	F	390	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	X	390	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	q	390	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	B	390	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	q	308	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	b	390	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	r	390	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	Z	284	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	o	284	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	V	64	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	T	284	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	a	284	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	339	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	o	390	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	V	284	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	64	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	s	284	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	B	284	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	R	400	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	Y	284	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	f	339	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	Y	390	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	O	339	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	64	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	J	339	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	M	339	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	a	390	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	j	339	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	k	64	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	p	284	ARG	NE-CZ-NH1	5.05	122.82	120.30
2	S	284	ARG	NE-CZ-NH1	5.05	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	339	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	339	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	L	64	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	d	339	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	J	156	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	a	400	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	q	284	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	f	156	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	b	400	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	N	339	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	U	400	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	N	264	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	q	400	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	K	339	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	R	284	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	Z	400	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	j	156	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	K	156	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	C	264	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	G	339	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	W	390	ARG	NE-CZ-NH1	5.01	122.80	120.30
2	r	400	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	A	339	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	52	TYR	Sidechain
2	B	64	ARG	Sidechain
2	F	52	TYR	Sidechain
2	F	64	ARG	Sidechain
2	Q	52	TYR	Sidechain
2	Q	64	ARG	Sidechain
2	R	52	TYR	Sidechain
2	R	64	ARG	Sidechain
2	S	52	TYR	Sidechain
2	S	64	ARG	Sidechain
2	T	52	TYR	Sidechain
2	T	64	ARG	Sidechain
2	U	52	TYR	Sidechain
2	U	64	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	V	52	TYR	Sidechain
2	V	64	ARG	Sidechain
2	W	52	TYR	Sidechain
2	W	64	ARG	Sidechain
2	X	52	TYR	Sidechain
2	X	64	ARG	Sidechain
2	Y	52	TYR	Sidechain
2	Y	64	ARG	Sidechain
2	Z	52	TYR	Sidechain
2	Z	64	ARG	Sidechain
2	a	52	TYR	Sidechain
2	a	64	ARG	Sidechain
2	b	52	TYR	Sidechain
2	b	64	ARG	Sidechain
2	o	52	TYR	Sidechain
2	o	64	ARG	Sidechain
2	p	52	TYR	Sidechain
2	p	64	ARG	Sidechain
2	q	52	TYR	Sidechain
2	q	64	ARG	Sidechain
2	r	52	TYR	Sidechain
2	r	64	ARG	Sidechain
2	s	52	TYR	Sidechain
2	s	64	ARG	Sidechain

## 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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	C	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	D	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	E	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	G	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	H	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	I	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	J	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	K	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	L	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	M	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	N	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	O	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	P	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	c	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	d	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	e	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	f	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	g	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	h	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	i	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	j	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
1	k	426/450 (95%)	421 (99%)	5 (1%)	0	100	100
2	B	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	F	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	Q	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	R	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	S	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	T	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	U	424/445 (95%)	414 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	W	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	X	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	Y	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	Z	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	a	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	b	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	o	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	p	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	q	424/445 (95%)	415 (98%)	9 (2%)	0	100	100
2	r	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	s	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
All	All	17854/18805 (95%)	17554 (98%)	300 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	C	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	D	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	E	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	G	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	H	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	I	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	J	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	K	366/382 (96%)	362 (99%)	4 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	M	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	N	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	O	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	P	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	c	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	d	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	e	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	f	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	g	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	h	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	i	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	j	366/382 (96%)	362 (99%)	4 (1%)	70	80
1	k	366/382 (96%)	362 (99%)	4 (1%)	70	80
2	B	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	F	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	Q	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	R	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	S	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	T	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	U	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	V	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	W	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	X	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	Y	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	Z	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	a	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	b	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	o	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	p	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	q	365/379 (96%)	360 (99%)	5 (1%)	62	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	r	365/379 (96%)	360 (99%)	5 (1%)	62	75
2	s	365/379 (96%)	360 (99%)	5 (1%)	62	75
All	All	15353/15987 (96%)	15166 (99%)	187 (1%)	66	78

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	141	PHE
1	A	367	ASP
1	A	425	MET
2	B	15	GLN
2	B	90	ASP
2	B	139	HIS
2	B	242	LEU
2	B	415	GLU
1	C	71	GLU
1	C	141	PHE
1	C	367	ASP
1	C	425	MET
1	D	71	GLU
1	D	141	PHE
1	D	367	ASP
1	D	425	MET
1	E	71	GLU
1	E	141	PHE
1	E	367	ASP
1	E	425	MET
2	F	15	GLN
2	F	90	ASP
2	F	139	HIS
2	F	242	LEU
2	F	415	GLU
1	G	71	GLU
1	G	141	PHE
1	G	367	ASP
1	G	425	MET
1	H	71	GLU
1	H	141	PHE
1	H	367	ASP
1	H	425	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	71	GLU
1	I	141	PHE
1	I	367	ASP
1	I	425	MET
1	J	71	GLU
1	J	141	PHE
1	J	367	ASP
1	J	425	MET
1	K	71	GLU
1	K	141	PHE
1	K	367	ASP
1	K	425	MET
1	L	71	GLU
1	L	141	PHE
1	L	367	ASP
1	L	425	MET
1	M	71	GLU
1	M	141	PHE
1	M	367	ASP
1	M	425	MET
1	N	71	GLU
1	N	141	PHE
1	N	367	ASP
1	N	425	MET
1	O	71	GLU
1	O	141	PHE
1	O	367	ASP
1	O	425	MET
1	P	71	GLU
1	P	141	PHE
1	P	367	ASP
1	P	425	MET
2	Q	15	GLN
2	Q	90	ASP
2	Q	139	HIS
2	Q	242	LEU
2	Q	415	GLU
2	R	15	GLN
2	R	90	ASP
2	R	139	HIS
2	R	242	LEU
2	R	415	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	S	15	GLN
2	S	90	ASP
2	S	139	HIS
2	S	242	LEU
2	S	415	GLU
2	T	15	GLN
2	T	90	ASP
2	T	139	HIS
2	T	242	LEU
2	T	415	GLU
2	U	15	GLN
2	U	90	ASP
2	U	139	HIS
2	U	242	LEU
2	U	415	GLU
2	V	15	GLN
2	V	90	ASP
2	V	139	HIS
2	V	242	LEU
2	V	415	GLU
2	W	15	GLN
2	W	90	ASP
2	W	139	HIS
2	W	242	LEU
2	W	415	GLU
2	X	15	GLN
2	X	90	ASP
2	X	139	HIS
2	X	242	LEU
2	X	415	GLU
2	Y	15	GLN
2	Y	90	ASP
2	Y	139	HIS
2	Y	242	LEU
2	Y	415	GLU
2	Z	15	GLN
2	Z	90	ASP
2	Z	139	HIS
2	Z	242	LEU
2	Z	415	GLU
2	a	15	GLN
2	a	90	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	a	139	HIS
2	a	242	LEU
2	a	415	GLU
2	b	15	GLN
2	b	90	ASP
2	b	139	HIS
2	b	242	LEU
2	b	415	GLU
1	c	71	GLU
1	c	141	PHE
1	c	367	ASP
1	c	425	MET
1	d	71	GLU
1	d	141	PHE
1	d	367	ASP
1	d	425	MET
1	e	71	GLU
1	e	141	PHE
1	e	367	ASP
1	e	425	MET
1	f	71	GLU
1	f	141	PHE
1	f	367	ASP
1	f	425	MET
1	g	71	GLU
1	g	141	PHE
1	g	367	ASP
1	g	425	MET
1	h	71	GLU
1	h	141	PHE
1	h	367	ASP
1	h	425	MET
1	i	71	GLU
1	i	141	PHE
1	i	367	ASP
1	i	425	MET
1	j	71	GLU
1	j	141	PHE
1	j	367	ASP
1	j	425	MET
1	k	71	GLU
1	k	141	PHE

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Mol	Chain	Res	Type
1	k	367	ASP
1	k	425	MET
2	o	15	GLN
2	o	90	ASP
2	o	139	HIS
2	o	242	LEU
2	o	415	GLU
2	p	15	GLN
2	p	90	ASP
2	p	139	HIS
2	p	242	LEU
2	p	415	GLU
2	q	15	GLN
2	q	90	ASP
2	q	139	HIS
2	q	242	LEU
2	q	415	GLU
2	r	15	GLN
2	r	90	ASP
2	r	139	HIS
2	r	242	LEU
2	r	415	GLU
2	s	15	GLN
2	s	90	ASP
2	s	139	HIS
2	s	242	LEU
2	s	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	394	GLN
1	D	249	ASN
1	D	283	HIS
1	D	356	ASN
1	G	61	HIS
1	G	88	HIS
1	G	128	GLN
1	G	249	ASN
1	G	356	ASN
1	H	293	ASN
1	I	249	ASN

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Mol	Chain	Res	Type
1	I	356	ASN
1	J	249	ASN
1	J	356	ASN
1	L	249	ASN
1	L	283	HIS
1	L	356	ASN
1	M	91	GLN
1	M	283	HIS
1	N	283	HIS
1	O	283	HIS
1	O	285	GLN
1	P	249	ASN
1	P	356	ASN
2	Q	394	GLN
2	R	394	GLN
2	S	394	GLN
2	T	281	GLN
2	T	339	ASN
2	T	394	GLN
2	U	394	GLN
2	V	394	GLN
2	W	394	GLN
2	X	394	GLN
2	Y	394	GLN
2	Z	85	GLN
1	d	249	ASN
1	d	356	ASN
1	e	128	GLN
1	e	249	ASN
1	e	356	ASN
1	f	285	GLN
1	g	249	ASN
1	g	356	ASN
1	h	249	ASN
1	h	356	ASN
1	j	88	HIS
1	j	249	ASN
1	j	356	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 23 are monoatomic - leaving 61 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
5	GDP	o	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
5	GDP	B	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
5	GDP	p	501	-	24,30,30	1.02	2 (8%)	30,47,47	1.47	3 (10%)
3	GTP	i	501	4	26,34,34	1.03	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	h	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	N	501	4	26,34,34	1.05	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	d	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	A	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	P	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	e	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
5	GDP	S	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.47	3 (10%)
3	GTP	M	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	j	501	4	26,34,34	1.05	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	k	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
5	GDP	R	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
6	TA1	B	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	R	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	V	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GTP	D	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
6	TA1	o	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	q	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	Z	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	S	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	a	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	p	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
3	GTP	G	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
5	GDP	Z	501	-	24,30,30	1.01	2 (8%)	30,47,47	1.48	3 (10%)
3	GTP	E	501	4	26,34,34	1.05	2 (7%)	32,54,54	1.54	6 (18%)
5	GDP	r	501	-	24,30,30	1.02	2 (8%)	30,47,47	1.47	3 (10%)
6	TA1	r	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	F	501	-	68,68,68	0.84	0	105,105,105	0.75	1 (0%)
3	GTP	C	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
5	GDP	Y	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
6	TA1	W	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
3	GTP	f	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	J	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	g	501	4	26,34,34	1.05	2 (7%)	32,54,54	1.54	6 (18%)
5	GDP	q	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.47	3 (10%)
6	TA1	Y	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
5	GDP	s	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
5	GDP	U	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
6	TA1	X	502	-	68,68,68	0.84	0	105,105,105	0.75	1 (0%)
6	TA1	s	502	-	68,68,68	0.83	0	105,105,105	0.74	1 (0%)
5	GDP	a	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
5	GDP	Q	501	-	24,30,30	1.02	2 (8%)	30,47,47	1.48	3 (10%)
6	TA1	Q	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
5	GDP	T	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
6	TA1	T	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
3	GTP	O	501	4	26,34,34	1.03	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	c	501	4	26,34,34	1.05	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	H	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
5	GDP	F	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
5	GDP	W	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GTP	K	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	I	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
3	GTP	L	501	4	26,34,34	1.04	2 (7%)	32,54,54	1.54	6 (18%)
5	GDP	b	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
5	GDP	X	501	-	24,30,30	1.03	2 (8%)	30,47,47	1.48	3 (10%)
6	TA1	b	502	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
6	TA1	U	501	-	68,68,68	0.83	0	105,105,105	0.75	1 (0%)
5	GDP	V	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)

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
5	GDP	o	501	-	-	3/12/32/32	0/3/3/3
5	GDP	B	501	-	-	3/12/32/32	0/3/3/3
5	GDP	p	501	-	-	3/12/32/32	0/3/3/3
3	GTP	i	501	4	-	2/18/38/38	0/3/3/3
3	GTP	h	501	4	-	2/18/38/38	0/3/3/3
3	GTP	N	501	4	-	2/18/38/38	0/3/3/3
3	GTP	d	501	4	-	2/18/38/38	0/3/3/3
3	GTP	A	501	4	-	2/18/38/38	0/3/3/3
3	GTP	P	501	4	-	2/18/38/38	0/3/3/3
3	GTP	e	501	4	-	2/18/38/38	0/3/3/3
5	GDP	S	501	-	-	3/12/32/32	0/3/3/3
3	GTP	M	501	4	-	2/18/38/38	0/3/3/3
3	GTP	j	501	4	-	2/18/38/38	0/3/3/3
3	GTP	k	501	4	-	2/18/38/38	0/3/3/3
5	GDP	R	501	-	-	3/12/32/32	0/3/3/3
6	TA1	B	502	-	-	0/41/127/127	0/7/7/7
6	TA1	R	502	-	-	0/41/127/127	0/7/7/7
6	TA1	V	502	-	-	0/41/127/127	0/7/7/7
3	GTP	D	501	4	-	2/18/38/38	0/3/3/3
6	TA1	o	502	-	-	0/41/127/127	0/7/7/7
6	TA1	q	502	-	-	0/41/127/127	0/7/7/7
6	TA1	Z	502	-	-	0/41/127/127	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TA1	S	502	-	-	0/41/127/127	0/7/7/7
6	TA1	a	502	-	-	0/41/127/127	0/7/7/7
6	TA1	p	502	-	-	0/41/127/127	0/7/7/7
3	GTP	G	501	4	-	2/18/38/38	0/3/3/3
5	GDP	Z	501	-	-	3/12/32/32	0/3/3/3
3	GTP	E	501	4	-	2/18/38/38	0/3/3/3
5	GDP	r	501	-	-	3/12/32/32	0/3/3/3
6	TA1	r	502	-	-	0/41/127/127	0/7/7/7
6	TA1	F	501	-	-	0/41/127/127	0/7/7/7
3	GTP	C	501	4	-	2/18/38/38	0/3/3/3
5	GDP	Y	501	-	-	3/12/32/32	0/3/3/3
6	TA1	W	502	-	-	0/41/127/127	0/7/7/7
3	GTP	f	501	4	-	2/18/38/38	0/3/3/3
3	GTP	J	501	4	-	2/18/38/38	0/3/3/3
3	GTP	g	501	4	-	2/18/38/38	0/3/3/3
5	GDP	q	501	-	-	3/12/32/32	0/3/3/3
6	TA1	Y	502	-	-	0/41/127/127	0/7/7/7
5	GDP	s	501	-	-	3/12/32/32	0/3/3/3
5	GDP	U	502	-	-	3/12/32/32	0/3/3/3
6	TA1	X	502	-	-	0/41/127/127	0/7/7/7
6	TA1	s	502	-	-	0/41/127/127	0/7/7/7
5	GDP	a	501	-	-	3/12/32/32	0/3/3/3
5	GDP	Q	501	-	-	3/12/32/32	0/3/3/3
6	TA1	Q	502	-	-	0/41/127/127	0/7/7/7
5	GDP	T	501	-	-	3/12/32/32	0/3/3/3
6	TA1	T	502	-	-	0/41/127/127	0/7/7/7
3	GTP	O	501	4	-	2/18/38/38	0/3/3/3
3	GTP	c	501	4	-	2/18/38/38	0/3/3/3
3	GTP	H	501	4	-	2/18/38/38	0/3/3/3
5	GDP	F	502	-	-	3/12/32/32	0/3/3/3
5	GDP	W	501	-	-	3/12/32/32	0/3/3/3
3	GTP	K	501	4	-	2/18/38/38	0/3/3/3
3	GTP	I	501	4	-	2/18/38/38	0/3/3/3
3	GTP	L	501	4	-	2/18/38/38	0/3/3/3
5	GDP	b	501	-	-	3/12/32/32	0/3/3/3
5	GDP	X	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TA1	b	502	-	-	0/41/127/127	0/7/7/7
6	TA1	U	501	-	-	0/41/127/127	0/7/7/7
5	GDP	V	501	-	-	3/12/32/32	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	501	GTP	C5-C4	-2.63	1.36	1.43
3	d	501	GTP	C5-C4	-2.62	1.36	1.43
3	f	501	GTP	C5-C4	-2.62	1.36	1.43
3	H	501	GTP	C5-C4	-2.62	1.36	1.43
3	E	501	GTP	C5-C4	-2.62	1.36	1.43
3	N	501	GTP	C5-C4	-2.61	1.36	1.43
3	h	501	GTP	C5-C4	-2.61	1.36	1.43
3	j	501	GTP	C5-C4	-2.61	1.36	1.43
3	A	501	GTP	C5-C4	-2.61	1.36	1.43
3	J	501	GTP	C5-C4	-2.61	1.36	1.43
3	K	501	GTP	C5-C4	-2.61	1.36	1.43
3	G	501	GTP	C5-C4	-2.60	1.36	1.43
3	k	501	GTP	C5-C4	-2.60	1.36	1.43
3	c	501	GTP	C5-C4	-2.60	1.36	1.43
3	i	501	GTP	C5-C4	-2.60	1.36	1.43
3	M	501	GTP	C5-C4	-2.60	1.36	1.43
3	C	501	GTP	C5-C4	-2.59	1.36	1.43
3	L	501	GTP	C5-C4	-2.59	1.36	1.43
3	P	501	GTP	C5-C4	-2.59	1.36	1.43
3	I	501	GTP	C5-C4	-2.59	1.36	1.43
3	O	501	GTP	C5-C4	-2.59	1.36	1.43
3	D	501	GTP	C5-C4	-2.58	1.36	1.43
3	e	501	GTP	C5-C4	-2.58	1.36	1.43
3	c	501	GTP	C6-N1	-2.53	1.34	1.37
3	N	501	GTP	C6-N1	-2.51	1.34	1.37
5	r	501	GDP	C8-N7	-2.51	1.30	1.35
3	e	501	GTP	C6-N1	-2.51	1.34	1.37
5	o	501	GDP	C8-N7	-2.50	1.30	1.35
5	F	502	GDP	C8-N7	-2.50	1.30	1.35
5	X	501	GDP	C8-N7	-2.50	1.30	1.35
5	T	501	GDP	C8-N7	-2.49	1.30	1.35
5	V	501	GDP	C8-N7	-2.49	1.30	1.35
5	Q	501	GDP	C8-N7	-2.49	1.30	1.35
5	R	501	GDP	C8-N7	-2.49	1.30	1.35
3	E	501	GTP	C6-N1	-2.49	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	j	501	GTP	C6-N1	-2.49	1.34	1.37
5	B	501	GDP	C8-N7	-2.48	1.30	1.35
3	G	501	GTP	C6-N1	-2.48	1.34	1.37
3	P	501	GTP	C6-N1	-2.48	1.34	1.37
3	h	501	GTP	C6-N1	-2.48	1.34	1.37
3	C	501	GTP	C6-N1	-2.48	1.34	1.37
5	S	501	GDP	C8-N7	-2.47	1.30	1.35
5	q	501	GDP	C8-N7	-2.47	1.30	1.35
5	b	501	GDP	C8-N7	-2.47	1.30	1.35
5	U	502	GDP	C8-N7	-2.47	1.30	1.35
5	s	501	GDP	C8-N7	-2.47	1.30	1.35
3	J	501	GTP	C6-N1	-2.47	1.34	1.37
3	f	501	GTP	C6-N1	-2.47	1.34	1.37
3	L	501	GTP	C6-N1	-2.47	1.34	1.37
3	D	501	GTP	C6-N1	-2.47	1.34	1.37
5	W	501	GDP	C8-N7	-2.47	1.30	1.35
3	A	501	GTP	C6-N1	-2.47	1.34	1.37
5	a	501	GDP	C8-N7	-2.46	1.30	1.35
3	K	501	GTP	C6-N1	-2.46	1.34	1.37
3	M	501	GTP	C6-N1	-2.46	1.34	1.37
3	g	501	GTP	C6-N1	-2.46	1.34	1.37
3	H	501	GTP	C6-N1	-2.46	1.34	1.37
3	d	501	GTP	C6-N1	-2.46	1.34	1.37
5	Y	501	GDP	C8-N7	-2.46	1.30	1.35
5	p	501	GDP	C8-N7	-2.46	1.30	1.35
3	I	501	GTP	C6-N1	-2.45	1.34	1.37
3	k	501	GTP	C6-N1	-2.44	1.34	1.37
5	Z	501	GDP	C8-N7	-2.43	1.30	1.35
3	i	501	GTP	C6-N1	-2.41	1.34	1.37
3	O	501	GTP	C6-N1	-2.41	1.34	1.37
5	Q	501	GDP	C5-C4	-2.02	1.37	1.43
5	p	501	GDP	C5-C4	-2.01	1.37	1.43
5	r	501	GDP	C5-C4	-2.01	1.38	1.43
5	Z	501	GDP	C5-C4	-2.01	1.38	1.43
5	X	501	GDP	C5-C4	-2.00	1.38	1.43

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	501	GDP	PA-O3A-PB	-4.68	116.76	132.83
5	o	501	GDP	PA-O3A-PB	-4.68	116.77	132.83
5	F	502	GDP	PA-O3A-PB	-4.68	116.78	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	501	GDP	PA-O3A-PB	-4.68	116.78	132.83
5	S	501	GDP	PA-O3A-PB	-4.67	116.79	132.83
5	s	501	GDP	PA-O3A-PB	-4.67	116.79	132.83
5	V	501	GDP	PA-O3A-PB	-4.67	116.79	132.83
5	a	501	GDP	PA-O3A-PB	-4.67	116.79	132.83
5	B	501	GDP	PA-O3A-PB	-4.67	116.80	132.83
5	U	502	GDP	PA-O3A-PB	-4.67	116.80	132.83
5	Q	501	GDP	PA-O3A-PB	-4.67	116.81	132.83
5	T	501	GDP	PA-O3A-PB	-4.67	116.82	132.83
5	p	501	GDP	PA-O3A-PB	-4.67	116.82	132.83
5	R	501	GDP	PA-O3A-PB	-4.66	116.82	132.83
5	Z	501	GDP	PA-O3A-PB	-4.66	116.82	132.83
5	b	501	GDP	PA-O3A-PB	-4.66	116.82	132.83
5	Y	501	GDP	PA-O3A-PB	-4.66	116.83	132.83
5	r	501	GDP	PA-O3A-PB	-4.66	116.84	132.83
5	q	501	GDP	PA-O3A-PB	-4.66	116.85	132.83
3	L	501	GTP	PB-O3B-PG	-4.03	119.00	132.83
3	G	501	GTP	PB-O3B-PG	-4.03	119.00	132.83
3	K	501	GTP	PB-O3B-PG	-4.03	119.01	132.83
3	h	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
3	d	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
3	M	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
3	e	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
3	C	501	GTP	PB-O3B-PG	-4.02	119.02	132.83
3	O	501	GTP	PB-O3B-PG	-4.02	119.03	132.83
3	i	501	GTP	PB-O3B-PG	-4.02	119.03	132.83
3	A	501	GTP	PB-O3B-PG	-4.02	119.03	132.83
3	k	501	GTP	PB-O3B-PG	-4.02	119.03	132.83
3	E	501	GTP	PB-O3B-PG	-4.02	119.04	132.83
3	j	501	GTP	PB-O3B-PG	-4.02	119.04	132.83
3	g	501	GTP	PB-O3B-PG	-4.02	119.04	132.83
3	f	501	GTP	PB-O3B-PG	-4.02	119.04	132.83
3	c	501	GTP	PB-O3B-PG	-4.02	119.04	132.83
3	H	501	GTP	PB-O3B-PG	-4.02	119.04	132.83
3	I	501	GTP	PB-O3B-PG	-4.02	119.05	132.83
3	N	501	GTP	PB-O3B-PG	-4.02	119.05	132.83
3	D	501	GTP	PB-O3B-PG	-4.01	119.05	132.83
3	J	501	GTP	PB-O3B-PG	-4.01	119.07	132.83
3	P	501	GTP	PB-O3B-PG	-4.01	119.08	132.83
3	H	501	GTP	O4'-C1'-C2'	-3.98	101.11	106.93
3	J	501	GTP	O4'-C1'-C2'	-3.98	101.11	106.93
3	E	501	GTP	O4'-C1'-C2'	-3.98	101.11	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	501	GTP	O4'-C1'-C2'	-3.98	101.11	106.93
3	P	501	GTP	O4'-C1'-C2'	-3.98	101.12	106.93
3	G	501	GTP	O4'-C1'-C2'	-3.97	101.12	106.93
3	N	501	GTP	O4'-C1'-C2'	-3.97	101.12	106.93
3	i	501	GTP	O4'-C1'-C2'	-3.97	101.12	106.93
3	C	501	GTP	O4'-C1'-C2'	-3.97	101.13	106.93
3	K	501	GTP	O4'-C1'-C2'	-3.97	101.13	106.93
3	h	501	GTP	O4'-C1'-C2'	-3.97	101.13	106.93
3	e	501	GTP	O4'-C1'-C2'	-3.97	101.13	106.93
3	A	501	GTP	O4'-C1'-C2'	-3.96	101.14	106.93
3	g	501	GTP	O4'-C1'-C2'	-3.96	101.14	106.93
3	M	501	GTP	O4'-C1'-C2'	-3.96	101.14	106.93
3	f	501	GTP	O4'-C1'-C2'	-3.96	101.14	106.93
3	d	501	GTP	O4'-C1'-C2'	-3.96	101.14	106.93
3	c	501	GTP	O4'-C1'-C2'	-3.96	101.15	106.93
3	I	501	GTP	O4'-C1'-C2'	-3.95	101.15	106.93
3	k	501	GTP	O4'-C1'-C2'	-3.95	101.16	106.93
3	L	501	GTP	O4'-C1'-C2'	-3.94	101.16	106.93
3	j	501	GTP	O4'-C1'-C2'	-3.93	101.18	106.93
3	D	501	GTP	O4'-C1'-C2'	-3.93	101.18	106.93
3	M	501	GTP	PA-O3A-PB	-3.22	121.77	132.83
3	k	501	GTP	PA-O3A-PB	-3.22	121.79	132.83
3	D	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
3	K	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
3	h	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
3	f	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
3	P	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
3	H	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
3	L	501	GTP	PA-O3A-PB	-3.21	121.81	132.83
3	i	501	GTP	PA-O3A-PB	-3.21	121.81	132.83
3	A	501	GTP	PA-O3A-PB	-3.21	121.82	132.83
3	I	501	GTP	PA-O3A-PB	-3.21	121.82	132.83
3	g	501	GTP	PA-O3A-PB	-3.21	121.82	132.83
3	J	501	GTP	PA-O3A-PB	-3.21	121.82	132.83
3	N	501	GTP	PA-O3A-PB	-3.21	121.82	132.83
3	j	501	GTP	PA-O3A-PB	-3.21	121.82	132.83
3	C	501	GTP	PA-O3A-PB	-3.21	121.82	132.83
3	E	501	GTP	PA-O3A-PB	-3.21	121.83	132.83
3	d	501	GTP	PA-O3A-PB	-3.20	121.83	132.83
3	G	501	GTP	PA-O3A-PB	-3.20	121.83	132.83
3	c	501	GTP	PA-O3A-PB	-3.20	121.83	132.83
3	e	501	GTP	PA-O3A-PB	-3.20	121.84	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	501	GTP	PA-O3A-PB	-3.20	121.85	132.83
3	D	501	GTP	O2G-PG-O3B	2.91	114.39	104.64
3	O	501	GTP	O2G-PG-O3B	2.90	114.38	104.64
3	G	501	GTP	O2G-PG-O3B	2.90	114.37	104.64
3	c	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	I	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	L	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	j	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	H	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	K	501	GTP	O2G-PG-O3B	2.90	114.36	104.64
3	f	501	GTP	O2G-PG-O3B	2.90	114.35	104.64
3	C	501	GTP	O2G-PG-O3B	2.90	114.35	104.64
3	A	501	GTP	O2G-PG-O3B	2.90	114.35	104.64
3	k	501	GTP	O2G-PG-O3B	2.90	114.35	104.64
3	d	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	N	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	E	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	h	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	g	501	GTP	O2G-PG-O3B	2.89	114.33	104.64
3	P	501	GTP	O2G-PG-O3B	2.89	114.32	104.64
3	e	501	GTP	O2G-PG-O3B	2.89	114.32	104.64
3	i	501	GTP	O2G-PG-O3B	2.89	114.32	104.64
3	M	501	GTP	O2G-PG-O3B	2.88	114.31	104.64
3	J	501	GTP	O2G-PG-O3B	2.88	114.29	104.64
5	F	502	GDP	O6-C6-N1	-2.88	117.25	120.65
5	Y	501	GDP	O6-C6-N1	-2.86	117.27	120.65
5	s	501	GDP	O6-C6-N1	-2.86	117.27	120.65
5	R	501	GDP	O6-C6-N1	-2.86	117.27	120.65
5	T	501	GDP	O6-C6-N1	-2.85	117.28	120.65
5	V	501	GDP	O6-C6-N1	-2.85	117.28	120.65
5	a	501	GDP	O6-C6-N1	-2.85	117.28	120.65
5	Q	501	GDP	O6-C6-N1	-2.85	117.28	120.65
5	U	502	GDP	O6-C6-N1	-2.85	117.28	120.65
5	b	501	GDP	O6-C6-N1	-2.85	117.28	120.65
5	B	501	GDP	O6-C6-N1	-2.85	117.29	120.65
5	Z	501	GDP	O6-C6-N1	-2.85	117.29	120.65
5	o	501	GDP	O6-C6-N1	-2.84	117.29	120.65
5	W	501	GDP	O6-C6-N1	-2.84	117.30	120.65
5	S	501	GDP	O6-C6-N1	-2.83	117.30	120.65
5	Q	501	GDP	O6-C6-C5	2.83	129.90	124.37
5	Y	501	GDP	O6-C6-C5	2.83	129.90	124.37
5	p	501	GDP	O6-C6-N1	-2.82	117.32	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	q	501	GDP	O6-C6-N1	-2.81	117.33	120.65
5	V	501	GDP	O6-C6-C5	2.81	129.87	124.37
5	X	501	GDP	O6-C6-N1	-2.81	117.33	120.65
5	Z	501	GDP	O6-C6-C5	2.81	129.86	124.37
5	o	501	GDP	O6-C6-C5	2.81	129.86	124.37
5	R	501	GDP	O6-C6-C5	2.81	129.85	124.37
5	U	502	GDP	O6-C6-C5	2.81	129.85	124.37
5	F	502	GDP	O6-C6-C5	2.80	129.85	124.37
5	r	501	GDP	O6-C6-N1	-2.80	117.34	120.65
5	B	501	GDP	O6-C6-C5	2.80	129.84	124.37
5	T	501	GDP	O6-C6-C5	2.80	129.83	124.37
5	p	501	GDP	O6-C6-C5	2.79	129.83	124.37
5	a	501	GDP	O6-C6-C5	2.79	129.82	124.37
5	r	501	GDP	O6-C6-C5	2.79	129.82	124.37
5	X	501	GDP	O6-C6-C5	2.79	129.81	124.37
5	b	501	GDP	O6-C6-C5	2.78	129.81	124.37
5	s	501	GDP	O6-C6-C5	2.78	129.81	124.37
5	S	501	GDP	O6-C6-C5	2.78	129.81	124.37
5	q	501	GDP	O6-C6-C5	2.78	129.80	124.37
5	W	501	GDP	O6-C6-C5	2.76	129.77	124.37
6	a	502	TA1	C02-O02-C03	2.60	122.71	117.79
6	F	501	TA1	C02-O02-C03	2.60	122.70	117.79
6	R	502	TA1	C02-O02-C03	2.59	122.70	117.79
6	S	502	TA1	C02-O02-C03	2.59	122.69	117.79
6	V	502	TA1	C02-O02-C03	2.59	122.69	117.79
6	b	502	TA1	C02-O02-C03	2.59	122.69	117.79
6	Y	502	TA1	C02-O02-C03	2.59	122.69	117.79
6	r	502	TA1	C02-O02-C03	2.59	122.68	117.79
6	B	502	TA1	C02-O02-C03	2.59	122.68	117.79
6	T	502	TA1	C02-O02-C03	2.58	122.68	117.79
6	p	502	TA1	C02-O02-C03	2.58	122.66	117.79
6	X	502	TA1	C02-O02-C03	2.57	122.66	117.79
6	Z	502	TA1	C02-O02-C03	2.57	122.66	117.79
6	o	502	TA1	C02-O02-C03	2.57	122.66	117.79
6	W	502	TA1	C02-O02-C03	2.57	122.65	117.79
6	q	502	TA1	C02-O02-C03	2.57	122.65	117.79
6	Q	502	TA1	C02-O02-C03	2.57	122.65	117.79
6	U	501	TA1	C02-O02-C03	2.57	122.64	117.79
6	s	502	TA1	C02-O02-C03	2.56	122.63	117.79
3	N	501	GTP	C3'-C2'-C1'	2.18	104.27	100.98
3	i	501	GTP	C3'-C2'-C1'	2.18	104.26	100.98
3	g	501	GTP	C3'-C2'-C1'	2.18	104.25	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	GTP	C3'-C2'-C1'	2.17	104.25	100.98
3	C	501	GTP	C3'-C2'-C1'	2.17	104.25	100.98
3	I	501	GTP	C3'-C2'-C1'	2.17	104.24	100.98
3	G	501	GTP	C3'-C2'-C1'	2.17	104.24	100.98
3	H	501	GTP	C3'-C2'-C1'	2.17	104.24	100.98
3	j	501	GTP	C3'-C2'-C1'	2.16	104.23	100.98
3	e	501	GTP	C3'-C2'-C1'	2.16	104.23	100.98
3	f	501	GTP	C3'-C2'-C1'	2.16	104.23	100.98
3	M	501	GTP	C3'-C2'-C1'	2.16	104.22	100.98
3	d	501	GTP	C3'-C2'-C1'	2.16	104.22	100.98
3	A	501	GTP	C3'-C2'-C1'	2.15	104.22	100.98
3	h	501	GTP	C3'-C2'-C1'	2.15	104.22	100.98
3	P	501	GTP	C3'-C2'-C1'	2.15	104.21	100.98
3	L	501	GTP	C3'-C2'-C1'	2.15	104.21	100.98
3	D	501	GTP	C3'-C2'-C1'	2.15	104.21	100.98
3	J	501	GTP	C3'-C2'-C1'	2.15	104.21	100.98
3	k	501	GTP	C3'-C2'-C1'	2.14	104.21	100.98
3	O	501	GTP	C3'-C2'-C1'	2.14	104.20	100.98
3	K	501	GTP	C3'-C2'-C1'	2.14	104.20	100.98
3	c	501	GTP	C3'-C2'-C1'	2.13	104.18	100.98
3	k	501	GTP	N1-C2-N3	2.08	127.21	123.32
3	M	501	GTP	N1-C2-N3	2.08	127.21	123.32
3	g	501	GTP	N1-C2-N3	2.08	127.20	123.32
3	I	501	GTP	N1-C2-N3	2.08	127.19	123.32
3	D	501	GTP	N1-C2-N3	2.07	127.18	123.32
3	j	501	GTP	N1-C2-N3	2.07	127.18	123.32
3	P	501	GTP	N1-C2-N3	2.06	127.17	123.32
3	E	501	GTP	N1-C2-N3	2.06	127.17	123.32
3	f	501	GTP	N1-C2-N3	2.06	127.16	123.32
3	K	501	GTP	N1-C2-N3	2.05	127.16	123.32
3	G	501	GTP	N1-C2-N3	2.05	127.15	123.32
3	O	501	GTP	N1-C2-N3	2.05	127.15	123.32
3	h	501	GTP	N1-C2-N3	2.05	127.15	123.32
3	L	501	GTP	N1-C2-N3	2.05	127.15	123.32
3	d	501	GTP	N1-C2-N3	2.05	127.15	123.32
3	A	501	GTP	N1-C2-N3	2.05	127.14	123.32
3	c	501	GTP	N1-C2-N3	2.05	127.14	123.32
3	i	501	GTP	N1-C2-N3	2.04	127.13	123.32
3	J	501	GTP	N1-C2-N3	2.03	127.11	123.32
3	e	501	GTP	N1-C2-N3	2.02	127.10	123.32
3	C	501	GTP	N1-C2-N3	2.02	127.09	123.32
3	N	501	GTP	N1-C2-N3	2.02	127.09	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	501	GTP	N1-C2-N3	2.01	127.08	123.32

