



## wwPDB EM Validation Summary Report ⓘ

Sep 26, 2023 – 12:58 pm BST

PDB ID : 7QUP  
EMDB ID : EMD-14150  
Title : D. melanogaster 13-protofilament microtubule  
Authors : Wagstaff, J.; Planelles-Herrero, V.J.; Derivery, E.; Lowe, J.  
Deposited on : 2022-01-18  
Resolution : 3.80 Å (reported)  
Based on initial model : 3J1T

This is a wwPDB EM Validation Summary 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:

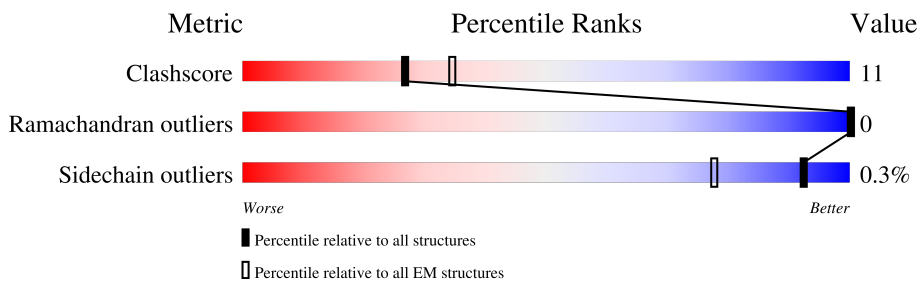
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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.



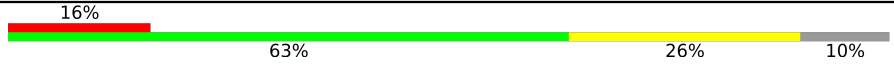
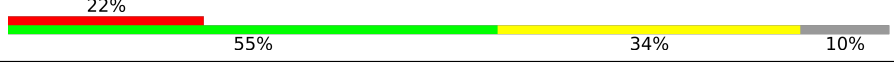
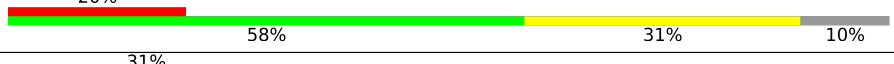


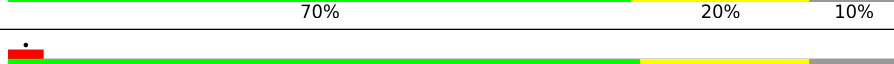
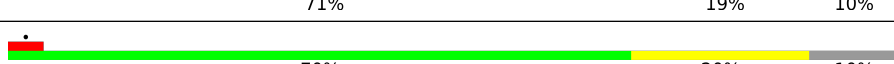
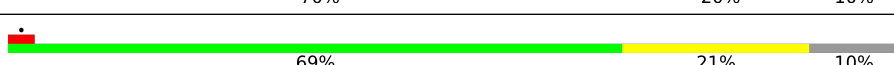
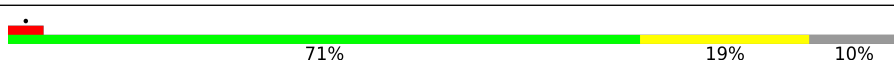


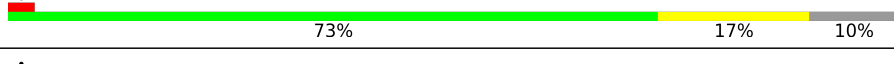
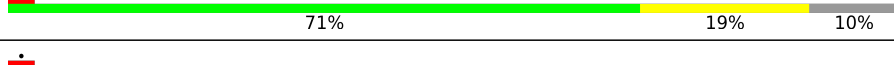

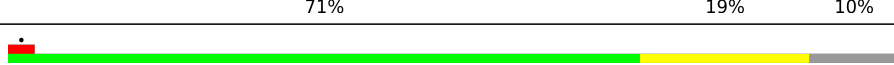










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	10A	475	
1	10C	475	
1	10E	475	
1	11A	475	
1	11C	475	
1	11E	475	
1	12A	475	
1	12C	475	







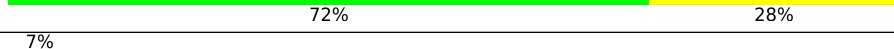
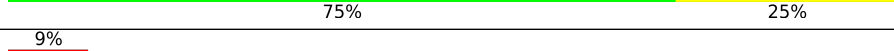
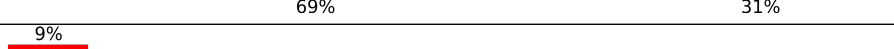
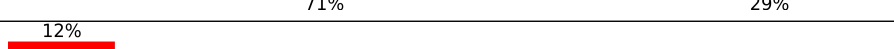
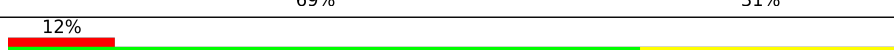

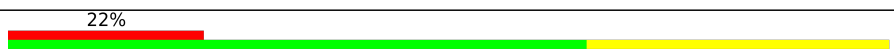

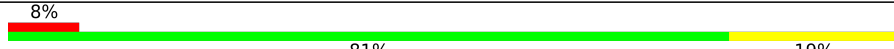





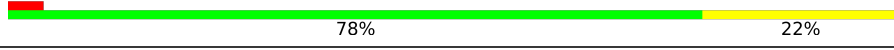
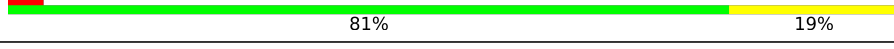



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Mol	Chain	Length	Quality of chain
1	12E	475	
1	13A	475	
1	13C	475	
1	13E	475	
1	1A	475	
1	1C	475	
1	1E	475	
1	2A	475	
1	2C	475	
1	2E	475	
1	3A	475	
1	3C	475	
1	3E	475	
1	4A	475	
1	4C	475	
1	4E	475	
1	5A	475	
1	5C	475	
1	5E	475	
1	6A	475	
1	6C	475	
1	6E	475	
1	7A	475	
1	7C	475	
1	7E	475	




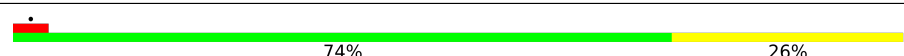
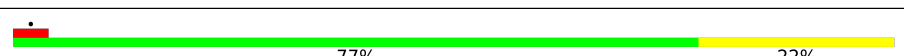
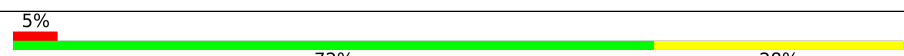
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Mol	Chain	Length	Quality of chain
1	8A	475	 66% 23% 10%
1	8C	475	 67% 23% 10%
1	8E	475	 63% 26% 10%
1	9A	475	 66% 24% 10%
1	9C	475	 65% 25% 10%
1	9E	475	 67% 22% 10%
2	10B	425	 6% 72% 28%
2	10D	425	 7% 75% 25%
2	11B	425	 9% 69% 31%
2	11D	425	 9% 71% 29%
2	12B	425	 12% 69% 31%
2	12D	425	 12% 71% 29%
2	13B	425	 21% 63% 36%
2	13D	425	 22% 65% 34%
2	1B	425	 8% 77% 23%
2	1D	425	 8% 81% 19%
2	2B	425	 6% 82% 18%
2	2D	425	 6% 79% 21%
2	3B	425	 5% 80% 20%
2	3D	425	 5% 76% 24%
2	4B	425	 5% 79% 21%
2	4D	425	 5% 78% 22%
2	5B	425	 5% 81% 19%
2	5D	425	 5% 80% 20%
2	6B	425	 5% 75% 24%

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Mol	Chain	Length	Quality of chain
2	6D	425	 76% 24%
2	7B	425	 77% 23%
2	7D	425	 75% 25%
2	8B	425	 74% 26%
2	8D	425	 73% 26%
2	9B	425	 77% 22%
2	9D	425	 72% 28%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 219271 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-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	10A	426	3342	2121	569	631	21	0	0
1	10C	426	3342	2121	569	631	21	0	0
1	10E	426	3342	2121	569	631	21	0	0
1	11A	426	3342	2121	569	631	21	0	0
1	11C	426	3342	2121	569	631	21	0	0
1	11E	426	3342	2121	569	631	21	0	0
1	12A	426	3342	2121	569	631	21	0	0
1	12C	426	3342	2121	569	631	21	0	0
1	12E	426	3342	2121	569	631	21	0	0
1	13A	426	3342	2121	569	631	21	0	0
1	13C	426	3342	2121	569	631	21	0	0
1	13E	426	3342	2121	569	631	21	0	0
1	1A	426	3342	2121	569	631	21	0	0
1	1C	426	3342	2121	569	631	21	0	0
1	1E	426	3342	2121	569	631	21	0	0
1	2A	426	3342	2121	569	631	21	0	0
1	2C	426	3342	2121	569	631	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2E	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	3A	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	3C	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	3E	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	4A	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	4C	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	4E	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	5A	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	5C	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	5E	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	6A	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	6C	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	6E	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	7A	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	7C	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	7E	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	8A	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	8C	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	8E	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	9A	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		
1	9C	426	Total	C	N	O	S	0	0
			3342	2121	569	631	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	9E	426	3342	2121	569	631	21	0	0

