



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 11:58 PM UTC

PDB ID : 8C5C / pdb_00008c5c
EMDB ID : EMD-16435
Title : microtubule decorated with tubulin oligomers in presence of APC C-terminal domain. (here only map corresponding to the 13-pf microtubule is represented)
Authors : Serre, L.; Arnal, I.
Deposited on : 2023-01-06
Resolution : 5.30 Å(reported)

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

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

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

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

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

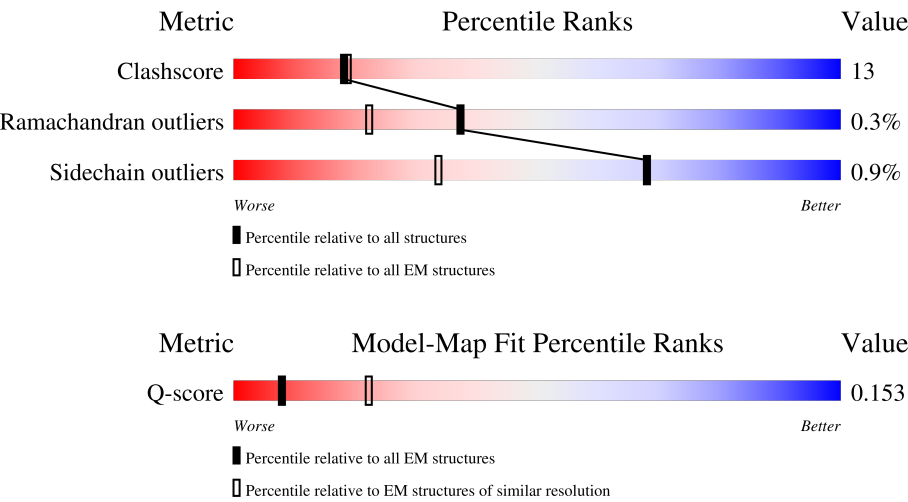
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.30 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.



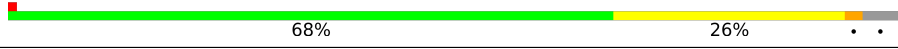
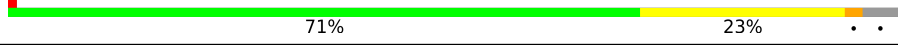
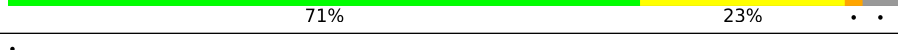
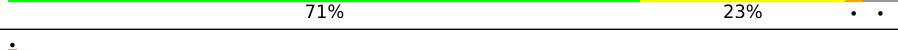
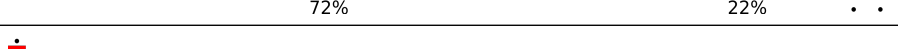
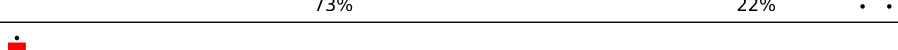
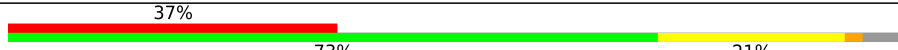
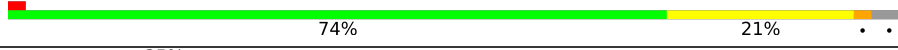
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	625 (4.80 - 5.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	446	
1	b	446	
1	c	446	
1	d	446	

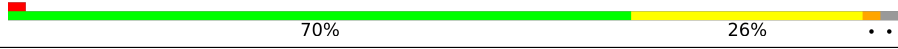
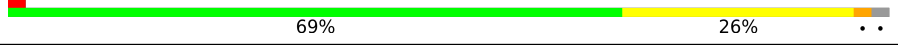
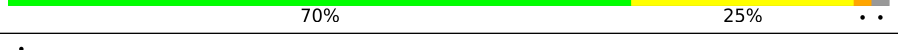
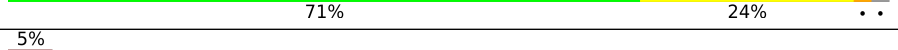
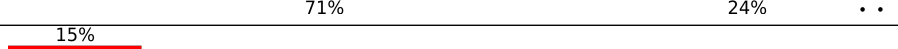
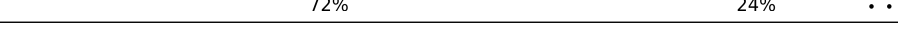
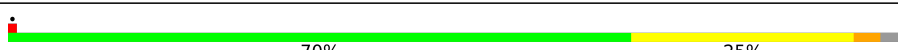
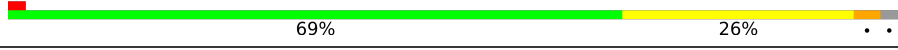
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Mol	Chain	Length	Quality of chain
1	e	446	
1	f	446	
1	g	446	
1	h	446	
1	i	446	
1	j	446	
1	k	446	
1	l	446	
1	m	446	
1	n	446	
1	o	446	
1	p	446	
1	q	446	
1	r	446	
1	s	446	
1	t	446	
1	u	446	
1	v	446	
1	w	446	
1	x	446	
1	y	446	
1	z	446	
2	A	451	
2	B	451	
2	C	451	

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Mol	Chain	Length	Quality of chain
2	D	451	
2	E	451	
2	F	451	
2	G	451	
2	H	451	
2	I	451	
2	J	451	
2	K	451	
2	L	451	
2	M	451	
2	N	451	
2	O	451	
2	P	451	
2	Q	451	
2	R	451	
2	S	451	
2	T	451	
2	U	451	
2	V	451	
2	W	451	
2	X	451	
2	Y	451	
2	Z	451	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TA1	c	601	-	-	X	-
3	TA1	i	601	-	-	X	-
4	GDP	a	602	-	-	X	-
4	GDP	b	602	-	-	X	-
4	GDP	c	602	-	-	X	-
4	GDP	d	602	-	-	X	-
4	GDP	e	602	-	-	X	-
4	GDP	f	602	-	-	X	-
4	GDP	g	602	-	-	X	-
4	GDP	h	602	-	-	X	-
4	GDP	i	602	-	-	X	-
4	GDP	j	602	-	-	X	-
4	GDP	k	602	-	-	X	-
4	GDP	l	602	-	-	X	-
4	GDP	m	602	-	-	X	-
6	GTP	N	502	-	-	X	-
6	GTP	O	502	-	-	X	-
6	GTP	P	502	-	-	X	-
6	GTP	Q	502	-	-	X	-
6	GTP	R	502	-	-	X	-
6	GTP	S	502	-	-	X	-
6	GTP	T	502	-	-	X	-
6	GTP	U	502	-	-	X	-
6	GTP	V	502	-	-	X	-
6	GTP	W	502	-	-	X	-
6	GTP	X	502	-	-	X	-
6	GTP	Y	502	-	-	X	-
6	GTP	Z	502	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 178971 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	b	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	c	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	d	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	e	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	f	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	g	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	h	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	i	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	j	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	k	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	l	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	m	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	n	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	o	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	p	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	q	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	r	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	s	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	t	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	u	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	v	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	w	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	x	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	y	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		
1	z	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		

- Molecule 2 is a protein called Tubulin alpha-1B chain.

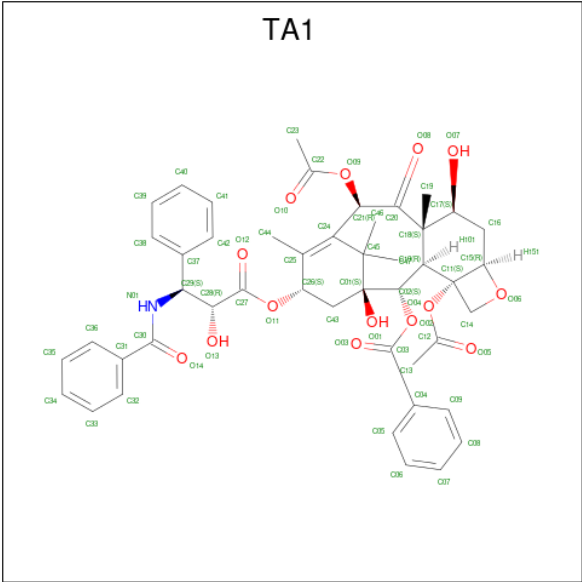
Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	O	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	P	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	Q	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	R	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	S	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	T	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	U	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	V	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		
2	W	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	Y	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	Z	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	A	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	B	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	C	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	D	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	E	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	F	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	G	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	H	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	I	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	J	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	K	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	L	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	M	441	Total 3446	C 2180	N 585	O 659	S 22	0	0

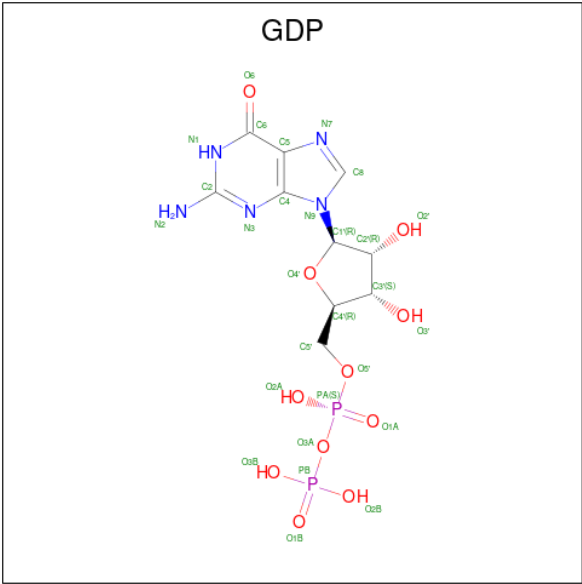
- Molecule 3 is TAXOL (CCD ID: TA1) (formula: $C_{47}H_{51}NO_{14}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	a	1	Total	C	N	O	0
			62	47	1	14	
3	b	1	Total	C	N	O	0
			62	47	1	14	
3	c	1	Total	C	N	O	0
			62	47	1	14	
3	d	1	Total	C	N	O	0
			62	47	1	14	
3	e	1	Total	C	N	O	0
			62	47	1	14	
3	f	1	Total	C	N	O	0
			62	47	1	14	
3	g	1	Total	C	N	O	0
			62	47	1	14	
3	h	1	Total	C	N	O	0
			62	47	1	14	
3	i	1	Total	C	N	O	0
			62	47	1	14	
3	j	1	Total	C	N	O	0
			62	47	1	14	
3	k	1	Total	C	N	O	0
			62	47	1	14	
3	l	1	Total	C	N	O	0
			62	47	1	14	
3	m	1	Total	C	N	O	0
			62	47	1	14	

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂)

(labeled as "Ligand of Interest" by depositor).

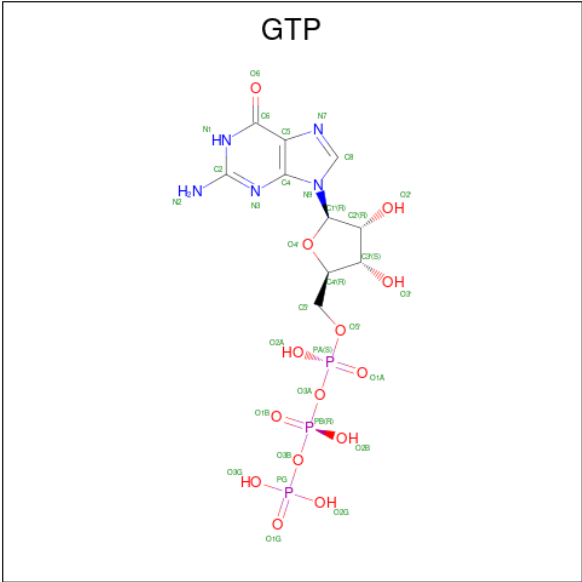


Mol	Chain	Residues	Atoms					AltConf
4	a	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	c	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	d	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	e	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	f	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	g	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	h	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	j	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	k	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	l	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	m	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	N	1	Total 1	Mg 1	0
5	O	1	Total 1	Mg 1	0
5	P	1	Total 1	Mg 1	0
5	Q	1	Total 1	Mg 1	0
5	R	1	Total 1	Mg 1	0
5	S	1	Total 1	Mg 1	0
5	T	1	Total 1	Mg 1	0
5	U	1	Total 1	Mg 1	0
5	V	1	Total 1	Mg 1	0
5	W	1	Total 1	Mg 1	0
5	X	1	Total 1	Mg 1	0
5	Y	1	Total 1	Mg 1	0
5	Z	1	Total 1	Mg 1	0

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

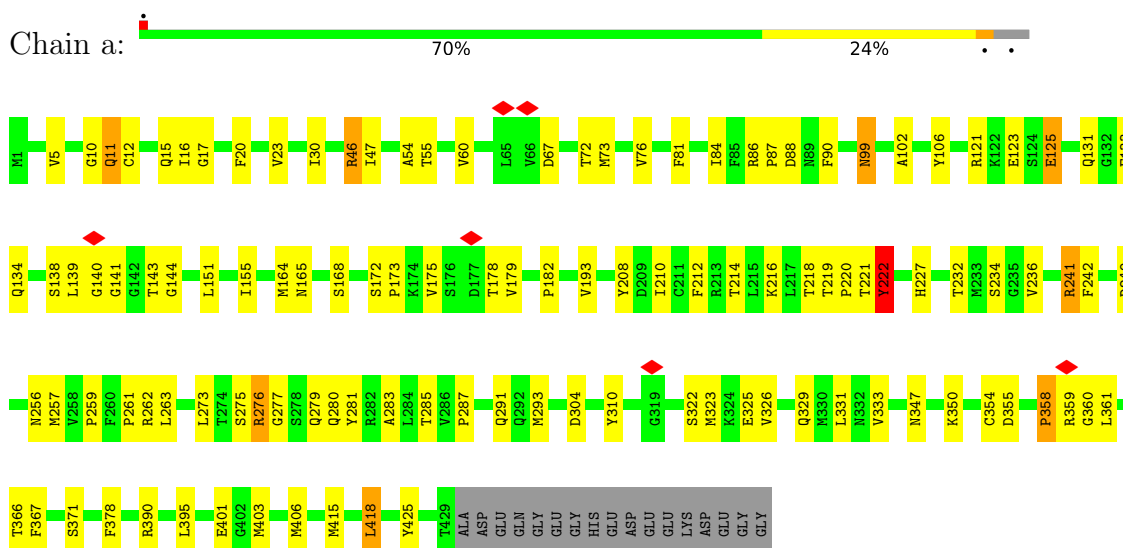


Mol	Chain	Residues	Atoms					AltConf
6	N	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	O	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	P	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	Q	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	R	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	S	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	T	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	U	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	V	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	W	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	X	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	Y	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	

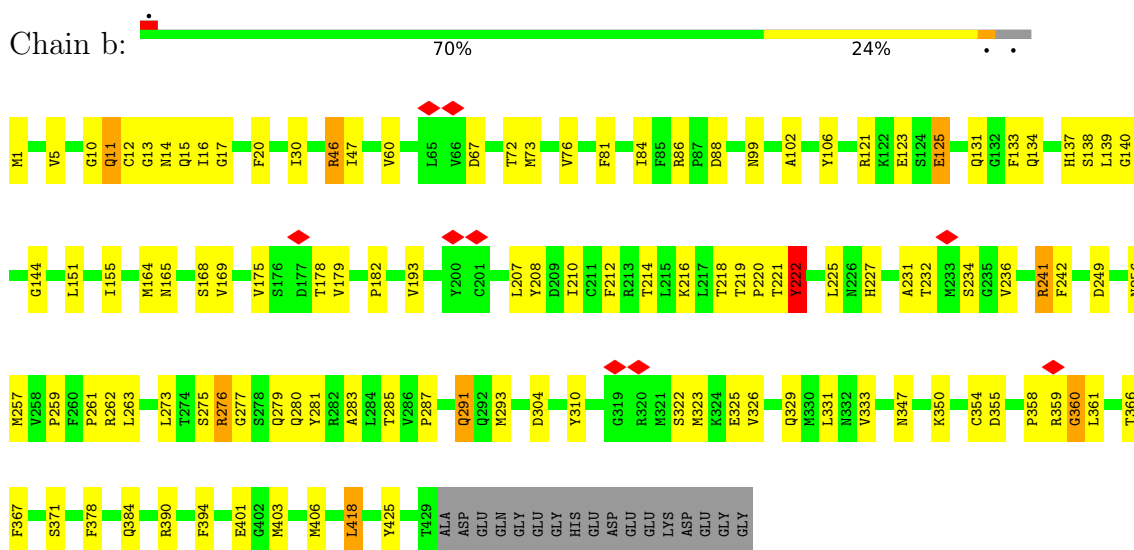
3 Residue-property plots

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

- Molecule 1: Tubulin beta chain



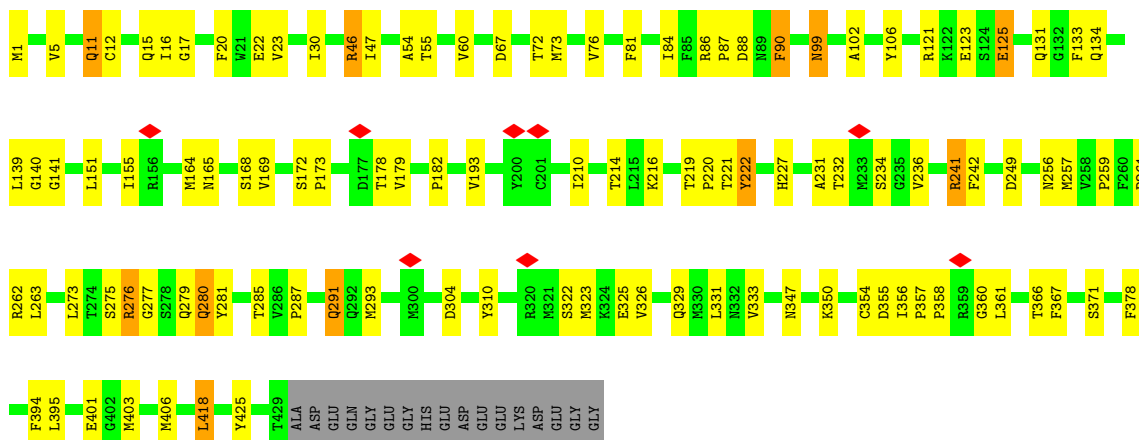
- Molecule 1: Tubulin beta chain



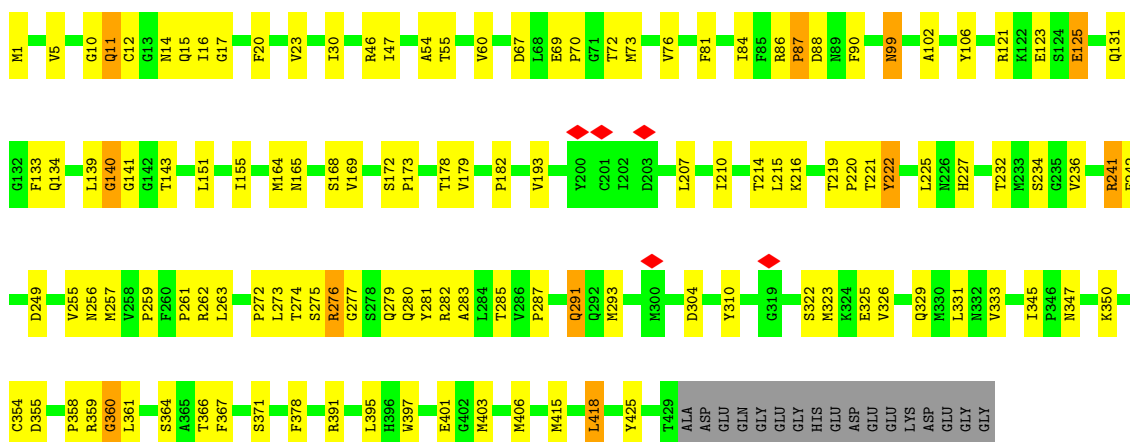
- Molecule 1: Tubulin beta chain



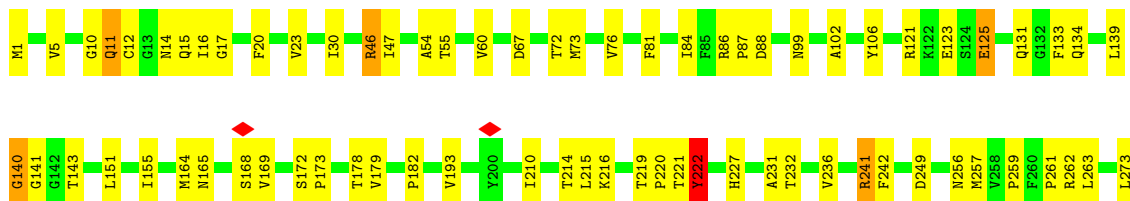
• Molecule 1: Tubulin beta chain

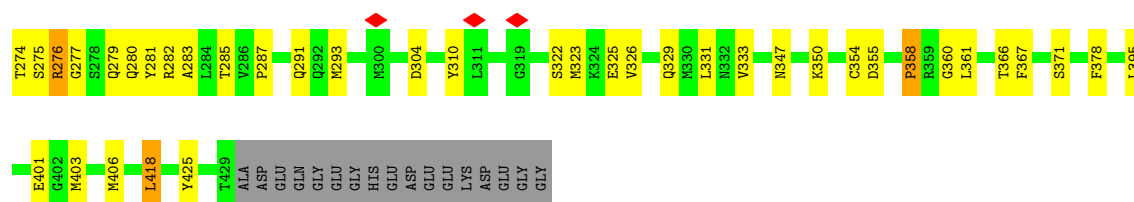


• Molecule 1: Tubulin beta chain

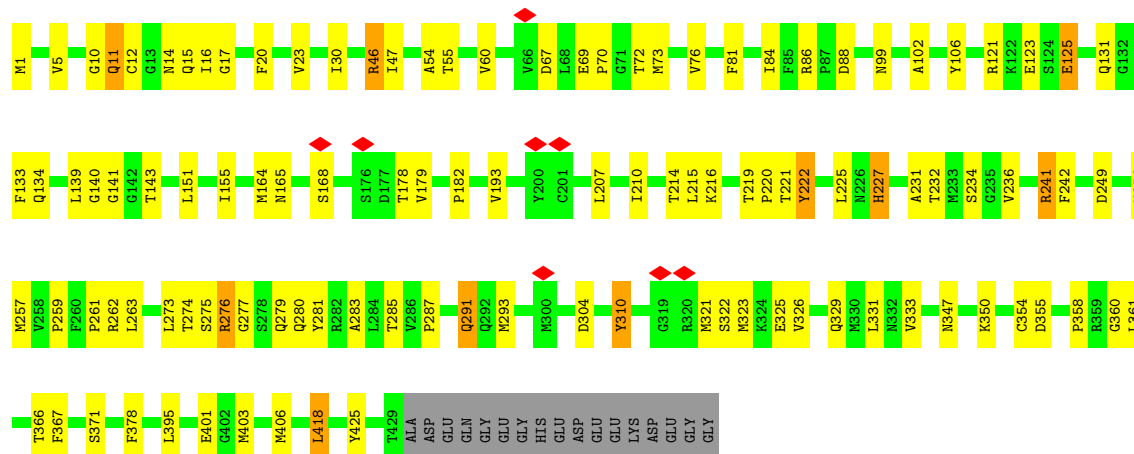


• Molecule 1: Tubulin beta chain

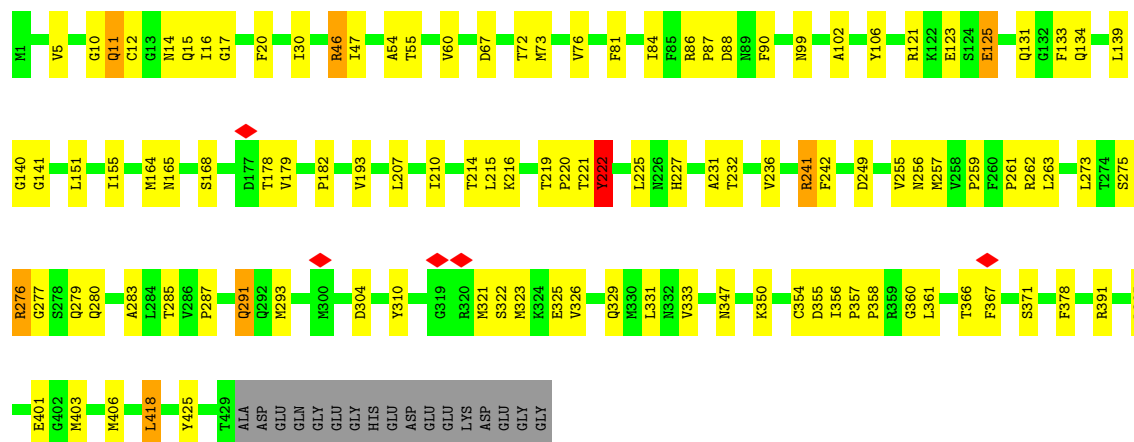




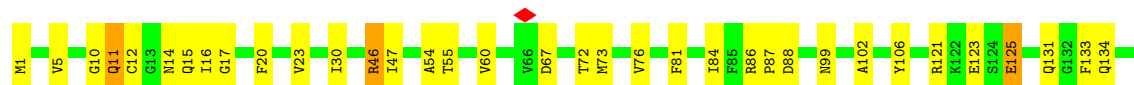
• Molecule 1: Tubulin beta chain

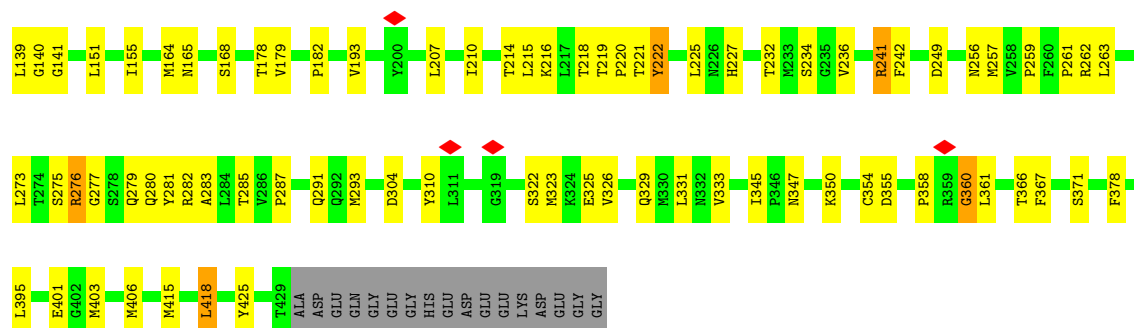


• Molecule 1: Tubulin beta chain

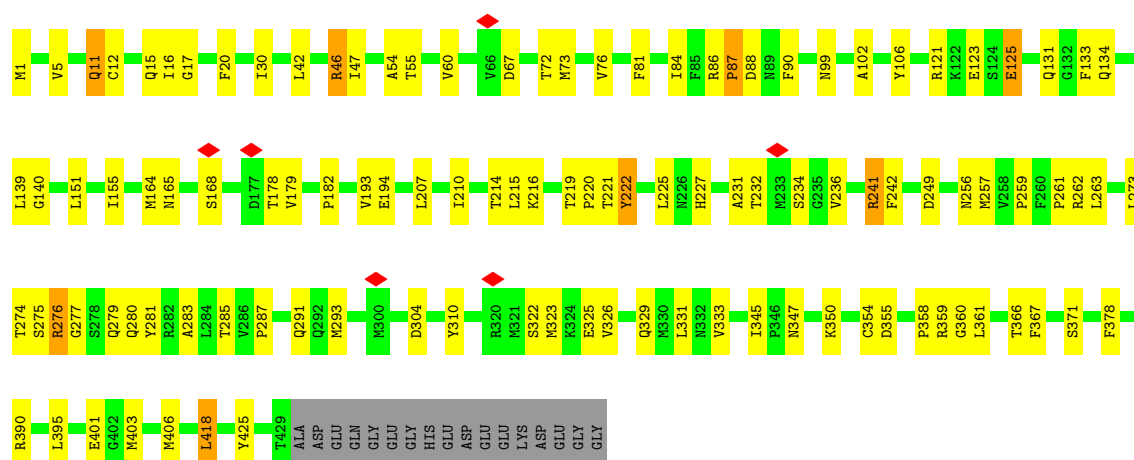


• Molecule 1: Tubulin beta chain

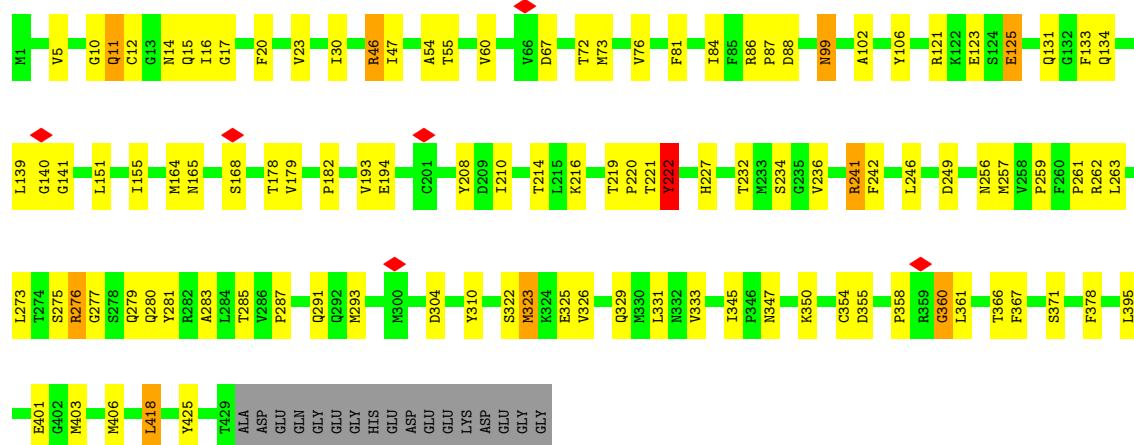
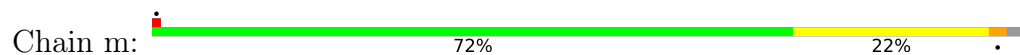




• Molecule 1: Tubulin beta chain

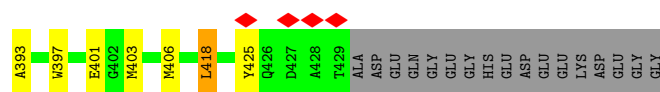


• Molecule 1: Tubulin beta chain

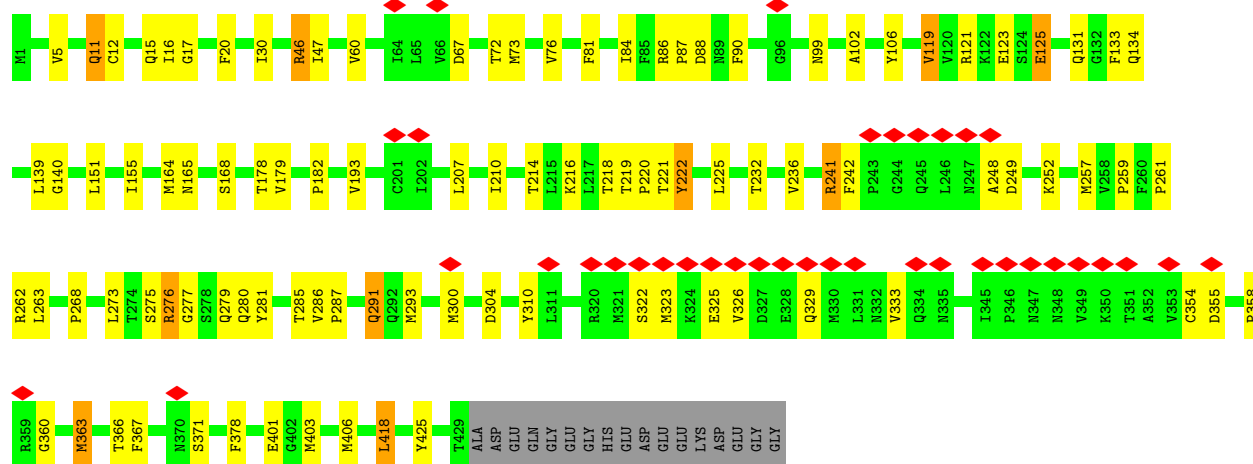
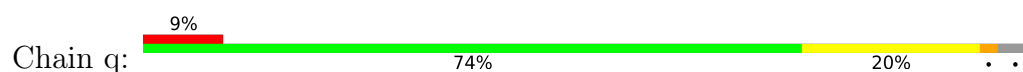


• Molecule 1: Tubulin beta chain

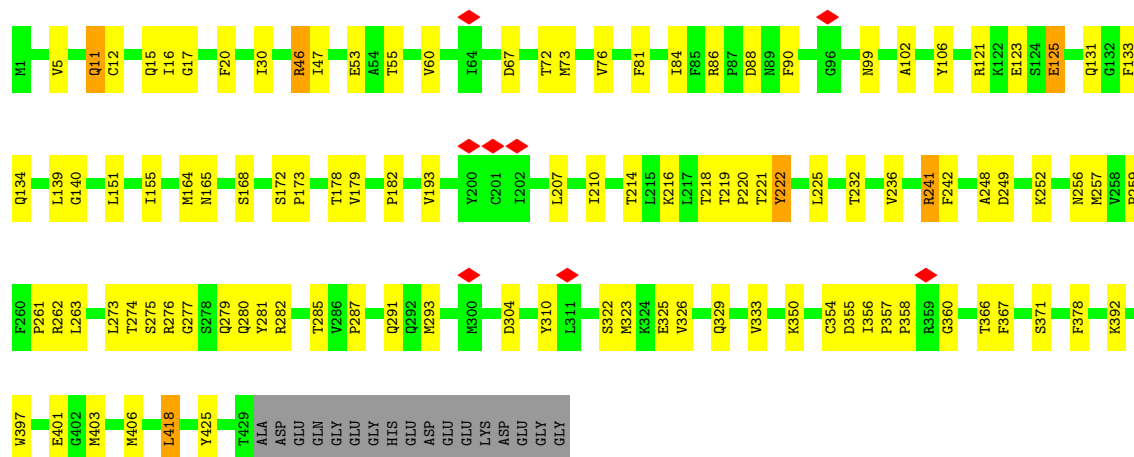




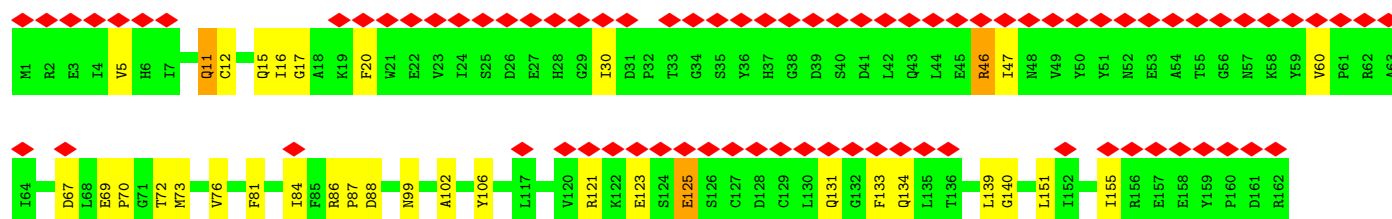
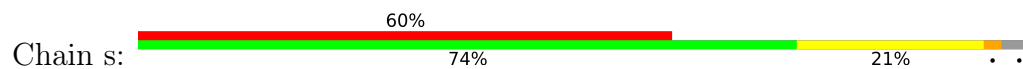
• Molecule 1: Tubulin beta chain