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GDP	C5'-O5'-PA-O3A
5	F	502	GDP	C5'-O5'-PA-O3A
5	Q	501	GDP	C5'-O5'-PA-O3A
5	R	501	GDP	C5'-O5'-PA-O3A
5	S	501	GDP	C5'-O5'-PA-O3A
5	T	501	GDP	C5'-O5'-PA-O3A
5	U	502	GDP	C5'-O5'-PA-O3A
5	V	501	GDP	C5'-O5'-PA-O3A
5	W	501	GDP	C5'-O5'-PA-O3A
5	X	501	GDP	C5'-O5'-PA-O3A
5	Y	501	GDP	C5'-O5'-PA-O3A
5	Z	501	GDP	C5'-O5'-PA-O3A
5	a	501	GDP	C5'-O5'-PA-O3A
5	b	501	GDP	C5'-O5'-PA-O3A
5	o	501	GDP	C5'-O5'-PA-O3A
5	p	501	GDP	C5'-O5'-PA-O3A
5	q	501	GDP	C5'-O5'-PA-O3A
5	r	501	GDP	C5'-O5'-PA-O3A
5	s	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O2A
5	F	502	GDP	C5'-O5'-PA-O2A
5	Q	501	GDP	C5'-O5'-PA-O2A
5	R	501	GDP	C5'-O5'-PA-O2A
5	S	501	GDP	C5'-O5'-PA-O2A
5	T	501	GDP	C5'-O5'-PA-O2A
5	U	502	GDP	C5'-O5'-PA-O2A
5	V	501	GDP	C5'-O5'-PA-O2A
5	W	501	GDP	C5'-O5'-PA-O2A
5	X	501	GDP	C5'-O5'-PA-O2A
5	Y	501	GDP	C5'-O5'-PA-O2A
5	Z	501	GDP	C5'-O5'-PA-O2A
5	a	501	GDP	C5'-O5'-PA-O2A
5	b	501	GDP	C5'-O5'-PA-O2A
5	o	501	GDP	C5'-O5'-PA-O2A
5	p	501	GDP	C5'-O5'-PA-O2A
5	q	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	r	501	GDP	C5'-O5'-PA-O2A
5	s	501	GDP	C5'-O5'-PA-O2A
3	A	501	GTP	C4'-C5'-O5'-PA
3	C	501	GTP	C4'-C5'-O5'-PA
3	D	501	GTP	C4'-C5'-O5'-PA
3	E	501	GTP	C4'-C5'-O5'-PA
3	G	501	GTP	C4'-C5'-O5'-PA
3	H	501	GTP	C4'-C5'-O5'-PA
3	I	501	GTP	C4'-C5'-O5'-PA
3	J	501	GTP	C4'-C5'-O5'-PA
3	K	501	GTP	C4'-C5'-O5'-PA
3	L	501	GTP	C4'-C5'-O5'-PA
3	M	501	GTP	C4'-C5'-O5'-PA
3	N	501	GTP	C4'-C5'-O5'-PA
3	O	501	GTP	C4'-C5'-O5'-PA
3	P	501	GTP	C4'-C5'-O5'-PA
3	c	501	GTP	C4'-C5'-O5'-PA
3	d	501	GTP	C4'-C5'-O5'-PA
3	e	501	GTP	C4'-C5'-O5'-PA
3	f	501	GTP	C4'-C5'-O5'-PA
3	g	501	GTP	C4'-C5'-O5'-PA
3	h	501	GTP	C4'-C5'-O5'-PA
3	i	501	GTP	C4'-C5'-O5'-PA
3	j	501	GTP	C4'-C5'-O5'-PA
3	k	501	GTP	C4'-C5'-O5'-PA
3	A	501	GTP	C3'-C4'-C5'-O5'
3	C	501	GTP	C3'-C4'-C5'-O5'
3	D	501	GTP	C3'-C4'-C5'-O5'
3	E	501	GTP	C3'-C4'-C5'-O5'
3	G	501	GTP	C3'-C4'-C5'-O5'
3	H	501	GTP	C3'-C4'-C5'-O5'
3	I	501	GTP	C3'-C4'-C5'-O5'
3	J	501	GTP	C3'-C4'-C5'-O5'
3	K	501	GTP	C3'-C4'-C5'-O5'
3	L	501	GTP	C3'-C4'-C5'-O5'
3	M	501	GTP	C3'-C4'-C5'-O5'
3	N	501	GTP	C3'-C4'-C5'-O5'
3	O	501	GTP	C3'-C4'-C5'-O5'
3	P	501	GTP	C3'-C4'-C5'-O5'
3	c	501	GTP	C3'-C4'-C5'-O5'
3	d	501	GTP	C3'-C4'-C5'-O5'
3	e	501	GTP	C3'-C4'-C5'-O5'

*Continued on next page...*

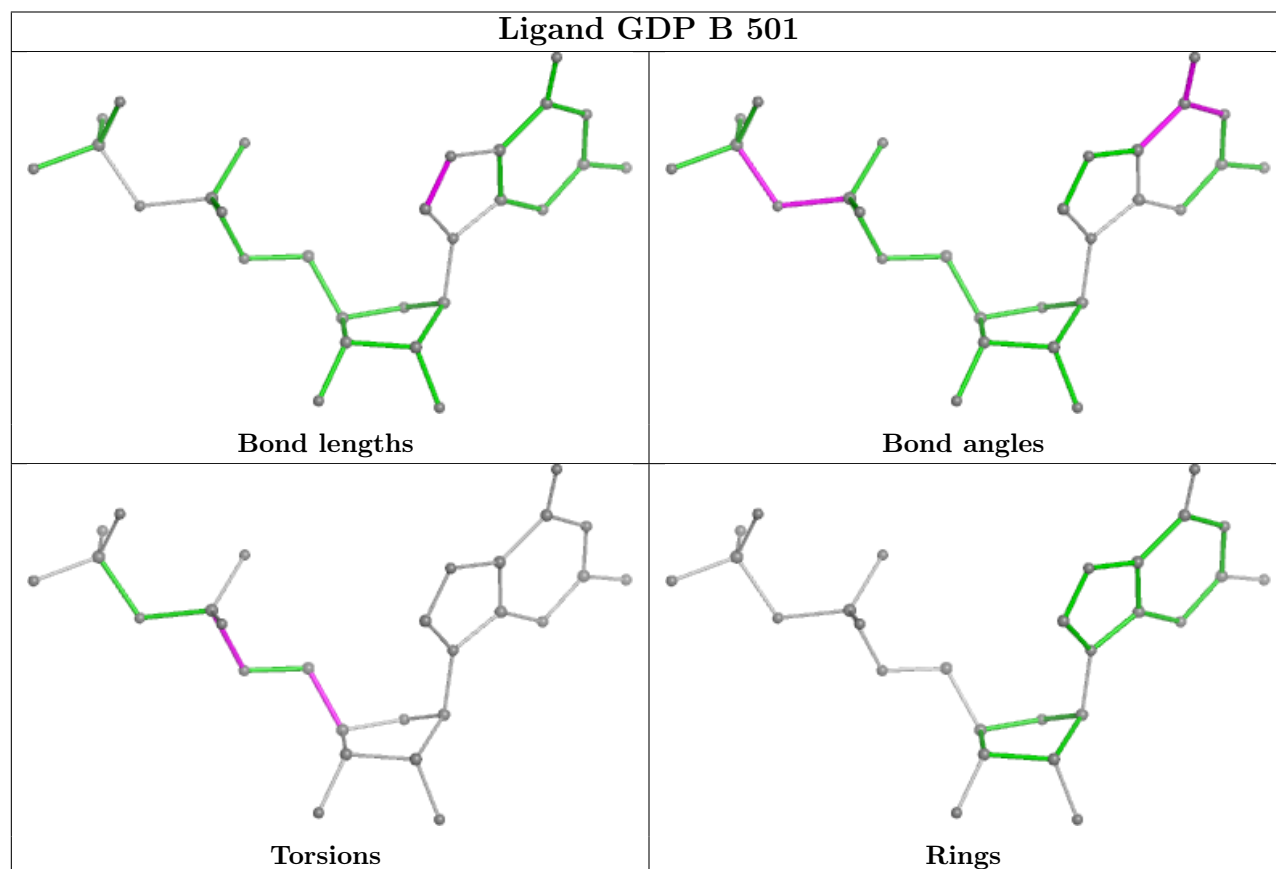
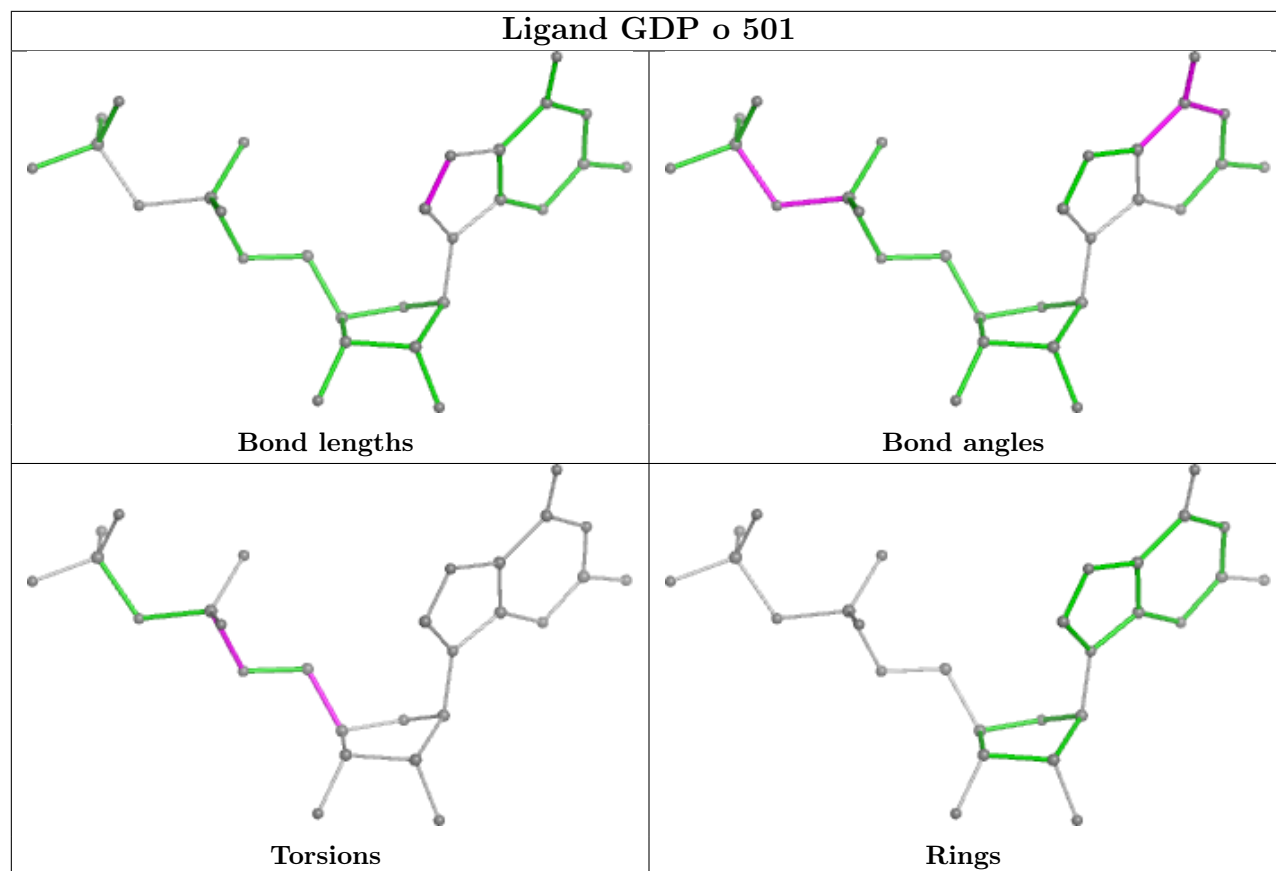
*Continued from previous page...*

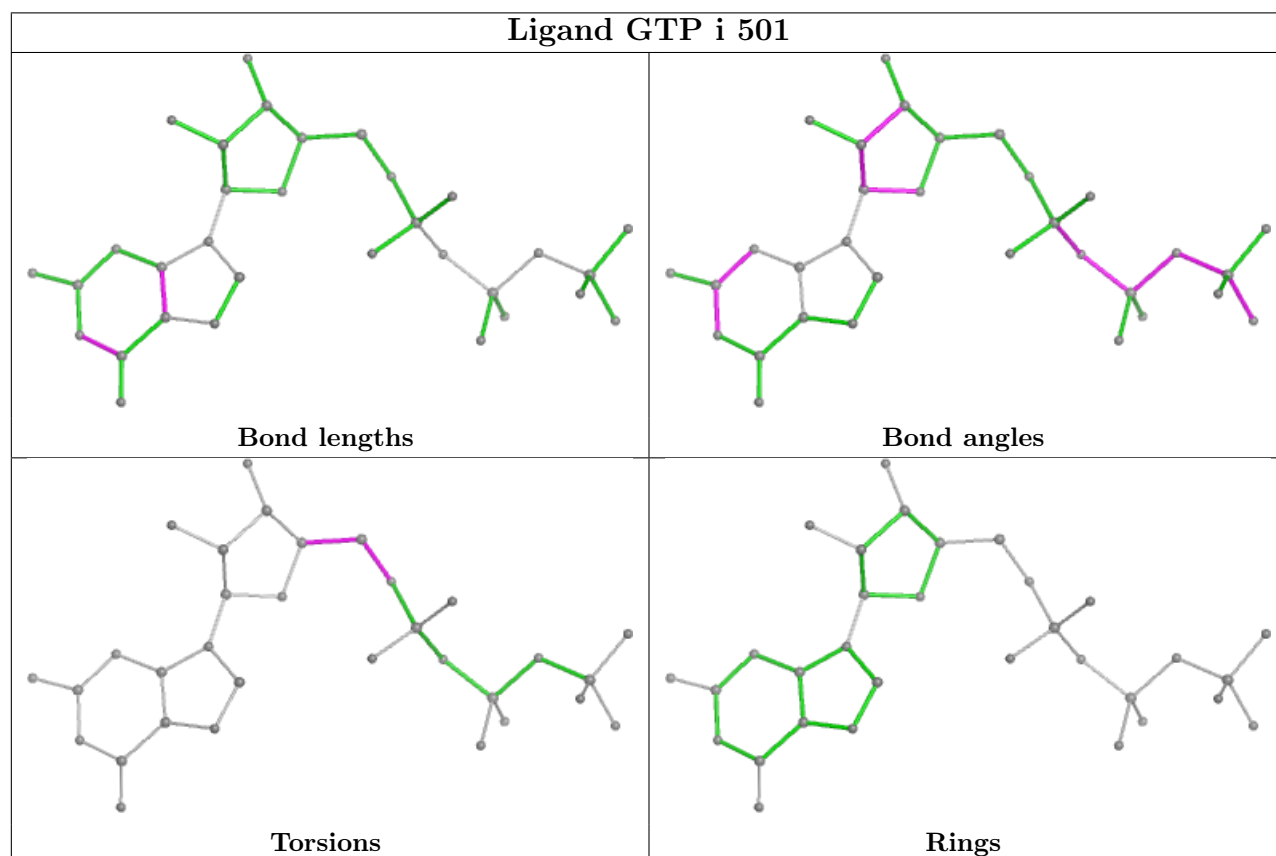
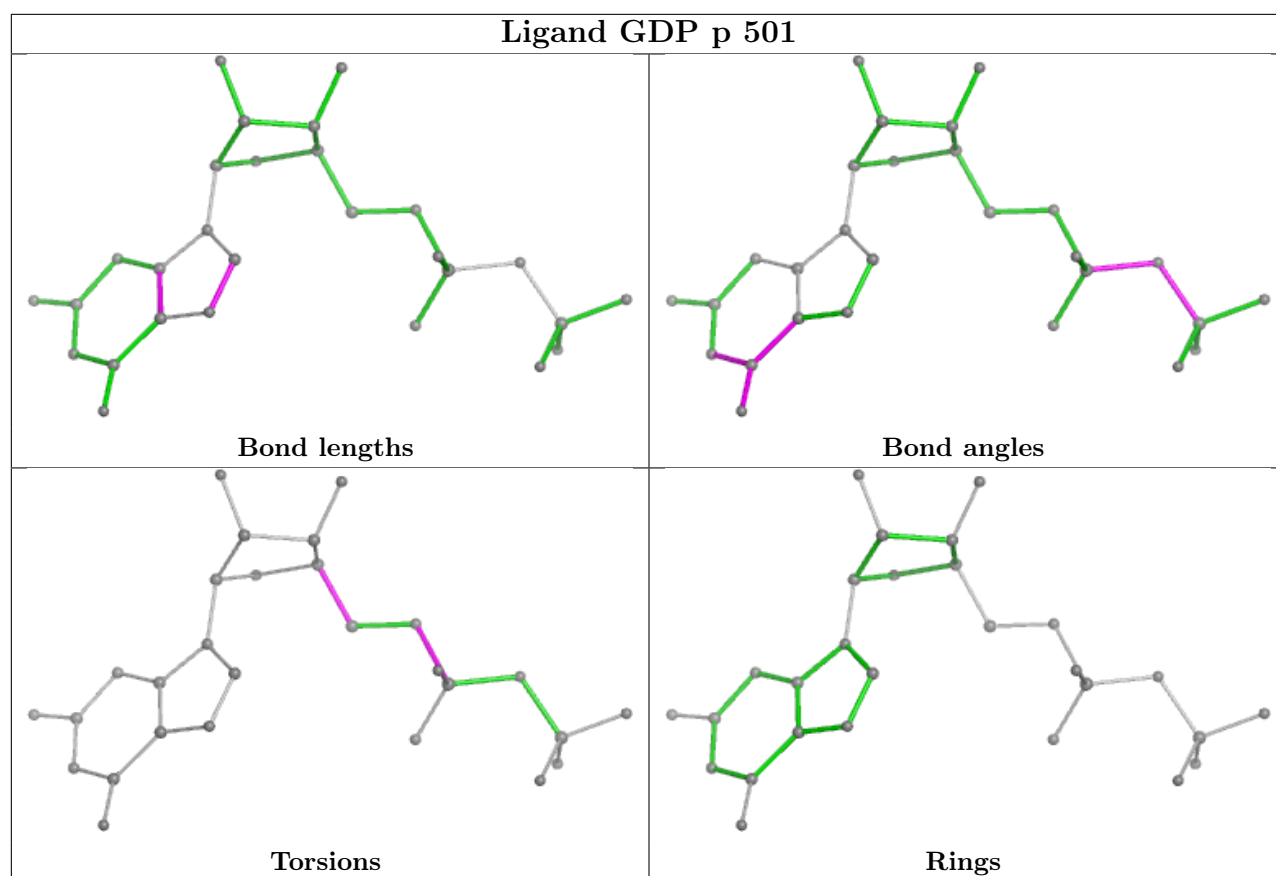
Mol	Chain	Res	Type	Atoms
3	f	501	GTP	C3'-C4'-C5'-O5'
3	g	501	GTP	C3'-C4'-C5'-O5'
3	h	501	GTP	C3'-C4'-C5'-O5'
3	i	501	GTP	C3'-C4'-C5'-O5'
3	j	501	GTP	C3'-C4'-C5'-O5'
3	k	501	GTP	C3'-C4'-C5'-O5'
5	B	501	GDP	O4'-C4'-C5'-O5'
5	F	502	GDP	O4'-C4'-C5'-O5'
5	Q	501	GDP	O4'-C4'-C5'-O5'
5	R	501	GDP	O4'-C4'-C5'-O5'
5	S	501	GDP	O4'-C4'-C5'-O5'
5	T	501	GDP	O4'-C4'-C5'-O5'
5	U	502	GDP	O4'-C4'-C5'-O5'
5	V	501	GDP	O4'-C4'-C5'-O5'
5	W	501	GDP	O4'-C4'-C5'-O5'
5	X	501	GDP	O4'-C4'-C5'-O5'
5	Y	501	GDP	O4'-C4'-C5'-O5'
5	Z	501	GDP	O4'-C4'-C5'-O5'
5	a	501	GDP	O4'-C4'-C5'-O5'
5	b	501	GDP	O4'-C4'-C5'-O5'
5	o	501	GDP	O4'-C4'-C5'-O5'
5	p	501	GDP	O4'-C4'-C5'-O5'
5	q	501	GDP	O4'-C4'-C5'-O5'
5	r	501	GDP	O4'-C4'-C5'-O5'
5	s	501	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

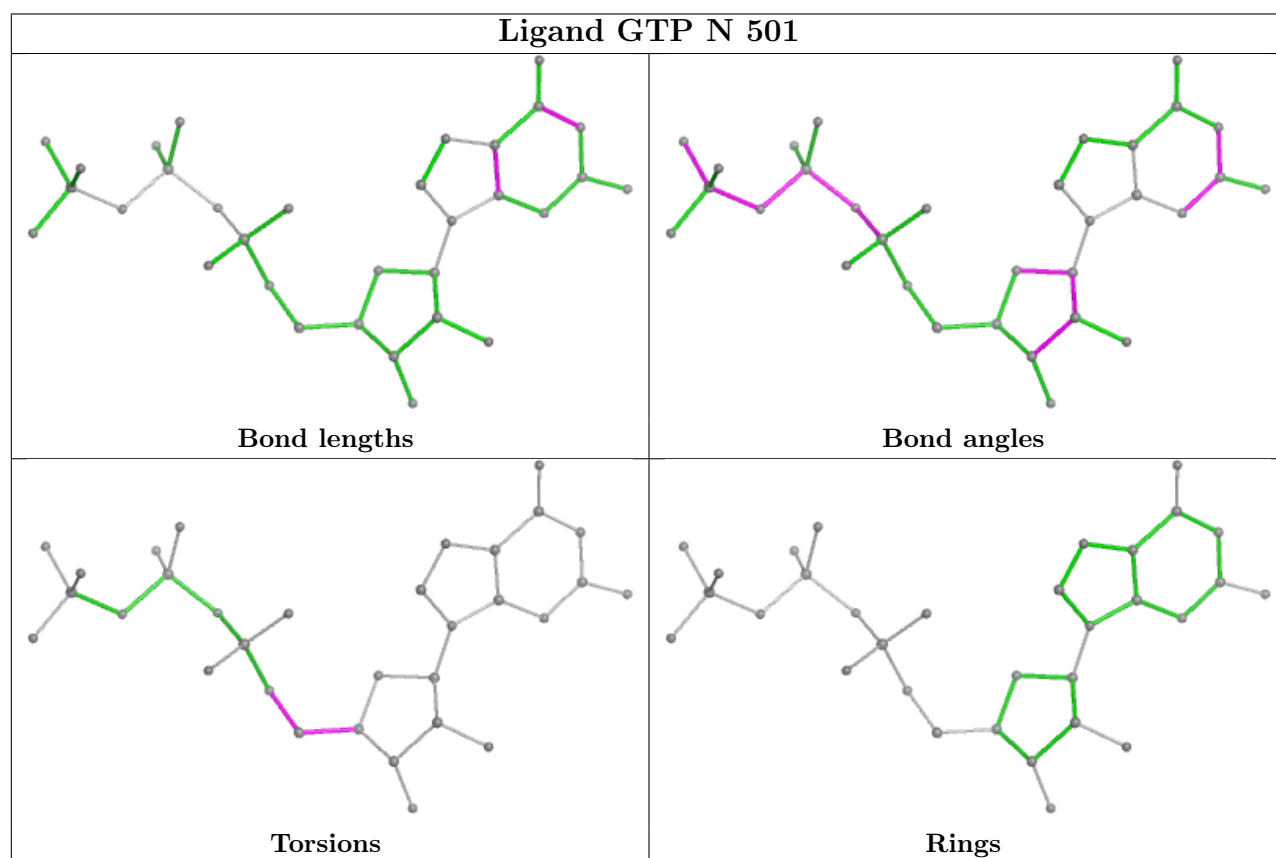
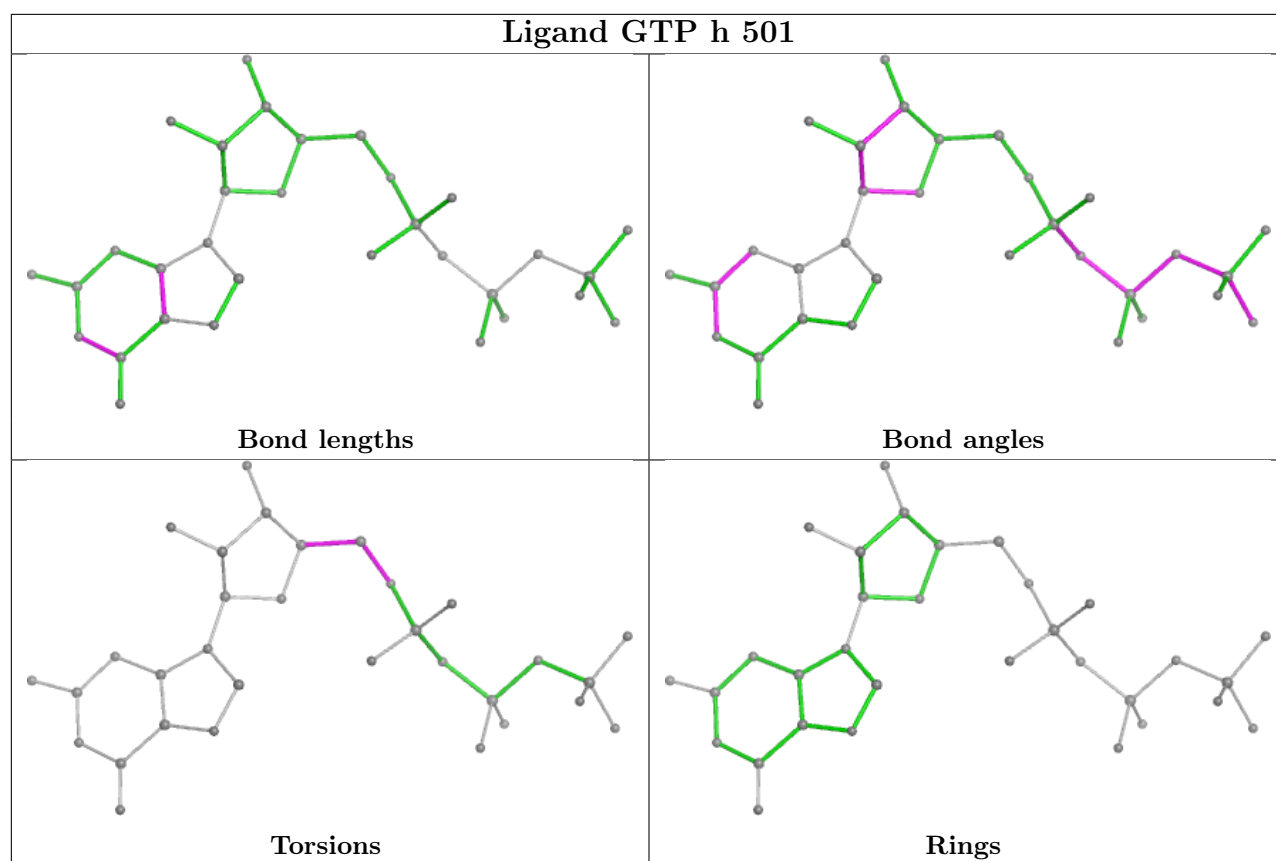
No monomer is involved in short contacts.

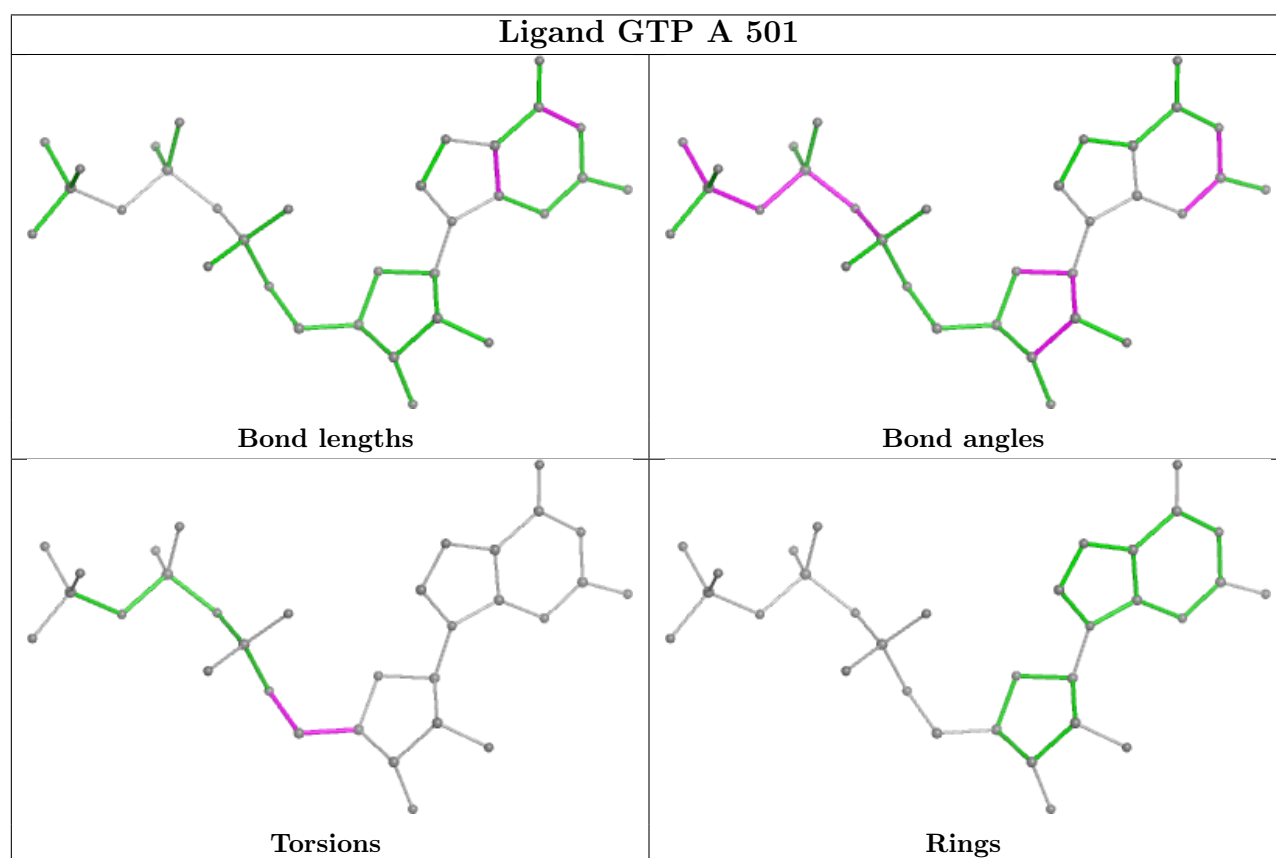
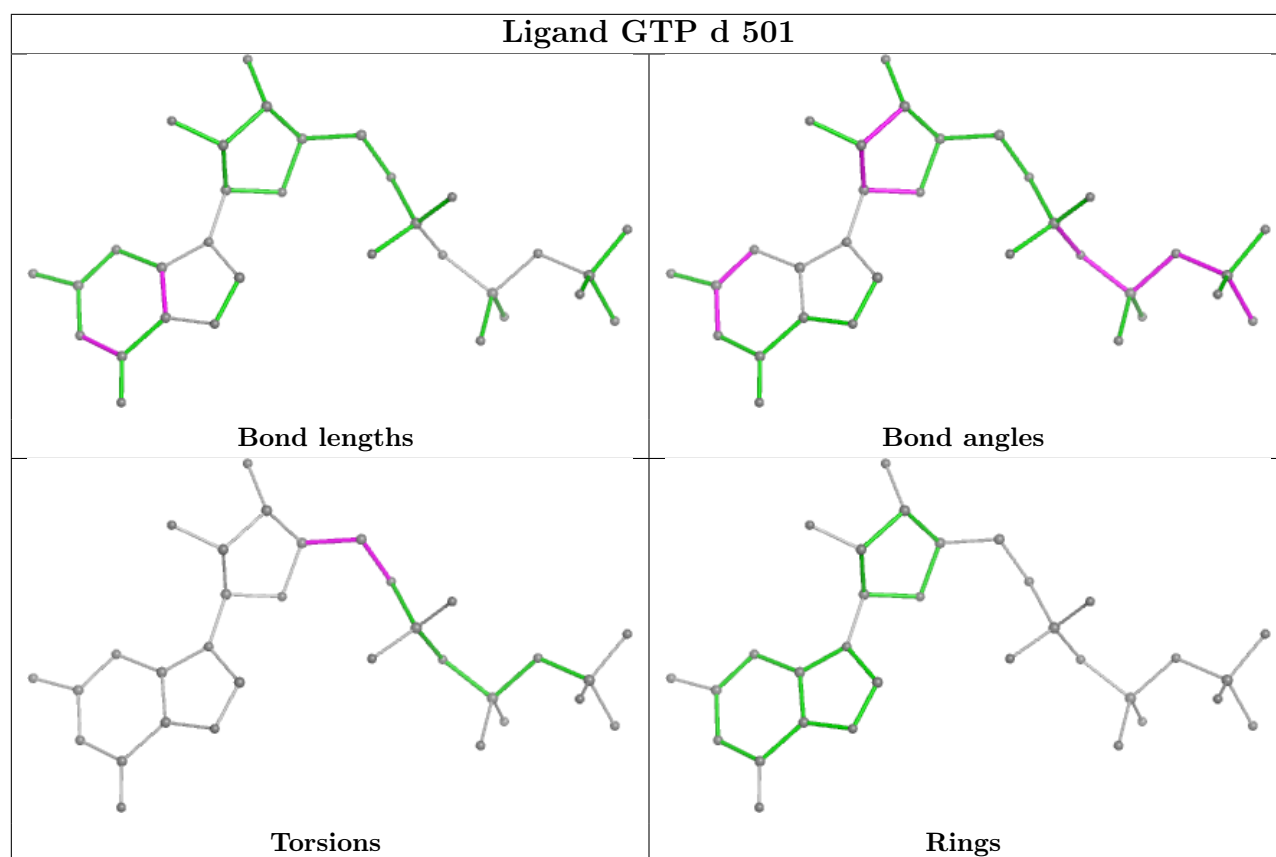
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

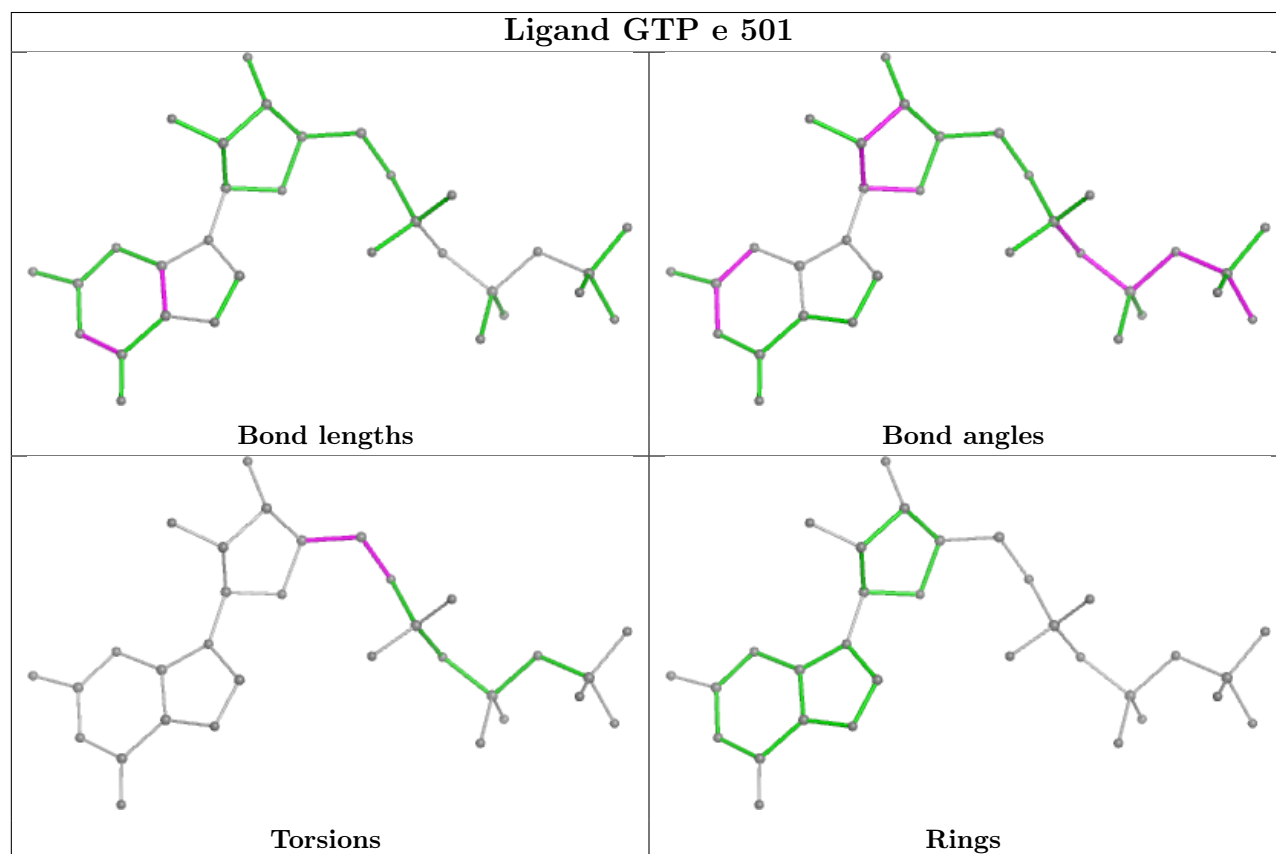
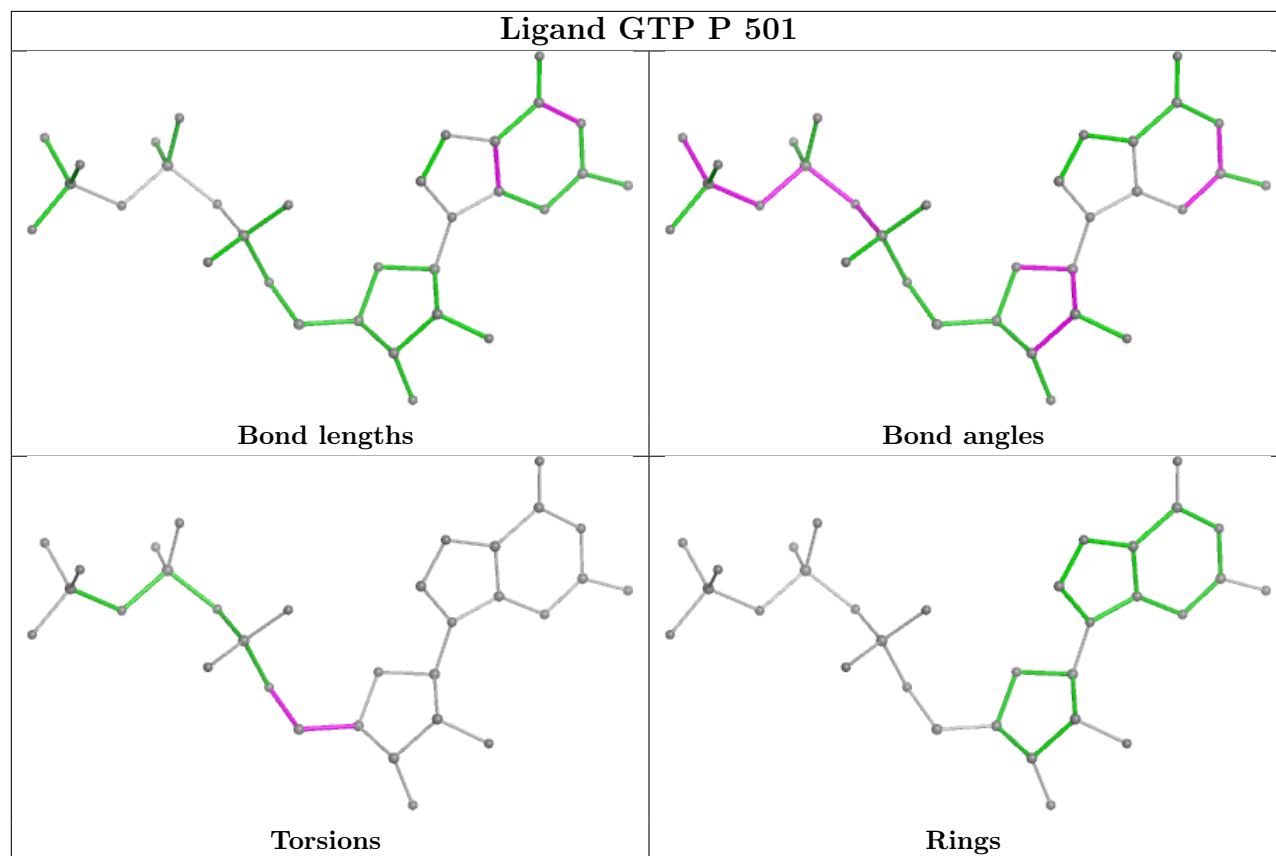