There are 1521 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
10A	-24	MET	-	initiating methionine	UNP P06603
10A	-23	HIS	-	expression tag	UNP P06603
10A	-22	HIS	-	expression tag	UNP P06603
10A	-21	HIS	-	expression tag	UNP P06603
10A	-20	HIS	-	expression tag	UNP P06603
10A	-19	HIS	-	expression tag	UNP P06603
10A	-18	HIS	-	expression tag	UNP P06603
10A	-17	GLU	-	expression tag	UNP P06603
10A	-16	ASP	-	expression tag	UNP P06603
10A	-15	GLN	-	expression tag	UNP P06603
10A	-14	VAL	-	expression tag	UNP P06603
10A	-13	ASP	-	expression tag	UNP P06603
10A	-12	PRO	-	expression tag	UNP P06603
10A	-11	ARG	-	expression tag	UNP P06603
10A	-10	LEU	-	expression tag	UNP P06603
10A	-9	ILE	-	expression tag	UNP P06603
10A	-8	ASP	-	expression tag	UNP P06603
10A	-7	GLY	-	expression tag	UNP P06603
10A	-6	LYS	-	expression tag	UNP P06603
10A	-5	GLY	-	expression tag	UNP P06603
10A	-4	GLY	-	expression tag	UNP P06603
10A	-3	GLY	-	expression tag	UNP P06603
10A	-2	GLY	-	expression tag	UNP P06603
10A	-1	ARG	-	expression tag	UNP P06603
10A	0	PRO	-	expression tag	UNP P06603
10A	437	MET	-	expression tag	UNP P06603
10A	438	ASP	-	expression tag	UNP P06603
10A	439	SER	-	expression tag	UNP P06603
10A	440	GLY	-	expression tag	UNP P06603
10A	441	ASP	-	expression tag	UNP P06603
10A	442	GLY	-	expression tag	UNP P06603
10A	443	GLU	-	expression tag	UNP P06603
10A	444	GLY	-	expression tag	UNP P06603
10A	445	GLU	-	expression tag	UNP P06603
10A	446	GLY	-	expression tag	UNP P06603
10A	447	ALA	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
10A	448	GLU	-	expression tag	UNP P06603
10A	449	GLU	-	expression tag	UNP P06603
10A	450	TYR	-	expression tag	UNP P06603
10C	-24	MET	-	initiating methionine	UNP P06603
10C	-23	HIS	-	expression tag	UNP P06603
10C	-22	HIS	-	expression tag	UNP P06603
10C	-21	HIS	-	expression tag	UNP P06603
10C	-20	HIS	-	expression tag	UNP P06603
10C	-19	HIS	-	expression tag	UNP P06603
10C	-18	HIS	-	expression tag	UNP P06603
10C	-17	GLU	-	expression tag	UNP P06603
10C	-16	ASP	-	expression tag	UNP P06603
10C	-15	GLN	-	expression tag	UNP P06603
10C	-14	VAL	-	expression tag	UNP P06603
10C	-13	ASP	-	expression tag	UNP P06603
10C	-12	PRO	-	expression tag	UNP P06603
10C	-11	ARG	-	expression tag	UNP P06603
10C	-10	LEU	-	expression tag	UNP P06603
10C	-9	ILE	-	expression tag	UNP P06603
10C	-8	ASP	-	expression tag	UNP P06603
10C	-7	GLY	-	expression tag	UNP P06603
10C	-6	LYS	-	expression tag	UNP P06603
10C	-5	GLY	-	expression tag	UNP P06603
10C	-4	GLY	-	expression tag	UNP P06603
10C	-3	GLY	-	expression tag	UNP P06603
10C	-2	GLY	-	expression tag	UNP P06603
10C	-1	ARG	-	expression tag	UNP P06603
10C	0	PRO	-	expression tag	UNP P06603
10C	437	MET	-	expression tag	UNP P06603
10C	438	ASP	-	expression tag	UNP P06603
10C	439	SER	-	expression tag	UNP P06603
10C	440	GLY	-	expression tag	UNP P06603
10C	441	ASP	-	expression tag	UNP P06603
10C	442	GLY	-	expression tag	UNP P06603
10C	443	GLU	-	expression tag	UNP P06603
10C	444	GLY	-	expression tag	UNP P06603
10C	445	GLU	-	expression tag	UNP P06603
10C	446	GLY	-	expression tag	UNP P06603
10C	447	ALA	-	expression tag	UNP P06603
10C	448	GLU	-	expression tag	UNP P06603
10C	449	GLU	-	expression tag	UNP P06603
10C	450	TYR	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
10E	-24	MET	-	initiating methionine	UNP P06603
10E	-23	HIS	-	expression tag	UNP P06603
10E	-22	HIS	-	expression tag	UNP P06603
10E	-21	HIS	-	expression tag	UNP P06603
10E	-20	HIS	-	expression tag	UNP P06603
10E	-19	HIS	-	expression tag	UNP P06603
10E	-18	HIS	-	expression tag	UNP P06603
10E	-17	GLU	-	expression tag	UNP P06603
10E	-16	ASP	-	expression tag	UNP P06603
10E	-15	GLN	-	expression tag	UNP P06603
10E	-14	VAL	-	expression tag	UNP P06603
10E	-13	ASP	-	expression tag	UNP P06603
10E	-12	PRO	-	expression tag	UNP P06603
10E	-11	ARG	-	expression tag	UNP P06603
10E	-10	LEU	-	expression tag	UNP P06603
10E	-9	ILE	-	expression tag	UNP P06603
10E	-8	ASP	-	expression tag	UNP P06603
10E	-7	GLY	-	expression tag	UNP P06603
10E	-6	LYS	-	expression tag	UNP P06603
10E	-5	GLY	-	expression tag	UNP P06603
10E	-4	GLY	-	expression tag	UNP P06603
10E	-3	GLY	-	expression tag	UNP P06603
10E	-2	GLY	-	expression tag	UNP P06603
10E	-1	ARG	-	expression tag	UNP P06603
10E	0	PRO	-	expression tag	UNP P06603
10E	437	MET	-	expression tag	UNP P06603
10E	438	ASP	-	expression tag	UNP P06603
10E	439	SER	-	expression tag	UNP P06603
10E	440	GLY	-	expression tag	UNP P06603
10E	441	ASP	-	expression tag	UNP P06603
10E	442	GLY	-	expression tag	UNP P06603
10E	443	GLU	-	expression tag	UNP P06603
10E	444	GLY	-	expression tag	UNP P06603
10E	445	GLU	-	expression tag	UNP P06603
10E	446	GLY	-	expression tag	UNP P06603
10E	447	ALA	-	expression tag	UNP P06603
10E	448	GLU	-	expression tag	UNP P06603
10E	449	GLU	-	expression tag	UNP P06603
10E	450	TYR	-	expression tag	UNP P06603
11A	-24	MET	-	initiating methionine	UNP P06603
11A	-23	HIS	-	expression tag	UNP P06603
11A	-22	HIS	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
11A	-21	HIS	-	expression tag	UNP P06603
11A	-20	HIS	-	expression tag	UNP P06603
11A	-19	HIS	-	expression tag	UNP P06603
11A	-18	HIS	-	expression tag	UNP P06603
11A	-17	GLU	-	expression tag	UNP P06603
11A	-16	ASP	-	expression tag	UNP P06603
11A	-15	GLN	-	expression tag	UNP P06603
11A	-14	VAL	-	expression tag	UNP P06603
11A	-13	ASP	-	expression tag	UNP P06603
11A	-12	PRO	-	expression tag	UNP P06603
11A	-11	ARG	-	expression tag	UNP P06603
11A	-10	LEU	-	expression tag	UNP P06603
11A	-9	ILE	-	expression tag	UNP P06603
11A	-8	ASP	-	expression tag	UNP P06603
11A	-7	GLY	-	expression tag	UNP P06603
11A	-6	LYS	-	expression tag	UNP P06603
11A	-5	GLY	-	expression tag	UNP P06603
11A	-4	GLY	-	expression tag	UNP P06603
11A	-3	GLY	-	expression tag	UNP P06603
11A	-2	GLY	-	expression tag	UNP P06603
11A	-1	ARG	-	expression tag	UNP P06603
11A	0	PRO	-	expression tag	UNP P06603
11A	437	MET	-	expression tag	UNP P06603
11A	438	ASP	-	expression tag	UNP P06603
11A	439	SER	-	expression tag	UNP P06603
11A	440	GLY	-	expression tag	UNP P06603
11A	441	ASP	-	expression tag	UNP P06603
11A	442	GLY	-	expression tag	UNP P06603
11A	443	GLU	-	expression tag	UNP P06603
11A	444	GLY	-	expression tag	UNP P06603
11A	445	GLU	-	expression tag	UNP P06603
11A	446	GLY	-	expression tag	UNP P06603
11A	447	ALA	-	expression tag	UNP P06603
11A	448	GLU	-	expression tag	UNP P06603
11A	449	GLU	-	expression tag	UNP P06603
11A	450	TYR	-	expression tag	UNP P06603
11C	-24	MET	-	initiating methionine	UNP P06603
11C	-23	HIS	-	expression tag	UNP P06603
11C	-22	HIS	-	expression tag	UNP P06603
11C	-21	HIS	-	expression tag	UNP P06603
11C	-20	HIS	-	expression tag	UNP P06603
11C	-19	HIS	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
11C	-18	HIS	-	expression tag	UNP P06603
11C	-17	GLU	-	expression tag	UNP P06603
11C	-16	ASP	-	expression tag	UNP P06603
11C	-15	GLN	-	expression tag	UNP P06603
11C	-14	VAL	-	expression tag	UNP P06603
11C	-13	ASP	-	expression tag	UNP P06603
11C	-12	PRO	-	expression tag	UNP P06603
11C	-11	ARG	-	expression tag	UNP P06603
11C	-10	LEU	-	expression tag	UNP P06603
11C	-9	ILE	-	expression tag	UNP P06603
11C	-8	ASP	-	expression tag	UNP P06603
11C	-7	GLY	-	expression tag	UNP P06603
11C	-6	LYS	-	expression tag	UNP P06603
11C	-5	GLY	-	expression tag	UNP P06603
11C	-4	GLY	-	expression tag	UNP P06603
11C	-3	GLY	-	expression tag	UNP P06603
11C	-2	GLY	-	expression tag	UNP P06603
11C	-1	ARG	-	expression tag	UNP P06603
11C	0	PRO	-	expression tag	UNP P06603
11C	437	MET	-	expression tag	UNP P06603
11C	438	ASP	-	expression tag	UNP P06603
11C	439	SER	-	expression tag	UNP P06603
11C	440	GLY	-	expression tag	UNP P06603
11C	441	ASP	-	expression tag	UNP P06603
11C	442	GLY	-	expression tag	UNP P06603
11C	443	GLU	-	expression tag	UNP P06603
11C	444	GLY	-	expression tag	UNP P06603
11C	445	GLU	-	expression tag	UNP P06603
11C	446	GLY	-	expression tag	UNP P06603
11C	447	ALA	-	expression tag	UNP P06603
11C	448	GLU	-	expression tag	UNP P06603
11C	449	GLU	-	expression tag	UNP P06603
11C	450	TYR	-	expression tag	UNP P06603
11E	-24	MET	-	initiating methionine	UNP P06603
11E	-23	HIS	-	expression tag	UNP P06603
11E	-22	HIS	-	expression tag	UNP P06603
11E	-21	HIS	-	expression tag	UNP P06603
11E	-20	HIS	-	expression tag	UNP P06603
11E	-19	HIS	-	expression tag	UNP P06603
11E	-18	HIS	-	expression tag	UNP P06603
11E	-17	GLU	-	expression tag	UNP P06603
11E	-16	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
11E	-15	GLN	-	expression tag	UNP P06603
11E	-14	VAL	-	expression tag	UNP P06603
11E	-13	ASP	-	expression tag	UNP P06603
11E	-12	PRO	-	expression tag	UNP P06603
11E	-11	ARG	-	expression tag	UNP P06603
11E	-10	LEU	-	expression tag	UNP P06603
11E	-9	ILE	-	expression tag	UNP P06603
11E	-8	ASP	-	expression tag	UNP P06603
11E	-7	GLY	-	expression tag	UNP P06603
11E	-6	LYS	-	expression tag	UNP P06603
11E	-5	GLY	-	expression tag	UNP P06603
11E	-4	GLY	-	expression tag	UNP P06603
11E	-3	GLY	-	expression tag	UNP P06603
11E	-2	GLY	-	expression tag	UNP P06603
11E	-1	ARG	-	expression tag	UNP P06603
11E	0	PRO	-	expression tag	UNP P06603
11E	437	MET	-	expression tag	UNP P06603
11E	438	ASP	-	expression tag	UNP P06603
11E	439	SER	-	expression tag	UNP P06603
11E	440	GLY	-	expression tag	UNP P06603
11E	441	ASP	-	expression tag	UNP P06603
11E	442	GLY	-	expression tag	UNP P06603
11E	443	GLU	-	expression tag	UNP P06603
11E	444	GLY	-	expression tag	UNP P06603
11E	445	GLU	-	expression tag	UNP P06603
11E	446	GLY	-	expression tag	UNP P06603
11E	447	ALA	-	expression tag	UNP P06603
11E	448	GLU	-	expression tag	UNP P06603
11E	449	GLU	-	expression tag	UNP P06603
11E	450	TYR	-	expression tag	UNP P06603
12A	-24	MET	-	initiating methionine	UNP P06603
12A	-23	HIS	-	expression tag	UNP P06603
12A	-22	HIS	-	expression tag	UNP P06603
12A	-21	HIS	-	expression tag	UNP P06603
12A	-20	HIS	-	expression tag	UNP P06603
12A	-19	HIS	-	expression tag	UNP P06603
12A	-18	HIS	-	expression tag	UNP P06603
12A	-17	GLU	-	expression tag	UNP P06603
12A	-16	ASP	-	expression tag	UNP P06603
12A	-15	GLN	-	expression tag	UNP P06603
12A	-14	VAL	-	expression tag	UNP P06603
12A	-13	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
12A	-12	PRO	-	expression tag	UNP P06603
12A	-11	ARG	-	expression tag	UNP P06603
12A	-10	LEU	-	expression tag	UNP P06603
12A	-9	ILE	-	expression tag	UNP P06603
12A	-8	ASP	-	expression tag	UNP P06603
12A	-7	GLY	-	expression tag	UNP P06603
12A	-6	LYS	-	expression tag	UNP P06603
12A	-5	GLY	-	expression tag	UNP P06603
12A	-4	GLY	-	expression tag	UNP P06603
12A	-3	GLY	-	expression tag	UNP P06603
12A	-2	GLY	-	expression tag	UNP P06603
12A	-1	ARG	-	expression tag	UNP P06603
12A	0	PRO	-	expression tag	UNP P06603
12A	437	MET	-	expression tag	UNP P06603
12A	438	ASP	-	expression tag	UNP P06603
12A	439	SER	-	expression tag	UNP P06603
12A	440	GLY	-	expression tag	UNP P06603
12A	441	ASP	-	expression tag	UNP P06603
12A	442	GLY	-	expression tag	UNP P06603
12A	443	GLU	-	expression tag	UNP P06603
12A	444	GLY	-	expression tag	UNP P06603
12A	445	GLU	-	expression tag	UNP P06603
12A	446	GLY	-	expression tag	UNP P06603
12A	447	ALA	-	expression tag	UNP P06603
12A	448	GLU	-	expression tag	UNP P06603
12A	449	GLU	-	expression tag	UNP P06603
12A	450	TYR	-	expression tag	UNP P06603
12C	-24	MET	-	initiating methionine	UNP P06603
12C	-23	HIS	-	expression tag	UNP P06603
12C	-22	HIS	-	expression tag	UNP P06603
12C	-21	HIS	-	expression tag	UNP P06603
12C	-20	HIS	-	expression tag	UNP P06603
12C	-19	HIS	-	expression tag	UNP P06603
12C	-18	HIS	-	expression tag	UNP P06603
12C	-17	GLU	-	expression tag	UNP P06603
12C	-16	ASP	-	expression tag	UNP P06603
12C	-15	GLN	-	expression tag	UNP P06603
12C	-14	VAL	-	expression tag	UNP P06603
12C	-13	ASP	-	expression tag	UNP P06603
12C	-12	PRO	-	expression tag	UNP P06603
12C	-11	ARG	-	expression tag	UNP P06603
12C	-10	LEU	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
12C	-9	ILE	-	expression tag	UNP P06603
12C	-8	ASP	-	expression tag	UNP P06603
12C	-7	GLY	-	expression tag	UNP P06603
12C	-6	LYS	-	expression tag	UNP P06603
12C	-5	GLY	-	expression tag	UNP P06603
12C	-4	GLY	-	expression tag	UNP P06603
12C	-3	GLY	-	expression tag	UNP P06603
12C	-2	GLY	-	expression tag	UNP P06603
12C	-1	ARG	-	expression tag	UNP P06603
12C	0	PRO	-	expression tag	UNP P06603
12C	437	MET	-	expression tag	UNP P06603
12C	438	ASP	-	expression tag	UNP P06603
12C	439	SER	-	expression tag	UNP P06603
12C	440	GLY	-	expression tag	UNP P06603
12C	441	ASP	-	expression tag	UNP P06603
12C	442	GLY	-	expression tag	UNP P06603
12C	443	GLU	-	expression tag	UNP P06603
12C	444	GLY	-	expression tag	UNP P06603
12C	445	GLU	-	expression tag	UNP P06603
12C	446	GLY	-	expression tag	UNP P06603
12C	447	ALA	-	expression tag	UNP P06603
12C	448	GLU	-	expression tag	UNP P06603
12C	449	GLU	-	expression tag	UNP P06603
12C	450	TYR	-	expression tag	UNP P06603
12E	-24	MET	-	initiating methionine	UNP P06603
12E	-23	HIS	-	expression tag	UNP P06603
12E	-22	HIS	-	expression tag	UNP P06603
12E	-21	HIS	-	expression tag	UNP P06603
12E	-20	HIS	-	expression tag	UNP P06603
12E	-19	HIS	-	expression tag	UNP P06603
12E	-18	HIS	-	expression tag	UNP P06603
12E	-17	GLU	-	expression tag	UNP P06603
12E	-16	ASP	-	expression tag	UNP P06603
12E	-15	GLN	-	expression tag	UNP P06603
12E	-14	VAL	-	expression tag	UNP P06603
12E	-13	ASP	-	expression tag	UNP P06603
12E	-12	PRO	-	expression tag	UNP P06603
12E	-11	ARG	-	expression tag	UNP P06603
12E	-10	LEU	-	expression tag	UNP P06603
12E	-9	ILE	-	expression tag	UNP P06603
12E	-8	ASP	-	expression tag	UNP P06603
12E	-7	GLY	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
12E	-6	LYS	-	expression tag	UNP P06603
12E	-5	GLY	-	expression tag	UNP P06603
12E	-4	GLY	-	expression tag	UNP P06603
12E	-3	GLY	-	expression tag	UNP P06603
12E	-2	GLY	-	expression tag	UNP P06603
12E	-1	ARG	-	expression tag	UNP P06603
12E	0	PRO	-	expression tag	UNP P06603
12E	437	MET	-	expression tag	UNP P06603
12E	438	ASP	-	expression tag	UNP P06603
12E	439	SER	-	expression tag	UNP P06603
12E	440	GLY	-	expression tag	UNP P06603
12E	441	ASP	-	expression tag	UNP P06603
12E	442	GLY	-	expression tag	UNP P06603
12E	443	GLU	-	expression tag	UNP P06603
12E	444	GLY	-	expression tag	UNP P06603
12E	445	GLU	-	expression tag	UNP P06603
12E	446	GLY	-	expression tag	UNP P06603
12E	447	ALA	-	expression tag	UNP P06603
12E	448	GLU	-	expression tag	UNP P06603
12E	449	GLU	-	expression tag	UNP P06603
12E	450	TYR	-	expression tag	UNP P06603
13A	-24	MET	-	initiating methionine	UNP P06603
13A	-23	HIS	-	expression tag	UNP P06603
13A	-22	HIS	-	expression tag	UNP P06603
13A	-21	HIS	-	expression tag	UNP P06603
13A	-20	HIS	-	expression tag	UNP P06603
13A	-19	HIS	-	expression tag	UNP P06603
13A	-18	HIS	-	expression tag	UNP P06603
13A	-17	GLU	-	expression tag	UNP P06603
13A	-16	ASP	-	expression tag	UNP P06603
13A	-15	GLN	-	expression tag	UNP P06603
13A	-14	VAL	-	expression tag	UNP P06603
13A	-13	ASP	-	expression tag	UNP P06603
13A	-12	PRO	-	expression tag	UNP P06603
13A	-11	ARG	-	expression tag	UNP P06603
13A	-10	LEU	-	expression tag	UNP P06603
13A	-9	ILE	-	expression tag	UNP P06603
13A	-8	ASP	-	expression tag	UNP P06603
13A	-7	GLY	-	expression tag	UNP P06603
13A	-6	LYS	-	expression tag	UNP P06603
13A	-5	GLY	-	expression tag	UNP P06603
13A	-4	GLY	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
13A	-3	GLY	-	expression tag	UNP P06603
13A	-2	GLY	-	expression tag	UNP P06603
13A	-1	ARG	-	expression tag	UNP P06603
13A	0	PRO	-	expression tag	UNP P06603
13A	437	MET	-	expression tag	UNP P06603
13A	438	ASP	-	expression tag	UNP P06603
13A	439	SER	-	expression tag	UNP P06603
13A	440	GLY	-	expression tag	UNP P06603
13A	441	ASP	-	expression tag	UNP P06603
13A	442	GLY	-	expression tag	UNP P06603
13A	443	GLU	-	expression tag	UNP P06603
13A	444	GLY	-	expression tag	UNP P06603
13A	445	GLU	-	expression tag	UNP P06603
13A	446	GLY	-	expression tag	UNP P06603
13A	447	ALA	-	expression tag	UNP P06603
13A	448	GLU	-	expression tag	UNP P06603
13A	449	GLU	-	expression tag	UNP P06603
13A	450	TYR	-	expression tag	UNP P06603
13C	-24	MET	-	initiating methionine	UNP P06603
13C	-23	HIS	-	expression tag	UNP P06603
13C	-22	HIS	-	expression tag	UNP P06603
13C	-21	HIS	-	expression tag	UNP P06603
13C	-20	HIS	-	expression tag	UNP P06603
13C	-19	HIS	-	expression tag	UNP P06603
13C	-18	HIS	-	expression tag	UNP P06603
13C	-17	GLU	-	expression tag	UNP P06603
13C	-16	ASP	-	expression tag	UNP P06603
13C	-15	GLN	-	expression tag	UNP P06603
13C	-14	VAL	-	expression tag	UNP P06603
13C	-13	ASP	-	expression tag	UNP P06603
13C	-12	PRO	-	expression tag	UNP P06603
13C	-11	ARG	-	expression tag	UNP P06603
13C	-10	LEU	-	expression tag	UNP P06603
13C	-9	ILE	-	expression tag	UNP P06603
13C	-8	ASP	-	expression tag	UNP P06603
13C	-7	GLY	-	expression tag	UNP P06603
13C	-6	LYS	-	expression tag	UNP P06603
13C	-5	GLY	-	expression tag	UNP P06603
13C	-4	GLY	-	expression tag	UNP P06603
13C	-3	GLY	-	expression tag	UNP P06603
13C	-2	GLY	-	expression tag	UNP P06603
13C	-1	ARG	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
13C	0	PRO	-	expression tag	UNP P06603
13C	437	MET	-	expression tag	UNP P06603
13C	438	ASP	-	expression tag	UNP P06603
13C	439	SER	-	expression tag	UNP P06603
13C	440	GLY	-	expression tag	UNP P06603
13C	441	ASP	-	expression tag	UNP P06603
13C	442	GLY	-	expression tag	UNP P06603
13C	443	GLU	-	expression tag	UNP P06603
13C	444	GLY	-	expression tag	UNP P06603
13C	445	GLU	-	expression tag	UNP P06603
13C	446	GLY	-	expression tag	UNP P06603
13C	447	ALA	-	expression tag	UNP P06603
13C	448	GLU	-	expression tag	UNP P06603
13C	449	GLU	-	expression tag	UNP P06603
13C	450	TYR	-	expression tag	UNP P06603
13E	-24	MET	-	initiating methionine	UNP P06603
13E	-23	HIS	-	expression tag	UNP P06603
13E	-22	HIS	-	expression tag	UNP P06603
13E	-21	HIS	-	expression tag	UNP P06603
13E	-20	HIS	-	expression tag	UNP P06603
13E	-19	HIS	-	expression tag	UNP P06603
13E	-18	HIS	-	expression tag	UNP P06603
13E	-17	GLU	-	expression tag	UNP P06603
13E	-16	ASP	-	expression tag	UNP P06603
13E	-15	GLN	-	expression tag	UNP P06603
13E	-14	VAL	-	expression tag	UNP P06603
13E	-13	ASP	-	expression tag	UNP P06603
13E	-12	PRO	-	expression tag	UNP P06603
13E	-11	ARG	-	expression tag	UNP P06603
13E	-10	LEU	-	expression tag	UNP P06603
13E	-9	ILE	-	expression tag	UNP P06603
13E	-8	ASP	-	expression tag	UNP P06603
13E	-7	GLY	-	expression tag	UNP P06603
13E	-6	LYS	-	expression tag	UNP P06603
13E	-5	GLY	-	expression tag	UNP P06603
13E	-4	GLY	-	expression tag	UNP P06603
13E	-3	GLY	-	expression tag	UNP P06603
13E	-2	GLY	-	expression tag	UNP P06603
13E	-1	ARG	-	expression tag	UNP P06603
13E	0	PRO	-	expression tag	UNP P06603
13E	437	MET	-	expression tag	UNP P06603
13E	438	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
13E	439	SER	-	expression tag	UNP P06603
13E	440	GLY	-	expression tag	UNP P06603
13E	441	ASP	-	expression tag	UNP P06603
13E	442	GLY	-	expression tag	UNP P06603
13E	443	GLU	-	expression tag	UNP P06603
13E	444	GLY	-	expression tag	UNP P06603
13E	445	GLU	-	expression tag	UNP P06603
13E	446	GLY	-	expression tag	UNP P06603
13E	447	ALA	-	expression tag	UNP P06603
13E	448	GLU	-	expression tag	UNP P06603
13E	449	GLU	-	expression tag	UNP P06603
13E	450	TYR	-	expression tag	UNP P06603
1A	-24	MET	-	initiating methionine	UNP P06603
1A	-23	HIS	-	expression tag	UNP P06603
1A	-22	HIS	-	expression tag	UNP P06603
1A	-21	HIS	-	expression tag	UNP P06603
1A	-20	HIS	-	expression tag	UNP P06603
1A	-19	HIS	-	expression tag	UNP P06603
1A	-18	HIS	-	expression tag	UNP P06603
1A	-17	GLU	-	expression tag	UNP P06603
1A	-16	ASP	-	expression tag	UNP P06603
1A	-15	GLN	-	expression tag	UNP P06603
1A	-14	VAL	-	expression tag	UNP P06603
1A	-13	ASP	-	expression tag	UNP P06603
1A	-12	PRO	-	expression tag	UNP P06603
1A	-11	ARG	-	expression tag	UNP P06603
1A	-10	LEU	-	expression tag	UNP P06603
1A	-9	ILE	-	expression tag	UNP P06603
1A	-8	ASP	-	expression tag	UNP P06603
1A	-7	GLY	-	expression tag	UNP P06603
1A	-6	LYS	-	expression tag	UNP P06603
1A	-5	GLY	-	expression tag	UNP P06603
1A	-4	GLY	-	expression tag	UNP P06603
1A	-3	GLY	-	expression tag	UNP P06603
1A	-2	GLY	-	expression tag	UNP P06603
1A	-1	ARG	-	expression tag	UNP P06603
1A	0	PRO	-	expression tag	UNP P06603
1A	437	MET	-	expression tag	UNP P06603
1A	438	ASP	-	expression tag	UNP P06603
1A	439	SER	-	expression tag	UNP P06603
1A	440	GLY	-	expression tag	UNP P06603
1A	441	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
1A	442	GLY	-	expression tag	UNP P06603
1A	443	GLU	-	expression tag	UNP P06603
1A	444	GLY	-	expression tag	UNP P06603
1A	445	GLU	-	expression tag	UNP P06603
1A	446	GLY	-	expression tag	UNP P06603
1A	447	ALA	-	expression tag	UNP P06603
1A	448	GLU	-	expression tag	UNP P06603
1A	449	GLU	-	expression tag	UNP P06603
1A	450	TYR	-	expression tag	UNP P06603
1C	-24	MET	-	initiating methionine	UNP P06603
1C	-23	HIS	-	expression tag	UNP P06603
1C	-22	HIS	-	expression tag	UNP P06603
1C	-21	HIS	-	expression tag	UNP P06603
1C	-20	HIS	-	expression tag	UNP P06603
1C	-19	HIS	-	expression tag	UNP P06603
1C	-18	HIS	-	expression tag	UNP P06603
1C	-17	GLU	-	expression tag	UNP P06603
1C	-16	ASP	-	expression tag	UNP P06603
1C	-15	GLN	-	expression tag	UNP P06603
1C	-14	VAL	-	expression tag	UNP P06603
1C	-13	ASP	-	expression tag	UNP P06603
1C	-12	PRO	-	expression tag	UNP P06603
1C	-11	ARG	-	expression tag	UNP P06603
1C	-10	LEU	-	expression tag	UNP P06603
1C	-9	ILE	-	expression tag	UNP P06603
1C	-8	ASP	-	expression tag	UNP P06603
1C	-7	GLY	-	expression tag	UNP P06603
1C	-6	LYS	-	expression tag	UNP P06603
1C	-5	GLY	-	expression tag	UNP P06603
1C	-4	GLY	-	expression tag	UNP P06603
1C	-3	GLY	-	expression tag	UNP P06603
1C	-2	GLY	-	expression tag	UNP P06603
1C	-1	ARG	-	expression tag	UNP P06603
1C	0	PRO	-	expression tag	UNP P06603
1C	437	MET	-	expression tag	UNP P06603
1C	438	ASP	-	expression tag	UNP P06603
1C	439	SER	-	expression tag	UNP P06603
1C	440	GLY	-	expression tag	UNP P06603
1C	441	ASP	-	expression tag	UNP P06603
1C	442	GLY	-	expression tag	UNP P06603
1C	443	GLU	-	expression tag	UNP P06603
1C	444	GLY	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
1C	445	GLU	-	expression tag	UNP P06603
1C	446	GLY	-	expression tag	UNP P06603
1C	447	ALA	-	expression tag	UNP P06603
1C	448	GLU	-	expression tag	UNP P06603
1C	449	GLU	-	expression tag	UNP P06603
1C	450	TYR	-	expression tag	UNP P06603
1E	-24	MET	-	initiating methionine	UNP P06603
1E	-23	HIS	-	expression tag	UNP P06603
1E	-22	HIS	-	expression tag	UNP P06603
1E	-21	HIS	-	expression tag	UNP P06603
1E	-20	HIS	-	expression tag	UNP P06603
1E	-19	HIS	-	expression tag	UNP P06603
1E	-18	HIS	-	expression tag	UNP P06603
1E	-17	GLU	-	expression tag	UNP P06603
1E	-16	ASP	-	expression tag	UNP P06603
1E	-15	GLN	-	expression tag	UNP P06603
1E	-14	VAL	-	expression tag	UNP P06603
1E	-13	ASP	-	expression tag	UNP P06603
1E	-12	PRO	-	expression tag	UNP P06603
1E	-11	ARG	-	expression tag	UNP P06603
1E	-10	LEU	-	expression tag	UNP P06603
1E	-9	ILE	-	expression tag	UNP P06603
1E	-8	ASP	-	expression tag	UNP P06603
1E	-7	GLY	-	expression tag	UNP P06603
1E	-6	LYS	-	expression tag	UNP P06603
1E	-5	GLY	-	expression tag	UNP P06603
1E	-4	GLY	-	expression tag	UNP P06603
1E	-3	GLY	-	expression tag	UNP P06603
1E	-2	GLY	-	expression tag	UNP P06603
1E	-1	ARG	-	expression tag	UNP P06603
1E	0	PRO	-	expression tag	UNP P06603
1E	437	MET	-	expression tag	UNP P06603
1E	438	ASP	-	expression tag	UNP P06603
1E	439	SER	-	expression tag	UNP P06603
1E	440	GLY	-	expression tag	UNP P06603
1E	441	ASP	-	expression tag	UNP P06603
1E	442	GLY	-	expression tag	UNP P06603
1E	443	GLU	-	expression tag	UNP P06603
1E	444	GLY	-	expression tag	UNP P06603
1E	445	GLU	-	expression tag	UNP P06603
1E	446	GLY	-	expression tag	UNP P06603
1E	447	ALA	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
1E	448	GLU	-	expression tag	UNP P06603
1E	449	GLU	-	expression tag	UNP P06603
1E	450	TYR	-	expression tag	UNP P06603
2A	-24	MET	-	initiating methionine	UNP P06603
2A	-23	HIS	-	expression tag	UNP P06603
2A	-22	HIS	-	expression tag	UNP P06603
2A	-21	HIS	-	expression tag	UNP P06603
2A	-20	HIS	-	expression tag	UNP P06603
2A	-19	HIS	-	expression tag	UNP P06603
2A	-18	HIS	-	expression tag	UNP P06603
2A	-17	GLU	-	expression tag	UNP P06603
2A	-16	ASP	-	expression tag	UNP P06603
2A	-15	GLN	-	expression tag	UNP P06603
2A	-14	VAL	-	expression tag	UNP P06603
2A	-13	ASP	-	expression tag	UNP P06603
2A	-12	PRO	-	expression tag	UNP P06603
2A	-11	ARG	-	expression tag	UNP P06603
2A	-10	LEU	-	expression tag	UNP P06603
2A	-9	ILE	-	expression tag	UNP P06603
2A	-8	ASP	-	expression tag	UNP P06603
2A	-7	GLY	-	expression tag	UNP P06603
2A	-6	LYS	-	expression tag	UNP P06603
2A	-5	GLY	-	expression tag	UNP P06603
2A	-4	GLY	-	expression tag	UNP P06603
2A	-3	GLY	-	expression tag	UNP P06603
2A	-2	GLY	-	expression tag	UNP P06603
2A	-1	ARG	-	expression tag	UNP P06603
2A	0	PRO	-	expression tag	UNP P06603
2A	437	MET	-	expression tag	UNP P06603
2A	438	ASP	-	expression tag	UNP P06603
2A	439	SER	-	expression tag	UNP P06603
2A	440	GLY	-	expression tag	UNP P06603
2A	441	ASP	-	expression tag	UNP P06603
2A	442	GLY	-	expression tag	UNP P06603
2A	443	GLU	-	expression tag	UNP P06603
2A	444	GLY	-	expression tag	UNP P06603
2A	445	GLU	-	expression tag	UNP P06603
2A	446	GLY	-	expression tag	UNP P06603
2A	447	ALA	-	expression tag	UNP P06603
2A	448	GLU	-	expression tag	UNP P06603
2A	449	GLU	-	expression tag	UNP P06603
2A	450	TYR	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
2C	-24	MET	-	initiating methionine	UNP P06603
2C	-23	HIS	-	expression tag	UNP P06603
2C	-22	HIS	-	expression tag	UNP P06603
2C	-21	HIS	-	expression tag	UNP P06603
2C	-20	HIS	-	expression tag	UNP P06603
2C	-19	HIS	-	expression tag	UNP P06603
2C	-18	HIS	-	expression tag	UNP P06603
2C	-17	GLU	-	expression tag	UNP P06603
2C	-16	ASP	-	expression tag	UNP P06603
2C	-15	GLN	-	expression tag	UNP P06603
2C	-14	VAL	-	expression tag	UNP P06603
2C	-13	ASP	-	expression tag	UNP P06603
2C	-12	PRO	-	expression tag	UNP P06603
2C	-11	ARG	-	expression tag	UNP P06603
2C	-10	LEU	-	expression tag	UNP P06603
2C	-9	ILE	-	expression tag	UNP P06603
2C	-8	ASP	-	expression tag	UNP P06603
2C	-7	GLY	-	expression tag	UNP P06603
2C	-6	LYS	-	expression tag	UNP P06603
2C	-5	GLY	-	expression tag	UNP P06603
2C	-4	GLY	-	expression tag	UNP P06603
2C	-3	GLY	-	expression tag	UNP P06603
2C	-2	GLY	-	expression tag	UNP P06603
2C	-1	ARG	-	expression tag	UNP P06603
2C	0	PRO	-	expression tag	UNP P06603
2C	437	MET	-	expression tag	UNP P06603
2C	438	ASP	-	expression tag	UNP P06603
2C	439	SER	-	expression tag	UNP P06603
2C	440	GLY	-	expression tag	UNP P06603
2C	441	ASP	-	expression tag	UNP P06603
2C	442	GLY	-	expression tag	UNP P06603
2C	443	GLU	-	expression tag	UNP P06603
2C	444	GLY	-	expression tag	UNP P06603
2C	445	GLU	-	expression tag	UNP P06603
2C	446	GLY	-	expression tag	UNP P06603
2C	447	ALA	-	expression tag	UNP P06603
2C	448	GLU	-	expression tag	UNP P06603
2C	449	GLU	-	expression tag	UNP P06603
2C	450	TYR	-	expression tag	UNP P06603
2E	-24	MET	-	initiating methionine	UNP P06603
2E	-23	HIS	-	expression tag	UNP P06603
2E	-22	HIS	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
2E	-21	HIS	-	expression tag	UNP P06603
2E	-20	HIS	-	expression tag	UNP P06603
2E	-19	HIS	-	expression tag	UNP P06603
2E	-18	HIS	-	expression tag	UNP P06603
2E	-17	GLU	-	expression tag	UNP P06603
2E	-16	ASP	-	expression tag	UNP P06603
2E	-15	GLN	-	expression tag	UNP P06603
2E	-14	VAL	-	expression tag	UNP P06603
2E	-13	ASP	-	expression tag	UNP P06603
2E	-12	PRO	-	expression tag	UNP P06603
2E	-11	ARG	-	expression tag	UNP P06603
2E	-10	LEU	-	expression tag	UNP P06603
2E	-9	ILE	-	expression tag	UNP P06603
2E	-8	ASP	-	expression tag	UNP P06603
2E	-7	GLY	-	expression tag	UNP P06603
2E	-6	LYS	-	expression tag	UNP P06603
2E	-5	GLY	-	expression tag	UNP P06603
2E	-4	GLY	-	expression tag	UNP P06603
2E	-3	GLY	-	expression tag	UNP P06603
2E	-2	GLY	-	expression tag	UNP P06603
2E	-1	ARG	-	expression tag	UNP P06603
2E	0	PRO	-	expression tag	UNP P06603
2E	437	MET	-	expression tag	UNP P06603
2E	438	ASP	-	expression tag	UNP P06603
2E	439	SER	-	expression tag	UNP P06603
2E	440	GLY	-	expression tag	UNP P06603
2E	441	ASP	-	expression tag	UNP P06603
2E	442	GLY	-	expression tag	UNP P06603
2E	443	GLU	-	expression tag	UNP P06603
2E	444	GLY	-	expression tag	UNP P06603
2E	445	GLU	-	expression tag	UNP P06603
2E	446	GLY	-	expression tag	UNP P06603
2E	447	ALA	-	expression tag	UNP P06603
2E	448	GLU	-	expression tag	UNP P06603
2E	449	GLU	-	expression tag	UNP P06603
2E	450	TYR	-	expression tag	UNP P06603
3A	-24	MET	-	initiating methionine	UNP P06603
3A	-23	HIS	-	expression tag	UNP P06603
3A	-22	HIS	-	expression tag	UNP P06603
3A	-21	HIS	-	expression tag	UNP P06603
3A	-20	HIS	-	expression tag	UNP P06603
3A	-19	HIS	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
3A	-18	HIS	-	expression tag	UNP P06603
3A	-17	GLU	-	expression tag	UNP P06603
3A	-16	ASP	-	expression tag	UNP P06603
3A	-15	GLN	-	expression tag	UNP P06603
3A	-14	VAL	-	expression tag	UNP P06603
3A	-13	ASP	-	expression tag	UNP P06603
3A	-12	PRO	-	expression tag	UNP P06603
3A	-11	ARG	-	expression tag	UNP P06603
3A	-10	LEU	-	expression tag	UNP P06603
3A	-9	ILE	-	expression tag	UNP P06603
3A	-8	ASP	-	expression tag	UNP P06603
3A	-7	GLY	-	expression tag	UNP P06603
3A	-6	LYS	-	expression tag	UNP P06603
3A	-5	GLY	-	expression tag	UNP P06603
3A	-4	GLY	-	expression tag	UNP P06603
3A	-3	GLY	-	expression tag	UNP P06603
3A	-2	GLY	-	expression tag	UNP P06603
3A	-1	ARG	-	expression tag	UNP P06603
3A	0	PRO	-	expression tag	UNP P06603
3A	437	MET	-	expression tag	UNP P06603
3A	438	ASP	-	expression tag	UNP P06603
3A	439	SER	-	expression tag	UNP P06603
3A	440	GLY	-	expression tag	UNP P06603
3A	441	ASP	-	expression tag	UNP P06603
3A	442	GLY	-	expression tag	UNP P06603
3A	443	GLU	-	expression tag	UNP P06603
3A	444	GLY	-	expression tag	UNP P06603
3A	445	GLU	-	expression tag	UNP P06603
3A	446	GLY	-	expression tag	UNP P06603
3A	447	ALA	-	expression tag	UNP P06603
3A	448	GLU	-	expression tag	UNP P06603
3A	449	GLU	-	expression tag	UNP P06603
3A	450	TYR	-	expression tag	UNP P06603
3C	-24	MET	-	initiating methionine	UNP P06603
3C	-23	HIS	-	expression tag	UNP P06603
3C	-22	HIS	-	expression tag	UNP P06603
3C	-21	HIS	-	expression tag	UNP P06603
3C	-20	HIS	-	expression tag	UNP P06603
3C	-19	HIS	-	expression tag	UNP P06603
3C	-18	HIS	-	expression tag	UNP P06603
3C	-17	GLU	-	expression tag	UNP P06603
3C	-16	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
3C	-15	GLN	-	expression tag	UNP P06603
3C	-14	VAL	-	expression tag	UNP P06603
3C	-13	ASP	-	expression tag	UNP P06603
3C	-12	PRO	-	expression tag	UNP P06603
3C	-11	ARG	-	expression tag	UNP P06603
3C	-10	LEU	-	expression tag	UNP P06603
3C	-9	ILE	-	expression tag	UNP P06603
3C	-8	ASP	-	expression tag	UNP P06603
3C	-7	GLY	-	expression tag	UNP P06603
3C	-6	LYS	-	expression tag	UNP P06603
3C	-5	GLY	-	expression tag	UNP P06603
3C	-4	GLY	-	expression tag	UNP P06603
3C	-3	GLY	-	expression tag	UNP P06603
3C	-2	GLY	-	expression tag	UNP P06603
3C	-1	ARG	-	expression tag	UNP P06603
3C	0	PRO	-	expression tag	UNP P06603
3C	437	MET	-	expression tag	UNP P06603
3C	438	ASP	-	expression tag	UNP P06603
3C	439	SER	-	expression tag	UNP P06603
3C	440	GLY	-	expression tag	UNP P06603
3C	441	ASP	-	expression tag	UNP P06603
3C	442	GLY	-	expression tag	UNP P06603
3C	443	GLU	-	expression tag	UNP P06603
3C	444	GLY	-	expression tag	UNP P06603
3C	445	GLU	-	expression tag	UNP P06603
3C	446	GLY	-	expression tag	UNP P06603
3C	447	ALA	-	expression tag	UNP P06603
3C	448	GLU	-	expression tag	UNP P06603
3C	449	GLU	-	expression tag	UNP P06603
3C	450	TYR	-	expression tag	UNP P06603
3E	-24	MET	-	initiating methionine	UNP P06603
3E	-23	HIS	-	expression tag	UNP P06603
3E	-22	HIS	-	expression tag	UNP P06603
3E	-21	HIS	-	expression tag	UNP P06603
3E	-20	HIS	-	expression tag	UNP P06603
3E	-19	HIS	-	expression tag	UNP P06603
3E	-18	HIS	-	expression tag	UNP P06603
3E	-17	GLU	-	expression tag	UNP P06603
3E	-16	ASP	-	expression tag	UNP P06603
3E	-15	GLN	-	expression tag	UNP P06603
3E	-14	VAL	-	expression tag	UNP P06603
3E	-13	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
3E	-12	PRO	-	expression tag	UNP P06603
3E	-11	ARG	-	expression tag	UNP P06603
3E	-10	LEU	-	expression tag	UNP P06603
3E	-9	ILE	-	expression tag	UNP P06603
3E	-8	ASP	-	expression tag	UNP P06603
3E	-7	GLY	-	expression tag	UNP P06603
3E	-6	LYS	-	expression tag	UNP P06603
3E	-5	GLY	-	expression tag	UNP P06603
3E	-4	GLY	-	expression tag	UNP P06603
3E	-3	GLY	-	expression tag	UNP P06603
3E	-2	GLY	-	expression tag	UNP P06603
3E	-1	ARG	-	expression tag	UNP P06603
3E	0	PRO	-	expression tag	UNP P06603
3E	437	MET	-	expression tag	UNP P06603
3E	438	ASP	-	expression tag	UNP P06603
3E	439	SER	-	expression tag	UNP P06603
3E	440	GLY	-	expression tag	UNP P06603
3E	441	ASP	-	expression tag	UNP P06603
3E	442	GLY	-	expression tag	UNP P06603
3E	443	GLU	-	expression tag	UNP P06603
3E	444	GLY	-	expression tag	UNP P06603
3E	445	GLU	-	expression tag	UNP P06603
3E	446	GLY	-	expression tag	UNP P06603
3E	447	ALA	-	expression tag	UNP P06603
3E	448	GLU	-	expression tag	UNP P06603
3E	449	GLU	-	expression tag	UNP P06603
3E	450	TYR	-	expression tag	UNP P06603
4A	-24	MET	-	initiating methionine	UNP P06603
4A	-23	HIS	-	expression tag	UNP P06603
4A	-22	HIS	-	expression tag	UNP P06603
4A	-21	HIS	-	expression tag	UNP P06603
4A	-20	HIS	-	expression tag	UNP P06603
4A	-19	HIS	-	expression tag	UNP P06603
4A	-18	HIS	-	expression tag	UNP P06603
4A	-17	GLU	-	expression tag	UNP P06603
4A	-16	ASP	-	expression tag	UNP P06603
4A	-15	GLN	-	expression tag	UNP P06603
4A	-14	VAL	-	expression tag	UNP P06603
4A	-13	ASP	-	expression tag	UNP P06603
4A	-12	PRO	-	expression tag	UNP P06603
4A	-11	ARG	-	expression tag	UNP P06603
4A	-10	LEU	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
4A	-9	ILE	-	expression tag	UNP P06603
4A	-8	ASP	-	expression tag	UNP P06603
4A	-7	GLY	-	expression tag	UNP P06603
4A	-6	LYS	-	expression tag	UNP P06603
4A	-5	GLY	-	expression tag	UNP P06603
4A	-4	GLY	-	expression tag	UNP P06603
4A	-3	GLY	-	expression tag	UNP P06603
4A	-2	GLY	-	expression tag	UNP P06603
4A	-1	ARG	-	expression tag	UNP P06603
4A	0	PRO	-	expression tag	UNP P06603
4A	437	MET	-	expression tag	UNP P06603
4A	438	ASP	-	expression tag	UNP P06603
4A	439	SER	-	expression tag	UNP P06603
4A	440	GLY	-	expression tag	UNP P06603
4A	441	ASP	-	expression tag	UNP P06603
4A	442	GLY	-	expression tag	UNP P06603
4A	443	GLU	-	expression tag	UNP P06603
4A	444	GLY	-	expression tag	UNP P06603
4A	445	GLU	-	expression tag	UNP P06603
4A	446	GLY	-	expression tag	UNP P06603
4A	447	ALA	-	expression tag	UNP P06603
4A	448	GLU	-	expression tag	UNP P06603
4A	449	GLU	-	expression tag	UNP P06603
4A	450	TYR	-	expression tag	UNP P06603
4C	-24	MET	-	initiating methionine	UNP P06603
4C	-23	HIS	-	expression tag	UNP P06603
4C	-22	HIS	-	expression tag	UNP P06603
4C	-21	HIS	-	expression tag	UNP P06603
4C	-20	HIS	-	expression tag	UNP P06603
4C	-19	HIS	-	expression tag	UNP P06603
4C	-18	HIS	-	expression tag	UNP P06603
4C	-17	GLU	-	expression tag	UNP P06603
4C	-16	ASP	-	expression tag	UNP P06603
4C	-15	GLN	-	expression tag	UNP P06603
4C	-14	VAL	-	expression tag	UNP P06603
4C	-13	ASP	-	expression tag	UNP P06603
4C	-12	PRO	-	expression tag	UNP P06603
4C	-11	ARG	-	expression tag	UNP P06603
4C	-10	LEU	-	expression tag	UNP P06603
4C	-9	ILE	-	expression tag	UNP P06603
4C	-8	ASP	-	expression tag	UNP P06603
4C	-7	GLY	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
4C	-6	LYS	-	expression tag	UNP P06603
4C	-5	GLY	-	expression tag	UNP P06603
4C	-4	GLY	-	expression tag	UNP P06603
4C	-3	GLY	-	expression tag	UNP P06603
4C	-2	GLY	-	expression tag	UNP P06603
4C	-1	ARG	-	expression tag	UNP P06603
4C	0	PRO	-	expression tag	UNP P06603
4C	437	MET	-	expression tag	UNP P06603
4C	438	ASP	-	expression tag	UNP P06603
4C	439	SER	-	expression tag	UNP P06603
4C	440	GLY	-	expression tag	UNP P06603
4C	441	ASP	-	expression tag	UNP P06603
4C	442	GLY	-	expression tag	UNP P06603
4C	443	GLU	-	expression tag	UNP P06603
4C	444	GLY	-	expression tag	UNP P06603
4C	445	GLU	-	expression tag	UNP P06603
4C	446	GLY	-	expression tag	UNP P06603
4C	447	ALA	-	expression tag	UNP P06603
4C	448	GLU	-	expression tag	UNP P06603
4C	449	GLU	-	expression tag	UNP P06603
4C	450	TYR	-	expression tag	UNP P06603
4E	-24	MET	-	initiating methionine	UNP P06603
4E	-23	HIS	-	expression tag	UNP P06603
4E	-22	HIS	-	expression tag	UNP P06603
4E	-21	HIS	-	expression tag	UNP P06603
4E	-20	HIS	-	expression tag	UNP P06603
4E	-19	HIS	-	expression tag	UNP P06603
4E	-18	HIS	-	expression tag	UNP P06603
4E	-17	GLU	-	expression tag	UNP P06603
4E	-16	ASP	-	expression tag	UNP P06603
4E	-15	GLN	-	expression tag	UNP P06603
4E	-14	VAL	-	expression tag	UNP P06603
4E	-13	ASP	-	expression tag	UNP P06603
4E	-12	PRO	-	expression tag	UNP P06603
4E	-11	ARG	-	expression tag	UNP P06603
4E	-10	LEU	-	expression tag	UNP P06603
4E	-9	ILE	-	expression tag	UNP P06603
4E	-8	ASP	-	expression tag	UNP P06603
4E	-7	GLY	-	expression tag	UNP P06603
4E	-6	LYS	-	expression tag	UNP P06603
4E	-5	GLY	-	expression tag	UNP P06603
4E	-4	GLY	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
4E	-3	GLY	-	expression tag	UNP P06603
4E	-2	GLY	-	expression tag	UNP P06603
4E	-1	ARG	-	expression tag	UNP P06603
4E	0	PRO	-	expression tag	UNP P06603
4E	437	MET	-	expression tag	UNP P06603
4E	438	ASP	-	expression tag	UNP P06603
4E	439	SER	-	expression tag	UNP P06603
4E	440	GLY	-	expression tag	UNP P06603
4E	441	ASP	-	expression tag	UNP P06603
4E	442	GLY	-	expression tag	UNP P06603
4E	443	GLU	-	expression tag	UNP P06603
4E	444	GLY	-	expression tag	UNP P06603
4E	445	GLU	-	expression tag	UNP P06603
4E	446	GLY	-	expression tag	UNP P06603
4E	447	ALA	-	expression tag	UNP P06603
4E	448	GLU	-	expression tag	UNP P06603
4E	449	GLU	-	expression tag	UNP P06603
4E	450	TYR	-	expression tag	UNP P06603
5A	-24	MET	-	initiating methionine	UNP P06603
5A	-23	HIS	-	expression tag	UNP P06603
5A	-22	HIS	-	expression tag	UNP P06603
5A	-21	HIS	-	expression tag	UNP P06603
5A	-20	HIS	-	expression tag	UNP P06603
5A	-19	HIS	-	expression tag	UNP P06603
5A	-18	HIS	-	expression tag	UNP P06603
5A	-17	GLU	-	expression tag	UNP P06603
5A	-16	ASP	-	expression tag	UNP P06603
5A	-15	GLN	-	expression tag	UNP P06603
5A	-14	VAL	-	expression tag	UNP P06603
5A	-13	ASP	-	expression tag	UNP P06603
5A	-12	PRO	-	expression tag	UNP P06603
5A	-11	ARG	-	expression tag	UNP P06603
5A	-10	LEU	-	expression tag	UNP P06603
5A	-9	ILE	-	expression tag	UNP P06603
5A	-8	ASP	-	expression tag	UNP P06603
5A	-7	GLY	-	expression tag	UNP P06603
5A	-6	LYS	-	expression tag	UNP P06603
5A	-5	GLY	-	expression tag	UNP P06603
5A	-4	GLY	-	expression tag	UNP P06603
5A	-3	GLY	-	expression tag	UNP P06603
5A	-2	GLY	-	expression tag	UNP P06603
5A	-1	ARG	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
5A	0	PRO	-	expression tag	UNP P06603
5A	437	MET	-	expression tag	UNP P06603
5A	438	ASP	-	expression tag	UNP P06603
5A	439	SER	-	expression tag	UNP P06603
5A	440	GLY	-	expression tag	UNP P06603
5A	441	ASP	-	expression tag	UNP P06603
5A	442	GLY	-	expression tag	UNP P06603
5A	443	GLU	-	expression tag	UNP P06603
5A	444	GLY	-	expression tag	UNP P06603
5A	445	GLU	-	expression tag	UNP P06603
5A	446	GLY	-	expression tag	UNP P06603
5A	447	ALA	-	expression tag	UNP P06603
5A	448	GLU	-	expression tag	UNP P06603
5A	449	GLU	-	expression tag	UNP P06603
5A	450	TYR	-	expression tag	UNP P06603
5C	-24	MET	-	initiating methionine	UNP P06603
5C	-23	HIS	-	expression tag	UNP P06603
5C	-22	HIS	-	expression tag	UNP P06603
5C	-21	HIS	-	expression tag	UNP P06603
5C	-20	HIS	-	expression tag	UNP P06603
5C	-19	HIS	-	expression tag	UNP P06603
5C	-18	HIS	-	expression tag	UNP P06603
5C	-17	GLU	-	expression tag	UNP P06603
5C	-16	ASP	-	expression tag	UNP P06603
5C	-15	GLN	-	expression tag	UNP P06603
5C	-14	VAL	-	expression tag	UNP P06603
5C	-13	ASP	-	expression tag	UNP P06603
5C	-12	PRO	-	expression tag	UNP P06603
5C	-11	ARG	-	expression tag	UNP P06603
5C	-10	LEU	-	expression tag	UNP P06603
5C	-9	ILE	-	expression tag	UNP P06603
5C	-8	ASP	-	expression tag	UNP P06603
5C	-7	GLY	-	expression tag	UNP P06603
5C	-6	LYS	-	expression tag	UNP P06603
5C	-5	GLY	-	expression tag	UNP P06603
5C	-4	GLY	-	expression tag	UNP P06603
5C	-3	GLY	-	expression tag	UNP P06603
5C	-2	GLY	-	expression tag	UNP P06603
5C	-1	ARG	-	expression tag	UNP P06603
5C	0	PRO	-	expression tag	UNP P06603
5C	437	MET	-	expression tag	UNP P06603
5C	438	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
5C	439	SER	-	expression tag	UNP P06603
5C	440	GLY	-	expression tag	UNP P06603
5C	441	ASP	-	expression tag	UNP P06603
5C	442	GLY	-	expression tag	UNP P06603
5C	443	GLU	-	expression tag	UNP P06603
5C	444	GLY	-	expression tag	UNP P06603
5C	445	GLU	-	expression tag	UNP P06603
5C	446	GLY	-	expression tag	UNP P06603
5C	447	ALA	-	expression tag	UNP P06603
5C	448	GLU	-	expression tag	UNP P06603
5C	449	GLU	-	expression tag	UNP P06603
5C	450	TYR	-	expression tag	UNP P06603
5E	-24	MET	-	initiating methionine	UNP P06603
5E	-23	HIS	-	expression tag	UNP P06603
5E	-22	HIS	-	expression tag	UNP P06603
5E	-21	HIS	-	expression tag	UNP P06603
5E	-20	HIS	-	expression tag	UNP P06603
5E	-19	HIS	-	expression tag	UNP P06603
5E	-18	HIS	-	expression tag	UNP P06603
5E	-17	GLU	-	expression tag	UNP P06603
5E	-16	ASP	-	expression tag	UNP P06603
5E	-15	GLN	-	expression tag	UNP P06603
5E	-14	VAL	-	expression tag	UNP P06603
5E	-13	ASP	-	expression tag	UNP P06603
5E	-12	PRO	-	expression tag	UNP P06603
5E	-11	ARG	-	expression tag	UNP P06603
5E	-10	LEU	-	expression tag	UNP P06603
5E	-9	ILE	-	expression tag	UNP P06603
5E	-8	ASP	-	expression tag	UNP P06603
5E	-7	GLY	-	expression tag	UNP P06603
5E	-6	LYS	-	expression tag	UNP P06603
5E	-5	GLY	-	expression tag	UNP P06603
5E	-4	GLY	-	expression tag	UNP P06603
5E	-3	GLY	-	expression tag	UNP P06603
5E	-2	GLY	-	expression tag	UNP P06603
5E	-1	ARG	-	expression tag	UNP P06603
5E	0	PRO	-	expression tag	UNP P06603
5E	437	MET	-	expression tag	UNP P06603
5E	438	ASP	-	expression tag	UNP P06603
5E	439	SER	-	expression tag	UNP P06603
5E	440	GLY	-	expression tag	UNP P06603
5E	441	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
5E	442	GLY	-	expression tag	UNP P06603
5E	443	GLU	-	expression tag	UNP P06603
5E	444	GLY	-	expression tag	UNP P06603
5E	445	GLU	-	expression tag	UNP P06603
5E	446	GLY	-	expression tag	UNP P06603
5E	447	ALA	-	expression tag	UNP P06603
5E	448	GLU	-	expression tag	UNP P06603
5E	449	GLU	-	expression tag	UNP P06603
5E	450	TYR	-	expression tag	UNP P06603
6A	-24	MET	-	initiating methionine	UNP P06603
6A	-23	HIS	-	expression tag	UNP P06603
6A	-22	HIS	-	expression tag	UNP P06603
6A	-21	HIS	-	expression tag	UNP P06603
6A	-20	HIS	-	expression tag	UNP P06603
6A	-19	HIS	-	expression tag	UNP P06603
6A	-18	HIS	-	expression tag	UNP P06603
6A	-17	GLU	-	expression tag	UNP P06603
6A	-16	ASP	-	expression tag	UNP P06603
6A	-15	GLN	-	expression tag	UNP P06603
6A	-14	VAL	-	expression tag	UNP P06603
6A	-13	ASP	-	expression tag	UNP P06603
6A	-12	PRO	-	expression tag	UNP P06603
6A	-11	ARG	-	expression tag	UNP P06603
6A	-10	LEU	-	expression tag	UNP P06603
6A	-9	ILE	-	expression tag	UNP P06603
6A	-8	ASP	-	expression tag	UNP P06603
6A	-7	GLY	-	expression tag	UNP P06603
6A	-6	LYS	-	expression tag	UNP P06603
6A	-5	GLY	-	expression tag	UNP P06603
6A	-4	GLY	-	expression tag	UNP P06603
6A	-3	GLY	-	expression tag	UNP P06603
6A	-2	GLY	-	expression tag	UNP P06603
6A	-1	ARG	-	expression tag	UNP P06603
6A	0	PRO	-	expression tag	UNP P06603
6A	437	MET	-	expression tag	UNP P06603
6A	438	ASP	-	expression tag	UNP P06603
6A	439	SER	-	expression tag	UNP P06603
6A	440	GLY	-	expression tag	UNP P06603
6A	441	ASP	-	expression tag	UNP P06603
6A	442	GLY	-	expression tag	UNP P06603
6A	443	GLU	-	expression tag	UNP P06603
6A	444	GLY	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
6A	445	GLU	-	expression tag	UNP P06603
6A	446	GLY	-	expression tag	UNP P06603
6A	447	ALA	-	expression tag	UNP P06603
6A	448	GLU	-	expression tag	UNP P06603
6A	449	GLU	-	expression tag	UNP P06603
6A	450	TYR	-	expression tag	UNP P06603
6C	-24	MET	-	initiating methionine	UNP P06603
6C	-23	HIS	-	expression tag	UNP P06603
6C	-22	HIS	-	expression tag	UNP P06603
6C	-21	HIS	-	expression tag	UNP P06603
6C	-20	HIS	-	expression tag	UNP P06603
6C	-19	HIS	-	expression tag	UNP P06603
6C	-18	HIS	-	expression tag	UNP P06603
6C	-17	GLU	-	expression tag	UNP P06603
6C	-16	ASP	-	expression tag	UNP P06603
6C	-15	GLN	-	expression tag	UNP P06603
6C	-14	VAL	-	expression tag	UNP P06603
6C	-13	ASP	-	expression tag	UNP P06603
6C	-12	PRO	-	expression tag	UNP P06603
6C	-11	ARG	-	expression tag	UNP P06603
6C	-10	LEU	-	expression tag	UNP P06603
6C	-9	ILE	-	expression tag	UNP P06603
6C	-8	ASP	-	expression tag	UNP P06603
6C	-7	GLY	-	expression tag	UNP P06603
6C	-6	LYS	-	expression tag	UNP P06603
6C	-5	GLY	-	expression tag	UNP P06603
6C	-4	GLY	-	expression tag	UNP P06603
6C	-3	GLY	-	expression tag	UNP P06603
6C	-2	GLY	-	expression tag	UNP P06603
6C	-1	ARG	-	expression tag	UNP P06603
6C	0	PRO	-	expression tag	UNP P06603
6C	437	MET	-	expression tag	UNP P06603
6C	438	ASP	-	expression tag	UNP P06603
6C	439	SER	-	expression tag	UNP P06603
6C	440	GLY	-	expression tag	UNP P06603
6C	441	ASP	-	expression tag	UNP P06603
6C	442	GLY	-	expression tag	UNP P06603
6C	443	GLU	-	expression tag	UNP P06603
6C	444	GLY	-	expression tag	UNP P06603
6C	445	GLU	-	expression tag	UNP P06603
6C	446	GLY	-	expression tag	UNP P06603
6C	447	ALA	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
6C	448	GLU	-	expression tag	UNP P06603
6C	449	GLU	-	expression tag	UNP P06603
6C	450	TYR	-	expression tag	UNP P06603
6E	-24	MET	-	initiating methionine	UNP P06603
6E	-23	HIS	-	expression tag	UNP P06603
6E	-22	HIS	-	expression tag	UNP P06603
6E	-21	HIS	-	expression tag	UNP P06603
6E	-20	HIS	-	expression tag	UNP P06603
6E	-19	HIS	-	expression tag	UNP P06603
6E	-18	HIS	-	expression tag	UNP P06603
6E	-17	GLU	-	expression tag	UNP P06603
6E	-16	ASP	-	expression tag	UNP P06603
6E	-15	GLN	-	expression tag	UNP P06603
6E	-14	VAL	-	expression tag	UNP P06603
6E	-13	ASP	-	expression tag	UNP P06603
6E	-12	PRO	-	expression tag	UNP P06603
6E	-11	ARG	-	expression tag	UNP P06603
6E	-10	LEU	-	expression tag	UNP P06603
6E	-9	ILE	-	expression tag	UNP P06603
6E	-8	ASP	-	expression tag	UNP P06603
6E	-7	GLY	-	expression tag	UNP P06603
6E	-6	LYS	-	expression tag	UNP P06603
6E	-5	GLY	-	expression tag	UNP P06603
6E	-4	GLY	-	expression tag	UNP P06603
6E	-3	GLY	-	expression tag	UNP P06603
6E	-2	GLY	-	expression tag	UNP P06603
6E	-1	ARG	-	expression tag	UNP P06603
6E	0	PRO	-	expression tag	UNP P06603
6E	437	MET	-	expression tag	UNP P06603
6E	438	ASP	-	expression tag	UNP P06603
6E	439	SER	-	expression tag	UNP P06603
6E	440	GLY	-	expression tag	UNP P06603
6E	441	ASP	-	expression tag	UNP P06603
6E	442	GLY	-	expression tag	UNP P06603
6E	443	GLU	-	expression tag	UNP P06603
6E	444	GLY	-	expression tag	UNP P06603
6E	445	GLU	-	expression tag	UNP P06603
6E	446	GLY	-	expression tag	UNP P06603
6E	447	ALA	-	expression tag	UNP P06603
6E	448	GLU	-	expression tag	UNP P06603
6E	449	GLU	-	expression tag	UNP P06603
6E	450	TYR	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
7A	-24	MET	-	initiating methionine	UNP P06603
7A	-23	HIS	-	expression tag	UNP P06603
7A	-22	HIS	-	expression tag	UNP P06603
7A	-21	HIS	-	expression tag	UNP P06603
7A	-20	HIS	-	expression tag	UNP P06603
7A	-19	HIS	-	expression tag	UNP P06603
7A	-18	HIS	-	expression tag	UNP P06603
7A	-17	GLU	-	expression tag	UNP P06603
7A	-16	ASP	-	expression tag	UNP P06603
7A	-15	GLN	-	expression tag	UNP P06603
7A	-14	VAL	-	expression tag	UNP P06603
7A	-13	ASP	-	expression tag	UNP P06603
7A	-12	PRO	-	expression tag	UNP P06603
7A	-11	ARG	-	expression tag	UNP P06603
7A	-10	LEU	-	expression tag	UNP P06603
7A	-9	ILE	-	expression tag	UNP P06603
7A	-8	ASP	-	expression tag	UNP P06603
7A	-7	GLY	-	expression tag	UNP P06603
7A	-6	LYS	-	expression tag	UNP P06603
7A	-5	GLY	-	expression tag	UNP P06603
7A	-4	GLY	-	expression tag	UNP P06603
7A	-3	GLY	-	expression tag	UNP P06603
7A	-2	GLY	-	expression tag	UNP P06603
7A	-1	ARG	-	expression tag	UNP P06603
7A	0	PRO	-	expression tag	UNP P06603
7A	437	MET	-	expression tag	UNP P06603
7A	438	ASP	-	expression tag	UNP P06603
7A	439	SER	-	expression tag	UNP P06603
7A	440	GLY	-	expression tag	UNP P06603
7A	441	ASP	-	expression tag	UNP P06603
7A	442	GLY	-	expression tag	UNP P06603
7A	443	GLU	-	expression tag	UNP P06603
7A	444	GLY	-	expression tag	UNP P06603
7A	445	GLU	-	expression tag	UNP P06603
7A	446	GLY	-	expression tag	UNP P06603
7A	447	ALA	-	expression tag	UNP P06603
7A	448	GLU	-	expression tag	UNP P06603
7A	449	GLU	-	expression tag	UNP P06603
7A	450	TYR	-	expression tag	UNP P06603
7C	-24	MET	-	initiating methionine	UNP P06603
7C	-23	HIS	-	expression tag	UNP P06603
7C	-22	HIS	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
7C	-21	HIS	-	expression tag	UNP P06603
7C	-20	HIS	-	expression tag	UNP P06603
7C	-19	HIS	-	expression tag	UNP P06603
7C	-18	HIS	-	expression tag	UNP P06603
7C	-17	GLU	-	expression tag	UNP P06603
7C	-16	ASP	-	expression tag	UNP P06603
7C	-15	GLN	-	expression tag	UNP P06603
7C	-14	VAL	-	expression tag	UNP P06603
7C	-13	ASP	-	expression tag	UNP P06603
7C	-12	PRO	-	expression tag	UNP P06603
7C	-11	ARG	-	expression tag	UNP P06603
7C	-10	LEU	-	expression tag	UNP P06603
7C	-9	ILE	-	expression tag	UNP P06603
7C	-8	ASP	-	expression tag	UNP P06603
7C	-7	GLY	-	expression tag	UNP P06603
7C	-6	LYS	-	expression tag	UNP P06603
7C	-5	GLY	-	expression tag	UNP P06603
7C	-4	GLY	-	expression tag	UNP P06603
7C	-3	GLY	-	expression tag	UNP P06603
7C	-2	GLY	-	expression tag	UNP P06603
7C	-1	ARG	-	expression tag	UNP P06603
7C	0	PRO	-	expression tag	UNP P06603
7C	437	MET	-	expression tag	UNP P06603
7C	438	ASP	-	expression tag	UNP P06603
7C	439	SER	-	expression tag	UNP P06603
7C	440	GLY	-	expression tag	UNP P06603
7C	441	ASP	-	expression tag	UNP P06603
7C	442	GLY	-	expression tag	UNP P06603
7C	443	GLU	-	expression tag	UNP P06603
7C	444	GLY	-	expression tag	UNP P06603
7C	445	GLU	-	expression tag	UNP P06603
7C	446	GLY	-	expression tag	UNP P06603
7C	447	ALA	-	expression tag	UNP P06603
7C	448	GLU	-	expression tag	UNP P06603
7C	449	GLU	-	expression tag	UNP P06603
7C	450	TYR	-	expression tag	UNP P06603
7E	-24	MET	-	initiating methionine	UNP P06603
7E	-23	HIS	-	expression tag	UNP P06603
7E	-22	HIS	-	expression tag	UNP P06603
7E	-21	HIS	-	expression tag	UNP P06603
7E	-20	HIS	-	expression tag	UNP P06603
7E	-19	HIS	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
7E	-18	HIS	-	expression tag	UNP P06603
7E	-17	GLU	-	expression tag	UNP P06603
7E	-16	ASP	-	expression tag	UNP P06603
7E	-15	GLN	-	expression tag	UNP P06603
7E	-14	VAL	-	expression tag	UNP P06603
7E	-13	ASP	-	expression tag	UNP P06603
7E	-12	PRO	-	expression tag	UNP P06603
7E	-11	ARG	-	expression tag	UNP P06603
7E	-10	LEU	-	expression tag	UNP P06603
7E	-9	ILE	-	expression tag	UNP P06603
7E	-8	ASP	-	expression tag	UNP P06603
7E	-7	GLY	-	expression tag	UNP P06603
7E	-6	LYS	-	expression tag	UNP P06603
7E	-5	GLY	-	expression tag	UNP P06603
7E	-4	GLY	-	expression tag	UNP P06603
7E	-3	GLY	-	expression tag	UNP P06603
7E	-2	GLY	-	expression tag	UNP P06603
7E	-1	ARG	-	expression tag	UNP P06603
7E	0	PRO	-	expression tag	UNP P06603
7E	437	MET	-	expression tag	UNP P06603
7E	438	ASP	-	expression tag	UNP P06603
7E	439	SER	-	expression tag	UNP P06603
7E	440	GLY	-	expression tag	UNP P06603
7E	441	ASP	-	expression tag	UNP P06603
7E	442	GLY	-	expression tag	UNP P06603
7E	443	GLU	-	expression tag	UNP P06603
7E	444	GLY	-	expression tag	UNP P06603
7E	445	GLU	-	expression tag	UNP P06603
7E	446	GLY	-	expression tag	UNP P06603
7E	447	ALA	-	expression tag	UNP P06603
7E	448	GLU	-	expression tag	UNP P06603
7E	449	GLU	-	expression tag	UNP P06603
7E	450	TYR	-	expression tag	UNP P06603
8A	-24	MET	-	initiating methionine	UNP P06603
8A	-23	HIS	-	expression tag	UNP P06603
8A	-22	HIS	-	expression tag	UNP P06603
8A	-21	HIS	-	expression tag	UNP P06603
8A	-20	HIS	-	expression tag	UNP P06603
8A	-19	HIS	-	expression tag	UNP P06603
8A	-18	HIS	-	expression tag	UNP P06603
8A	-17	GLU	-	expression tag	UNP P06603
8A	-16	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
8A	-15	GLN	-	expression tag	UNP P06603
8A	-14	VAL	-	expression tag	UNP P06603
8A	-13	ASP	-	expression tag	UNP P06603
8A	-12	PRO	-	expression tag	UNP P06603
8A	-11	ARG	-	expression tag	UNP P06603
8A	-10	LEU	-	expression tag	UNP P06603
8A	-9	ILE	-	expression tag	UNP P06603
8A	-8	ASP	-	expression tag	UNP P06603
8A	-7	GLY	-	expression tag	UNP P06603
8A	-6	LYS	-	expression tag	UNP P06603
8A	-5	GLY	-	expression tag	UNP P06603
8A	-4	GLY	-	expression tag	UNP P06603
8A	-3	GLY	-	expression tag	UNP P06603
8A	-2	GLY	-	expression tag	UNP P06603
8A	-1	ARG	-	expression tag	UNP P06603
8A	0	PRO	-	expression tag	UNP P06603
8A	437	MET	-	expression tag	UNP P06603
8A	438	ASP	-	expression tag	UNP P06603
8A	439	SER	-	expression tag	UNP P06603
8A	440	GLY	-	expression tag	UNP P06603
8A	441	ASP	-	expression tag	UNP P06603
8A	442	GLY	-	expression tag	UNP P06603
8A	443	GLU	-	expression tag	UNP P06603
8A	444	GLY	-	expression tag	UNP P06603
8A	445	GLU	-	expression tag	UNP P06603
8A	446	GLY	-	expression tag	UNP P06603
8A	447	ALA	-	expression tag	UNP P06603
8A	448	GLU	-	expression tag	UNP P06603
8A	449	GLU	-	expression tag	UNP P06603
8A	450	TYR	-	expression tag	UNP P06603
8C	-24	MET	-	initiating methionine	UNP P06603
8C	-23	HIS	-	expression tag	UNP P06603
8C	-22	HIS	-	expression tag	UNP P06603
8C	-21	HIS	-	expression tag	UNP P06603
8C	-20	HIS	-	expression tag	UNP P06603
8C	-19	HIS	-	expression tag	UNP P06603
8C	-18	HIS	-	expression tag	UNP P06603
8C	-17	GLU	-	expression tag	UNP P06603
8C	-16	ASP	-	expression tag	UNP P06603
8C	-15	GLN	-	expression tag	UNP P06603
8C	-14	VAL	-	expression tag	UNP P06603
8C	-13	ASP	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
8C	-12	PRO	-	expression tag	UNP P06603
8C	-11	ARG	-	expression tag	UNP P06603
8C	-10	LEU	-	expression tag	UNP P06603
8C	-9	ILE	-	expression tag	UNP P06603
8C	-8	ASP	-	expression tag	UNP P06603
8C	-7	GLY	-	expression tag	UNP P06603
8C	-6	LYS	-	expression tag	UNP P06603
8C	-5	GLY	-	expression tag	UNP P06603
8C	-4	GLY	-	expression tag	UNP P06603
8C	-3	GLY	-	expression tag	UNP P06603
8C	-2	GLY	-	expression tag	UNP P06603
8C	-1	ARG	-	expression tag	UNP P06603
8C	0	PRO	-	expression tag	UNP P06603
8C	437	MET	-	expression tag	UNP P06603
8C	438	ASP	-	expression tag	UNP P06603
8C	439	SER	-	expression tag	UNP P06603
8C	440	GLY	-	expression tag	UNP P06603
8C	441	ASP	-	expression tag	UNP P06603
8C	442	GLY	-	expression tag	UNP P06603
8C	443	GLU	-	expression tag	UNP P06603
8C	444	GLY	-	expression tag	UNP P06603
8C	445	GLU	-	expression tag	UNP P06603
8C	446	GLY	-	expression tag	UNP P06603
8C	447	ALA	-	expression tag	UNP P06603
8C	448	GLU	-	expression tag	UNP P06603
8C	449	GLU	-	expression tag	UNP P06603
8C	450	TYR	-	expression tag	UNP P06603
8E	-24	MET	-	initiating methionine	UNP P06603
8E	-23	HIS	-	expression tag	UNP P06603
8E	-22	HIS	-	expression tag	UNP P06603
8E	-21	HIS	-	expression tag	UNP P06603
8E	-20	HIS	-	expression tag	UNP P06603
8E	-19	HIS	-	expression tag	UNP P06603
8E	-18	HIS	-	expression tag	UNP P06603
8E	-17	GLU	-	expression tag	UNP P06603
8E	-16	ASP	-	expression tag	UNP P06603
8E	-15	GLN	-	expression tag	UNP P06603
8E	-14	VAL	-	expression tag	UNP P06603
8E	-13	ASP	-	expression tag	UNP P06603
8E	-12	PRO	-	expression tag	UNP P06603
8E	-11	ARG	-	expression tag	UNP P06603
8E	-10	LEU	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
8E	-9	ILE	-	expression tag	UNP P06603
8E	-8	ASP	-	expression tag	UNP P06603
8E	-7	GLY	-	expression tag	UNP P06603
8E	-6	LYS	-	expression tag	UNP P06603
8E	-5	GLY	-	expression tag	UNP P06603
8E	-4	GLY	-	expression tag	UNP P06603
8E	-3	GLY	-	expression tag	UNP P06603
8E	-2	GLY	-	expression tag	UNP P06603
8E	-1	ARG	-	expression tag	UNP P06603
8E	0	PRO	-	expression tag	UNP P06603
8E	437	MET	-	expression tag	UNP P06603
8E	438	ASP	-	expression tag	UNP P06603
8E	439	SER	-	expression tag	UNP P06603
8E	440	GLY	-	expression tag	UNP P06603
8E	441	ASP	-	expression tag	UNP P06603
8E	442	GLY	-	expression tag	UNP P06603
8E	443	GLU	-	expression tag	UNP P06603
8E	444	GLY	-	expression tag	UNP P06603
8E	445	GLU	-	expression tag	UNP P06603
8E	446	GLY	-	expression tag	UNP P06603
8E	447	ALA	-	expression tag	UNP P06603
8E	448	GLU	-	expression tag	UNP P06603
8E	449	GLU	-	expression tag	UNP P06603
8E	450	TYR	-	expression tag	UNP P06603
9A	-24	MET	-	initiating methionine	UNP P06603
9A	-23	HIS	-	expression tag	UNP P06603
9A	-22	HIS	-	expression tag	UNP P06603
9A	-21	HIS	-	expression tag	UNP P06603
9A	-20	HIS	-	expression tag	UNP P06603
9A	-19	HIS	-	expression tag	UNP P06603
9A	-18	HIS	-	expression tag	UNP P06603
9A	-17	GLU	-	expression tag	UNP P06603
9A	-16	ASP	-	expression tag	UNP P06603
9A	-15	GLN	-	expression tag	UNP P06603
9A	-14	VAL	-	expression tag	UNP P06603
9A	-13	ASP	-	expression tag	UNP P06603
9A	-12	PRO	-	expression tag	UNP P06603
9A	-11	ARG	-	expression tag	UNP P06603
9A	-10	LEU	-	expression tag	UNP P06603
9A	-9	ILE	-	expression tag	UNP P06603
9A	-8	ASP	-	expression tag	UNP P06603
9A	-7	GLY	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
9A	-6	LYS	-	expression tag	UNP P06603
9A	-5	GLY	-	expression tag	UNP P06603
9A	-4	GLY	-	expression tag	UNP P06603
9A	-3	GLY	-	expression tag	UNP P06603
9A	-2	GLY	-	expression tag	UNP P06603
9A	-1	ARG	-	expression tag	UNP P06603
9A	0	PRO	-	expression tag	UNP P06603
9A	437	MET	-	expression tag	UNP P06603
9A	438	ASP	-	expression tag	UNP P06603
9A	439	SER	-	expression tag	UNP P06603
9A	440	GLY	-	expression tag	UNP P06603
9A	441	ASP	-	expression tag	UNP P06603
9A	442	GLY	-	expression tag	UNP P06603
9A	443	GLU	-	expression tag	UNP P06603
9A	444	GLY	-	expression tag	UNP P06603
9A	445	GLU	-	expression tag	UNP P06603
9A	446	GLY	-	expression tag	UNP P06603
9A	447	ALA	-	expression tag	UNP P06603
9A	448	GLU	-	expression tag	UNP P06603
9A	449	GLU	-	expression tag	UNP P06603
9A	450	TYR	-	expression tag	UNP P06603
9C	-24	MET	-	initiating methionine	UNP P06603
9C	-23	HIS	-	expression tag	UNP P06603
9C	-22	HIS	-	expression tag	UNP P06603
9C	-21	HIS	-	expression tag	UNP P06603
9C	-20	HIS	-	expression tag	UNP P06603
9C	-19	HIS	-	expression tag	UNP P06603
9C	-18	HIS	-	expression tag	UNP P06603
9C	-17	GLU	-	expression tag	UNP P06603
9C	-16	ASP	-	expression tag	UNP P06603
9C	-15	GLN	-	expression tag	UNP P06603
9C	-14	VAL	-	expression tag	UNP P06603
9C	-13	ASP	-	expression tag	UNP P06603
9C	-12	PRO	-	expression tag	UNP P06603
9C	-11	ARG	-	expression tag	UNP P06603
9C	-10	LEU	-	expression tag	UNP P06603
9C	-9	ILE	-	expression tag	UNP P06603
9C	-8	ASP	-	expression tag	UNP P06603
9C	-7	GLY	-	expression tag	UNP P06603
9C	-6	LYS	-	expression tag	UNP P06603
9C	-5	GLY	-	expression tag	UNP P06603
9C	-4	GLY	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
9C	-3	GLY	-	expression tag	UNP P06603
9C	-2	GLY	-	expression tag	UNP P06603
9C	-1	ARG	-	expression tag	UNP P06603
9C	0	PRO	-	expression tag	UNP P06603
9C	437	MET	-	expression tag	UNP P06603
9C	438	ASP	-	expression tag	UNP P06603
9C	439	SER	-	expression tag	UNP P06603
9C	440	GLY	-	expression tag	UNP P06603
9C	441	ASP	-	expression tag	UNP P06603
9C	442	GLY	-	expression tag	UNP P06603
9C	443	GLU	-	expression tag	UNP P06603
9C	444	GLY	-	expression tag	UNP P06603
9C	445	GLU	-	expression tag	UNP P06603
9C	446	GLY	-	expression tag	UNP P06603
9C	447	ALA	-	expression tag	UNP P06603
9C	448	GLU	-	expression tag	UNP P06603
9C	449	GLU	-	expression tag	UNP P06603
9C	450	TYR	-	expression tag	UNP P06603
9E	-24	MET	-	initiating methionine	UNP P06603
9E	-23	HIS	-	expression tag	UNP P06603
9E	-22	HIS	-	expression tag	UNP P06603
9E	-21	HIS	-	expression tag	UNP P06603
9E	-20	HIS	-	expression tag	UNP P06603
9E	-19	HIS	-	expression tag	UNP P06603
9E	-18	HIS	-	expression tag	UNP P06603
9E	-17	GLU	-	expression tag	UNP P06603
9E	-16	ASP	-	expression tag	UNP P06603
9E	-15	GLN	-	expression tag	UNP P06603
9E	-14	VAL	-	expression tag	UNP P06603
9E	-13	ASP	-	expression tag	UNP P06603
9E	-12	PRO	-	expression tag	UNP P06603
9E	-11	ARG	-	expression tag	UNP P06603
9E	-10	LEU	-	expression tag	UNP P06603
9E	-9	ILE	-	expression tag	UNP P06603
9E	-8	ASP	-	expression tag	UNP P06603
9E	-7	GLY	-	expression tag	UNP P06603
9E	-6	LYS	-	expression tag	UNP P06603
9E	-5	GLY	-	expression tag	UNP P06603
9E	-4	GLY	-	expression tag	UNP P06603
9E	-3	GLY	-	expression tag	UNP P06603
9E	-2	GLY	-	expression tag	UNP P06603
9E	-1	ARG	-	expression tag	UNP P06603