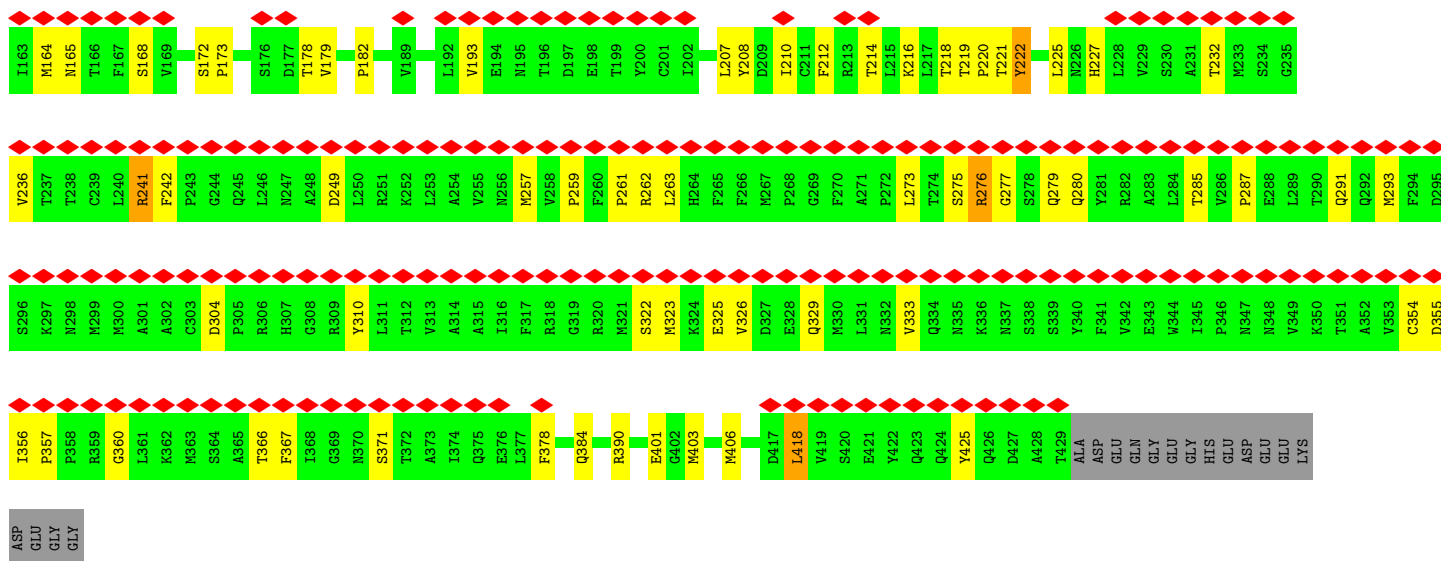


• Molecule 1: Tubulin beta chain

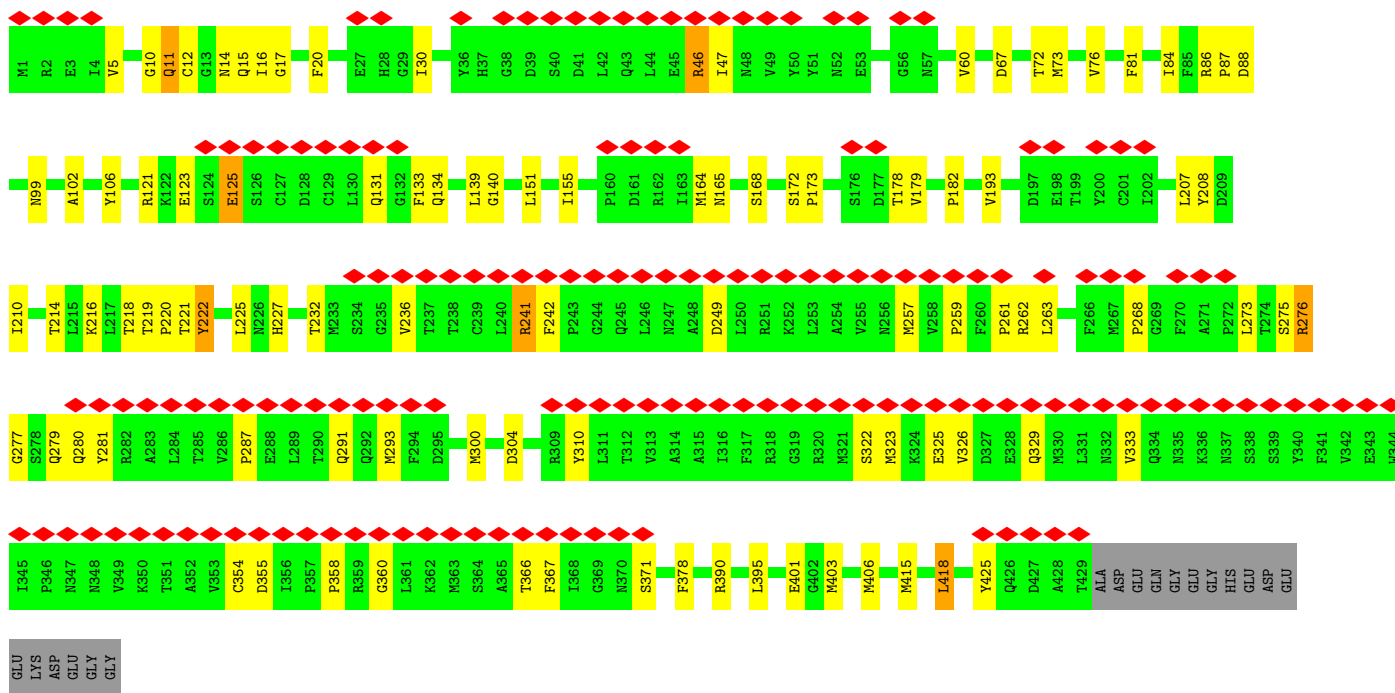


• Molecule 1: Tubulin beta chain

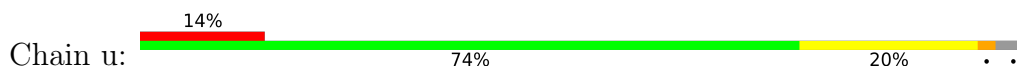




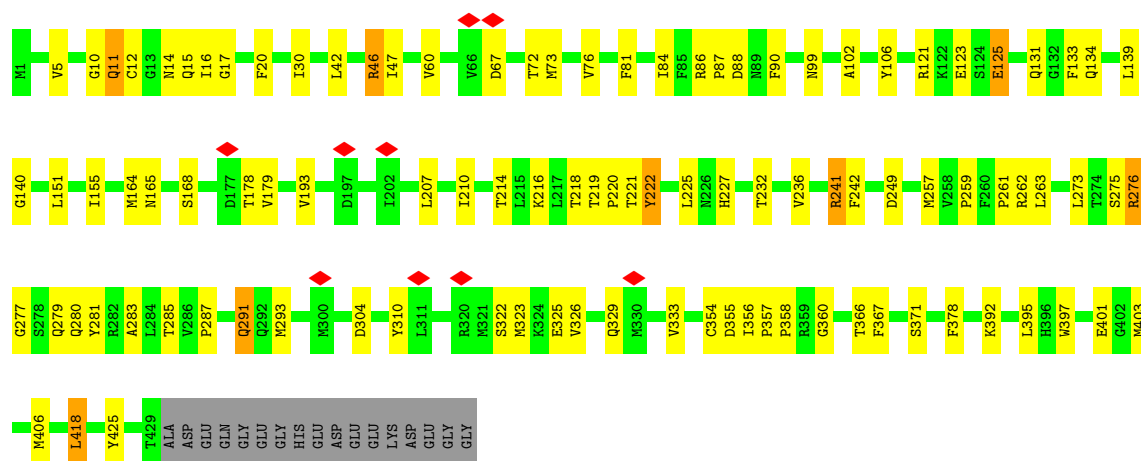
• Molecule 1: Tubulin beta chain



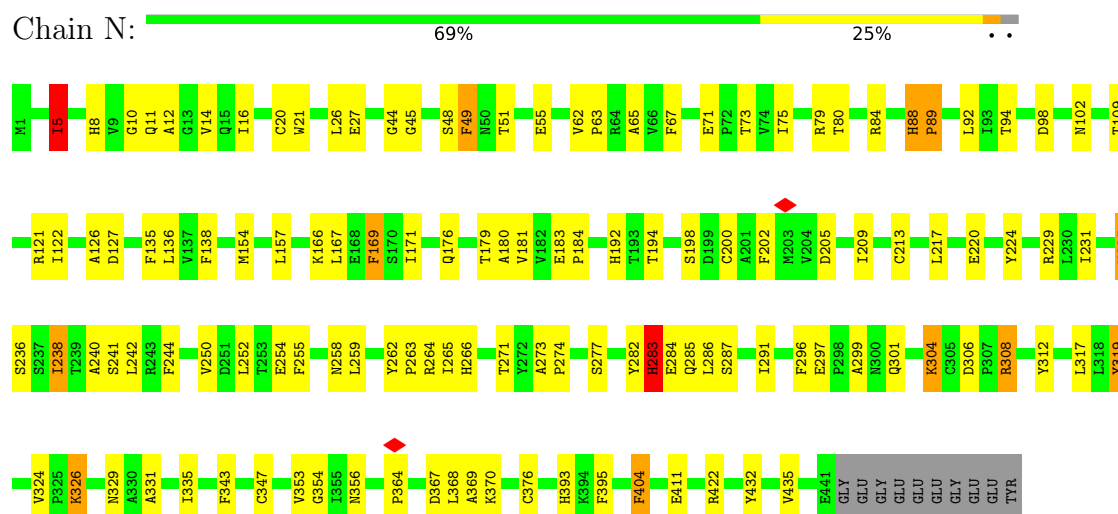
• Molecule 1: Tubulin beta chain



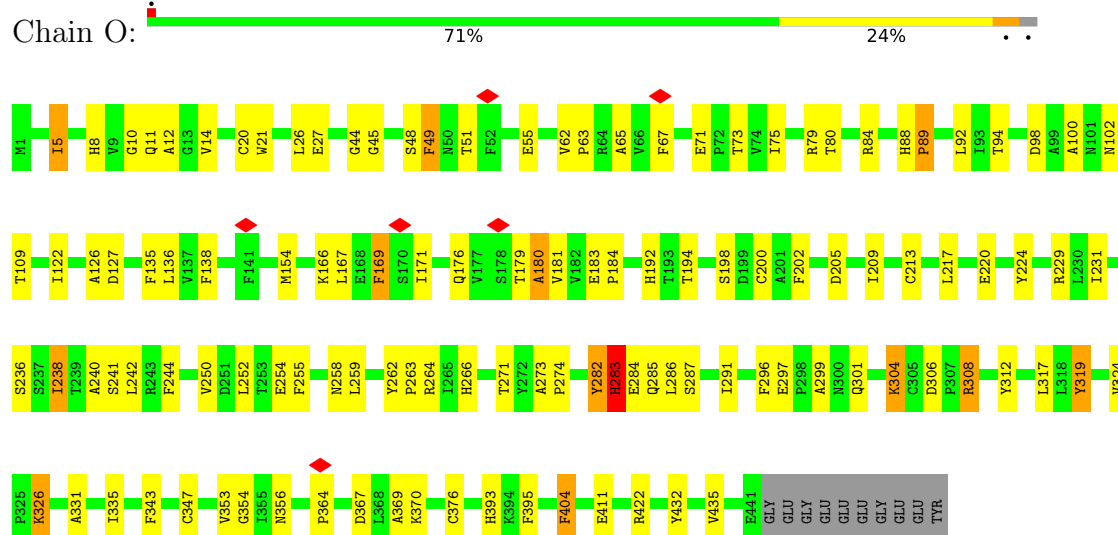




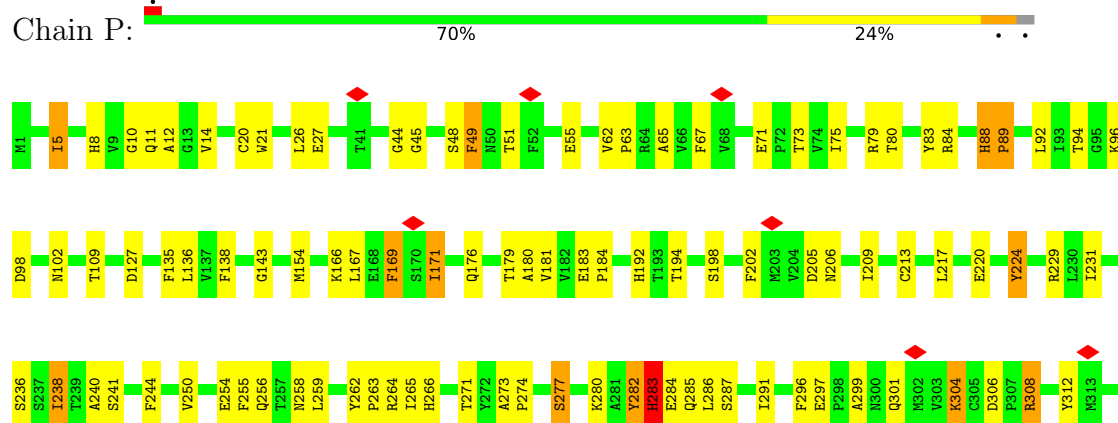
- Molecule 2: Tubulin alpha-1B chain

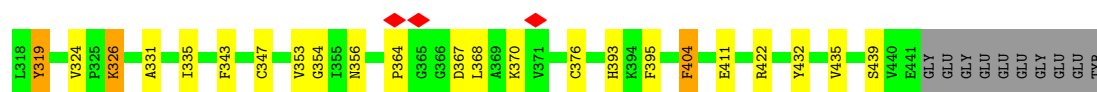


- Molecule 2: Tubulin alpha-1B chain



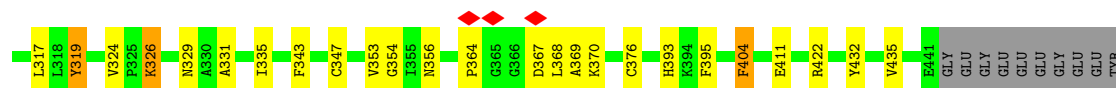
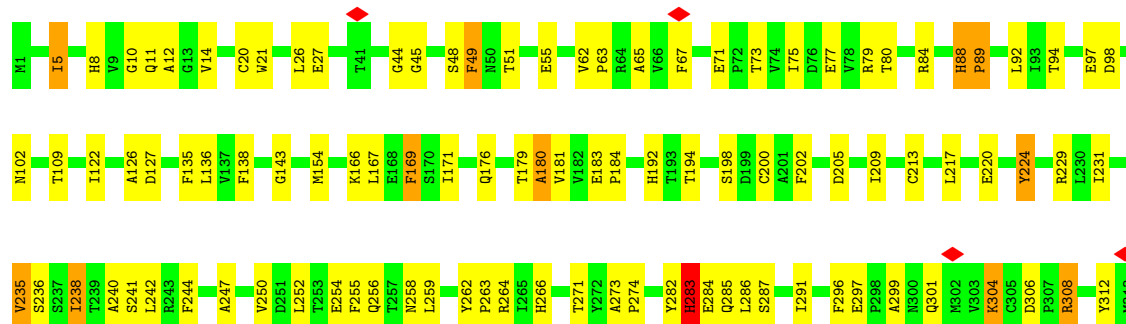
- Molecule 2: Tubulin alpha-1B chain





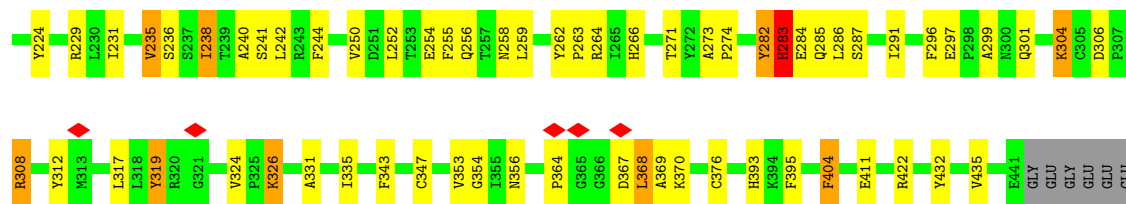
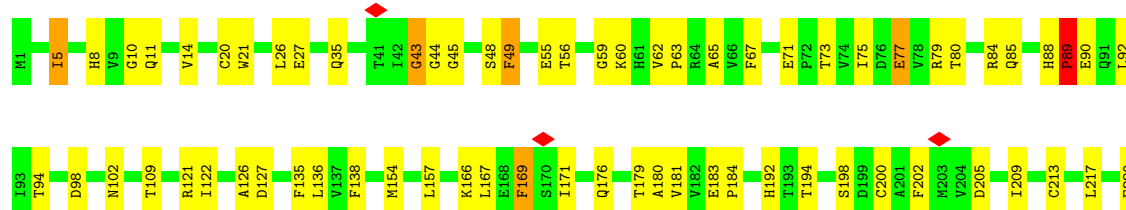
• Molecule 2: Tubulin alpha-1B chain