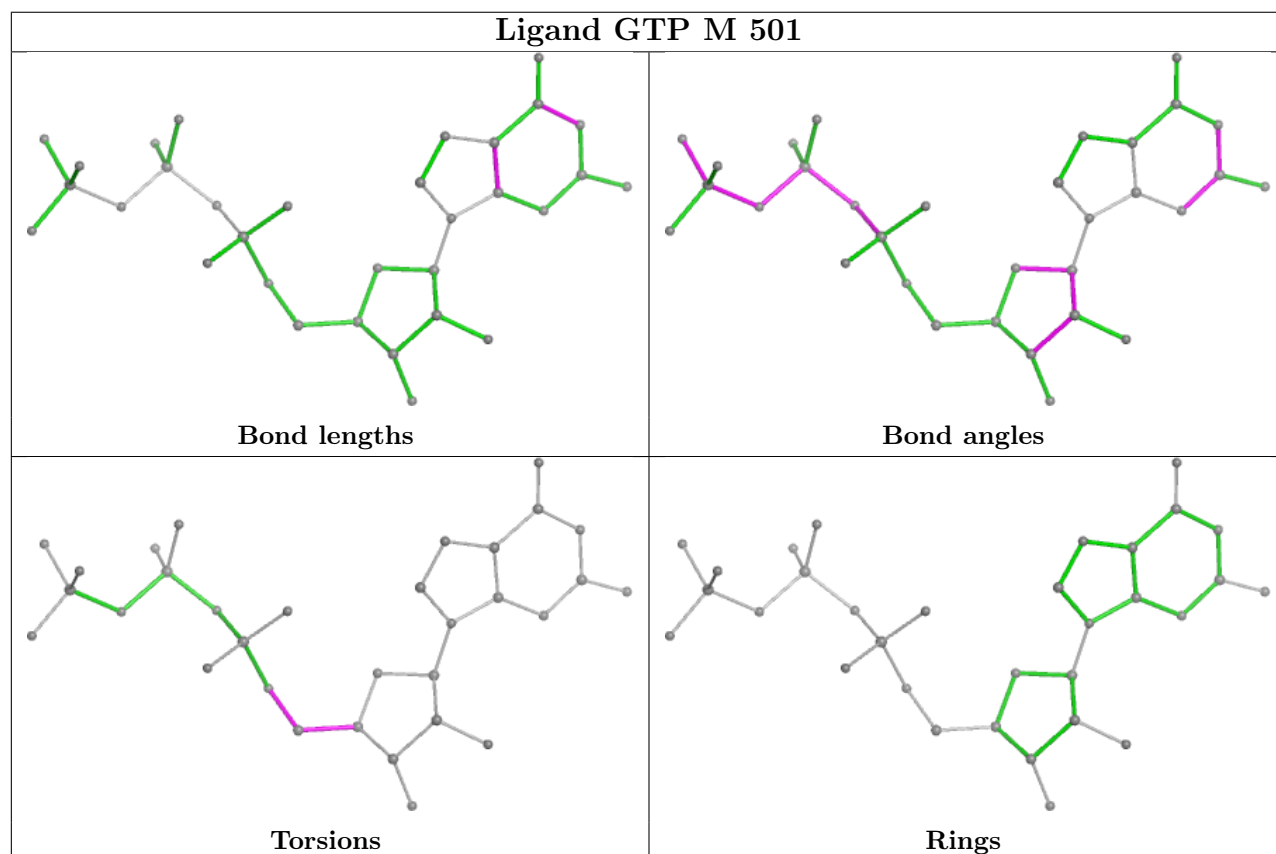
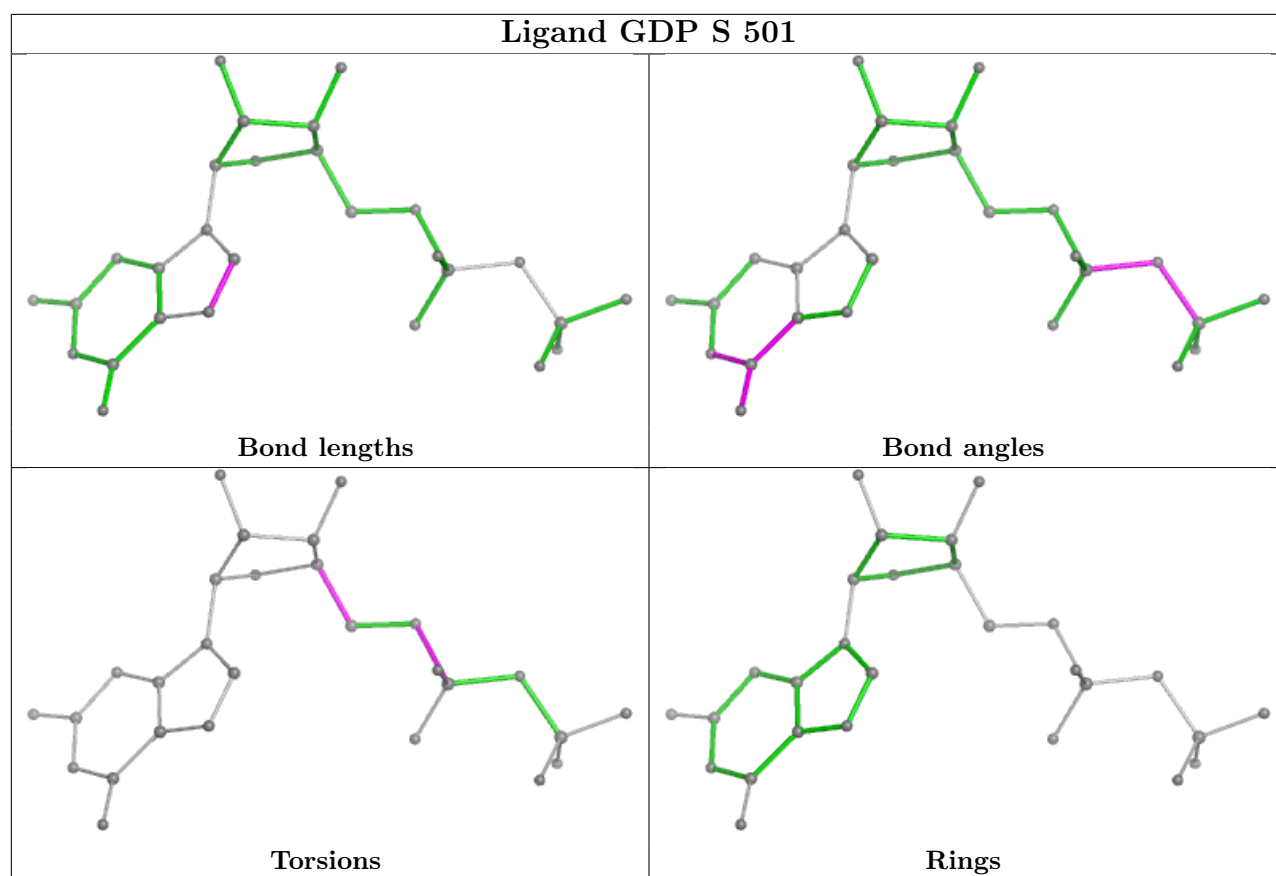


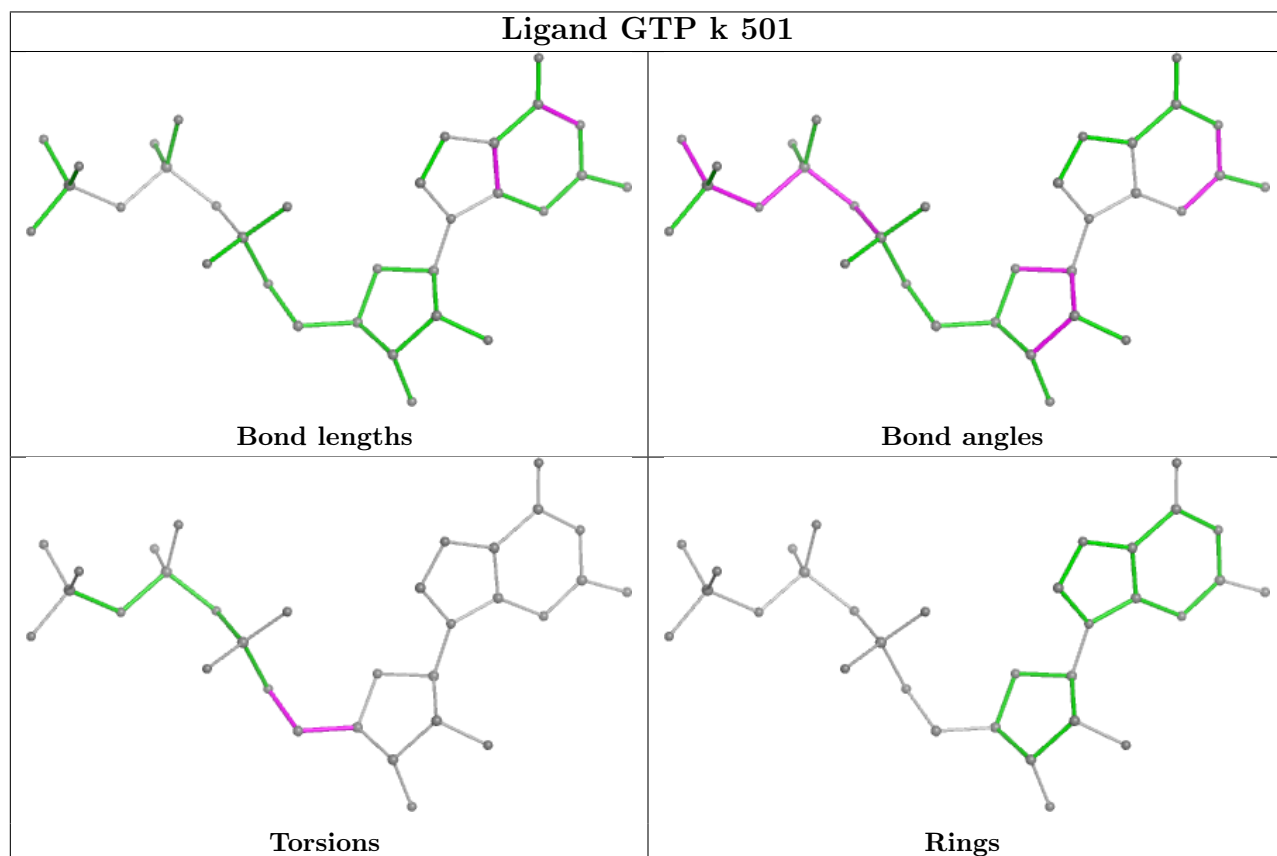
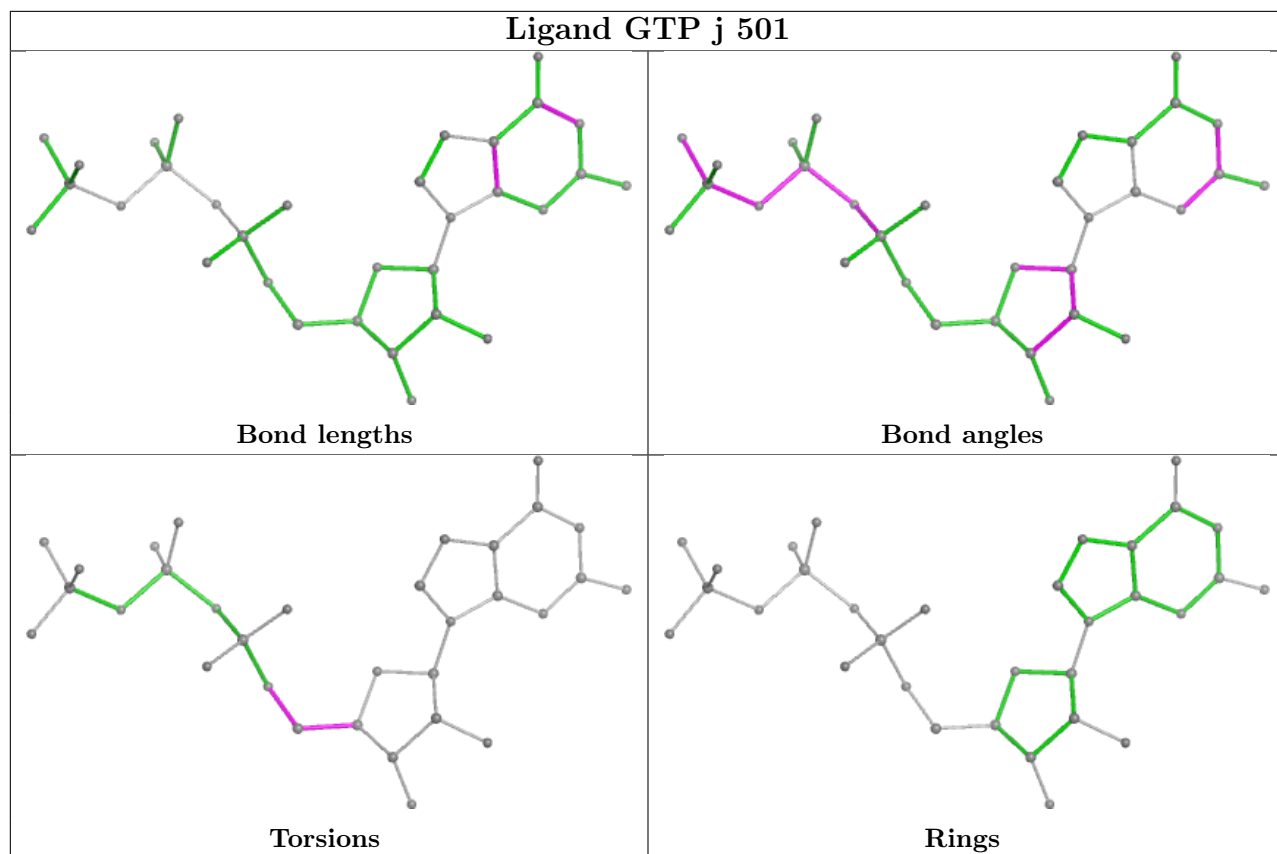