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Chain	Residue	Modelled	Actual	Comment	Reference
9E	0	PRO	-	expression tag	UNP P06603
9E	437	MET	-	expression tag	UNP P06603
9E	438	ASP	-	expression tag	UNP P06603
9E	439	SER	-	expression tag	UNP P06603
9E	440	GLY	-	expression tag	UNP P06603
9E	441	ASP	-	expression tag	UNP P06603
9E	442	GLY	-	expression tag	UNP P06603
9E	443	GLU	-	expression tag	UNP P06603
9E	444	GLY	-	expression tag	UNP P06603
9E	445	GLU	-	expression tag	UNP P06603
9E	446	GLY	-	expression tag	UNP P06603
9E	447	ALA	-	expression tag	UNP P06603
9E	448	GLU	-	expression tag	UNP P06603
9E	449	GLU	-	expression tag	UNP P06603
9E	450	TYR	-	expression tag	UNP P06603

- Molecule 2 is a protein called Tubulin beta-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	10B	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	10D	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	11B	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	11D	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	12B	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	12D	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	13B	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	13D	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	1B	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	1D	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	2B	425	Total 3343	C 2102	N 573	O 643	S 25	0	0
2	2D	425	Total 3343	C 2102	N 573	O 643	S 25	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	3B	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	3D	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	4B	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	4D	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	5B	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	5D	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	6B	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	6D	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	7B	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	7D	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	8B	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	8D	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	9B	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		
2	9D	425	Total	C	N	O	S	0	0
			3343	2102	573	643	25		

- 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	10A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	10C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	10E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	11A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	11C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	11E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	12A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	12C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	12E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	13A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	13C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	13E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1C	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
3	1E	1	32	10	5	14	3	0
3	2A	1	32	10	5	14	3	0
3	2C	1	32	10	5	14	3	0
3	2E	1	32	10	5	14	3	0
3	3A	1	32	10	5	14	3	0
3	3C	1	32	10	5	14	3	0
3	3E	1	32	10	5	14	3	0
3	4A	1	32	10	5	14	3	0
3	4C	1	32	10	5	14	3	0
3	4E	1	32	10	5	14	3	0
3	5A	1	32	10	5	14	3	0
3	5C	1	32	10	5	14	3	0
3	5E	1	32	10	5	14	3	0
3	6A	1	32	10	5	14	3	0
3	6C	1	32	10	5	14	3	0
3	6E	1	32	10	5	14	3	0
3	7A	1	32	10	5	14	3	0
3	7C	1	32	10	5	14	3	0
3	7E	1	32	10	5	14	3	0
3	8A	1	32	10	5	14	3	0
3	8C	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
3	8E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	9A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	9C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	9E	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	10A	1	Total	Mg	0
			1	1	
4	10C	1	Total	Mg	0
			1	1	
4	10E	1	Total	Mg	0
			1	1	
4	11A	1	Total	Mg	0
			1	1	
4	11C	1	Total	Mg	0
			1	1	
4	11E	1	Total	Mg	0
			1	1	
4	12A	1	Total	Mg	0
			1	1	
4	12C	1	Total	Mg	0
			1	1	
4	12E	1	Total	Mg	0
			1	1	
4	13A	1	Total	Mg	0
			1	1	
4	13C	1	Total	Mg	0
			1	1	
4	13E	1	Total	Mg	0
			1	1	
4	1A	1	Total	Mg	0
			1	1	
4	1C	1	Total	Mg	0
			1	1	
4	1E	1	Total	Mg	0
			1	1	

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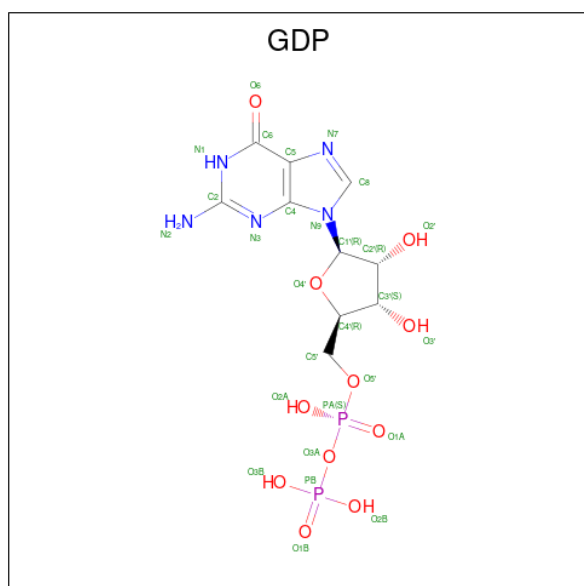
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	2A	1	1	1	0
4	2C	1	1	1	0
4	2E	1	1	1	0
4	3A	1	1	1	0
4	3C	1	1	1	0
4	3E	1	1	1	0
4	4A	1	1	1	0
4	4C	1	1	1	0
4	4E	1	1	1	0
4	5A	1	1	1	0
4	5C	1	1	1	0
4	5E	1	1	1	0
4	6A	1	1	1	0
4	6C	1	1	1	0
4	6E	1	1	1	0
4	7A	1	1	1	0
4	7C	1	1	1	0
4	7E	1	1	1	0
4	8A	1	1	1	0
4	8C	1	1	1	0
4	8E	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
4	9A	1	Total	Mg	0
			1	1	
4	9C	1	Total	Mg	0
			1	1	
4	9E	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	
5	10B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	10D	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	11B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	11D	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	12B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	12D	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	13B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	13D	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

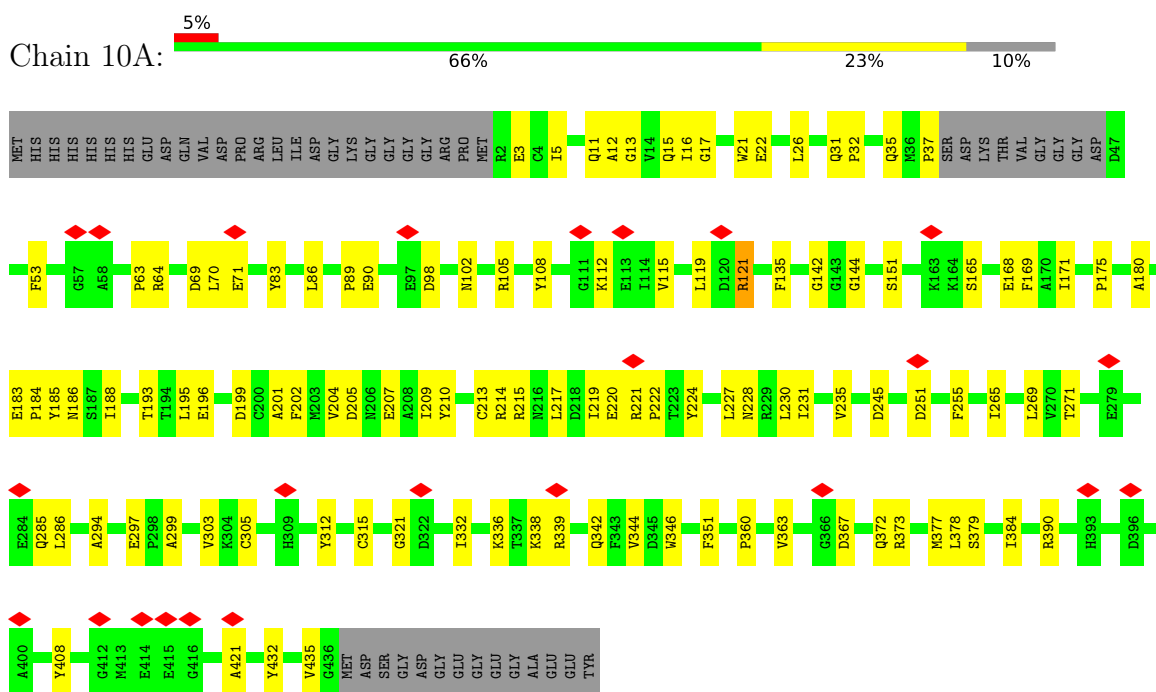
*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
5	1B	1	Total 28	C 10	N 5	O 11	P 2	0
5	1D	1	Total 28	C 10	N 5	O 11	P 2	0
5	2B	1	Total 28	C 10	N 5	O 11	P 2	0
5	2D	1	Total 28	C 10	N 5	O 11	P 2	0
5	3B	1	Total 28	C 10	N 5	O 11	P 2	0
5	3D	1	Total 28	C 10	N 5	O 11	P 2	0
5	4B	1	Total 28	C 10	N 5	O 11	P 2	0
5	4D	1	Total 28	C 10	N 5	O 11	P 2	0
5	5B	1	Total 28	C 10	N 5	O 11	P 2	0
5	5D	1	Total 28	C 10	N 5	O 11	P 2	0
5	6B	1	Total 28	C 10	N 5	O 11	P 2	0
5	6D	1	Total 28	C 10	N 5	O 11	P 2	0
5	7B	1	Total 28	C 10	N 5	O 11	P 2	0
5	7D	1	Total 28	C 10	N 5	O 11	P 2	0
5	8B	1	Total 28	C 10	N 5	O 11	P 2	0
5	8D	1	Total 28	C 10	N 5	O 11	P 2	0
5	9B	1	Total 28	C 10	N 5	O 11	P 2	0
5	9D	1	Total 28	C 10	N 5	O 11	P 2	0

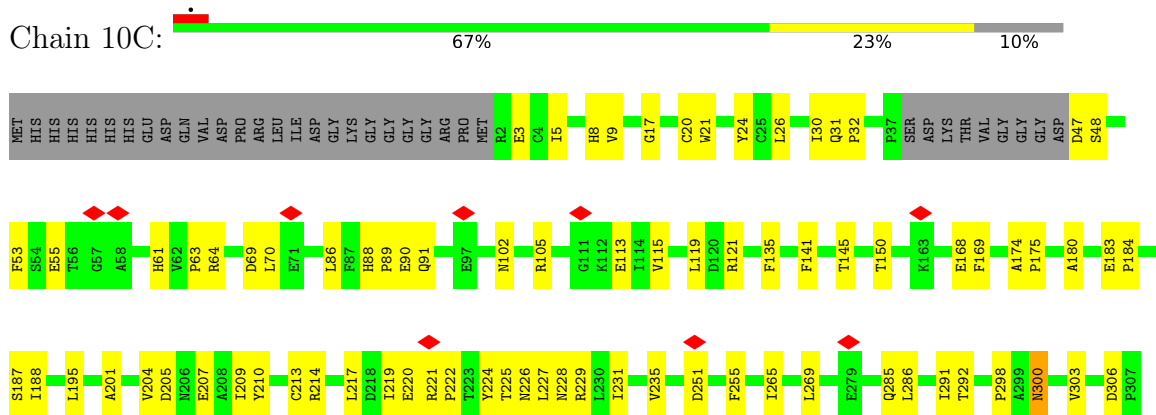
### 3 Residue-property plots [i](#)

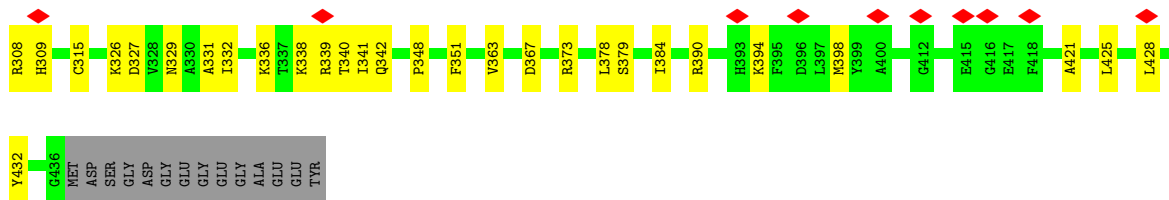
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-1 chain

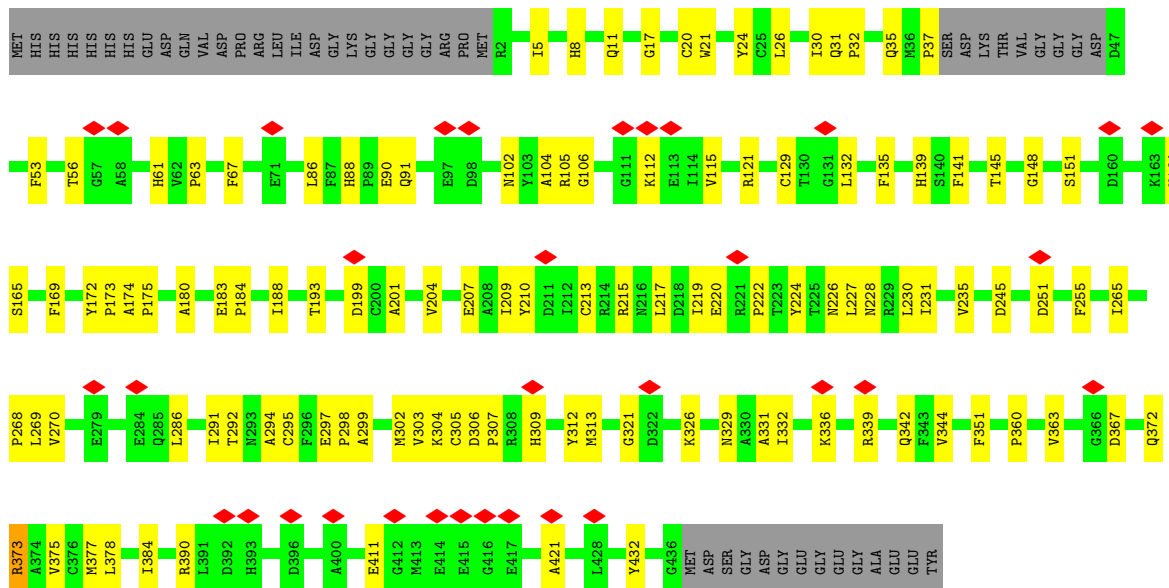


- Molecule 1: Tubulin alpha-1 chain

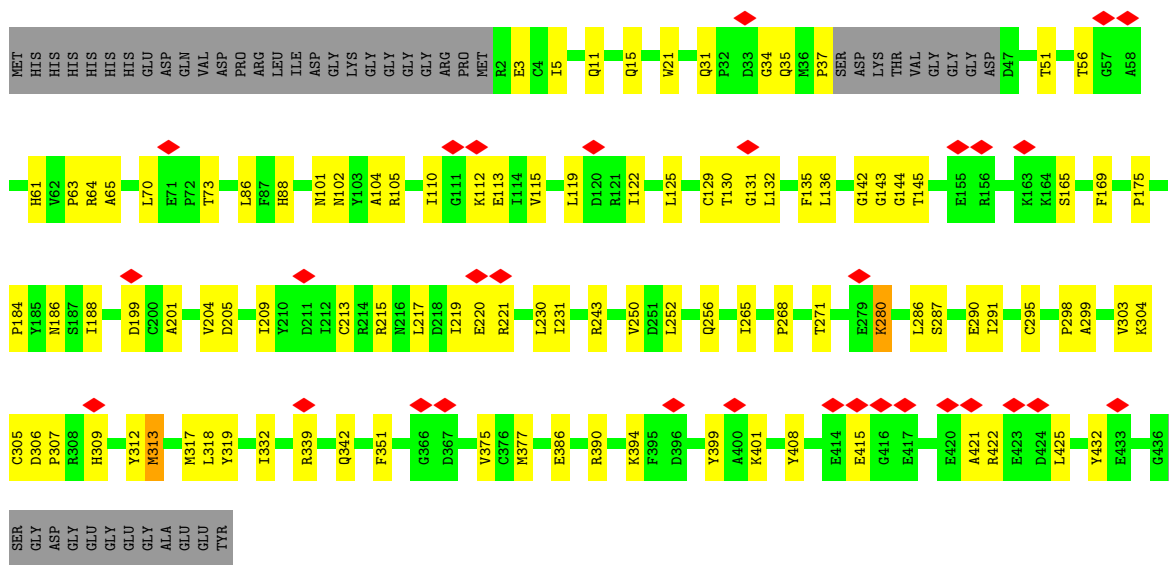
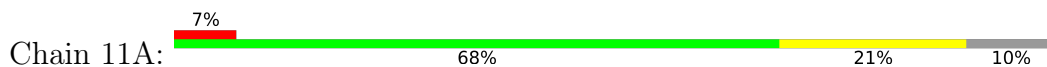