Chain Q: 69% 25%



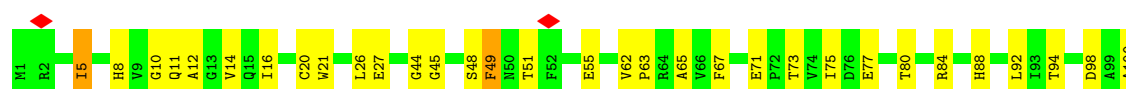
• Molecule 2: Tubulin alpha-1B chain

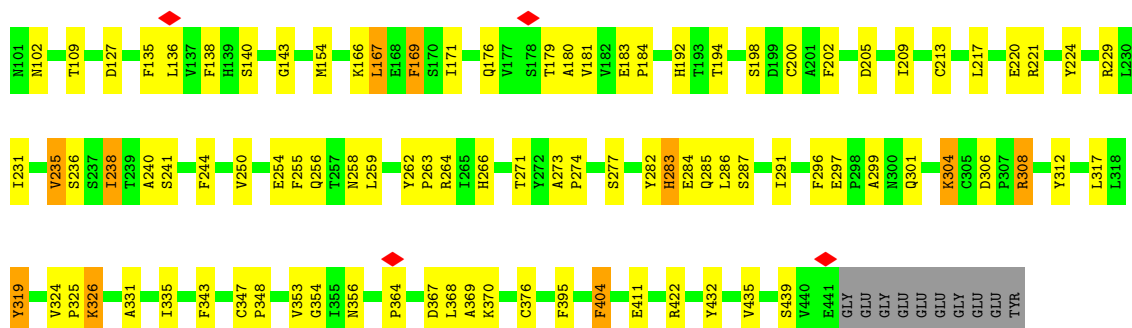
Chain R: 69% 25%



• Molecule 2: Tubulin alpha-1B chain

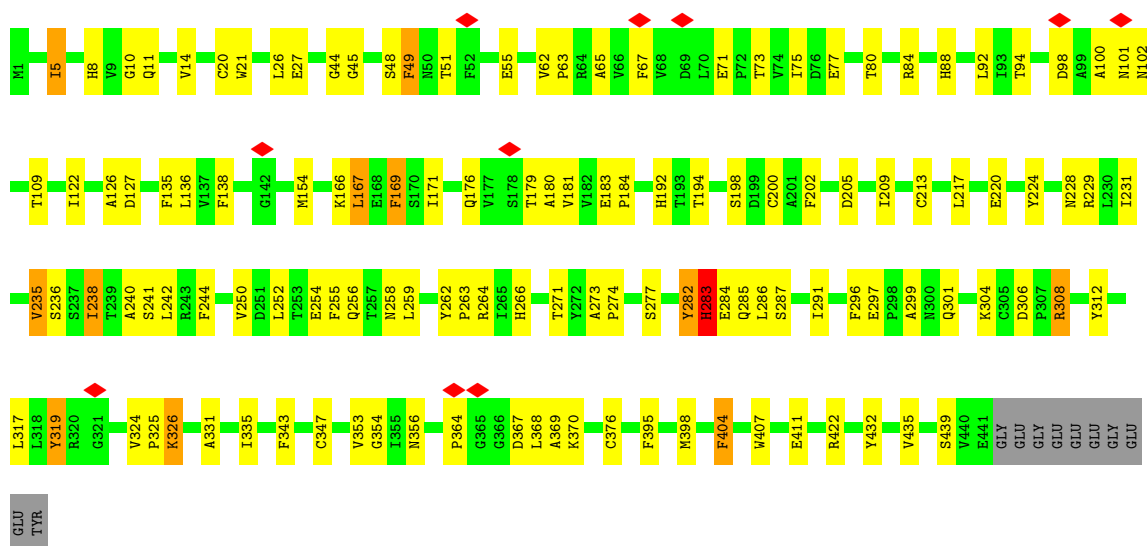
Chain S: 70% 25%





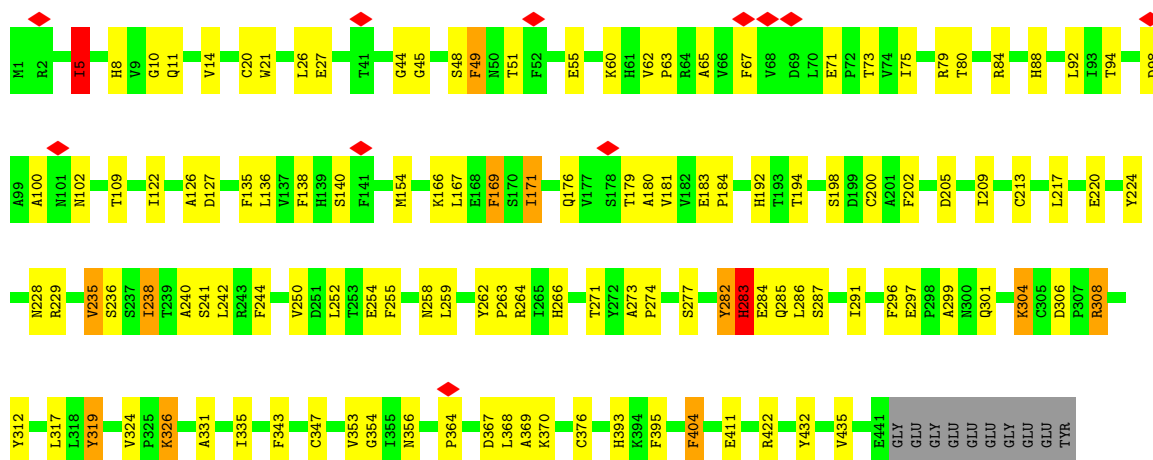
• Molecule 2: Tubulin alpha-1B chain

Chain T: 69% 26%



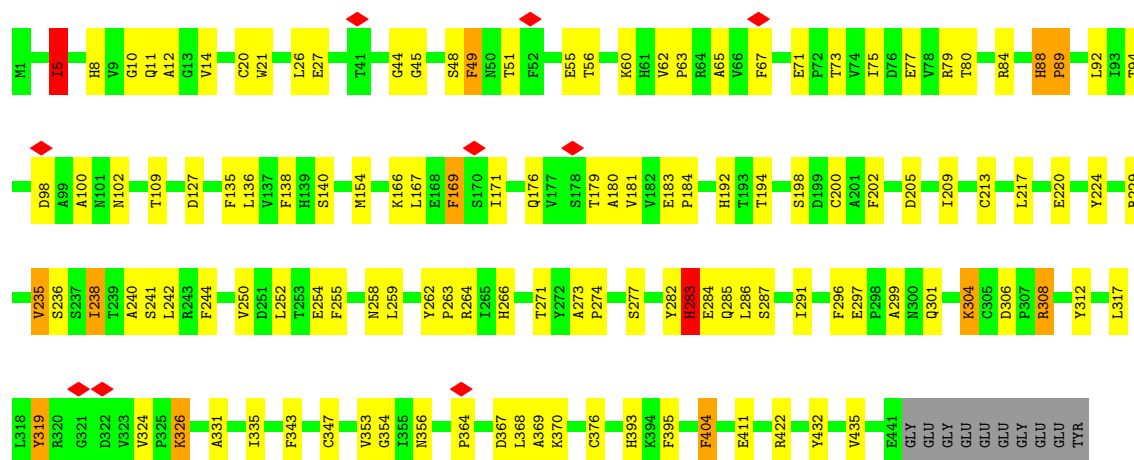
• Molecule 2: Tubulin alpha-1B chain

Chain U: 70% 25%



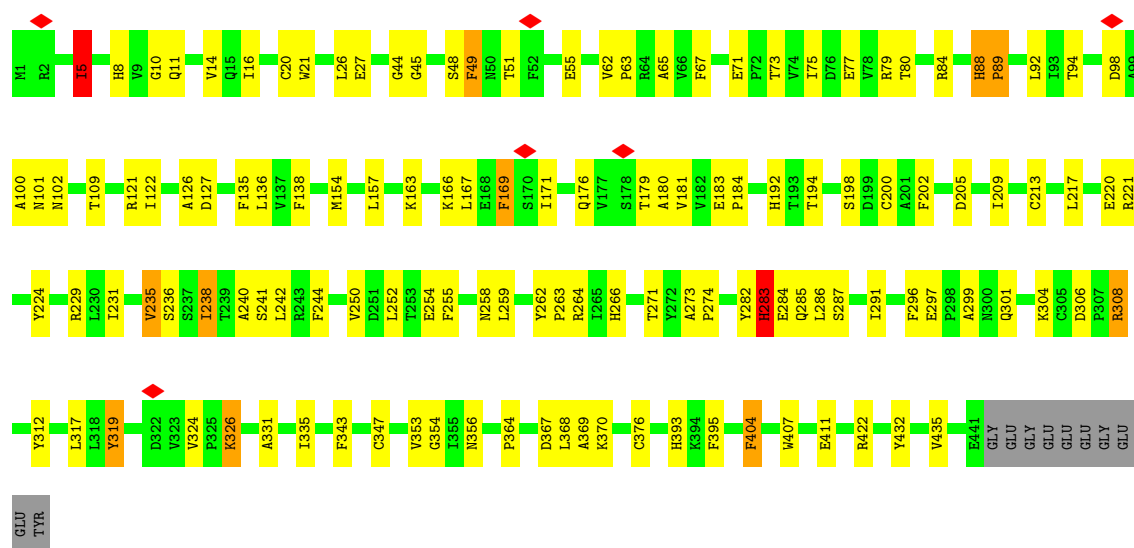
• Molecule 2: Tubulin alpha-1B chain

Chain V:  70% 25%



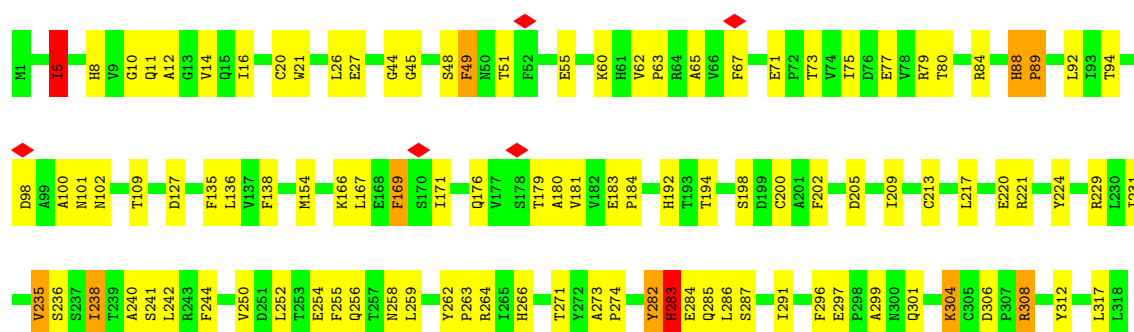
• Molecule 2: Tubulin alpha-1B chain

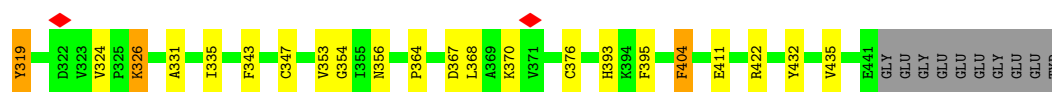
Chain W:  69% 26%



• Molecule 2: Tubulin alpha-1B chain

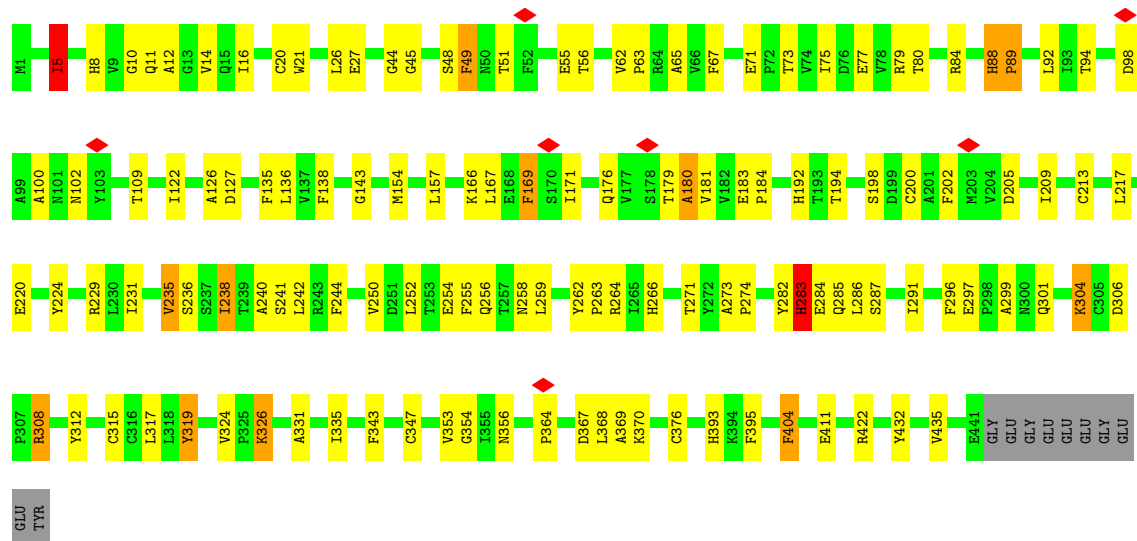
Chain X:  70% 25%





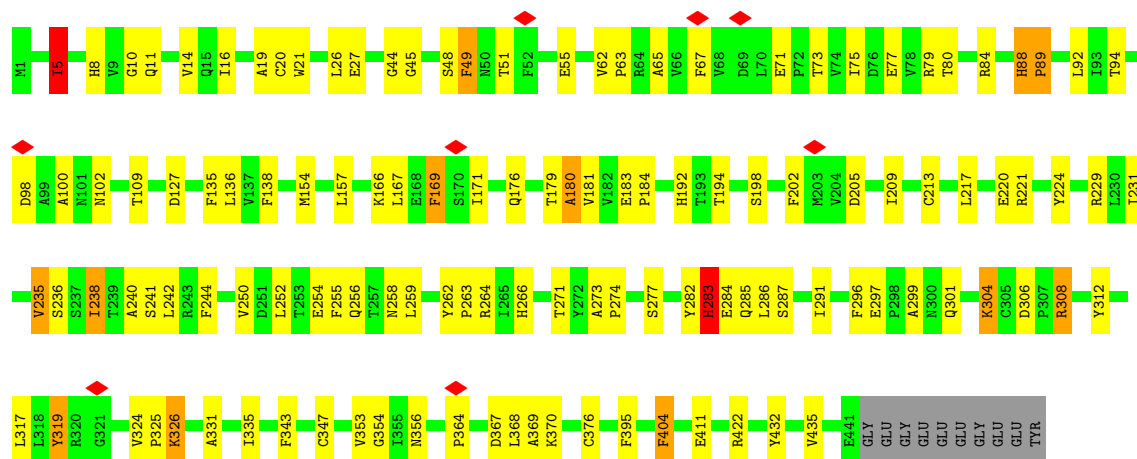
• Molecule 2: Tubulin alpha-1B chain

Chain Y: 69% 26%



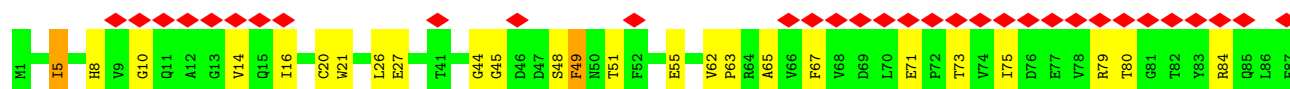
• Molecule 2: Tubulin alpha-1B chain

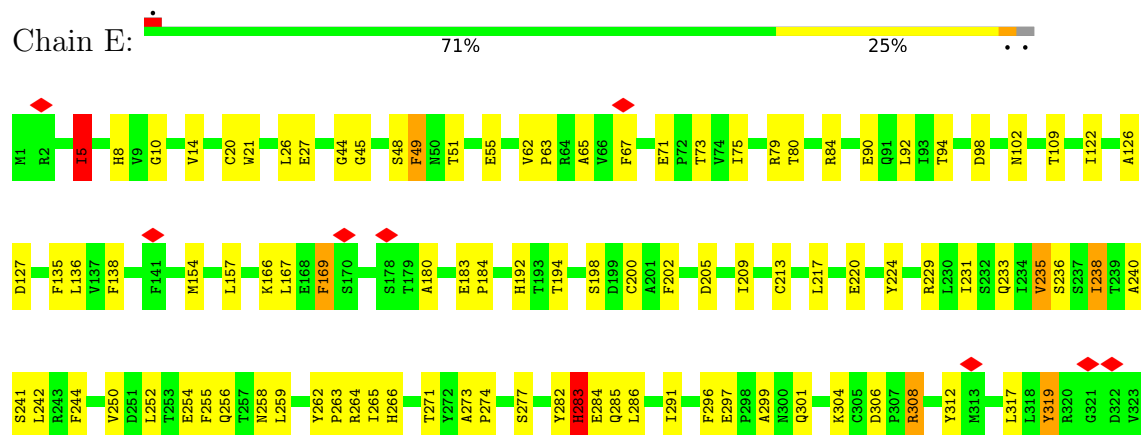
Chain Z: 70% 25%

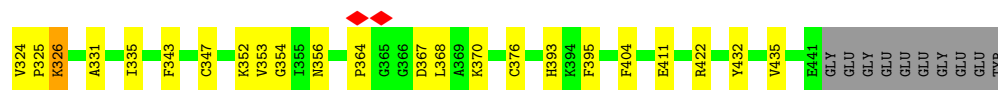


• Molecule 2: Tubulin alpha-1B chain

Chain A: 35% 71% 24%

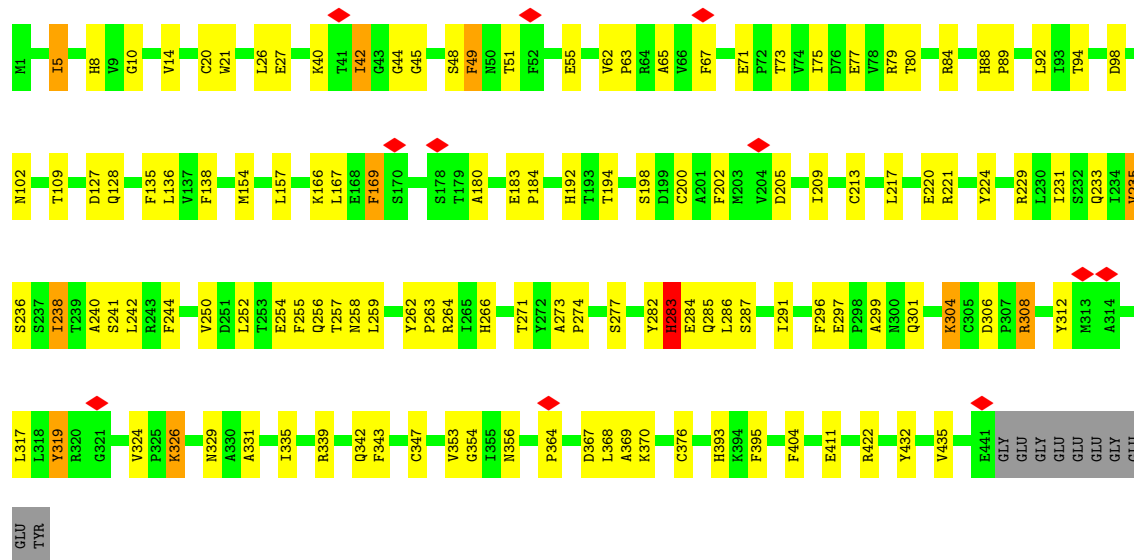






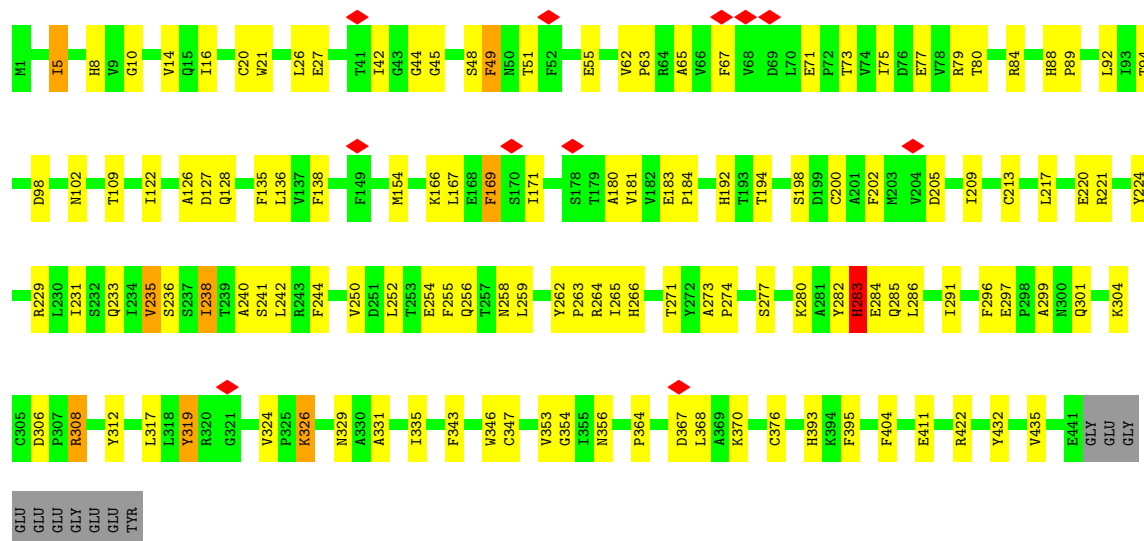
• Molecule 2: Tubulin alpha-1B chain

Chain F: 70% 26% ..



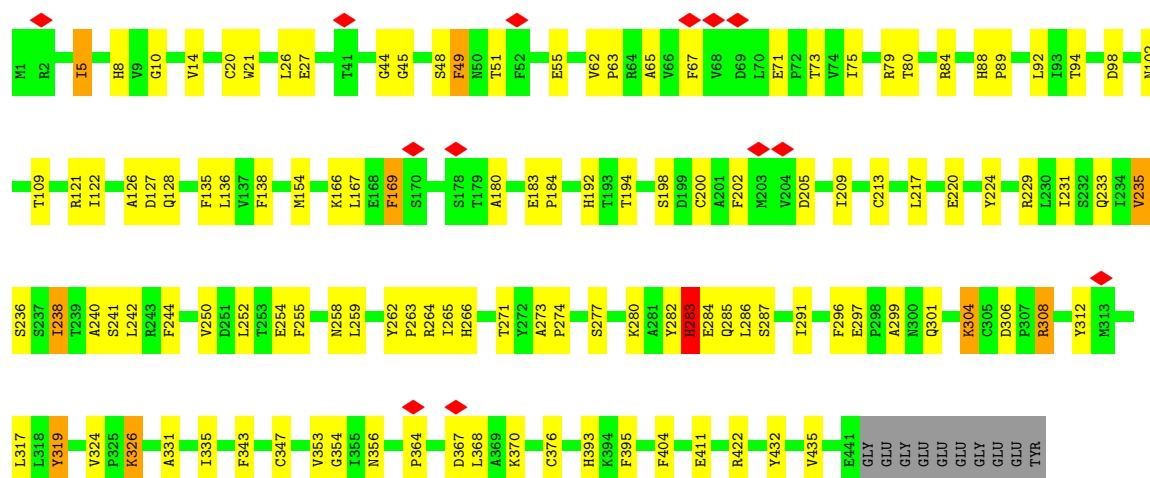
• Molecule 2: Tubulin alpha-1B chain

Chain G: 69% 26% ..



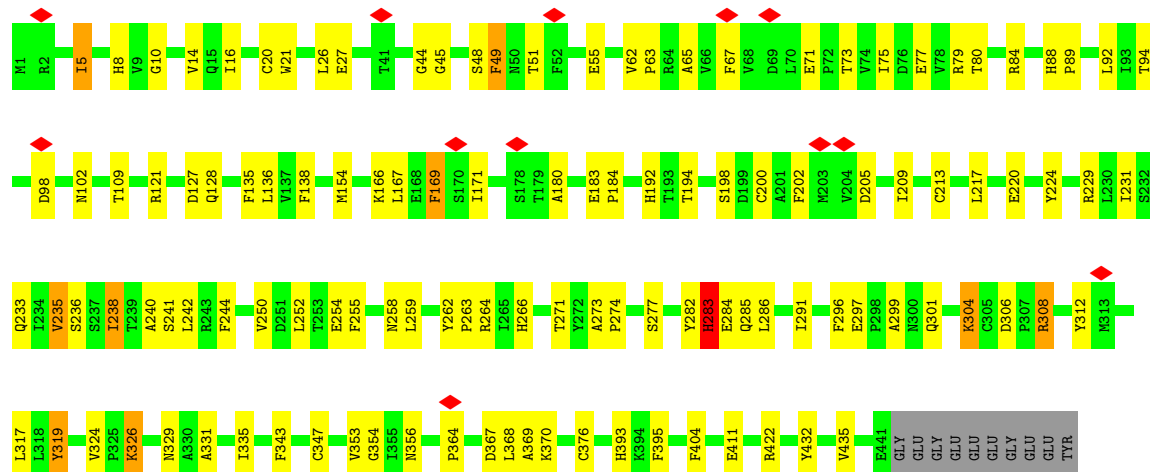
• Molecule 2: Tubulin alpha-1B chain

Chain H: 71% 25% ..



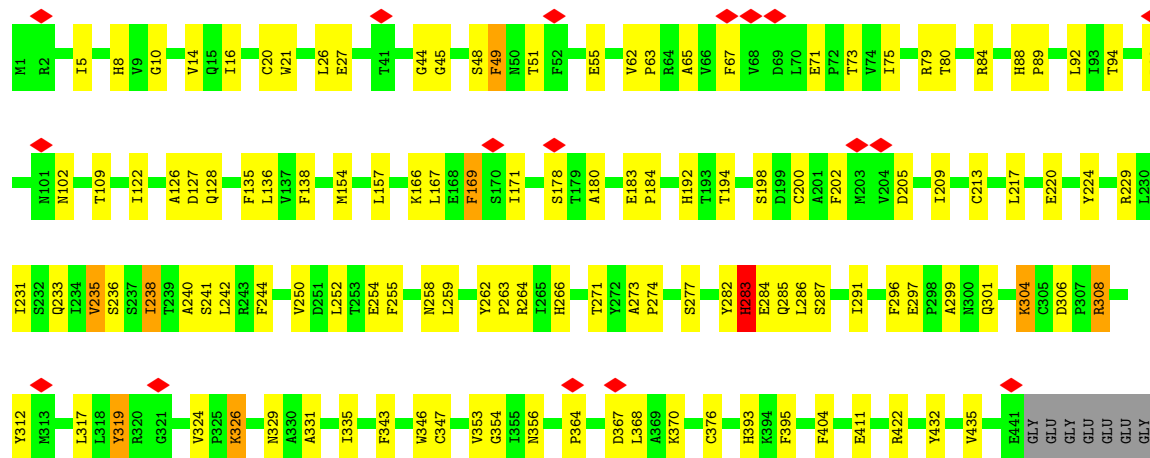
• Molecule 2: Tubulin alpha-1B chain

Chain I: 71% 25%



• Molecule 2: Tubulin alpha-1B chain

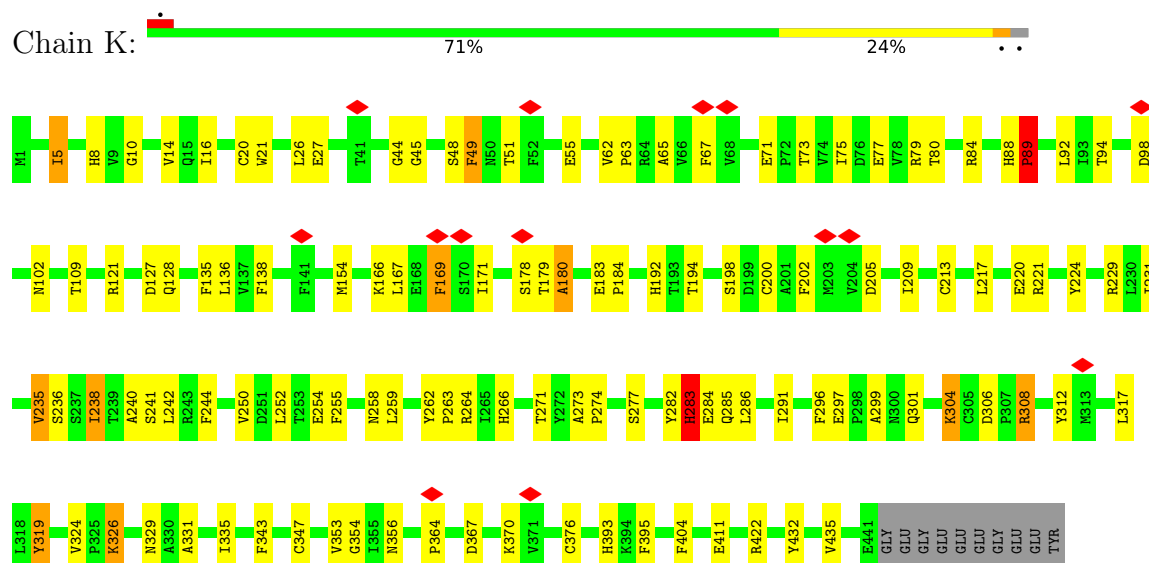
Chain J: 70% 25%



GLU
GLU
TYR

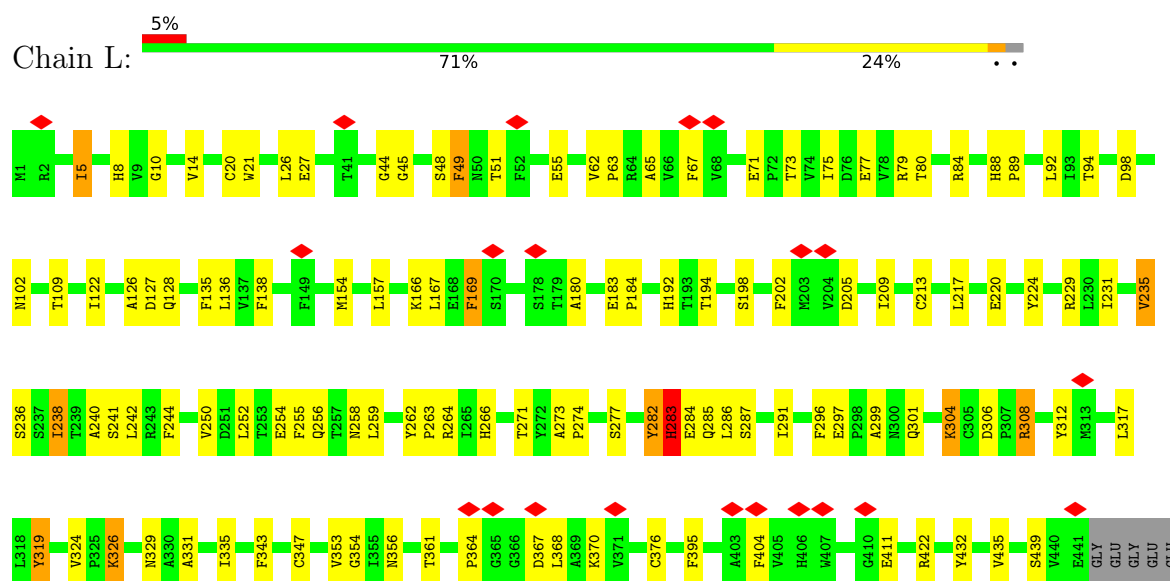
• Molecule 2: Tubulin alpha-1B chain

Chain K:



• Molecule 2: Tubulin alpha-1B chain

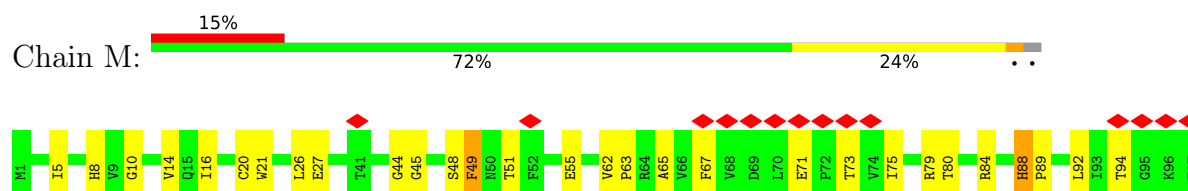
Chain L:

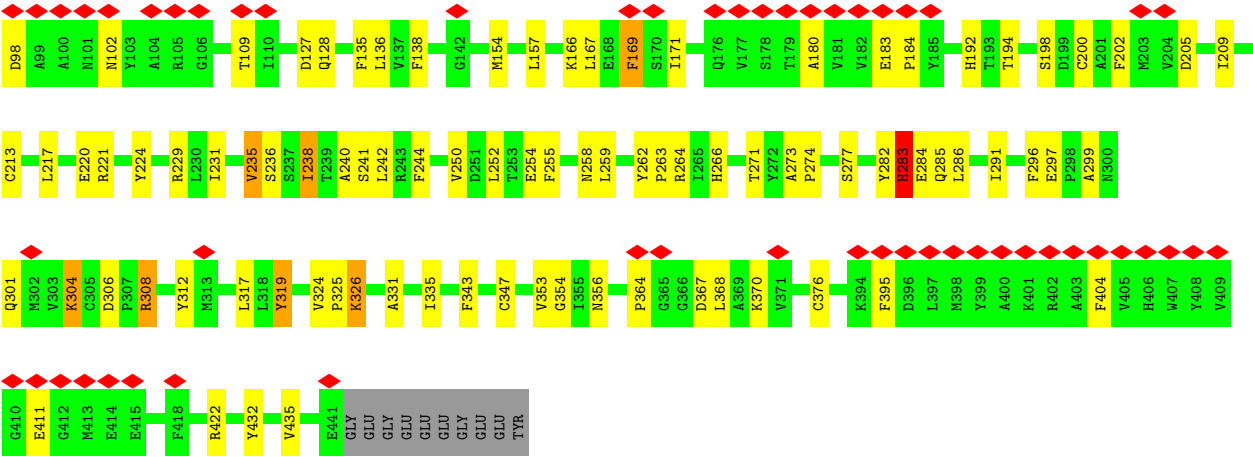


GLU
GLU
GLU
TYR

• Molecule 2: Tubulin alpha-1B chain

Chain M:





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-27.68°, rise=9.54 Å, axial sym=C1	Depositor
Number of segments used	11670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	627.2, 627.2, 627.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.96, 1.96, 1.96	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, TA1, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.74	0/3451	1.51	31/4674 (0.7%)
1	b	0.73	0/3451	1.51	29/4674 (0.6%)
1	c	0.75	1/3451 (0.0%)	1.52	33/4674 (0.7%)
1	d	0.76	2/3451 (0.1%)	1.52	35/4674 (0.7%)
1	e	1.01	4/3451 (0.1%)	1.59	36/4674 (0.8%)
1	f	0.75	1/3451 (0.0%)	1.50	31/4674 (0.7%)
1	g	0.76	0/3451	1.51	32/4674 (0.7%)
1	h	0.75	0/3451	1.51	29/4674 (0.6%)
1	i	0.74	0/3451	1.50	29/4674 (0.6%)
1	j	0.75	0/3451	1.50	30/4674 (0.6%)
1	k	0.76	0/3451	1.50	28/4674 (0.6%)
1	l	0.74	0/3451	1.51	31/4674 (0.7%)
1	m	0.74	0/3451	1.51	28/4674 (0.6%)
1	n	0.75	1/3451 (0.0%)	1.52	34/4674 (0.7%)
1	o	0.75	1/3451 (0.0%)	1.52	36/4674 (0.8%)
1	p	0.73	0/3451	1.52	31/4674 (0.7%)
1	q	0.74	0/3451	1.51	35/4674 (0.7%)
1	r	0.73	0/3451	1.52	32/4674 (0.7%)
1	s	0.72	0/3451	1.50	30/4674 (0.6%)
1	t	0.74	0/3451	1.50	27/4674 (0.6%)
1	u	0.73	0/3451	1.51	31/4674 (0.7%)
1	v	0.73	0/3451	1.51	34/4674 (0.7%)
1	w	0.73	0/3451	1.51	32/4674 (0.7%)
1	x	0.74	1/3451 (0.0%)	1.52	34/4674 (0.7%)
1	y	0.74	1/3451 (0.0%)	1.52	32/4674 (0.7%)
1	z	0.75	1/3451 (0.0%)	1.52	34/4674 (0.7%)
2	A	0.80	1/3524 (0.0%)	1.51	34/4784 (0.7%)
2	B	0.78	0/3524	1.50	32/4784 (0.7%)
2	C	0.77	0/3524	1.53	43/4784 (0.9%)
2	D	0.79	1/3524 (0.0%)	1.55	46/4784 (1.0%)
2	E	0.79	1/3524 (0.0%)	1.53	39/4784 (0.8%)
2	F	0.78	0/3524	1.55	43/4784 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	G	0.78	0/3524	1.54	41/4784 (0.9%)
2	H	0.79	0/3524	1.54	40/4784 (0.8%)
2	I	0.78	0/3524	1.53	43/4784 (0.9%)
2	J	0.78	0/3524	1.52	40/4784 (0.8%)
2	K	0.79	1/3524 (0.0%)	1.54	45/4784 (0.9%)
2	L	0.76	0/3524	1.52	38/4784 (0.8%)
2	M	0.77	1/3524 (0.0%)	1.52	34/4784 (0.7%)
2	N	0.78	1/3524 (0.0%)	1.53	40/4784 (0.8%)
2	O	0.77	0/3524	1.53	38/4784 (0.8%)
2	P	0.81	4/3524 (0.1%)	1.56	38/4784 (0.8%)
2	Q	0.79	1/3524 (0.0%)	1.55	42/4784 (0.9%)
2	R	1.09	1/3524 (0.0%)	1.55	41/4784 (0.9%)
2	S	0.77	0/3524	1.52	38/4784 (0.8%)
2	T	0.79	1/3524 (0.0%)	1.54	40/4784 (0.8%)
2	U	0.77	0/3524	1.53	37/4784 (0.8%)
2	V	0.77	1/3524 (0.0%)	1.53	39/4784 (0.8%)
2	W	0.78	1/3524 (0.0%)	1.53	41/4784 (0.9%)
2	X	0.79	2/3524 (0.1%)	1.53	38/4784 (0.8%)
2	Y	0.79	1/3524 (0.0%)	1.53	41/4784 (0.9%)
2	Z	0.80	2/3524 (0.1%)	1.53	40/4784 (0.8%)
All	All	0.78	33/181350 (0.0%)	1.52	1855/245908 (0.8%)

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
1	e	0	1
1	h	0	1
1	i	0	1
2	A	0	1
2	B	0	1
2	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	M	0	1
2	N	0	1
2	O	0	1
2	P	0	1
2	Q	0	1
2	R	0	1
2	S	0	1
2	T	0	1
2	U	0	1
2	V	0	1
2	W	0	1
2	X	0	1
2	Y	0	1
2	Z	0	1
All	All	0	29

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	43	GLY	C-N	44.65	1.98	1.33
1	e	294	PHE	C-N	34.87	1.83	1.33
2	A	88	HIS	CE1-NE2	12.88	1.45	1.32
2	W	88	HIS	CE1-NE2	-9.48	1.23	1.32
2	N	88	HIS	CE1-NE2	-9.35	1.23	1.32

The worst 5 of 1855 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	283	HIS	CA-CB-CG	18.53	132.33	113.80
1	p	99	ASN	CB-CA-C	17.35	136.37	111.73
1	e	294	PHE	CA-C-N	-16.20	95.10	122.64
1	e	294	PHE	C-N-CA	-16.20	95.10	122.64
1	r	99	ASN	CB-CA-C	15.89	134.45	111.89

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	347	CYS	Peptide
2	O	347	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	e	285	THR	Mainchain
1	h	222	TYR	Sidechain
1	i	310	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3376	0	3257	111	0
1	b	3376	0	3256	148	0
1	c	3376	0	3256	136	0
1	d	3376	0	3257	129	0
1	e	3376	0	3256	133	0
1	f	3376	0	3257	121	0
1	g	3376	0	3257	111	0
1	h	3376	0	3256	112	0
1	i	3376	0	3257	105	0
1	j	3376	0	3257	104	0
1	k	3376	0	3257	101	0
1	l	3376	0	3257	105	0
1	m	3376	0	3257	114	0
1	n	3376	0	3257	76	0
1	o	3376	0	3257	72	0
1	p	3376	0	3257	68	0
1	q	3376	0	3257	81	0
1	r	3376	0	3257	80	0
1	s	3376	0	3257	81	0
1	t	3376	0	3257	88	0
1	u	3376	0	3257	76	0
1	v	3376	0	3257	79	0
1	w	3376	0	3257	82	0
1	x	3376	0	3257	77	0
1	y	3376	0	3257	74	0
1	z	3376	0	3257	72	0
2	A	3446	0	3355	110	0
2	B	3446	0	3355	104	0
2	C	3446	0	3355	89	0
2	D	3446	0	3355	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3446	0	3355	83	0
2	F	3446	0	3355	106	0
2	G	3446	0	3355	119	0
2	H	3446	0	3355	108	0
2	I	3446	0	3355	103	0
2	J	3446	0	3355	104	0
2	K	3446	0	3355	100	0
2	L	3446	0	3355	106	0
2	M	3446	0	3355	101	0
2	N	3446	0	3355	116	0
2	O	3446	0	3355	113	0
2	P	3446	0	3355	109	0
2	Q	3446	0	3355	115	0
2	R	3446	0	3354	117	0
2	S	3446	0	3355	132	0
2	T	3446	0	3355	126	0
2	U	3446	0	3355	121	0
2	V	3446	0	3355	110	0
2	W	3446	0	3355	116	0
2	X	3446	0	3355	115	0
2	Y	3446	0	3355	118	0
2	Z	3446	0	3355	117	0
3	a	62	0	51	18	0
3	b	62	0	51	11	0
3	c	62	0	51	23	0
3	d	62	0	51	19	0
3	e	62	0	51	19	0
3	f	62	0	51	10	0
3	g	62	0	50	18	0
3	h	62	0	51	18	0
3	i	62	0	51	24	0
3	j	62	0	51	14	0
3	k	62	0	51	16	0
3	l	62	0	51	17	0
3	m	62	0	51	15	0
4	a	28	0	12	19	0
4	b	28	0	10	61	0
4	c	28	0	12	40	0
4	d	28	0	12	35	0
4	e	28	0	12	33	0
4	f	28	0	12	31	0
4	g	28	0	12	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	h	28	0	12	29	0
4	i	28	0	12	12	0
4	j	28	0	12	15	0
4	k	28	0	12	13	0
4	l	28	0	12	16	0
4	m	28	0	12	30	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
5	U	1	0	0	0	0
5	V	1	0	0	0	0
5	W	1	0	0	0	0
5	X	1	0	0	0	0
5	Y	1	0	0	0	0
5	Z	1	0	0	0	0
6	N	32	0	12	30	0
6	O	32	0	12	27	0
6	P	32	0	12	17	0
6	Q	32	0	12	23	0
6	R	32	0	12	19	0
6	S	32	0	12	31	0
6	T	32	0	11	31	0
6	U	32	0	12	38	0
6	V	32	0	12	28	0
6	W	32	0	12	28	0
6	X	32	0	12	29	0
6	Y	32	0	12	31	0
6	Z	32	0	12	30	0
All	All	178971	0	172878	4628	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 4628 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:88:HIS:CD2	2:L:283:HIS:CB	1.77	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:222:TYR:CE1	4:e:602:GDP:C2	1.86	1.62
1:e:222:TYR:HE1	4:e:602:GDP:C2	1.13	1.60
1:f:222:TYR:HE1	4:f:602:GDP:C2	0.98	1.59
1:f:222:TYR:CE1	4:f:602:GDP:C2	1.87	1.59

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	427/446 (96%)	389 (91%)	36 (8%)	2 (0%)	24	63
1	b	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	c	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	d	427/446 (96%)	389 (91%)	36 (8%)	2 (0%)	24	63
1	e	427/446 (96%)	388 (91%)	37 (9%)	2 (0%)	24	63
1	f	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	24	63
1	g	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	24	63
1	h	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	i	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	j	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	k	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	l	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	m	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	n	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	o	427/446 (96%)	392 (92%)	33 (8%)	2 (0%)	24	63
1	p	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	q	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	r	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	24	63
1	s	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	24	63
1	t	427/446 (96%)	392 (92%)	33 (8%)	2 (0%)	24	63
1	u	427/446 (96%)	392 (92%)	33 (8%)	2 (0%)	24	63
1	v	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	24	63
1	w	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	24	63
1	x	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	y	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	24	63
1	z	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	24	63
2	A	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	B	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	C	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	D	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	E	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	F	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	G	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	H	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	I	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	J	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	K	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	L	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	M	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	N	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	O	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	P	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	Q	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	R	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	S	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	T	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	U	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	439/451 (97%)	402 (92%)	36 (8%)	1 (0%)	43	77
2	W	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	43	77
2	X	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	Y	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
2	Z	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	43	77
All	All	22516/23322 (96%)	20640 (92%)	1798 (8%)	78 (0%)	37	71

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	304	LYS
2	F	304	LYS
2	G	304	LYS
2	H	304	LYS
2	J	304	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	b	371/383 (97%)	366 (99%)	5 (1%)	61	72
1	c	371/383 (97%)	366 (99%)	5 (1%)	61	72
1	d	371/383 (97%)	364 (98%)	7 (2%)	50	66
1	e	371/383 (97%)	366 (99%)	5 (1%)	61	72
1	f	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	g	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	h	371/383 (97%)	366 (99%)	5 (1%)	61	72
1	i	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	j	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	k	371/383 (97%)	367 (99%)	4 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	m	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	n	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	o	371/383 (97%)	366 (99%)	5 (1%)	61	72
1	p	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	q	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	r	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	s	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	t	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	u	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	v	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	w	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	x	371/383 (97%)	367 (99%)	4 (1%)	65	74
1	y	371/383 (97%)	365 (98%)	6 (2%)	55	69
1	z	371/383 (97%)	367 (99%)	4 (1%)	65	74
2	A	372/379 (98%)	371 (100%)	1 (0%)	86	84
2	B	372/379 (98%)	371 (100%)	1 (0%)	86	84
2	C	372/379 (98%)	369 (99%)	3 (1%)	73	78
2	D	372/379 (98%)	369 (99%)	3 (1%)	73	78
2	E	372/379 (98%)	370 (100%)	2 (0%)	81	82
2	F	372/379 (98%)	370 (100%)	2 (0%)	81	82
2	G	372/379 (98%)	370 (100%)	2 (0%)	81	82
2	H	372/379 (98%)	371 (100%)	1 (0%)	86	84
2	I	372/379 (98%)	371 (100%)	1 (0%)	86	84
2	J	372/379 (98%)	371 (100%)	1 (0%)	86	84
2	K	372/379 (98%)	370 (100%)	2 (0%)	81	82
2	L	372/379 (98%)	370 (100%)	2 (0%)	81	82
2	M	372/379 (98%)	371 (100%)	1 (0%)	86	84
2	N	372/379 (98%)	369 (99%)	3 (1%)	73	78
2	O	372/379 (98%)	370 (100%)	2 (0%)	81	82
2	P	372/379 (98%)	369 (99%)	3 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	372/379 (98%)	370 (100%)	2 (0%)	81	82
2	R	372/379 (98%)	369 (99%)	3 (1%)	73	78
2	S	372/379 (98%)	371 (100%)	1 (0%)	86	84
2	T	372/379 (98%)	371 (100%)	1 (0%)	86	84
2	U	372/379 (98%)	368 (99%)	4 (1%)	65	74
2	V	372/379 (98%)	368 (99%)	4 (1%)	65	74
2	W	372/379 (98%)	369 (99%)	3 (1%)	73	78
2	X	372/379 (98%)	368 (99%)	4 (1%)	65	74
2	Y	372/379 (98%)	369 (99%)	3 (1%)	73	78
2	Z	372/379 (98%)	369 (99%)	3 (1%)	73	78
All	All	19318/19812 (98%)	19146 (99%)	172 (1%)	68	77

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	361	THR
1	t	276	ARG
1	n	406	MET
1	q	222	TYR
1	v	222	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 275 such sidechains are listed below:

Mol	Chain	Res	Type
1	s	57	ASN
1	t	329	GLN
1	x	329	GLN
2	T	258	ASN
2	S	309	HIS

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 52 ligands modelled in this entry, 13 are monoatomic - leaving 39 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	$\# Z > 2$
6	GTP	Z	502	5	33,34,34	2.18	9 (27%)	50,54,54	2.26	13 (26%)
4	GDP	e	602	-	29,30,30	1.44	4 (13%)	45,47,47	2.22	15 (33%)
4	GDP	c	602	-	29,30,30	1.66	7 (24%)	45,47,47	2.15	18 (40%)
4	GDP	j	602	-	29,30,30	1.46	3 (10%)	45,47,47	2.19	17 (37%)
4	GDP	a	602	-	29,30,30	1.58	5 (17%)	45,47,47	2.45	14 (31%)
4	GDP	m	602	-	29,30,30	1.38	5 (17%)	45,47,47	2.28	14 (31%)
4	GDP	d	602	-	29,30,30	1.56	5 (17%)	45,47,47	2.49	17 (37%)
3	TA1	h	601	-	68,68,68	1.22	7 (10%)	105,105,105	1.69	17 (16%)
4	GDP	b	602	-	29,30,30	2.10	4 (13%)	45,47,47	2.06	15 (33%)
3	TA1	m	601	-	68,68,68	1.31	7 (10%)	105,105,105	1.52	18 (17%)
3	TA1	j	601	-	68,68,68	1.07	4 (5%)	105,105,105	1.37	15 (14%)
6	GTP	N	502	5	33,34,34	1.38	4 (12%)	50,54,54	1.51	11 (22%)
6	GTP	S	502	5	33,34,34	1.34	5 (15%)	50,54,54	2.01	15 (30%)
4	GDP	g	602	-	29,30,30	1.53	5 (17%)	45,47,47	2.29	17 (37%)
6	GTP	U	502	5	33,34,34	1.82	6 (18%)	50,54,54	2.09	15 (30%)
6	GTP	Q	502	5	33,34,34	2.08	11 (33%)	50,54,54	2.00	15 (30%)
6	GTP	Y	502	5	33,34,34	1.16	2 (6%)	50,54,54	1.62	9 (18%)
3	TA1	l	601	-	68,68,68	1.10	4 (5%)	105,105,105	1.24	15 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDP	i	602	-	29,30,30	1.76	6 (20%)	45,47,47	2.21	18 (40%)
4	GDP	h	602	-	29,30,30	1.46	4 (13%)	45,47,47	2.33	20 (44%)
3	TA1	b	601	-	68,68,68	1.21	7 (10%)	105,105,105	1.40	14 (13%)
6	GTP	R	502	5	33,34,34	1.99	8 (24%)	50,54,54	2.19	15 (30%)
3	TA1	a	601	-	68,68,68	1.04	3 (4%)	105,105,105	1.23	10 (9%)
4	GDP	k	602	-	29,30,30	1.43	3 (10%)	45,47,47	2.22	15 (33%)
3	TA1	f	601	-	68,68,68	1.55	11 (16%)	105,105,105	1.63	21 (20%)
3	TA1	c	601	-	68,68,68	1.11	5 (7%)	105,105,105	1.48	18 (17%)
4	GDP	l	602	-	29,30,30	1.32	3 (10%)	45,47,47	2.23	15 (33%)
6	GTP	P	502	5	33,34,34	1.87	8 (24%)	50,54,54	2.48	17 (34%)
6	GTP	T	502	5	33,34,34	2.44	12 (36%)	50,54,54	2.94	24 (48%)
4	GDP	f	602	-	29,30,30	1.55	3 (10%)	45,47,47	2.35	18 (40%)
6	GTP	V	502	5	33,34,34	1.14	2 (6%)	50,54,54	1.75	14 (28%)
3	TA1	d	601	-	68,68,68	1.17	7 (10%)	105,105,105	1.29	14 (13%)
6	GTP	W	502	5	33,34,34	2.22	9 (27%)	50,54,54	2.30	17 (34%)
3	TA1	g	601	-	68,68,68	1.72	15 (22%)	105,105,105	3.29	39 (37%)
6	GTP	O	502	5	33,34,34	1.00	2 (6%)	50,54,54	1.46	9 (18%)
3	TA1	k	601	-	68,68,68	1.68	13 (19%)	105,105,105	2.00	23 (21%)
3	TA1	i	601	-	68,68,68	1.05	5 (7%)	105,105,105	1.28	11 (10%)
6	GTP	X	502	5	33,34,34	1.16	4 (12%)	50,54,54	1.22	5 (10%)
3	TA1	e	601	-	68,68,68	1.23	6 (8%)	105,105,105	1.48	19 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GTP	Z	502	5	-	7/22/38/38	0/3/3/3
4	GDP	e	602	-	-	5/16/32/32	0/3/3/3
4	GDP	c	602	-	-	4/16/32/32	0/3/3/3
4	GDP	j	602	-	-	5/16/32/32	0/3/3/3
4	GDP	a	602	-	-	4/16/32/32	0/3/3/3
4	GDP	m	602	-	-	5/16/32/32	0/3/3/3
4	GDP	d	602	-	-	4/16/32/32	0/3/3/3
3	TA1	h	601	-	-	12/41/127/127	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	b	602	-	-	5/16/32/32	0/3/3/3
3	TA1	m	601	-	-	10/41/127/127	0/7/7/7
3	TA1	j	601	-	-	10/41/127/127	0/7/7/7
6	GTP	N	502	5	-	4/22/38/38	0/3/3/3
6	GTP	S	502	5	-	4/22/38/38	0/3/3/3
4	GDP	g	602	-	-	5/16/32/32	0/3/3/3
6	GTP	U	502	5	-	3/22/38/38	0/3/3/3
6	GTP	Q	502	5	-	5/22/38/38	0/3/3/3
6	GTP	Y	502	5	-	4/22/38/38	0/3/3/3
3	TA1	l	601	-	-	9/41/127/127	0/7/7/7
4	GDP	i	602	-	-	4/16/32/32	0/3/3/3
4	GDP	h	602	-	-	5/16/32/32	0/3/3/3
3	TA1	b	601	-	-	10/41/127/127	0/7/7/7
6	GTP	R	502	5	-	2/22/38/38	0/3/3/3
3	TA1	a	601	-	-	8/41/127/127	0/7/7/7
4	GDP	k	602	-	-	5/16/32/32	0/3/3/3
3	TA1	f	601	-	-	6/41/127/127	0/7/7/7
3	TA1	c	601	-	-	9/41/127/127	0/7/7/7
4	GDP	l	602	-	-	5/16/32/32	0/3/3/3
6	GTP	P	502	5	-	5/22/38/38	0/3/3/3
6	GTP	T	502	5	-	2/22/38/38	0/3/3/3
4	GDP	f	602	-	-	4/16/32/32	0/3/3/3
6	GTP	V	502	5	-	4/22/38/38	0/3/3/3
3	TA1	d	601	-	-	8/41/127/127	0/7/7/7
6	GTP	W	502	5	-	4/22/38/38	0/3/3/3
3	TA1	g	601	-	-	14/41/127/127	0/7/7/7
6	GTP	O	502	5	-	3/22/38/38	0/3/3/3
3	TA1	k	601	-	-	9/41/127/127	0/7/7/7
3	TA1	i	601	-	-	12/41/127/127	0/7/7/7
6	GTP	X	502	5	-	4/22/38/38	0/3/3/3
3	TA1	e	601	-	-	8/41/127/127	0/7/7/7

The worst 5 of 233 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	602	GDP	PA-O3A	8.35	1.68	1.59
6	Z	502	GTP	C1'-N9	6.54	1.66	1.47
6	W	502	GTP	C4-N3	6.45	1.49	1.34
6	T	502	GTP	C1'-N9	6.40	1.65	1.47
6	W	502	GTP	C6-N1	6.06	1.50	1.38

The worst 5 of 626 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	601	TA1	C42-C37-C29	15.02	144.64	120.78
3	g	601	TA1	C38-C37-C29	-14.25	98.14	120.78
3	g	601	TA1	C05-C04-C03	-8.57	101.51	120.40
6	T	502	GTP	C5-C4-N3	-8.14	115.44	128.39
3	g	601	TA1	C09-C04-C05	7.91	128.63	118.57

There are no chirality outliers.

5 of 236 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	c	601	TA1	O02-C03-C04-C05
3	g	601	TA1	C27-C28-C29-N01
4	a	602	GDP	PA-O3A-PB-O2B
4	a	602	GDP	C5'-O5'-PA-O3A
4	a	602	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

39 monomers are involved in 933 short contacts:

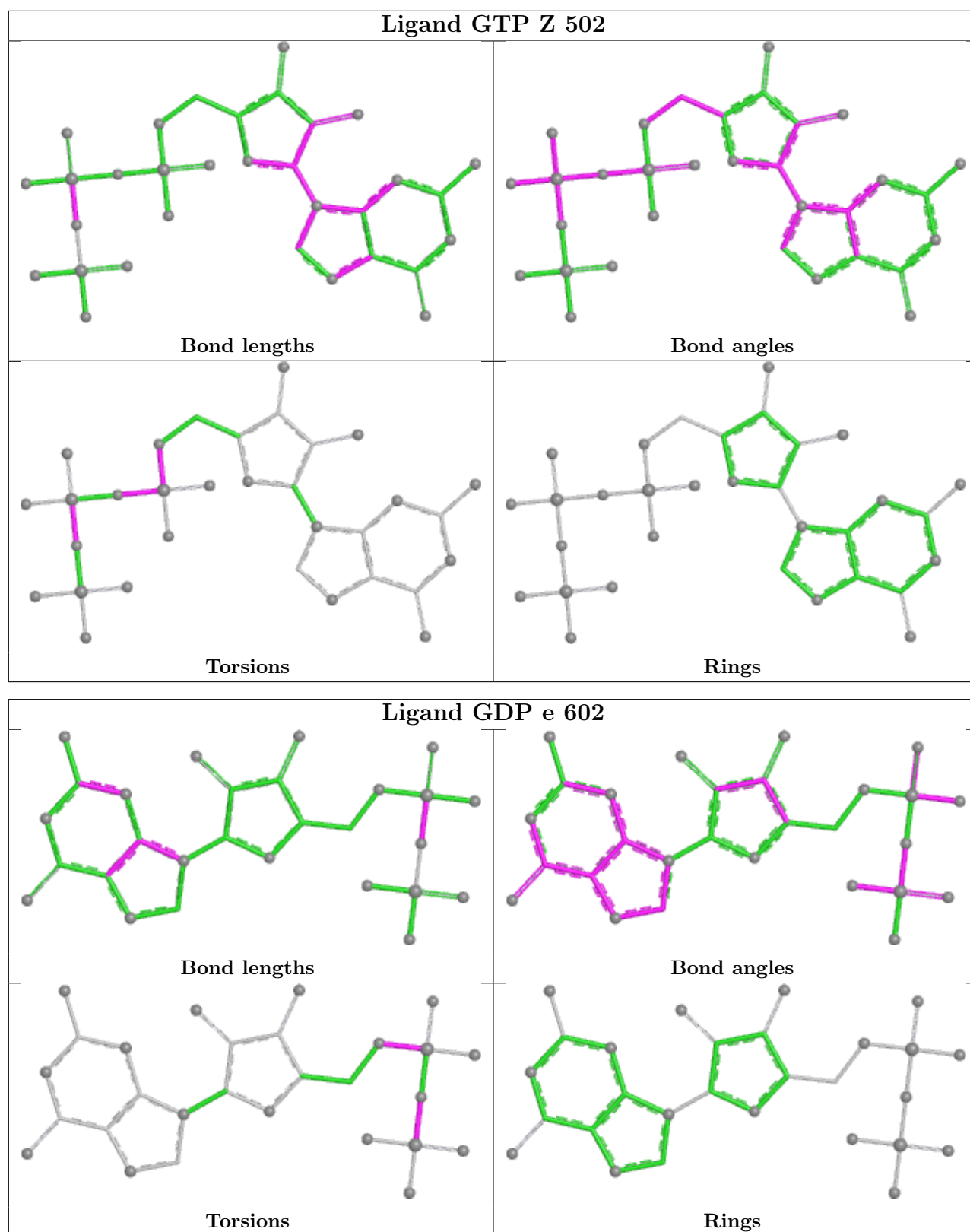
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	502	GTP	30	0
4	e	602	GDP	33	0
4	c	602	GDP	40	0
4	j	602	GDP	15	0
4	a	602	GDP	19	0
4	m	602	GDP	30	0
4	d	602	GDP	35	0
3	h	601	TA1	18	0
4	b	602	GDP	61	0
3	m	601	TA1	15	0
3	j	601	TA1	14	0
6	N	502	GTP	30	0
6	S	502	GTP	31	0

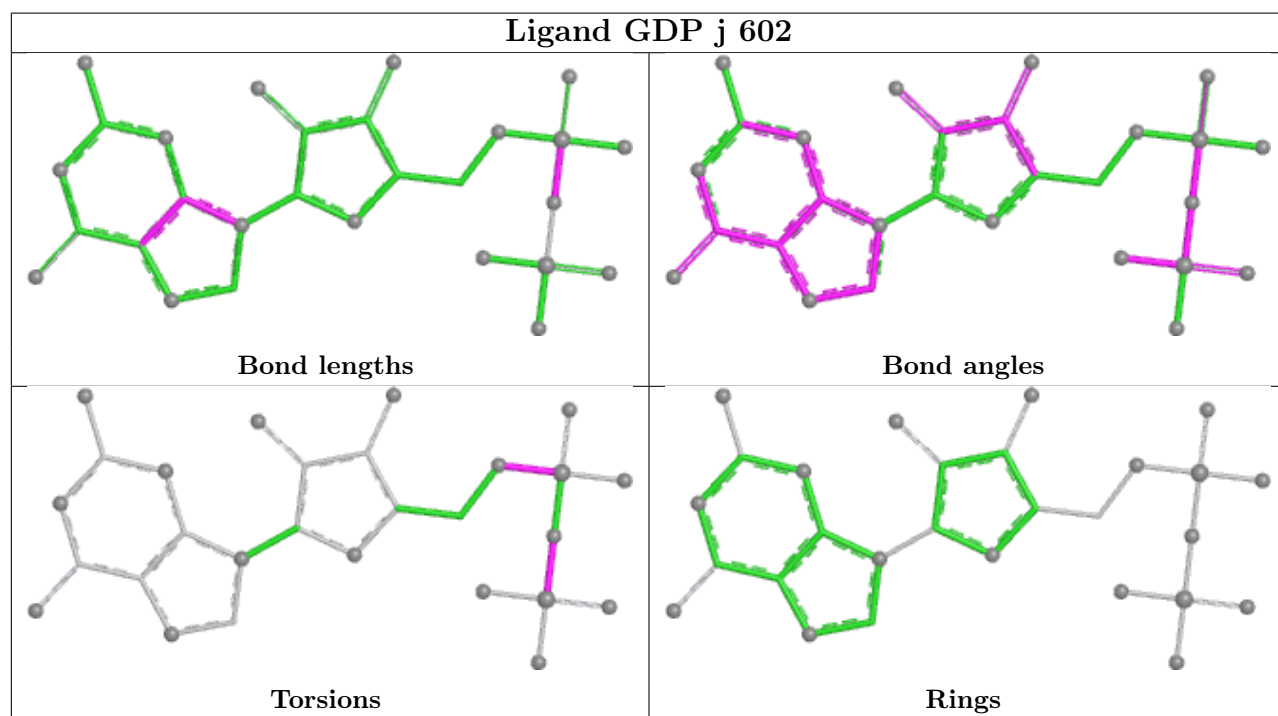
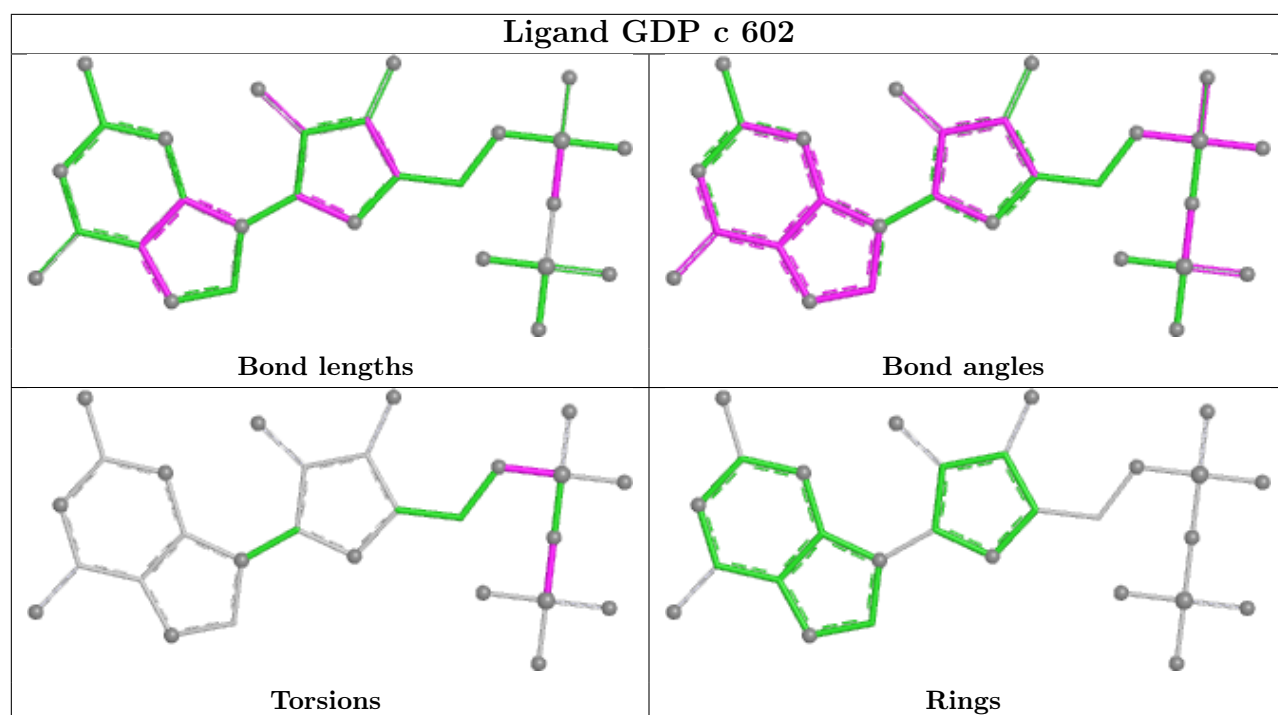
Continued on next page...

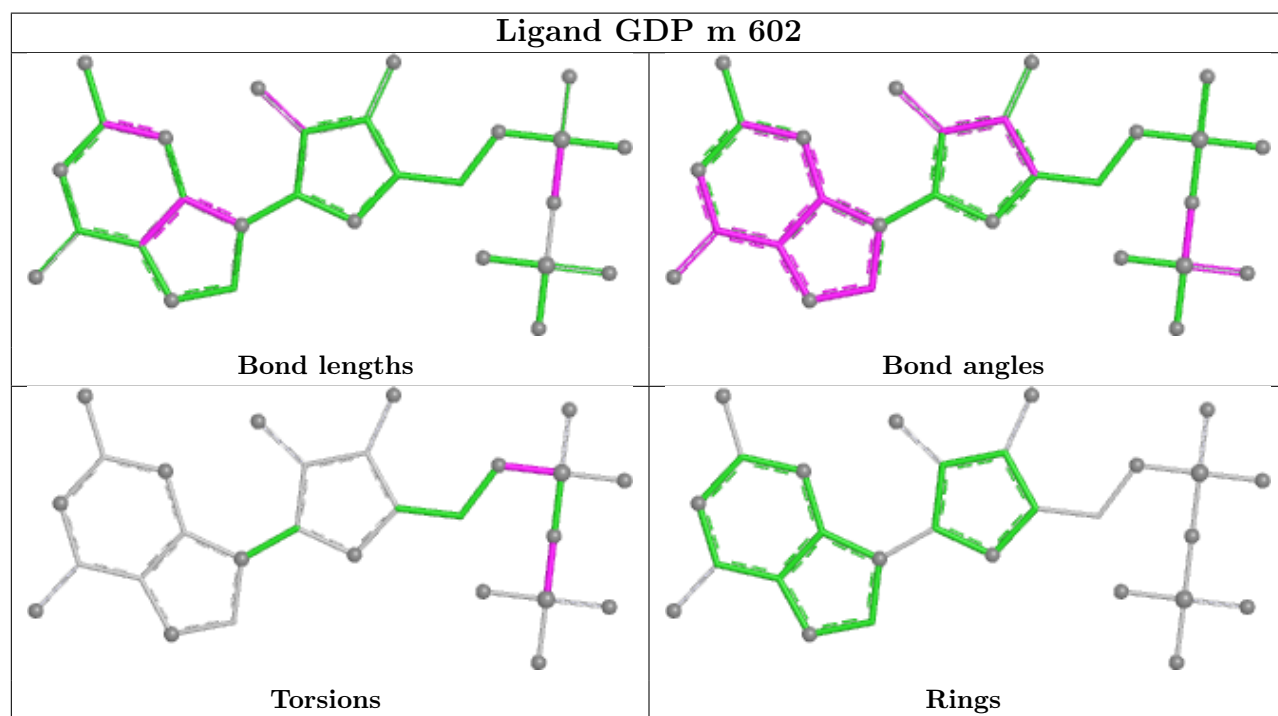
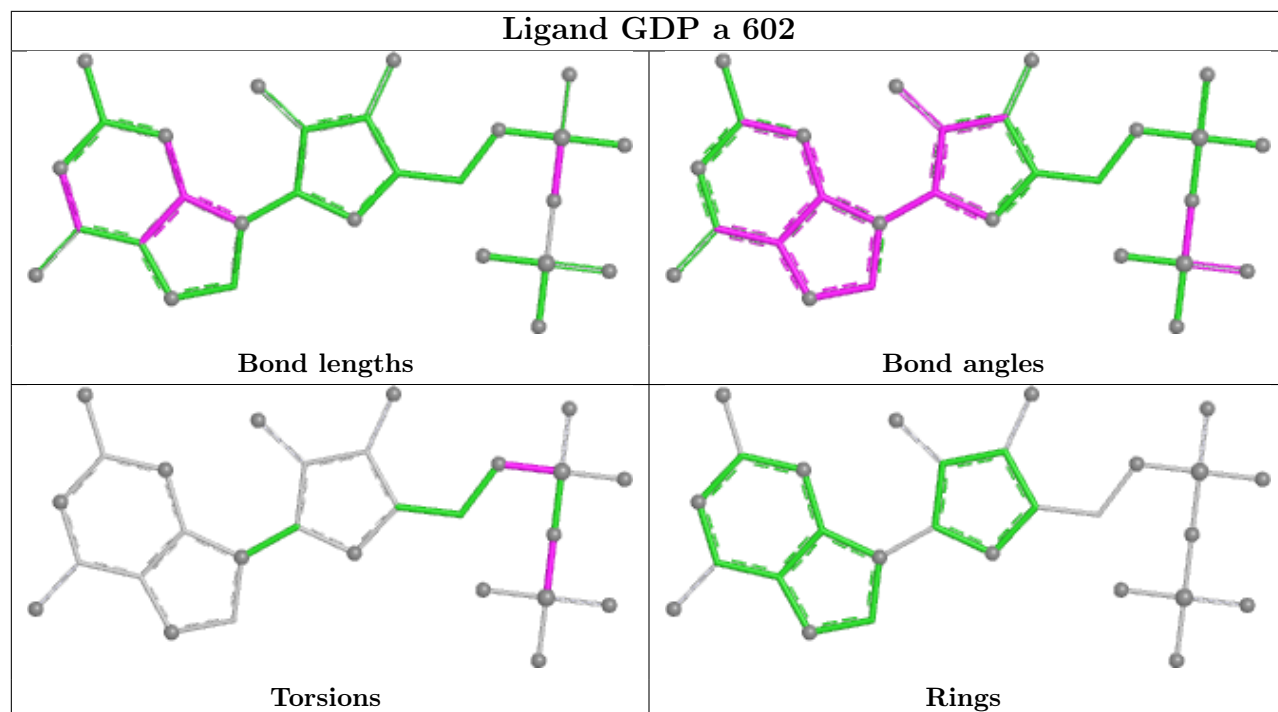
Continued from previous page...

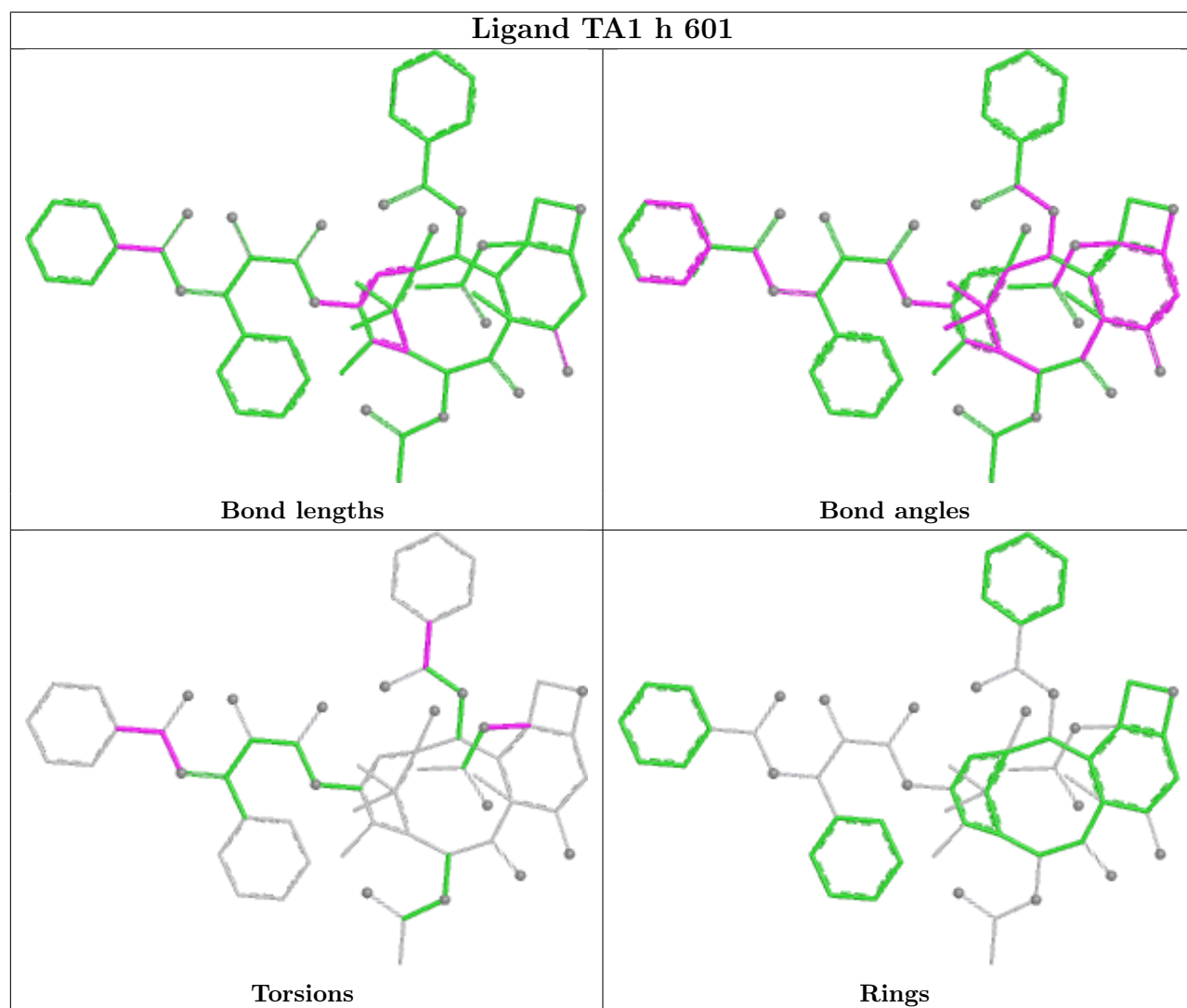
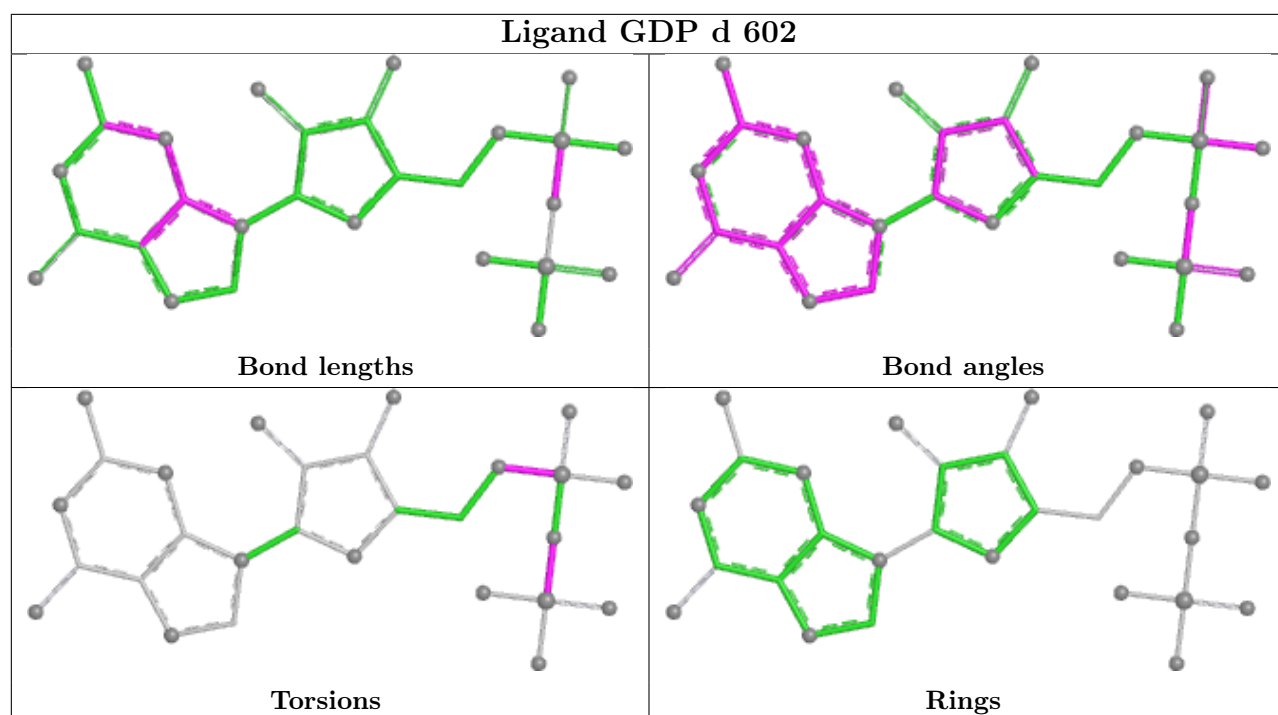
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	g	602	GDP	15	0
6	U	502	GTP	38	0
6	Q	502	GTP	23	0
6	Y	502	GTP	31	0
3	l	601	TA1	17	0
4	i	602	GDP	12	0
4	h	602	GDP	29	0
3	b	601	TA1	11	0
6	R	502	GTP	19	0
3	a	601	TA1	18	0
4	k	602	GDP	13	0
3	f	601	TA1	10	0
3	c	601	TA1	23	0
4	l	602	GDP	16	0
6	P	502	GTP	17	0
6	T	502	GTP	31	0
4	f	602	GDP	31	0
6	V	502	GTP	28	0
3	d	601	TA1	19	0
6	W	502	GTP	28	0
3	g	601	TA1	18	0
6	O	502	GTP	27	0
3	k	601	TA1	16	0
3	i	601	TA1	24	0
6	X	502	GTP	29	0
3	e	601	TA1	19	0

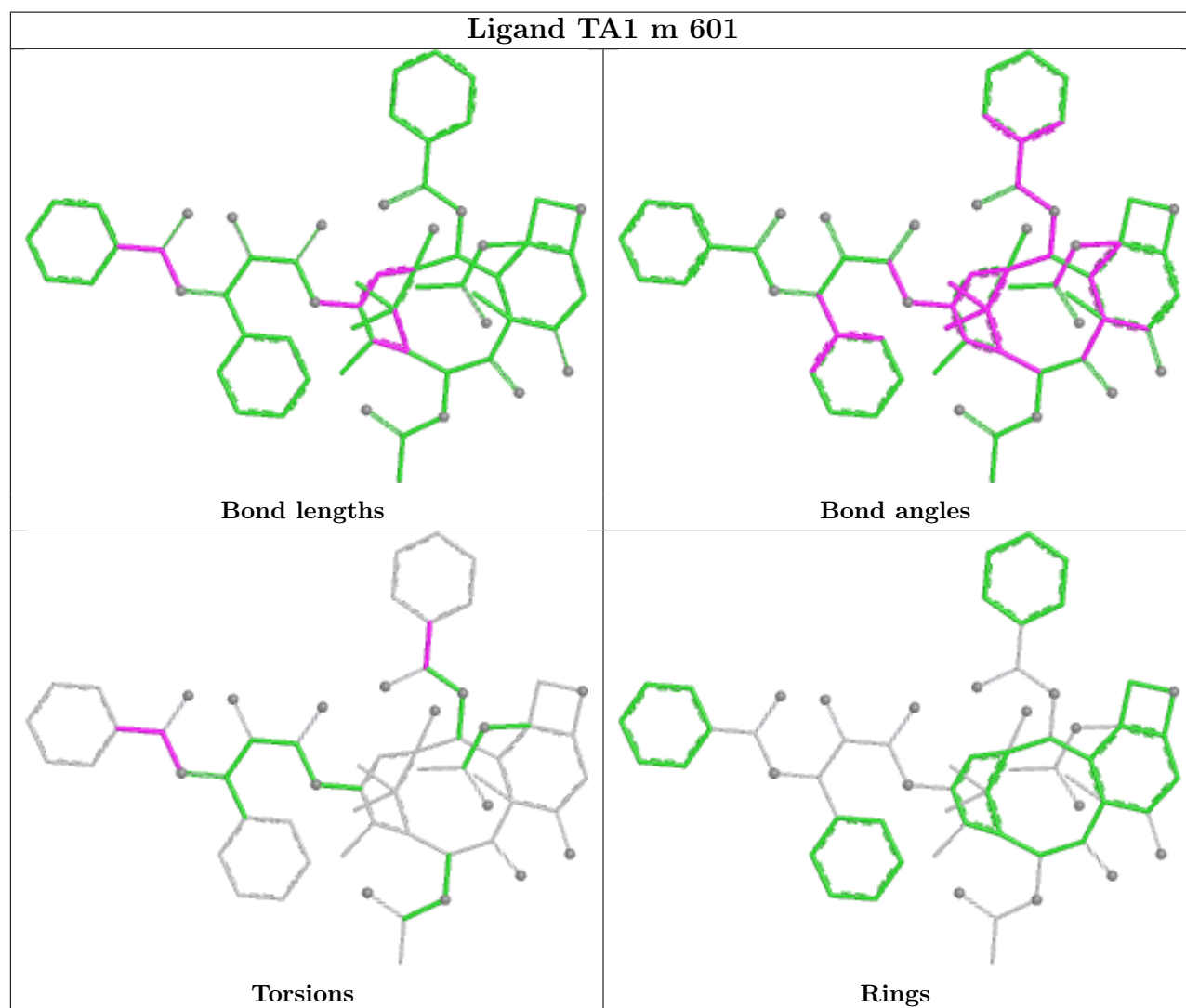
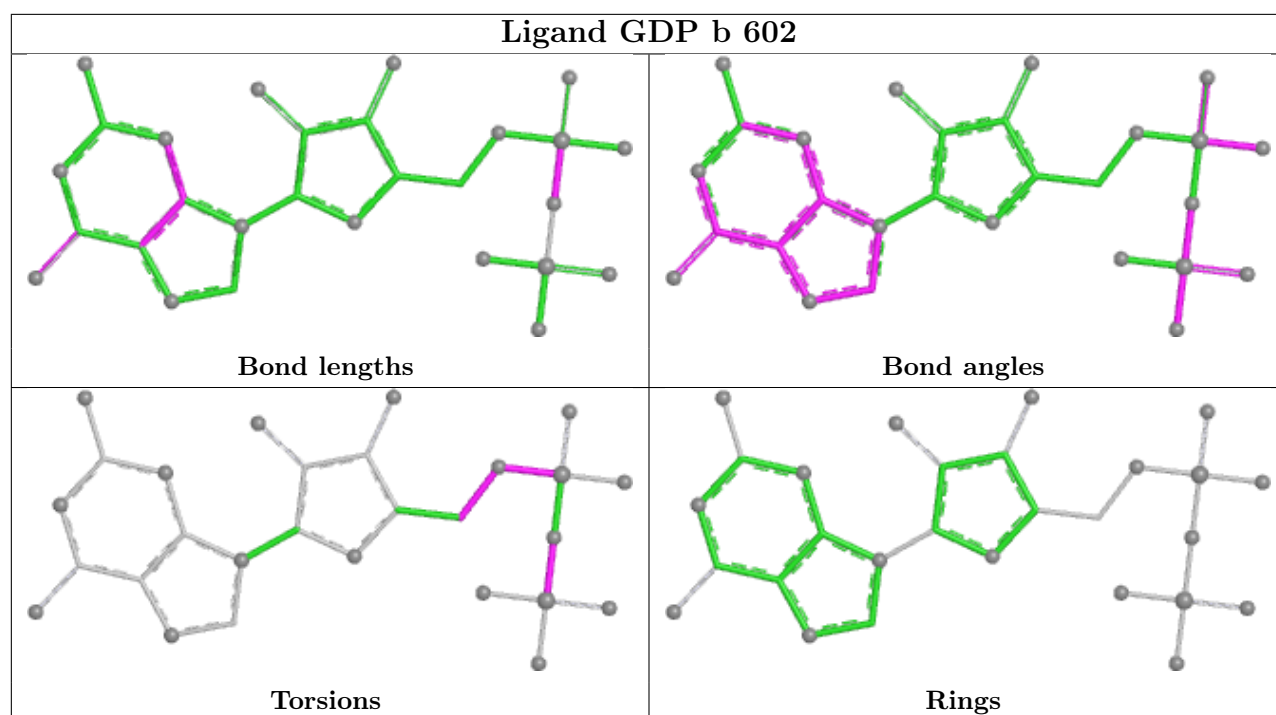
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