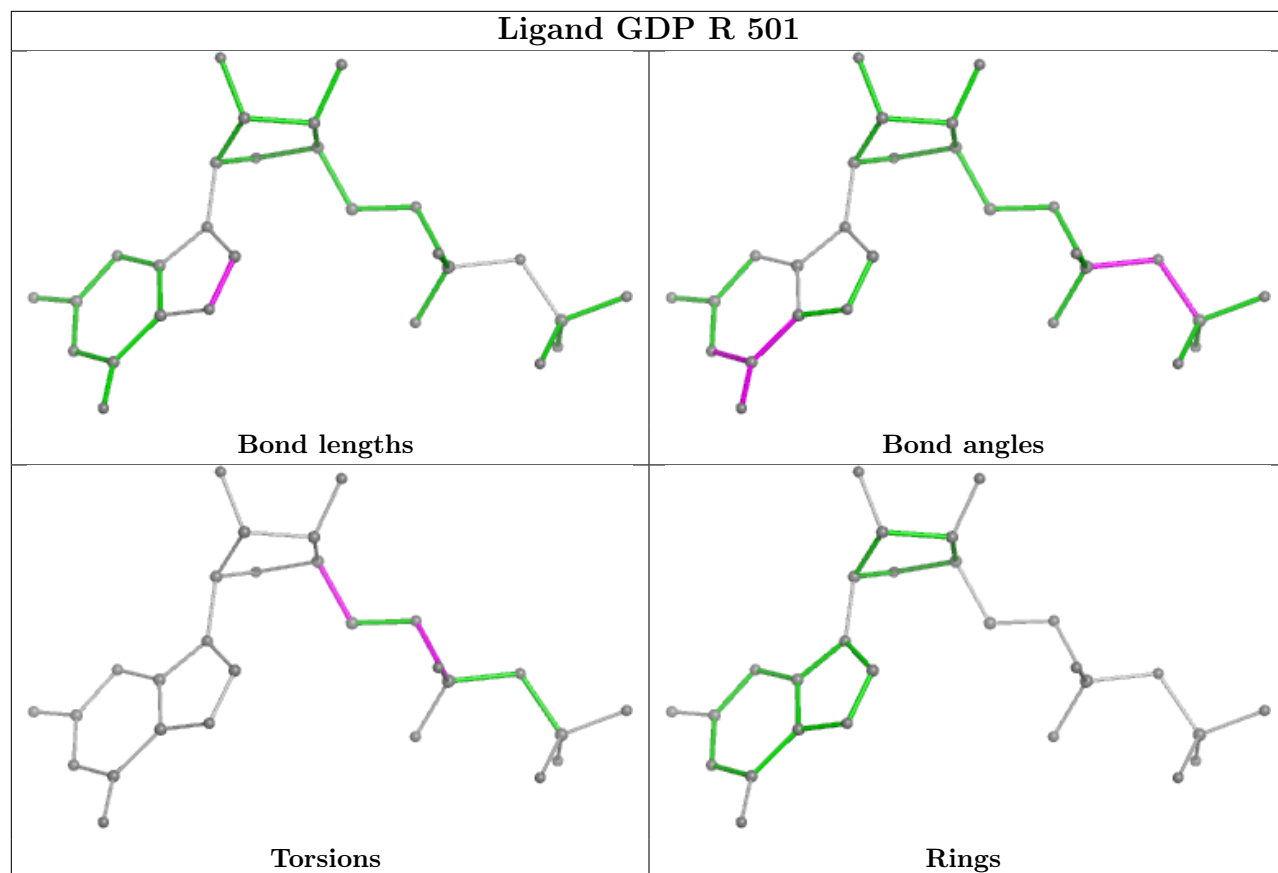


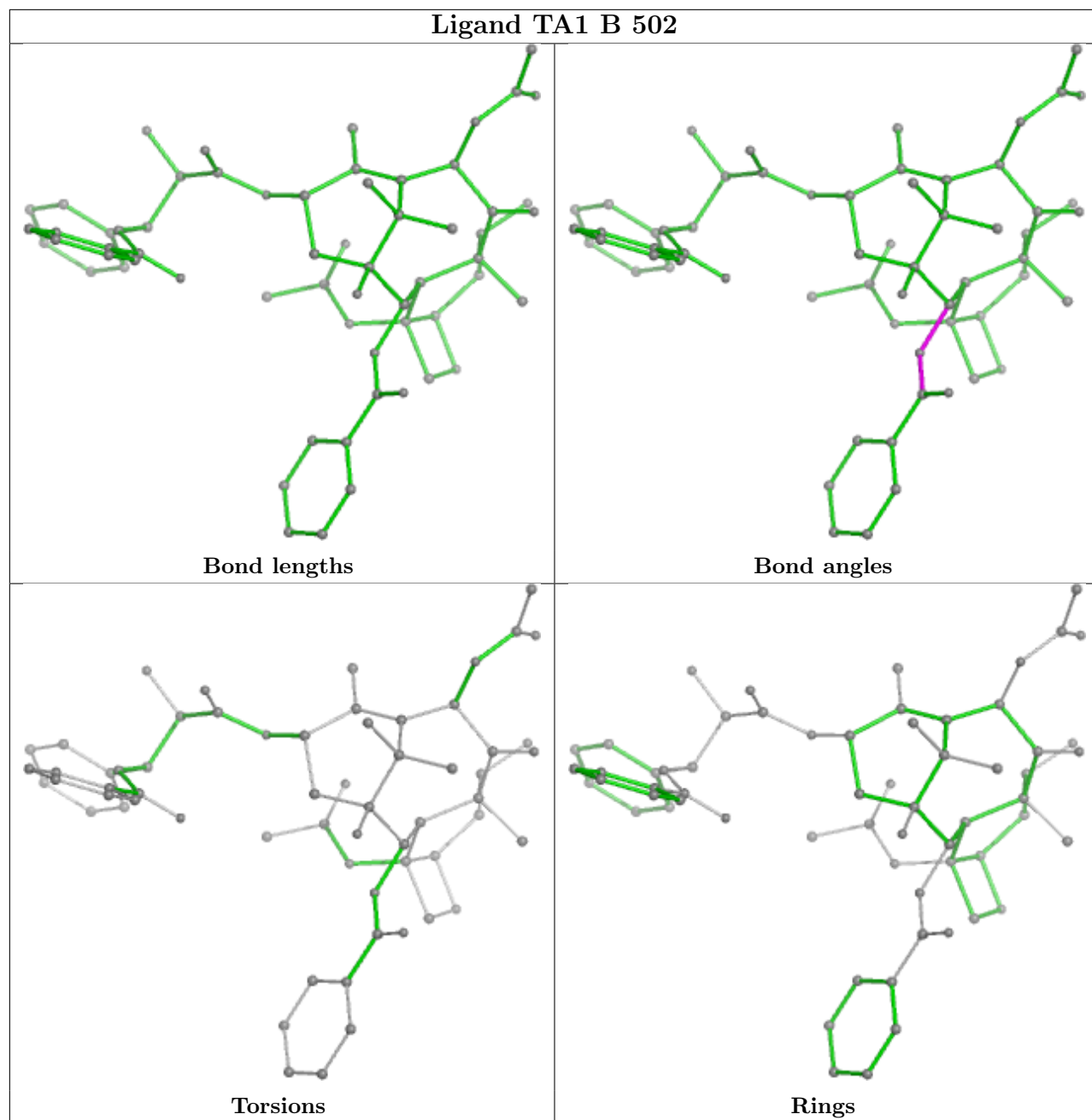


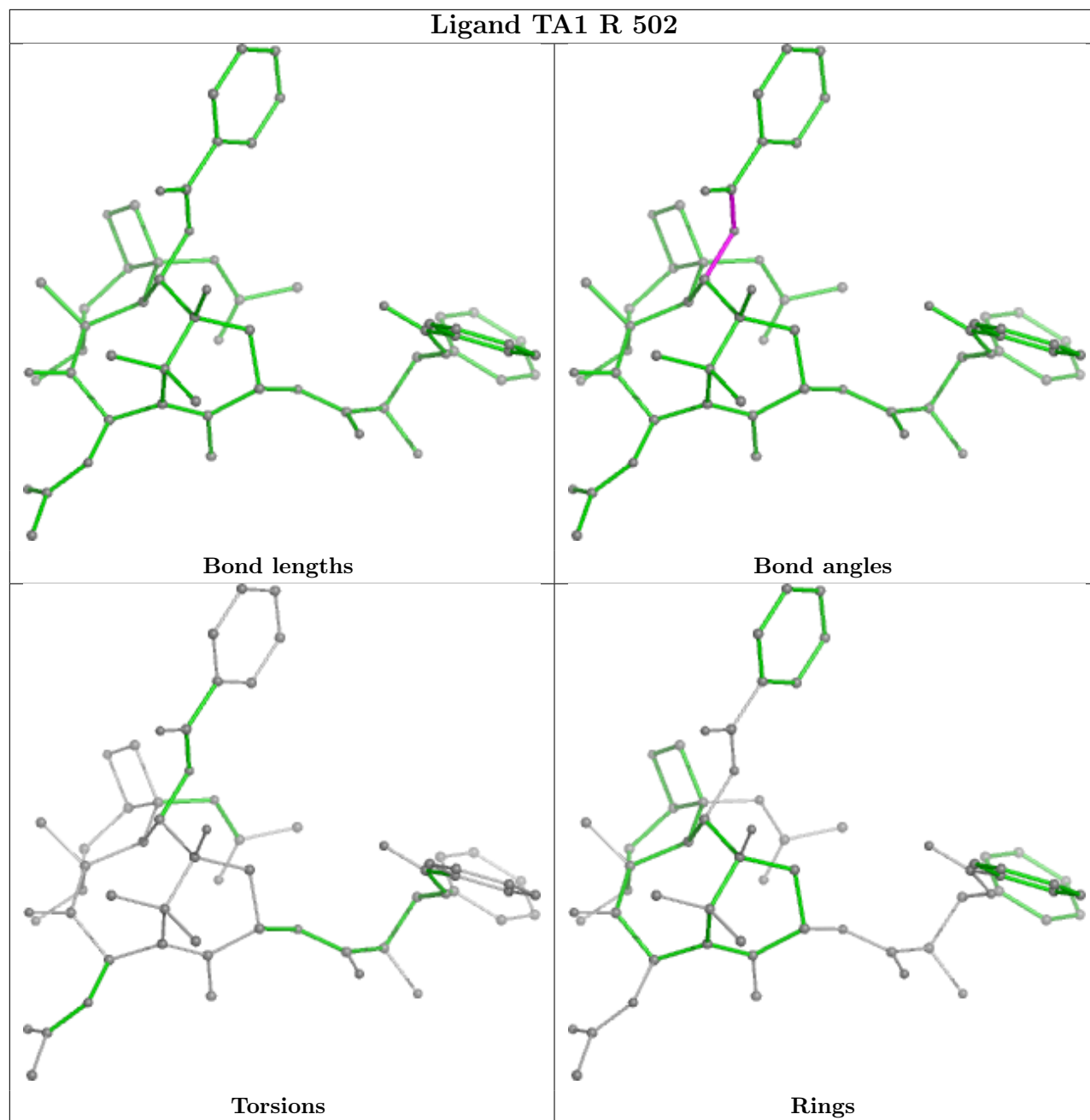




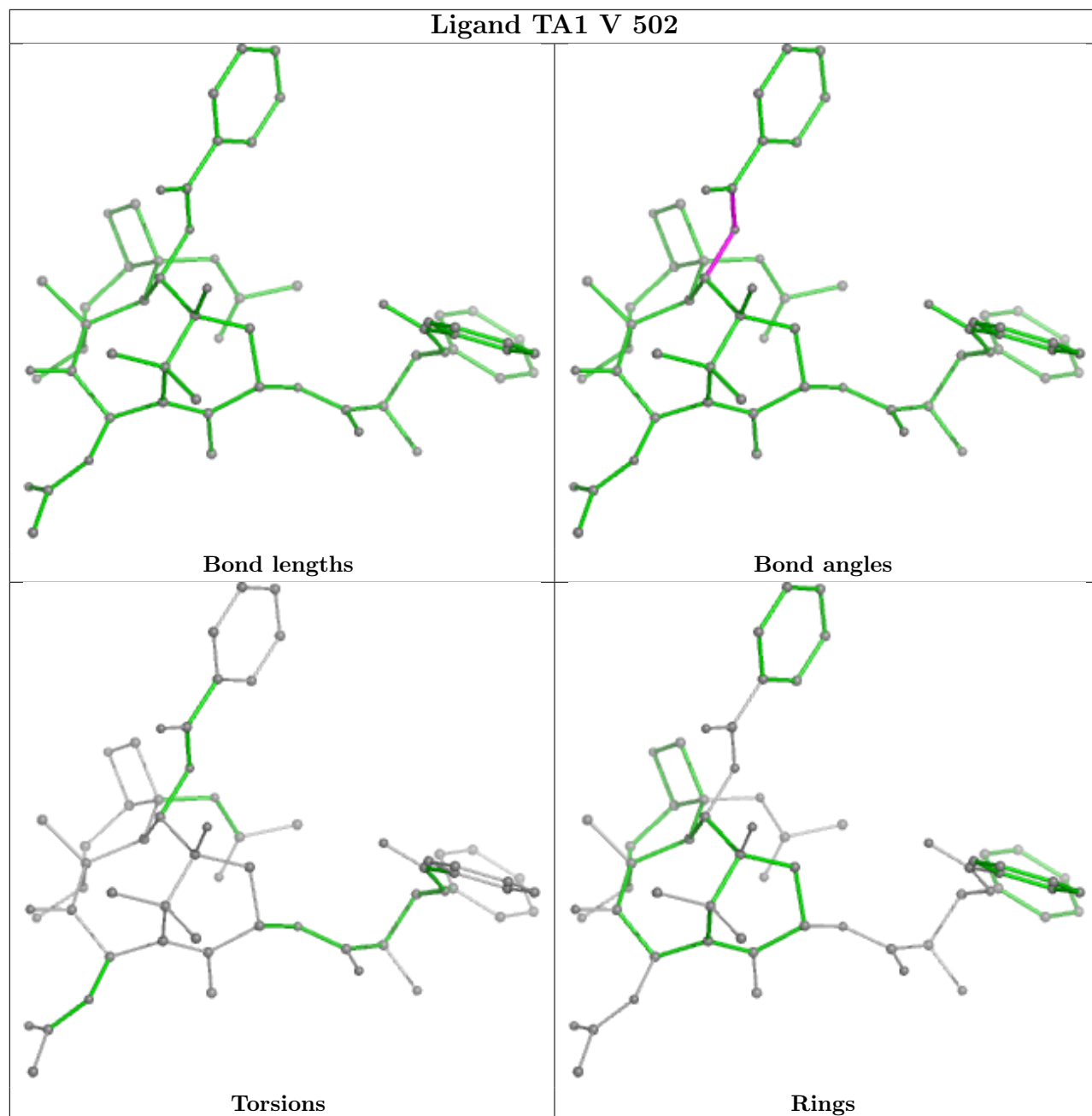


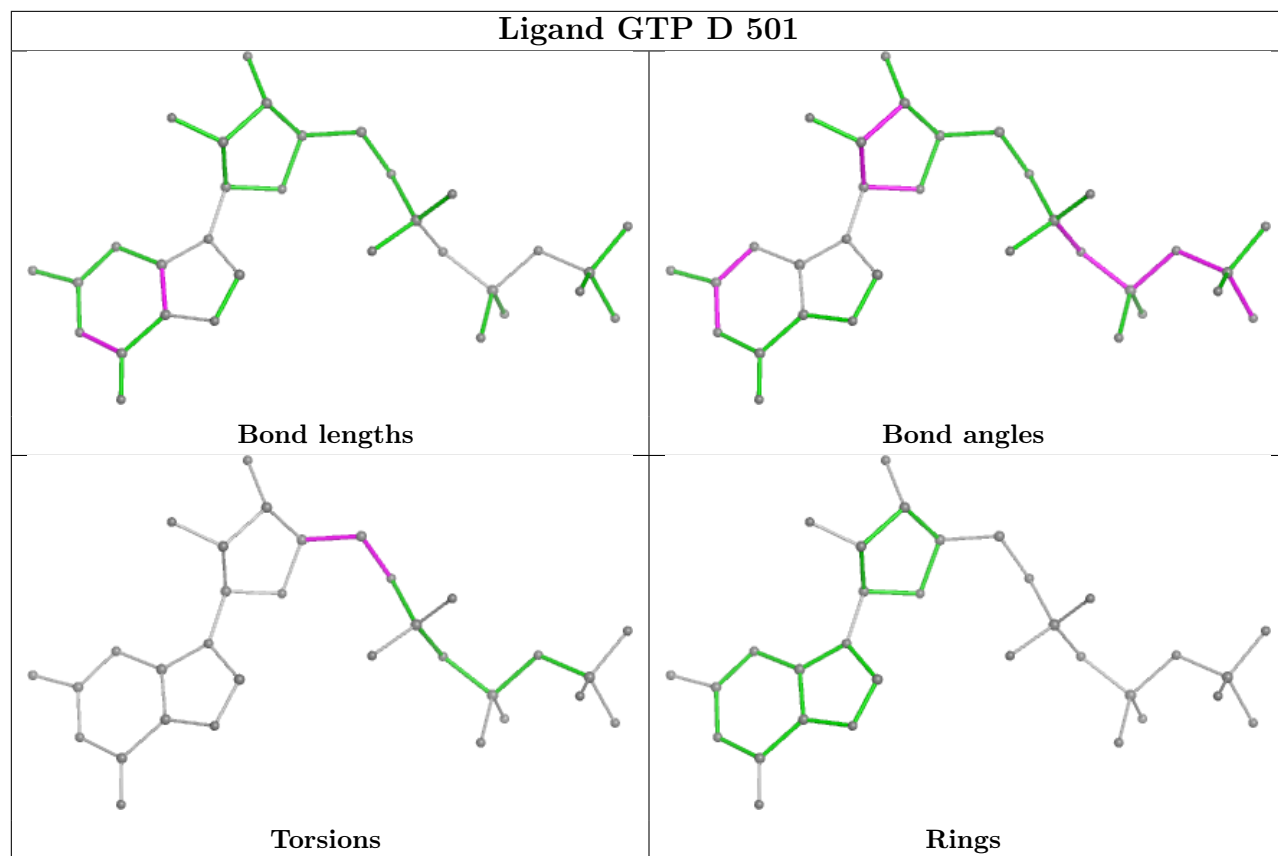


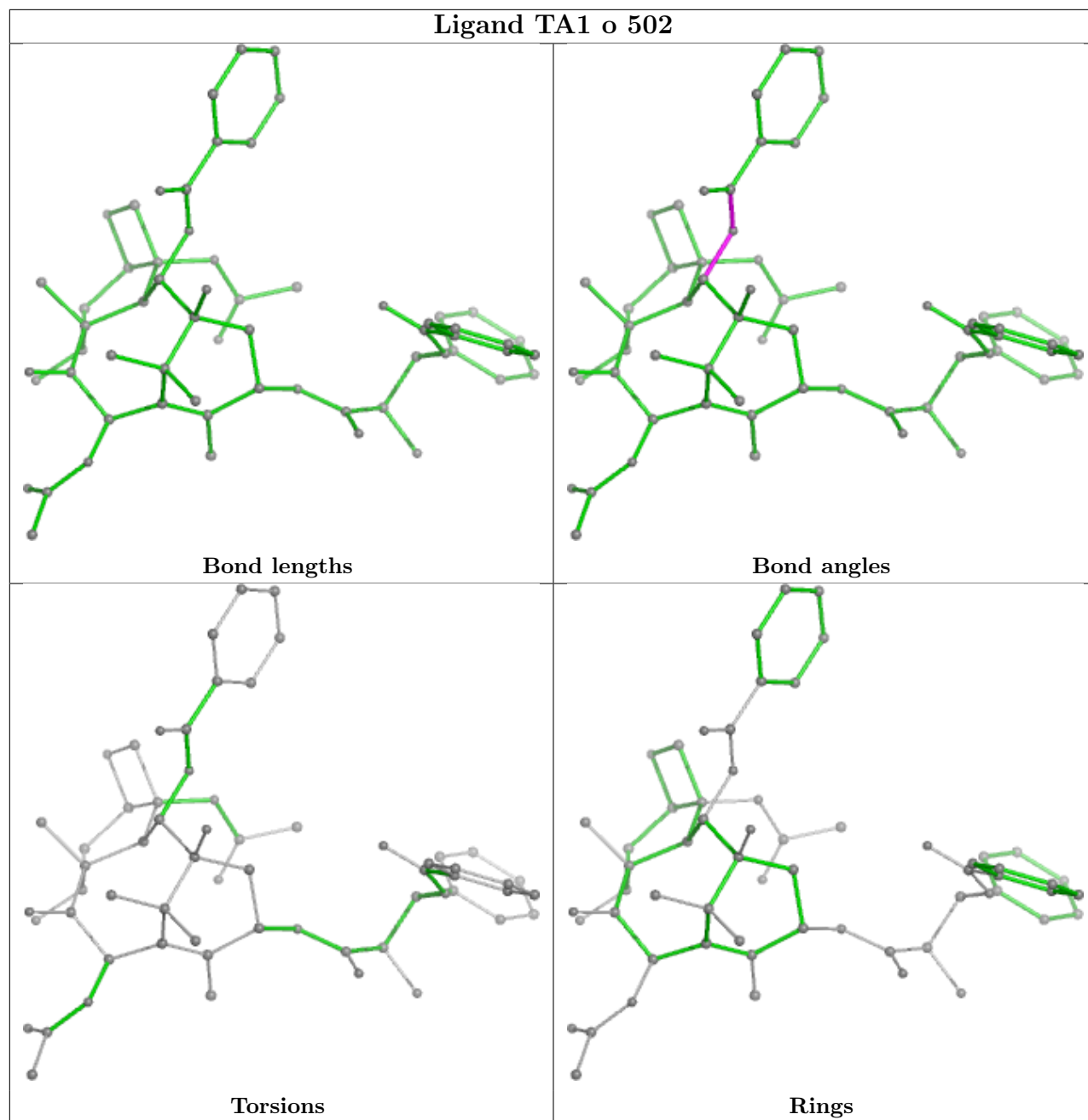


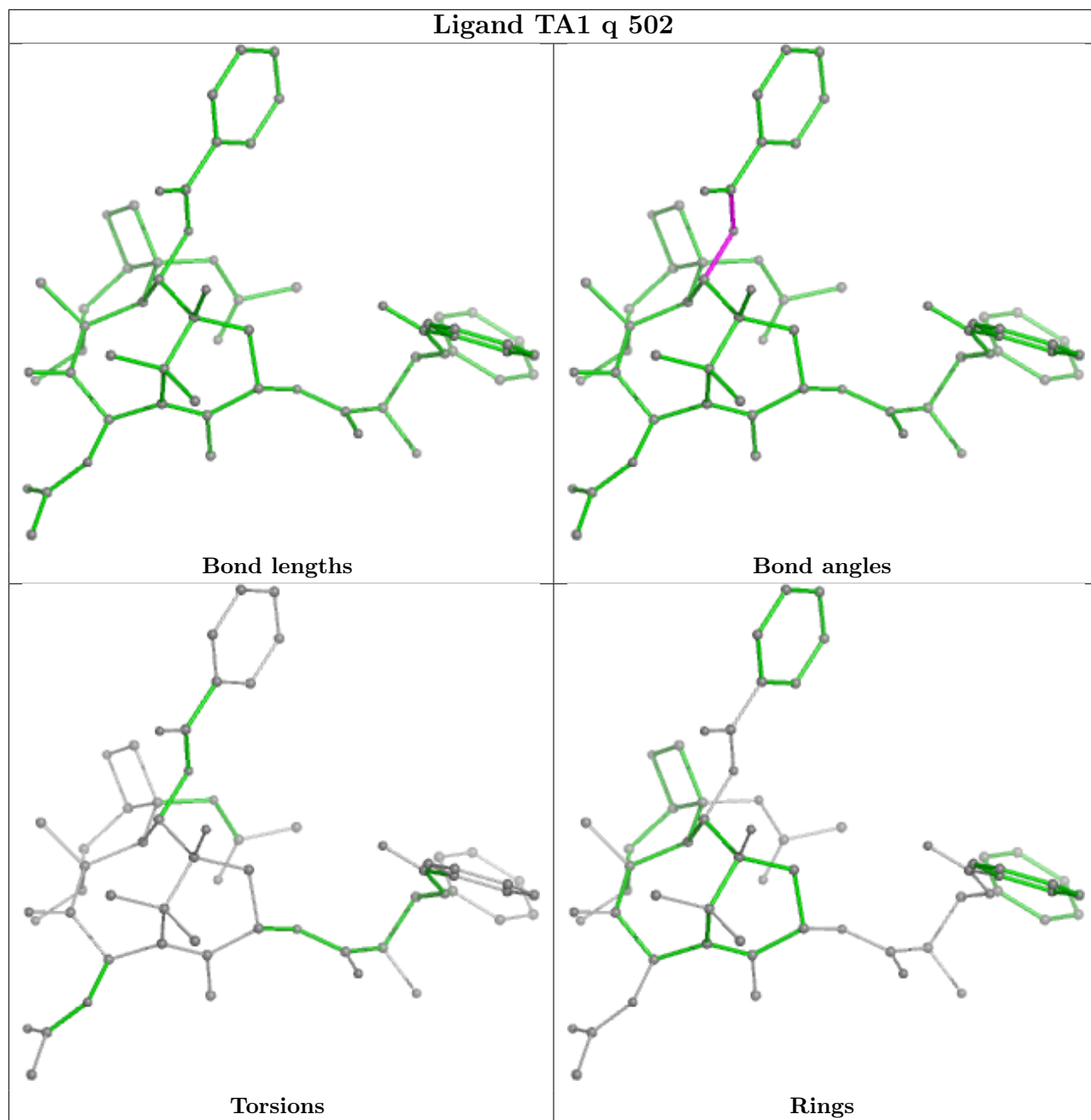


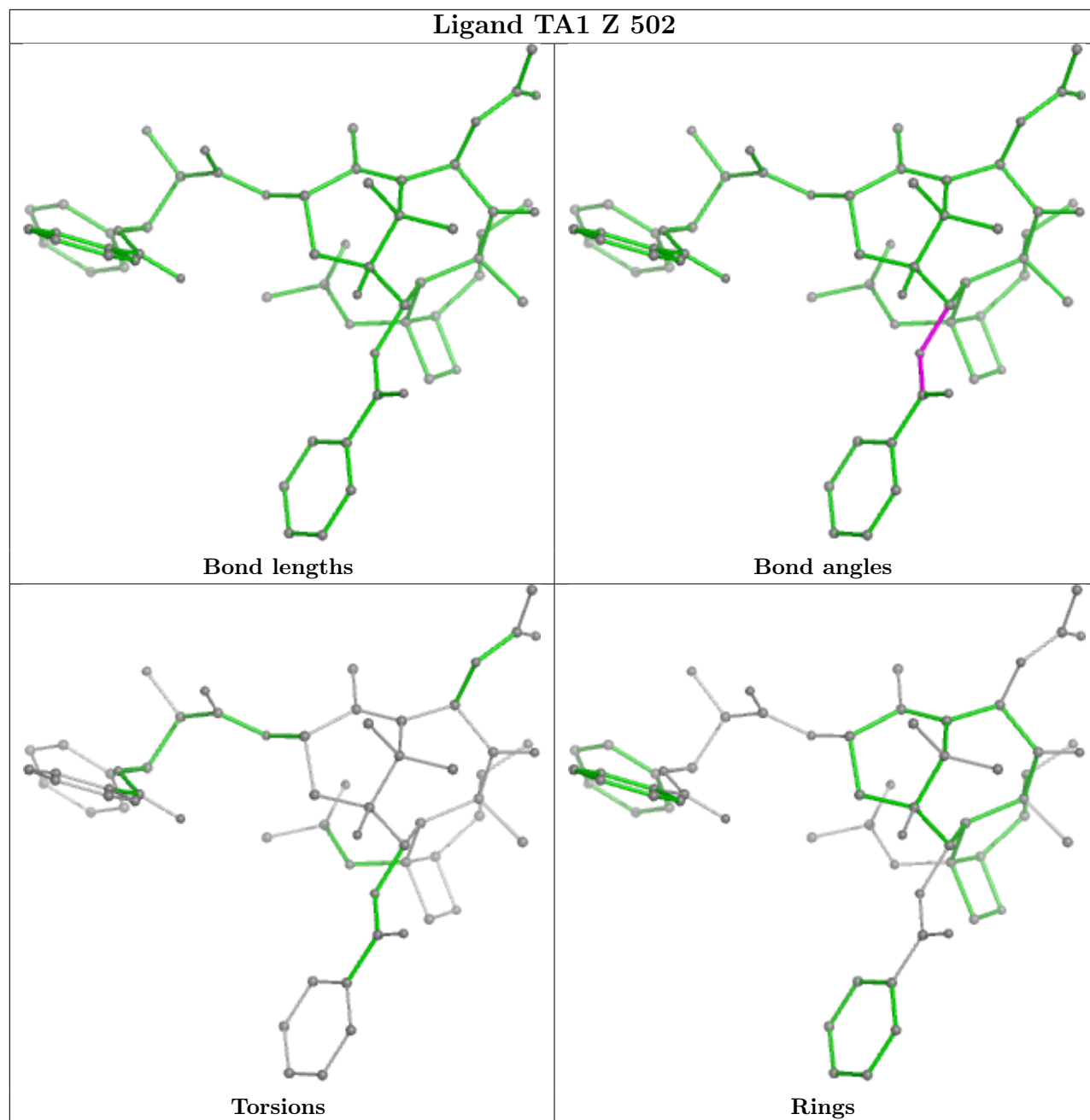


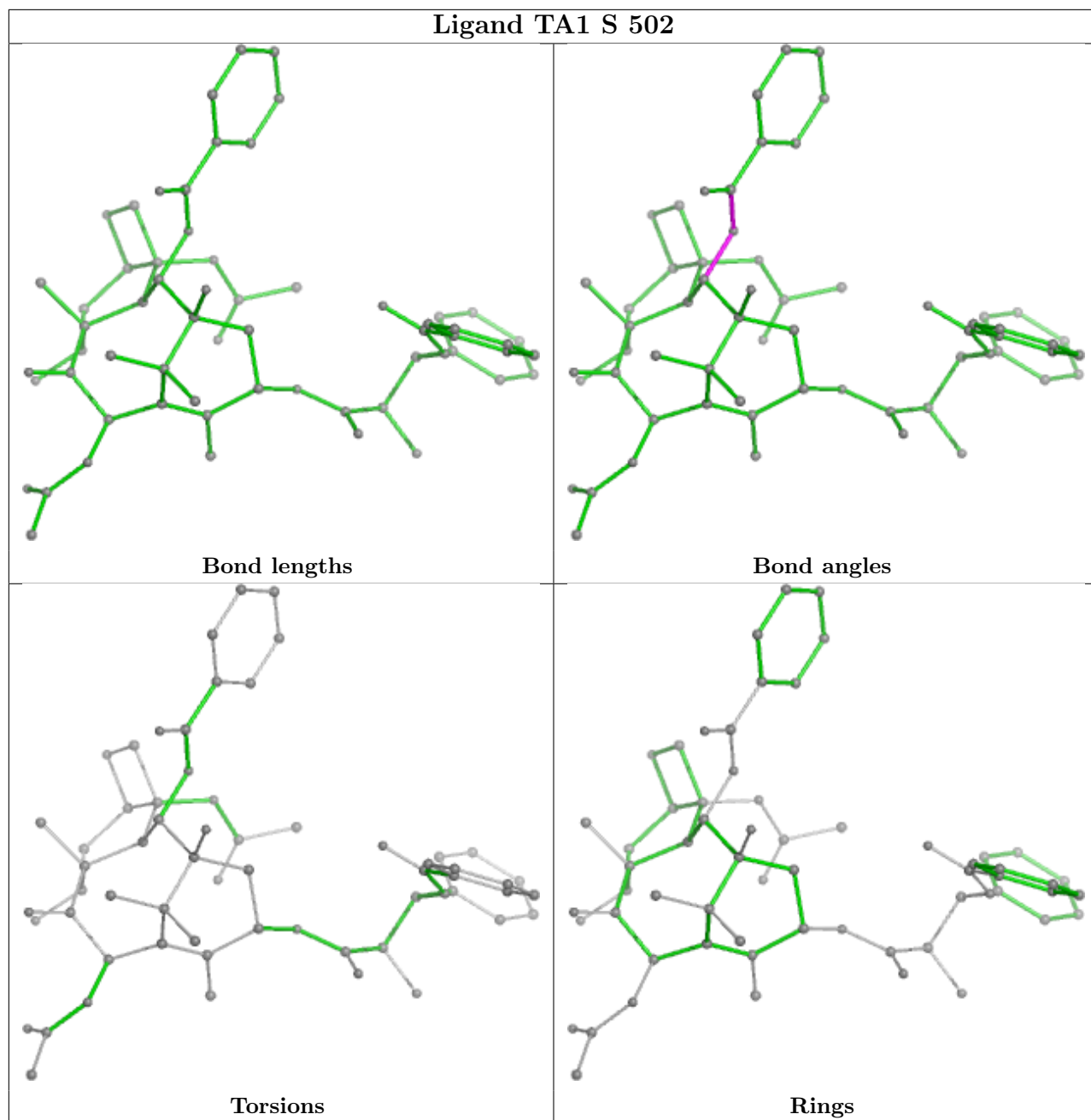


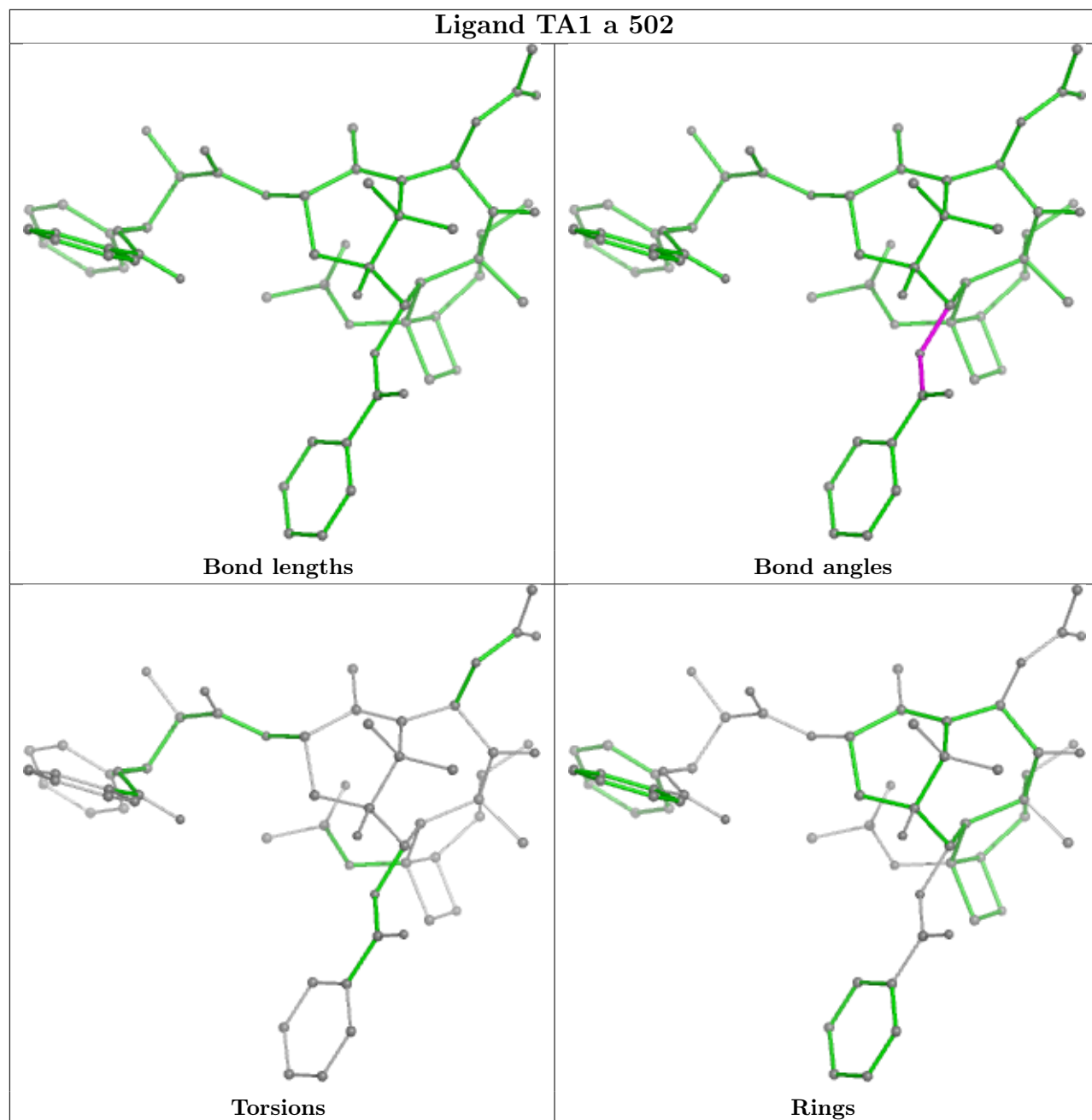


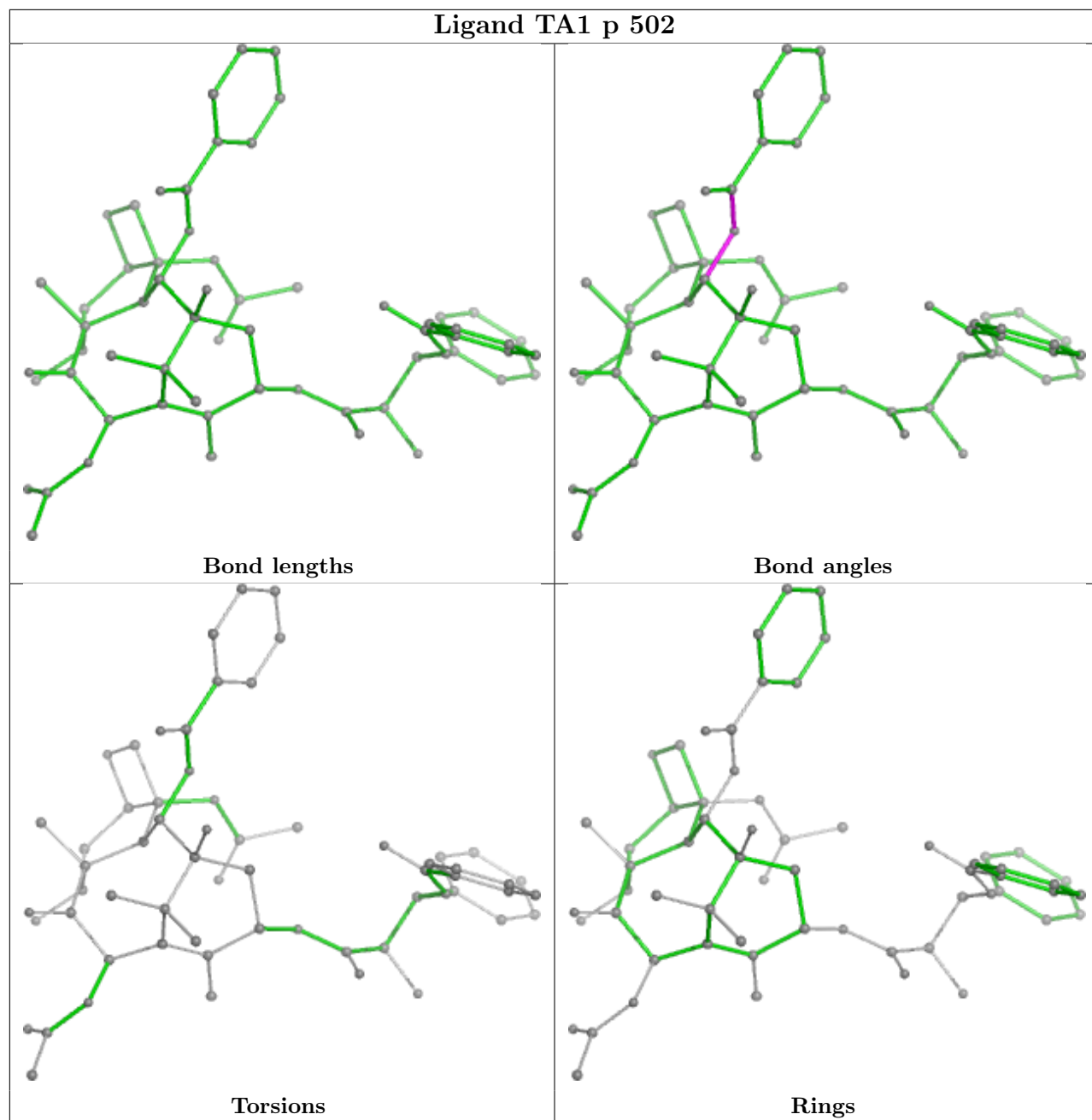




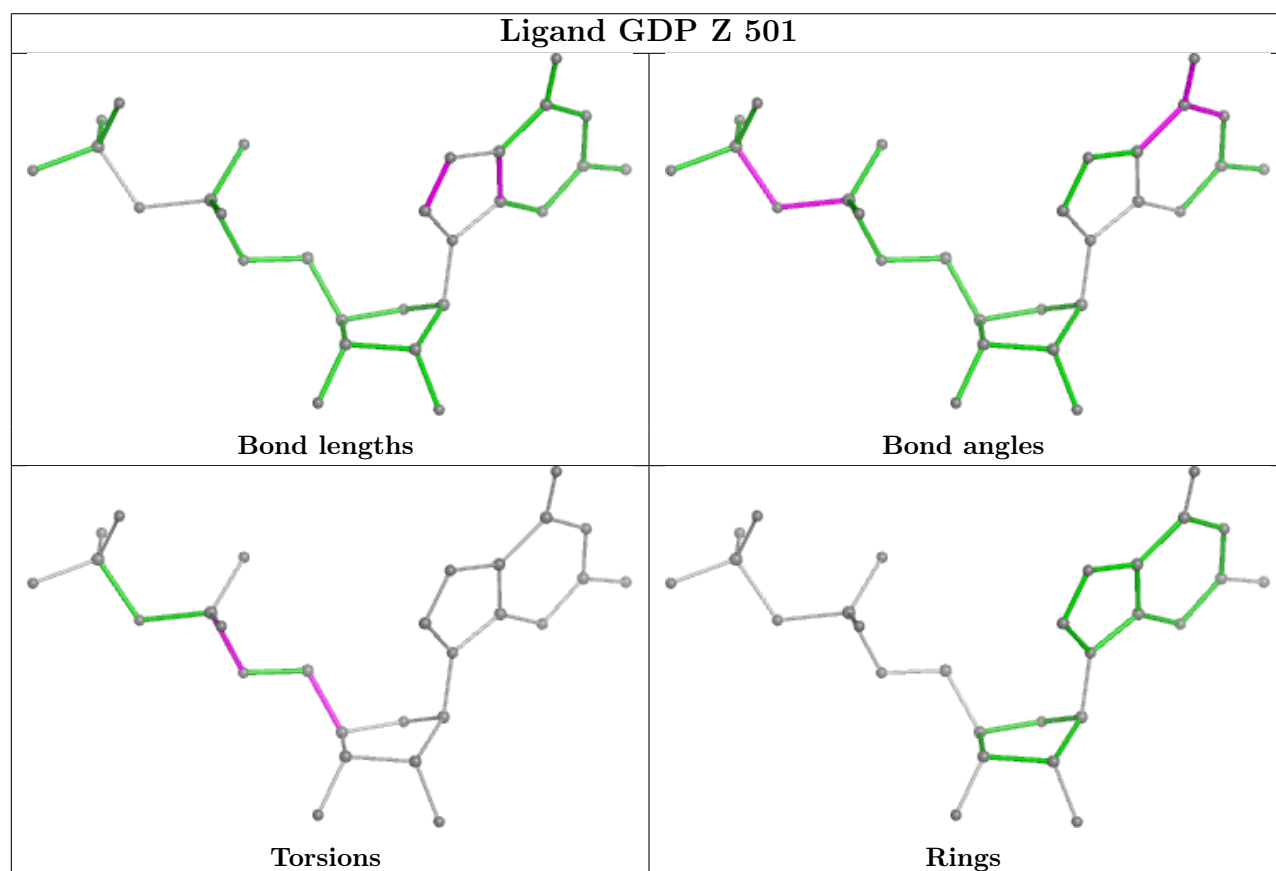
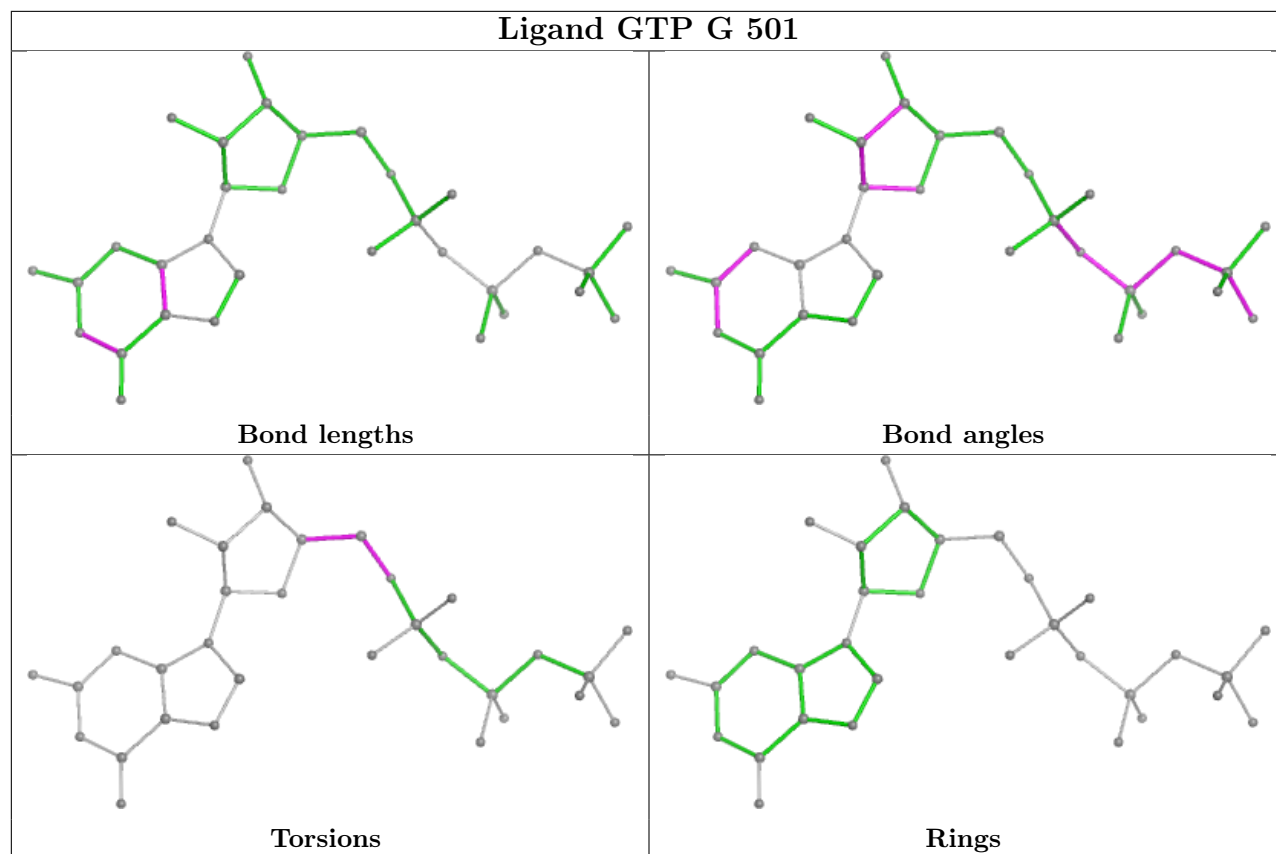


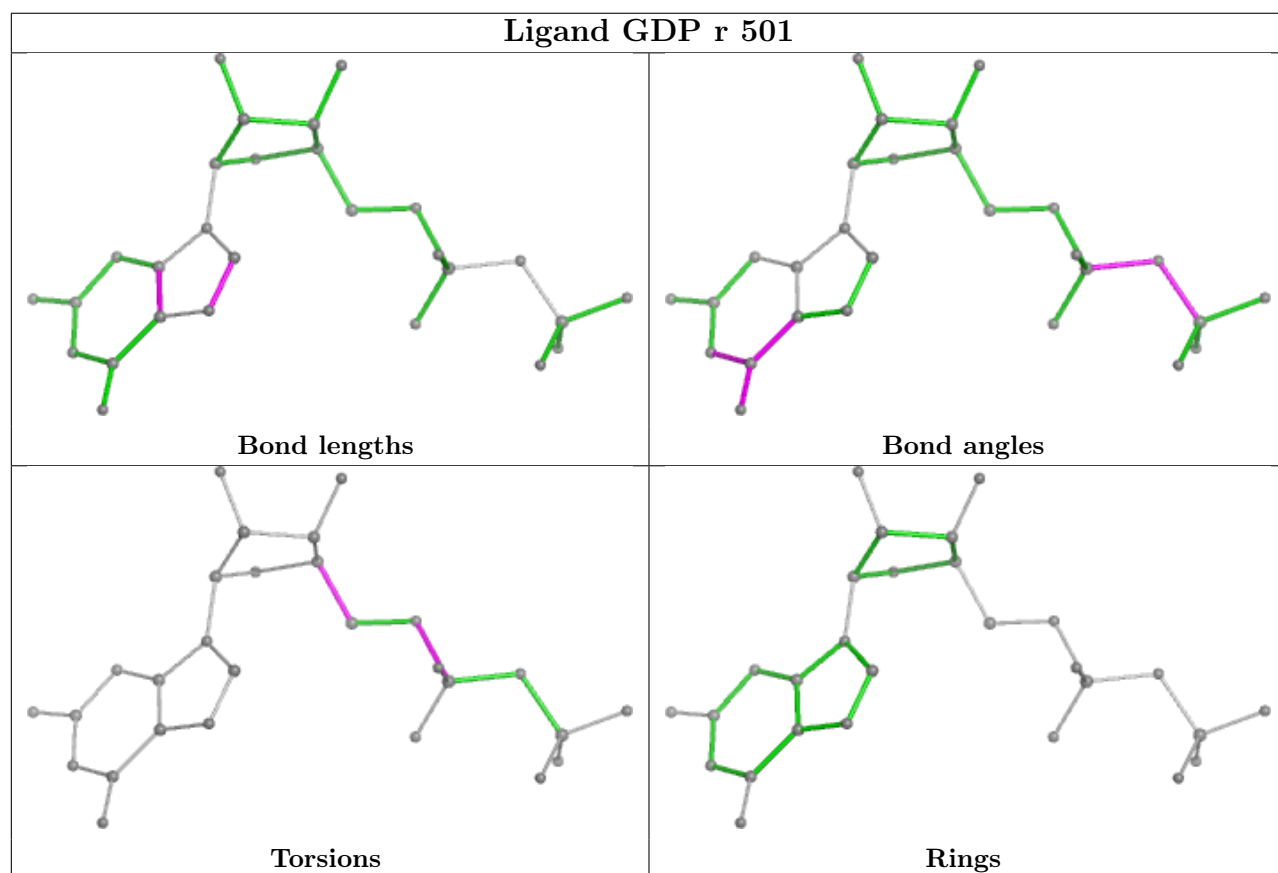
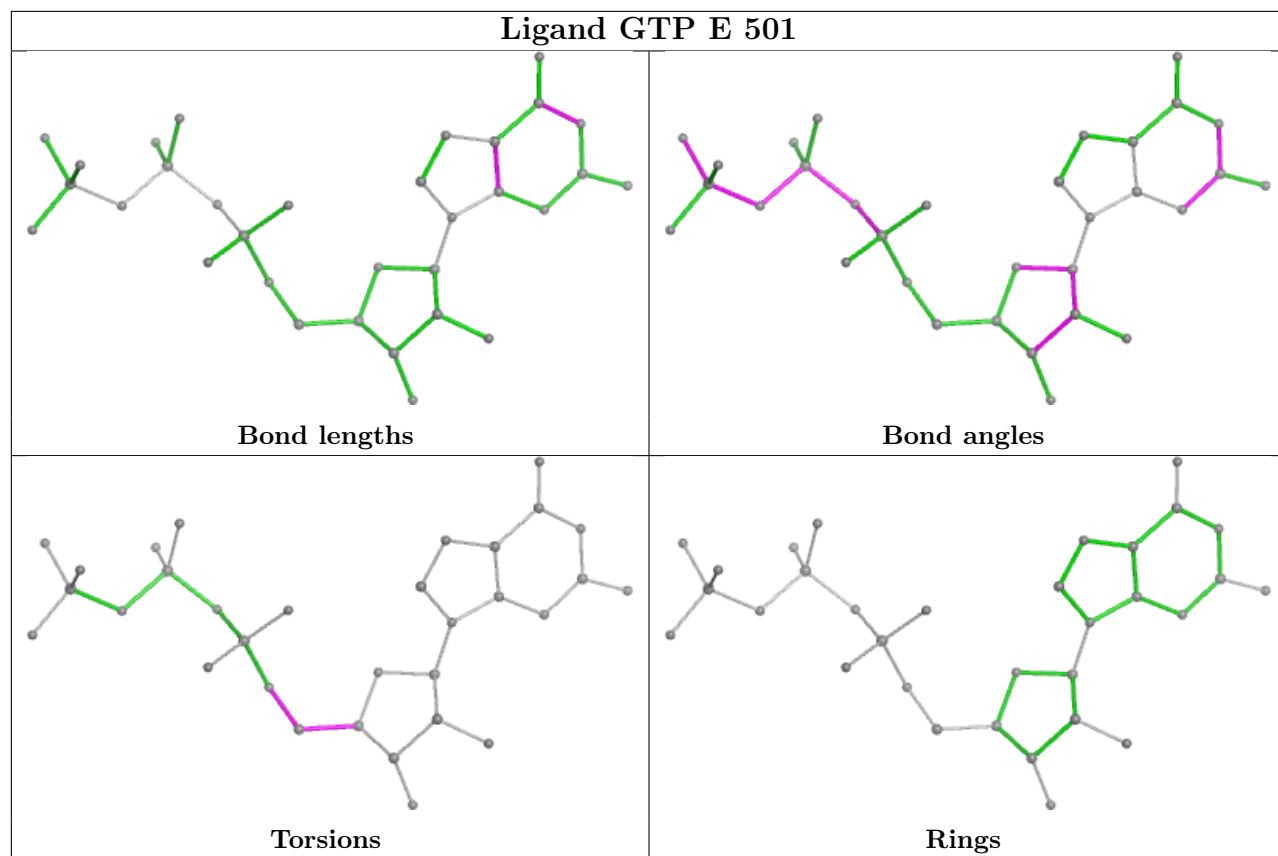