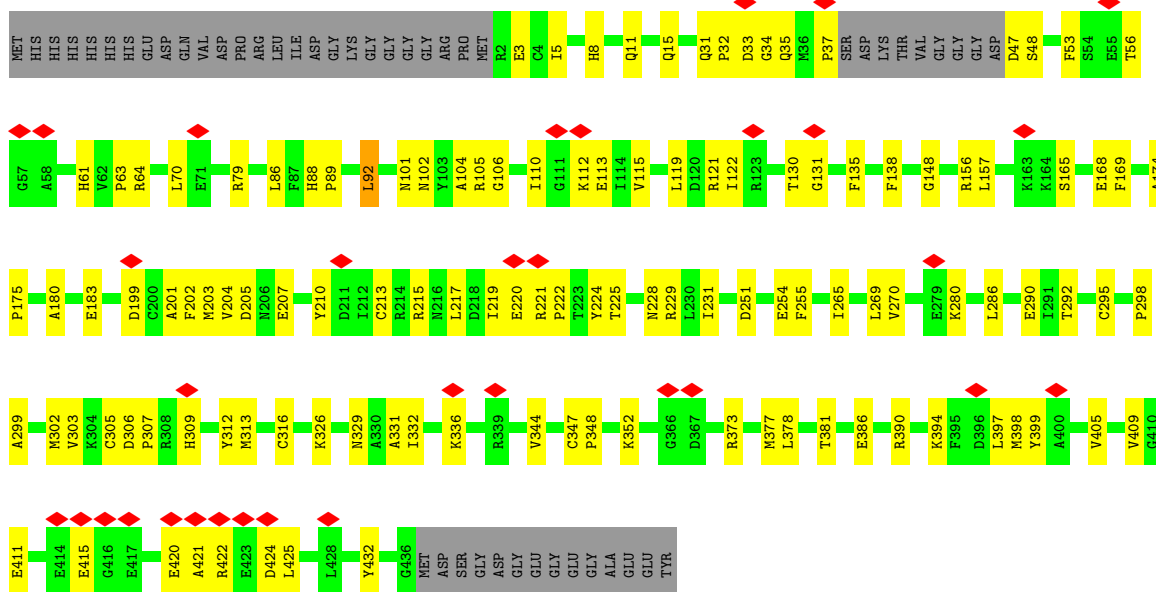
• Molecule 1: Tubulin alpha-1 chain



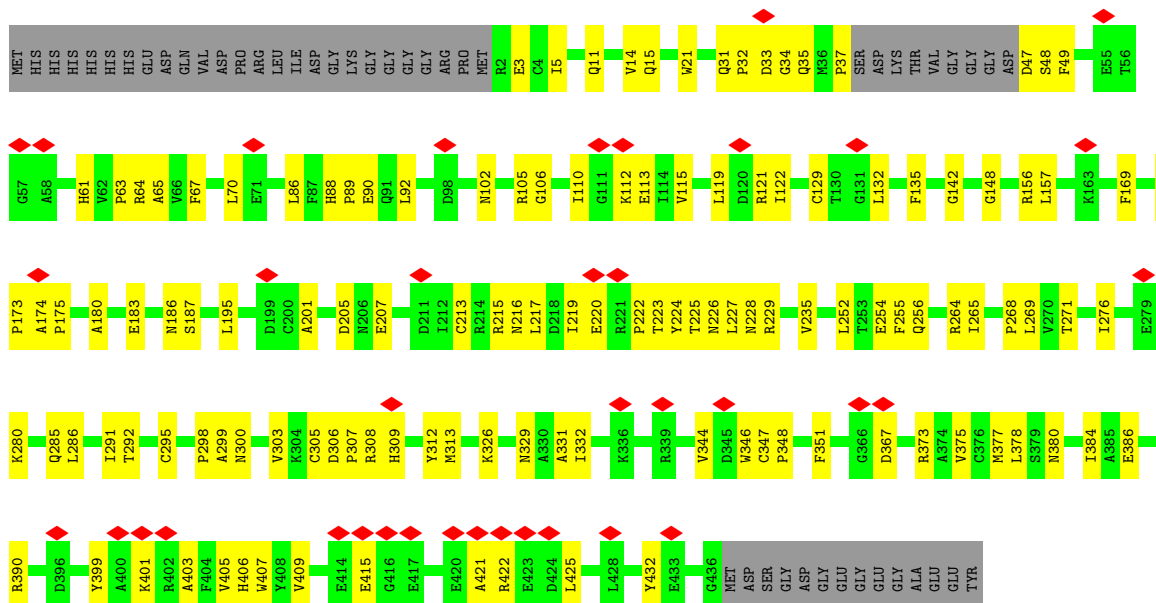
• Molecule 1: Tubulin alpha-1 chain



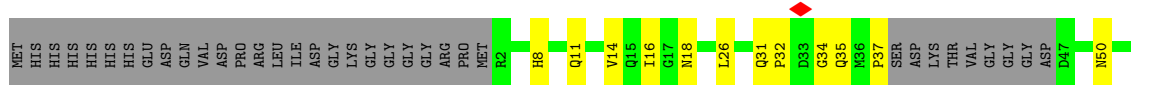
• Molecule 1: Tubulin alpha-1 chain



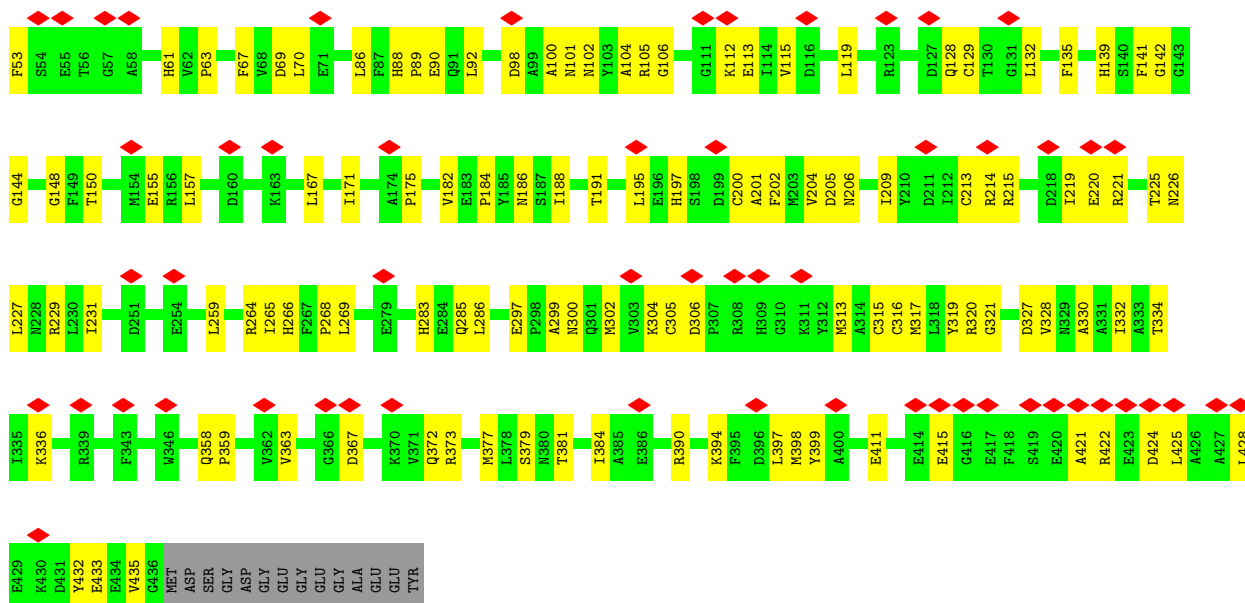
• Molecule 1: Tubulin alpha-1 chain



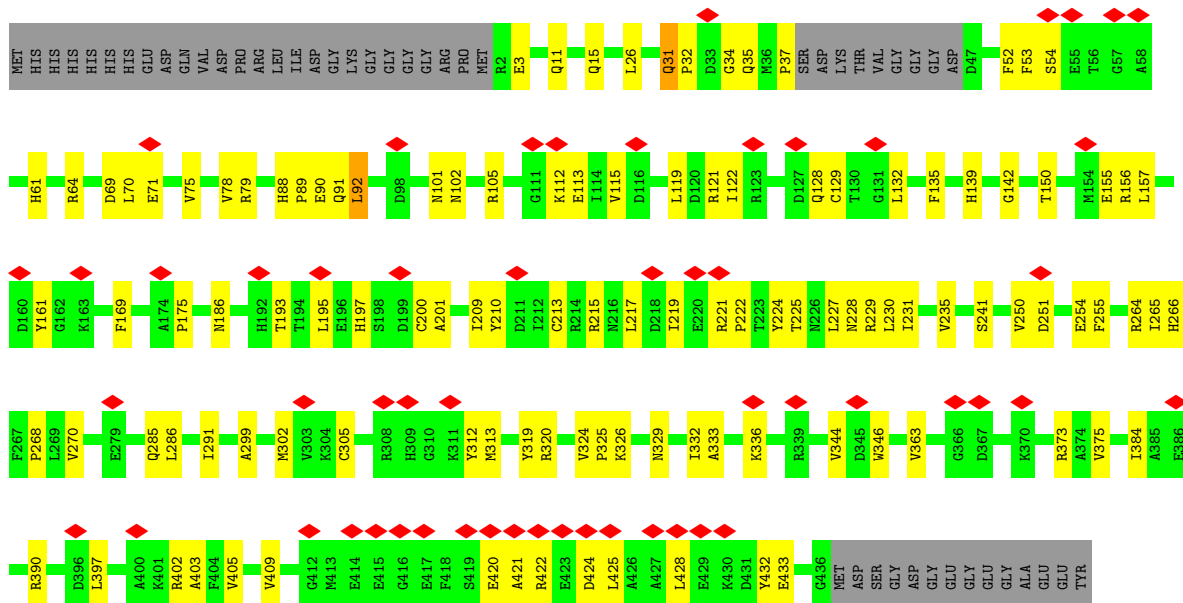
• Molecule 1: Tubulin alpha-1 chain



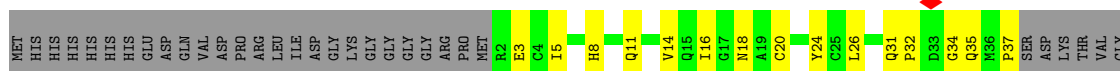


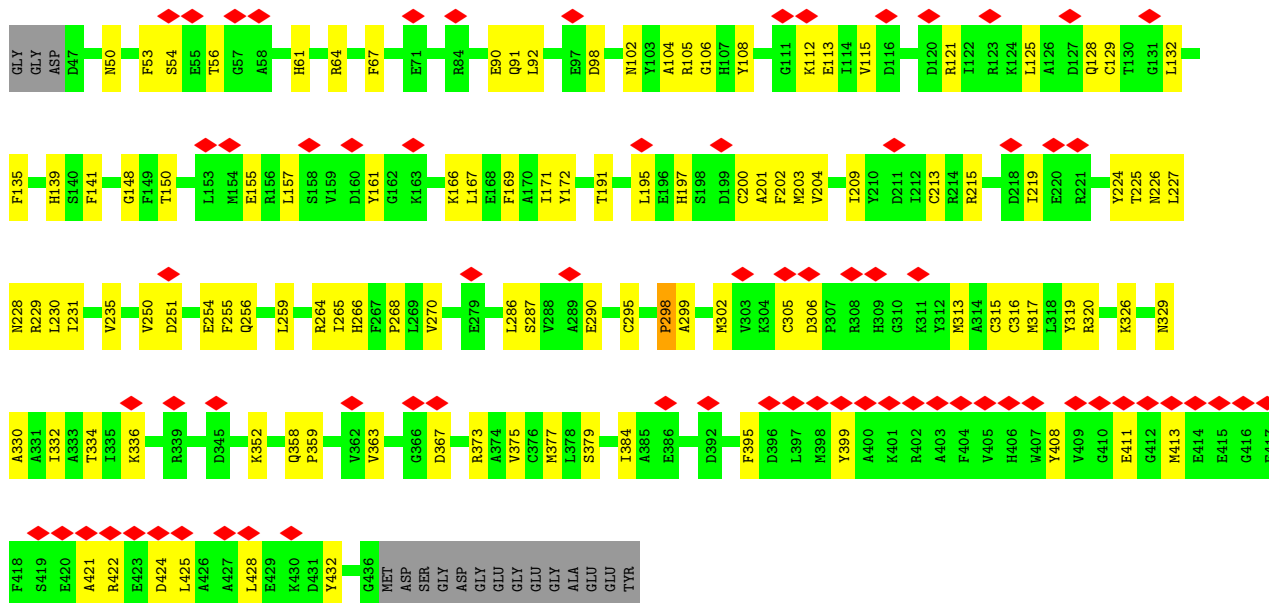


• Molecule 1: Tubulin alpha-1 chain

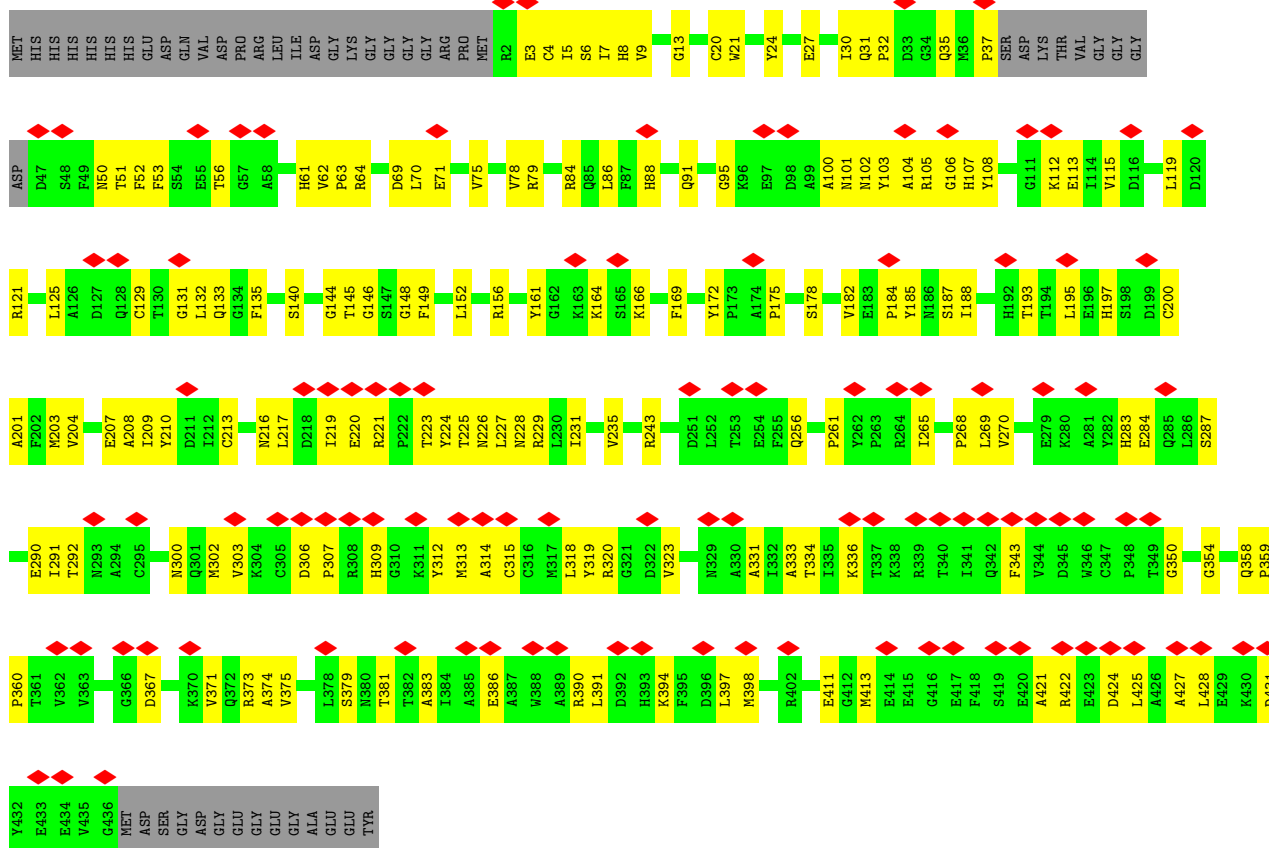


• Molecule 1: Tubulin alpha-1 chain

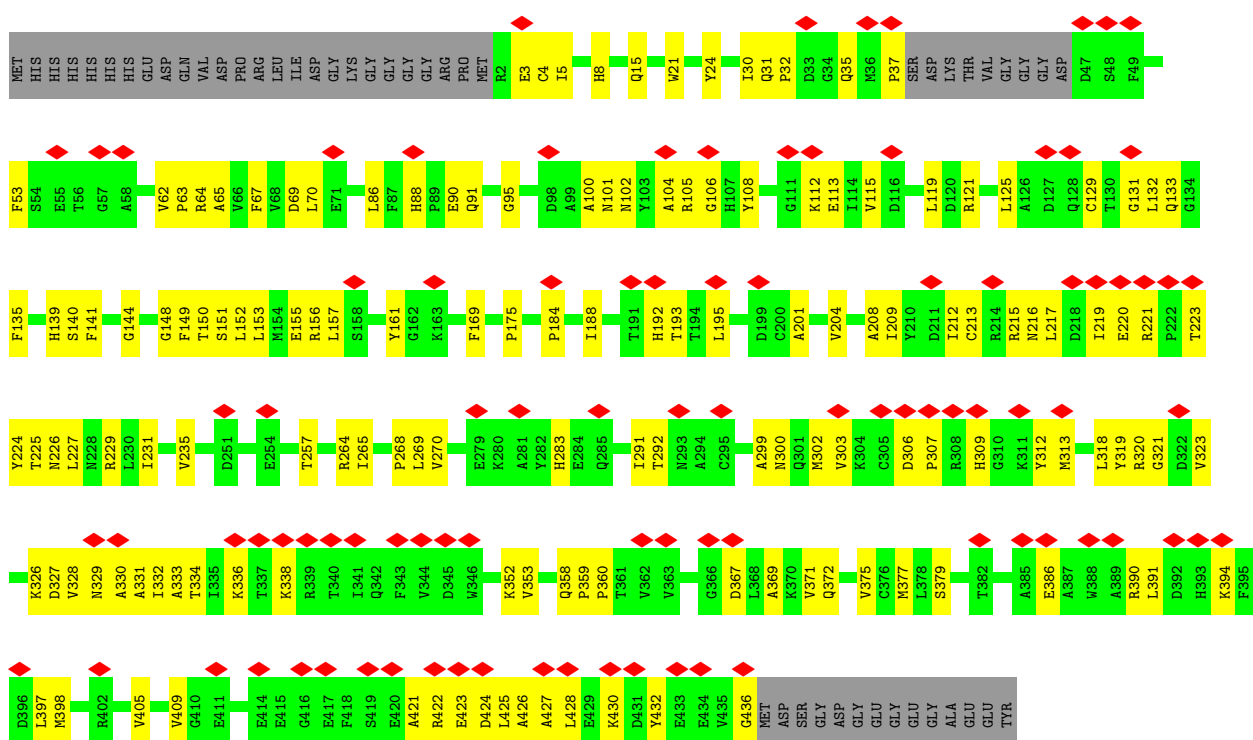




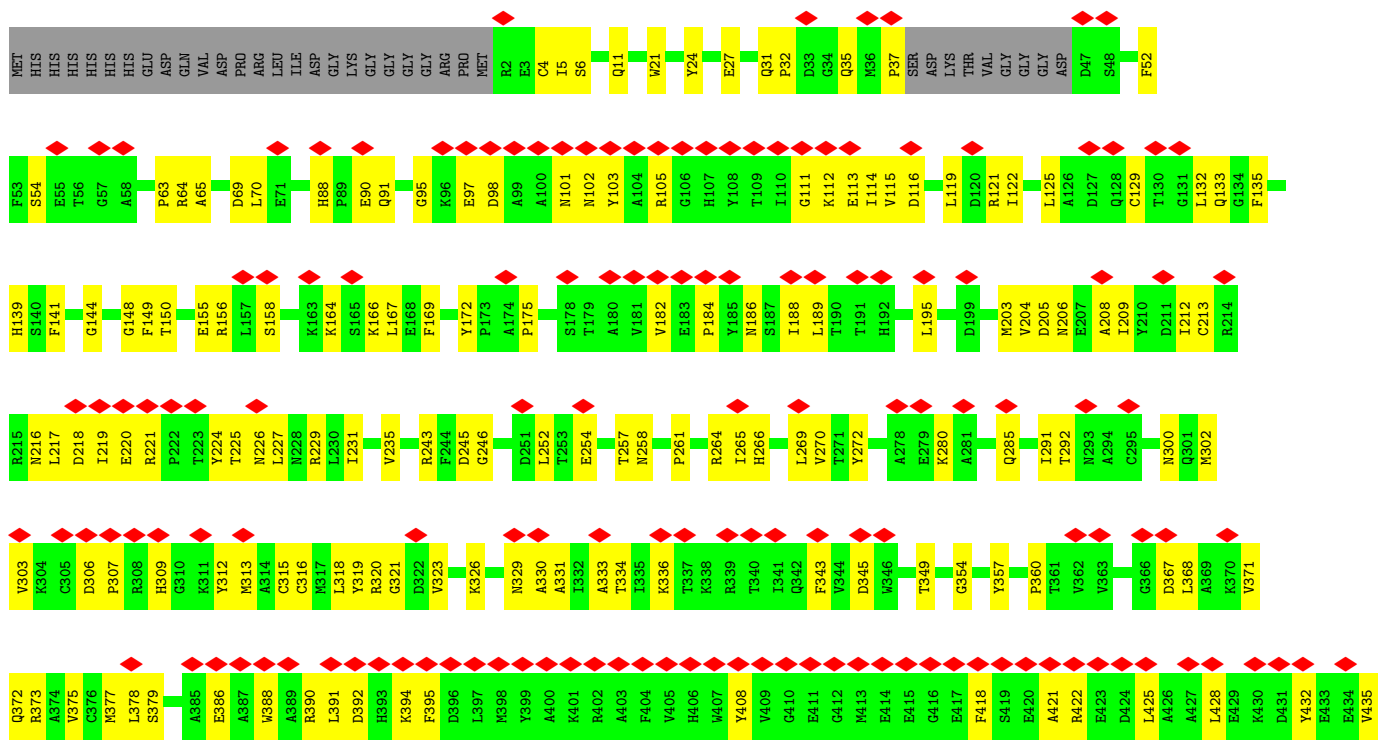
• Molecule 1: Tubulin alpha-1 chain

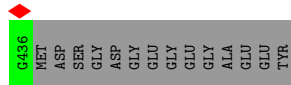


• Molecule 1: Tubulin alpha-1 chain

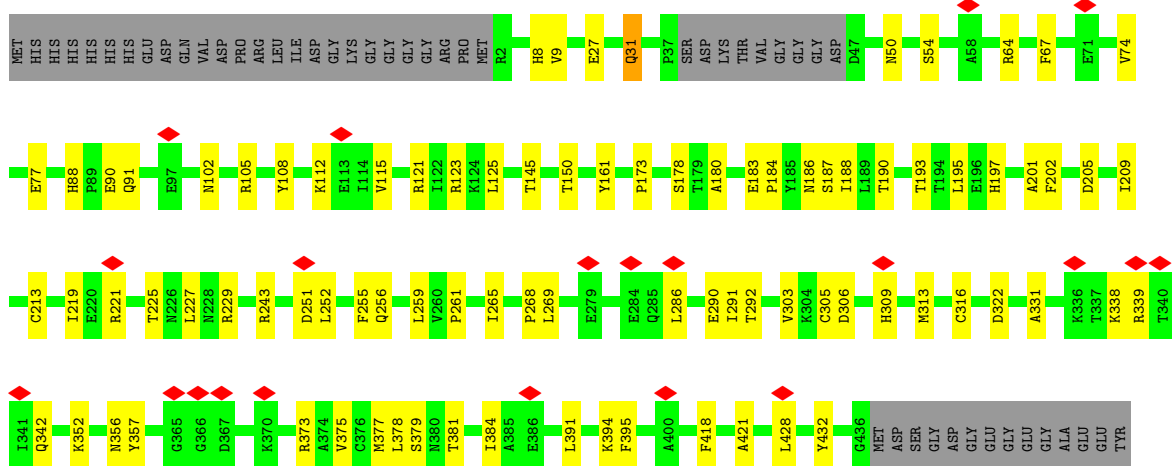


Molecule 1: Tubulin alpha-1 chain

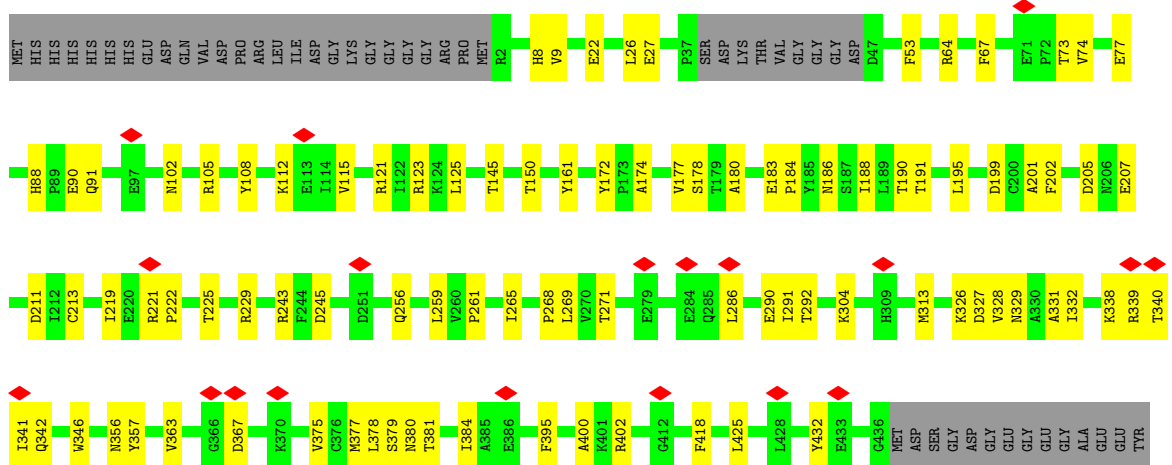




• Molecule 1: Tubulin alpha-1 chain



• Molecule 1: Tubulin alpha-1 chain



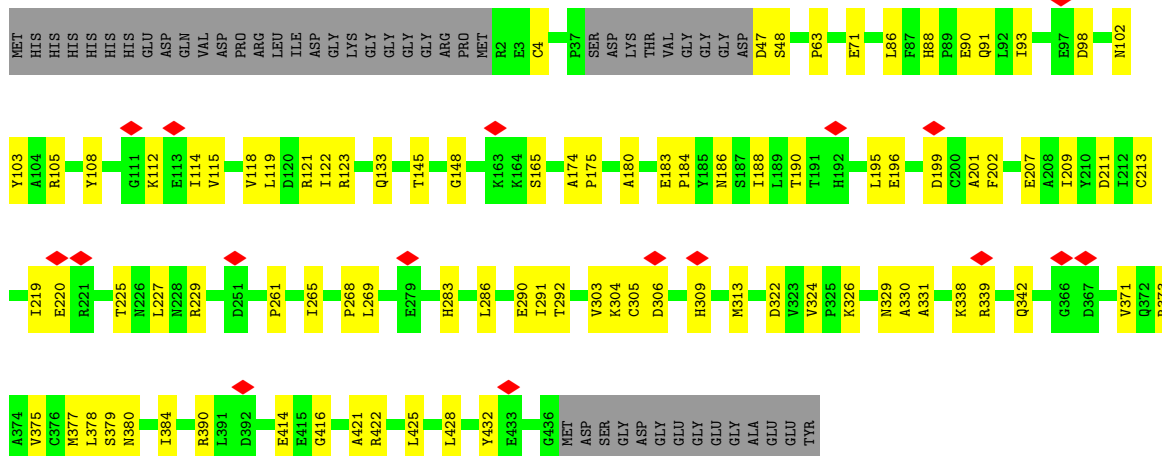
• Molecule 1: Tubulin alpha-1 chain





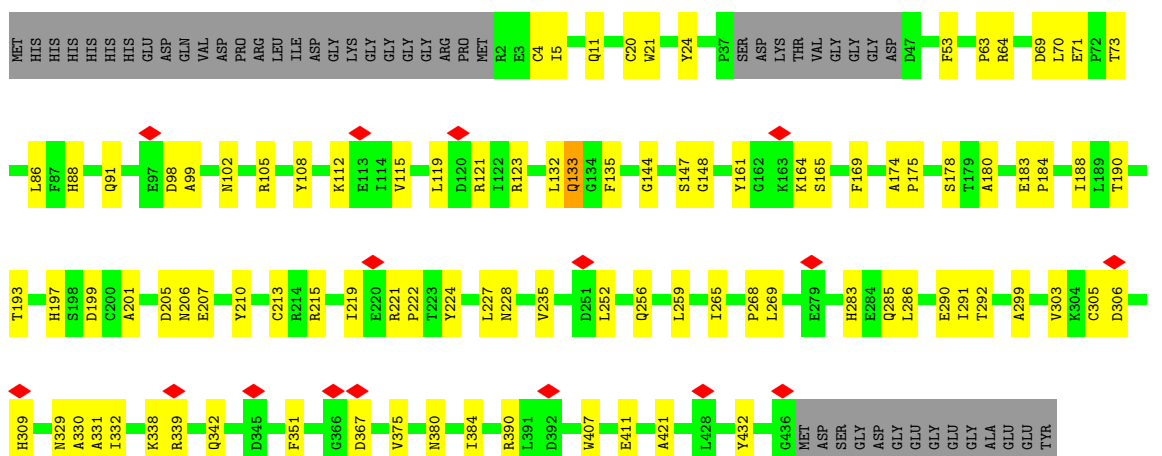
• Molecule 1: Tubulin alpha-1 chain

Chain 2E:



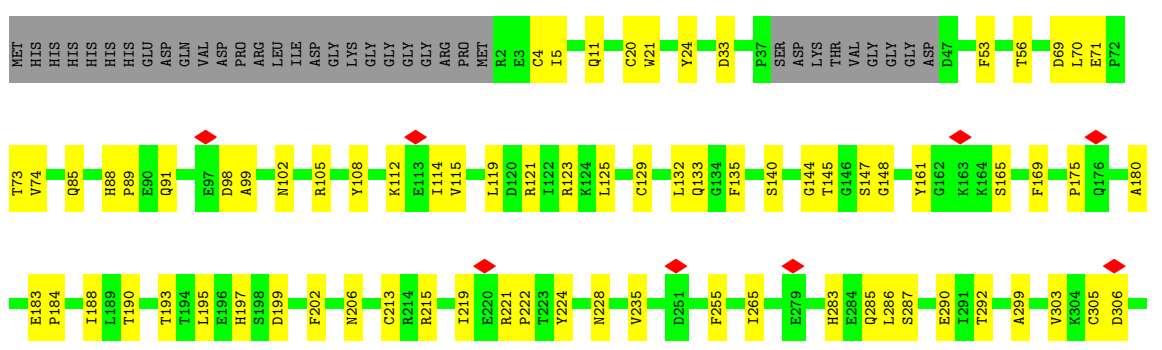
• Molecule 1: Tubulin alpha-1 chain

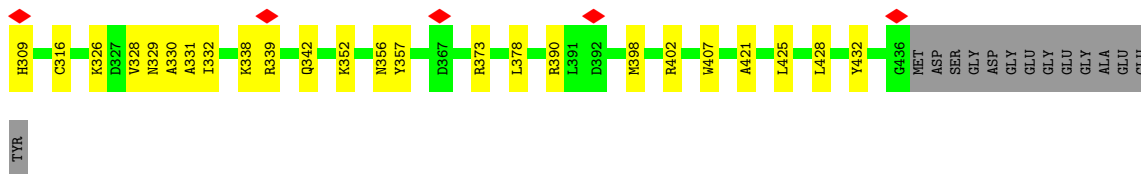
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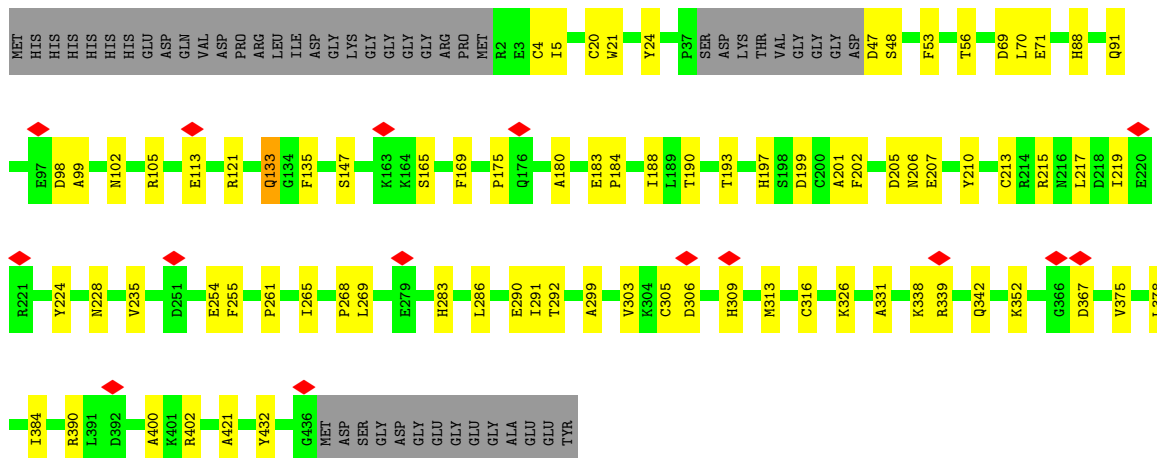
• Molecule 1: Tubulin alpha-1 chain

Chain 3C:

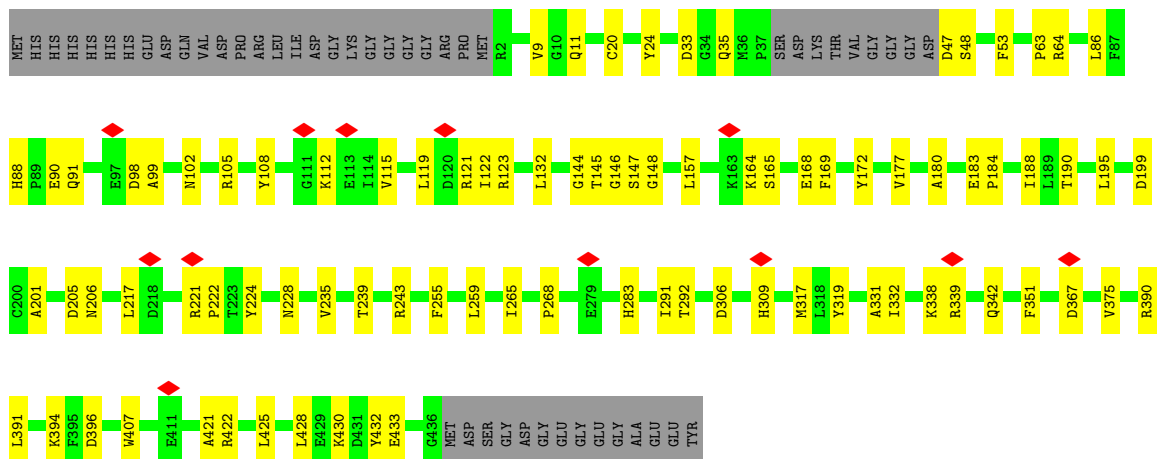




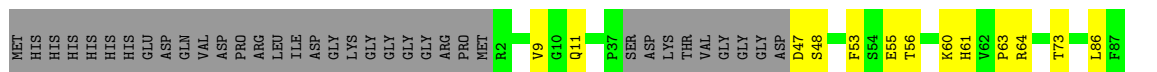
• Molecule 1: Tubulin alpha-1 chain



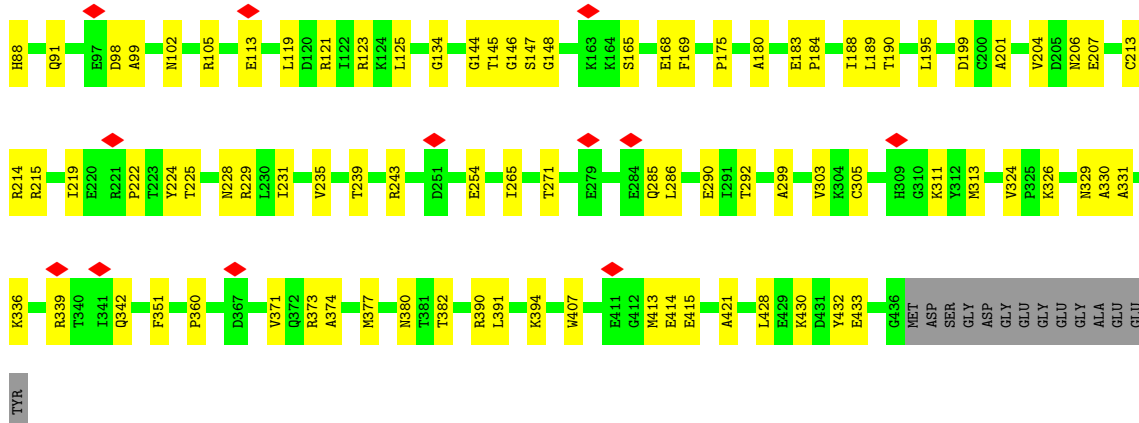
• Molecule 1: Tubulin alpha-1 chain



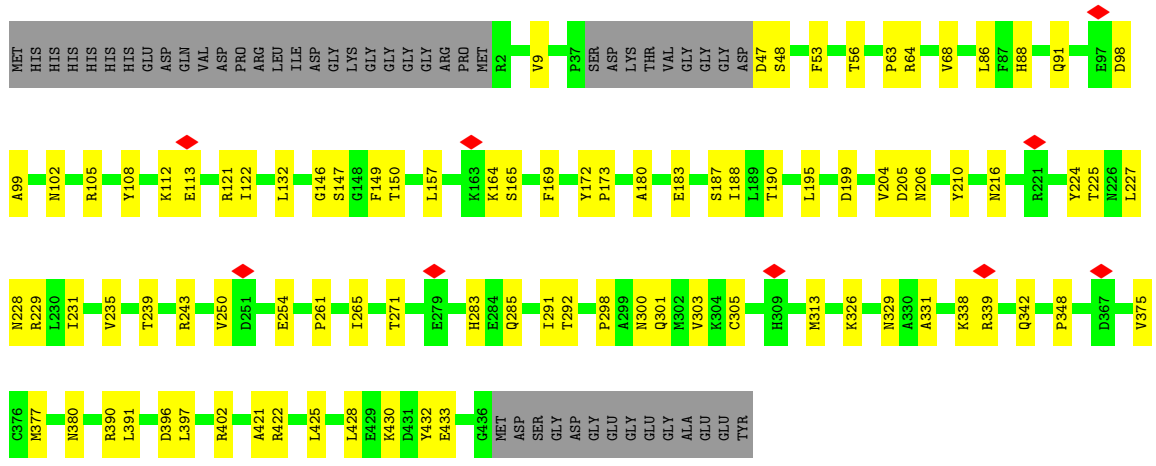
• Molecule 1: Tubulin alpha-1 chain



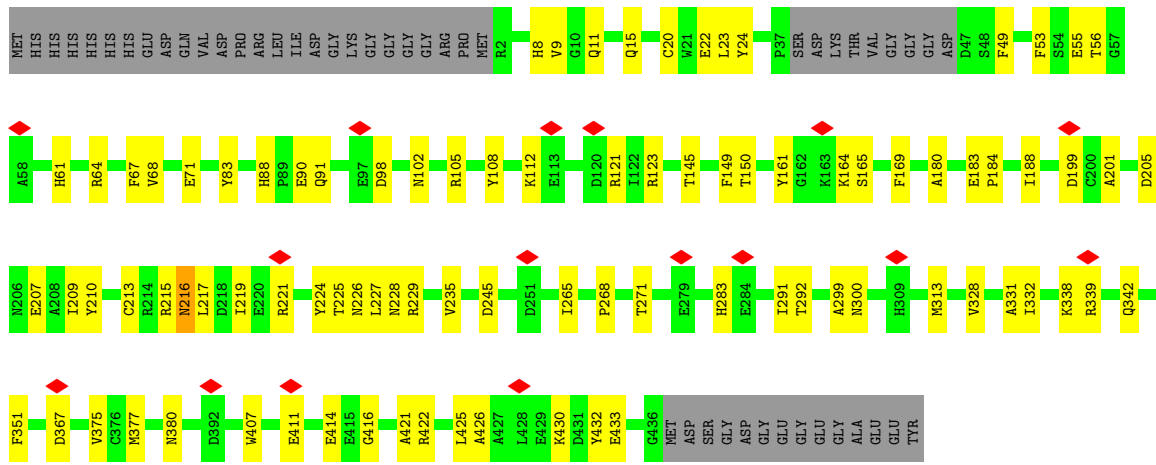





• Molecule 1: Tubulin alpha-1 chain

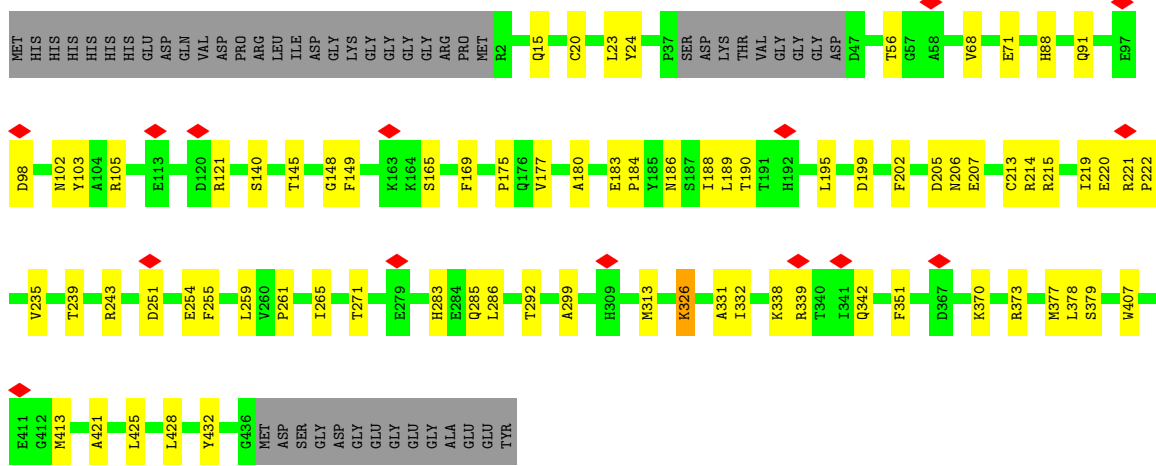


• Molecule 1: Tubulin alpha-1 chain



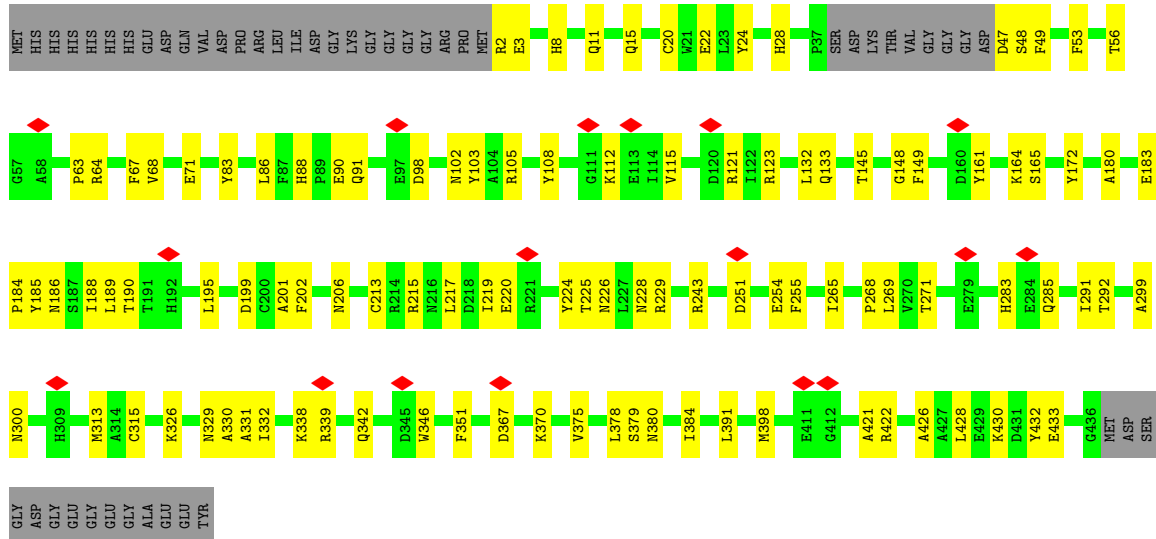
• Molecule 1: Tubulin alpha-1 chain

Chain 5C: 



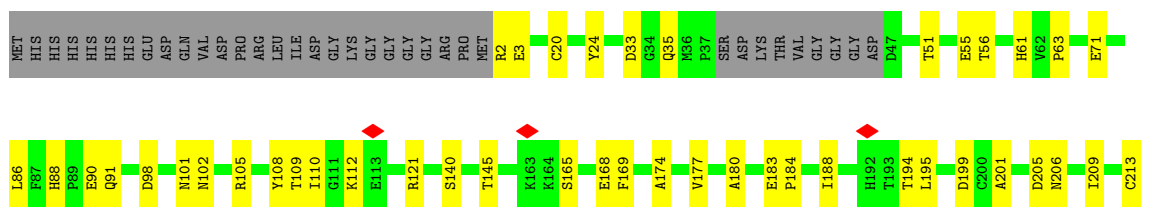
• Molecule 1: Tubulin alpha-1 chain

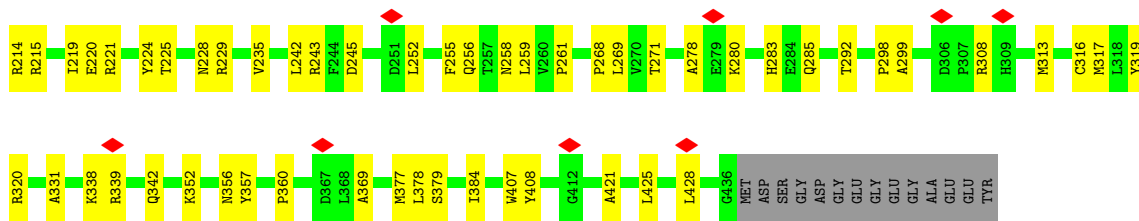
Chain 5E: 