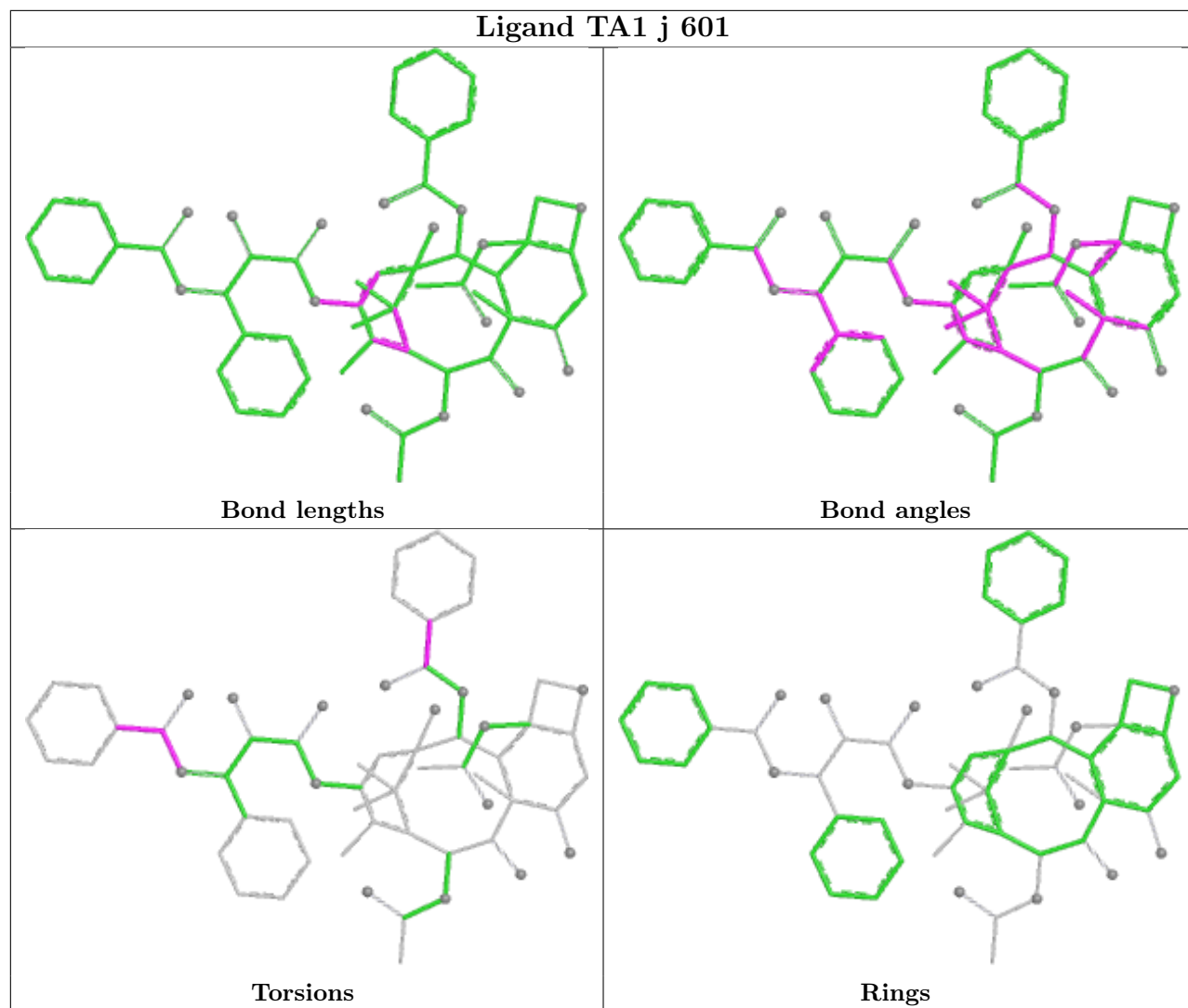


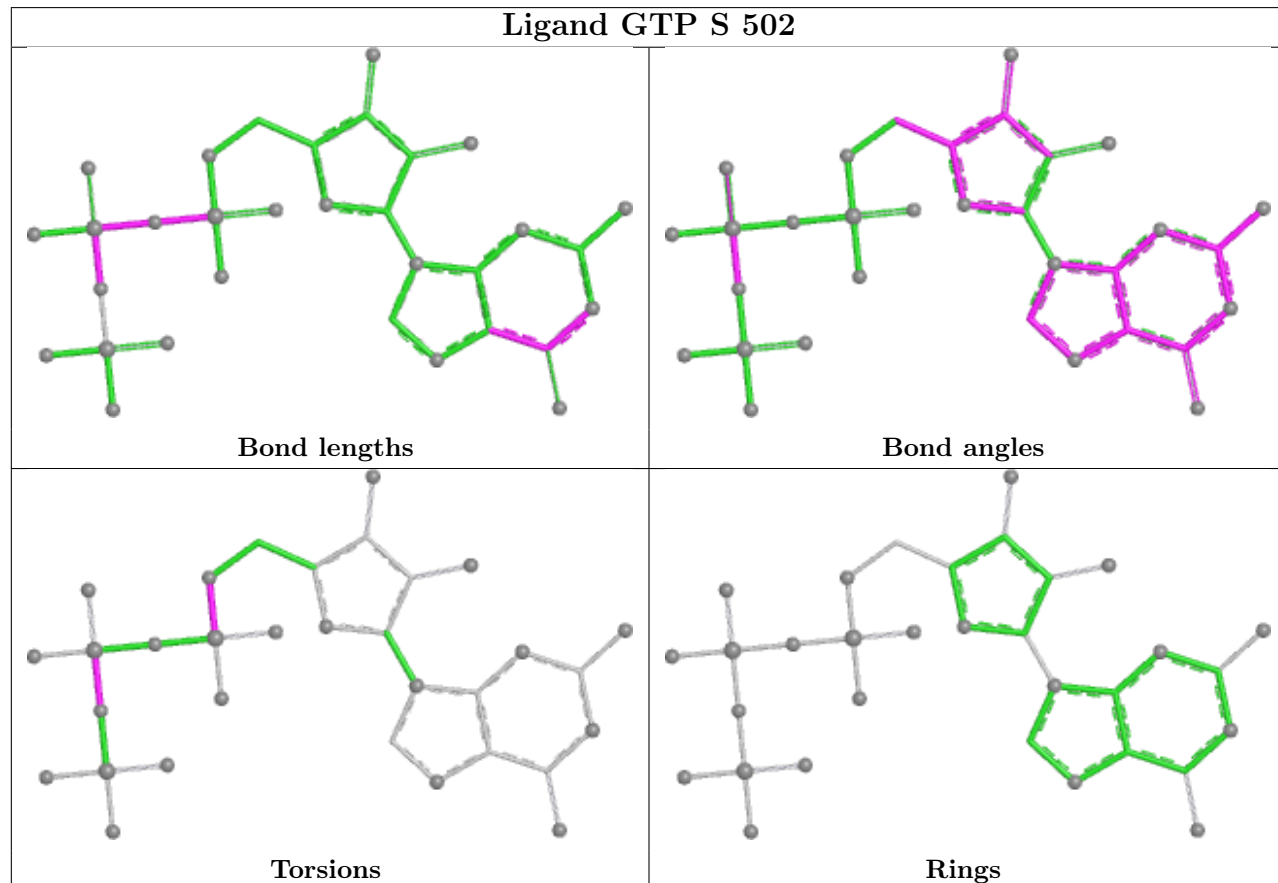
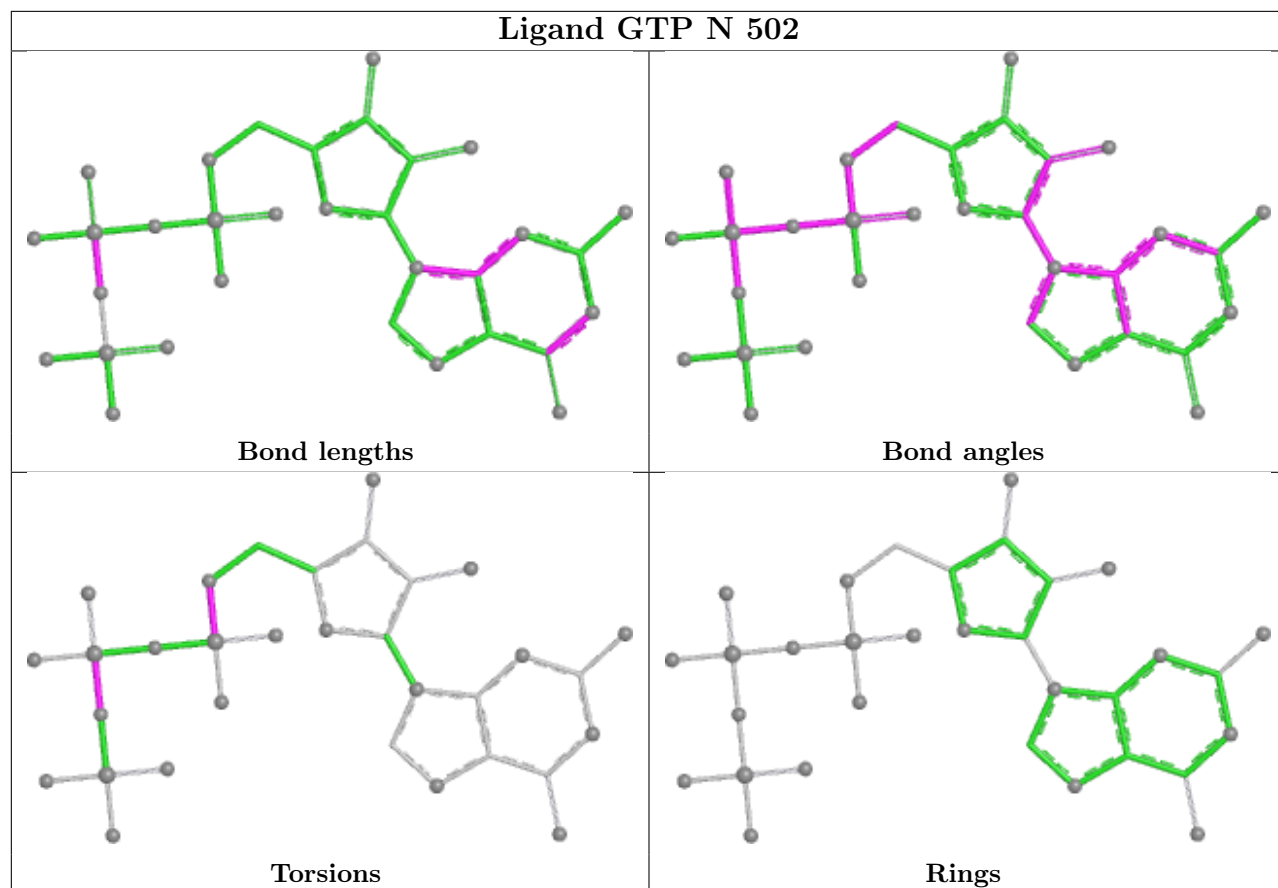


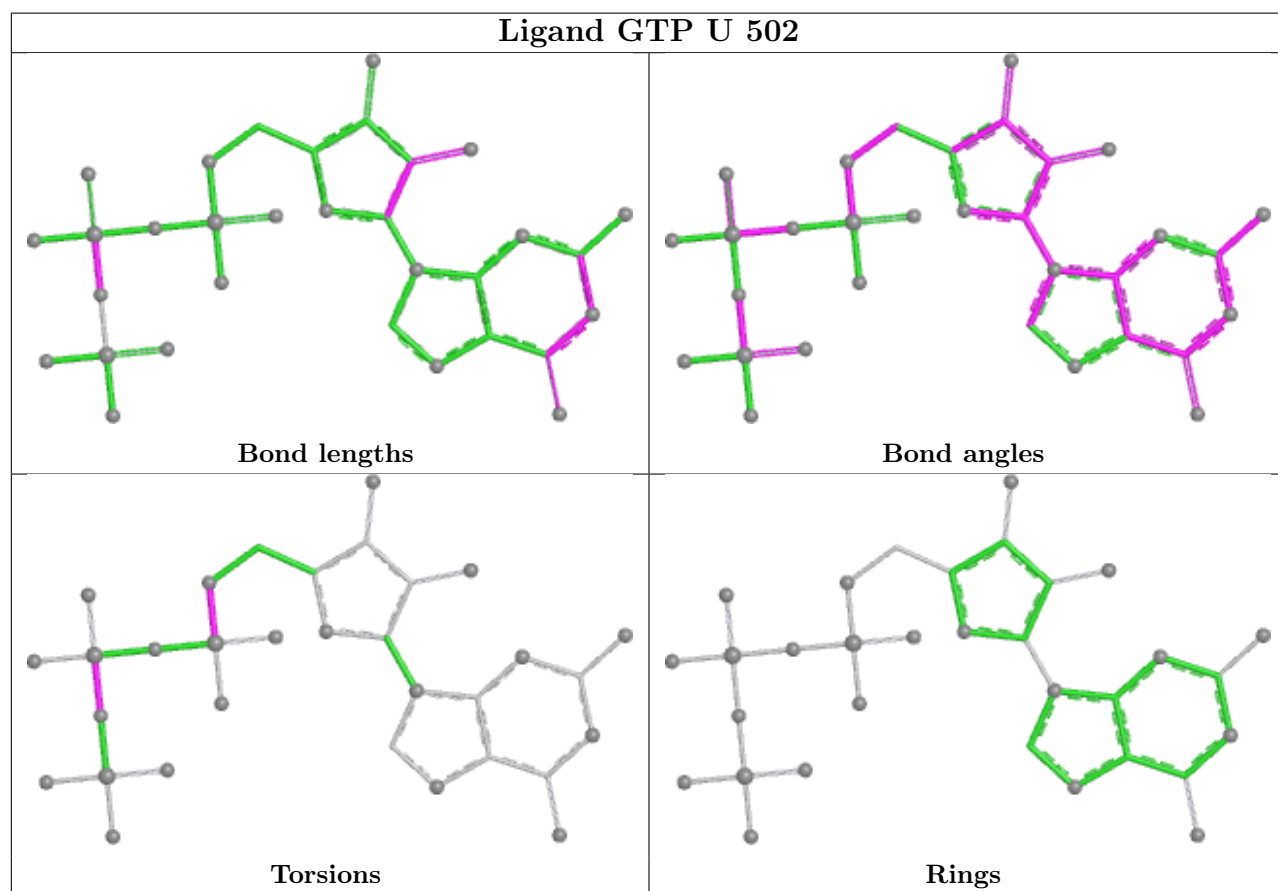
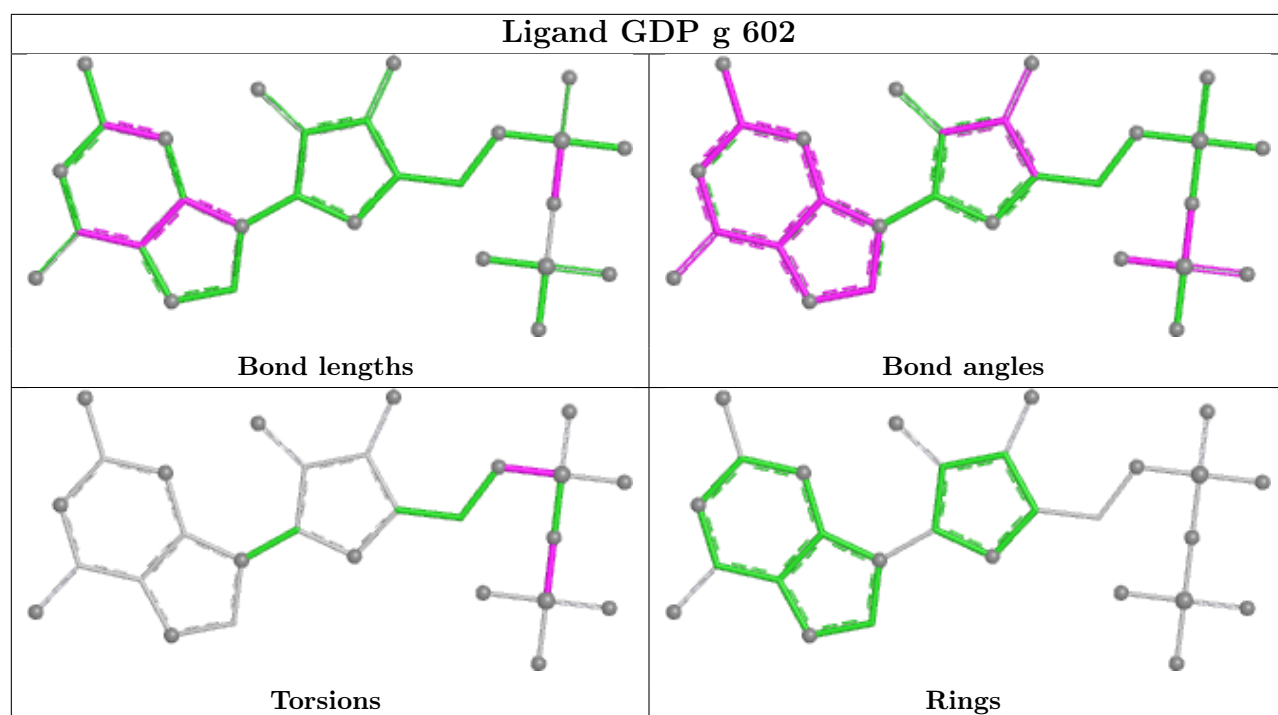


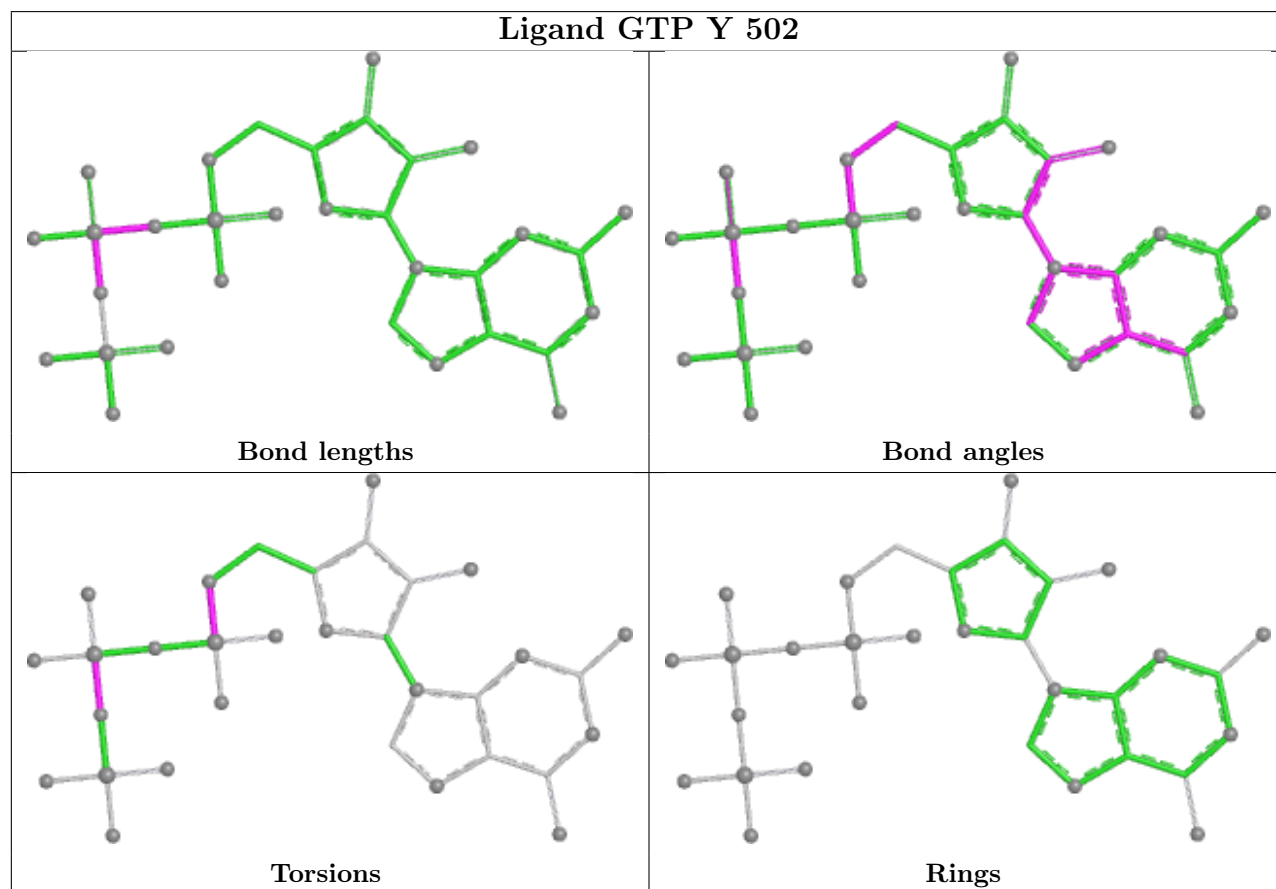
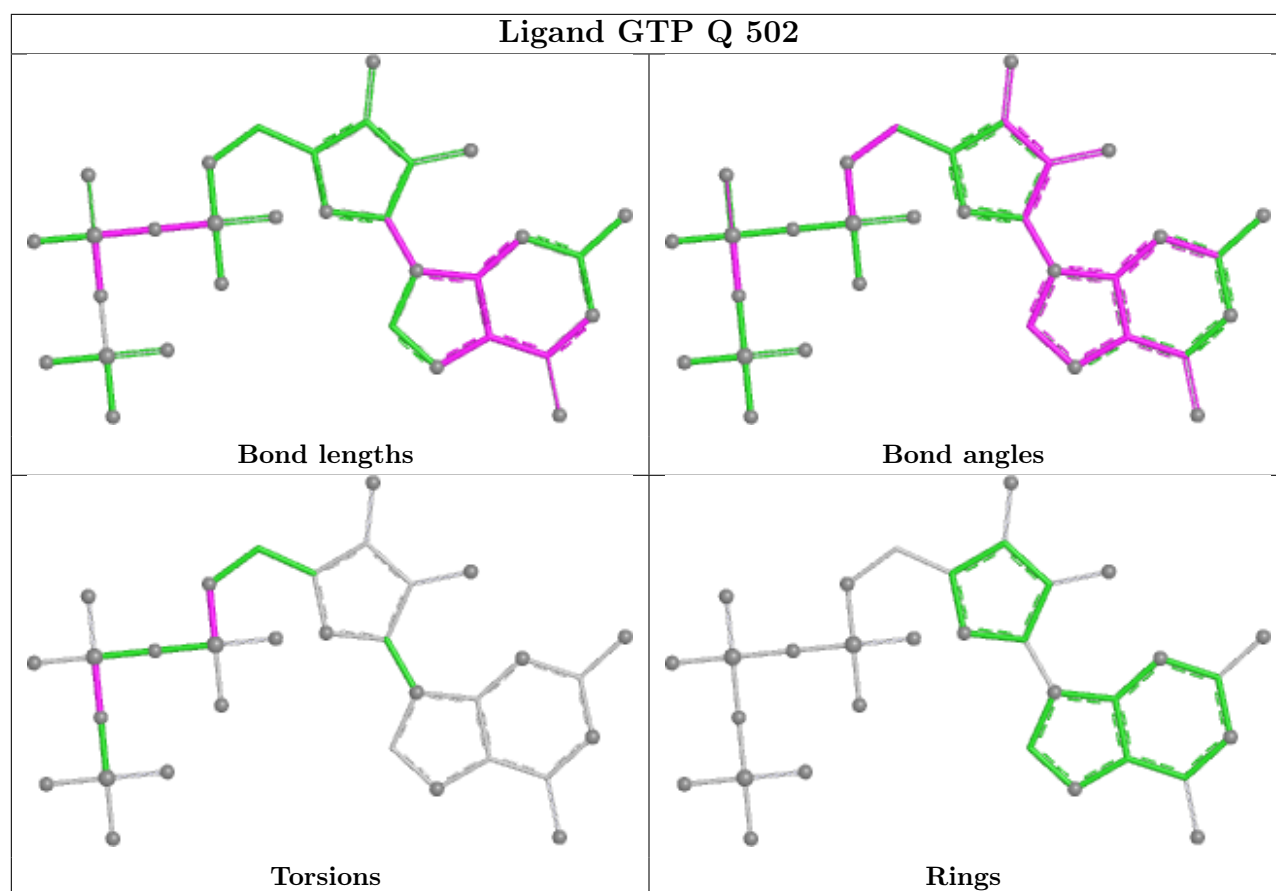


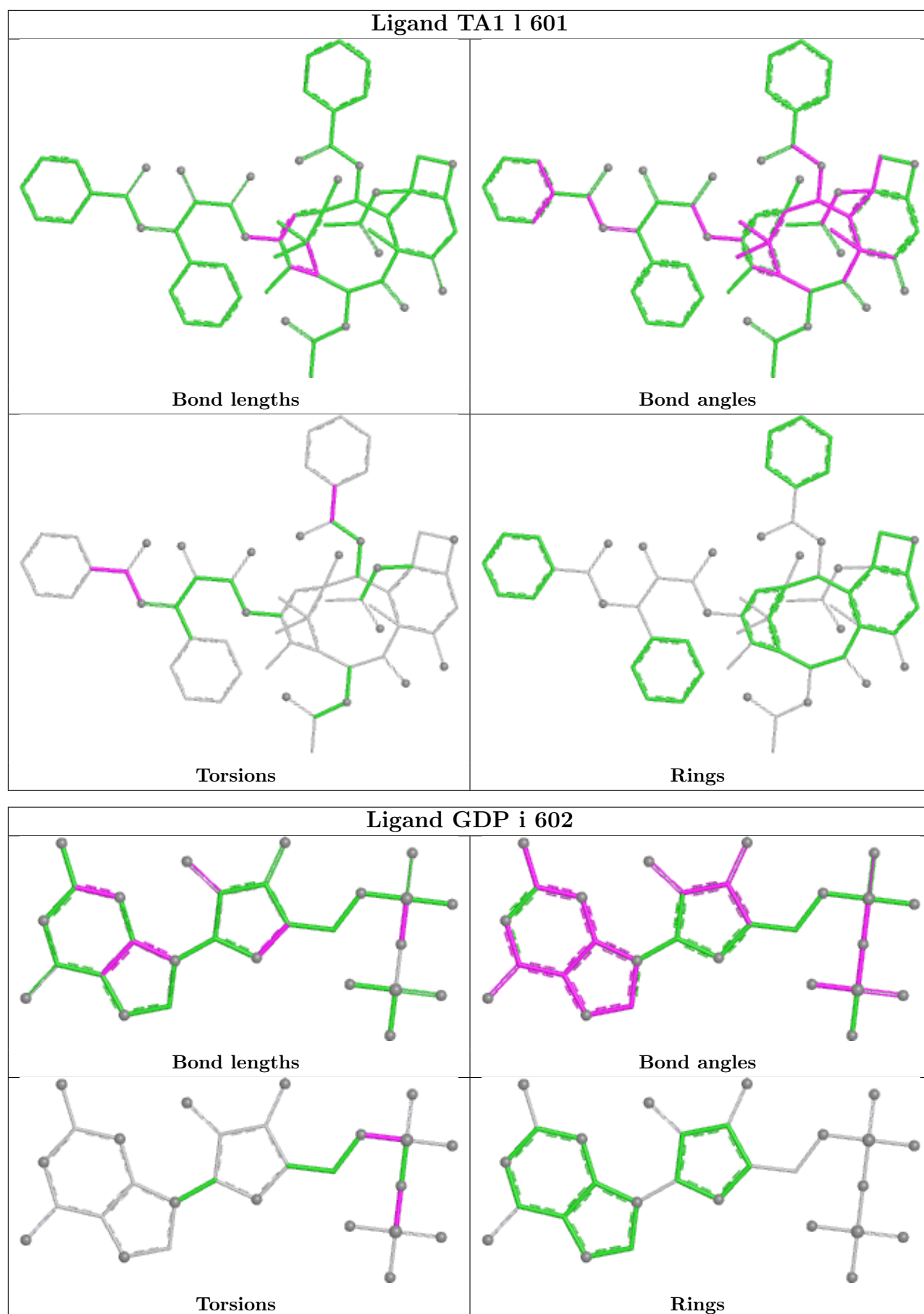


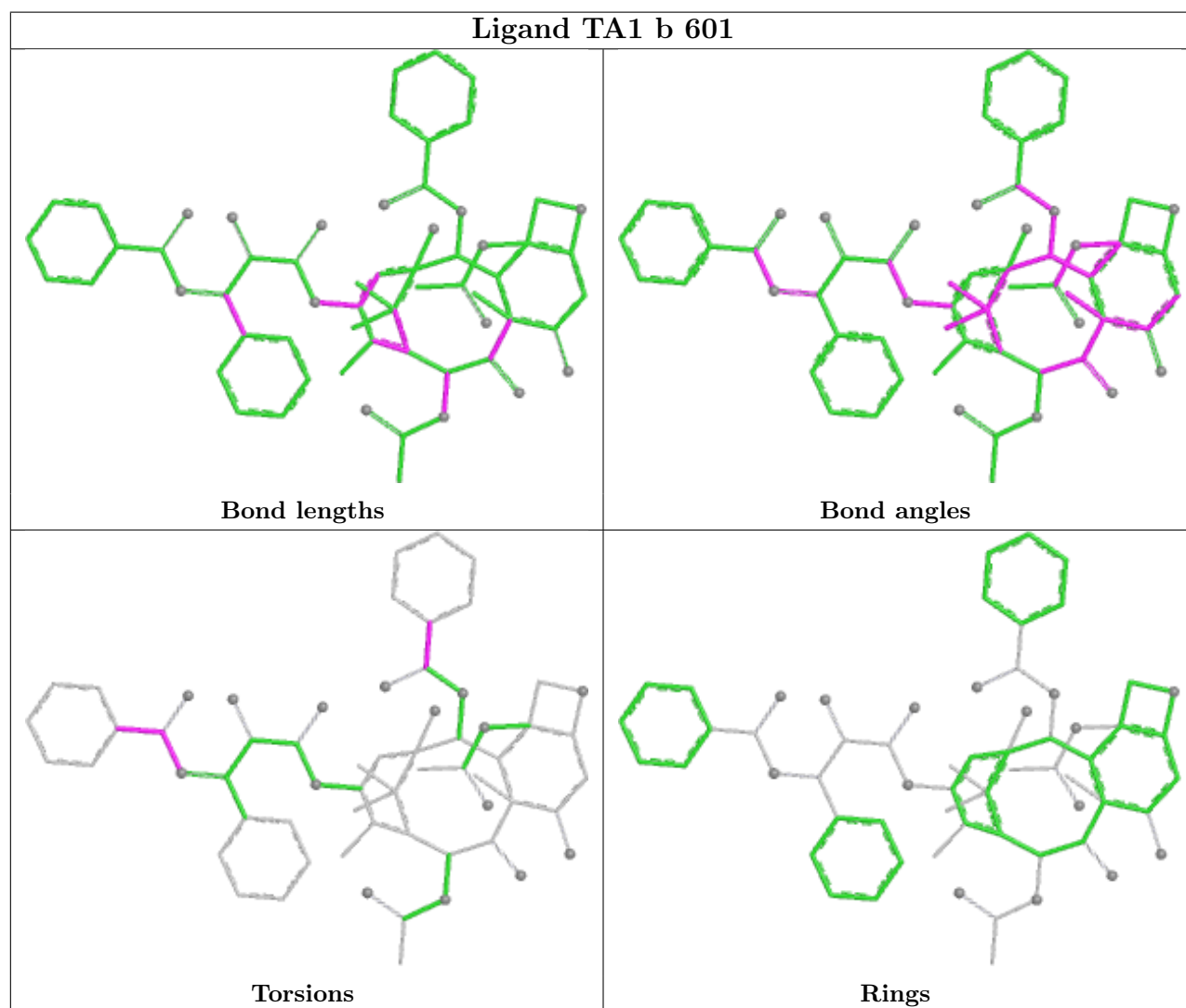
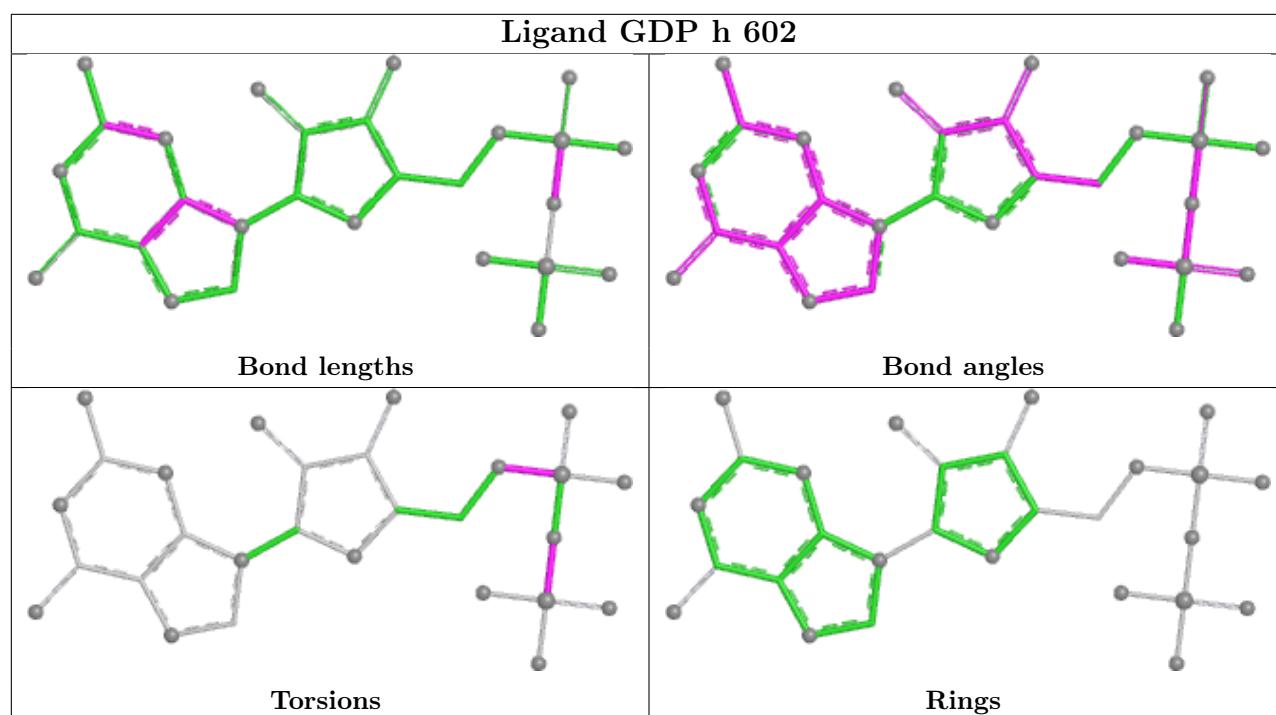