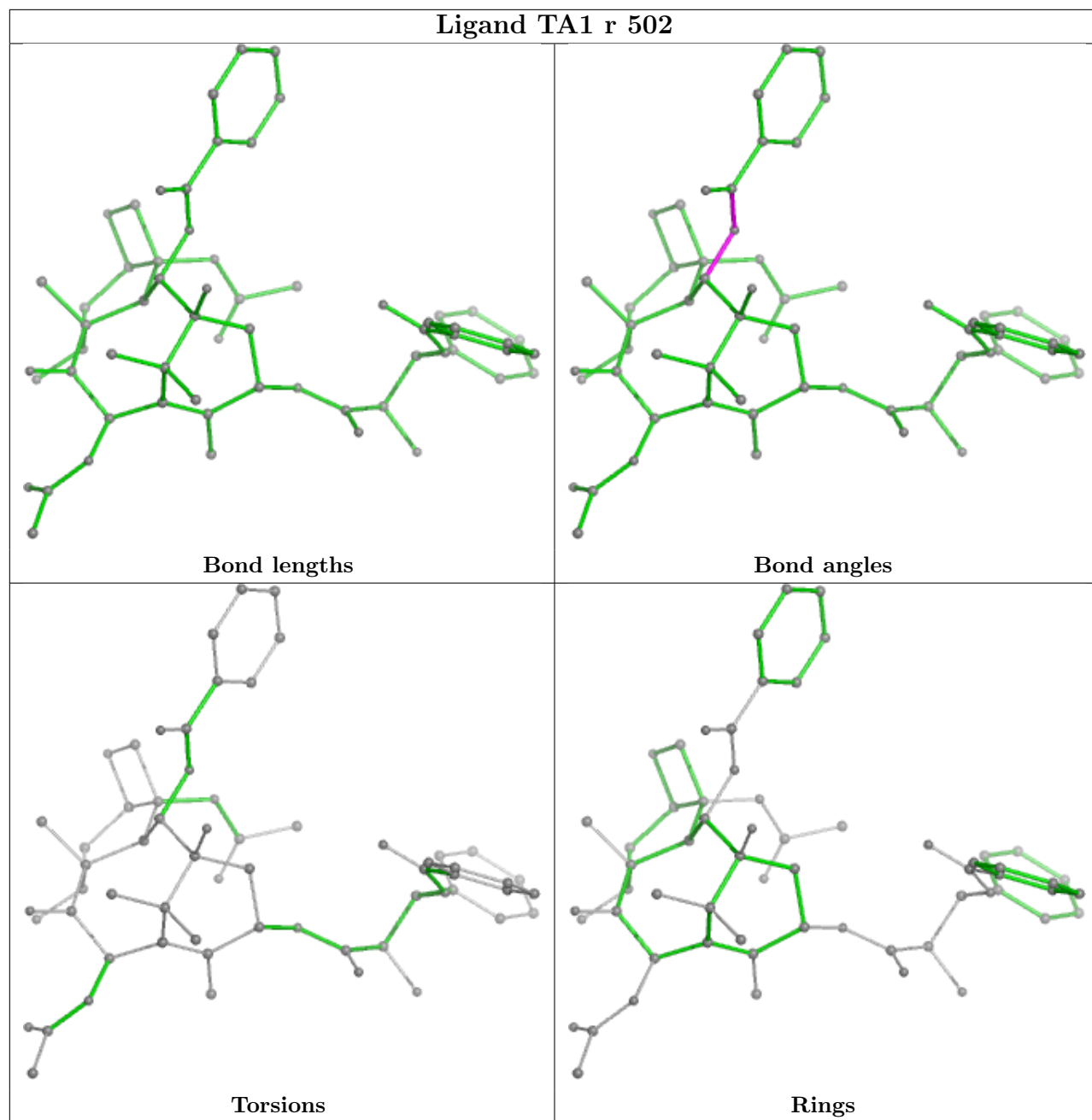


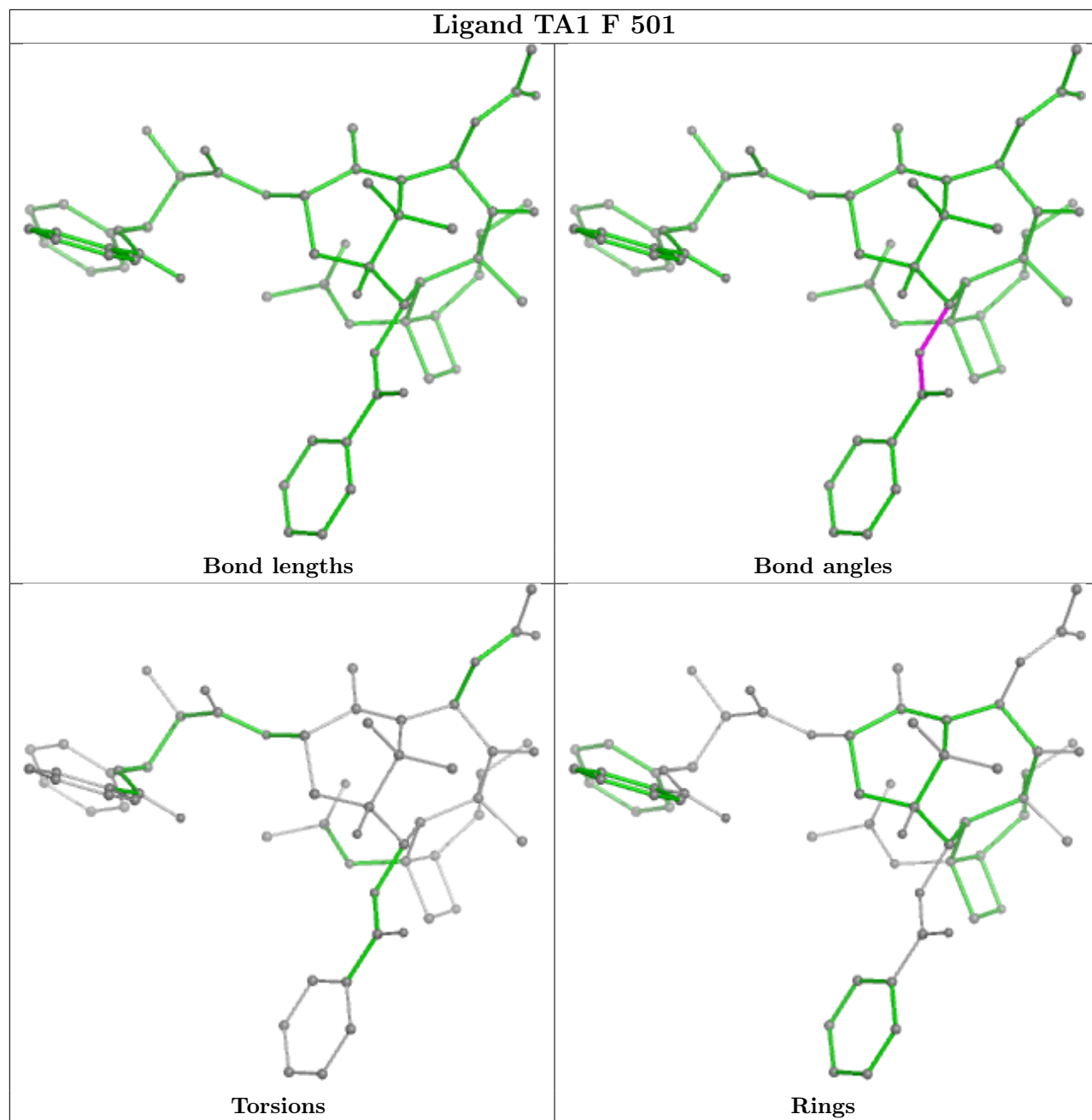


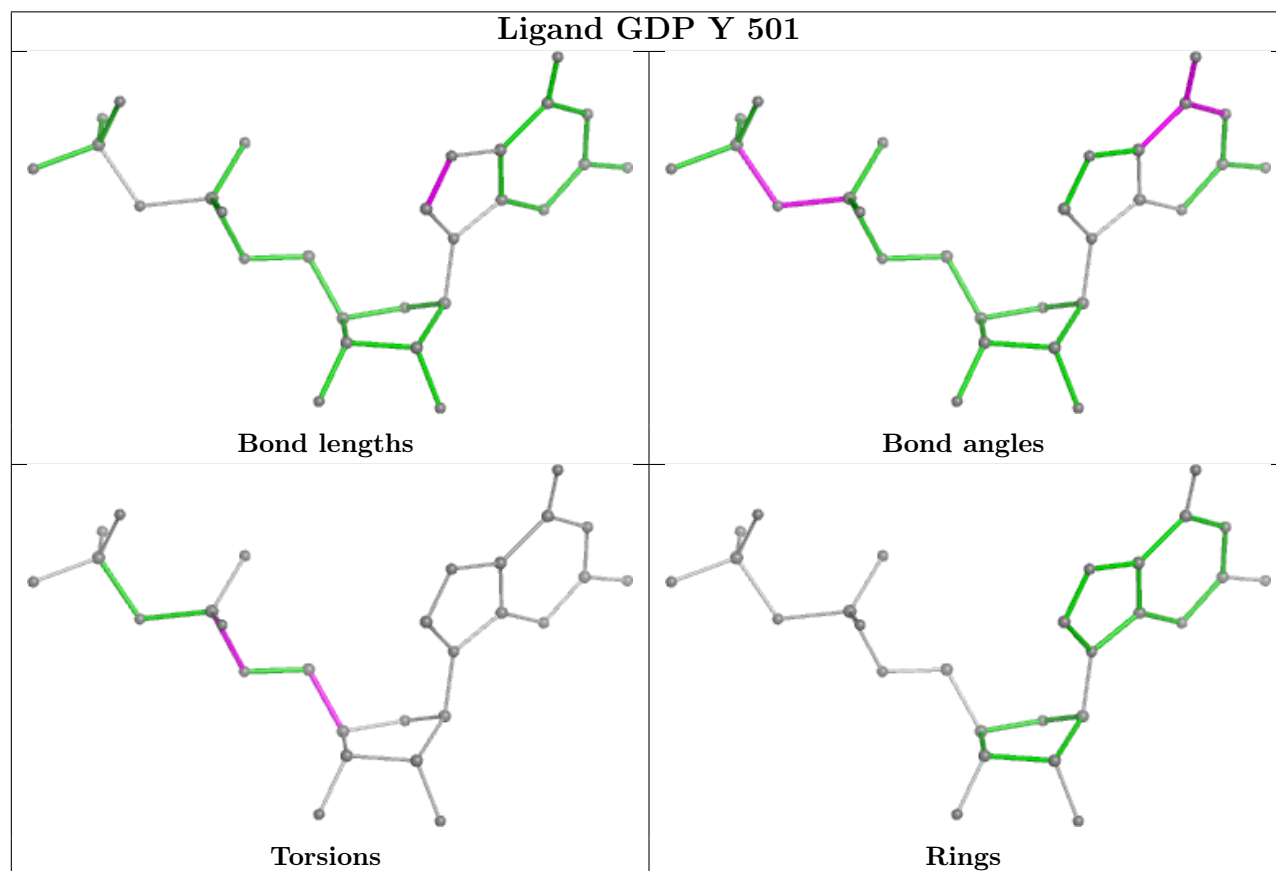
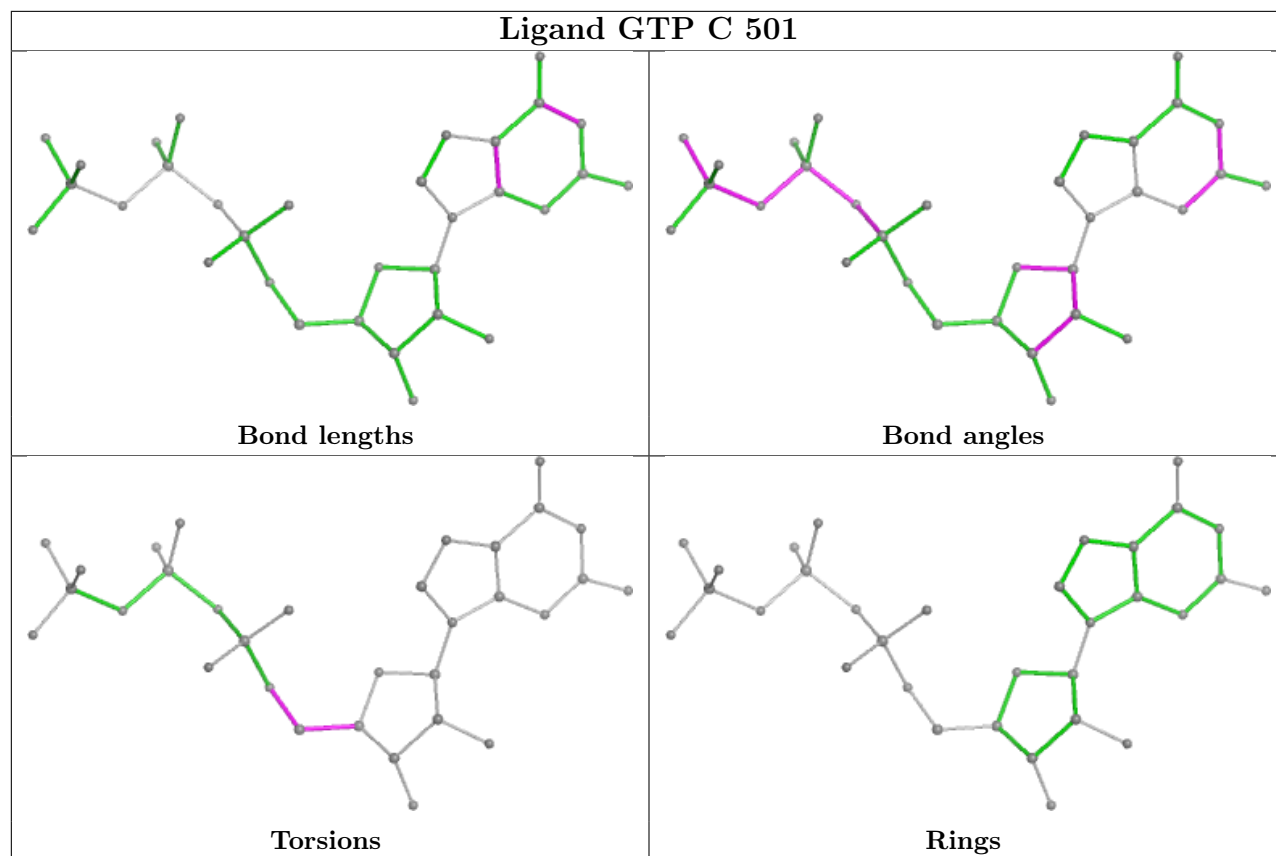


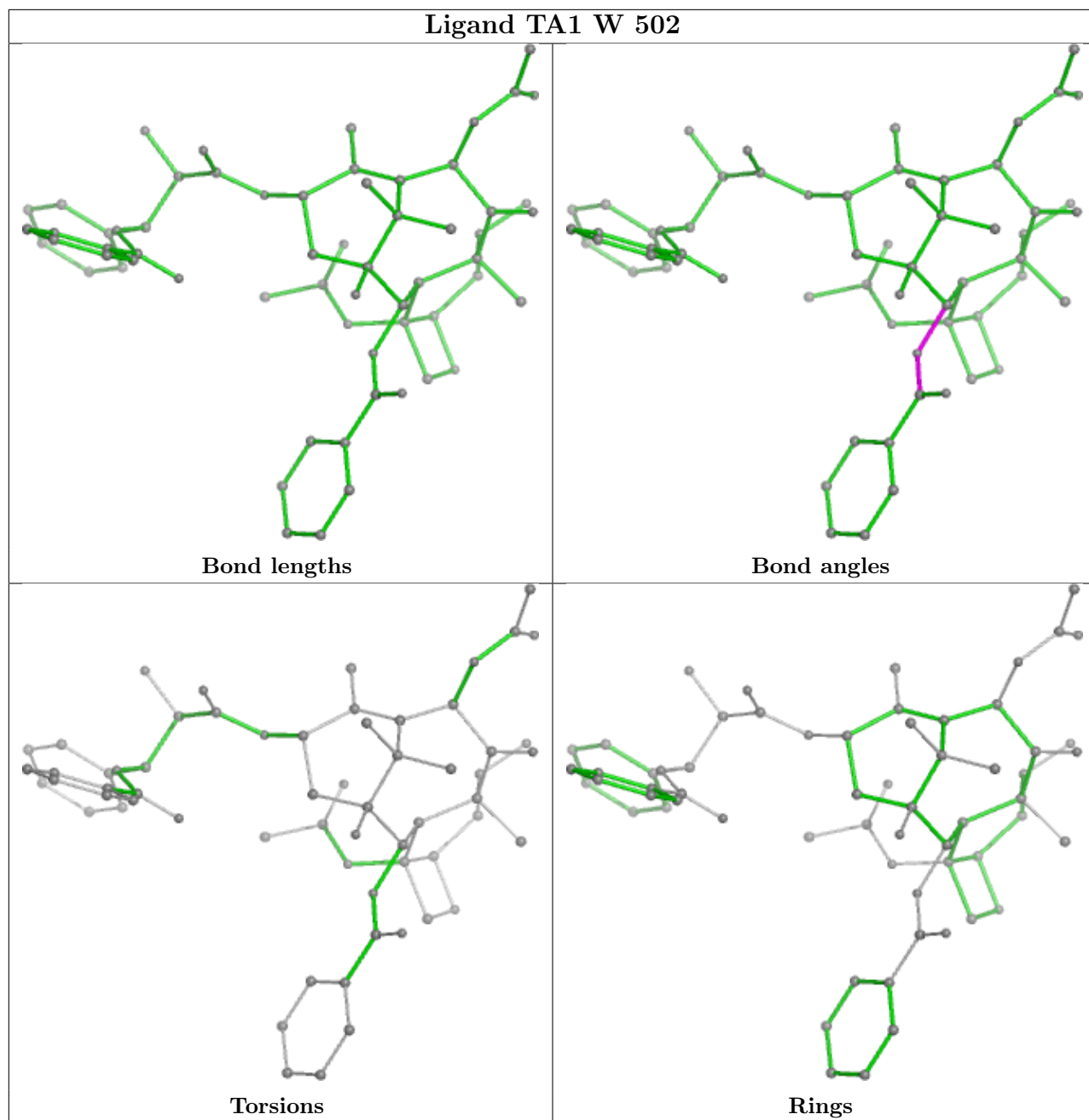


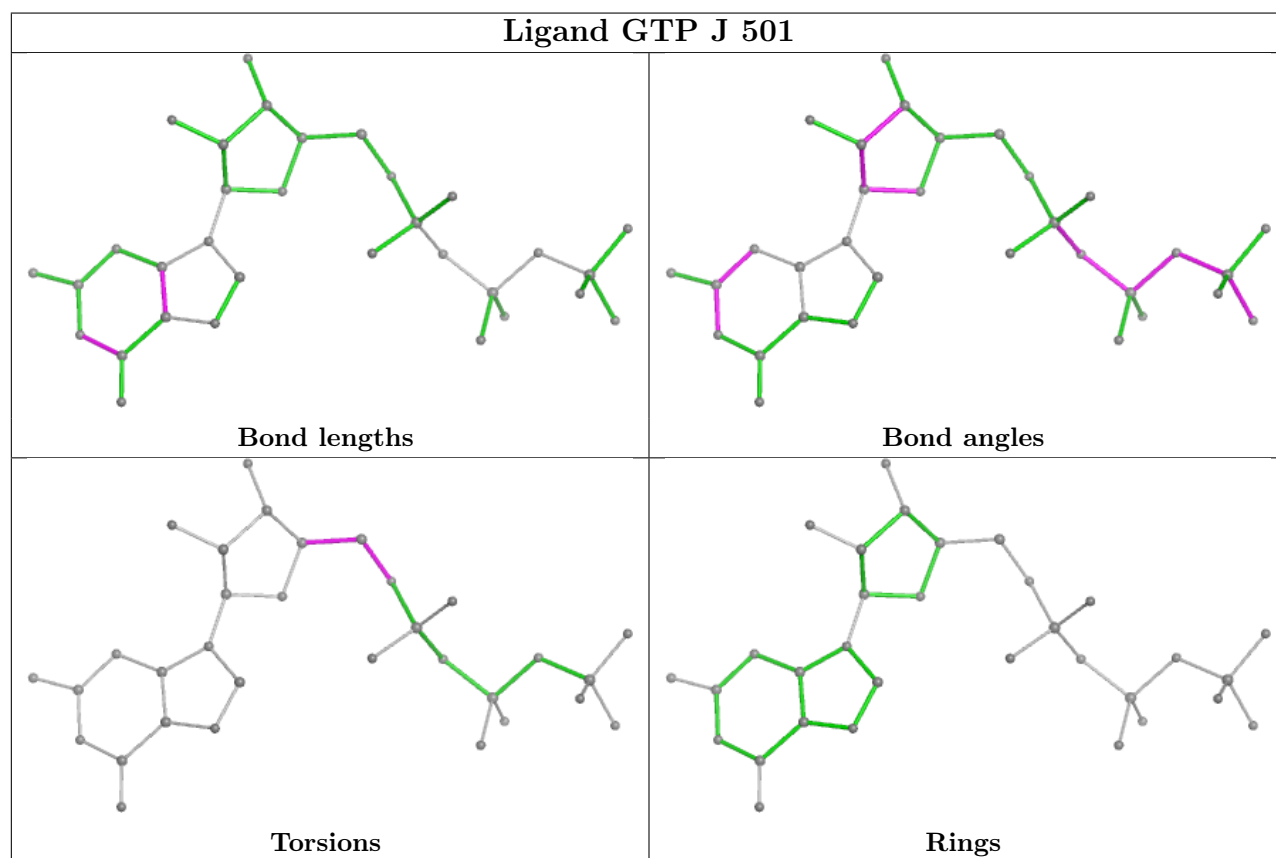
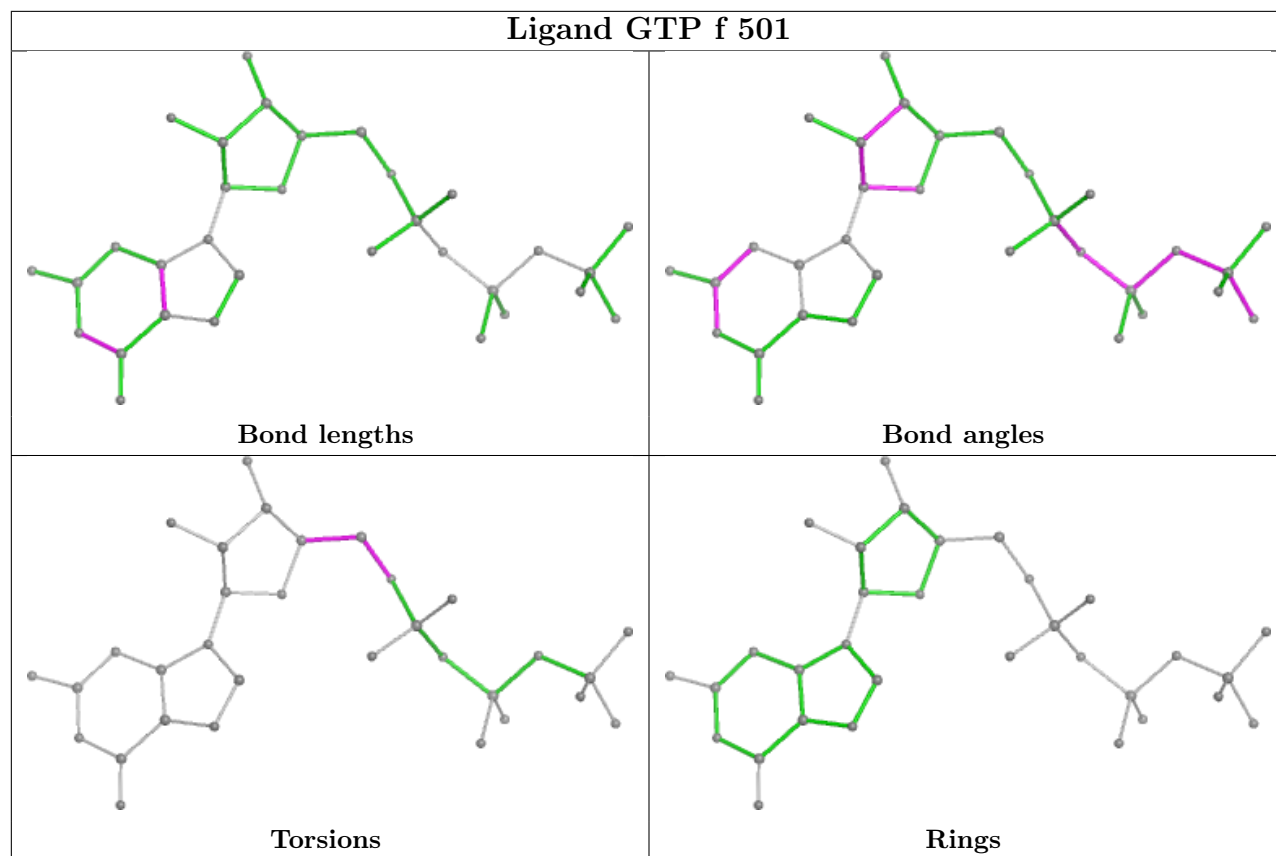


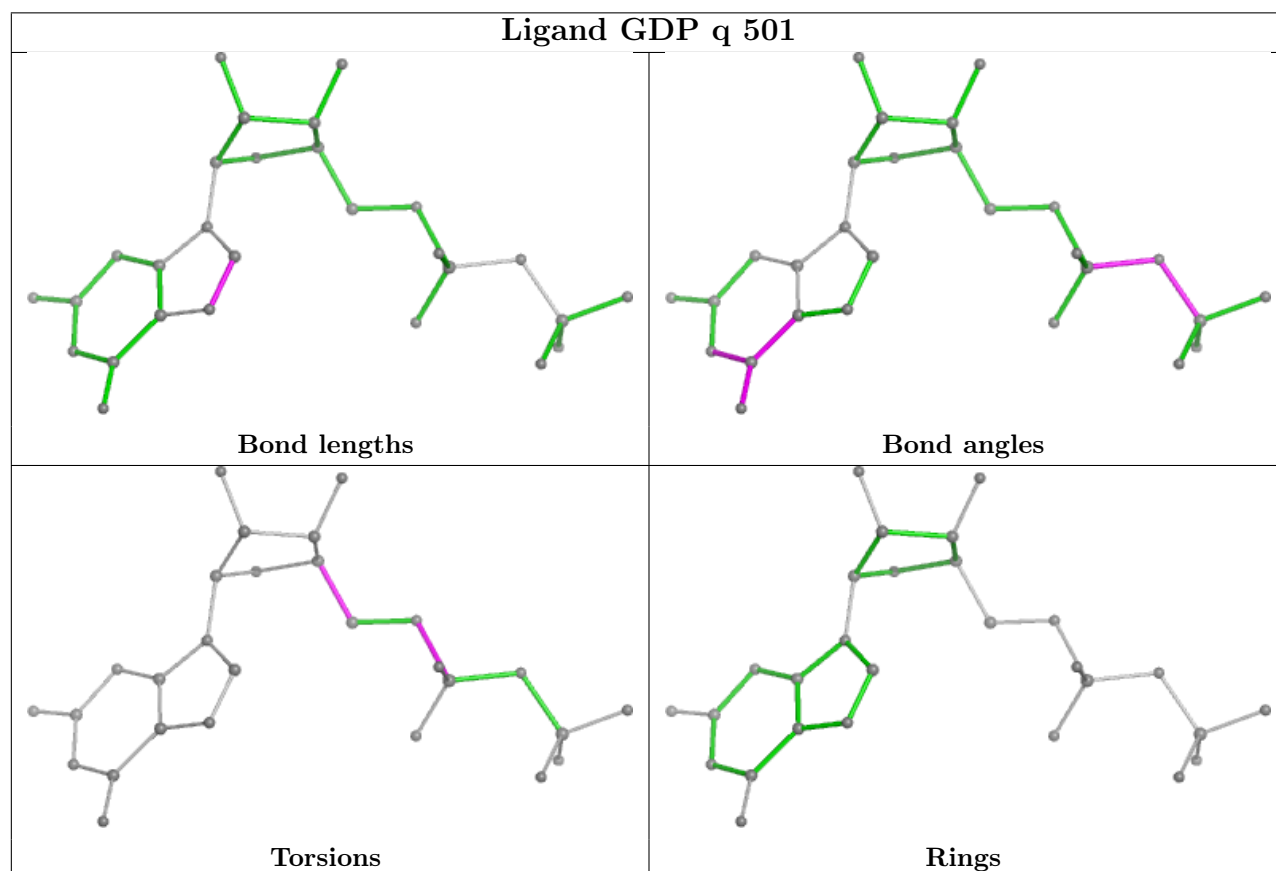
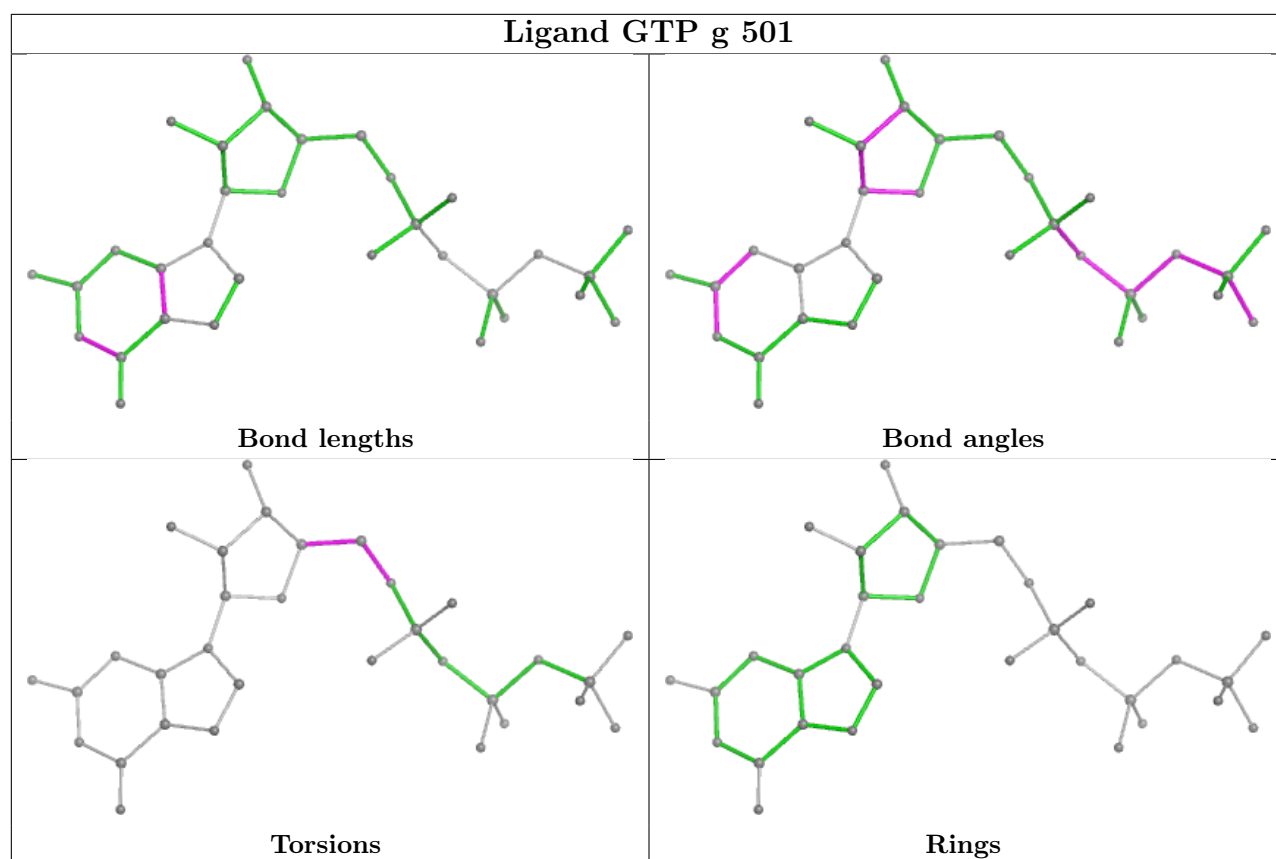




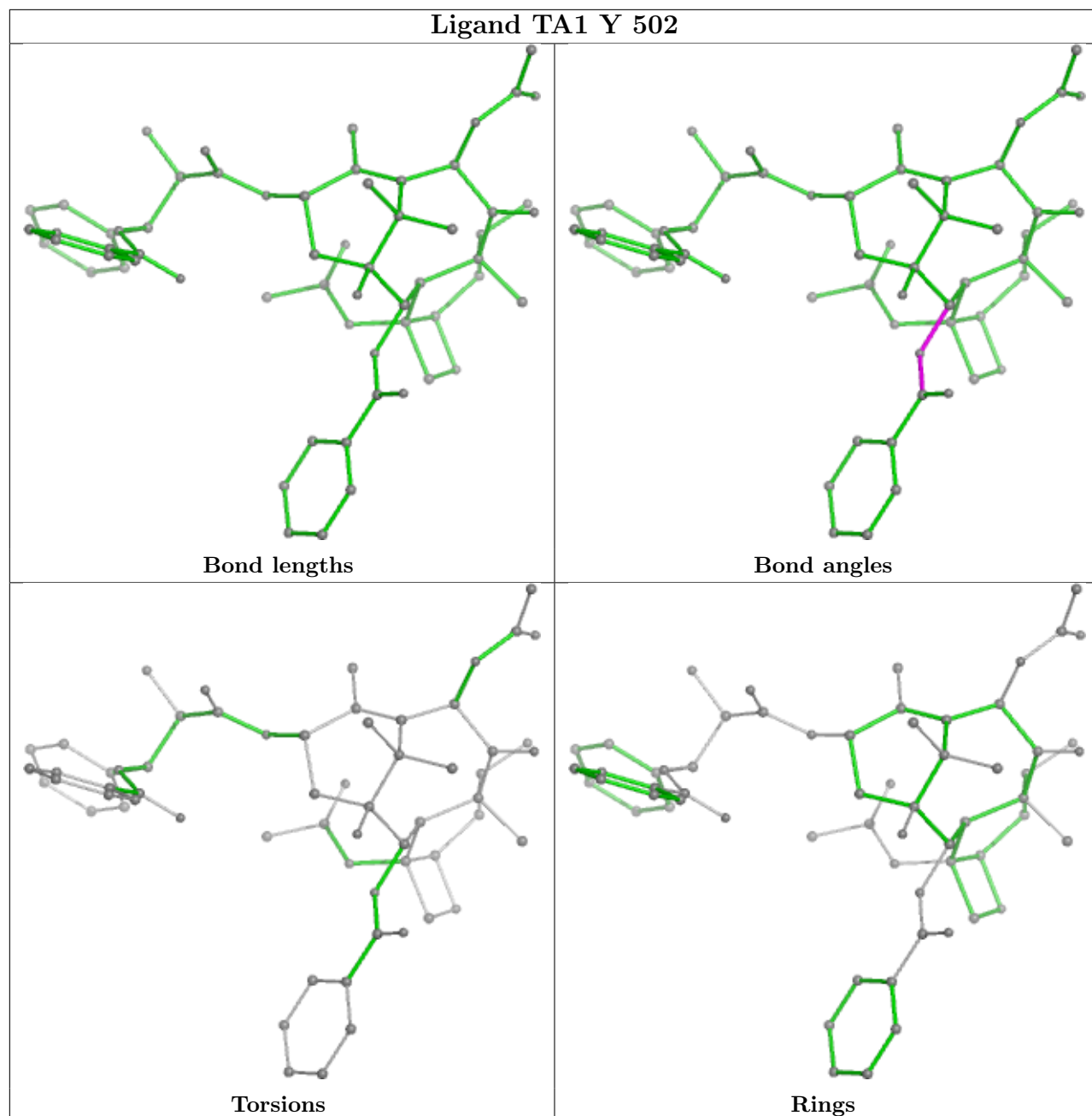


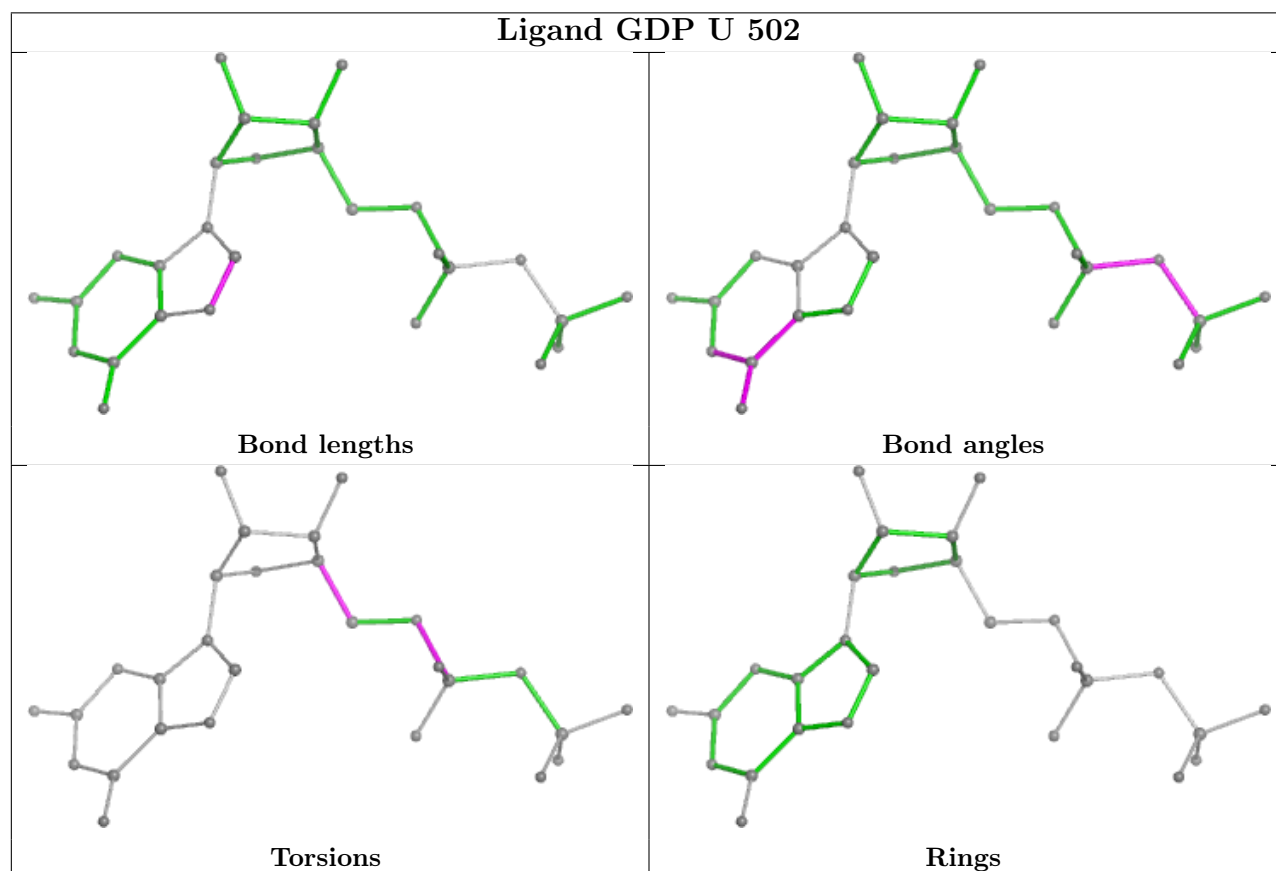
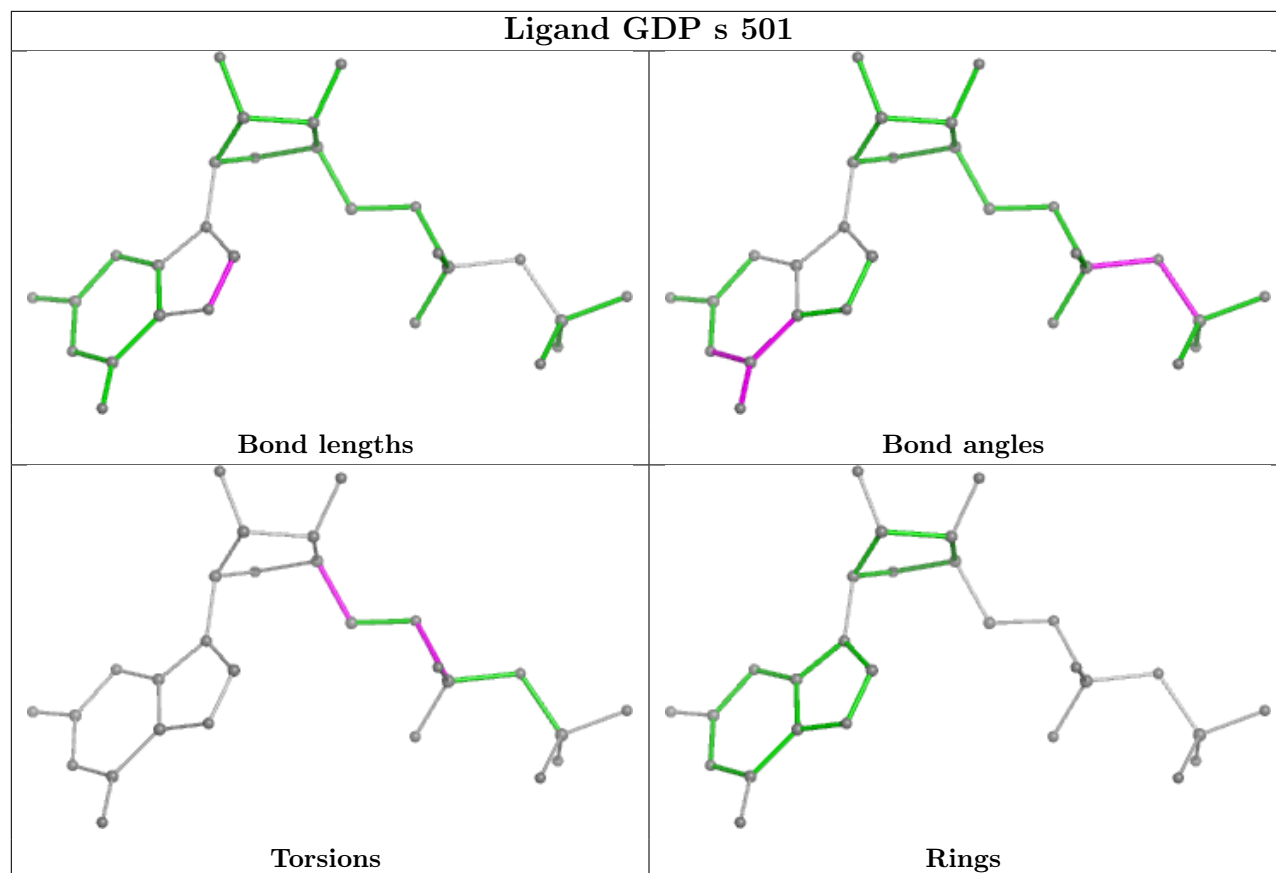