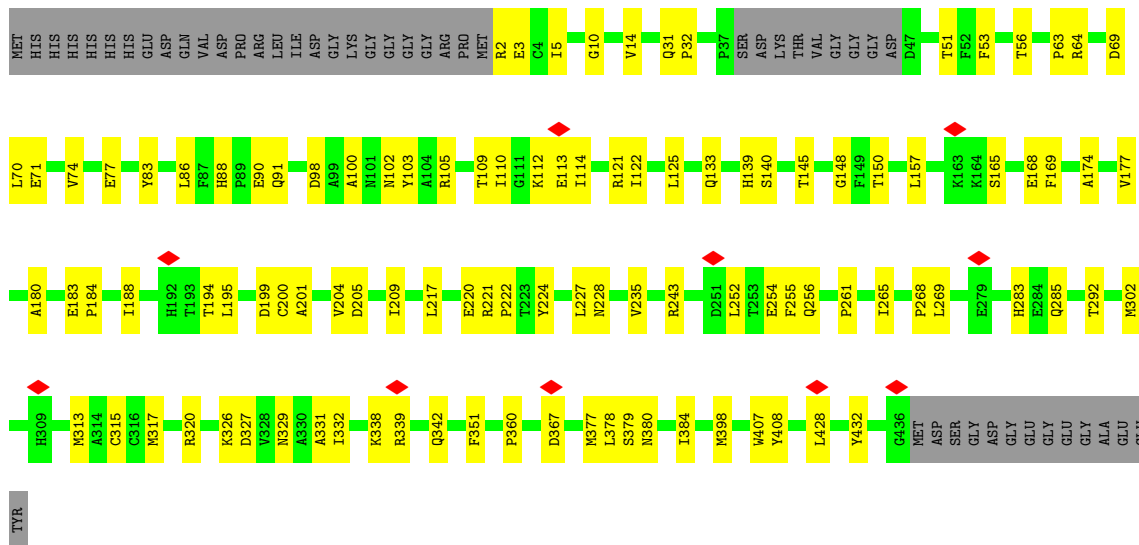
• Molecule 1: Tubulin alpha-1 chain

Chain 6A: 

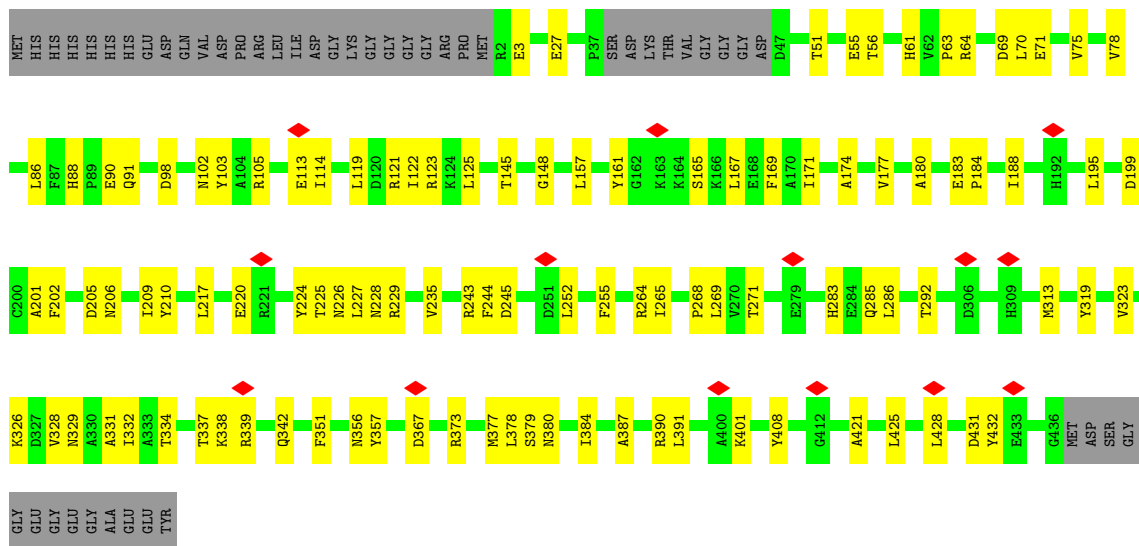




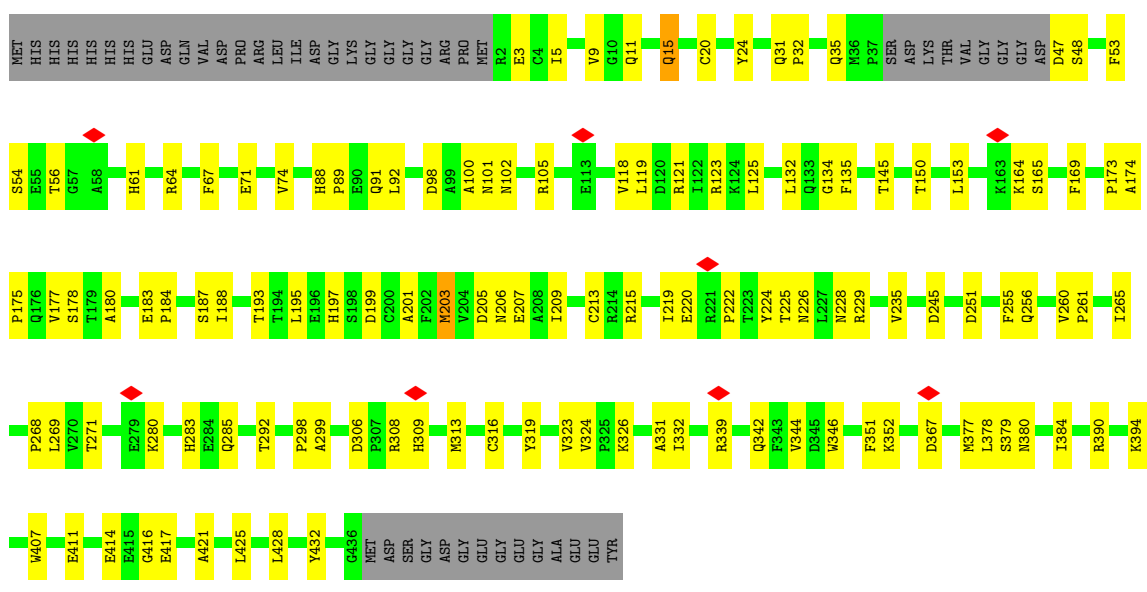
• Molecule 1: Tubulin alpha-1 chain



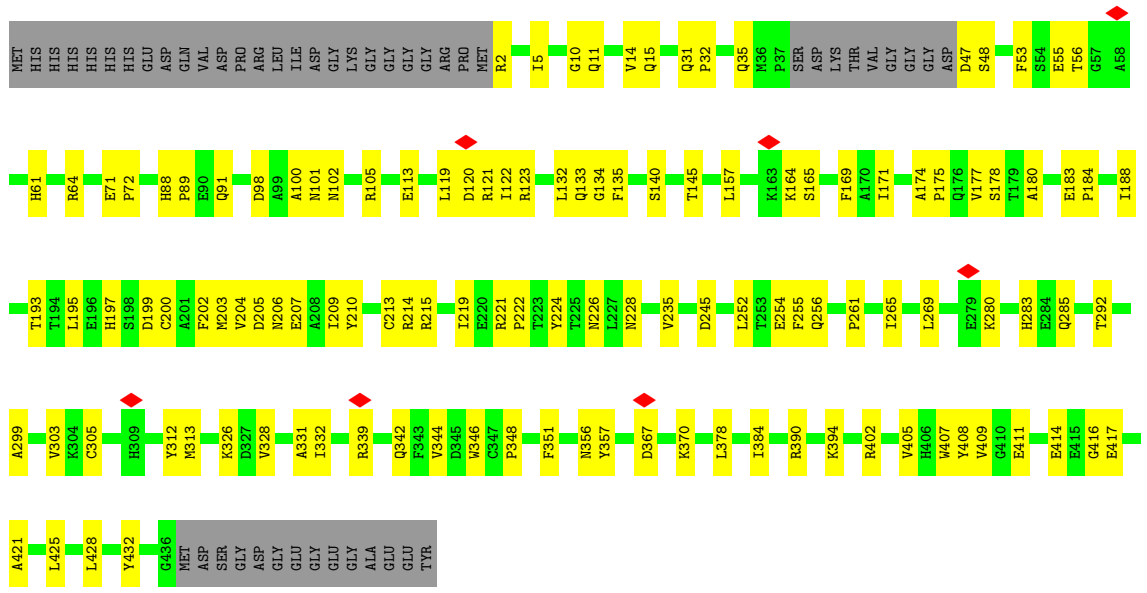
• Molecule 1: Tubulin alpha-1 chain



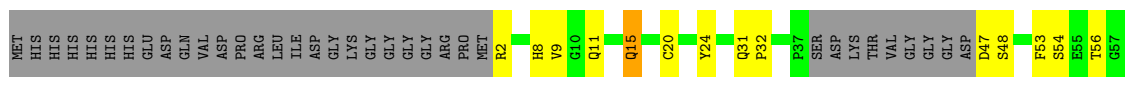
• Molecule 1: Tubulin alpha-1 chain



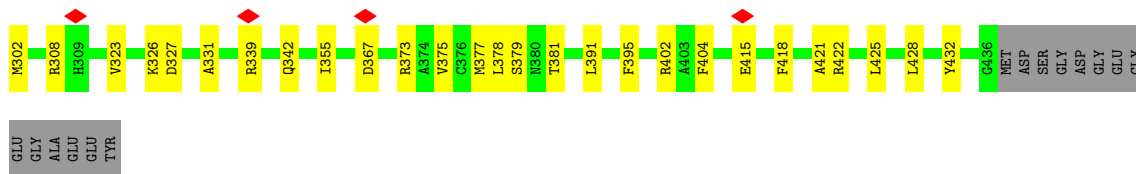
• Molecule 1: Tubulin alpha-1 chain



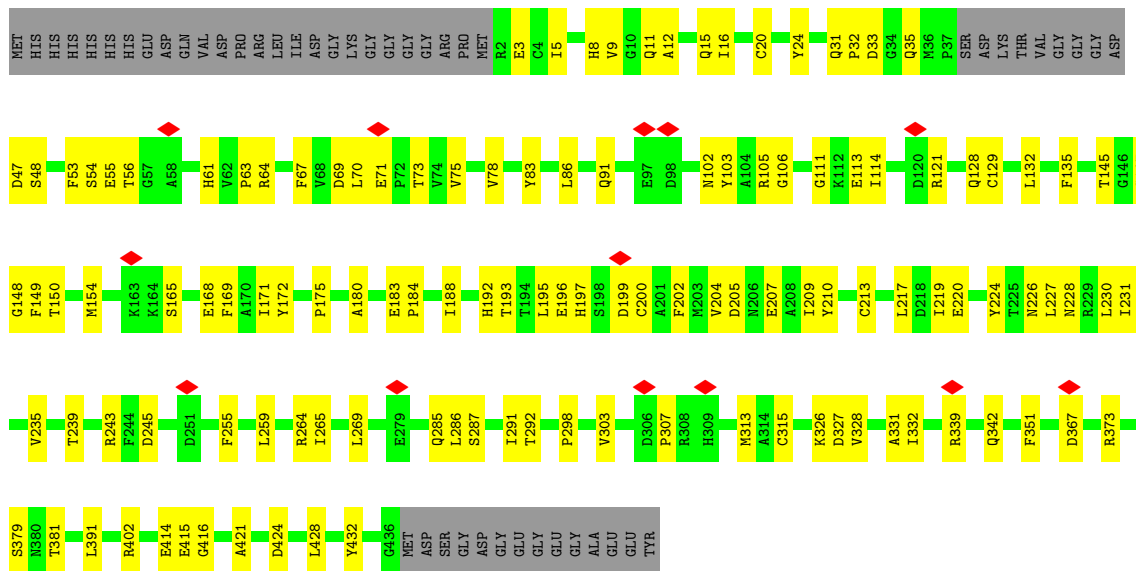
• Molecule 1: Tubulin alpha-1 chain



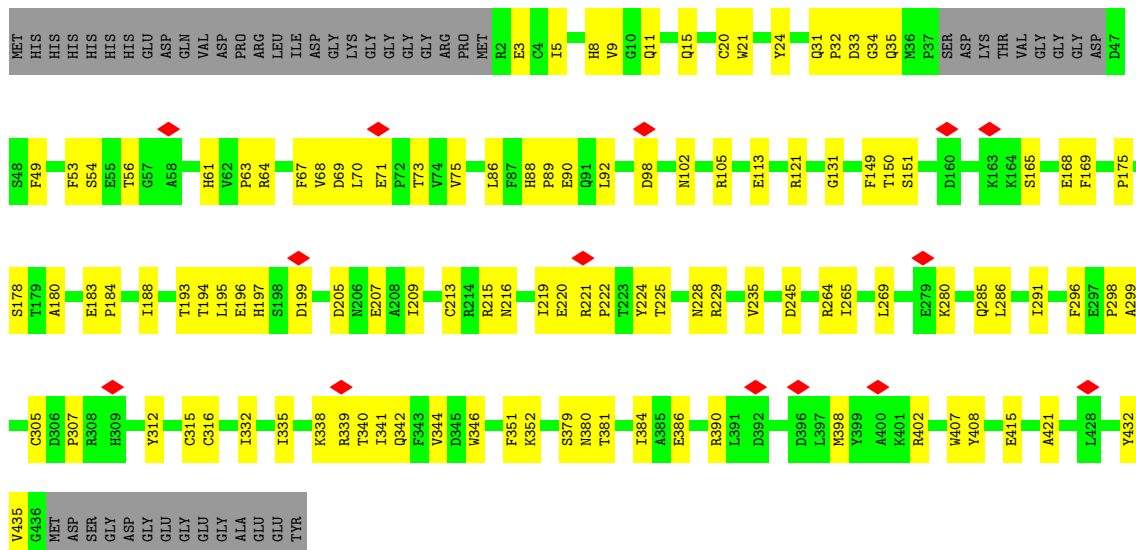




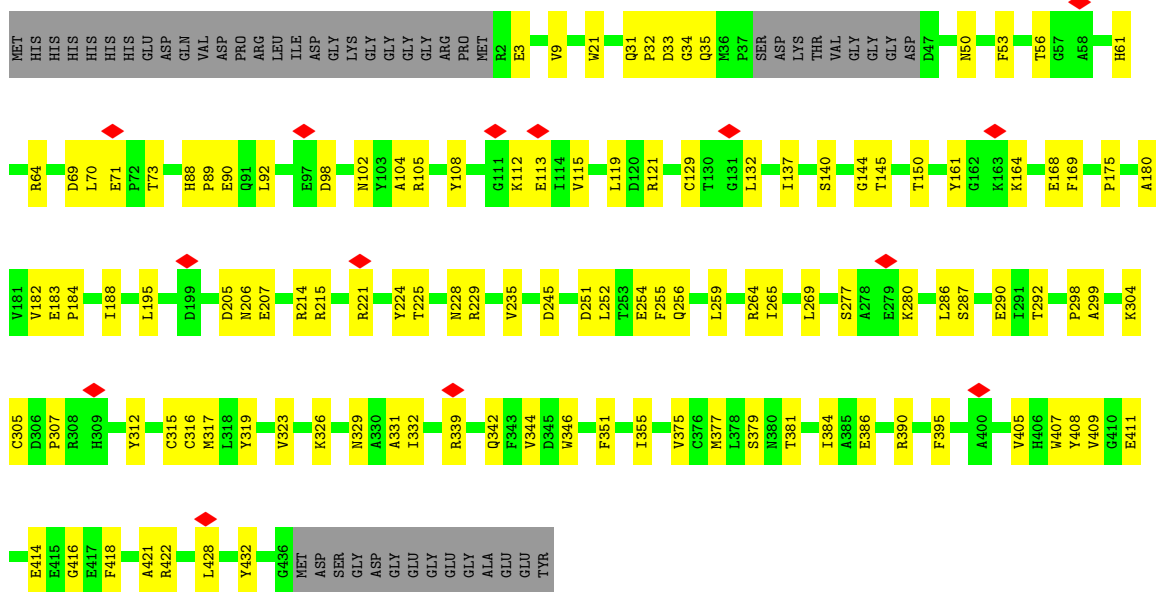
• Molecule 1: Tubulin alpha-1 chain



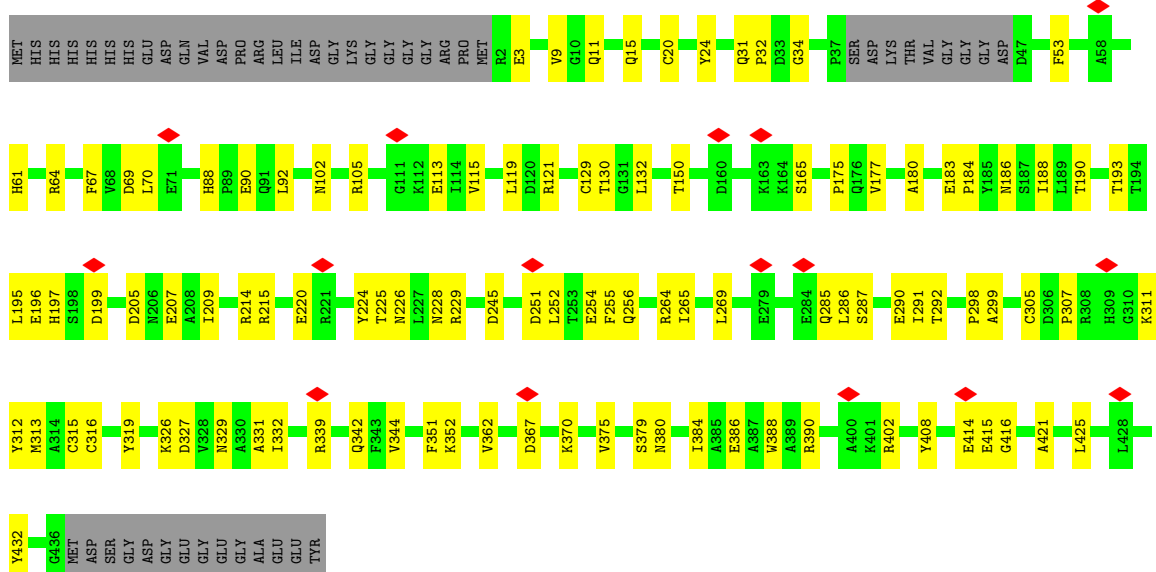
• Molecule 1: Tubulin alpha-1 chain



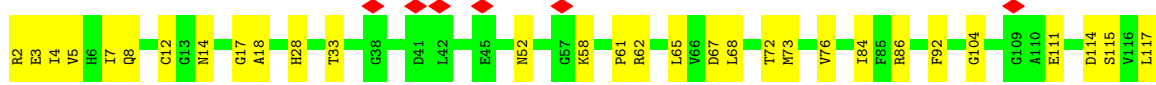
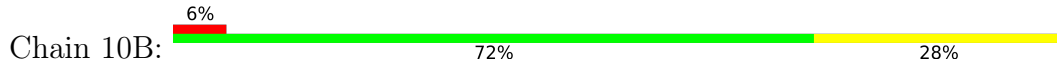
• Molecule 1: Tubulin alpha-1 chain



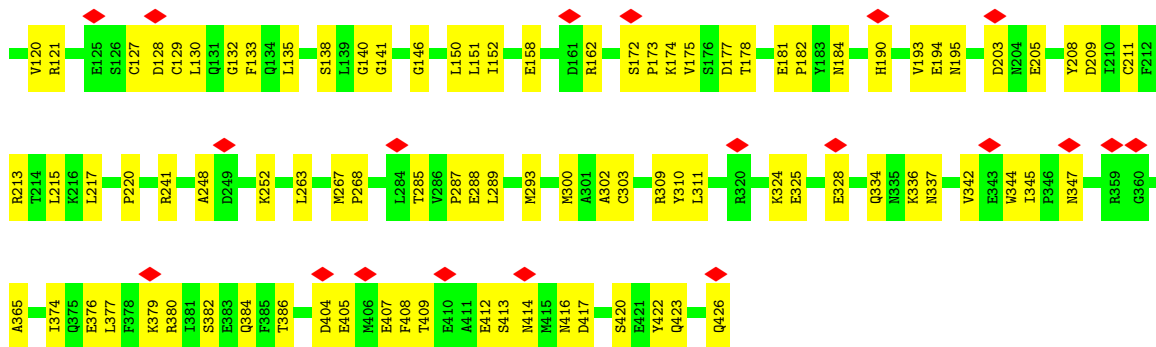
• Molecule 1: Tubulin alpha-1 chain



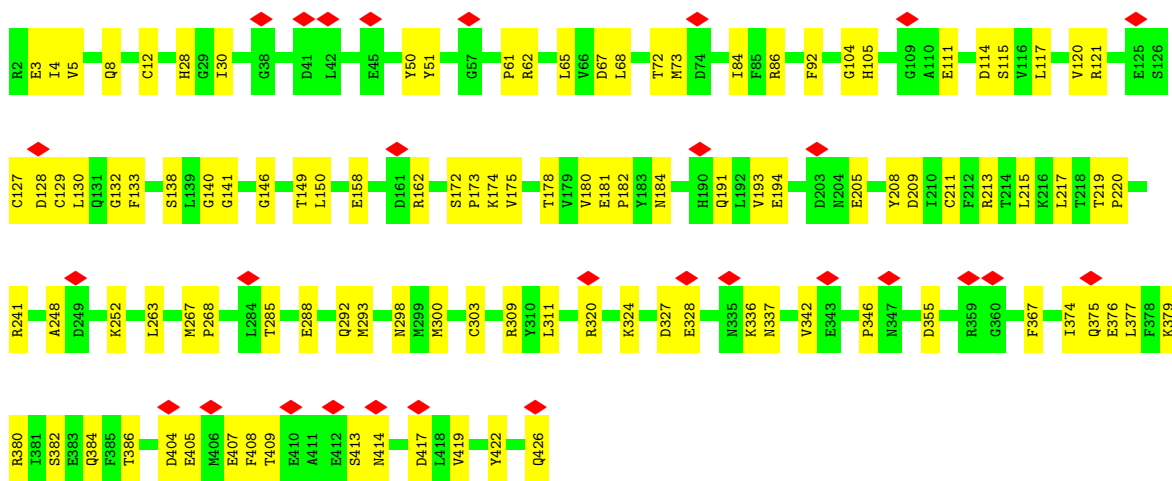
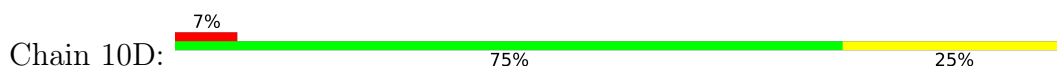
• Molecule 2: Tubulin beta-1 chain



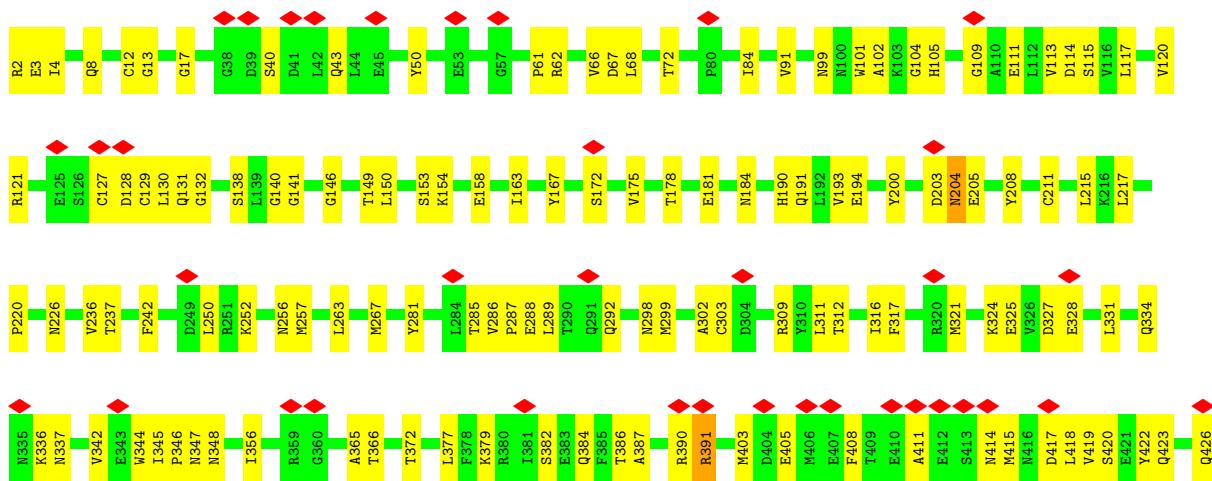




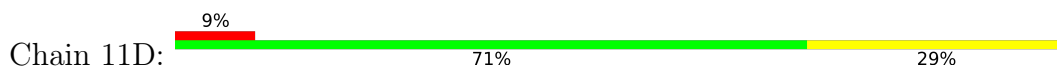
• Molecule 2: Tubulin beta-1 chain

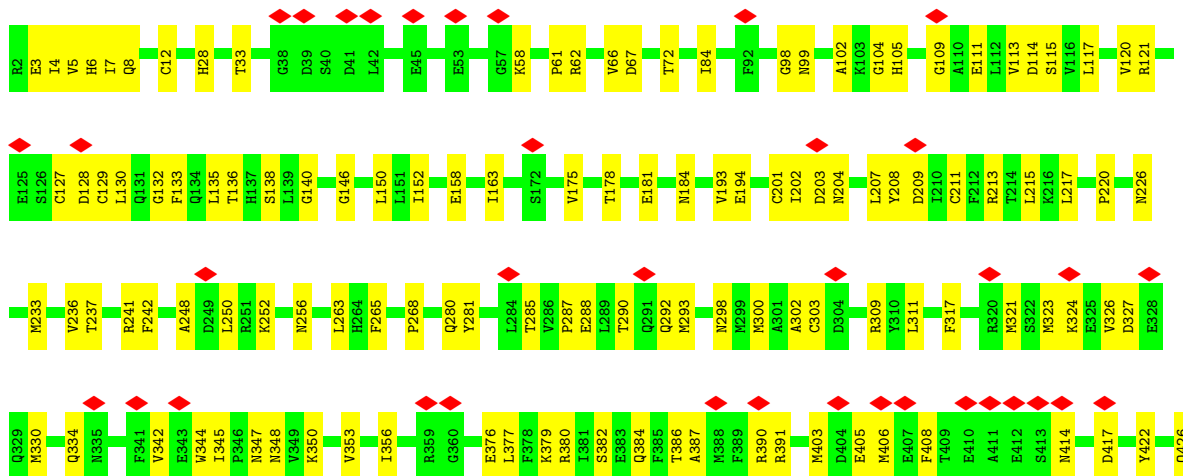


• Molecule 2: Tubulin beta-1 chain

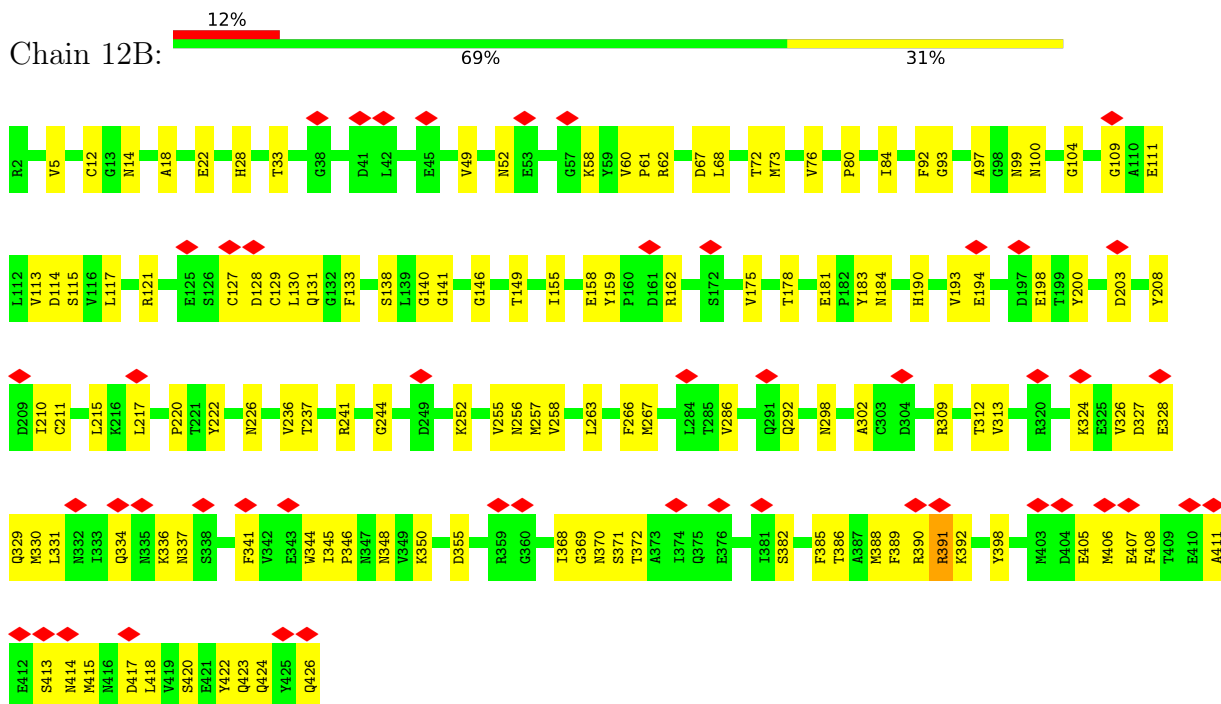


• Molecule 2: Tubulin beta-1 chain

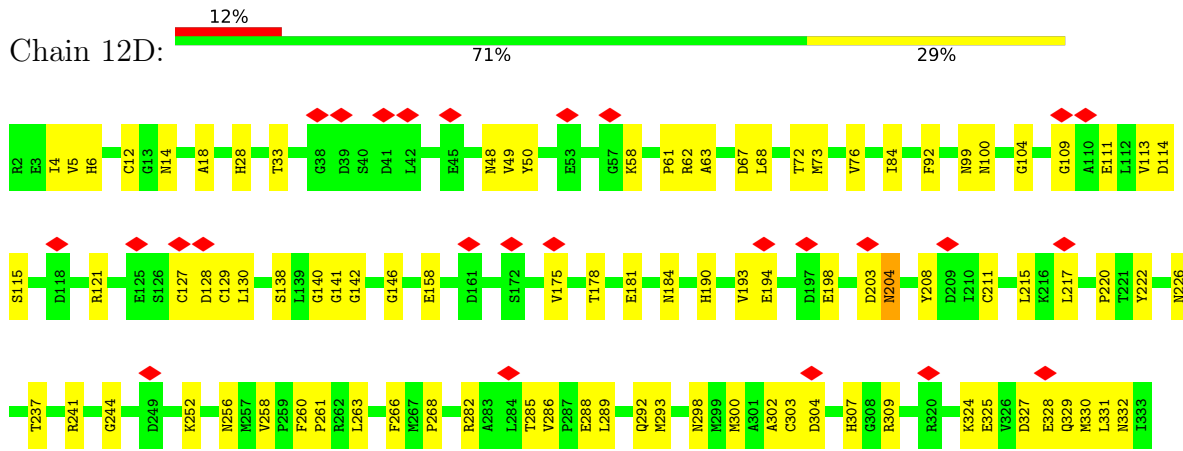




• Molecule 2: Tubulin beta-1 chain



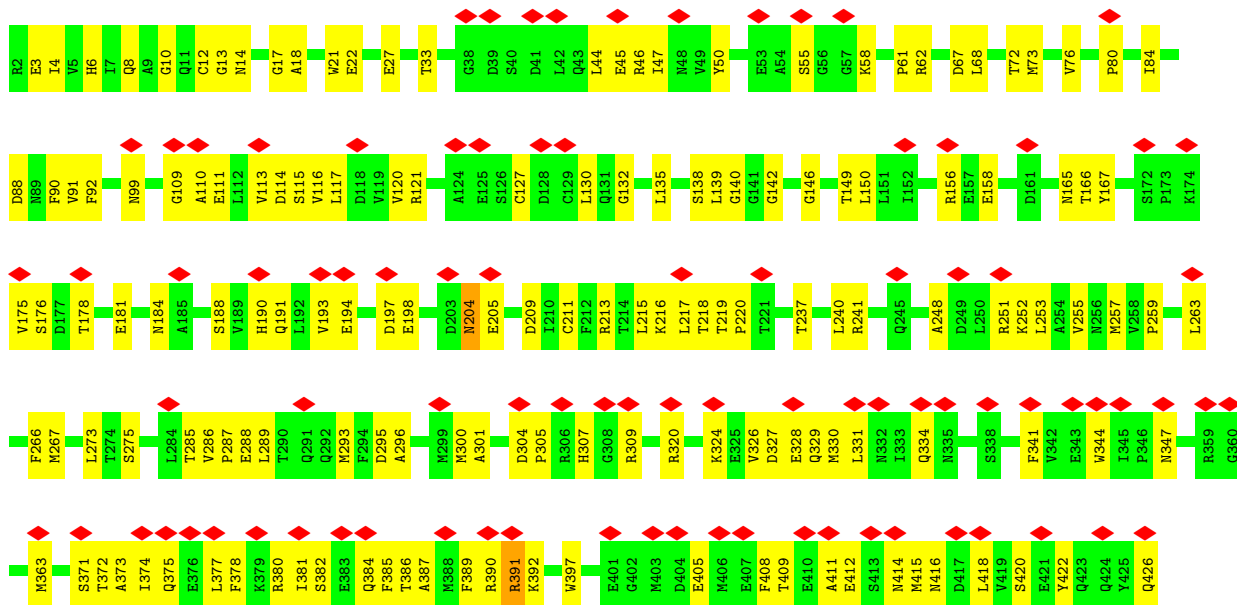
• Molecule 2: Tubulin beta-1 chain





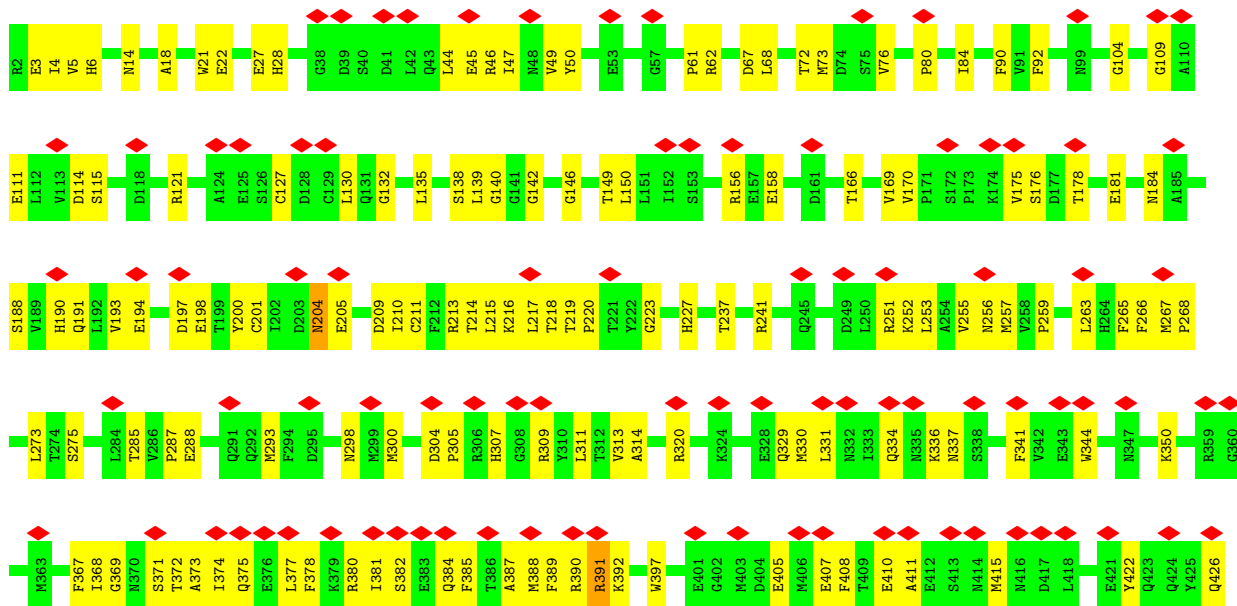
- Molecule 2: Tubulin beta-1 chain

Chain 13B:



- Molecule 2: Tubulin beta-1 chain

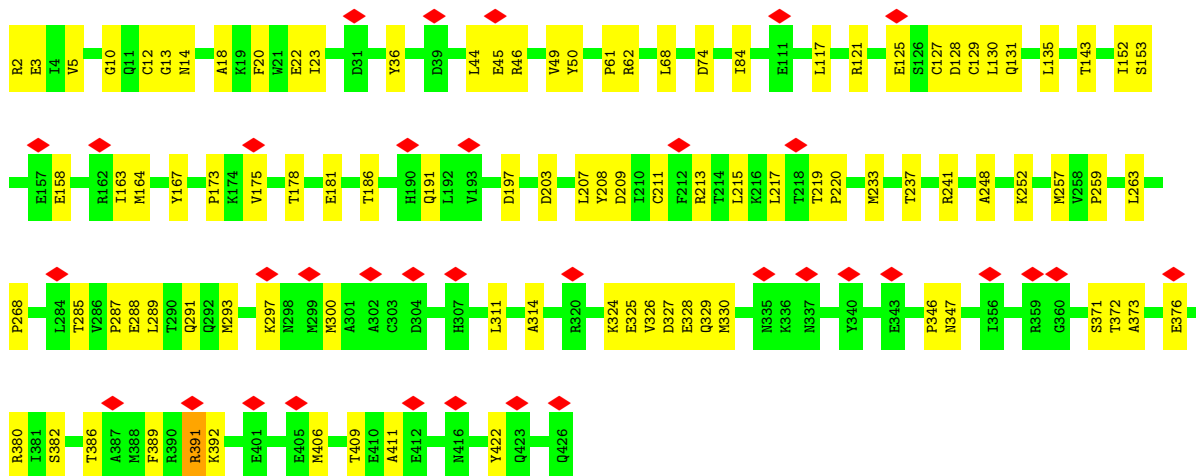
Chain 13D:



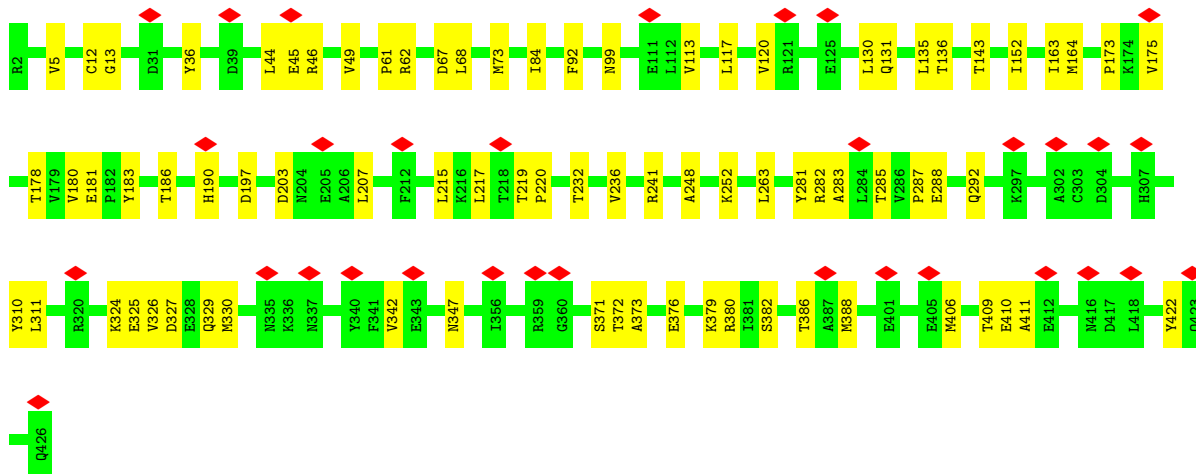
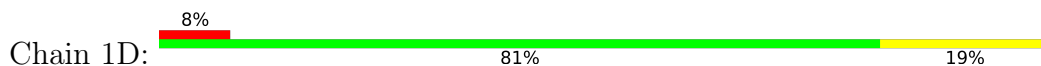
- Molecule 2: Tubulin beta-1 chain

Chain 1B:

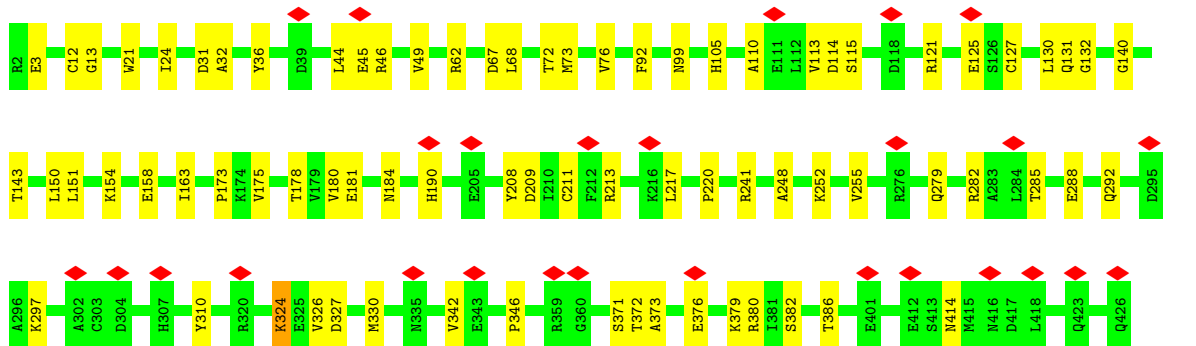
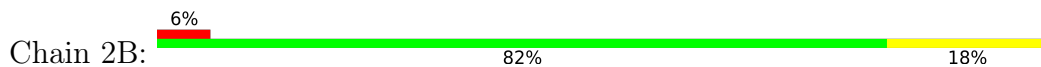




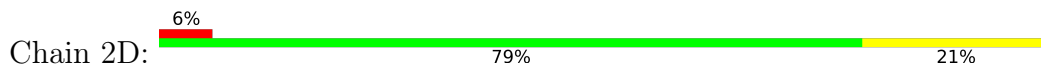
• Molecule 2: Tubulin beta-1 chain

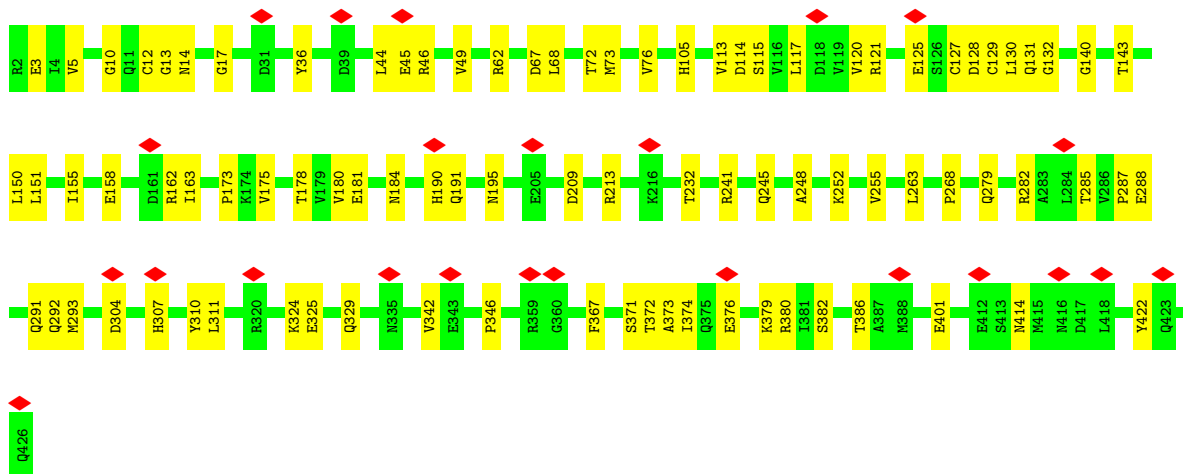


• Molecule 2: Tubulin beta-1 chain

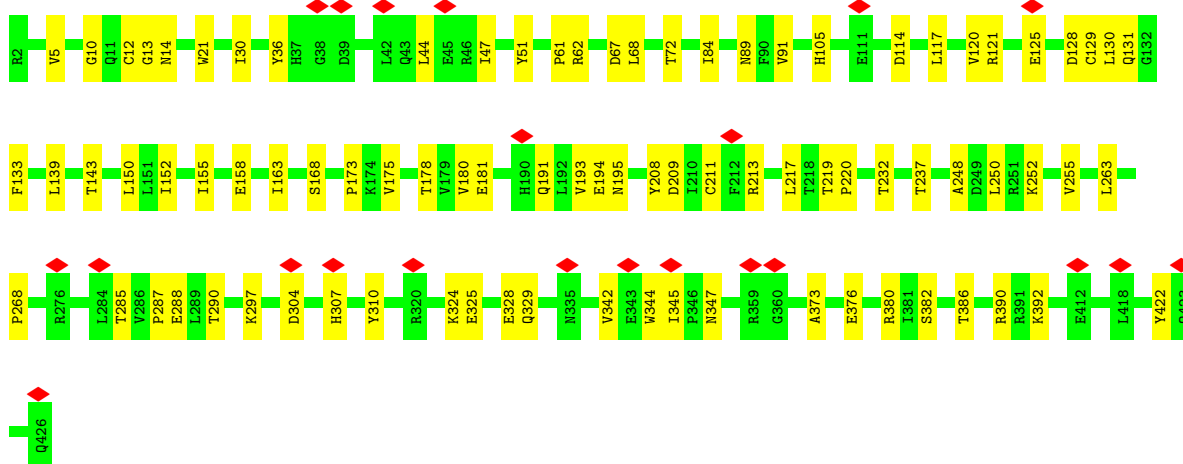
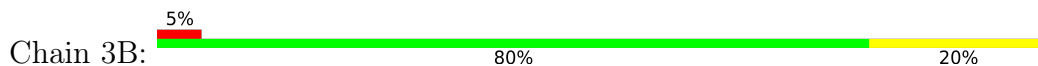


• Molecule 2: Tubulin beta-1 chain

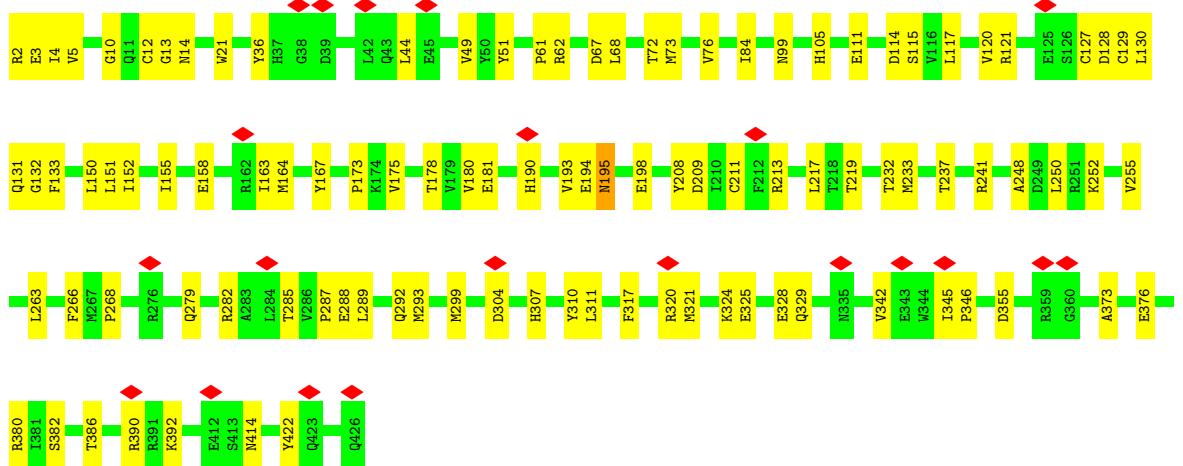
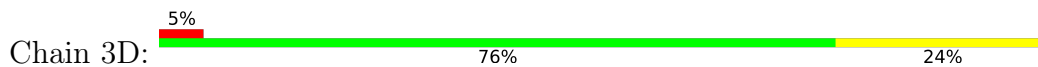




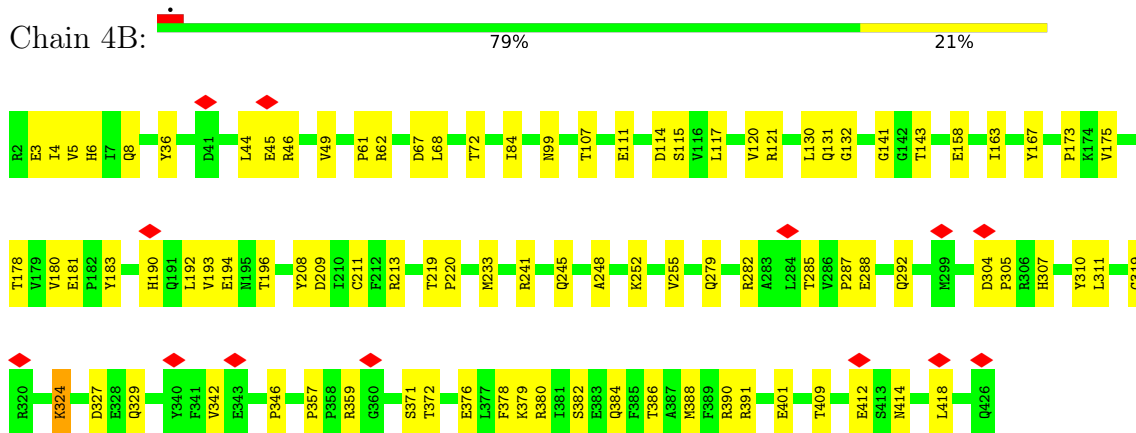
• Molecule 2: Tubulin beta-1 chain



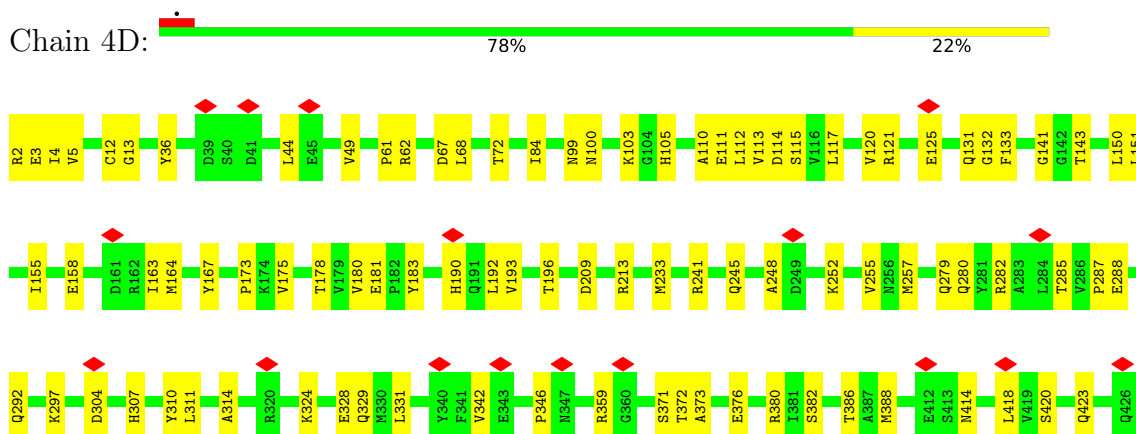
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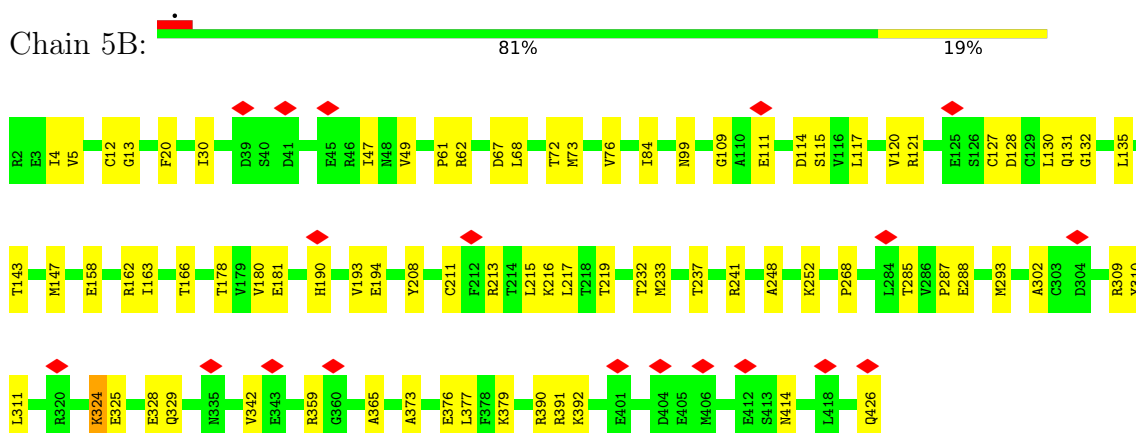
• Molecule 2: Tubulin beta-1 chain



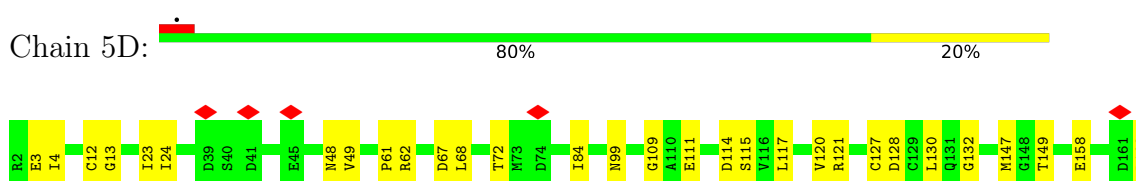
• Molecule 2: Tubulin beta-1 chain

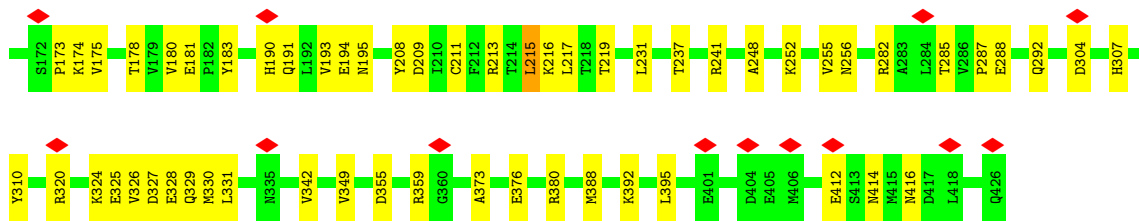


• Molecule 2: Tubulin beta-1 chain

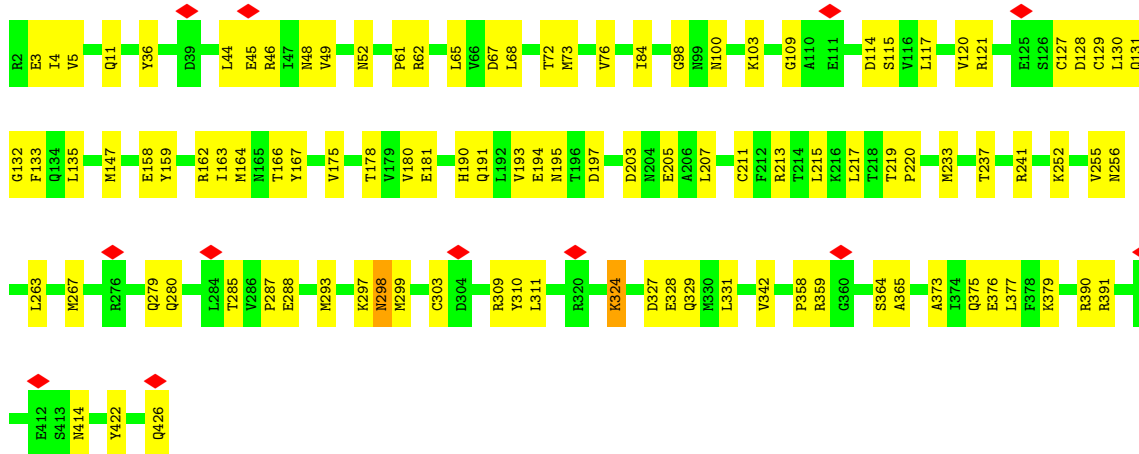
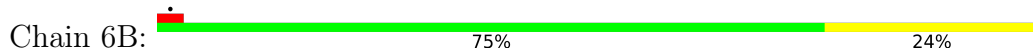


• Molecule 2: Tubulin beta-1 chain

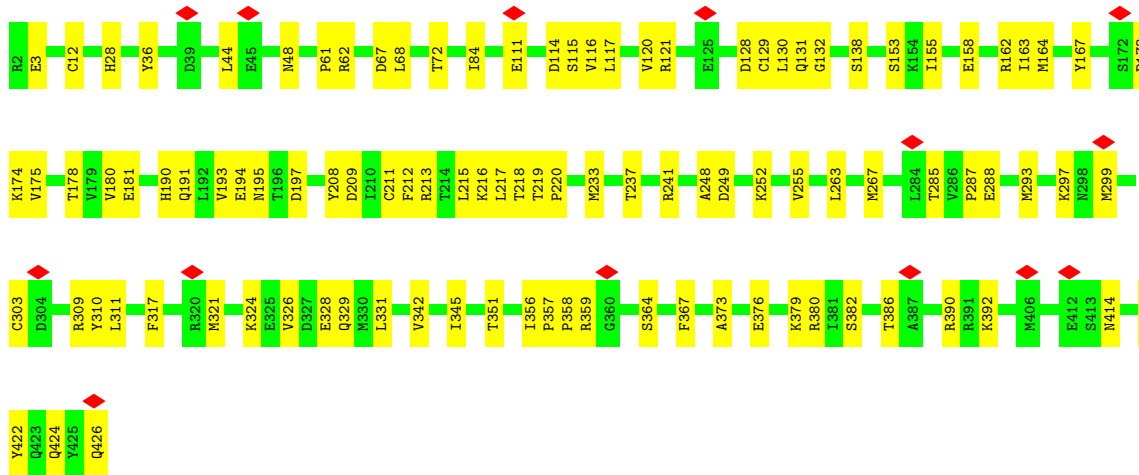
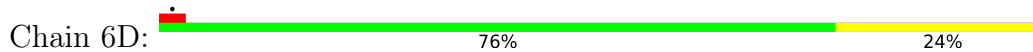




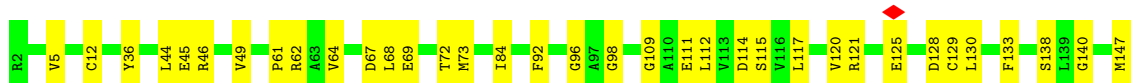
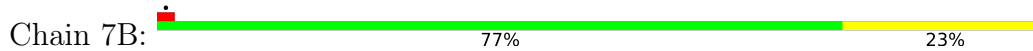
• Molecule 2: Tubulin beta-1 chain

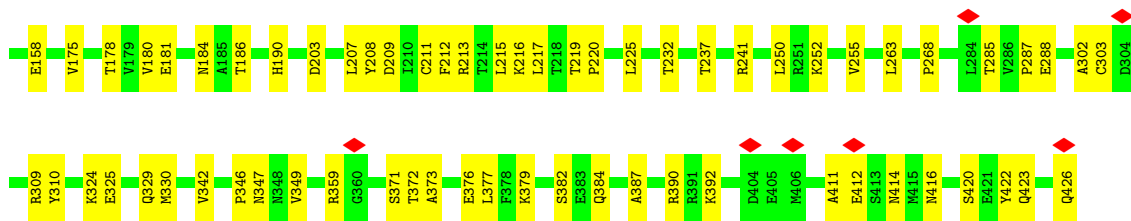


• Molecule 2: Tubulin beta-1 chain

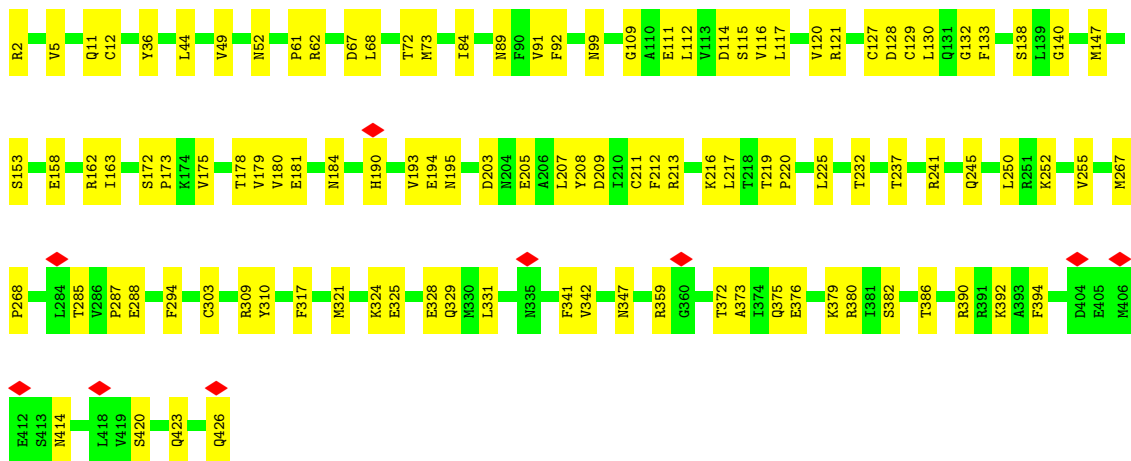
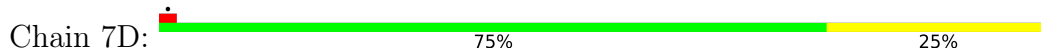


• Molecule 2: Tubulin beta-1 chain

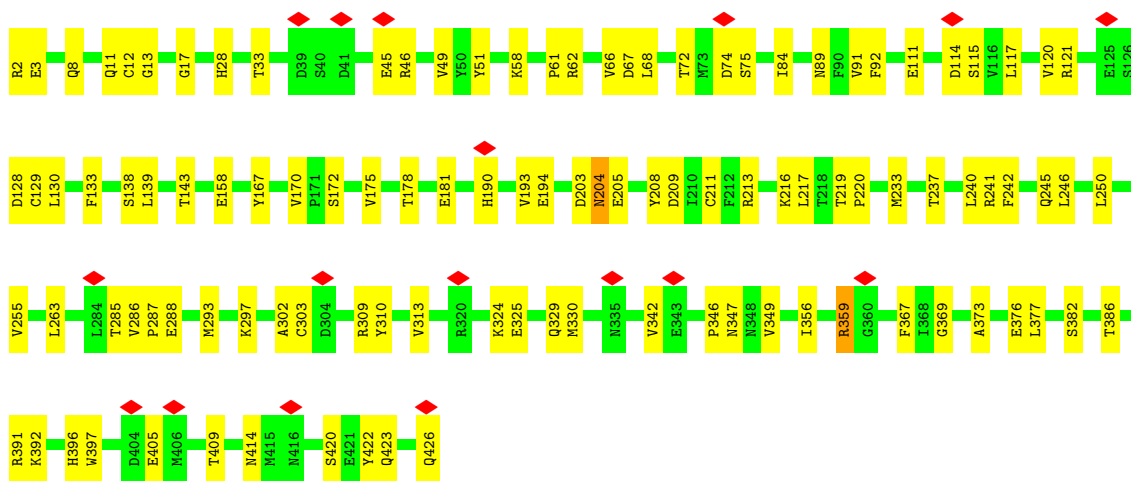
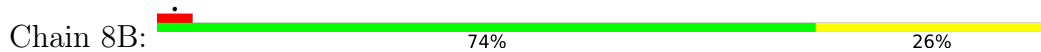




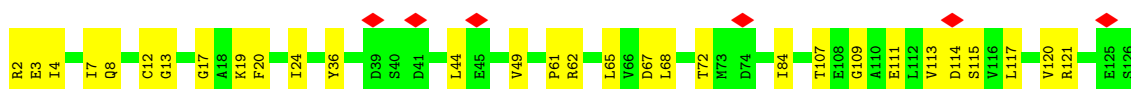
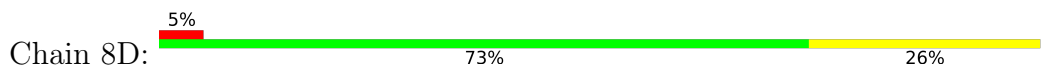
• Molecule 2: Tubulin beta-1 chain



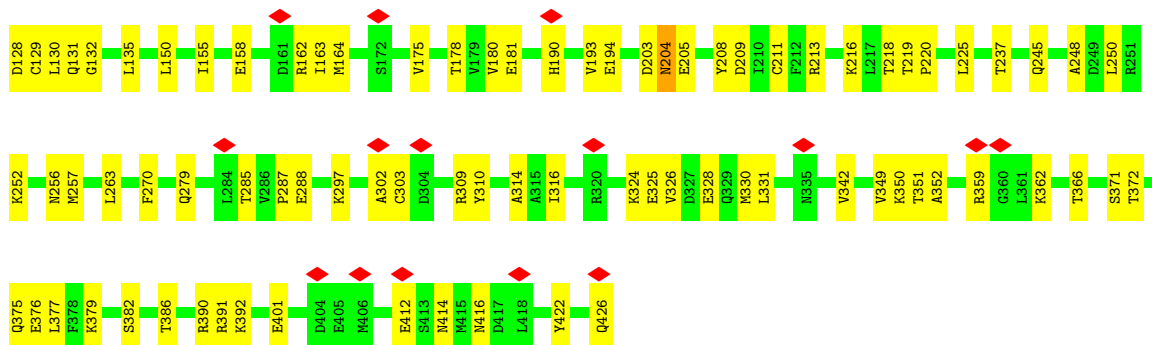
• Molecule 2: Tubulin beta-1 chain



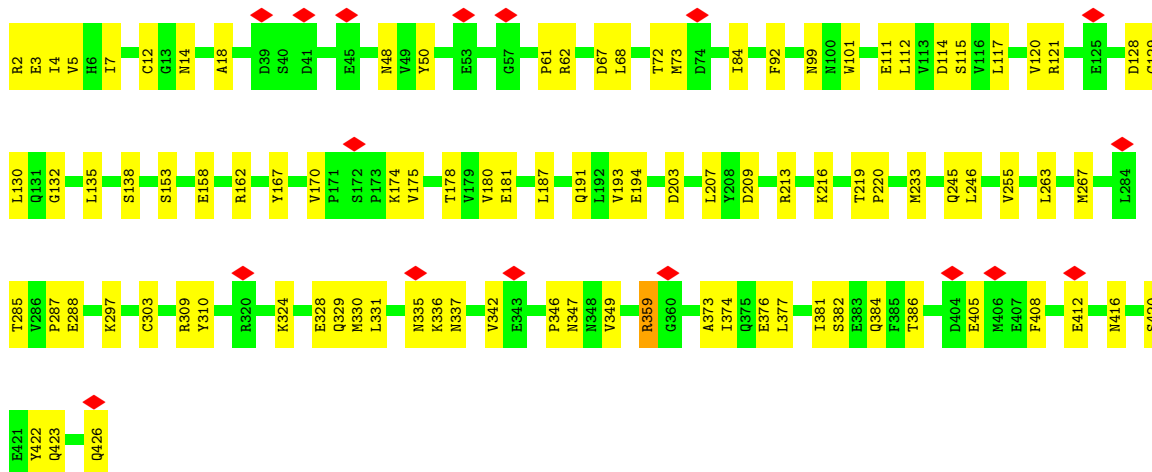
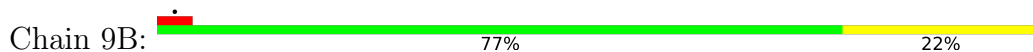
• Molecule 2: Tubulin beta-1 chain



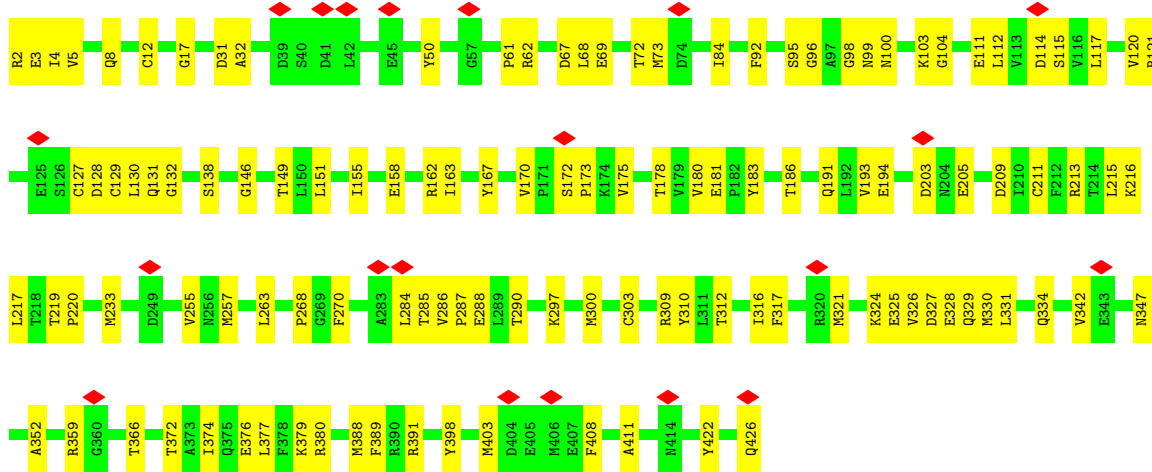
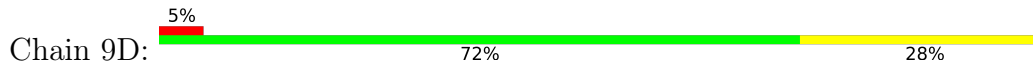




• Molecule 2: Tubulin beta-1 chain



• Molecule 2: Tubulin beta-1 chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39594	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.806	Depositor
Minimum map value	-3.037	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.233	Depositor
Recommended contour level	0.582	Depositor
Map size (Å)	431.984, 431.984, 431.984	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.102, 1.102, 1.102	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: GDP, GTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	10A	0.37	0/3419	0.59	2/4643 (0.0%)
1	10C	0.33	0/3419	0.54	0/4643
1	10E	0.34	0/3419	0.56	1/4643 (0.0%)
1	11A	0.33	0/3419	0.56	0/4643
1	11C	0.35	0/3419	0.59	1/4643 (0.0%)
1	11E	0.33	0/3419	0.56	1/4643 (0.0%)
1	12A	0.34	0/3419	0.57	1/4643 (0.0%)
1	12C	0.35	0/3419	0.59	2/4643 (0.0%)
1	12E	0.33	0/3419	0.58	2/4643 (0.0%)
1	13A	0.34	0/3419	0.58	0/4643
1	13C	0.36	0/3419	0.60	1/4643 (0.0%)
1	13E	0.34	0/3419	0.56	0/4643
1	1A	0.31	0/3419	0.52	0/4643
1	1C	0.32	0/3419	0.53	0/4643
1	1E	0.31	0/3419	0.52	0/4643
1	2A	0.31	0/3419	0.52	0/4643
1	2C	0.30	0/3419	0.51	0/4643
1	2E	0.30	0/3419	0.51	0/4643
1	3A	0.30	0/3419	0.50	0/4643
1	3C	0.30	0/3419	0.51	0/4643
1	3E	0.30	0/3419	0.50	0/4643
1	4A	0.31	0/3419	0.51	0/4643
1	4C	0.31	0/3419	0.50	0/4643
1	4E	0.31	0/3419	0.51	0/4643
1	5A	0.31	0/3419	0.51	0/4643
1	5C	0.32	0/3419	0.52	1/4643 (0.0%)
1	5E	0.31	0/3419	0.52	0/4643
1	6A	0.32	0/3419	0.52	0/4643
1	6C	0.33	0/3419	0.53	0/4643
1	6E	0.32	0/3419	0.53	0/4643
1	7A	0.35	0/3419	0.55	1/4643 (0.0%)
1	7C	0.35	0/3419	0.55	0/4643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	7E	0.35	0/3419	0.56	1/4643 (0.0%)
1	8A	0.33	0/3419	0.55	1/4643 (0.0%)
1	8C	0.34	0/3419	0.56	0/4643
1	8E	0.33	0/3419	0.54	0/4643
1	9A	0.32	0/3419	0.54	0/4643
1	9C	0.33	0/3419	0.55	1/4643 (0.0%)
1	9E	0.32	0/3419	0.54	0/4643
2	10B	0.33	0/3417	0.57	1/4627 (0.0%)
2	10D	0.33	0/3417	0.56	0/4627
2	11B	0.34	0/3417	0.57	0/4627
2	11D	0.31	0/3417	0.57	0/4627
2	12B	0.35	0/3417	0.60	0/4627
2	12D	0.33	0/3417	0.59	0/4627
2	13B	0.33	0/3417	0.58	0/4627
2	13D	0.33	0/3417	0.58	0/4627
2	1B	0.31	0/3417	0.54	1/4627 (0.0%)
2	1D	0.31	0/3417	0.54	0/4627
2	2B	0.31	0/3417	0.53	0/4627
2	2D	0.31	0/3417	0.53	0/4627
2	3B	0.31	0/3417	0.53	0/4627
2	3D	0.31	0/3417	0.53	0/4627
2	4B	0.31	0/3417	0.53	0/4627
2	4D	0.34	0/3417	0.54	0/4627
2	5B	0.31	0/3417	0.54	0/4627
2	5D	0.32	0/3417	0.54	1/4627 (0.0%)
2	6B	0.33	0/3417	0.55	0/4627
2	6D	0.31	0/3417	0.54	0/4627
2	7B	0.35	0/3417	0.57	0/4627
2	7D	0.34	0/3417	0.57	0/4627
2	8B	0.32	0/3417	0.55	0/4627
2	8D	0.32	0/3417	0.57	0/4627
2	9B	0.33	0/3417	0.56	0/4627
2	9D	0.31	0/3417	0.55	0/4627
All	All	0.33	0/222183	0.55	19/301379 (0.0%)

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	12B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	4D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10A	121	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	9C	92	LEU	CA-CB-CG	8.02	133.74	115.30
2	10B	177	ASP	CB-CG-OD1	7.41	124.97	118.30
1	10A	360	PRO	CA-N-CD	-6.86	101.90	111.50
1	8A	322	ASP	CB-CG-OD1	6.83	124.44	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	12B	60	VAL	Peptide
2	4D	3	GLU	Peptide

## 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	10A	3342	0	3257	74	0
1	10C	3342	0	3257	83	0
1	10E	3342	0	3257	80	0
1	11A	3342	0	3257	69	0
1	11C	3342	0	3257	99	0
1	11E	3342	0	3257	87	0
1	12A	3342	0	3257	91	0
1	12C	3342	0	3257	85	0
1	12E	3342	0	3257	84	0
1	13A	3342	0	3258	128	0
1	13C	3342	0	3257	115	0
1	13E	3342	0	3258	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	3342	0	3257	62	0
1	1C	3342	0	3257	66	0
1	1E	3342	0	3257	62	0
1	2A	3342	0	3256	62	0
1	2C	3342	0	3256	64	0
1	2E	3342	0	3256	61	0
1	3A	3342	0	3256	69	0
1	3C	3342	0	3256	75	0
1	3E	3342	0	3256	53	0
1	4A	3342	0	3256	57	0
1	4C	3342	0	3256	73	0
1	4E	3342	0	3256	58	0
1	5A	3342	0	3257	62	0
1	5C	3342	0	3257	56	0
1	5E	3342	0	3257	73	0
1	6A	3342	0	3257	69	0
1	6C	3342	0	3257	83	0
1	6E	3342	0	3257	75	0
1	7A	3342	0	3257	91	0
1	7C	3342	0	3257	91	0
1	7E	3342	0	3257	85	0
1	8A	3342	0	3257	80	0
1	8C	3342	0	3256	78	0
1	8E	3342	0	3257	89	0
1	9A	3342	0	3257	84	0
1	9C	3342	0	3257	83	0
1	9E	3342	0	3257	71	0
2	10B	3343	0	3230	86	0
2	10D	3343	0	3230	85	0
2	11B	3343	0	3230	100	0
2	11D	3343	0	3230	88	0
2	12B	3343	0	3230	113	0
2	12D	3343	0	3230	95	0
2	13B	3343	0	3230	119	0
2	13D	3343	0	3230	111	0
2	1B	3343	0	3230	69	0
2	1D	3343	0	3230	58	0
2	2B	3343	0	3230	55	0
2	2D	3343	0	3230	62	0
2	3B	3343	0	3230	60	0
2	3D	3343	0	3230	75	0
2	4B	3343	0	3230	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4D	3343	0	3230	63	0
2	5B	3343	0	3230	58	0
2	5D	3343	0	3230	64	0
2	6B	3343	0	3230	75	0
2	6D	3343	0	3230	75	0
2	7B	3343	0	3230	71	0
2	7D	3343	0	3230	79	0
2	8B	3343	0	3230	87	0
2	8D	3343	0	3230	84	0
2	9B	3343	0	3230	77	0
2	9D	3343	0	3230	82	0
3	10A	32	0	12	2	0
3	10C	32	0	12	1	0
3	10E	32	0	12	2	0
3	11A	32	0	12	5	0
3	11C	32	0	12	1	0
3	11E	32	0	12	1	0
3	12A	32	0	12	1	0
3	12C	32	0	12	2	0
3	12E	32	0	12	1	0
3	13A	32	0	12	1	0
3	13C	32	0	12	2	0
3	13E	32	0	12	1	0
3	1A	32	0	12	1	0
3	1C	32	0	12	1	0
3	1E	32	0	12	1	0
3	2A	32	0	12	2	0
3	2C	32	0	12	2	0
3	2E	32	0	12	1	0
3	3A	32	0	12	2	0
3	3C	32	0	12	3	0
3	3E	32	0	12	1	0
3	4A	32	0	12	2	0
3	4C	32	0	12	2	0
3	4E	32	0	12	1	0
3	5A	32	0	12	3	0
3	5C	32	0	12	2	0
3	5E	32	0	12	5	0
3	6A	32	0	12	4	0
3	6C	32	0	12	4	0
3	6E	32	0	12	3	0
3	7A	32	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7C	32	0	12	4	0
3	7E	32	0	12	6	0
3	8A	32	0	12	2	0
3	8C	32	0	12	4	0
3	8E	32	0	12	6	0
3	9A	32	0	12	1	0
3	9C	32	0	12	3	0
3	9E	32	0	12	0	0
4	10A	1	0	0	0	0
4	10C	1	0	0	0	0
4	10E	1	0	0	0	0
4	11A	1	0	0	0	0
4	11C	1	0	0	0	0
4	11E	1	0	0	0	0
4	12A	1	0	0	0	0
4	12C	1	0	0	0	0
4	12E	1	0	0	0	0
4	13A	1	0	0	0	0
4	13C	1	0	0	0	0
4	13E	1	0	0	0	0
4	1A	1	0	0	0	0
4	1C	1	0	0	0	0
4	1E	1	0	0	0	0
4	2A	1	0	0	0	0
4	2C	1	0	0	0	0
4	2E	1	0	0	0	0
4	3A	1	0	0	0	0
4	3C	1	0	0	0	0
4	3E	1	0	0	0	0
4	4A	1	0	0	0	0
4	4C	1	0	0	0	0
4	4E	1	0	0	0	0
4	5A	1	0	0	0	0
4	5C	1	0	0	0	0
4	5E	1	0	0	0	0
4	6A	1	0	0	0	0
4	6C	1	0	0	0	0
4	6E	1	0	0	0	0
4	7A	1	0	0	0	0
4	7C	1	0	0	0	0
4	7E	1	0	0	0	0
4	8A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	8C	1	0	0	0	0
4	8E	1	0	0	0	0
4	9A	1	0	0	0	0
4	9C	1	0	0	0	0
4	9E	1	0	0	0	0
5	10B	28	0	12	1	0
5	10D	28	0	12	1	0
5	11B	28	0	12	2	0
5	11D	28	0	12	1	0
5	12B	28	0	12	2	0
5	12D	28	0	12	3	0
5	13B	28	0	12	0	0
5	13D	28	0	12	0	0
5	1B	28	0	12	0	0
5	1D	28	0	12	0	0
5	2B	28	0	12	0	0
5	2D	28	0	12	1	0
5	3B	28	0	12	0	0
5	3D	28	0	12	0	0
5	4B	28	0	12	1	0
5	4D	28	0	12	1	0
5	5B	28	0	12	0	0
5	5D	28	0	12	0	0
5	6B	28	0	12	1	0
5	6D	28	0	12	0	0
5	7B	28	0	12	0	0
5	7D	28	0	12	0	0
5	8B	28	0	12	1	0
5	8D	28	0	12	0	0
5	9B	28	0	12	0	0
5	9D	28	0	12	0	0
All	All	219271	0	211775	4753	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 11.