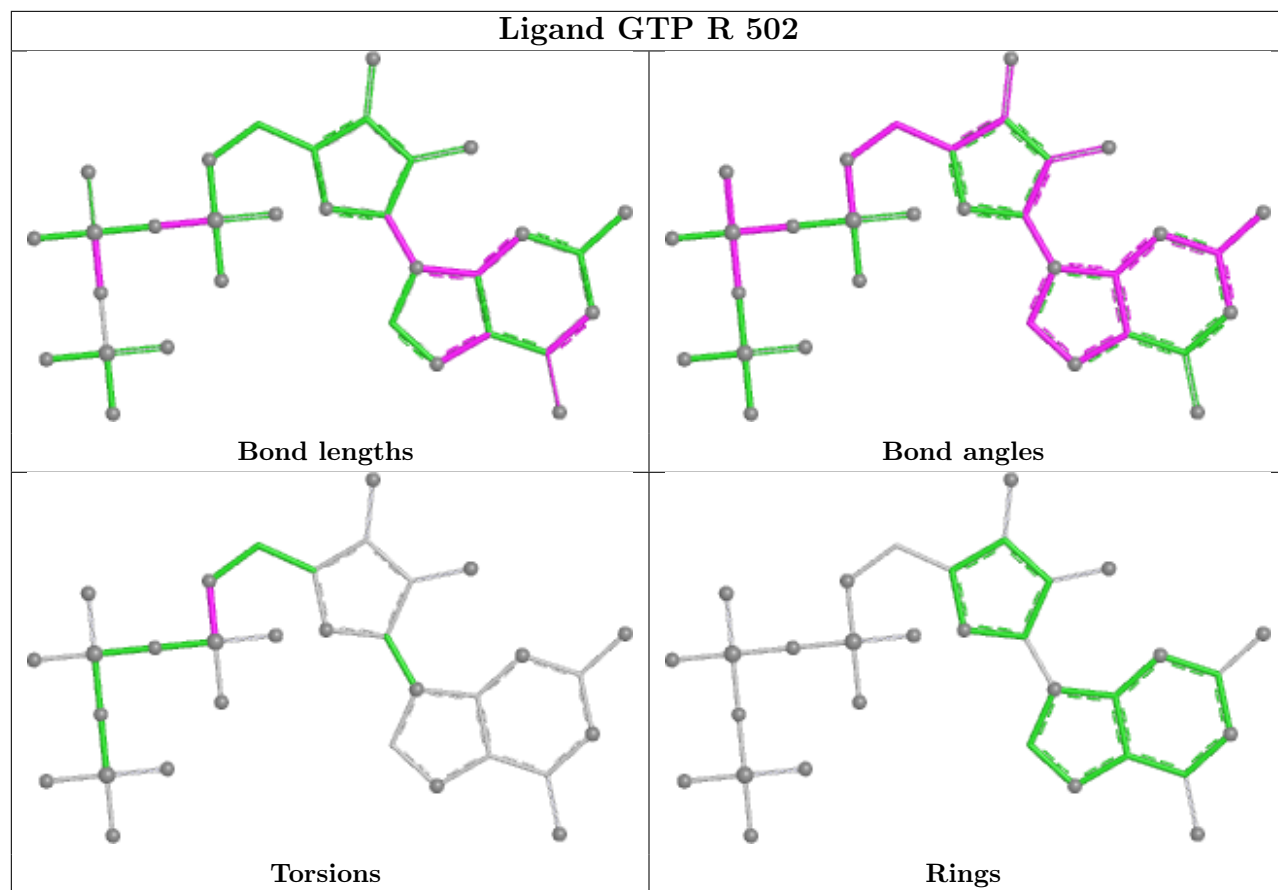


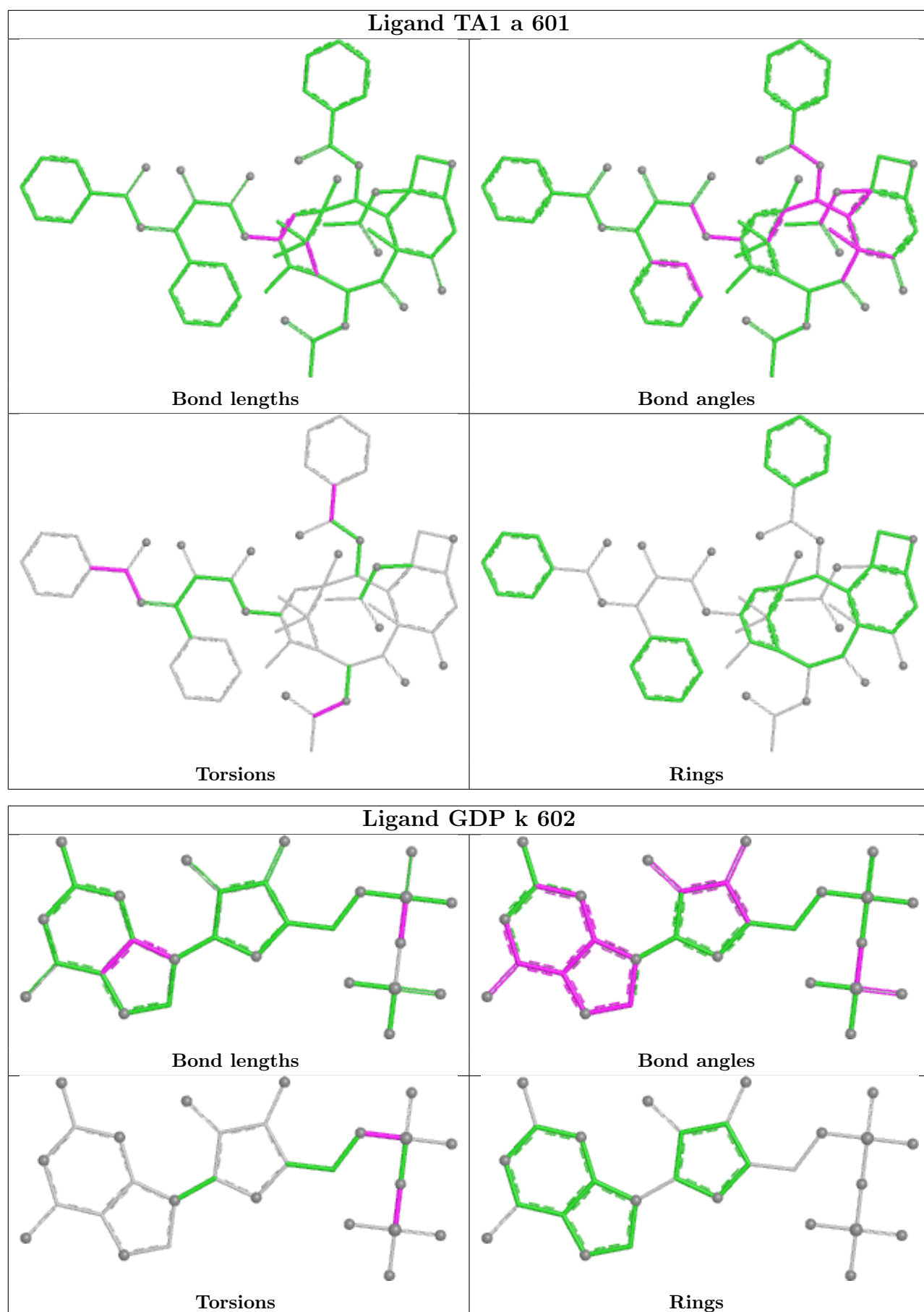




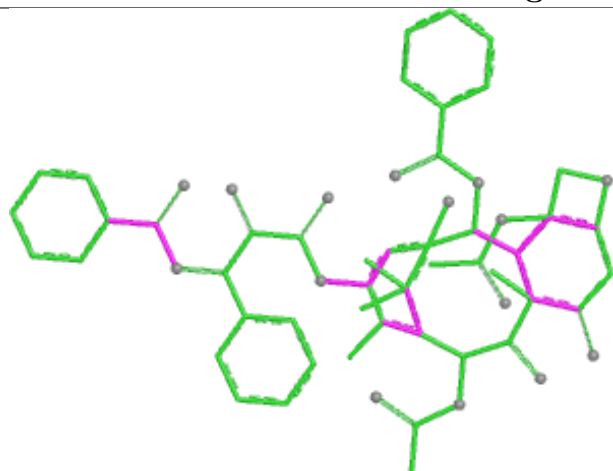




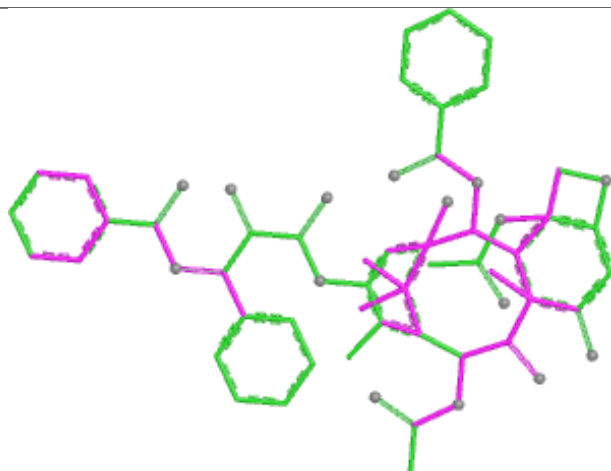




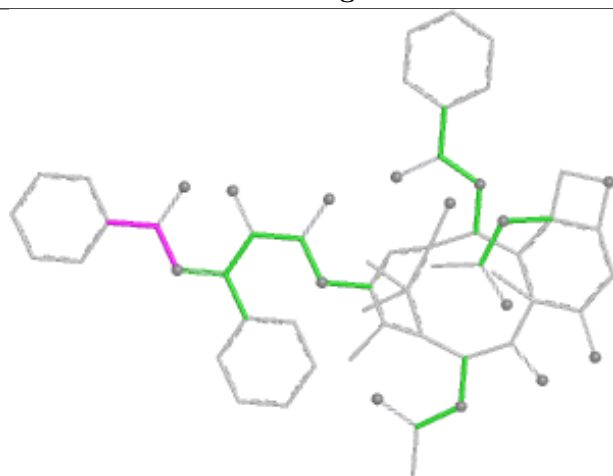
Ligand TA1 f 601



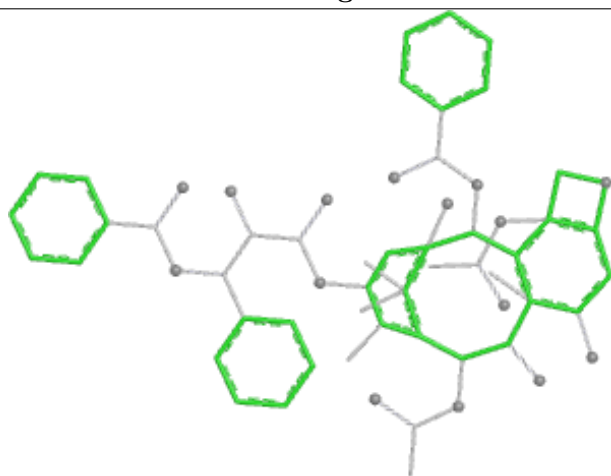
Bond lengths



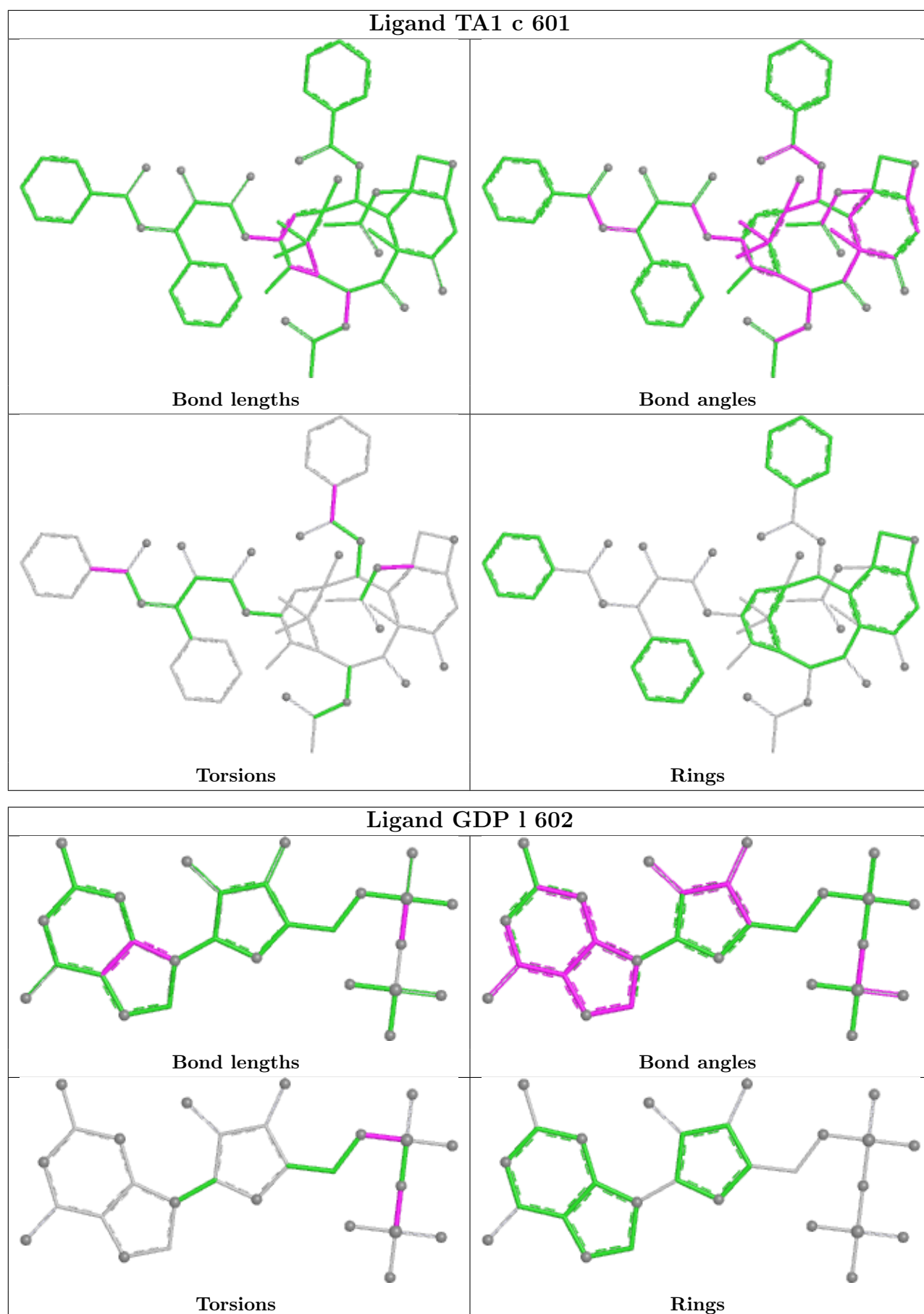
Bond angles



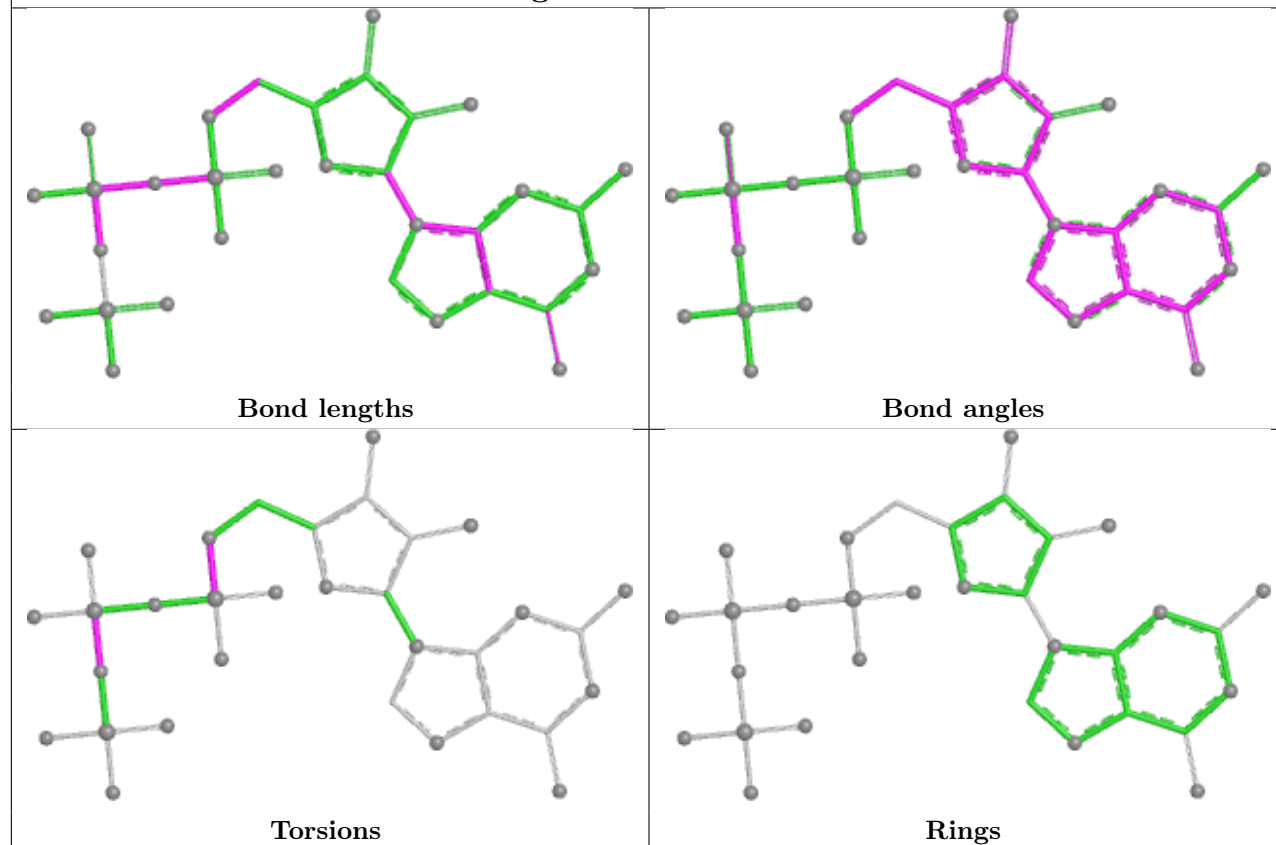
Torsions



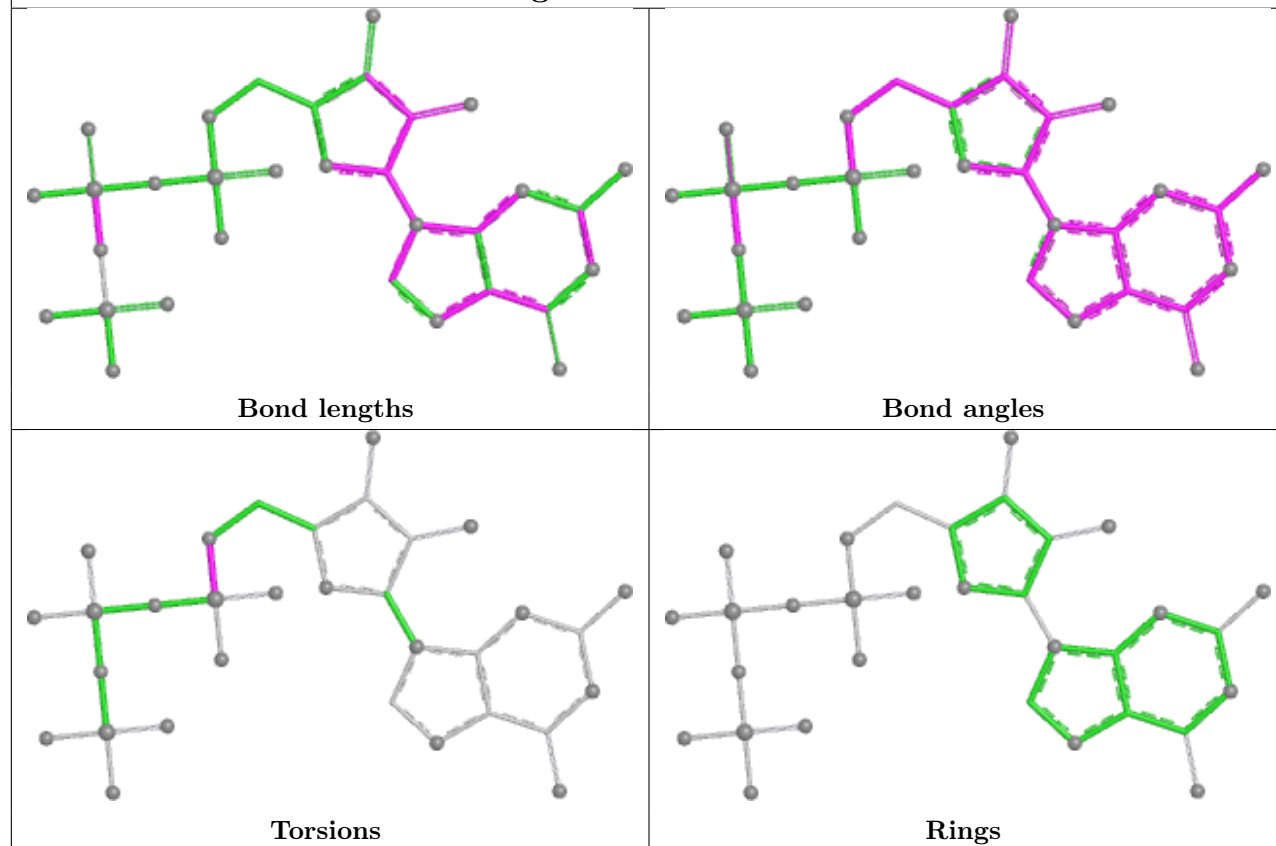
Rings

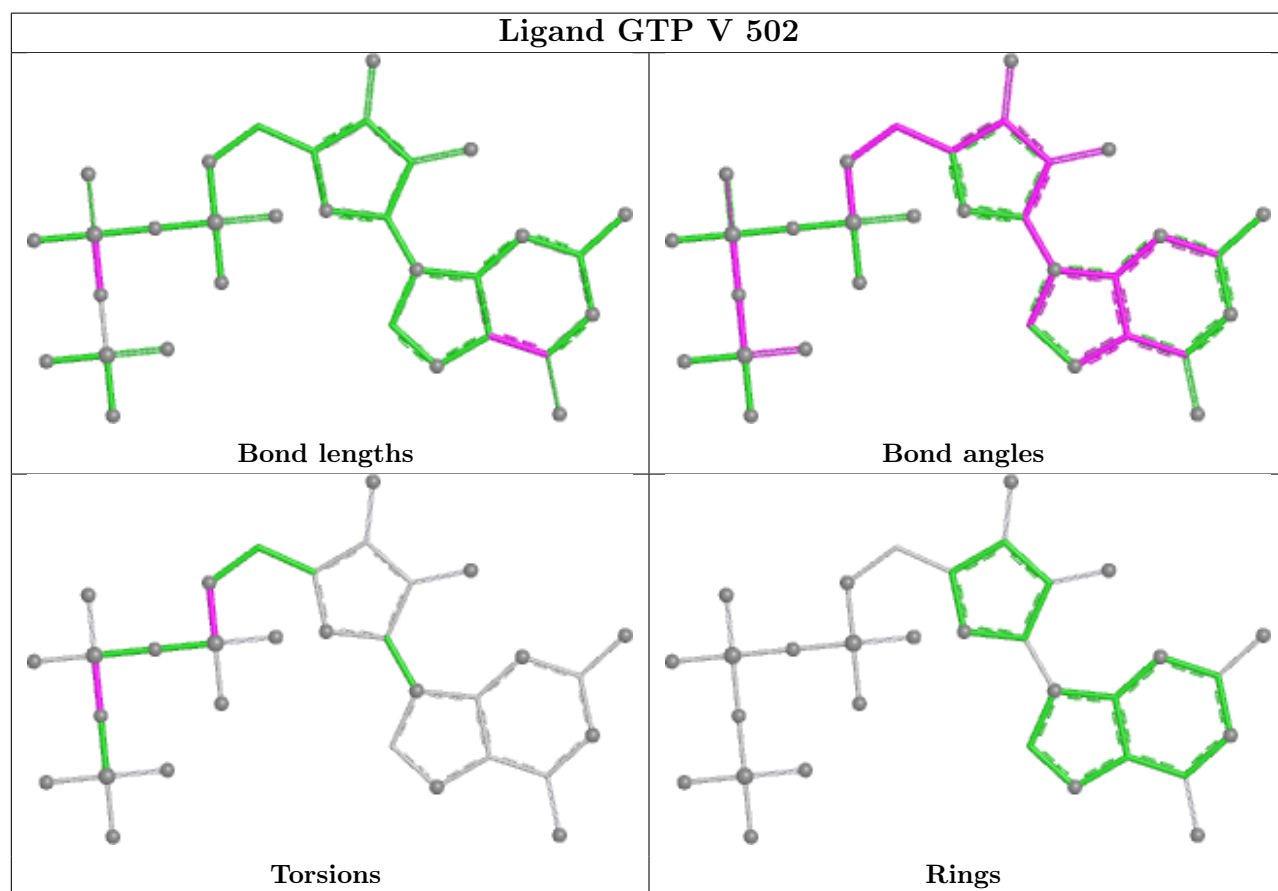
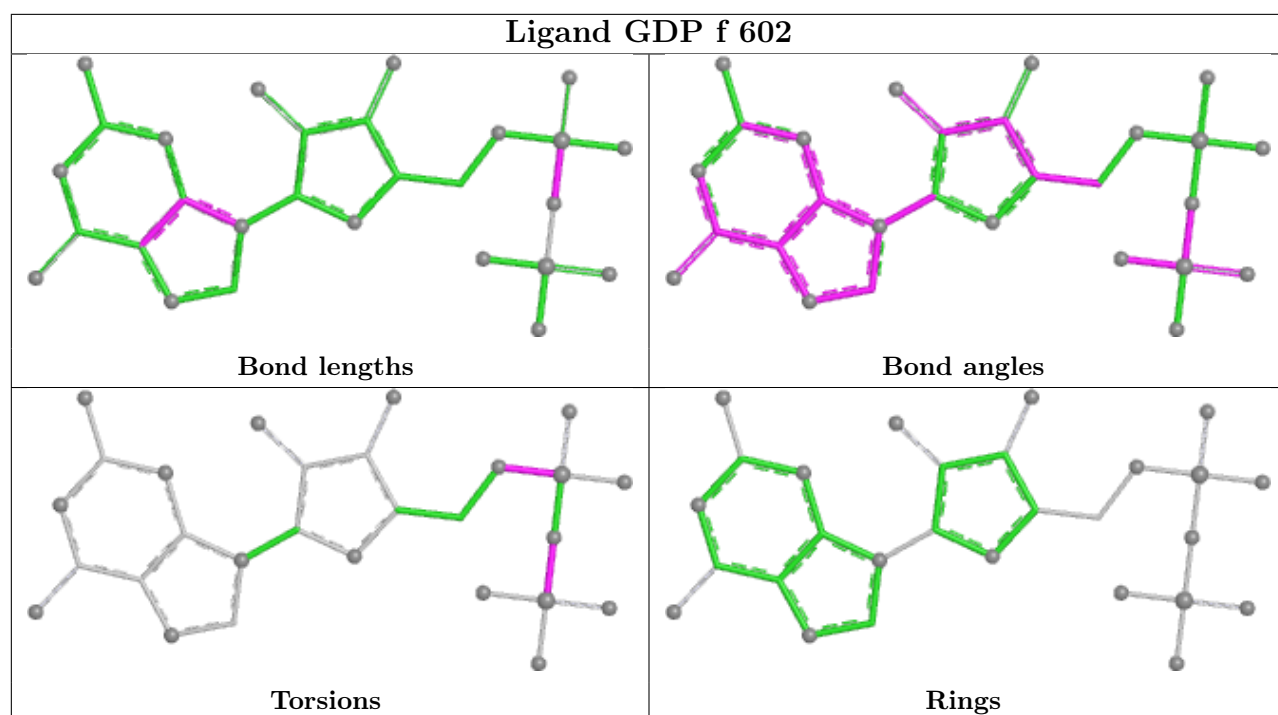