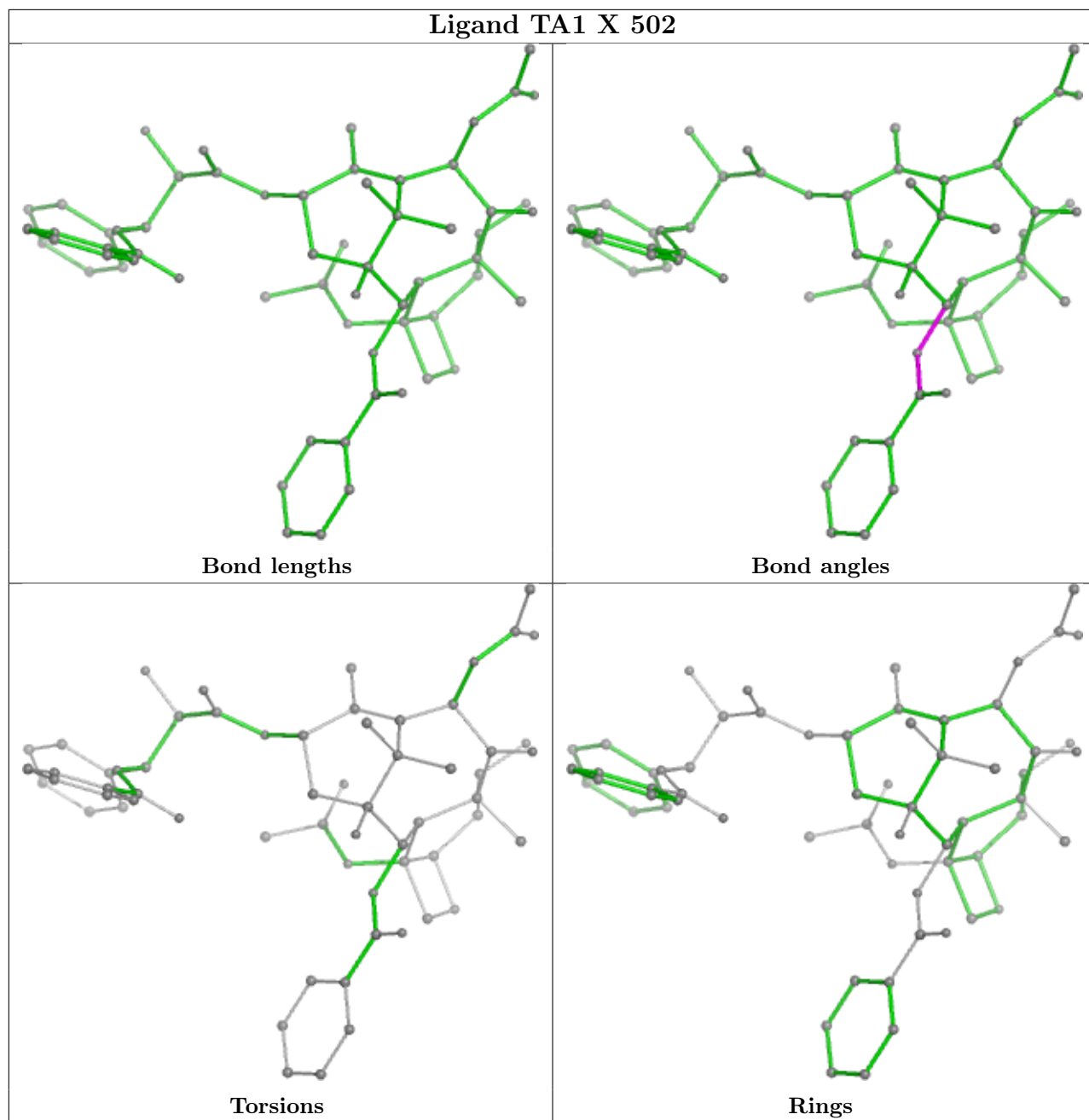


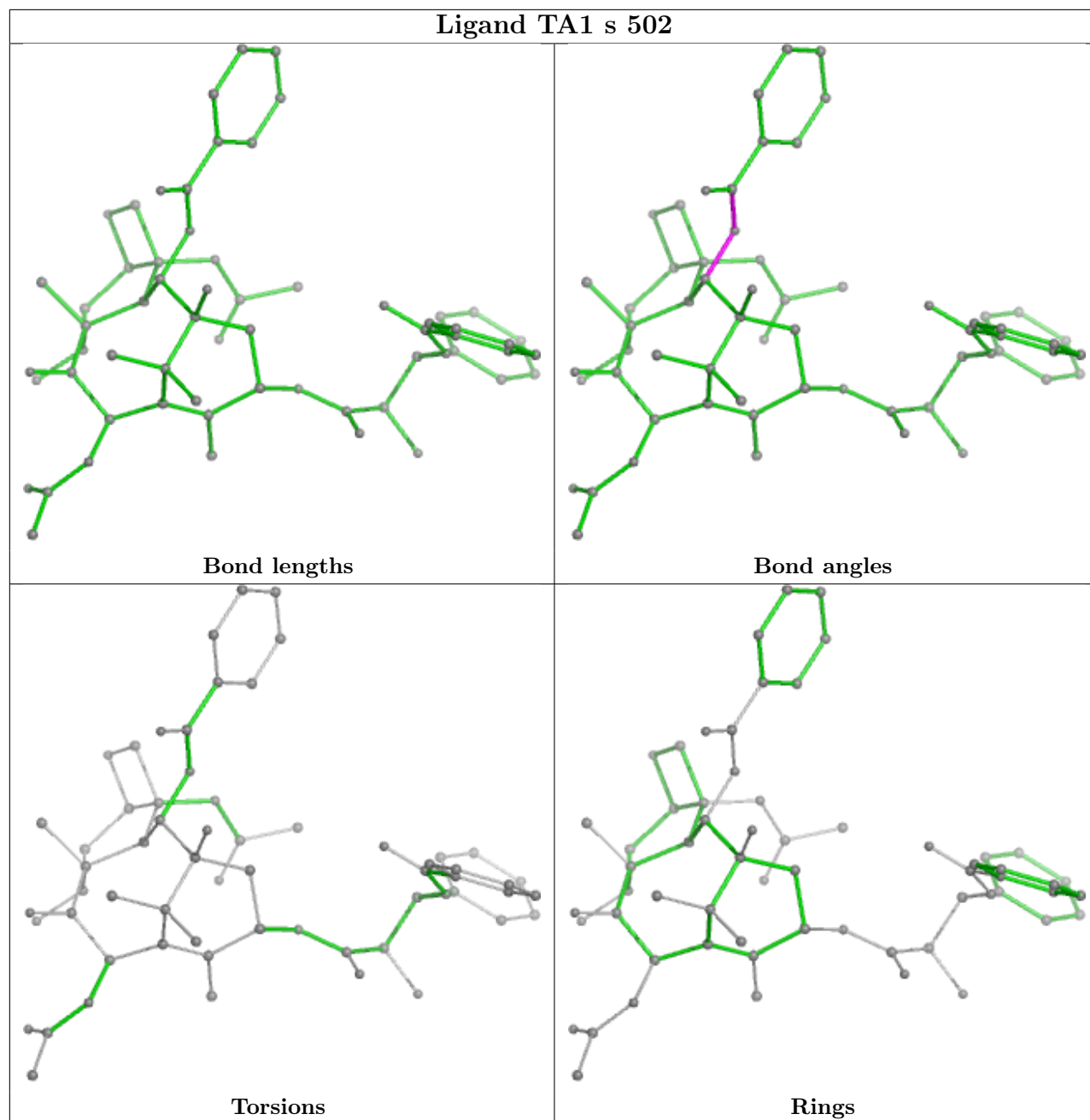


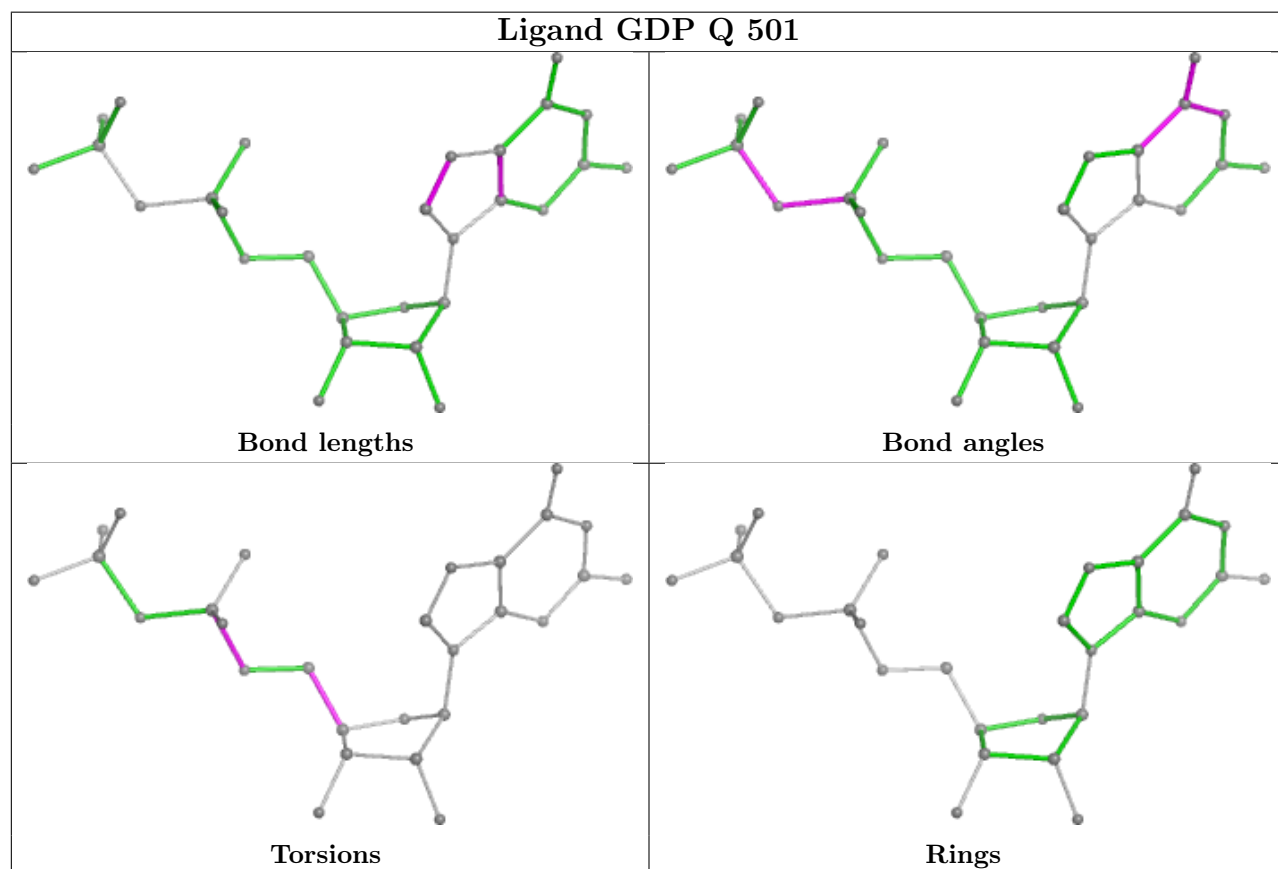
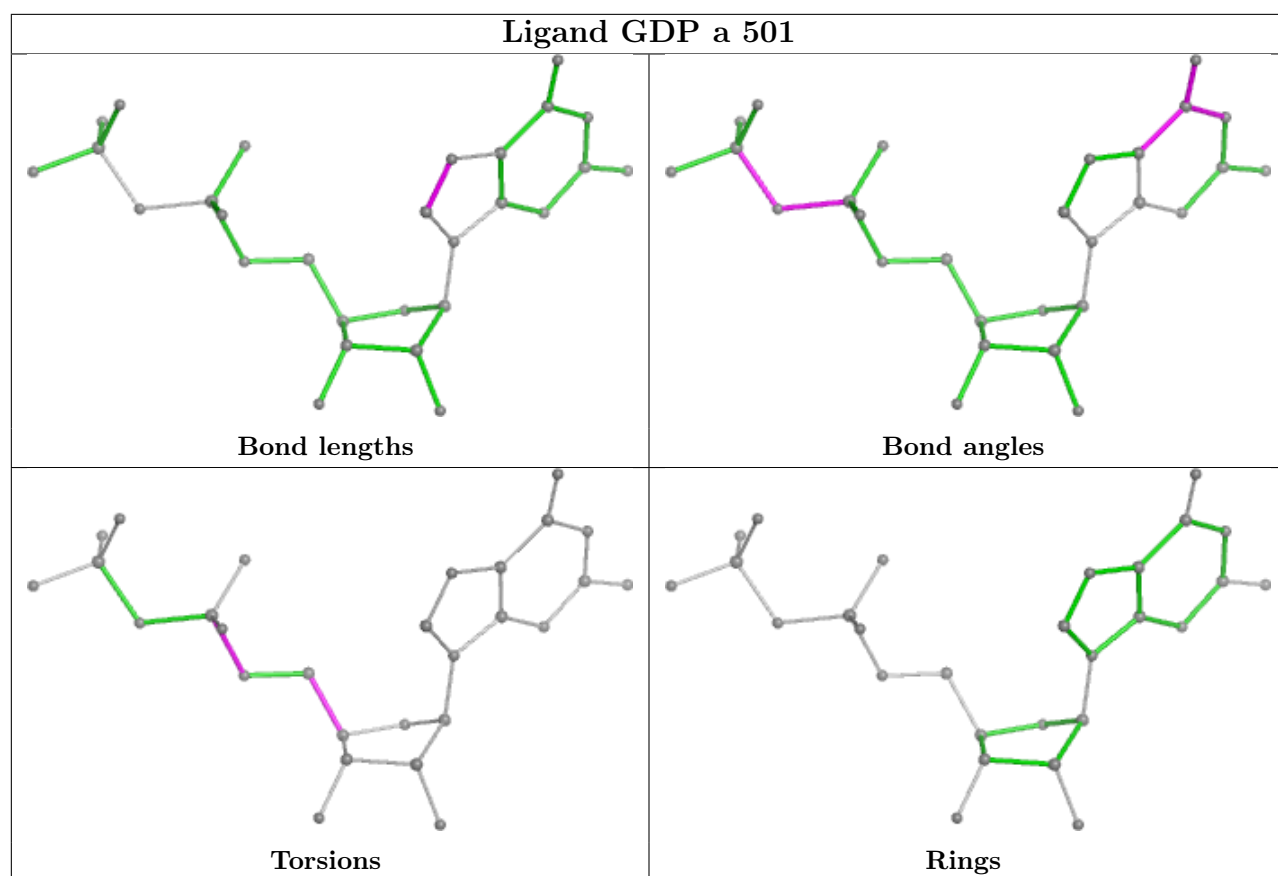


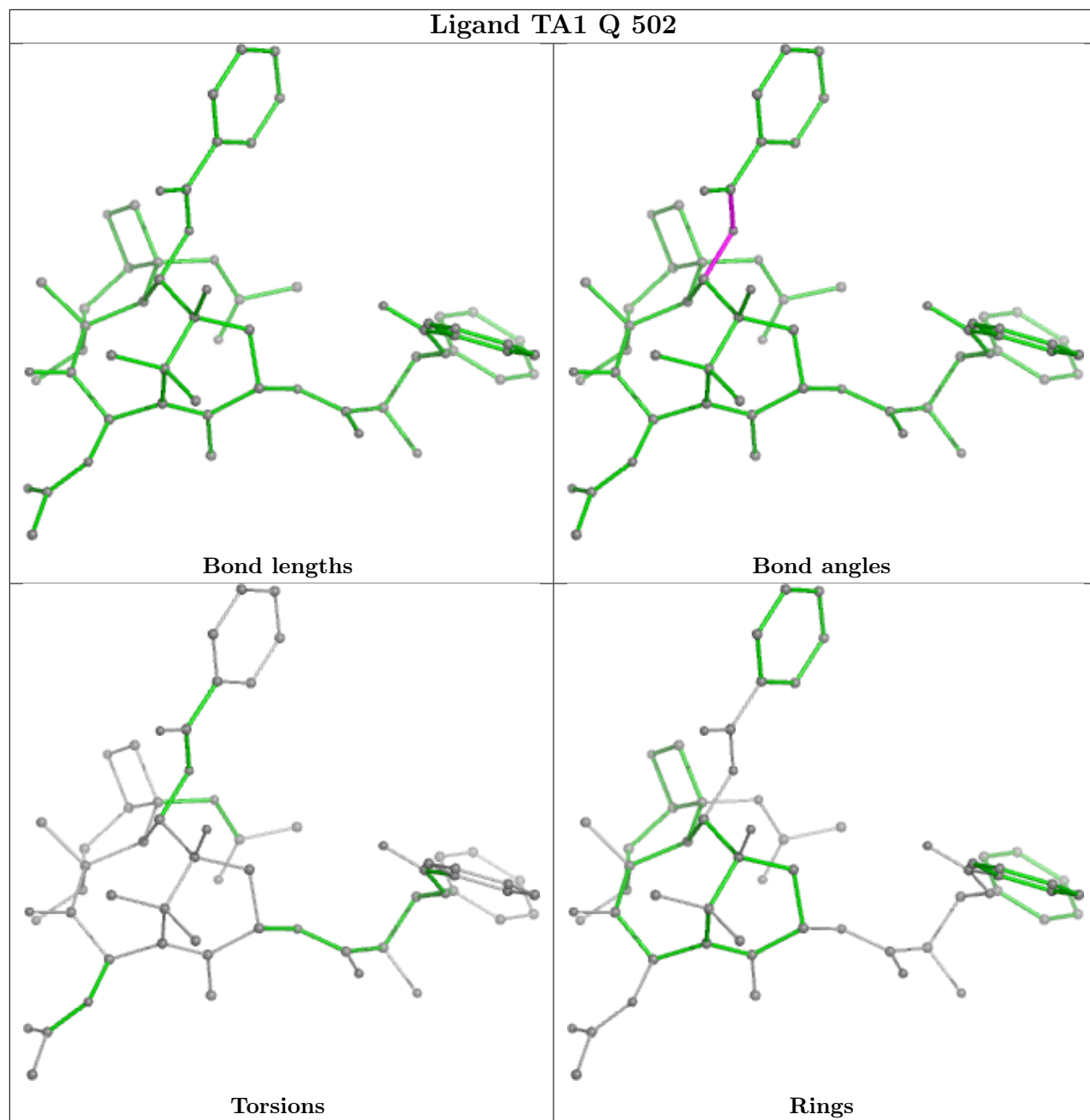


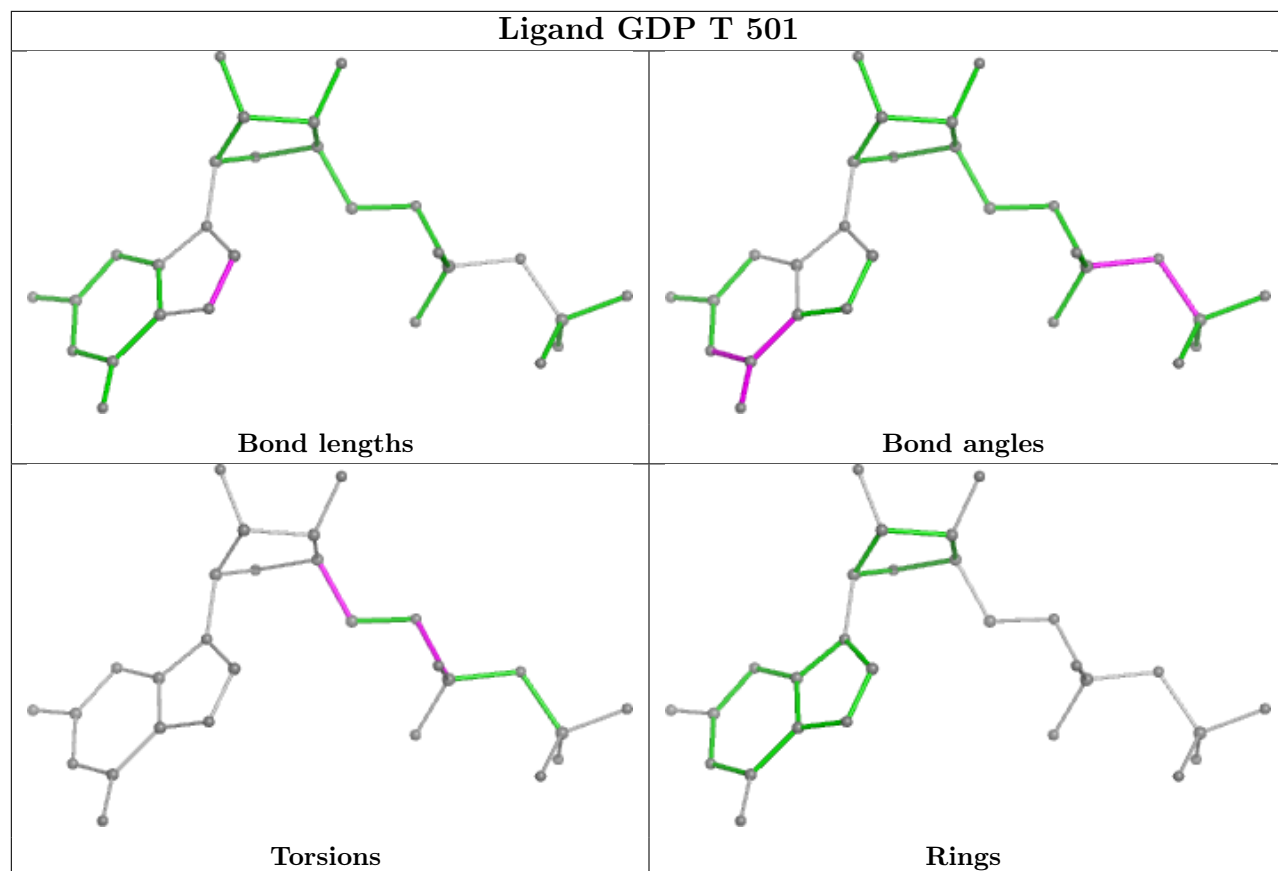


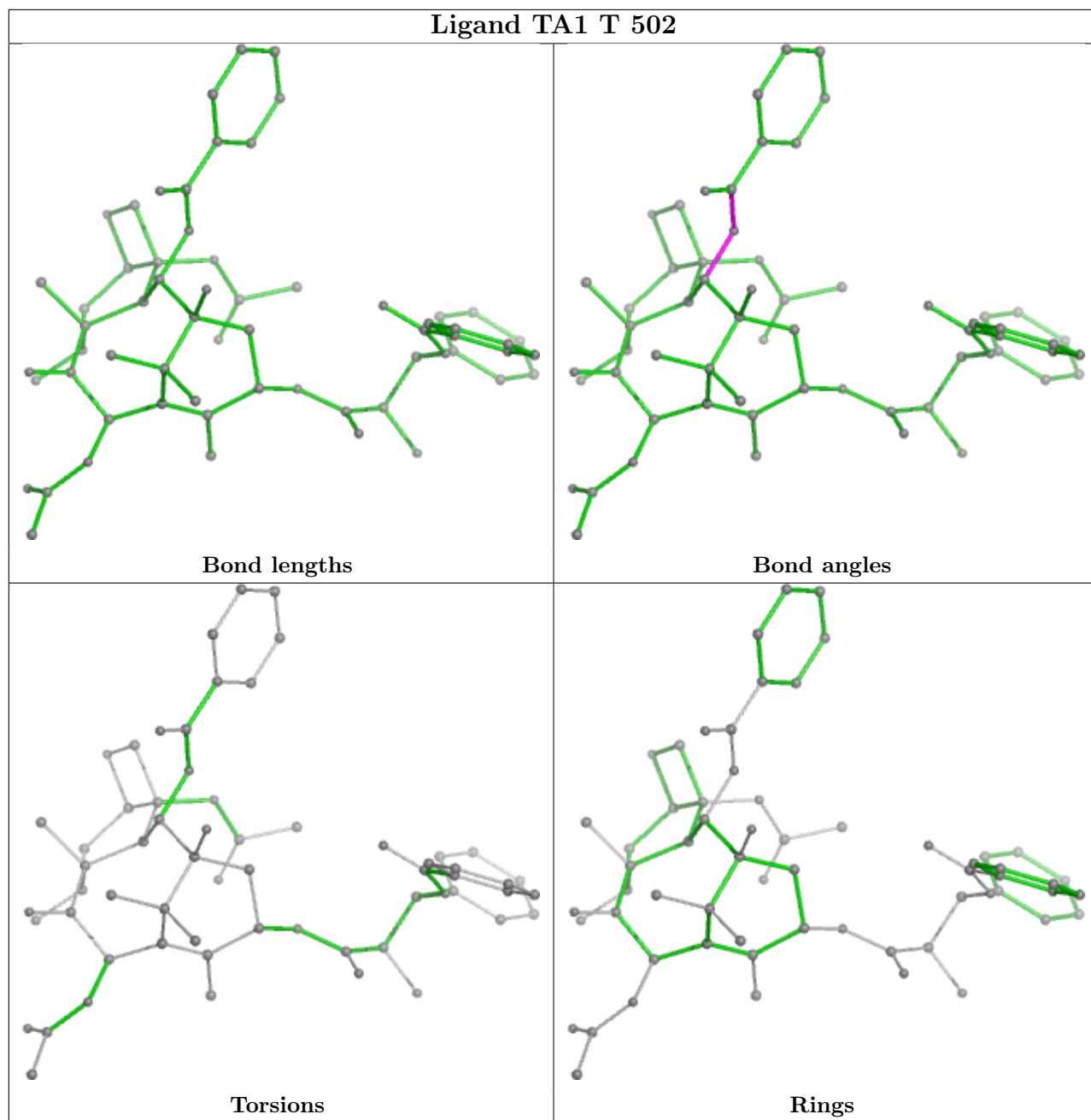




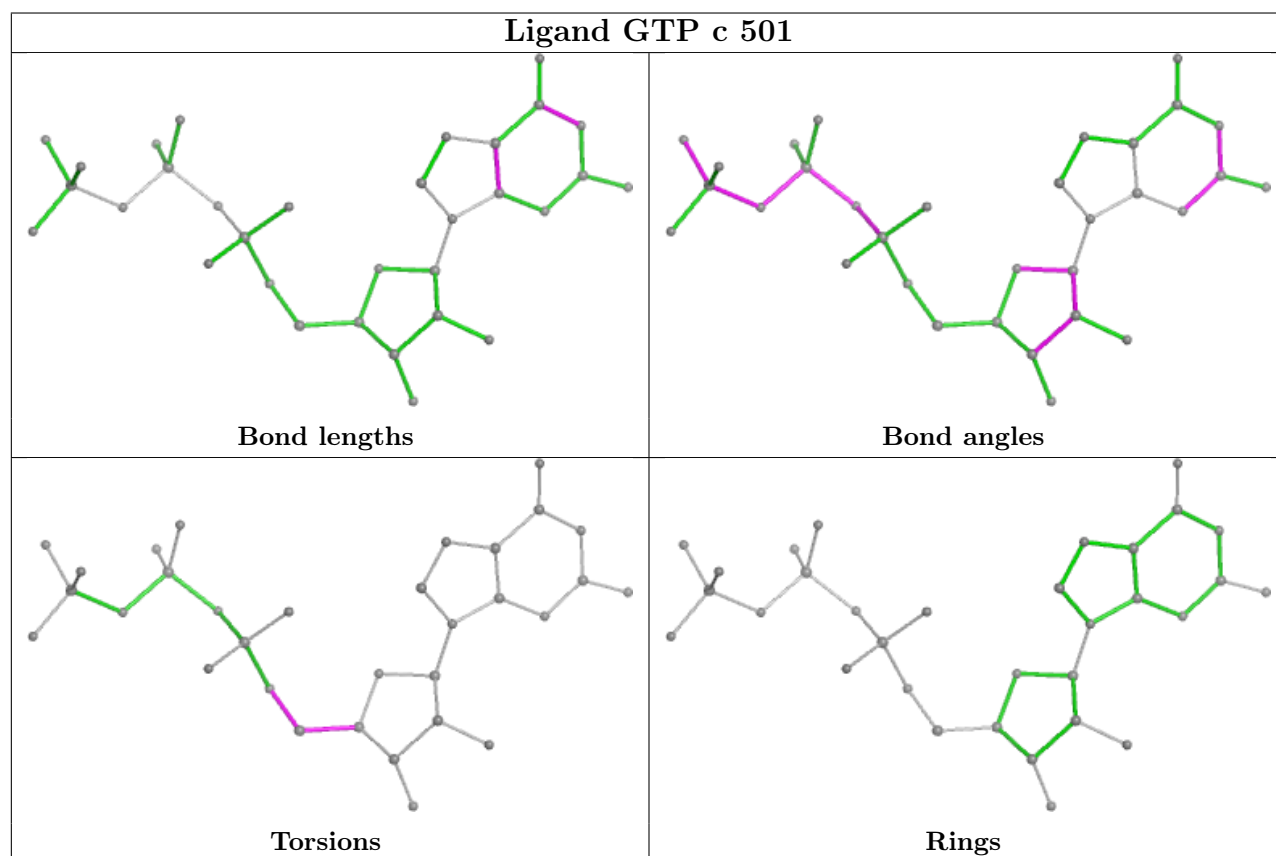
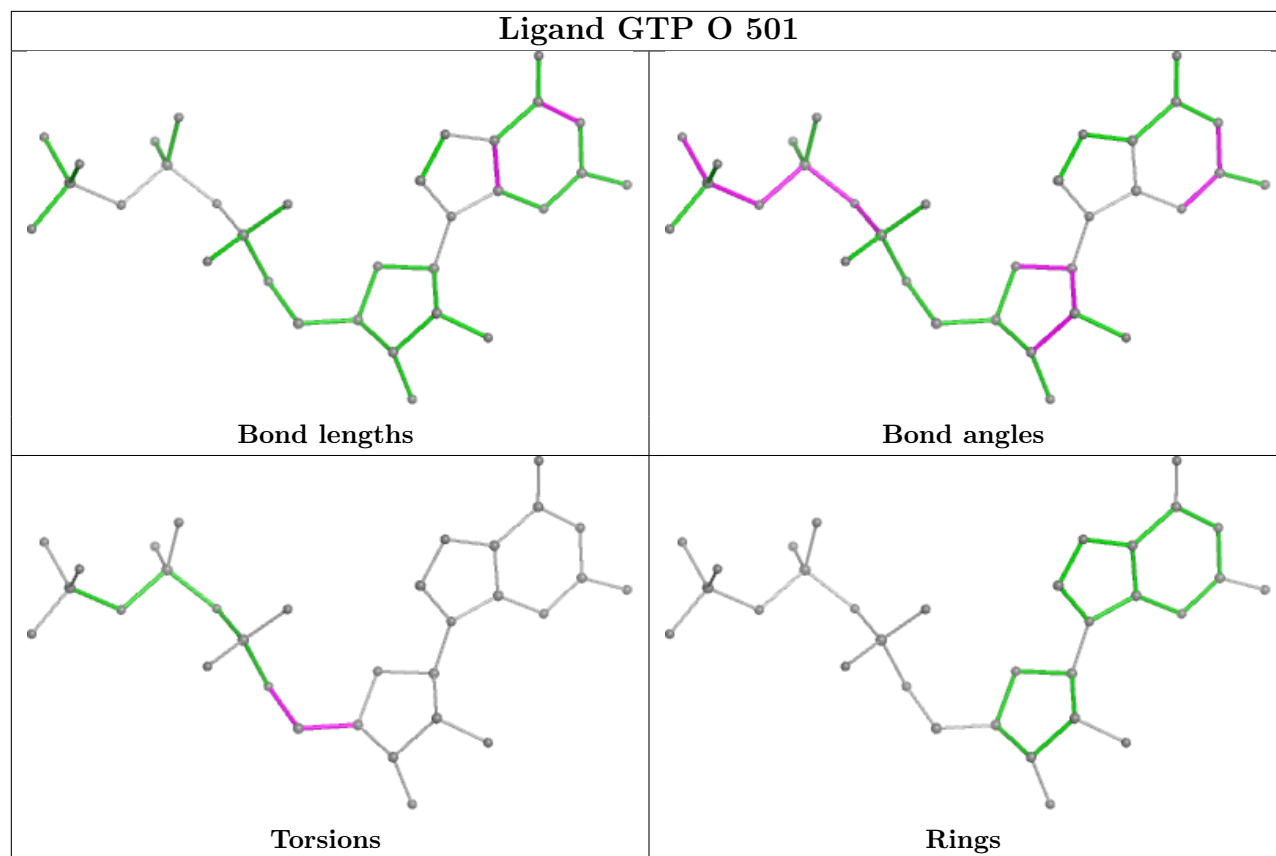


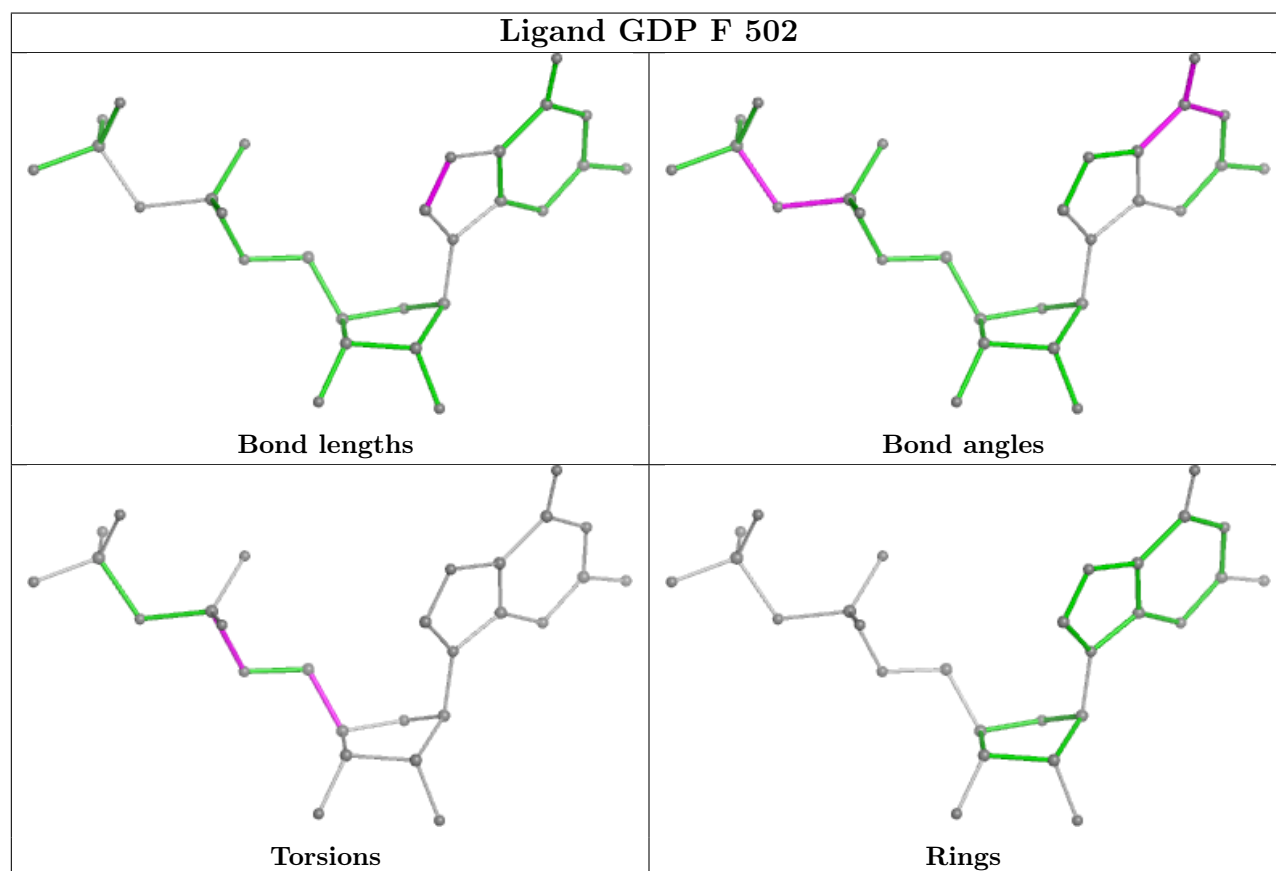
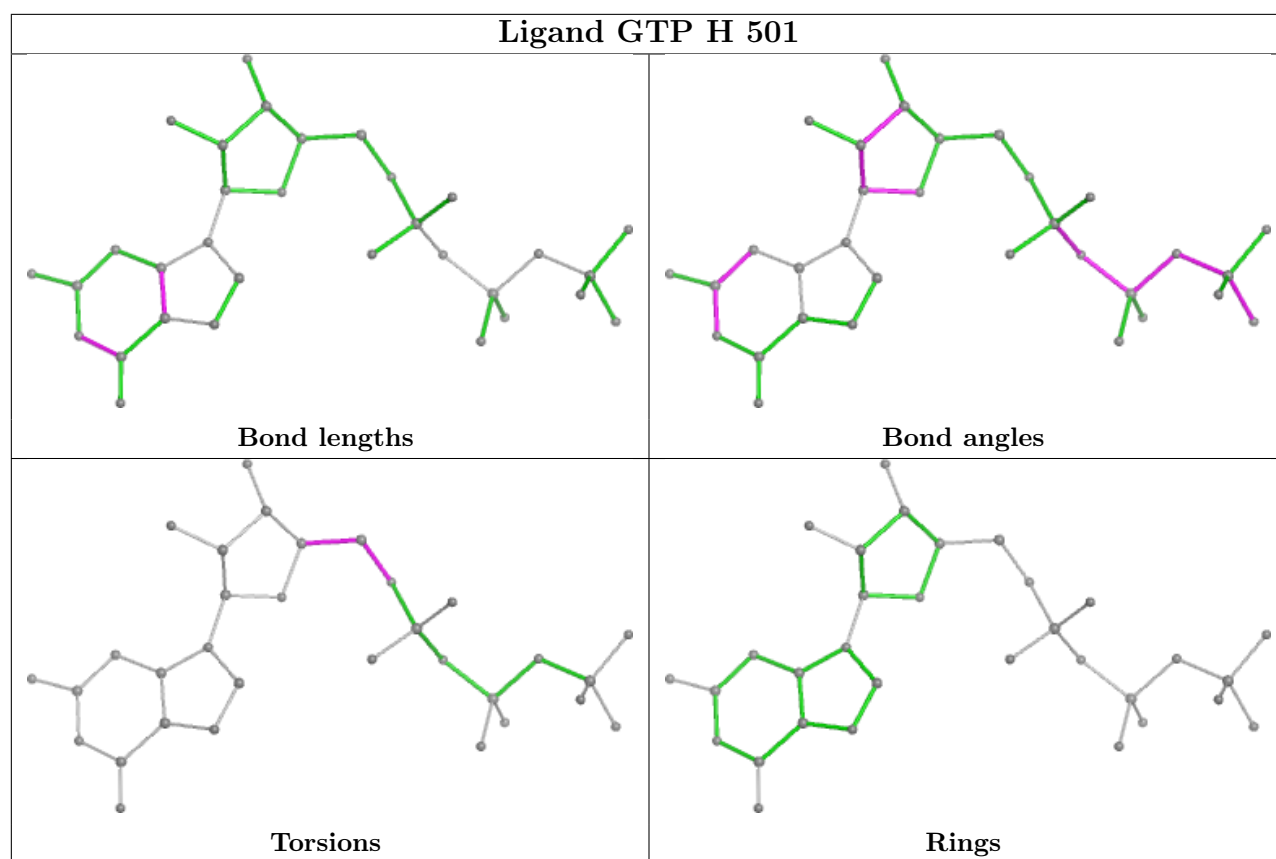