The worst 5 of 4753 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)
1:11C:302:MET:HG3	1:11C:303:VAL:HG23	1.45	0.98
1:13C:216:ASN:ND2	1:13C:300:ASN:OD1	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1E:102:ASN:HD22	1:1E:105:ARG:HD3	1.35	0.89
1:6E:71:GLU:HB2	1:6E:98:ASP:HB3	1.54	0.88
2:9D:61:PRO:HD3	2:9D:84:ILE:HG22	1.56	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	10A	422/475 (89%)	409 (97%)	13 (3%)	0	100	100
1	10C	422/475 (89%)	409 (97%)	13 (3%)	0	100	100
1	10E	422/475 (89%)	407 (96%)	15 (4%)	0	100	100
1	11A	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
1	11C	422/475 (89%)	404 (96%)	18 (4%)	0	100	100
1	11E	422/475 (89%)	401 (95%)	21 (5%)	0	100	100
1	12A	422/475 (89%)	409 (97%)	13 (3%)	0	100	100
1	12C	422/475 (89%)	410 (97%)	12 (3%)	0	100	100
1	12E	422/475 (89%)	406 (96%)	16 (4%)	0	100	100
1	13A	422/475 (89%)	402 (95%)	20 (5%)	0	100	100
1	13C	422/475 (89%)	403 (96%)	19 (4%)	0	100	100
1	13E	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
1	1A	422/475 (89%)	406 (96%)	16 (4%)	0	100	100
1	1C	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
1	1E	422/475 (89%)	404 (96%)	18 (4%)	0	100	100
1	2A	422/475 (89%)	407 (96%)	15 (4%)	0	100	100
1	2C	422/475 (89%)	407 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2E	422/475 (89%)	408 (97%)	14 (3%)	0	100	100
1	3A	422/475 (89%)	404 (96%)	18 (4%)	0	100	100
1	3C	422/475 (89%)	406 (96%)	16 (4%)	0	100	100
1	3E	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
1	4A	422/475 (89%)	408 (97%)	14 (3%)	0	100	100
1	4C	422/475 (89%)	406 (96%)	16 (4%)	0	100	100
1	4E	422/475 (89%)	406 (96%)	16 (4%)	0	100	100
1	5A	422/475 (89%)	407 (96%)	15 (4%)	0	100	100
1	5C	422/475 (89%)	411 (97%)	11 (3%)	0	100	100
1	5E	422/475 (89%)	409 (97%)	13 (3%)	0	100	100
1	6A	422/475 (89%)	403 (96%)	19 (4%)	0	100	100
1	6C	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
1	6E	422/475 (89%)	404 (96%)	18 (4%)	0	100	100
1	7A	422/475 (89%)	403 (96%)	19 (4%)	0	100	100
1	7C	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
1	7E	422/475 (89%)	404 (96%)	18 (4%)	0	100	100
1	8A	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
1	8C	422/475 (89%)	403 (96%)	19 (4%)	0	100	100
1	8E	422/475 (89%)	403 (96%)	19 (4%)	0	100	100
1	9A	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
1	9C	422/475 (89%)	408 (97%)	14 (3%)	0	100	100
1	9E	422/475 (89%)	405 (96%)	17 (4%)	0	100	100
2	10B	423/425 (100%)	405 (96%)	18 (4%)	0	100	100
2	10D	423/425 (100%)	404 (96%)	19 (4%)	0	100	100
2	11B	423/425 (100%)	403 (95%)	20 (5%)	0	100	100
2	11D	423/425 (100%)	405 (96%)	18 (4%)	0	100	100
2	12B	423/425 (100%)	398 (94%)	25 (6%)	0	100	100
2	12D	423/425 (100%)	398 (94%)	25 (6%)	0	100	100
2	13B	423/425 (100%)	396 (94%)	27 (6%)	0	100	100
2	13D	423/425 (100%)	400 (95%)	23 (5%)	0	100	100
2	1B	423/425 (100%)	411 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1D	423/425 (100%)	404 (96%)	19 (4%)	0	100	100
2	2B	423/425 (100%)	411 (97%)	12 (3%)	0	100	100
2	2D	423/425 (100%)	407 (96%)	16 (4%)	0	100	100
2	3B	423/425 (100%)	412 (97%)	11 (3%)	0	100	100
2	3D	423/425 (100%)	412 (97%)	11 (3%)	0	100	100
2	4B	423/425 (100%)	408 (96%)	15 (4%)	0	100	100
2	4D	423/425 (100%)	411 (97%)	12 (3%)	0	100	100
2	5B	423/425 (100%)	404 (96%)	19 (4%)	0	100	100
2	5D	423/425 (100%)	405 (96%)	18 (4%)	0	100	100
2	6B	423/425 (100%)	399 (94%)	24 (6%)	0	100	100
2	6D	423/425 (100%)	397 (94%)	26 (6%)	0	100	100
2	7B	423/425 (100%)	401 (95%)	22 (5%)	0	100	100
2	7D	423/425 (100%)	402 (95%)	21 (5%)	0	100	100
2	8B	423/425 (100%)	404 (96%)	19 (4%)	0	100	100
2	8D	423/425 (100%)	406 (96%)	17 (4%)	0	100	100
2	9B	423/425 (100%)	412 (97%)	11 (3%)	0	100	100
2	9D	423/425 (100%)	405 (96%)	18 (4%)	0	100	100
All	All	27456/29575 (93%)	26342 (96%)	1114 (4%)	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	10A	359/395 (91%)	359 (100%)	0	100	100
1	10C	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	10E	359/395 (91%)	357 (99%)	2 (1%)	86	92
1	11A	359/395 (91%)	357 (99%)	2 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11C	359/395 (91%)	359 (100%)	0	100	100
1	11E	359/395 (91%)	359 (100%)	0	100	100
1	12A	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	12C	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	12E	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	13A	359/395 (91%)	359 (100%)	0	100	100
1	13C	359/395 (91%)	359 (100%)	0	100	100
1	13E	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	1A	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	1C	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	1E	359/395 (91%)	359 (100%)	0	100	100
1	2A	359/395 (91%)	359 (100%)	0	100	100
1	2C	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	2E	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	3A	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	3C	359/395 (91%)	359 (100%)	0	100	100
1	3E	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	4A	359/395 (91%)	359 (100%)	0	100	100
1	4C	359/395 (91%)	359 (100%)	0	100	100
1	4E	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	5A	359/395 (91%)	357 (99%)	2 (1%)	86	92
1	5C	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	5E	359/395 (91%)	359 (100%)	0	100	100
1	6A	359/395 (91%)	359 (100%)	0	100	100
1	6C	359/395 (91%)	359 (100%)	0	100	100
1	6E	359/395 (91%)	359 (100%)	0	100	100
1	7A	359/395 (91%)	357 (99%)	2 (1%)	86	92
1	7C	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	7E	359/395 (91%)	359 (100%)	0	100	100
1	8A	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	8C	359/395 (91%)	359 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8E	359/395 (91%)	358 (100%)	1 (0%)	92	96
1	9A	359/395 (91%)	359 (100%)	0	100	100
1	9C	359/395 (91%)	359 (100%)	0	100	100
1	9E	359/395 (91%)	359 (100%)	0	100	100
2	10B	364/364 (100%)	364 (100%)	0	100	100
2	10D	364/364 (100%)	364 (100%)	0	100	100
2	11B	364/364 (100%)	362 (100%)	2 (0%)	88	94
2	11D	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	12B	364/364 (100%)	362 (100%)	2 (0%)	88	94
2	12D	364/364 (100%)	362 (100%)	2 (0%)	88	94
2	13B	364/364 (100%)	360 (99%)	4 (1%)	73	85
2	13D	364/364 (100%)	361 (99%)	3 (1%)	81	89
2	1B	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	1D	364/364 (100%)	364 (100%)	0	100	100
2	2B	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	2D	364/364 (100%)	364 (100%)	0	100	100
2	3B	364/364 (100%)	364 (100%)	0	100	100
2	3D	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	4B	364/364 (100%)	362 (100%)	2 (0%)	88	94
2	4D	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	5B	364/364 (100%)	362 (100%)	2 (0%)	88	94
2	5D	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	6B	364/364 (100%)	361 (99%)	3 (1%)	81	89
2	6D	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	7B	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	7D	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	8B	364/364 (100%)	362 (100%)	2 (0%)	88	94
2	8D	364/364 (100%)	362 (100%)	2 (0%)	88	94
2	9B	364/364 (100%)	363 (100%)	1 (0%)	92	96
2	9D	364/364 (100%)	363 (100%)	1 (0%)	92	96
All	All	23465/24869 (94%)	23406 (100%)	59 (0%)	92	96

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2E	422	ARG
2	8D	359	ARG
1	4E	326	LYS
2	8D	204	ASN
1	7C	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	8B	6	HIS
2	8B	204	ASN
1	9A	88	HIS
1	4A	88	HIS
1	3E	133	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 104 ligands modelled in this entry, 39 are monoatomic - leaving 65 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	12D	600	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	5 (16%)
5	GDP	3B	600	-	24,30,30	0.96	1 (4%)	30,47,47	1.41	4 (13%)
3	GTP	7E	500	1	26,34,34	1.27	2 (7%)	32,54,54	1.65	6 (18%)
3	GTP	1C	500	4,1	26,34,34	1.22	2 (7%)	32,54,54	1.73	7 (21%)
3	GTP	6C	500	4,1	26,34,34	1.19	2 (7%)	32,54,54	1.66	6 (18%)
3	GTP	12E	500	4,1	26,34,34	1.22	1 (3%)	32,54,54	1.53	6 (18%)
3	GTP	9A	500	4,1	26,34,34	1.25	2 (7%)	32,54,54	1.68	8 (25%)
5	GDP	11D	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.37	4 (13%)
5	GDP	9D	600	-	24,30,30	0.95	1 (4%)	30,47,47	1.43	4 (13%)
5	GDP	11B	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.39	4 (13%)
5	GDP	6D	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.41	5 (16%)
3	GTP	4A	500	4,1	26,34,34	1.20	2 (7%)	32,54,54	1.96	7 (21%)
3	GTP	6A	500	4,1	26,34,34	1.18	2 (7%)	32,54,54	1.64	6 (18%)
3	GTP	8A	500	4,1	26,34,34	1.22	2 (7%)	32,54,54	1.68	7 (21%)
3	GTP	1E	500	4,1	26,34,34	1.23	2 (7%)	32,54,54	1.69	7 (21%)
3	GTP	11A	500	4,1	26,34,34	1.23	2 (7%)	32,54,54	1.59	7 (21%)
3	GTP	12A	500	4,1	26,34,34	1.25	2 (7%)	32,54,54	1.65	7 (21%)
5	GDP	13B	600	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
5	GDP	12B	600	-	24,30,30	0.94	1 (4%)	30,47,47	1.40	5 (16%)
5	GDP	3D	600	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
5	GDP	4B	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.41	4 (13%)
3	GTP	4E	500	4,1	26,34,34	1.19	2 (7%)	32,54,54	1.93	7 (21%)
3	GTP	5A	500	4,1	26,34,34	1.22	1 (3%)	32,54,54	1.66	6 (18%)
3	GTP	4C	500	4,1	26,34,34	1.19	2 (7%)	32,54,54	1.93	7 (21%)
5	GDP	10D	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.52	4 (13%)
5	GDP	4D	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.41	4 (13%)
3	GTP	5E	500	4,1	26,34,34	1.23	1 (3%)	32,54,54	1.66	6 (18%)
3	GTP	8C	500	4,1	26,34,34	1.27	3 (11%)	32,54,54	1.64	5 (15%)
3	GTP	6E	500	4,1	26,34,34	1.21	2 (7%)	32,54,54	1.67	7 (21%)
5	GDP	9B	600	-	24,30,30	0.96	1 (4%)	30,47,47	1.40	4 (13%)
3	GTP	11E	500	4,1	26,34,34	1.25	2 (7%)	32,54,54	1.60	7 (21%)
5	GDP	1B	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.43	5 (16%)
5	GDP	5D	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.42	5 (16%)
3	GTP	3E	500	4,1	26,34,34	1.18	2 (7%)	32,54,54	1.89	7 (21%)
5	GDP	5B	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.46	5 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GTP	9C	500	4,1	26,34,34	1.23	2 (7%)	32,54,54	1.69	7 (21%)
3	GTP	10C	500	4,1	26,34,34	1.23	2 (7%)	32,54,54	1.56	7 (21%)
3	GTP	12C	500	4,1	26,34,34	1.23	2 (7%)	32,54,54	1.72	7 (21%)
3	GTP	9E	500	4,1	26,34,34	1.24	2 (7%)	32,54,54	1.66	7 (21%)
5	GDP	2B	600	-	24,30,30	0.99	1 (4%)	30,47,47	1.42	4 (13%)
5	GDP	8D	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.37	4 (13%)
3	GTP	7C	500	4,1	26,34,34	1.26	2 (7%)	32,54,54	1.78	8 (25%)
5	GDP	7B	600	-	24,30,30	1.01	1 (4%)	30,47,47	1.44	4 (13%)
3	GTP	10E	500	4,1	26,34,34	1.22	2 (7%)	32,54,54	1.57	6 (18%)
3	GTP	13C	500	4,1	26,34,34	1.27	1 (3%)	32,54,54	1.87	9 (28%)
3	GTP	2A	500	4,1	26,34,34	1.23	2 (7%)	32,54,54	1.74	7 (21%)
3	GTP	10A	500	4,1	26,34,34	1.24	2 (7%)	32,54,54	1.60	7 (21%)
3	GTP	1A	500	4,1	26,34,34	1.23	2 (7%)	32,54,54	1.71	7 (21%)
3	GTP	8E	500	4,1	26,34,34	1.41	3 (11%)	32,54,54	1.76	8 (25%)
5	GDP	8B	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.39	4 (13%)
3	GTP	3A	500	4,1	26,34,34	1.18	2 (7%)	32,54,54	1.90	7 (21%)
3	GTP	11C	500	4,1	26,34,34	1.24	2 (7%)	32,54,54	1.63	7 (21%)
3	GTP	3C	500	4,1	26,34,34	1.19	2 (7%)	32,54,54	1.86	7 (21%)
5	GDP	2D	600	-	24,30,30	0.99	1 (4%)	30,47,47	1.42	4 (13%)
3	GTP	13A	500	4,1	26,34,34	1.24	1 (3%)	32,54,54	1.71	8 (25%)
3	GTP	7A	500	4,1	26,34,34	1.28	2 (7%)	32,54,54	1.64	6 (18%)
5	GDP	1D	600	-	24,30,30	0.98	1 (4%)	30,47,47	1.42	5 (16%)
5	GDP	13D	600	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
5	GDP	7D	600	-	24,30,30	1.01	1 (4%)	30,47,47	1.43	4 (13%)
3	GTP	2C	500	4,1	26,34,34	1.23	2 (7%)	32,54,54	1.74	7 (21%)
5	GDP	10B	600	-	24,30,30	0.96	1 (4%)	30,47,47	1.53	4 (13%)
3	GTP	13E	500	4,1	26,34,34	1.23	1 (3%)	32,54,54	1.68	8 (25%)
3	GTP	5C	500	4,1	26,34,34	1.26	1 (3%)	32,54,54	1.78	8 (25%)
5	GDP	6B	600	-	24,30,30	0.97	1 (4%)	30,47,47	1.43	5 (16%)
3	GTP	2E	500	4,1	26,34,34	1.24	2 (7%)	32,54,54	1.74	7 (21%)

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	12D	600	-	-	2/12/32/32	0/3/3/3
5	GDP	3B	600	-	-	2/12/32/32	0/3/3/3
3	GTP	7E	500	1	-	5/18/38/38	0/3/3/3
3	GTP	1C	500	4,1	-	6/18/38/38	0/3/3/3
3	GTP	6C	500	4,1	-	4/18/38/38	0/3/3/3
3	GTP	12E	500	4,1	-	2/18/38/38	0/3/3/3
3	GTP	9A	500	4,1	-	6/18/38/38	0/3/3/3
5	GDP	11D	600	-	-	2/12/32/32	0/3/3/3
5	GDP	9D	600	-	-	2/12/32/32	0/3/3/3
5	GDP	11B	600	-	-	2/12/32/32	0/3/3/3
5	GDP	6D	600	-	-	4/12/32/32	0/3/3/3
3	GTP	4A	500	4,1	-	3/18/38/38	0/3/3/3
3	GTP	6A	500	4,1	-	4/18/38/38	0/3/3/3
3	GTP	8A	500	4,1	-	5/18/38/38	0/3/3/3
3	GTP	1E	500	4,1	-	7/18/38/38	0/3/3/3
3	GTP	11A	500	4,1	-	8/18/38/38	0/3/3/3
3	GTP	12A	500	4,1	-	1/18/38/38	0/3/3/3
5	GDP	13B	600	-	-	2/12/32/32	0/3/3/3
5	GDP	12B	600	-	-	2/12/32/32	0/3/3/3
5	GDP	3D	600	-	-	2/12/32/32	0/3/3/3
5	GDP	4B	600	-	-	5/12/32/32	0/3/3/3
3	GTP	4E	500	4,1	-	4/18/38/38	0/3/3/3
3	GTP	5A	500	4,1	-	4/18/38/38	0/3/3/3
3	GTP	4C	500	4,1	-	3/18/38/38	0/3/3/3
5	GDP	10D	600	-	-	2/12/32/32	0/3/3/3
5	GDP	4D	600	-	-	6/12/32/32	0/3/3/3
3	GTP	5E	500	4,1	-	5/18/38/38	0/3/3/3
3	GTP	8C	500	4,1	-	5/18/38/38	0/3/3/3
3	GTP	6E	500	4,1	-	4/18/38/38	0/3/3/3
5	GDP	9B	600	-	-	4/12/32/32	0/3/3/3
3	GTP	11E	500	4,1	-	8/18/38/38	0/3/3/3
5	GDP	1B	600	-	-	1/12/32/32	0/3/3/3
5	GDP	5D	600	-	-	5/12/32/32	0/3/3/3
3	GTP	3E	500	4,1	-	3/18/38/38	0/3/3/3
5	GDP	5B	600	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	9C	500	4,1	-	3/18/38/38	0/3/3/3
3	GTP	10C	500	4,1	-	7/18/38/38	0/3/3/3
3	GTP	12C	500	4,1	-	2/18/38/38	0/3/3/3
3	GTP	9E	500	4,1	-	3/18/38/38	0/3/3/3
5	GDP	2B	600	-	-	5/12/32/32	0/3/3/3
5	GDP	8D	600	-	-	4/12/32/32	0/3/3/3
3	GTP	7C	500	4,1	-	4/18/38/38	0/3/3/3
5	GDP	7B	600	-	-	4/12/32/32	0/3/3/3
3	GTP	10E	500	4,1	-	7/18/38/38	0/3/3/3
3	GTP	13C	500	4,1	-	3/18/38/38	0/3/3/3
3	GTP	2A	500	4,1	-	4/18/38/38	0/3/3/3
3	GTP	10A	500	4,1	-	7/18/38/38	0/3/3/3
3	GTP	1A	500	4,1	-	6/18/38/38	0/3/3/3
3	GTP	8E	500	4,1	-	6/18/38/38	0/3/3/3
5	GDP	8B	600	-	-	2/12/32/32	0/3/3/3
3	GTP	3A	500	4,1	-	4/18/38/38	0/3/3/3
3	GTP	11C	500	4,1	-	7/18/38/38	0/3/3/3
3	GTP	3C	500	4,1	-	4/18/38/38	0/3/3/3
5	GDP	2D	600	-	-	2/12/32/32	0/3/3/3
3	GTP	13A	500	4,1	-	6/18/38/38	0/3/3/3
3	GTP	7A	500	4,1	-	4/18/38/38	0/3/3/3
5	GDP	1D	600	-	-	1/12/32/32	0/3/3/3
5	GDP	13D	600	-	-	2/12/32/32	0/3/3/3
5	GDP	7D	600	-	-	5/12/32/32	0/3/3/3
3	GTP	2C	500	4,1	-	4/18/38/38	0/3/3/3
5	GDP	10B	600	-	-	2/12/32/32	0/3/3/3
3	GTP	13E	500	4,1	-	5/18/38/38	0/3/3/3
3	GTP	5C	500	4,1	-	4/18/38/38	0/3/3/3
5	GDP	6B	600	-	-	4/12/32/32	0/3/3/3
3	GTP	2E	500	4,1	-	4/18/38/38	0/3/3/3

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	12A	500	GTP	C5-C6	-4.54	1.38	1.47
3	7E	500	GTP	C5-C6	-4.52	1.38	1.47

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	13A	500	GTP	C5-C6	-4.51	1.38	1.47
3	13E	500	GTP	C5-C6	-4.47	1.38	1.47
3	7A	500	GTP	C5-C6	-4.47	1.38	1.47

The worst 5 of 383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4A	500	GTP	PA-O3A-PB	-6.13	111.78	132.83
3	4E	500	GTP	PA-O3A-PB	-5.98	112.30	132.83
3	4C	500	GTP	PA-O3A-PB	-5.91	112.55	132.83
3	7C	500	GTP	PA-O3A-PB	-5.69	113.29	132.83
3	3A	500	GTP	PA-O3A-PB	-5.63	113.52	132.83

There are no chirality outliers.

5 of 260 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	10A	500	GTP	C5'-O5'-PA-O1A
3	10C	500	GTP	C5'-O5'-PA-O1A
3	10E	500	GTP	C5'-O5'-PA-O1A
3	11A	500	GTP	C5'-O5'-PA-O1A
3	11A	500	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

49 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	12D	600	GDP	3	0
3	7E	500	GTP	6	0
3	1C	500	GTP	1	0
3	6C	500	GTP	4	0
3	12E	500	GTP	1	0
3	9A	500	GTP	1	0
5	11D	600	GDP	1	0
5	11B	600	GDP	2	0
3	4A	500	GTP	2	0
3	6A	500	GTP	4	0
3	8A	500	GTP	2	0
3	1E	500	GTP	1	0
3	11A	500	GTP	5	0
3	12A	500	GTP	1	0

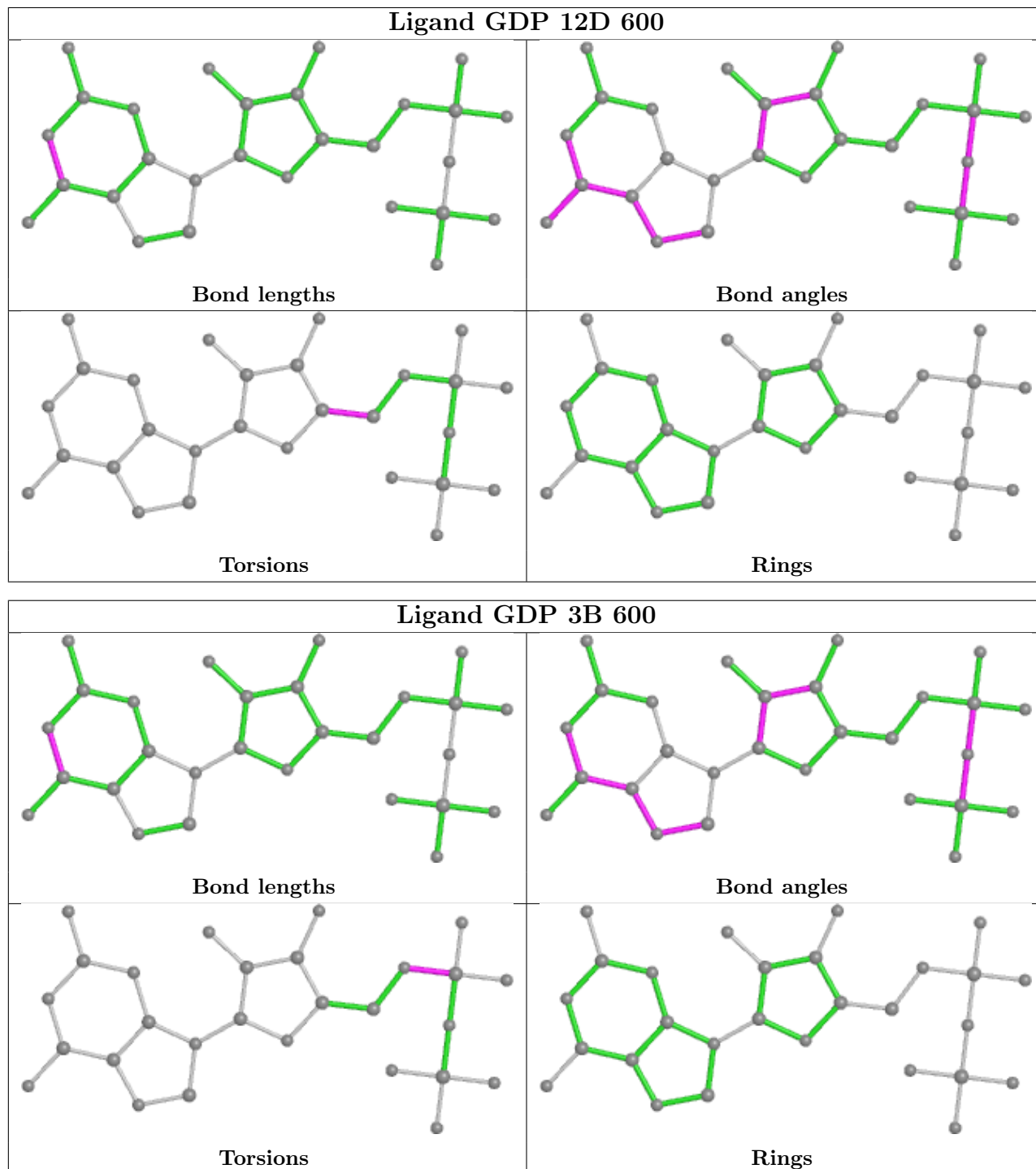
*Continued on next page...*

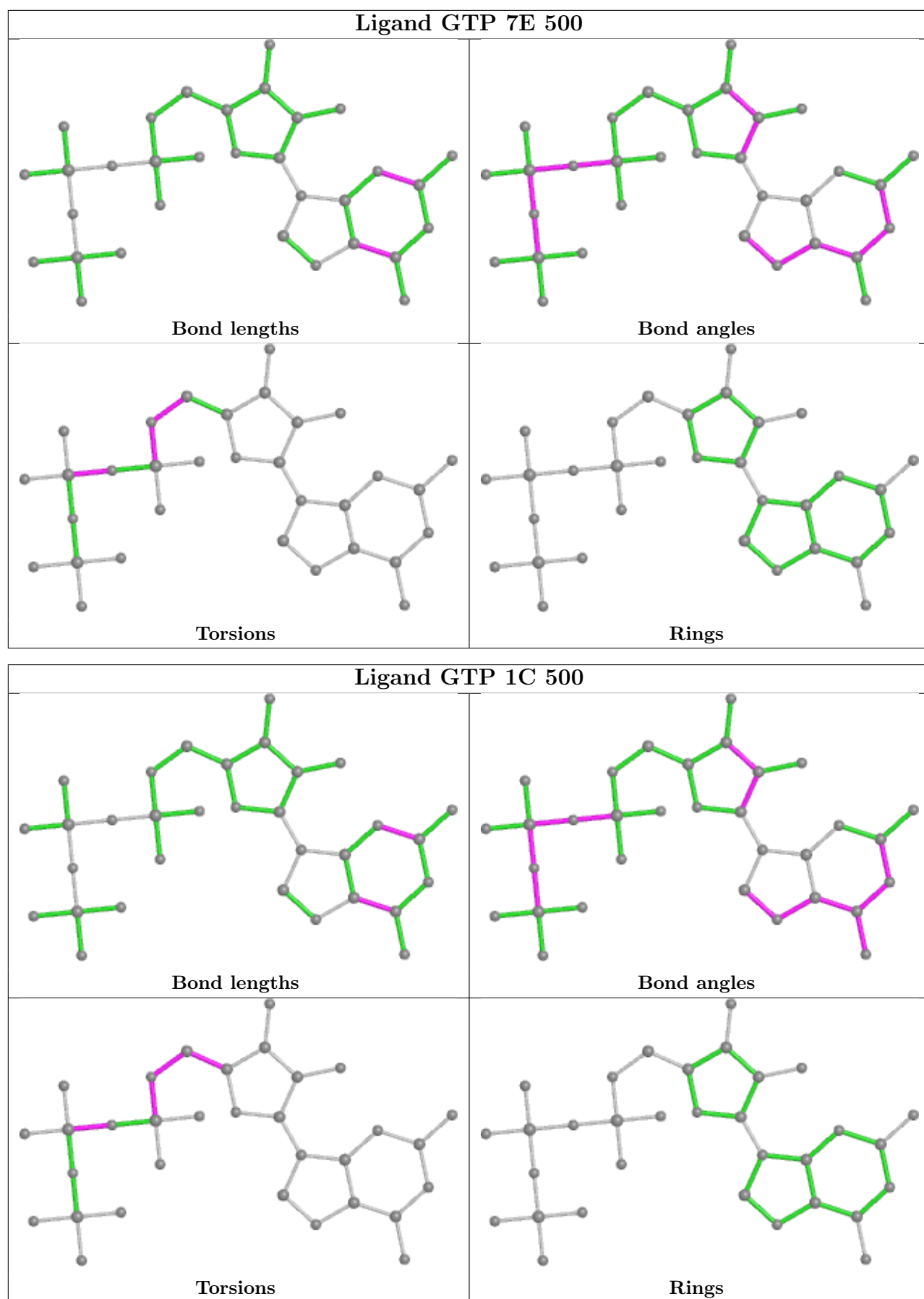
*Continued from previous page...*

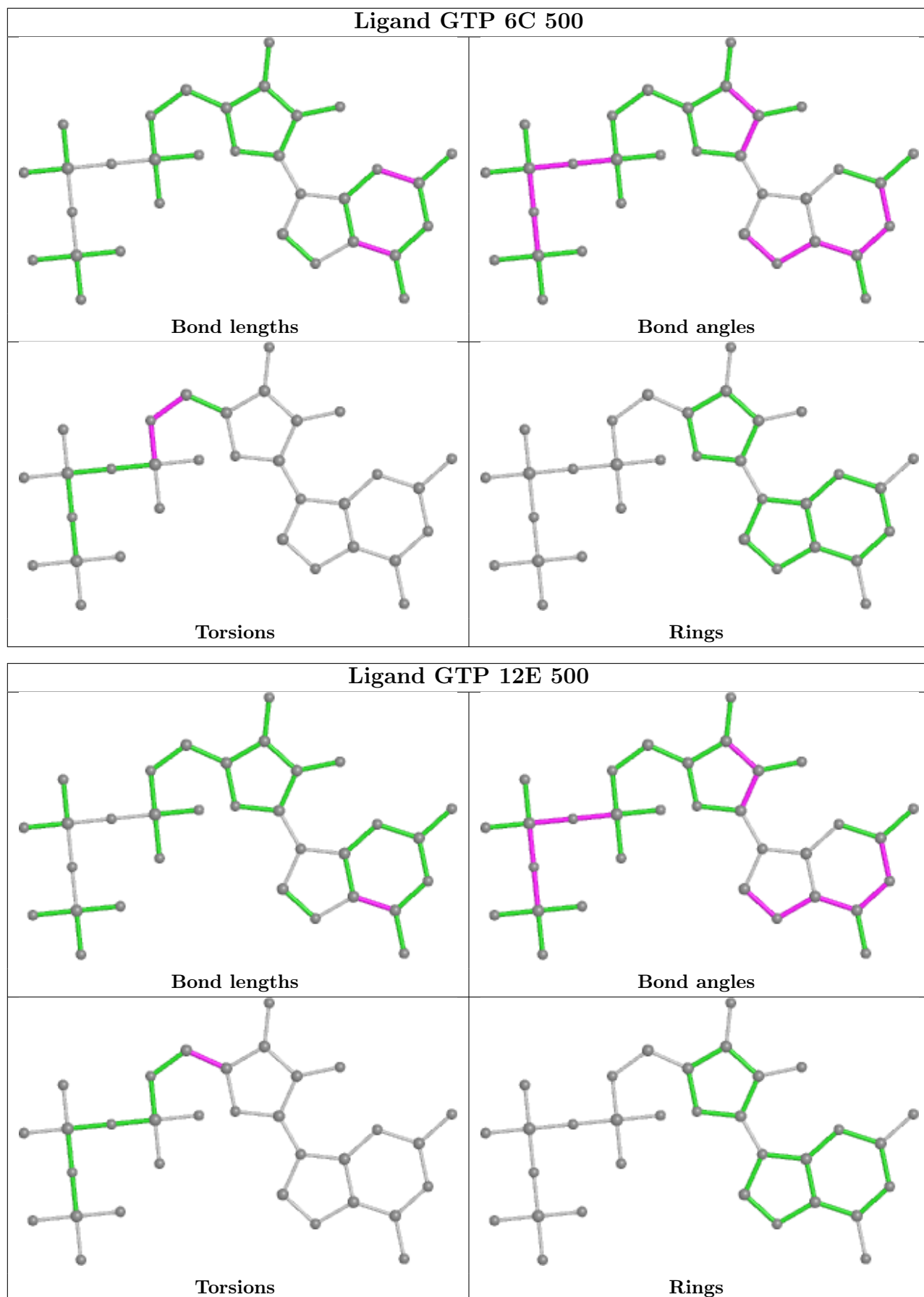
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	12B	600	GDP	2	0
5	4B	600	GDP	1	0
3	4E	500	GTP	1	0
3	5A	500	GTP	3	0
3	4C	500	GTP	2	0
5	10D	600	GDP	1	0
5	4D	600	GDP	1	0
3	5E	500	GTP	5	0
3	8C	500	GTP	4	0
3	6E	500	GTP	3	0
3	11E	500	GTP	1	0
3	3E	500	GTP	1	0
3	9C	500	GTP	3	0
3	10C	500	GTP	1	0
3	12C	500	GTP	2	0
3	7C	500	GTP	4	0
3	10E	500	GTP	2	0
3	13C	500	GTP	2	0
3	2A	500	GTP	2	0
3	10A	500	GTP	2	0
3	1A	500	GTP	1	0
3	8E	500	GTP	6	0
5	8B	600	GDP	1	0
3	3A	500	GTP	2	0
3	11C	500	GTP	1	0
3	3C	500	GTP	3	0
5	2D	600	GDP	1	0
3	13A	500	GTP	1	0
3	7A	500	GTP	5	0
3	2C	500	GTP	2	0
5	10B	600	GDP	1	0
3	13E	500	GTP	1	0
3	5C	500	GTP	2	0
5	6B	600	GDP	1	0
3	2E	500	GTP	1	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