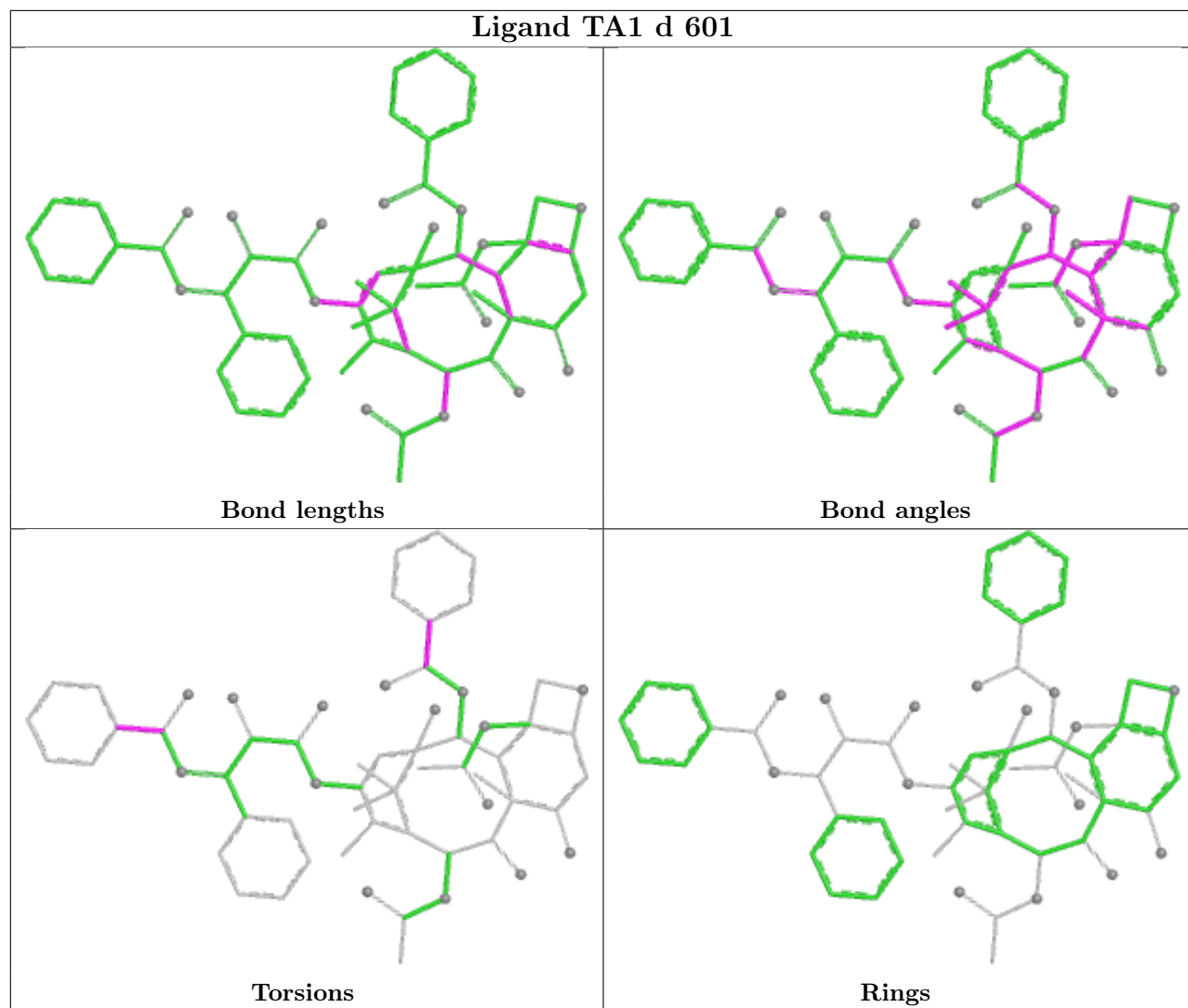
Ligand GTP P 502

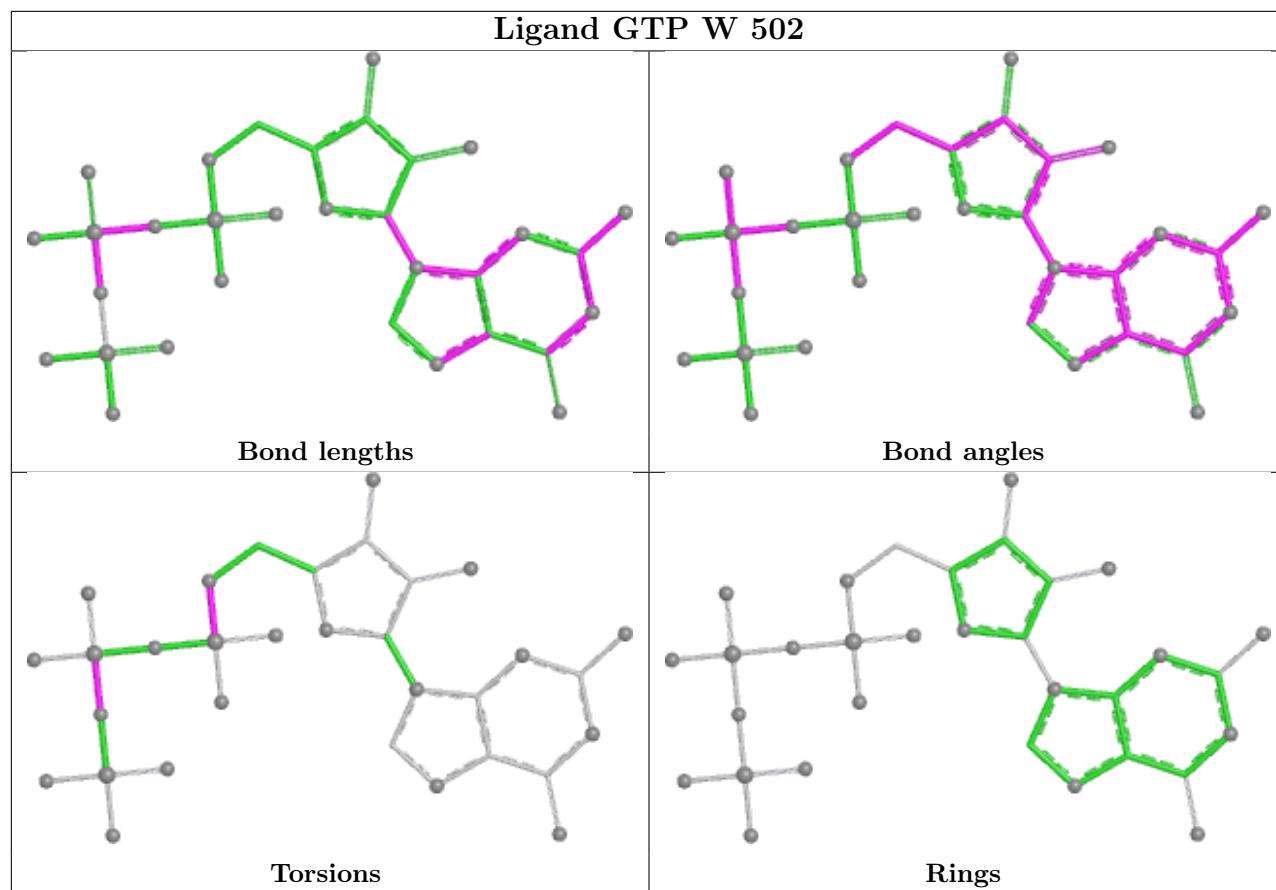


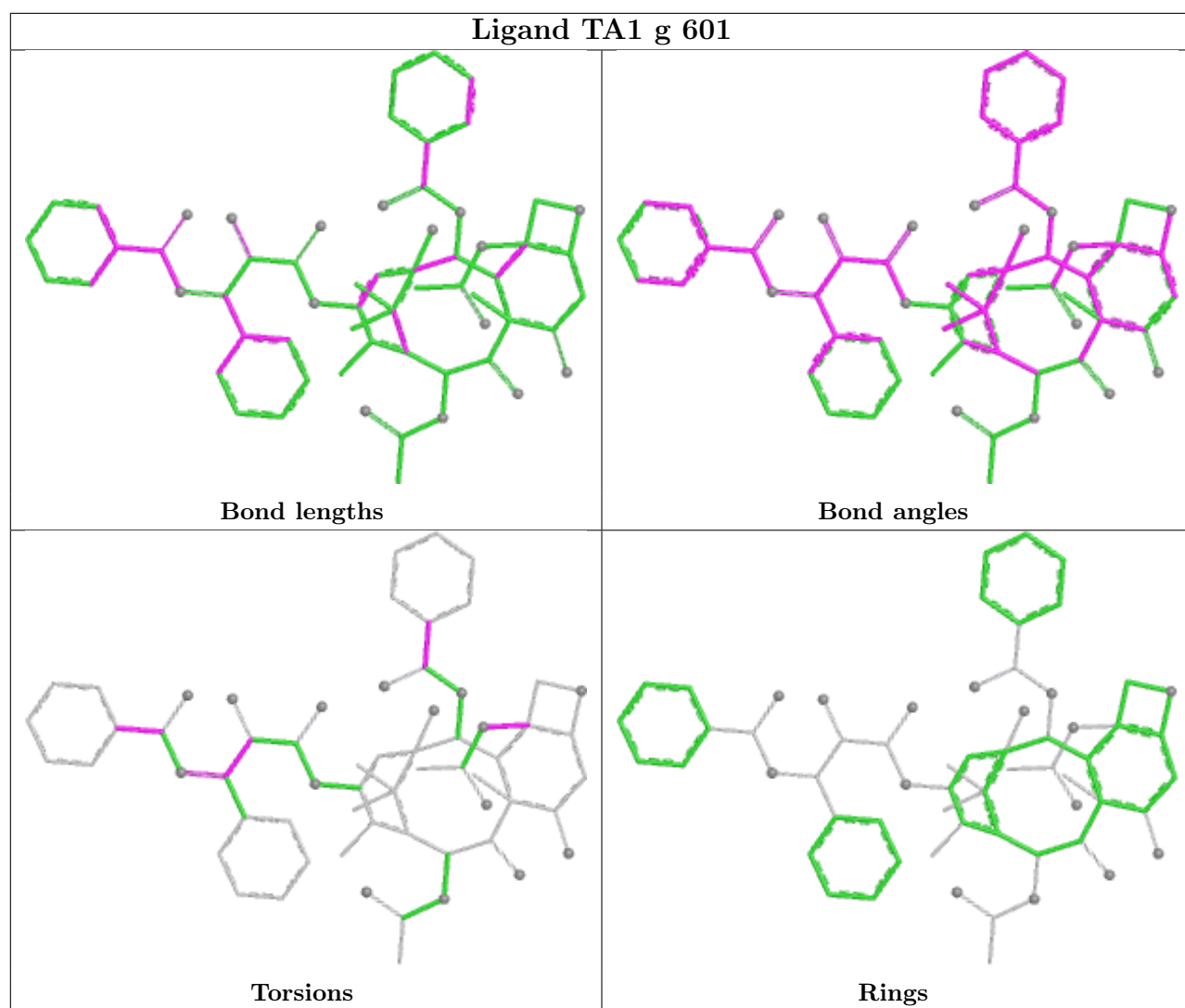
Ligand GTP T 502

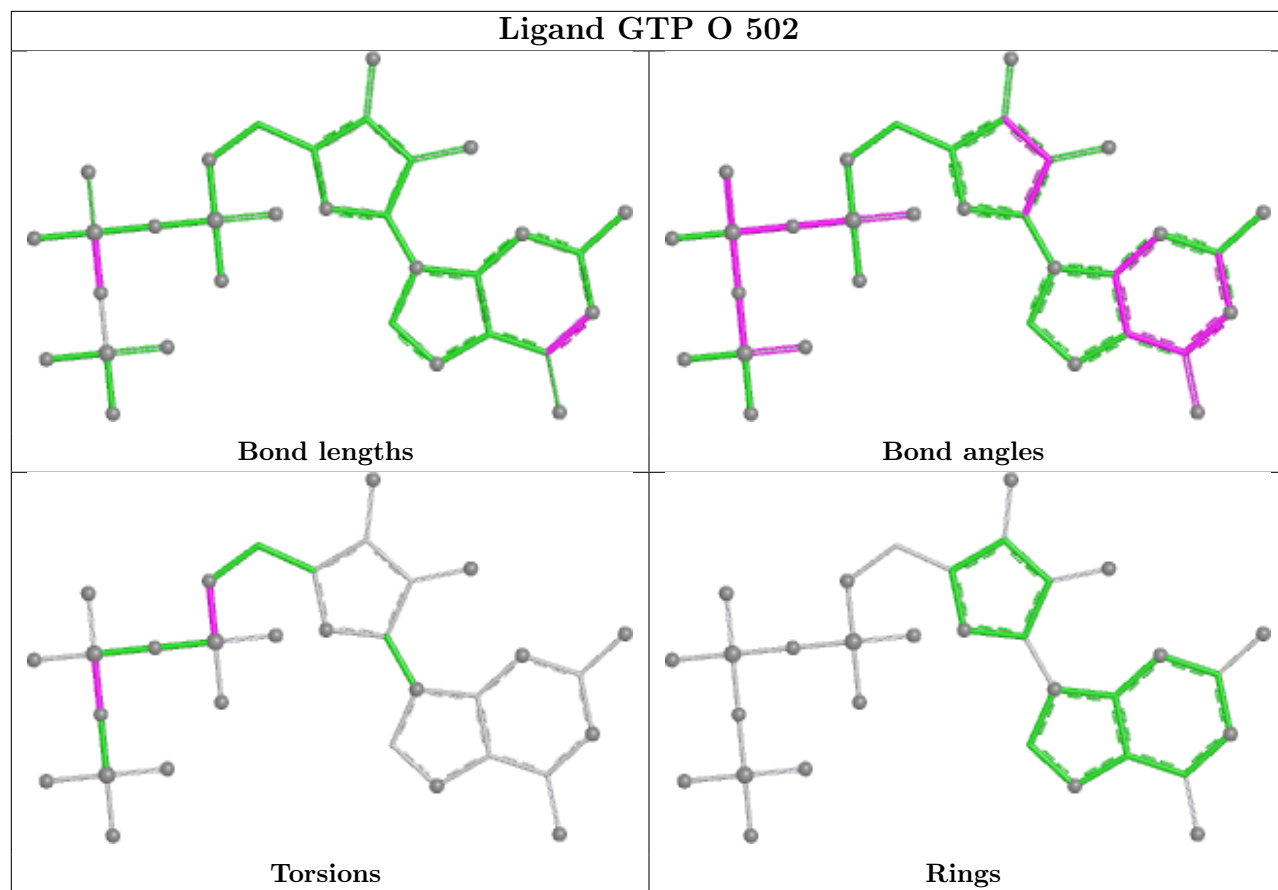


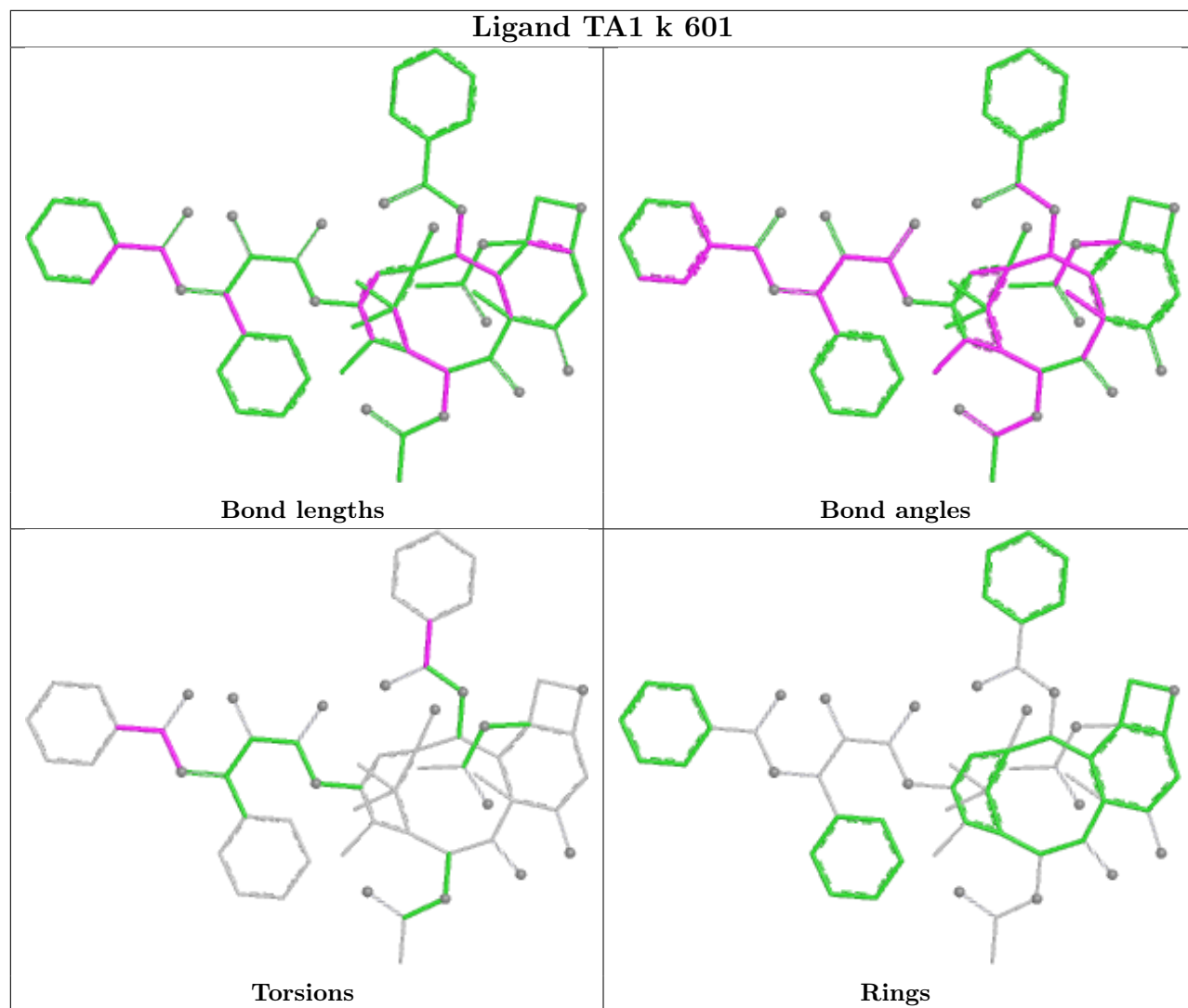




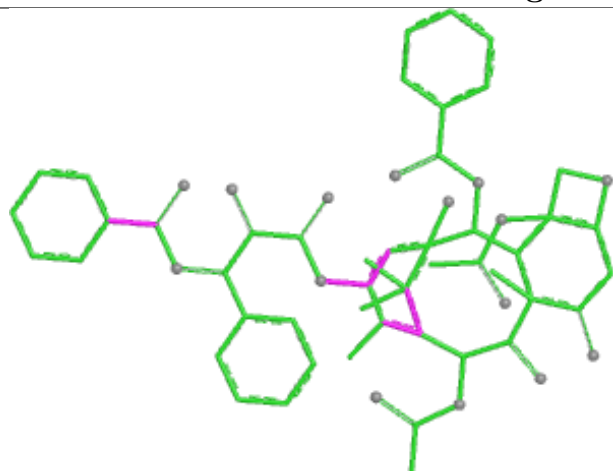




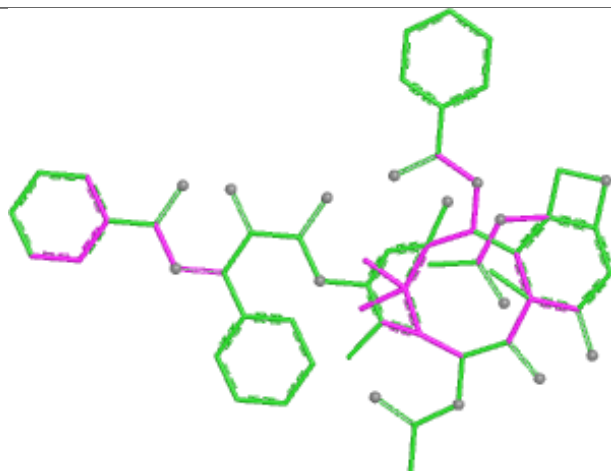




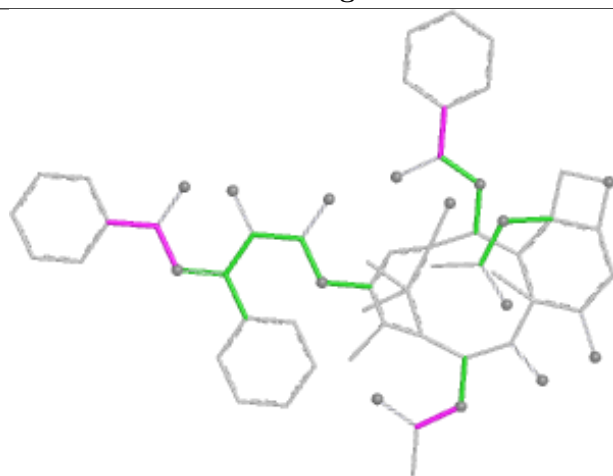
Ligand TA1 i 601



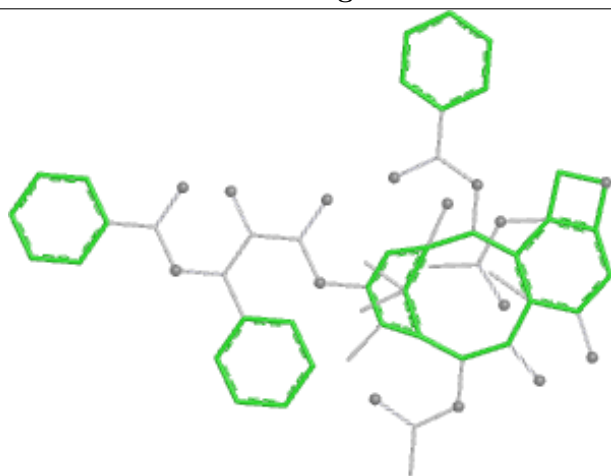
Bond lengths



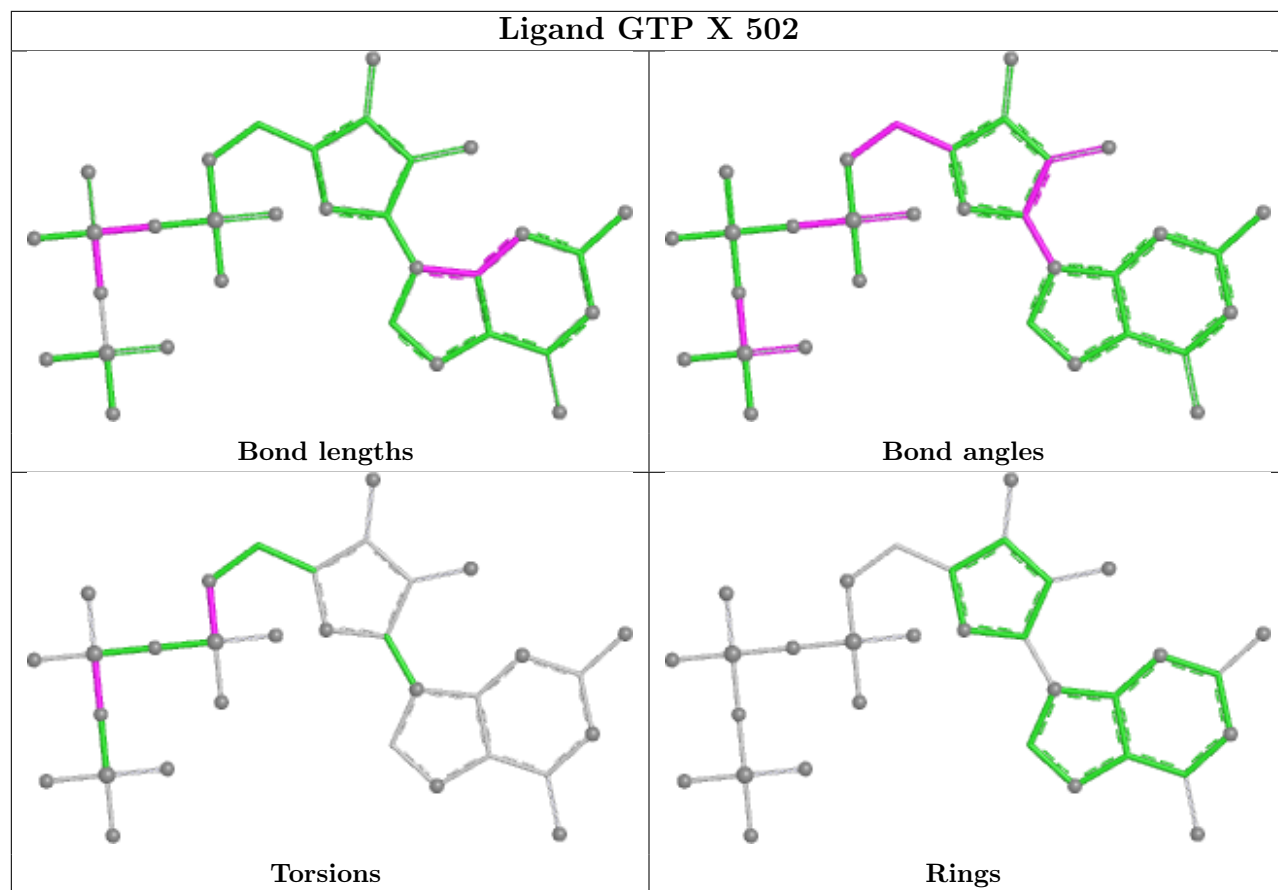
Bond angles

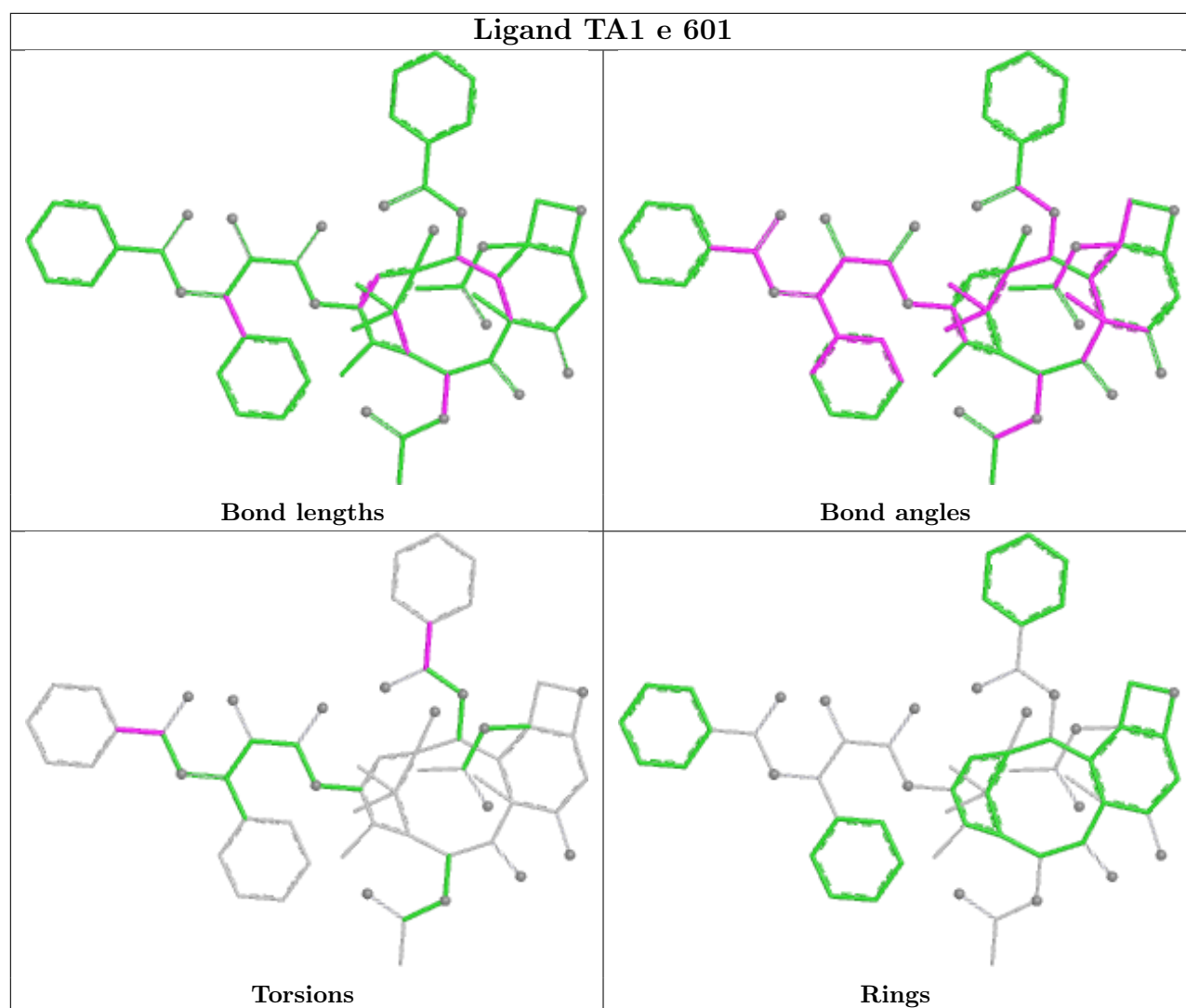


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	R	1
1	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	43:GLY	C	44:GLY	N	1.98
1	e	294:PHE	C	295:ASP	N	1.83

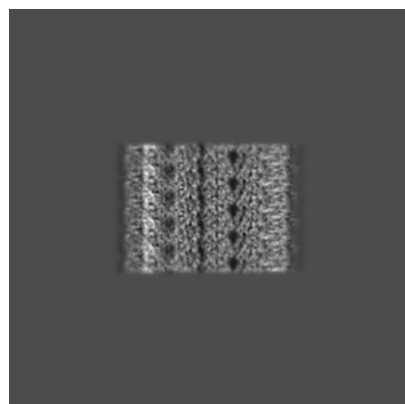
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16435. These allow visual inspection of the internal detail of the map and identification of artifacts.

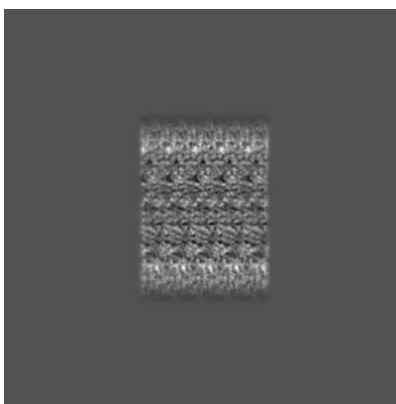
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

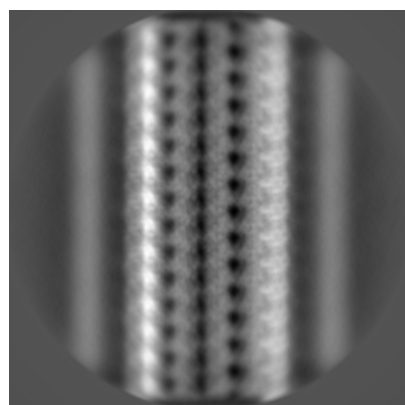


Y

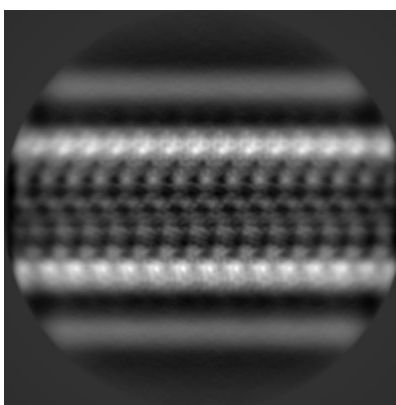


Z

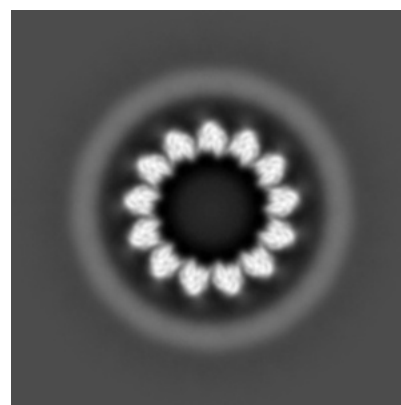
6.1.2 Raw map



X



Y

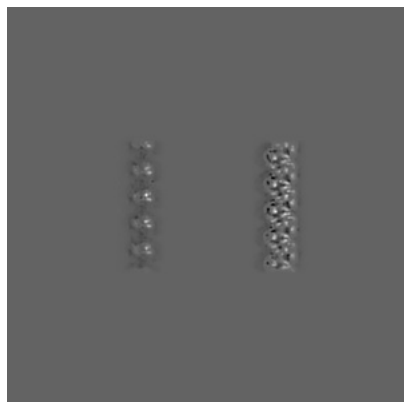


Z

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

6.2 Central slices [i](#)

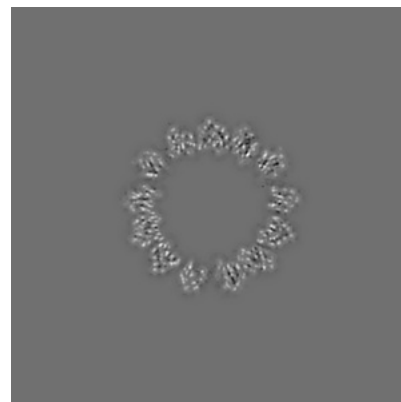
6.2.1 Primary map



X Index: 160

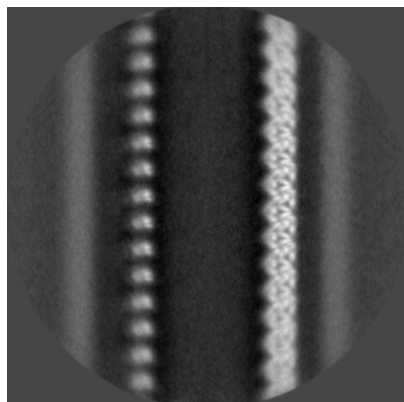


Y Index: 160

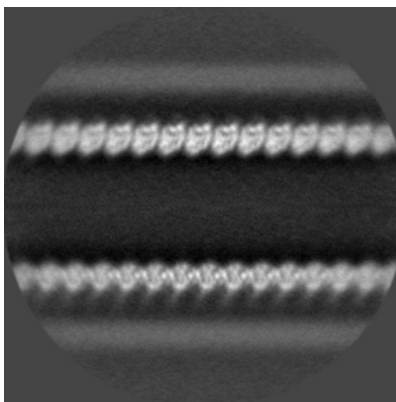


Z Index: 160

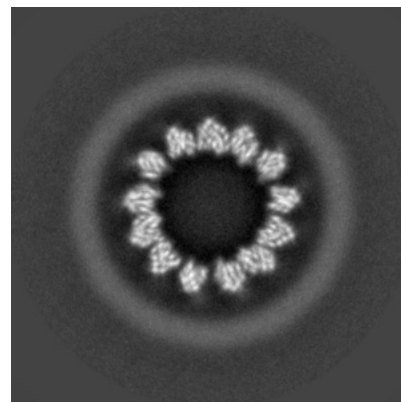
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 111

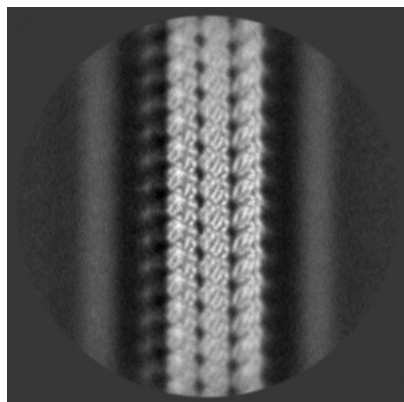


Y Index: 109

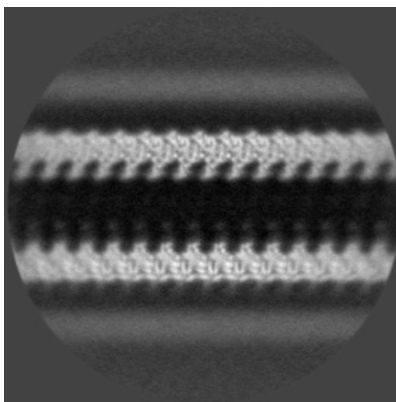


Z Index: 159

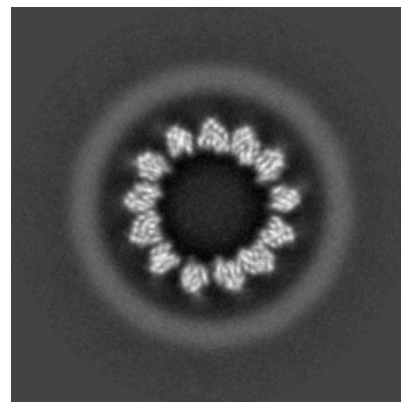
6.3.2 Raw map



X Index: 213



Y Index: 196

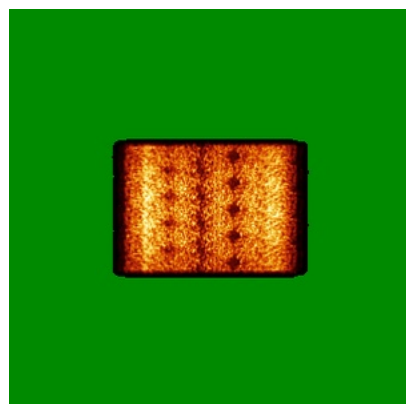


Z Index: 141

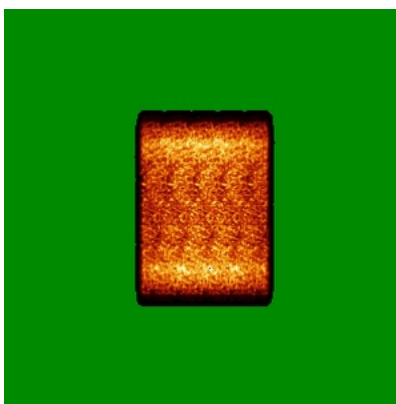
The images above show the largest variance slices of the map in three orthogonal directions.