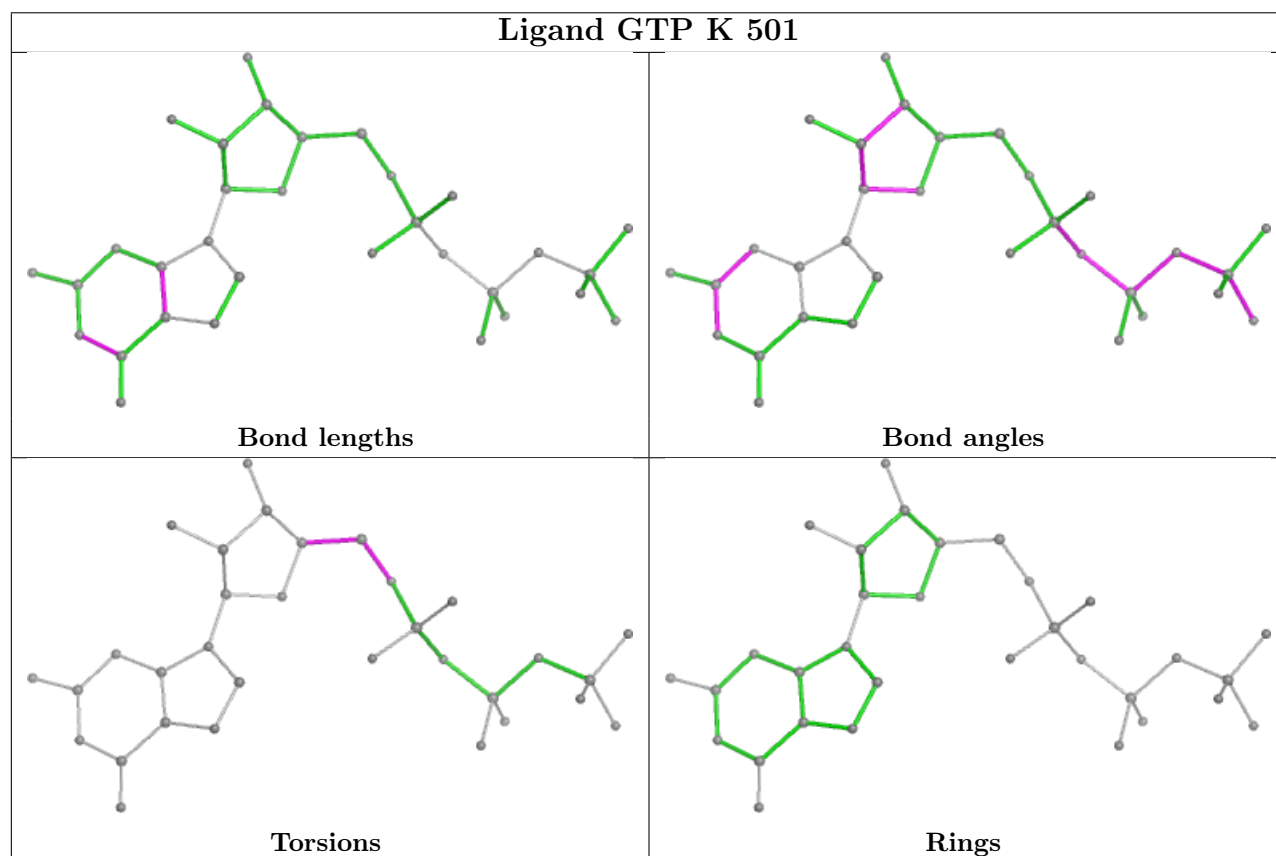
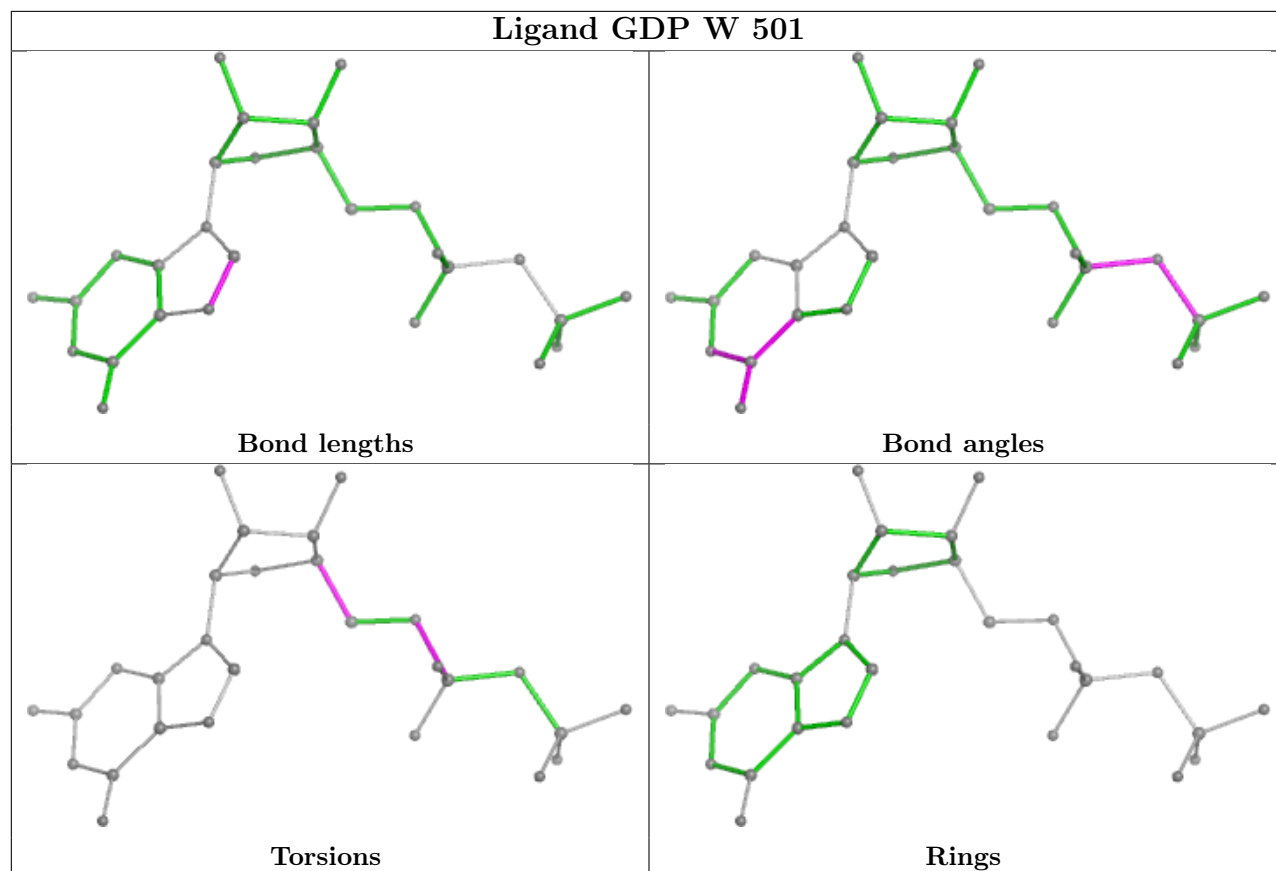


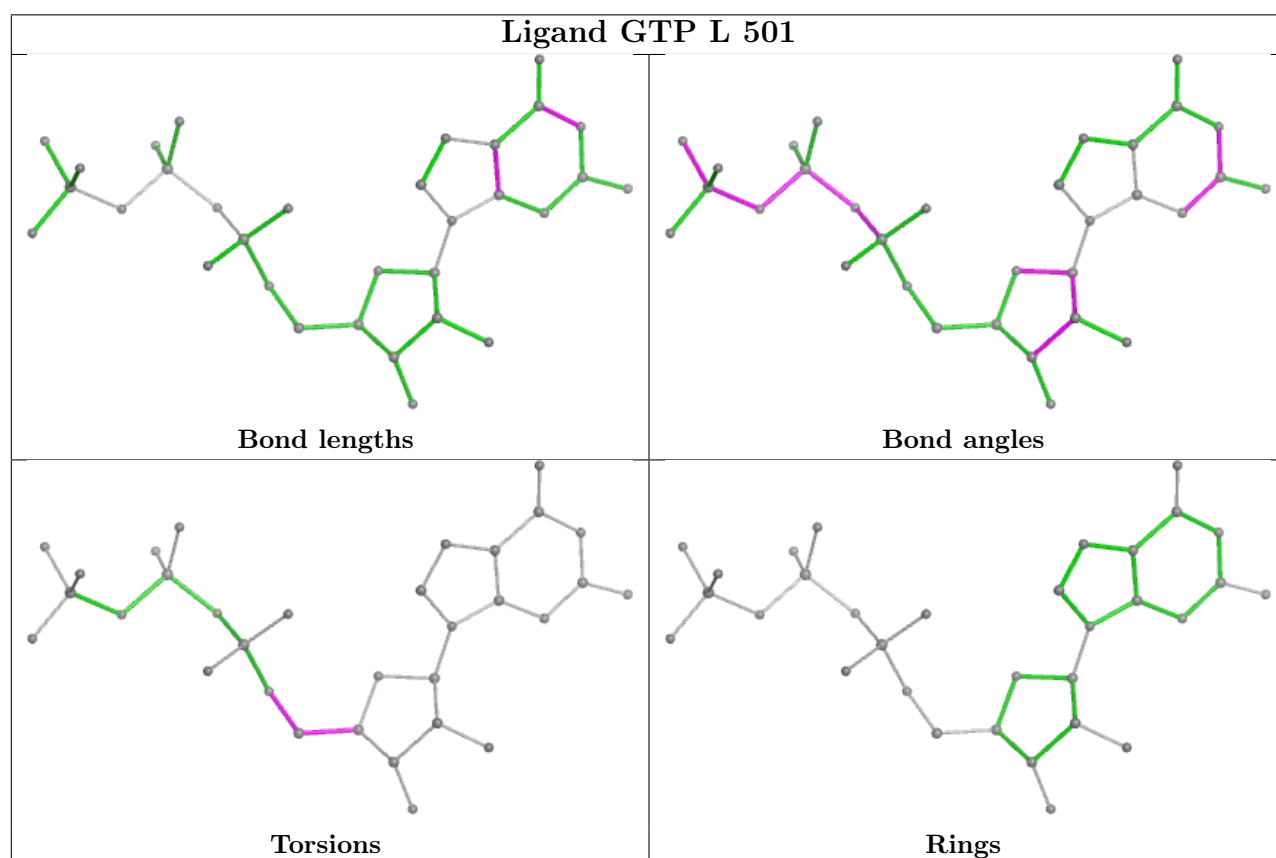
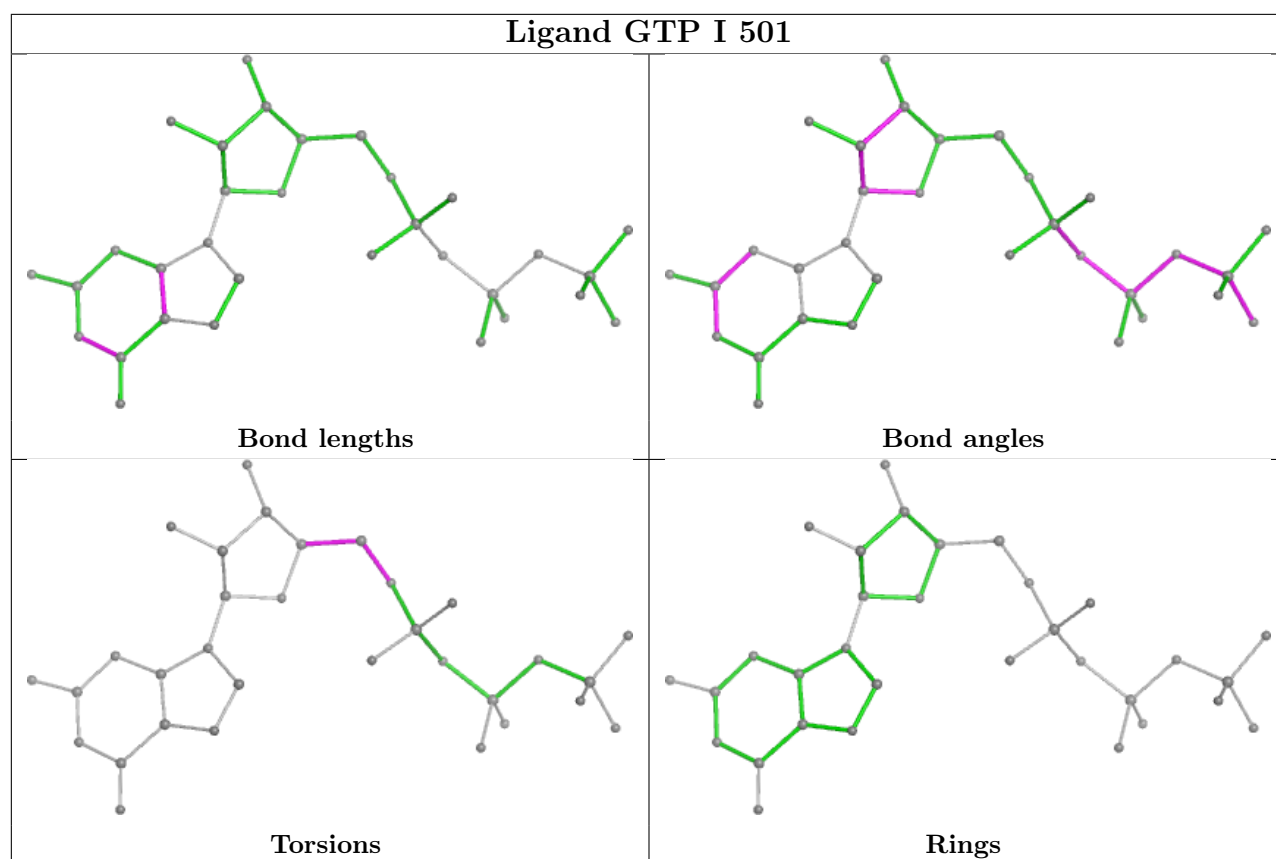


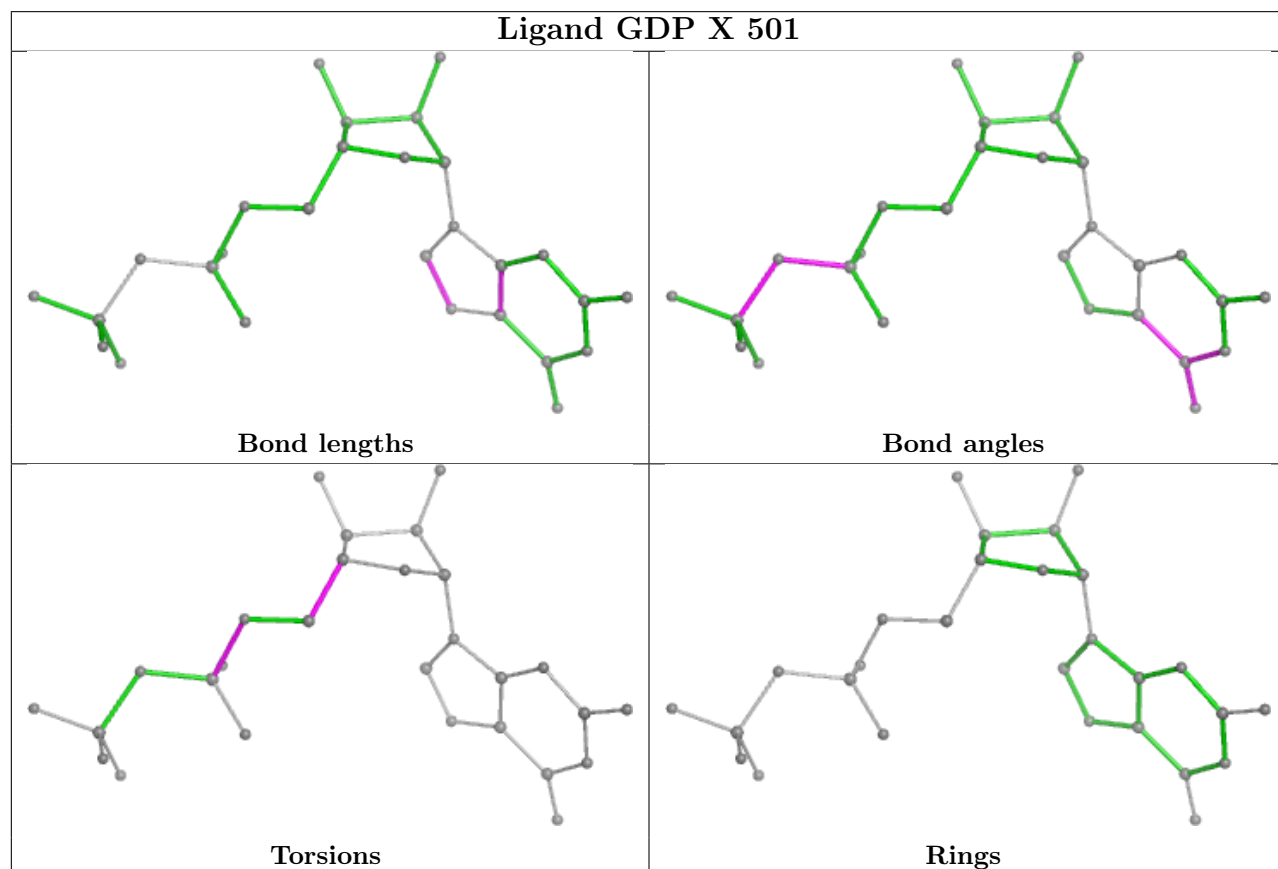
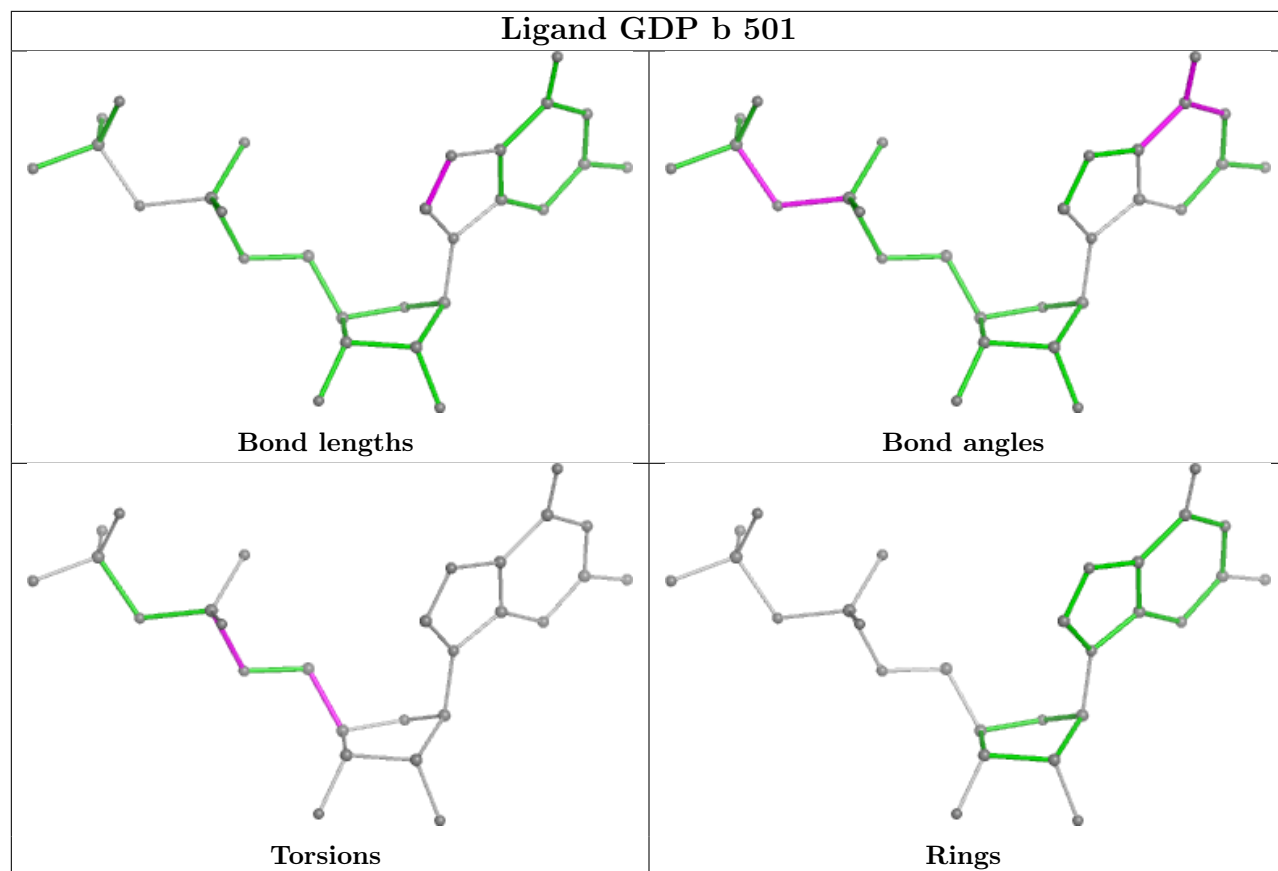


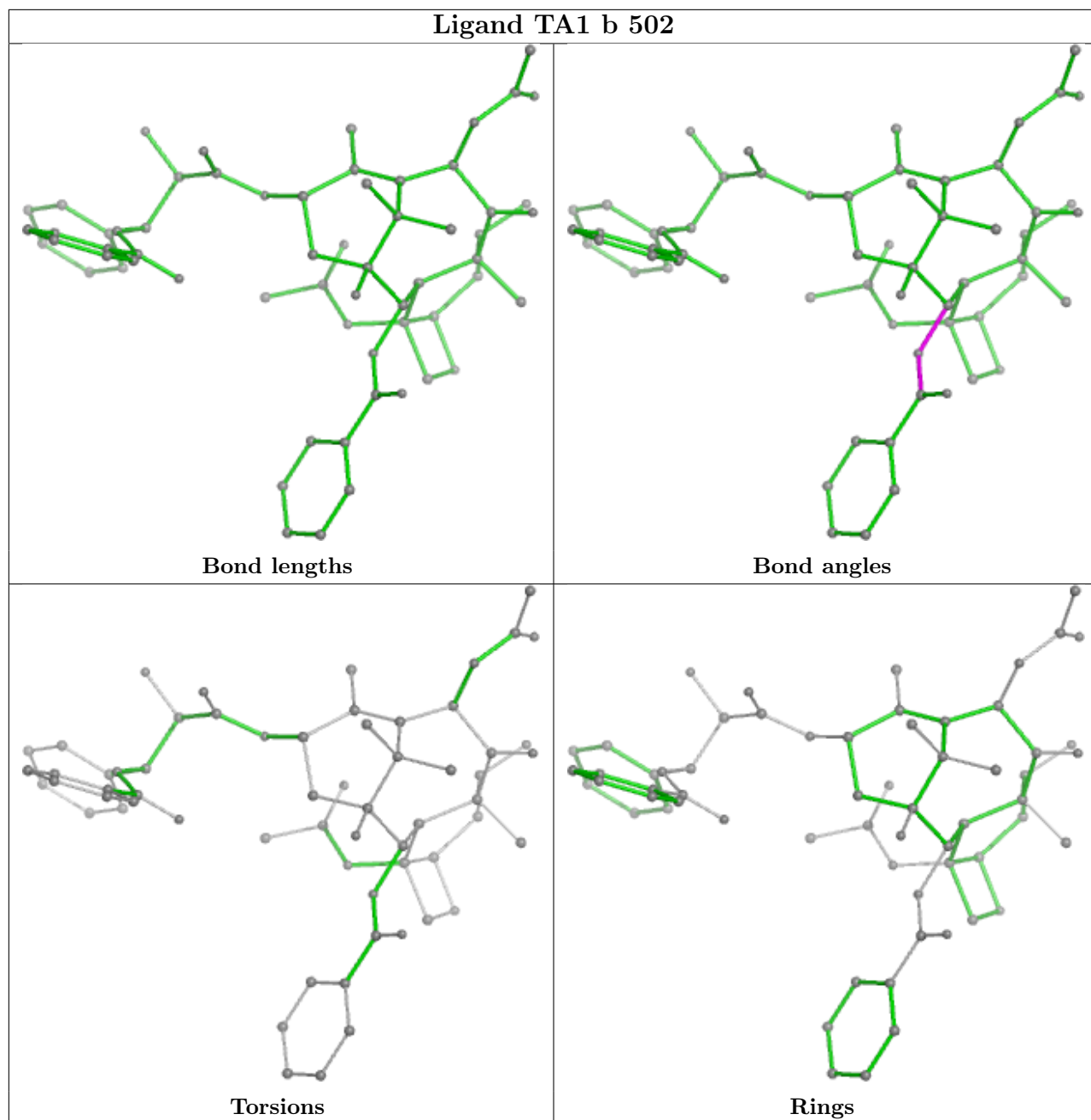


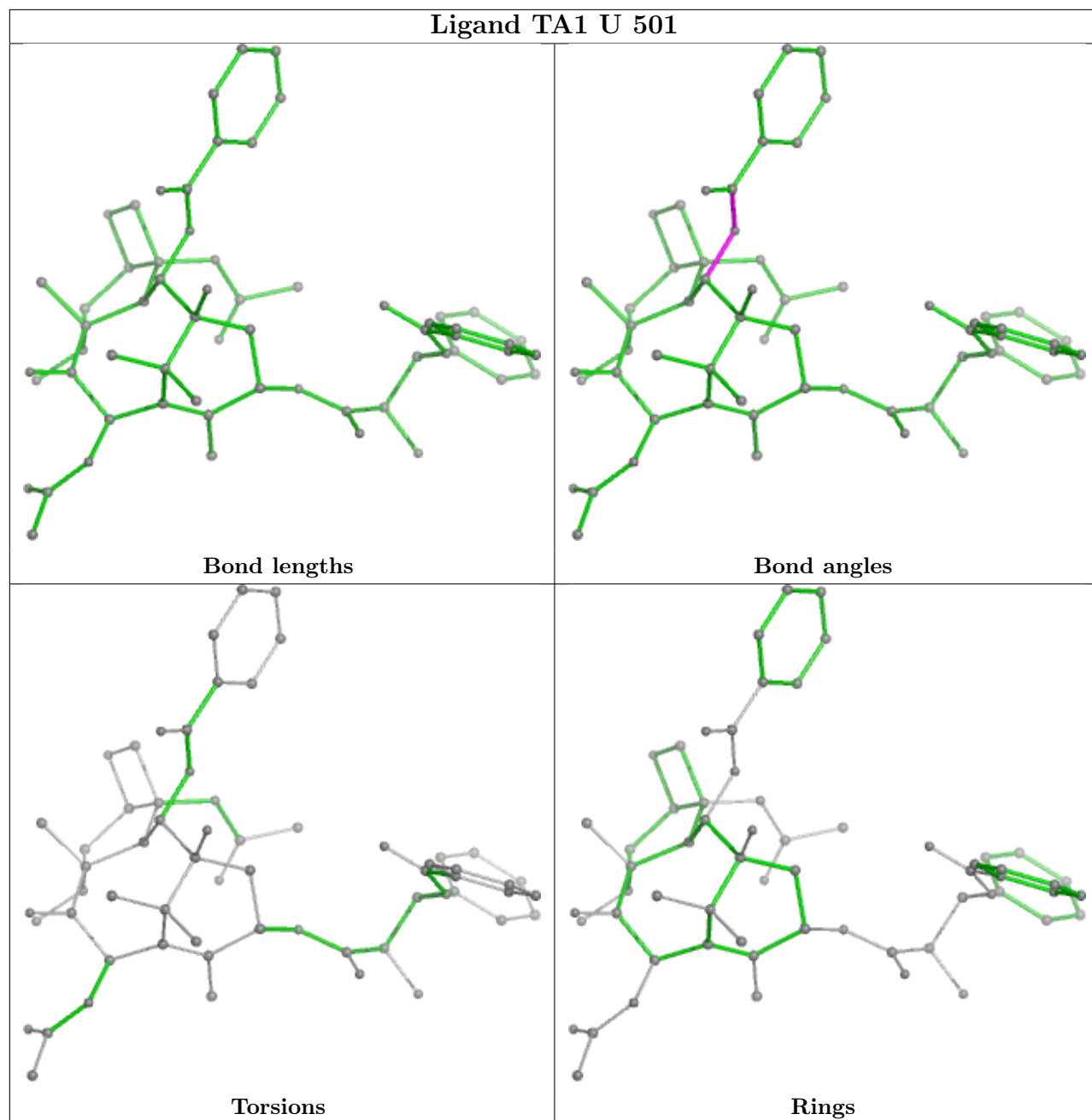


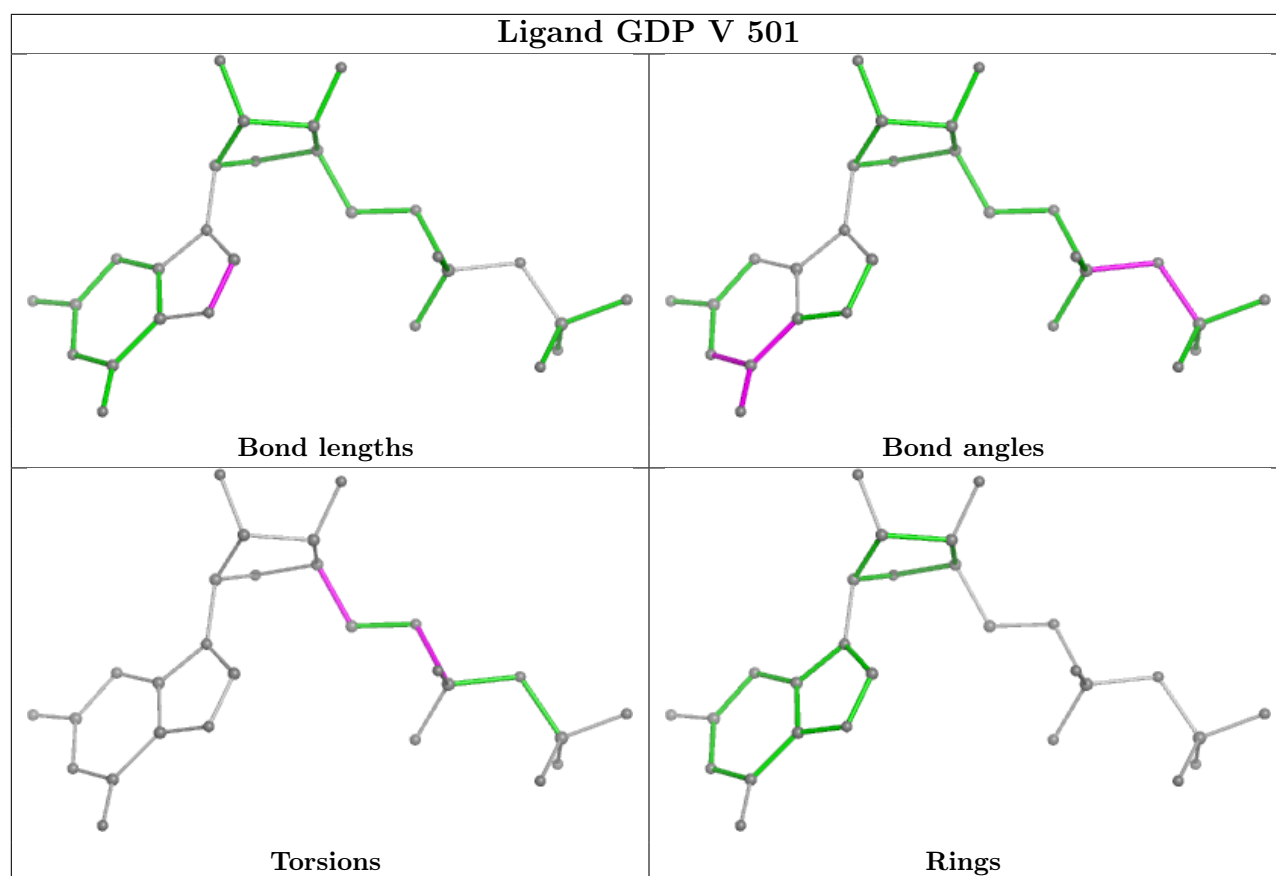












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



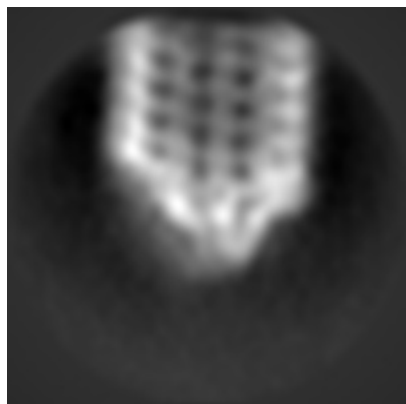
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19862. These allow visual inspection of the internal detail of the map and identification of artifacts.