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

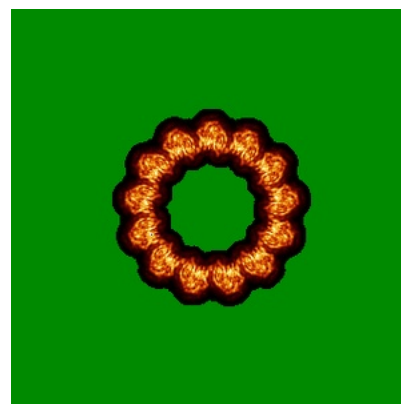
6.4.1 Primary map



X

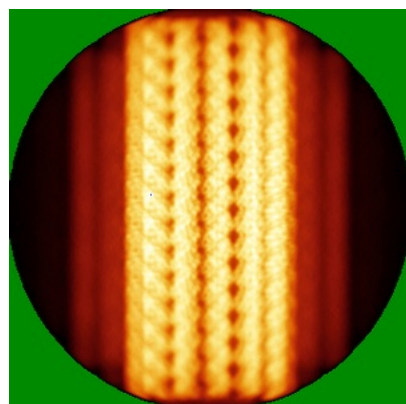


Y

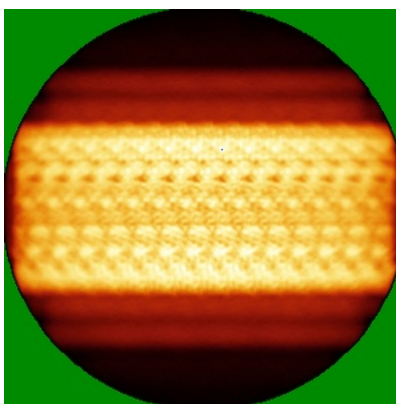


Z

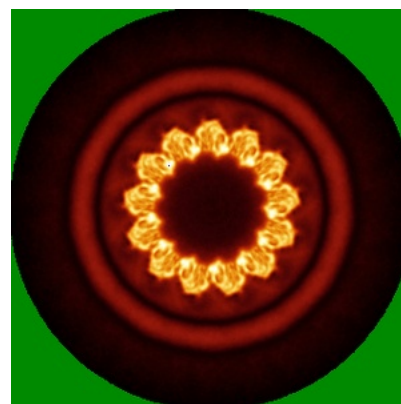
6.4.2 Raw map



X



Y

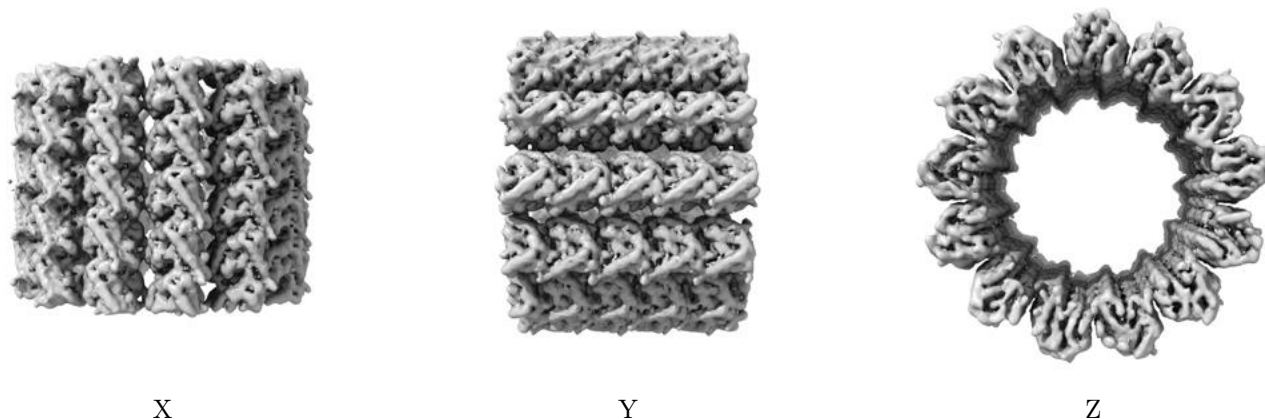


Z

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

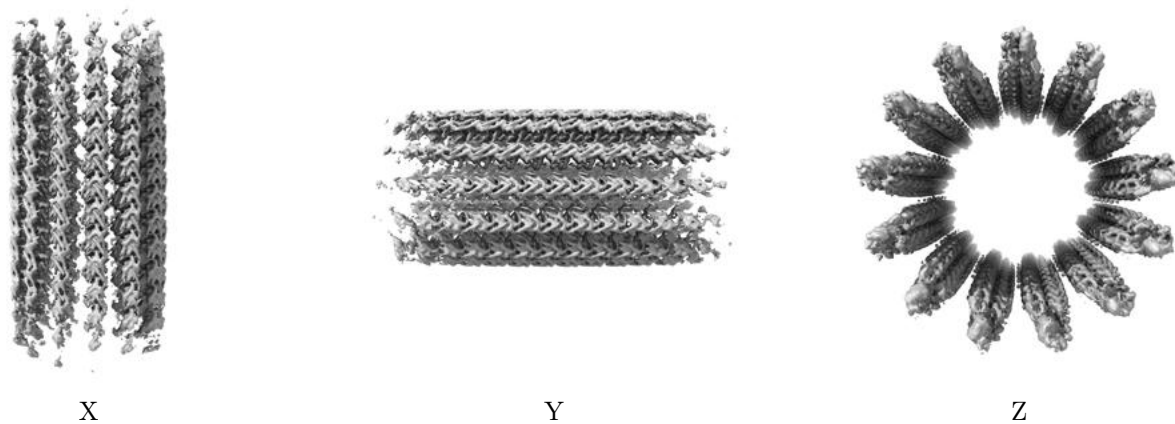
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

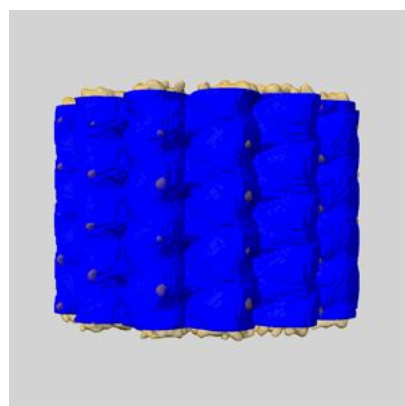
6.6 Mask visualisation [i](#)

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

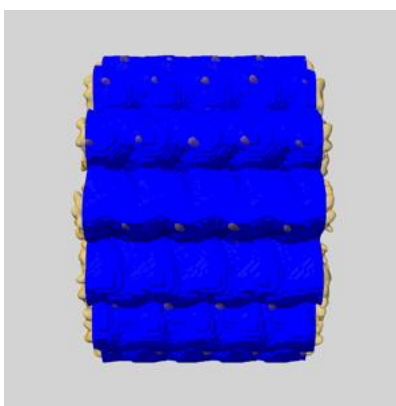
A mask typically either:

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

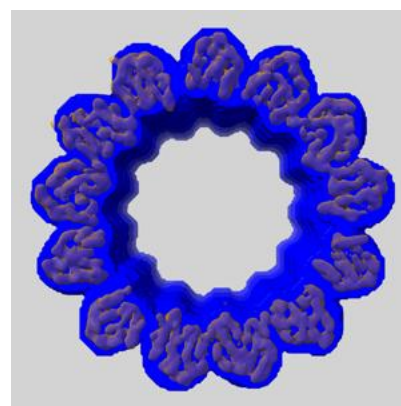
6.6.1 emd_16435_msk_1.map [i](#)



X



Y

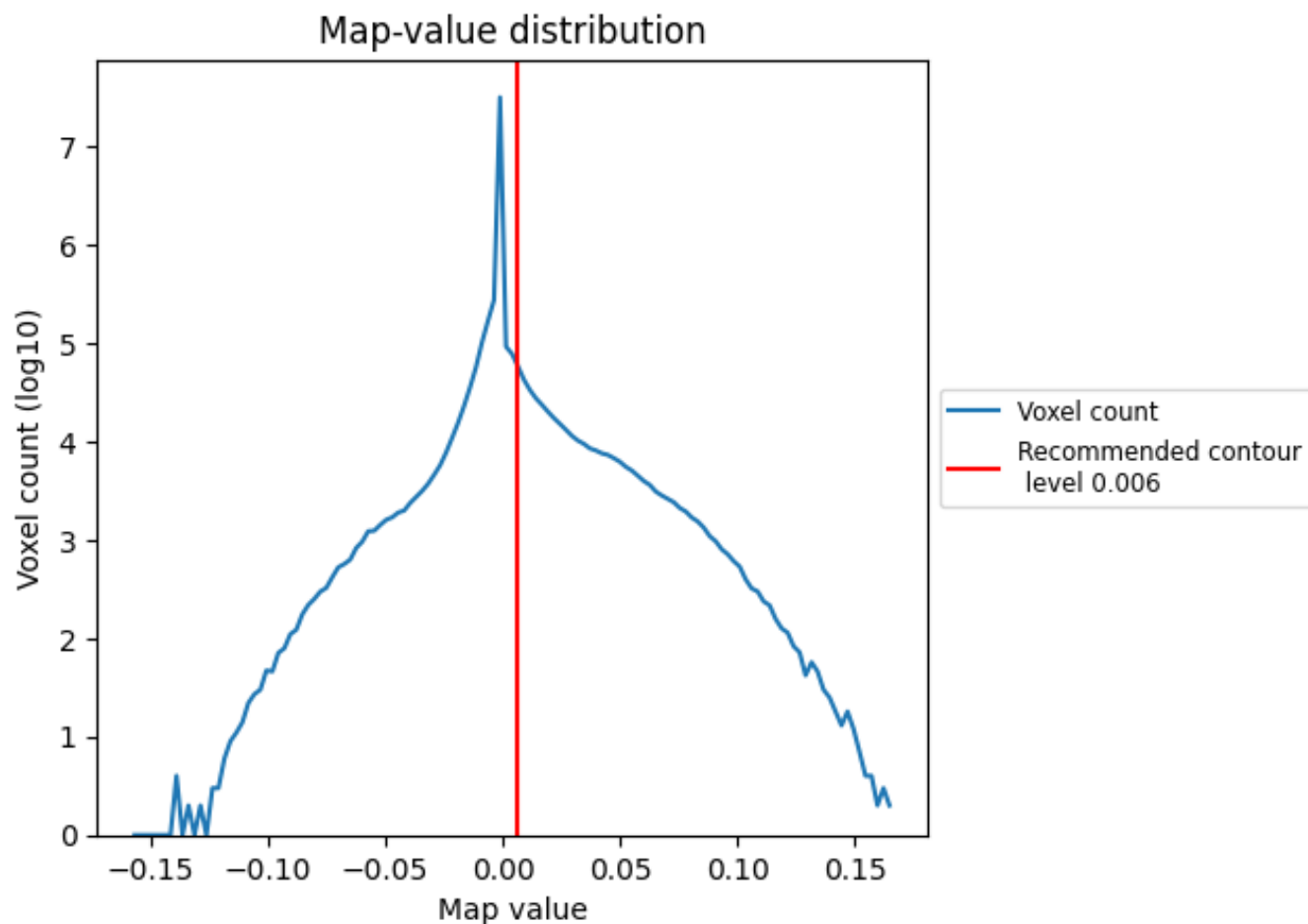


Z

7 Map analysis [i](#)

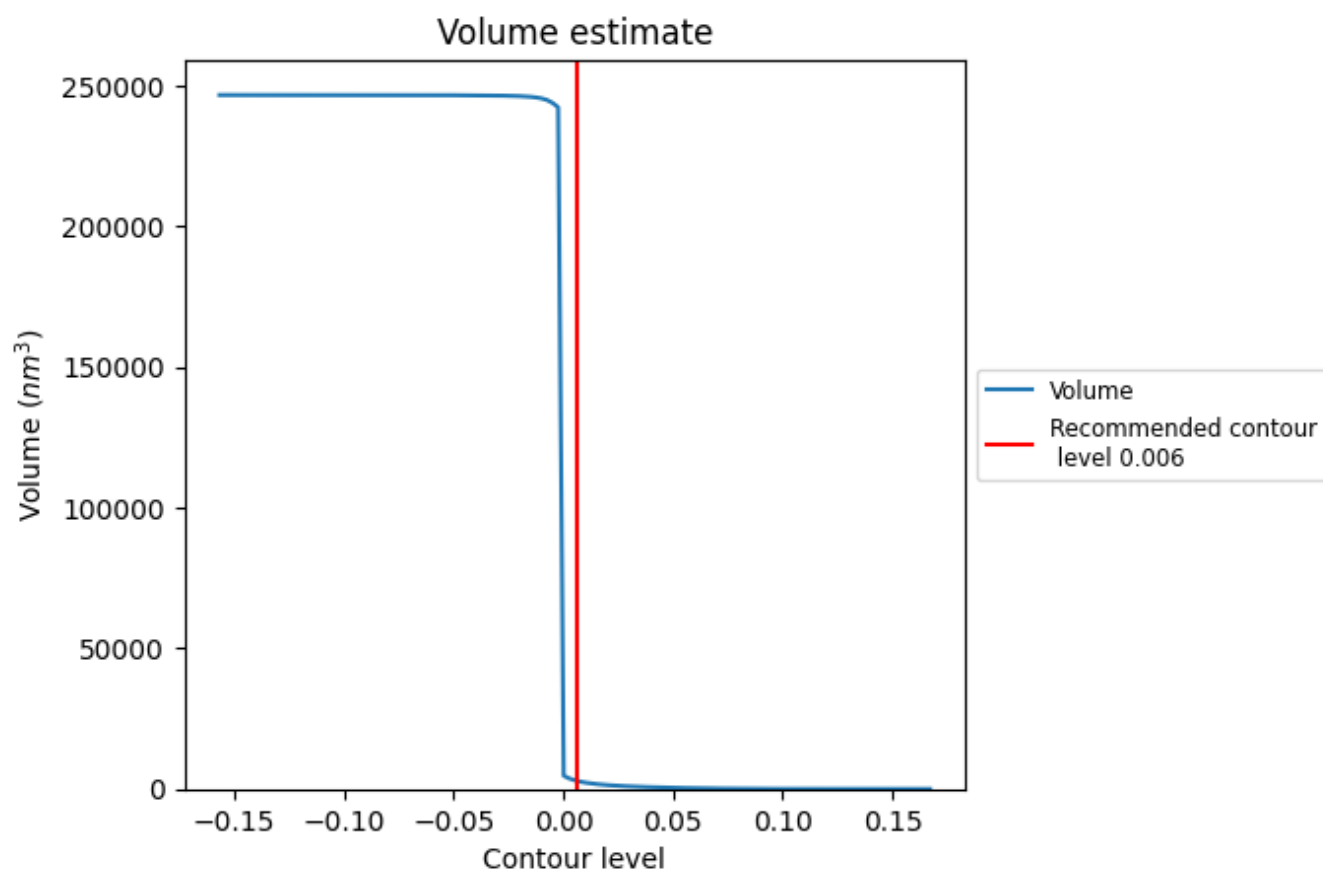
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

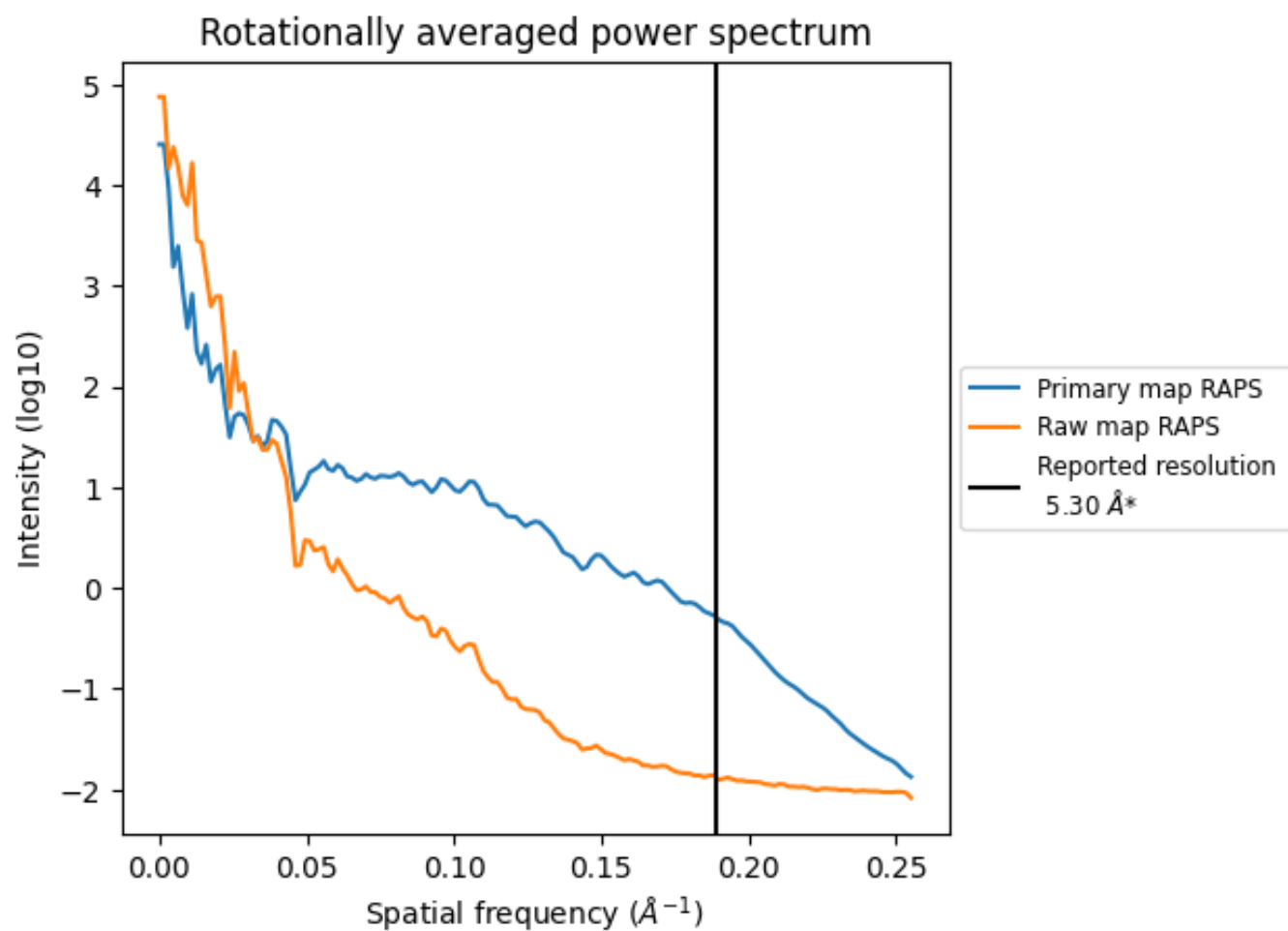
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2953 nm^3 ; this corresponds to an approximate mass of 2668 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](#)

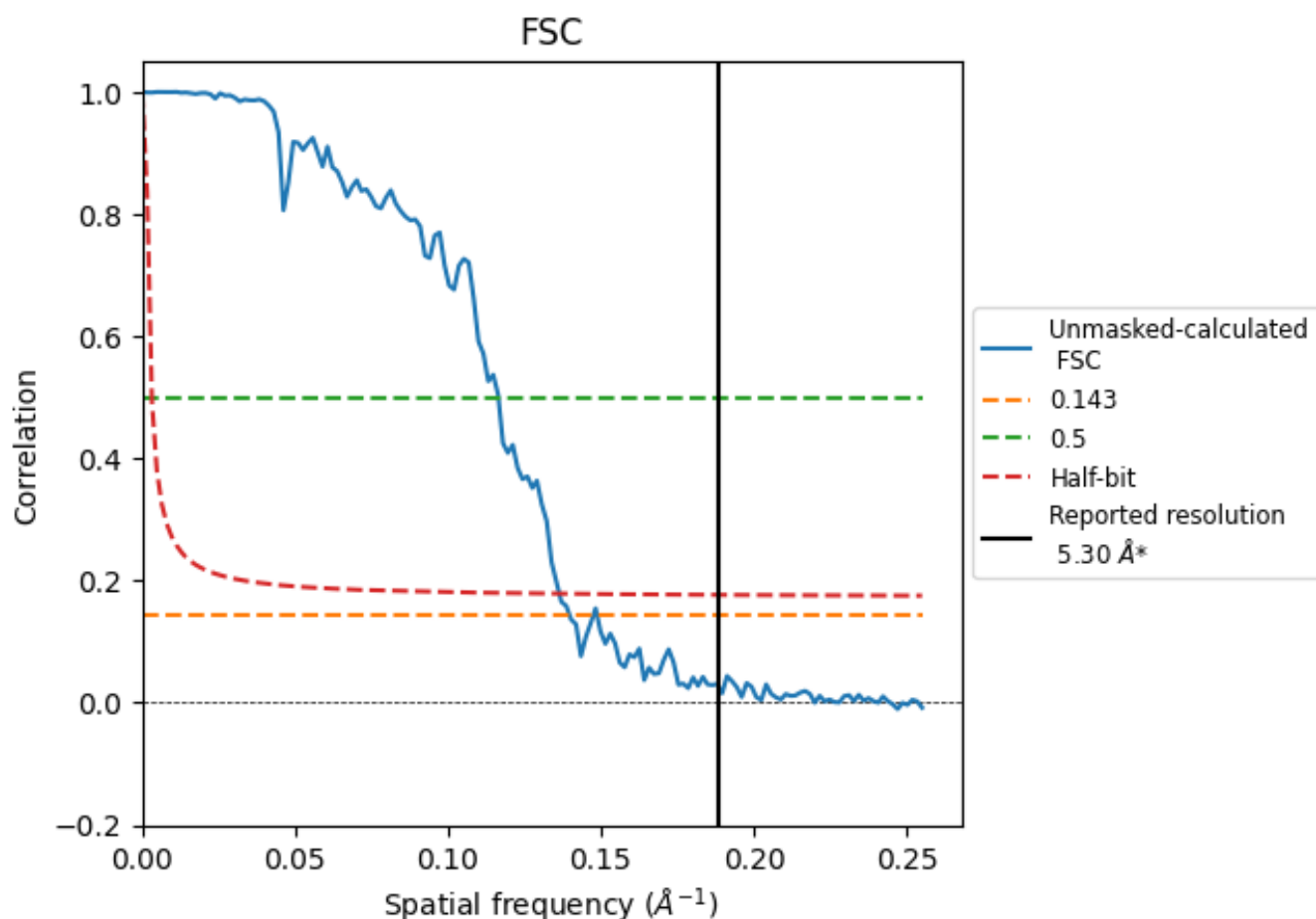


*Reported resolution corresponds to spatial frequency of 0.189 Å⁻¹

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 0.189 Å⁻¹

8.2 Resolution estimates [i](#)

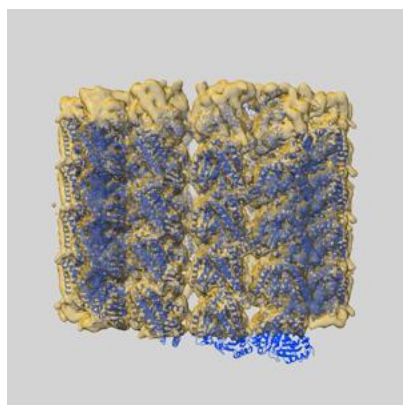
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.15	8.58	7.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.15 differs from the reported value 5.3 by more than 10 %

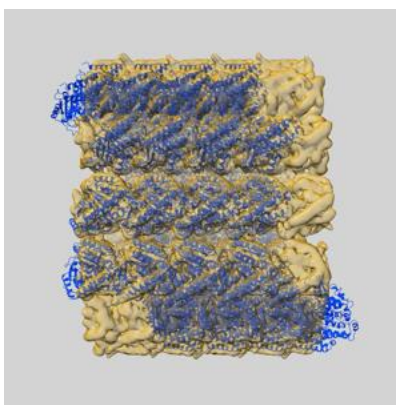
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16435 and PDB model 8C5C. Per-residue inclusion information can be found in section [3](#) on page [13](#).

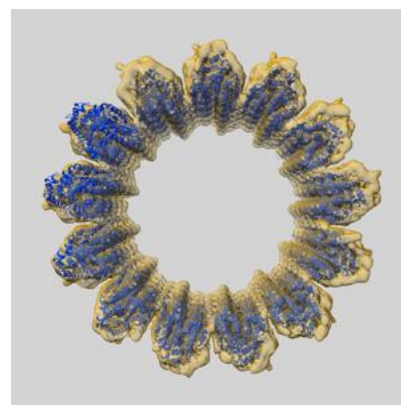
9.1 Map-model overlay [i](#)



X



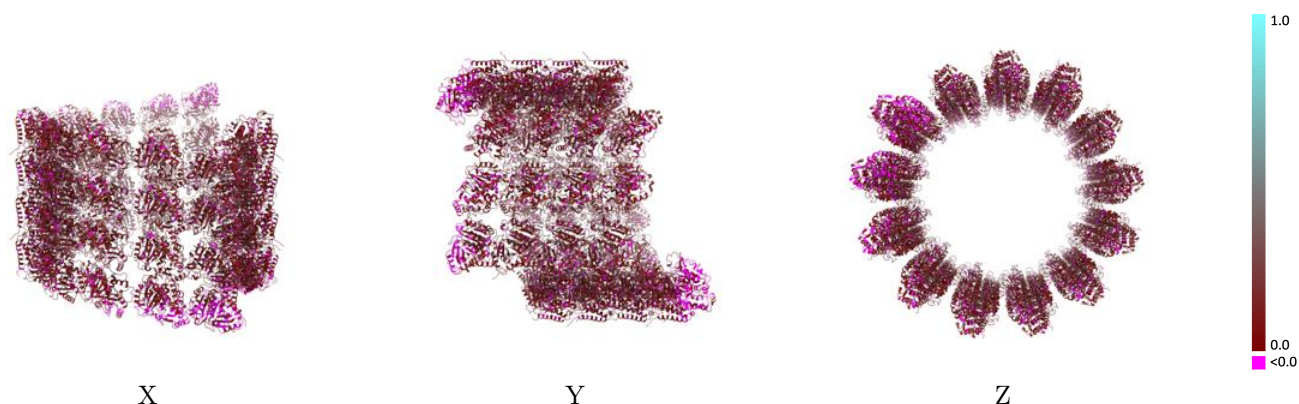
Y



Z

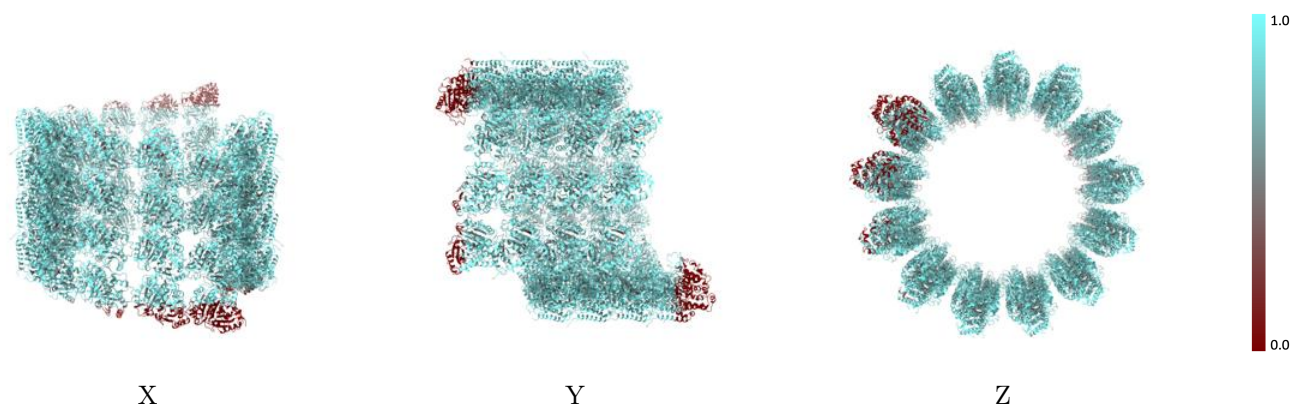
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



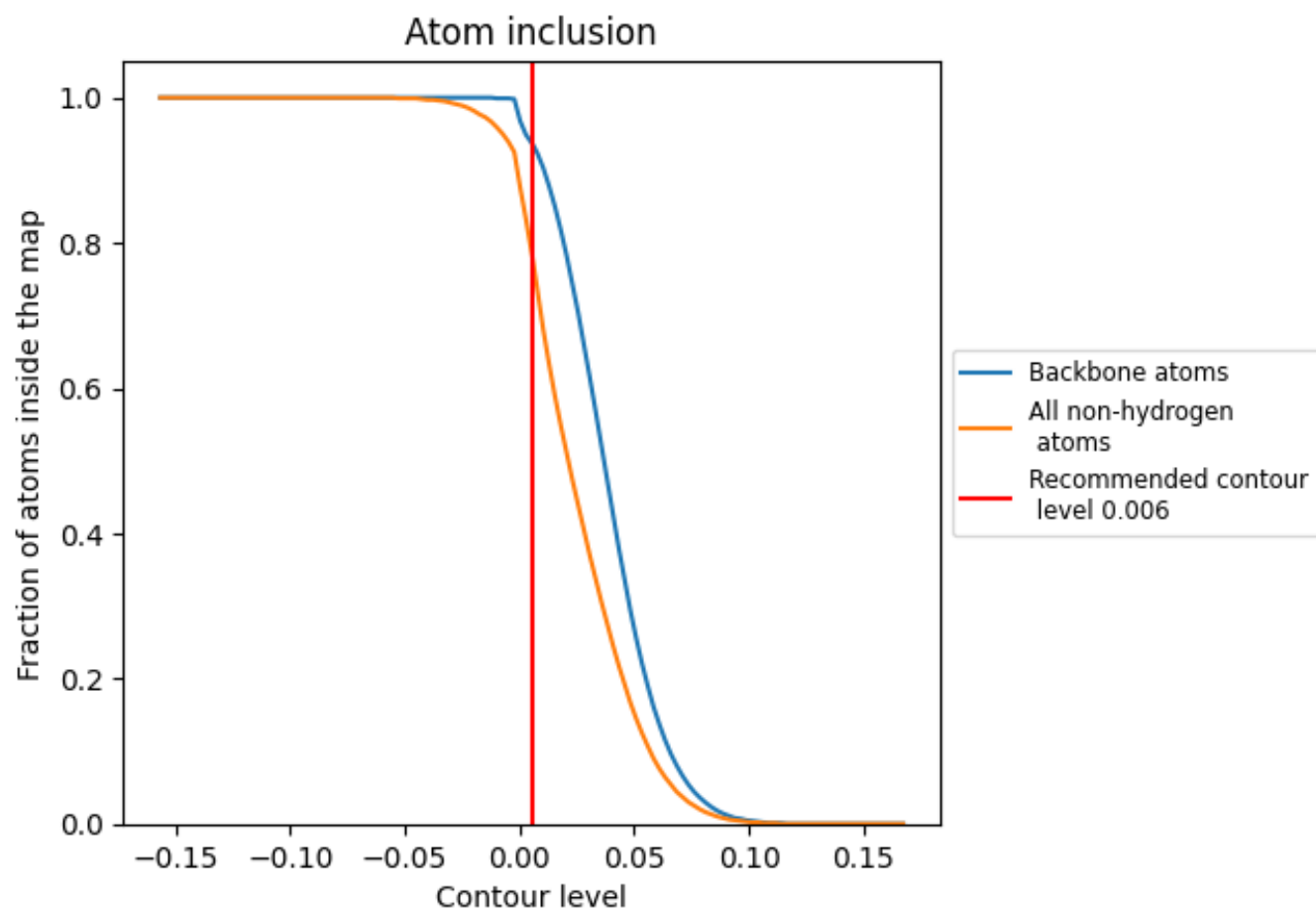
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 77% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.1530
A	 0.5240	 0.0860
B	 0.3220	 0.0470
C	 0.8080	 0.1670
D	 0.8120	 0.1620
E	 0.8100	 0.1620
F	 0.8060	 0.1670
G	 0.8140	 0.1680
H	 0.8040	 0.1630
I	 0.8090	 0.1650
J	 0.8070	 0.1640
K	 0.8030	 0.1550
L	 0.7950	 0.1470
M	 0.7050	 0.1290
N	 0.8170	 0.1740
O	 0.8160	 0.1730
P	 0.8100	 0.1600
Q	 0.8140	 0.1630
R	 0.8090	 0.1650
S	 0.8120	 0.1610
T	 0.8120	 0.1650
U	 0.8150	 0.1680
V	 0.8110	 0.1690
W	 0.8130	 0.1680
X	 0.8150	 0.1710
Y	 0.8130	 0.1730
Z	 0.8240	 0.1750
a	 0.8180	 0.1650
b	 0.8080	 0.1580
c	 0.8120	 0.1690
d	 0.8080	 0.1700
e	 0.8030	 0.1680
f	 0.8150	 0.1720
g	 0.8170	 0.1720
h	 0.8130	 0.1750



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Chain	Atom inclusion	Q-score
i	 0.8090	 0.1700
j	 0.8140	 0.1740
k	 0.8150	 0.1740
l	 0.8110	 0.1700
m	 0.8200	 0.1750
n	 0.8130	 0.1670
o	 0.8020	 0.1670
p	 0.5880	 0.0790
q	 0.7550	 0.1220
r	 0.8070	 0.1470
s	 0.3060	 0.0360
t	 0.5120	 0.0650
u	 0.7100	 0.1120
v	 0.8010	 0.1460
w	 0.8170	 0.1540
x	 0.8090	 0.1590
y	 0.8090	 0.1630
z	 0.8010	 0.1680