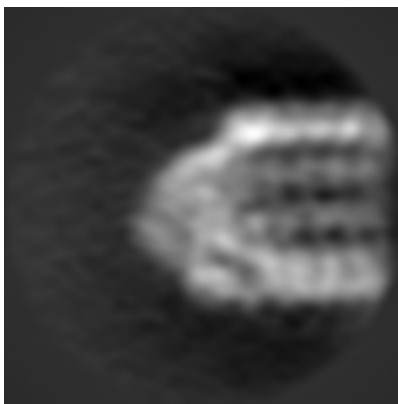
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

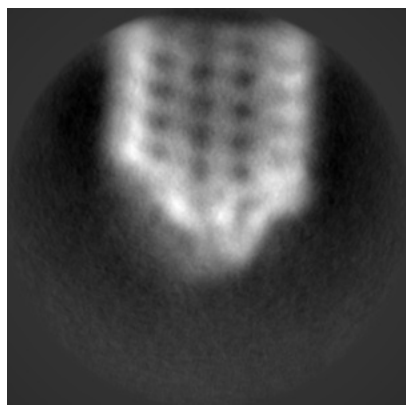


Y

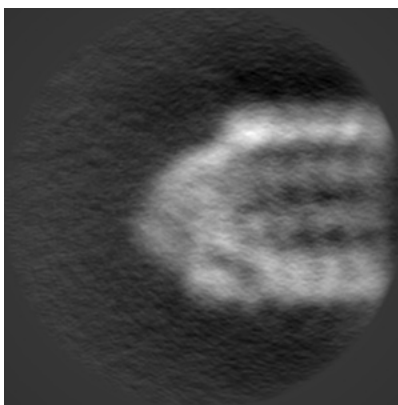


Z

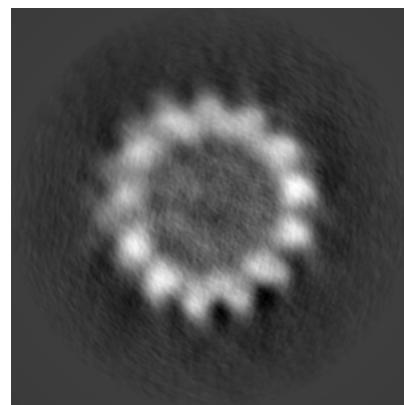
#### 6.1.2 Raw map



X



Y

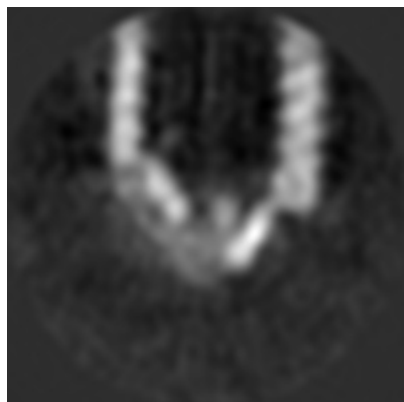


Z

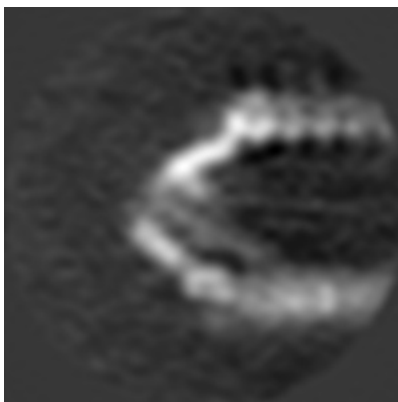
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 128

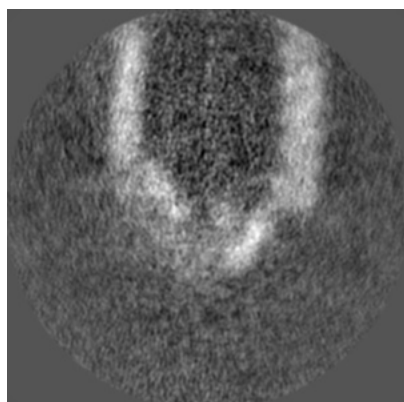


Y Index: 128

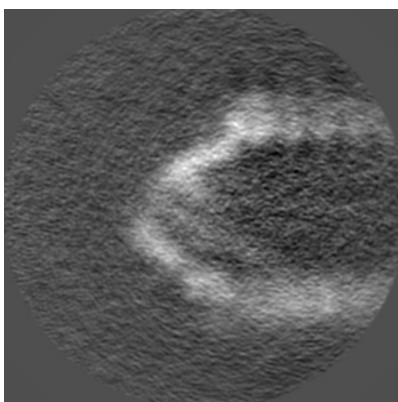


Z Index: 128

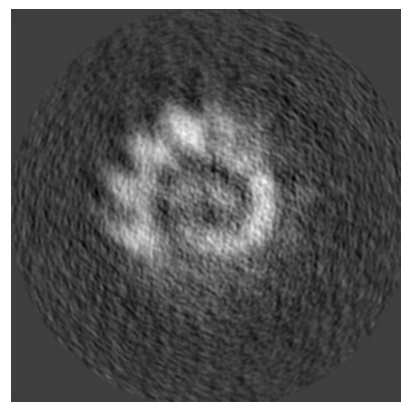
### 6.2.2 Raw map



X Index: 128



Y Index: 128

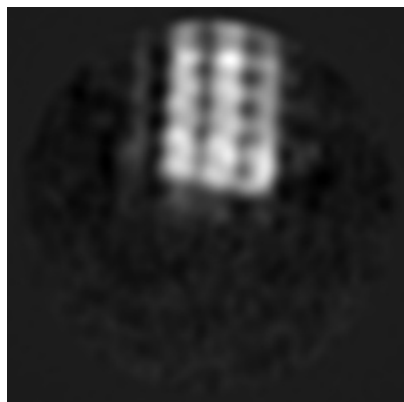


Z Index: 128

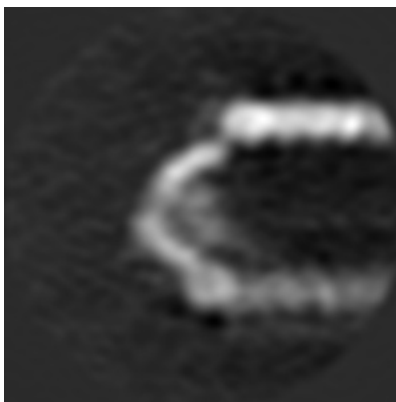
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 179

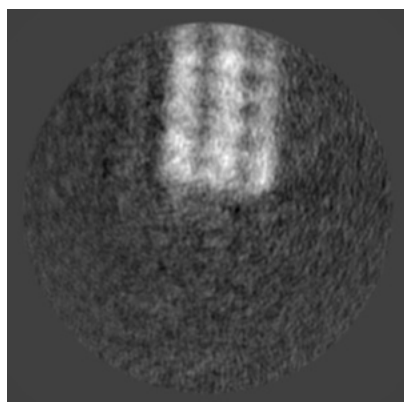


Y Index: 140

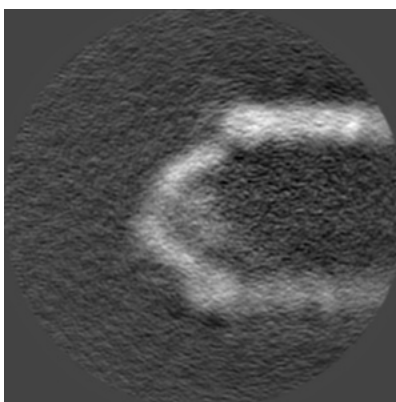


Z Index: 162

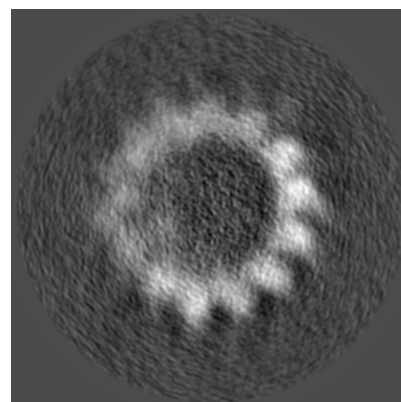
### 6.3.2 Raw map



X Index: 180



Y Index: 140

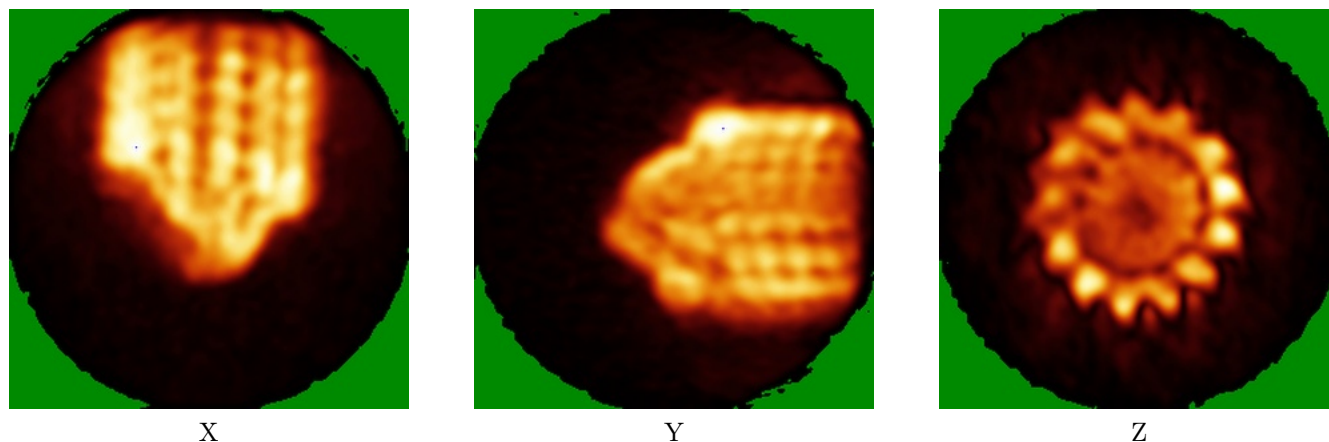


Z Index: 162

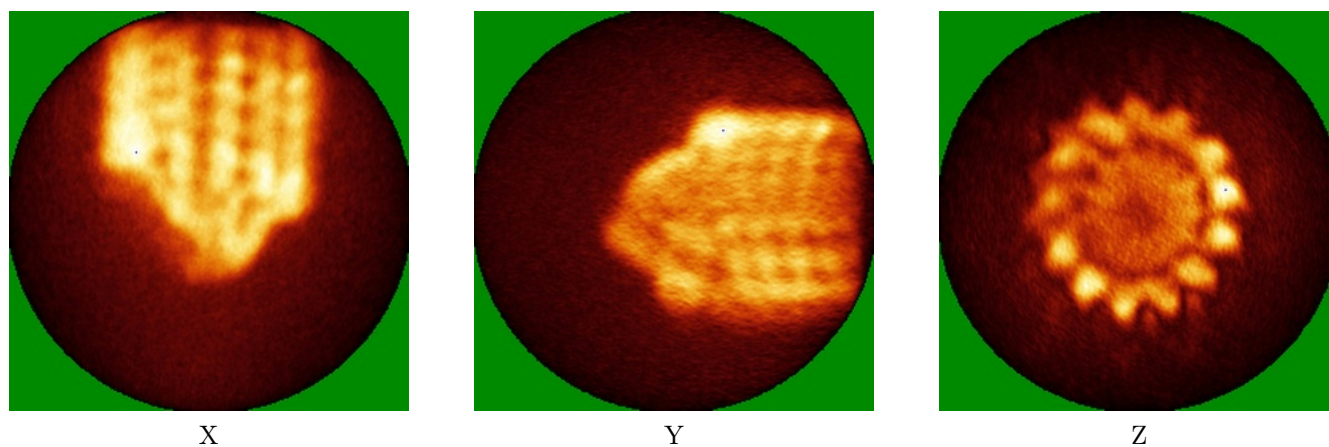
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



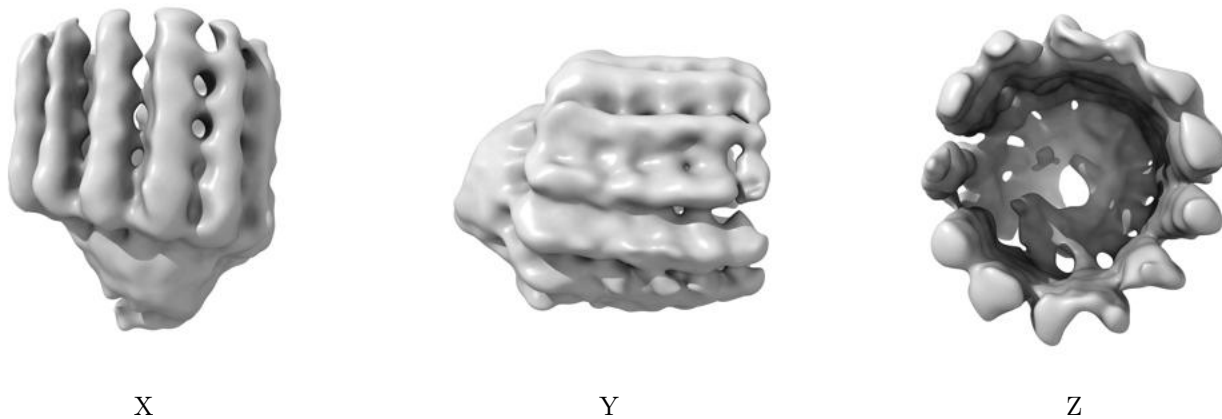
### 6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 0.0157. 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



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.

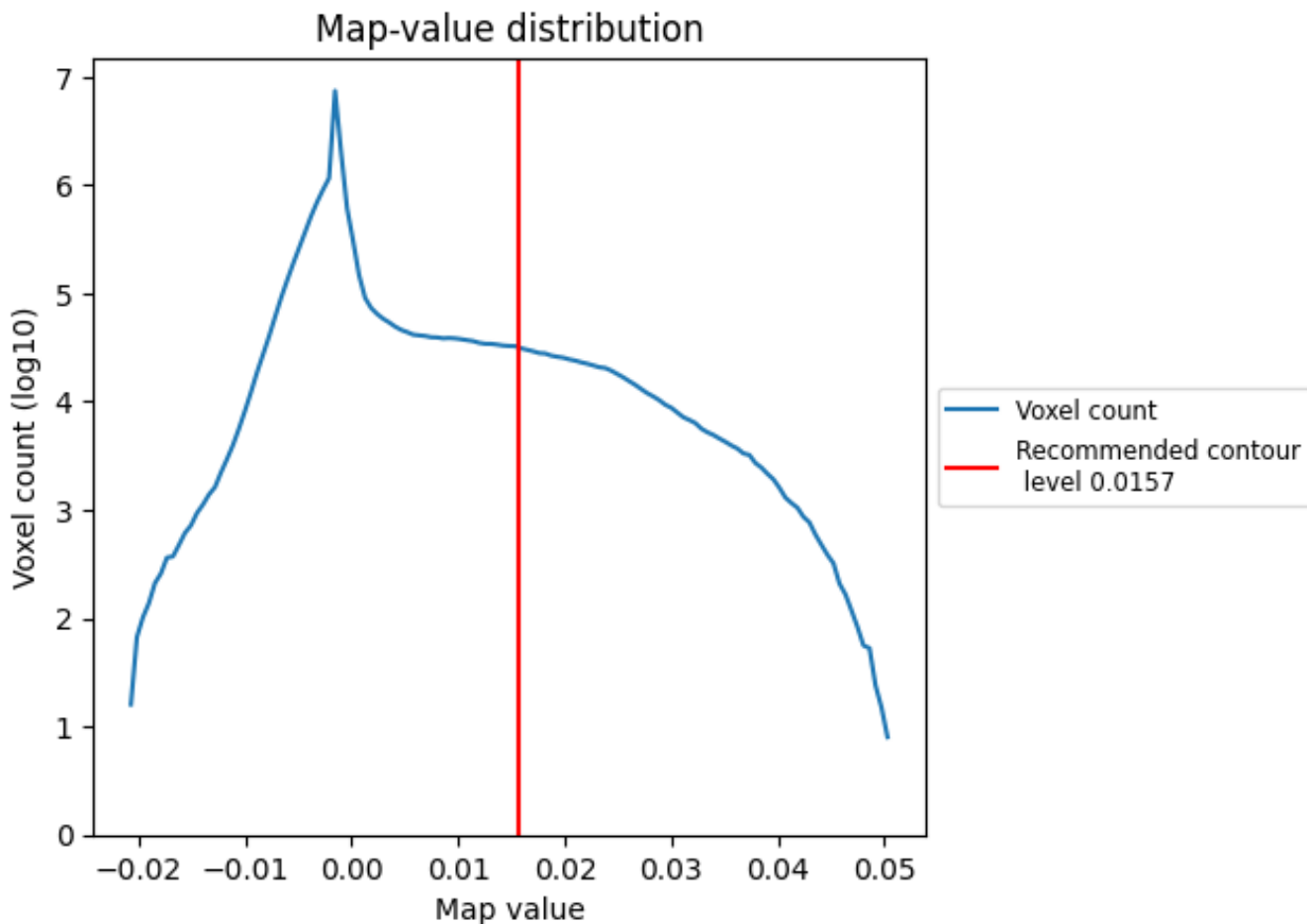
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

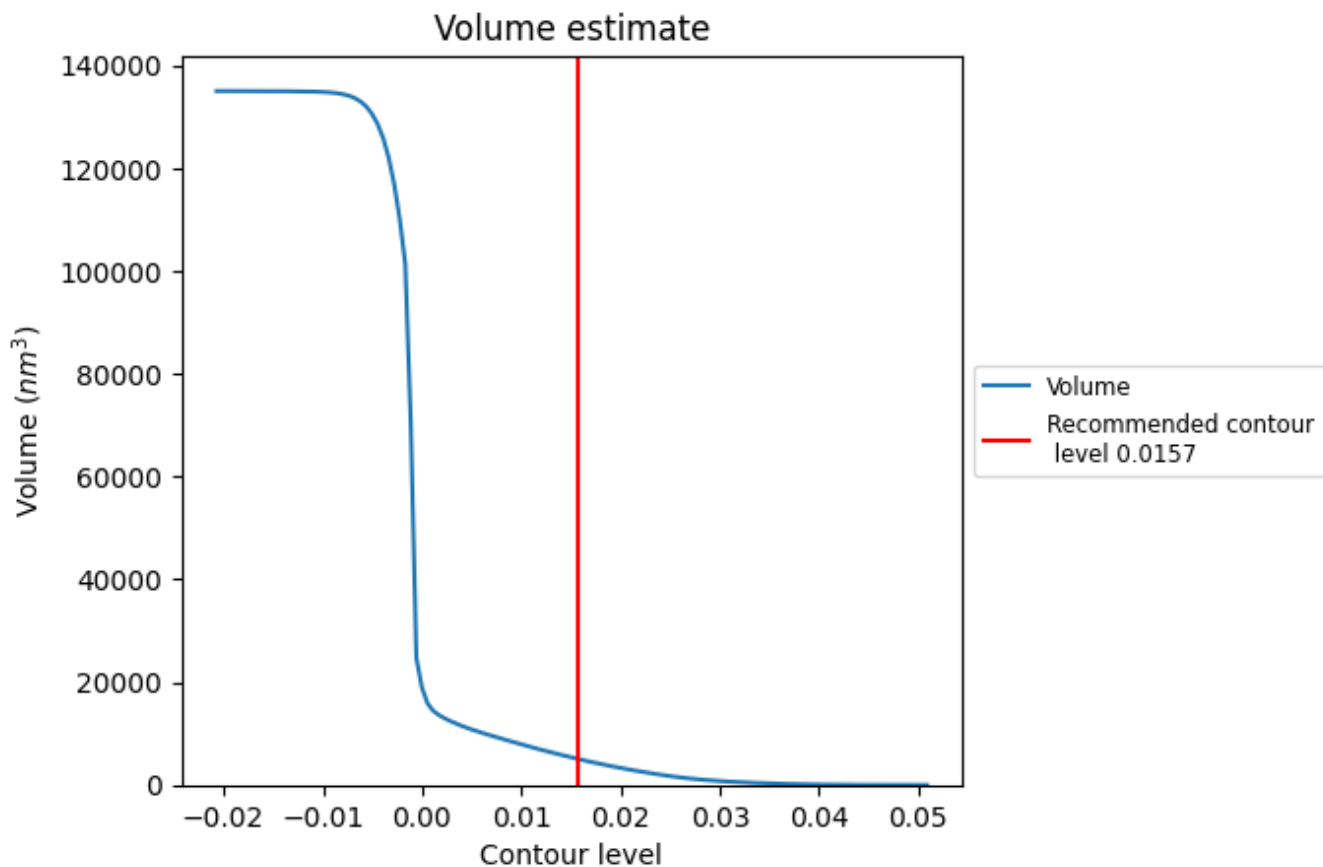
This section contains the results of statistical analysis of the map.

### 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.

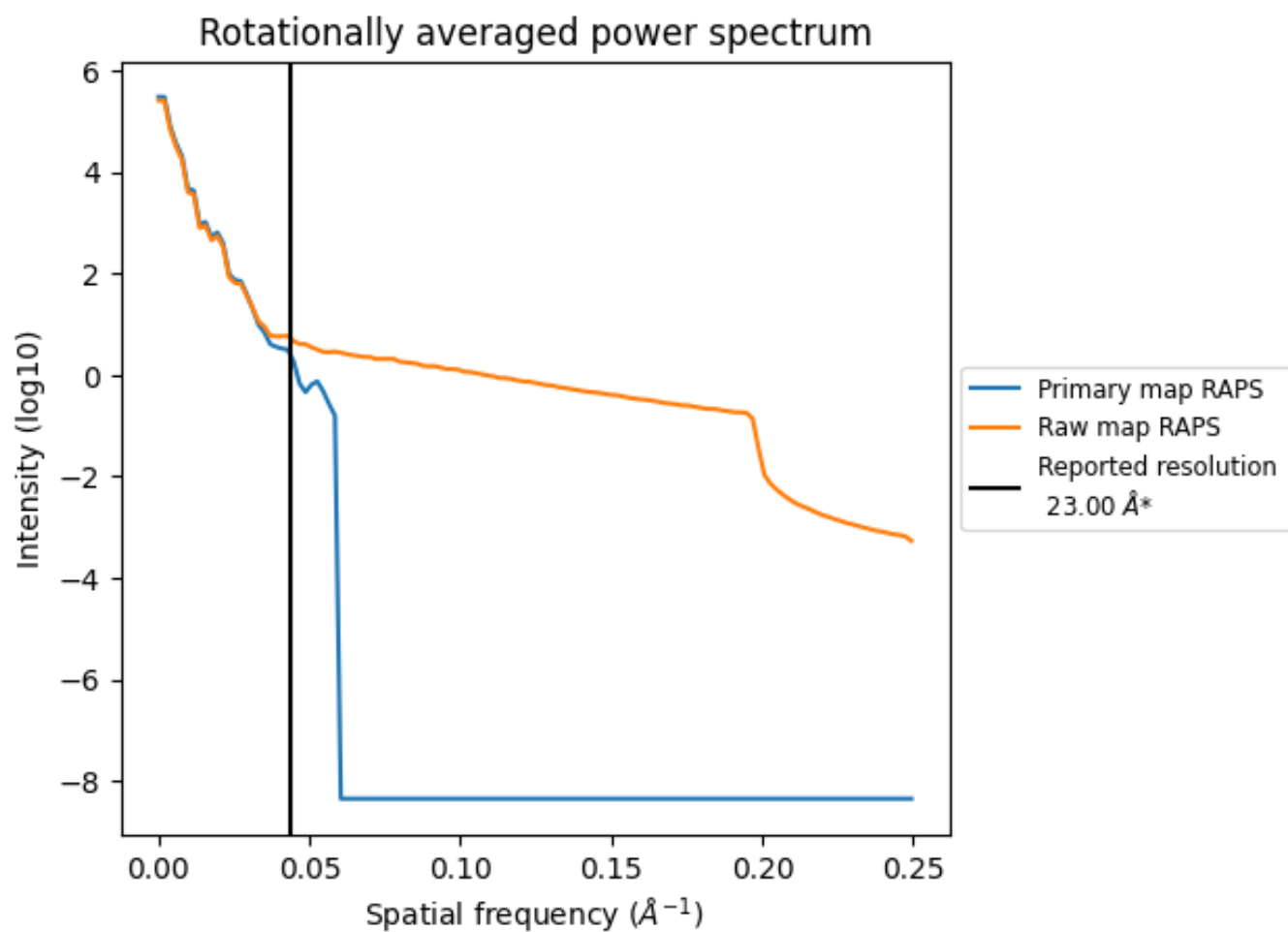
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 5060  $\text{nm}^3$ ; this corresponds to an approximate mass of 4571 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



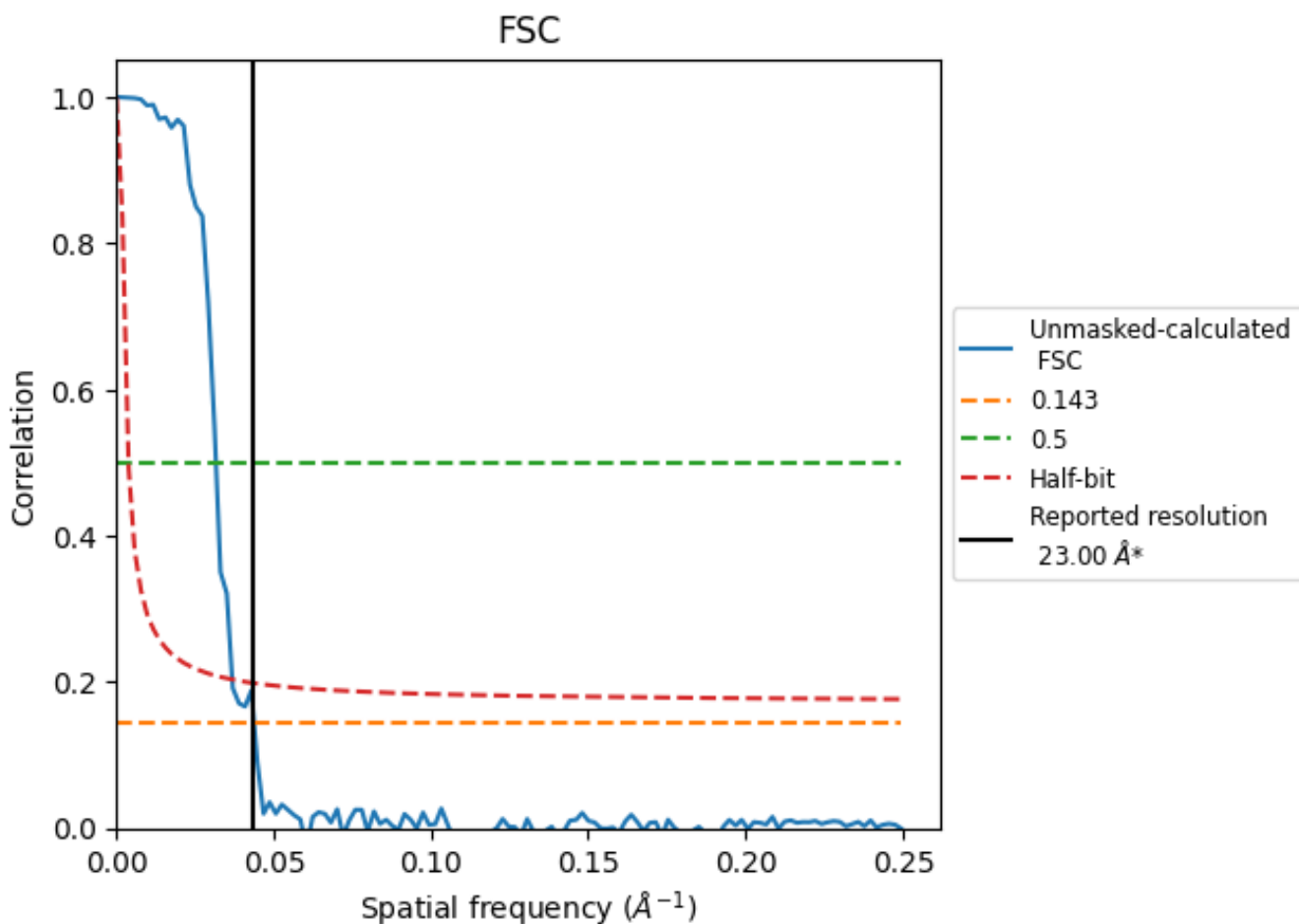
\*Reported resolution corresponds to spatial frequency of 0.043 Å<sup>-1</sup>



## 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 0.043 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

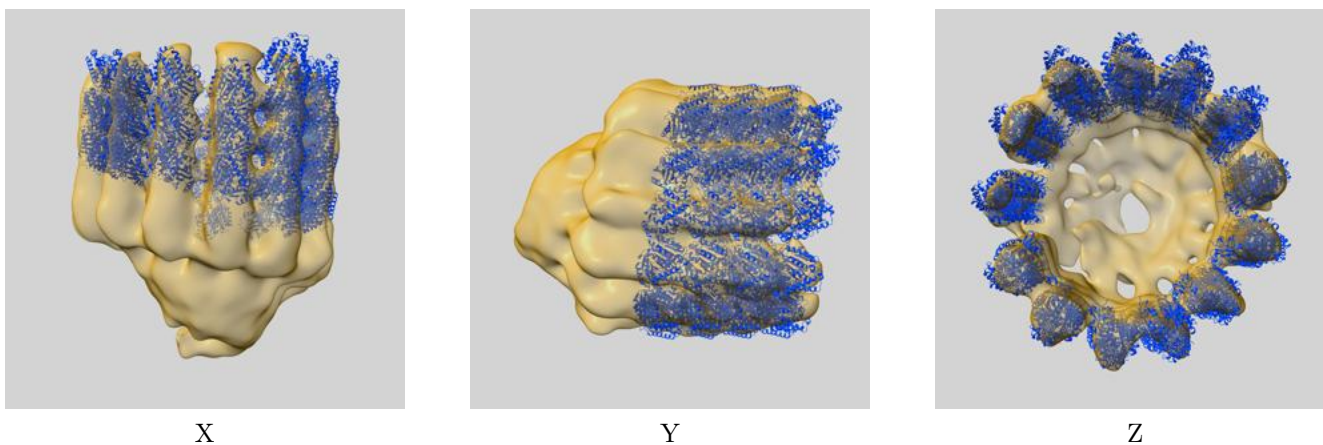
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	23.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	22.83	31.55	27.10

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

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

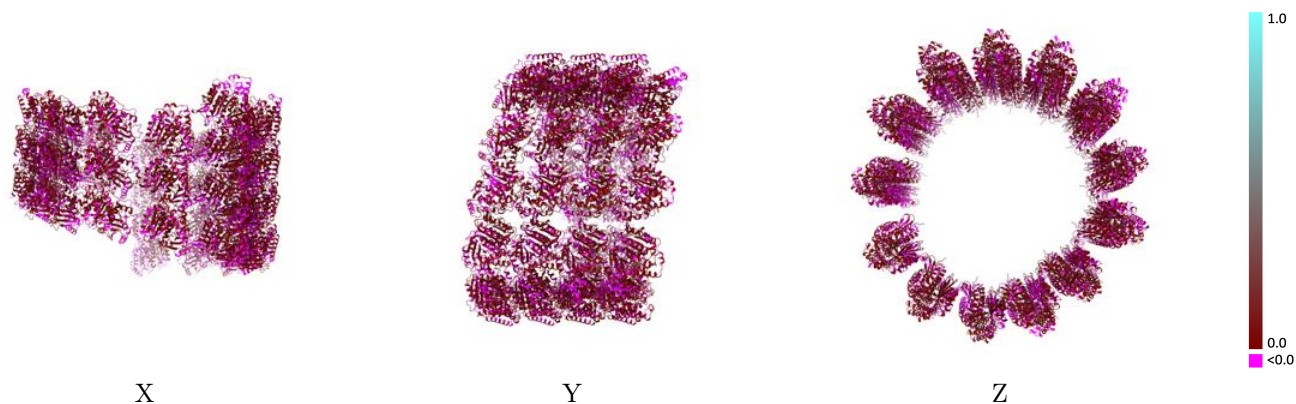
This section contains information regarding the fit between EMDB map EMD-19862 and PDB model 9EOK. Per-residue inclusion information can be found in section 3 on page 13.

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



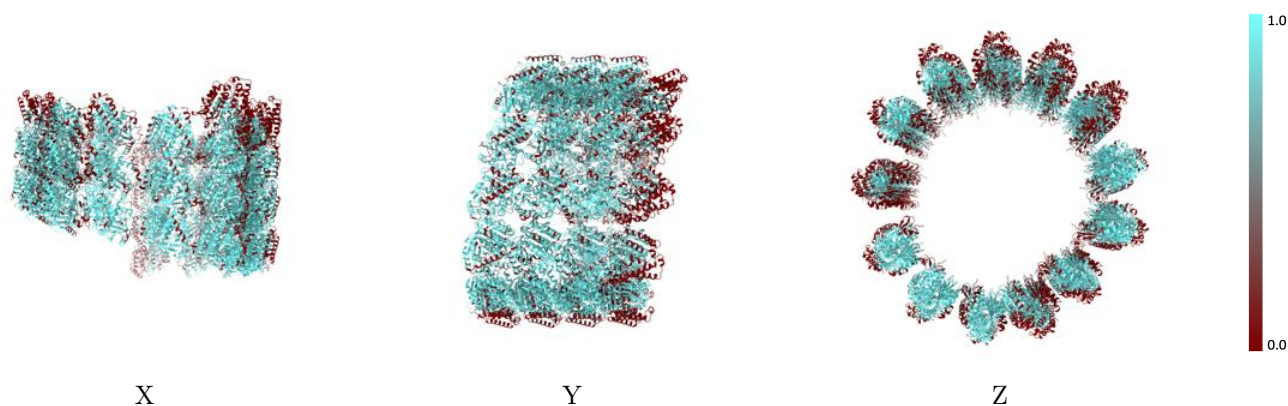
The images above show the 3D surface view of the map at the recommended contour level 0.0157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



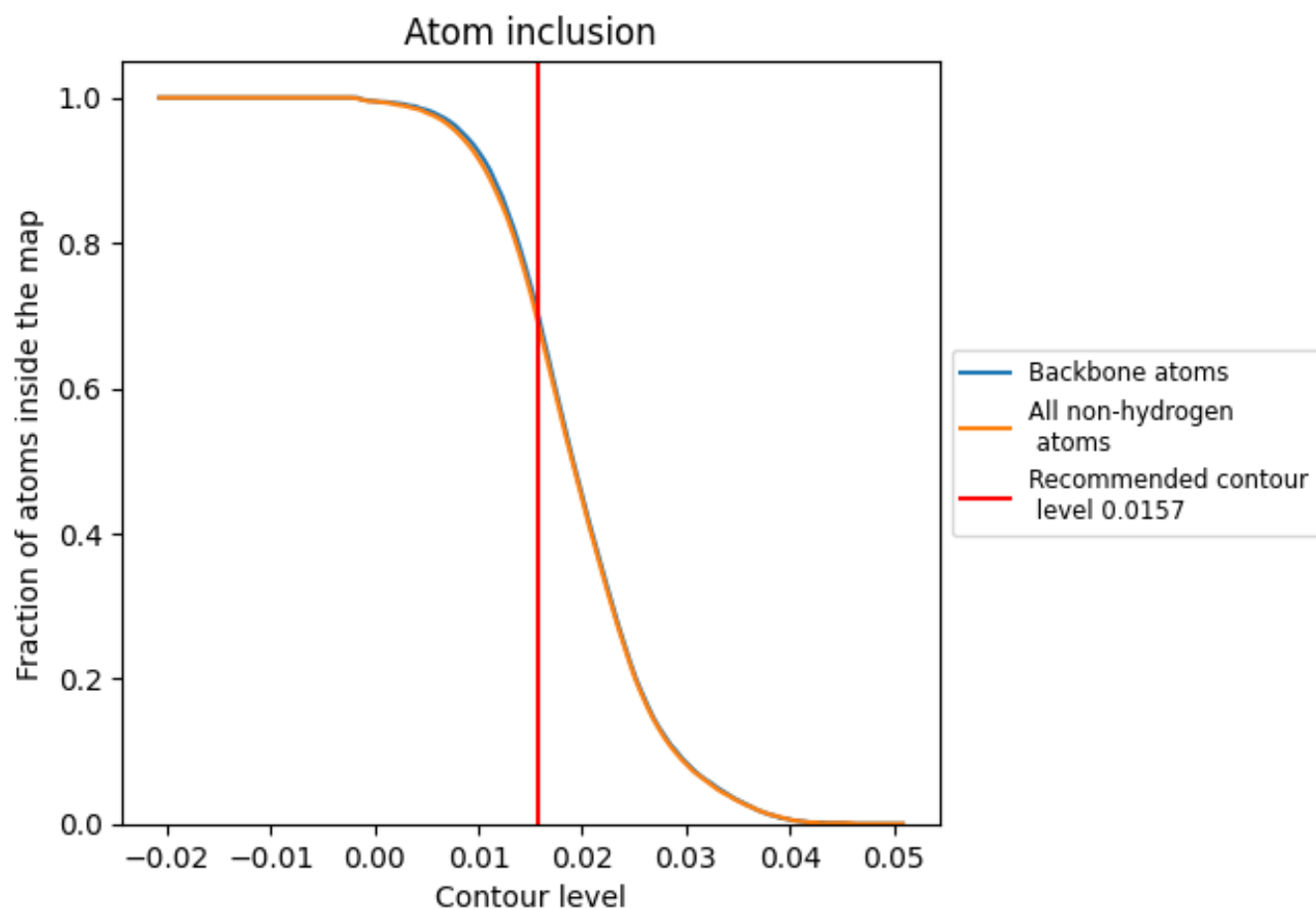
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0157).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.0157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.0360
A	 0.3640	 0.0190
B	 0.5850	 0.0330
C	 0.7340	 0.0330
D	 0.7730	 0.0370
E	 0.5630	 0.0340
F	 0.2140	 0.0230
G	 0.7930	 0.0360
H	 0.7940	 0.0400
I	 0.8330	 0.0360
J	 0.8780	 0.0360
K	 0.8300	 0.0370
L	 0.7820	 0.0370
M	 0.8120	 0.0390
N	 0.8360	 0.0330
O	 0.9170	 0.0360
P	 0.8570	 0.0350
Q	 0.7610	 0.0350
R	 0.8070	 0.0400
S	 0.7990	 0.0390
T	 0.8330	 0.0460
U	 0.8250	 0.0410
V	 0.8720	 0.0380
W	 0.7940	 0.0370
X	 0.7390	 0.0390
Y	 0.7500	 0.0360
Z	 0.7530	 0.0350
a	 0.8550	 0.0410
b	 0.6820	 0.0350
c	 0.7650	 0.0320
d	 0.7850	 0.0440
e	 0.7930	 0.0400
f	 0.7600	 0.0400
g	 0.7620	 0.0390
h	 0.8250	 0.0330



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Chain	Atom inclusion	Q-score
i	 0.6170	 0.0360
j	 0.5830	 0.0400
k	 0.3460	 0.0250
o	 0.5250	 0.0260
p	 0.4760	 0.0380
q	 0.2780	 0.0390
r	 0.2480	 0.0290
s	 0.3130	 0.0250