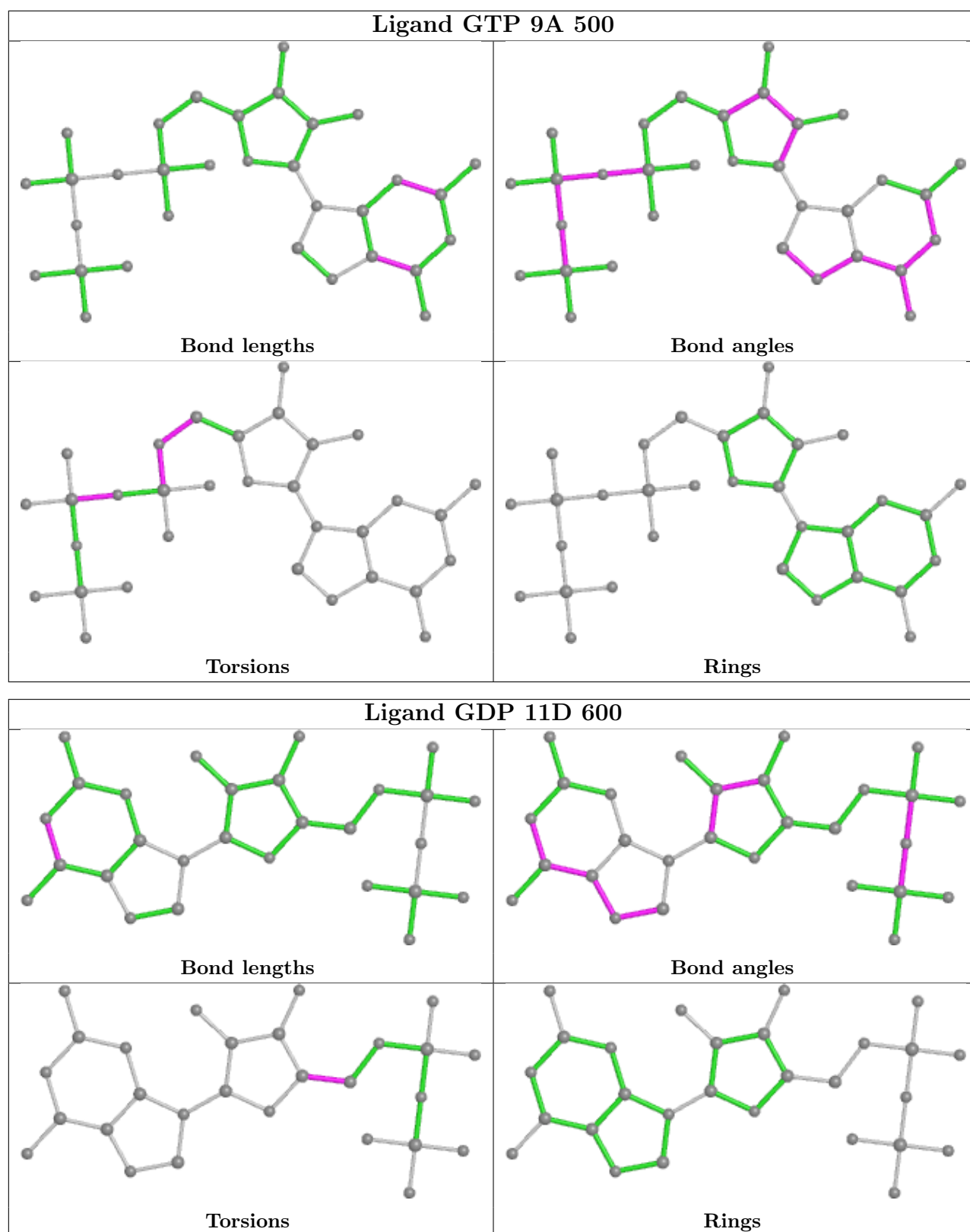
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

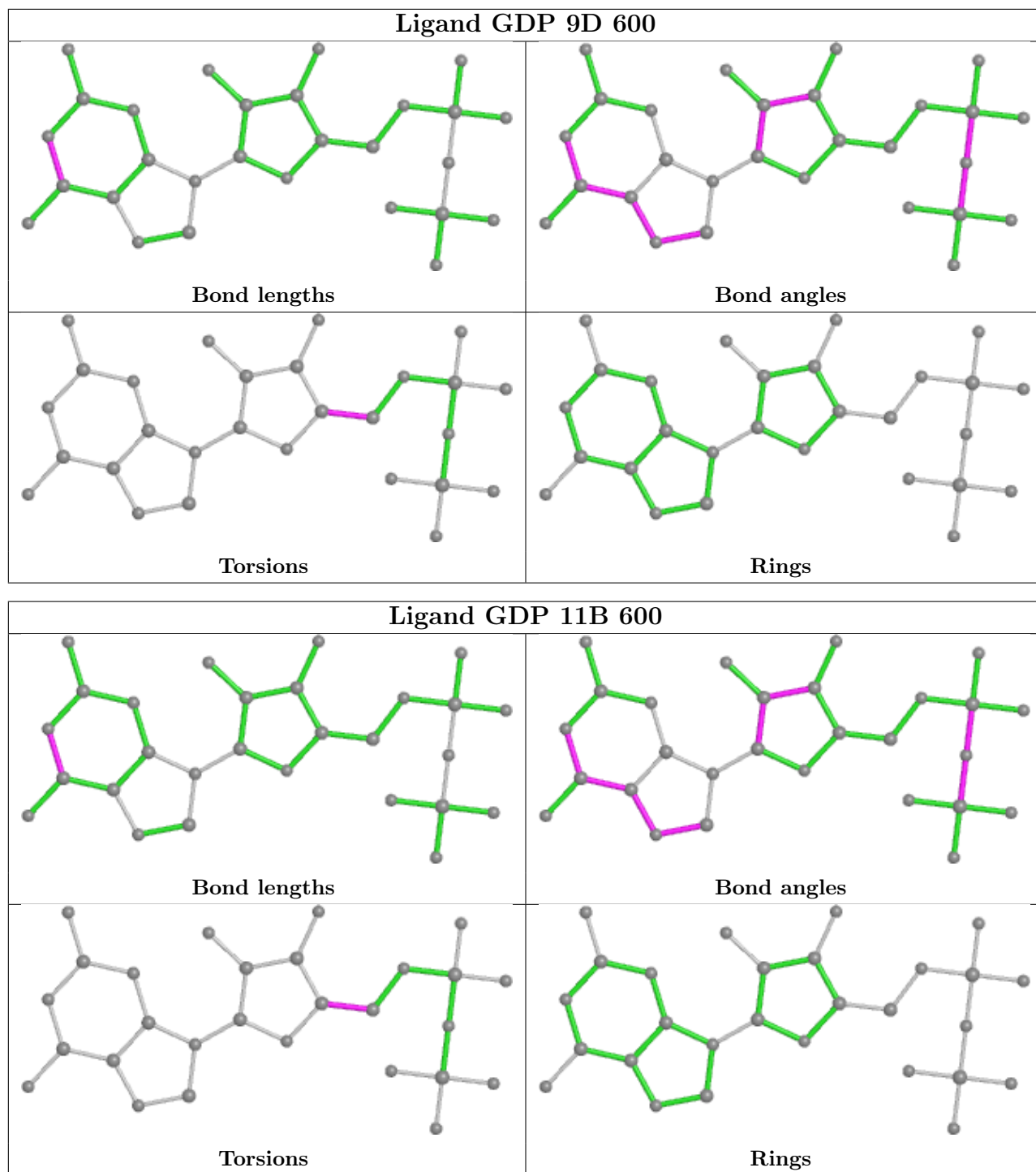


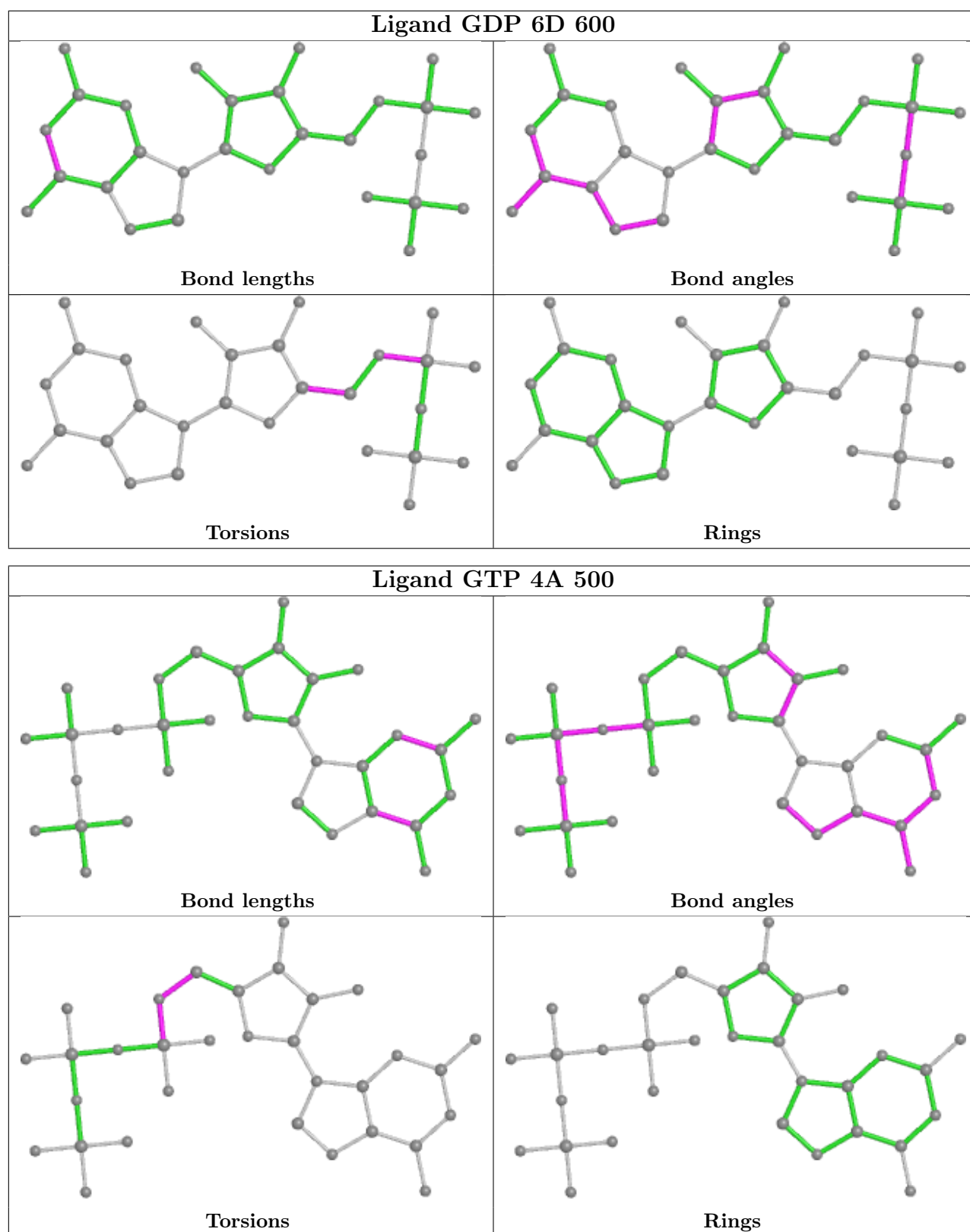


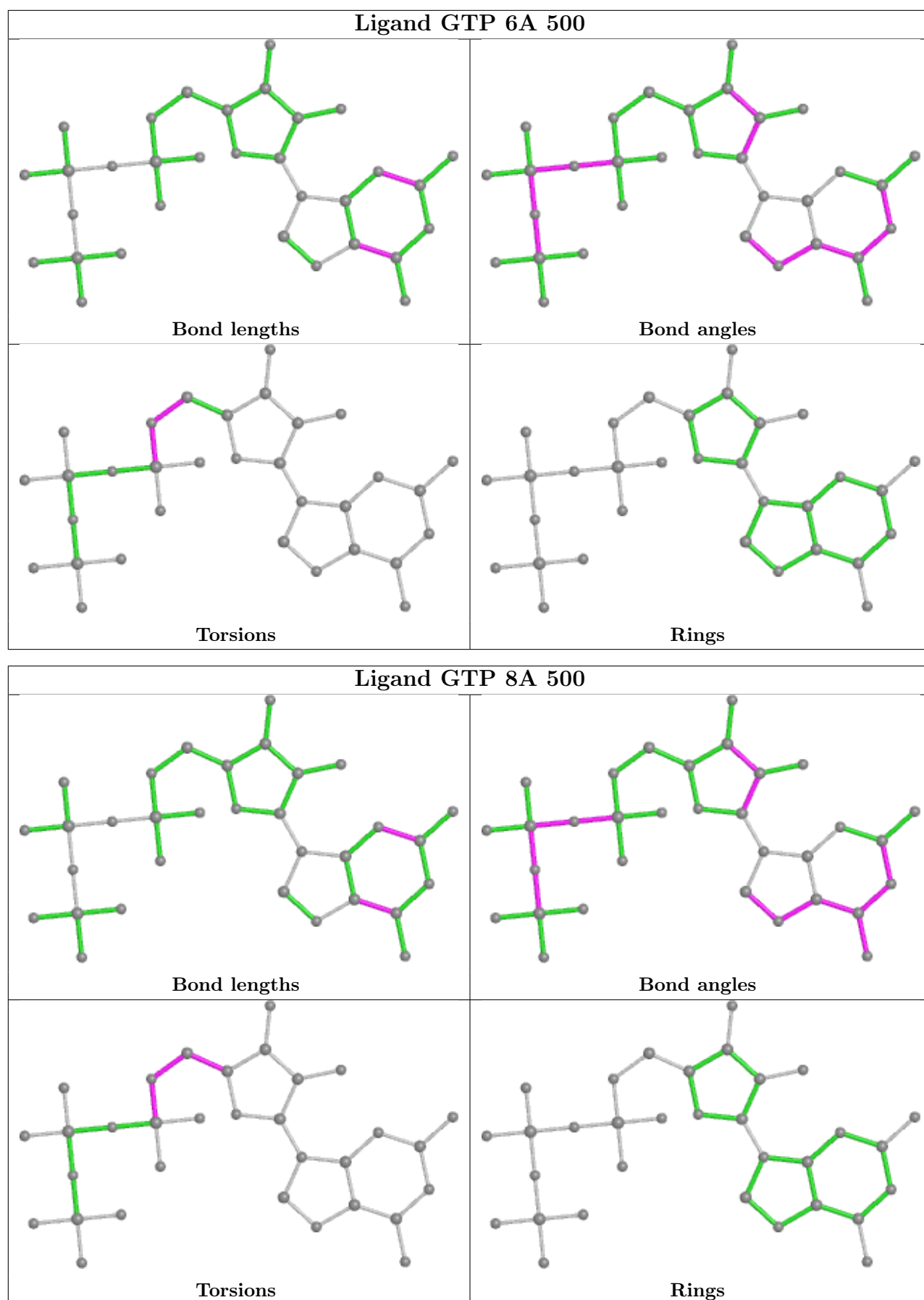


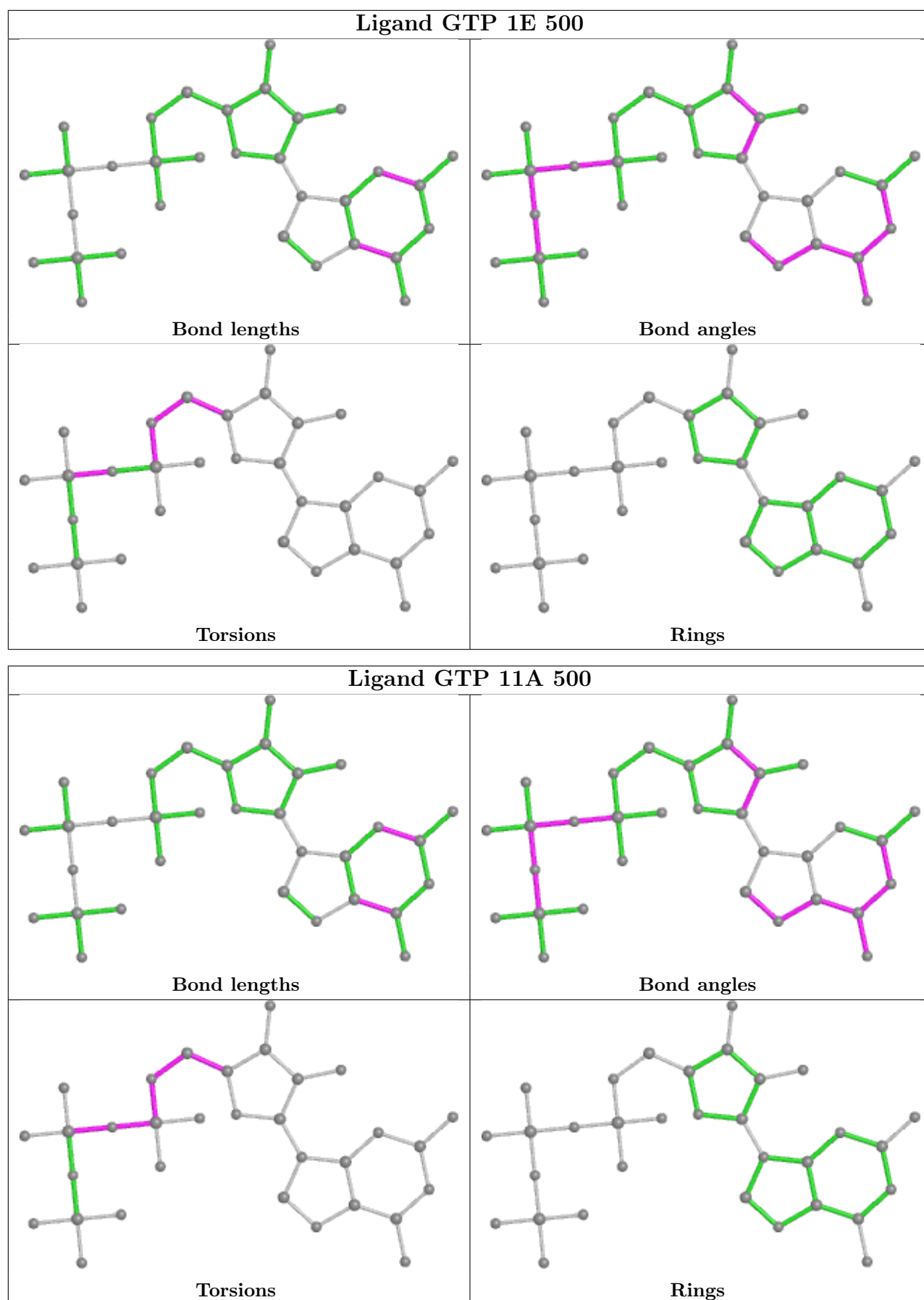


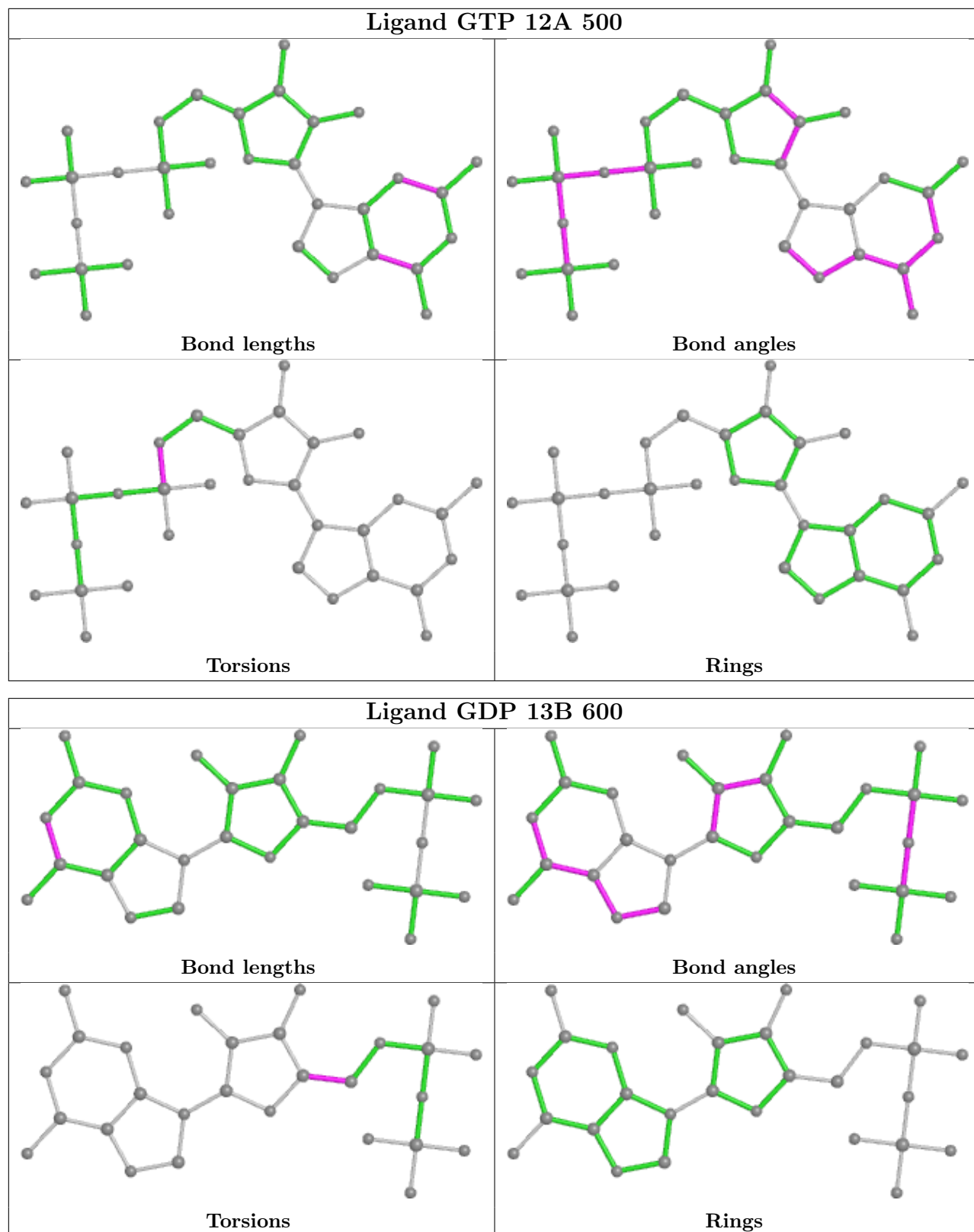


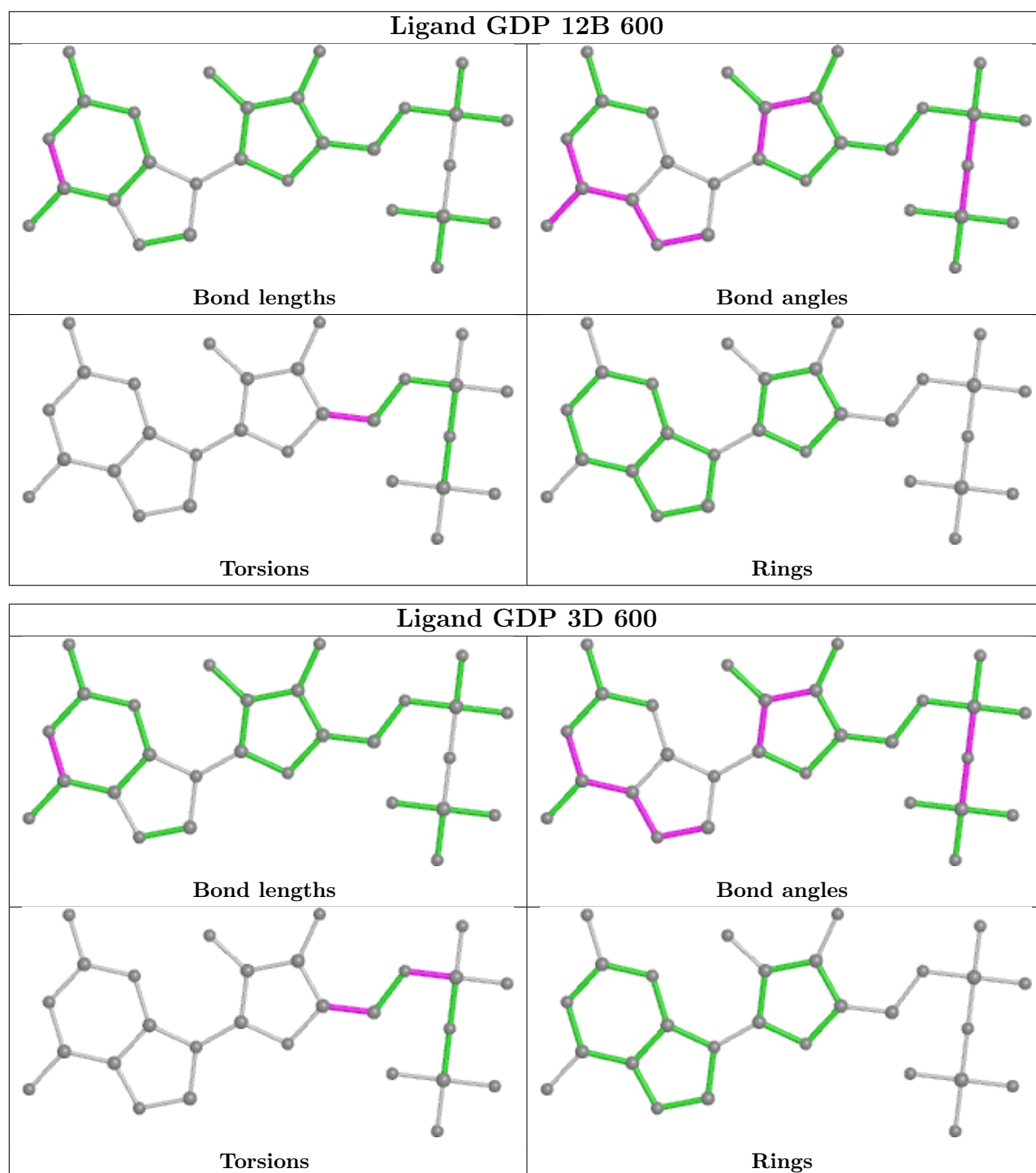


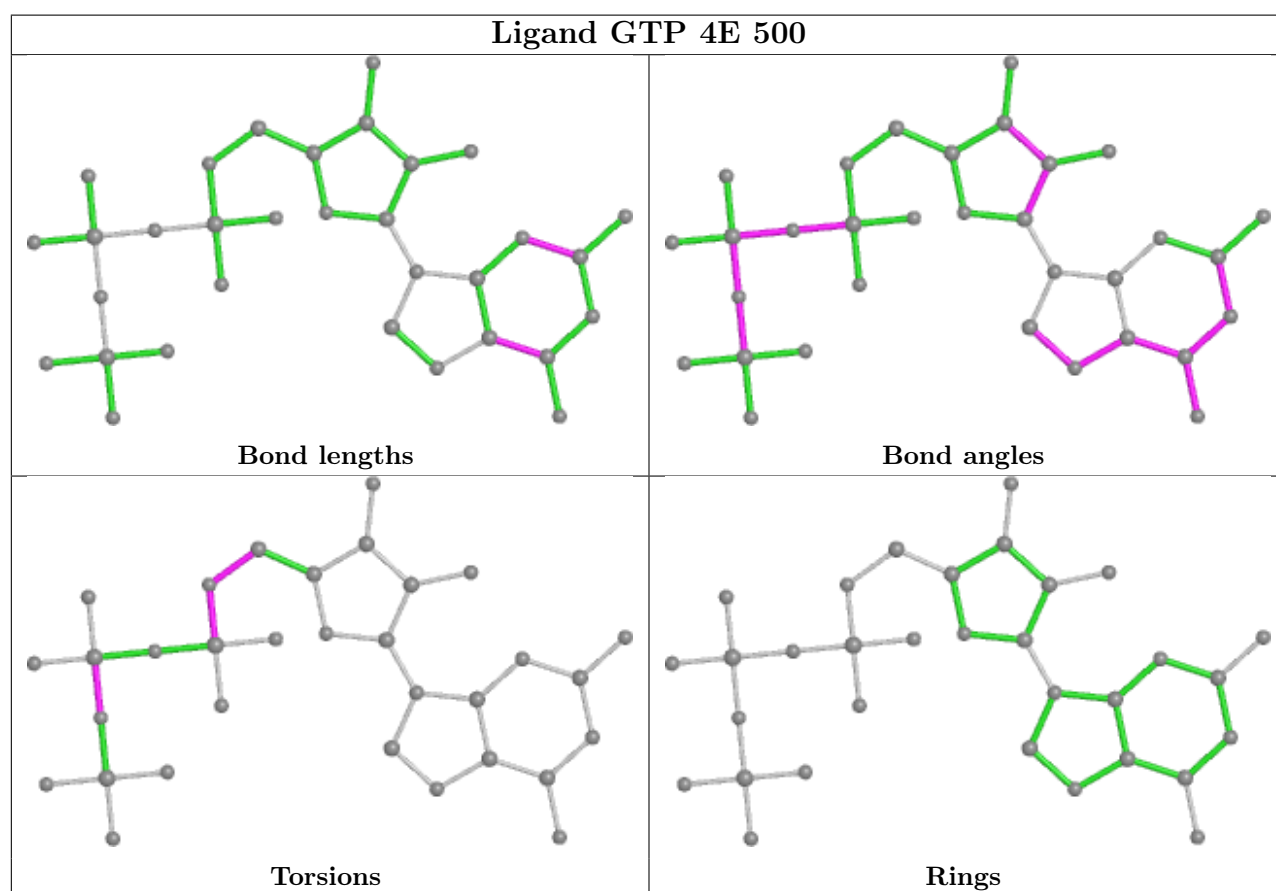
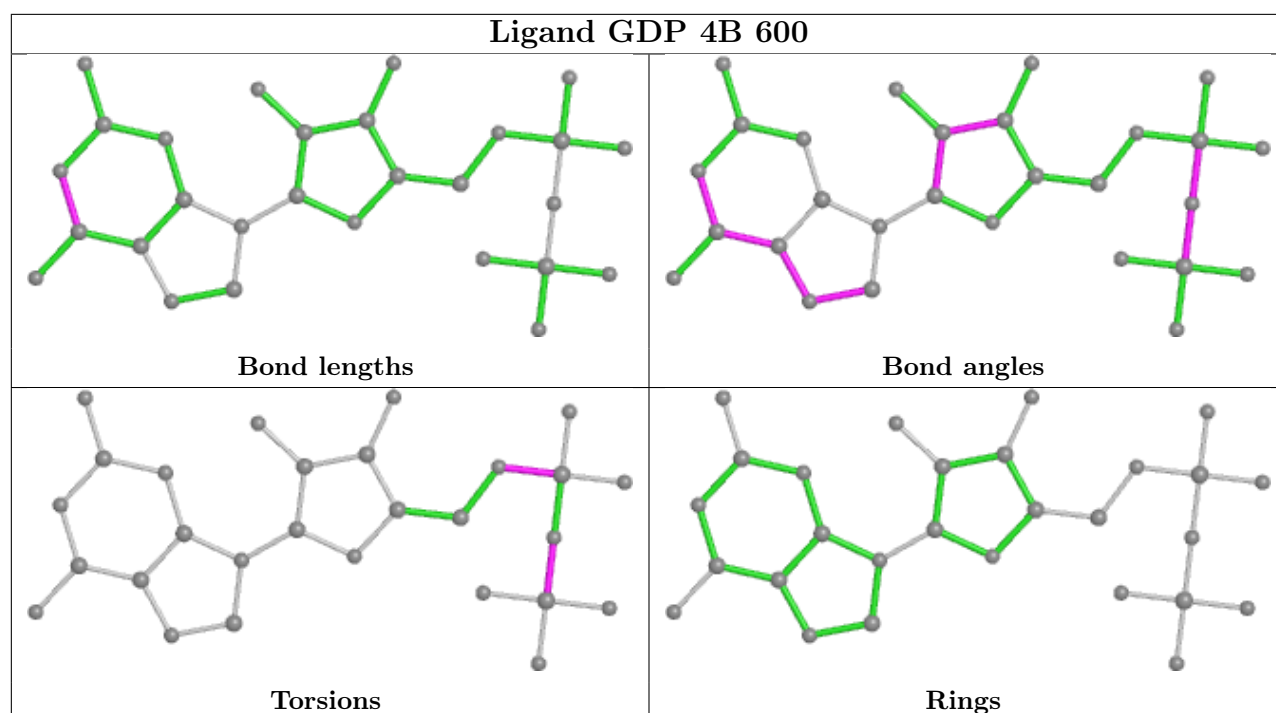




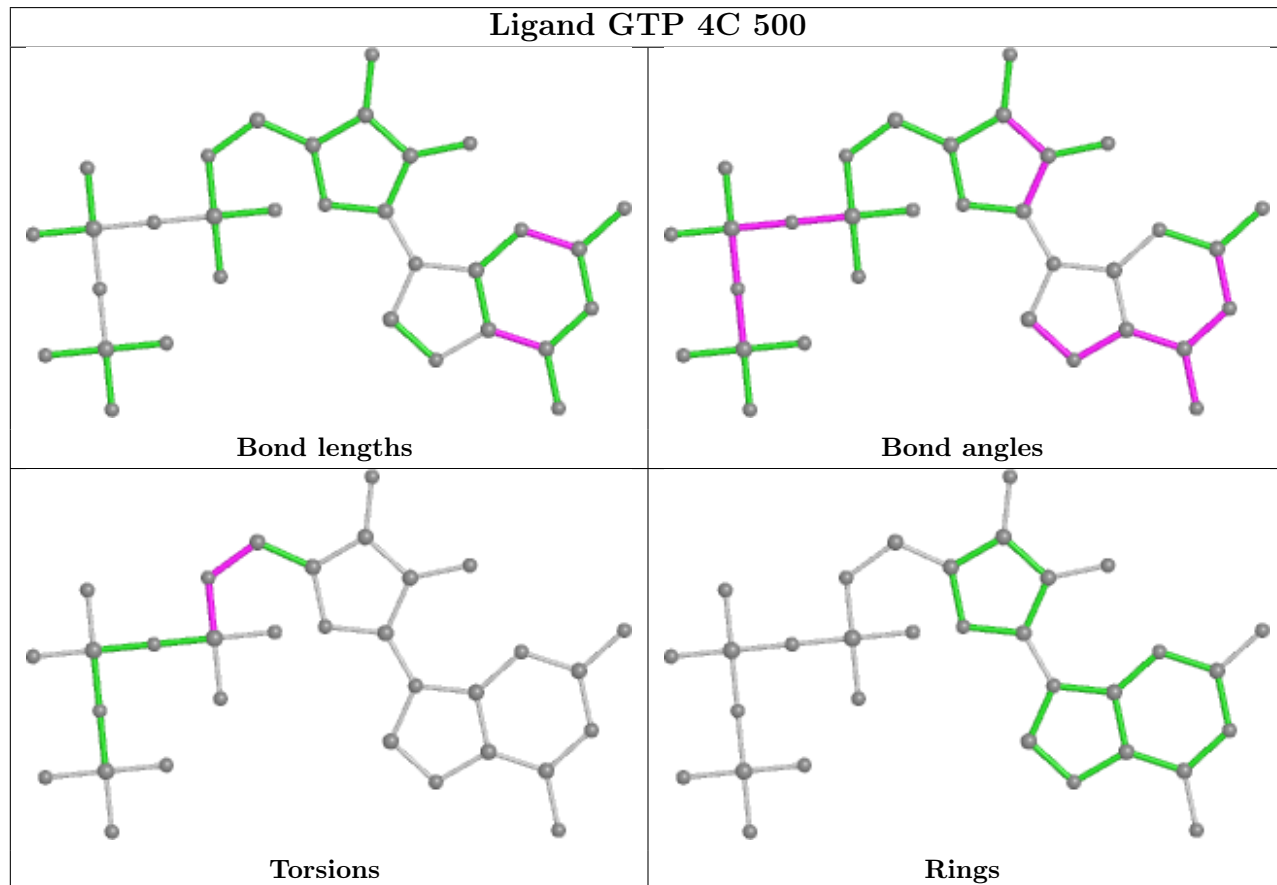
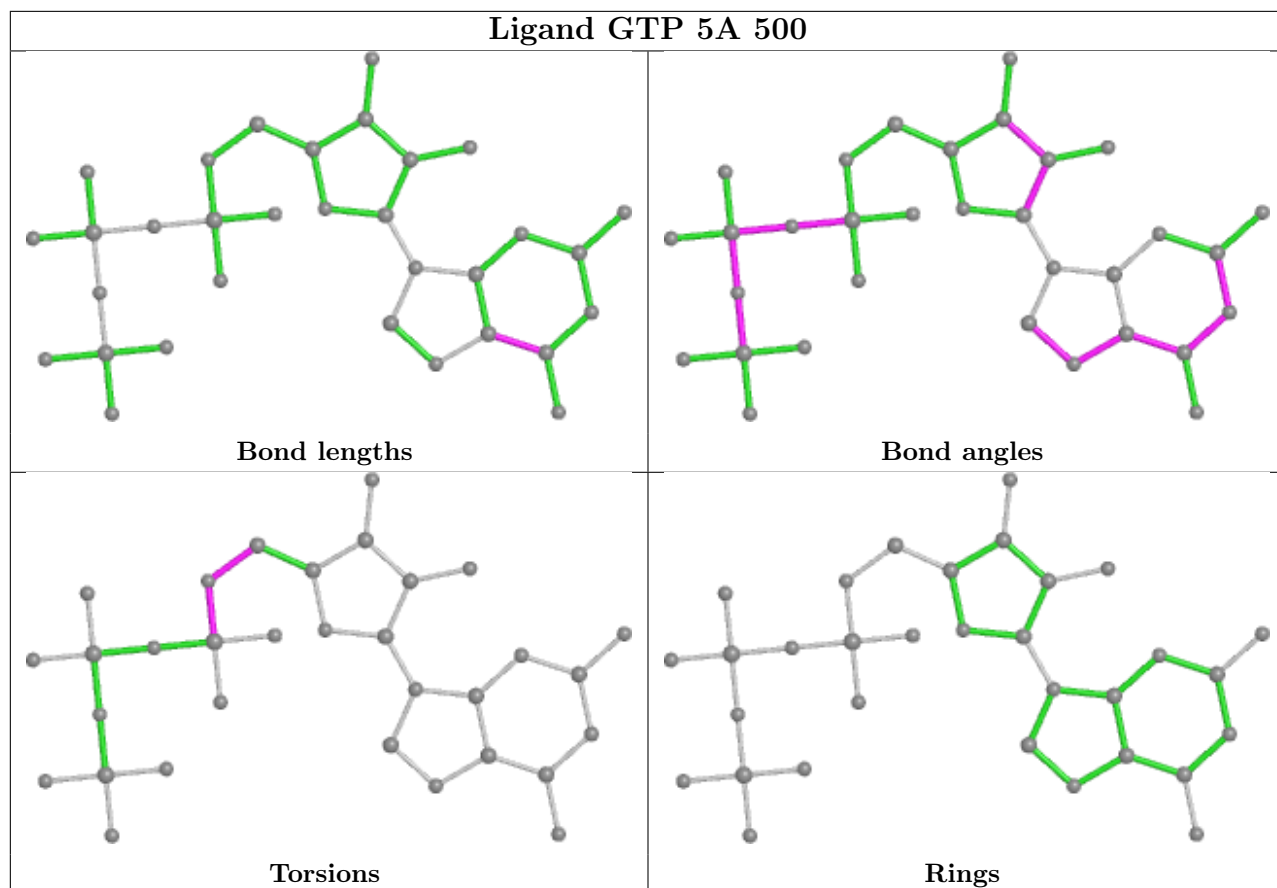


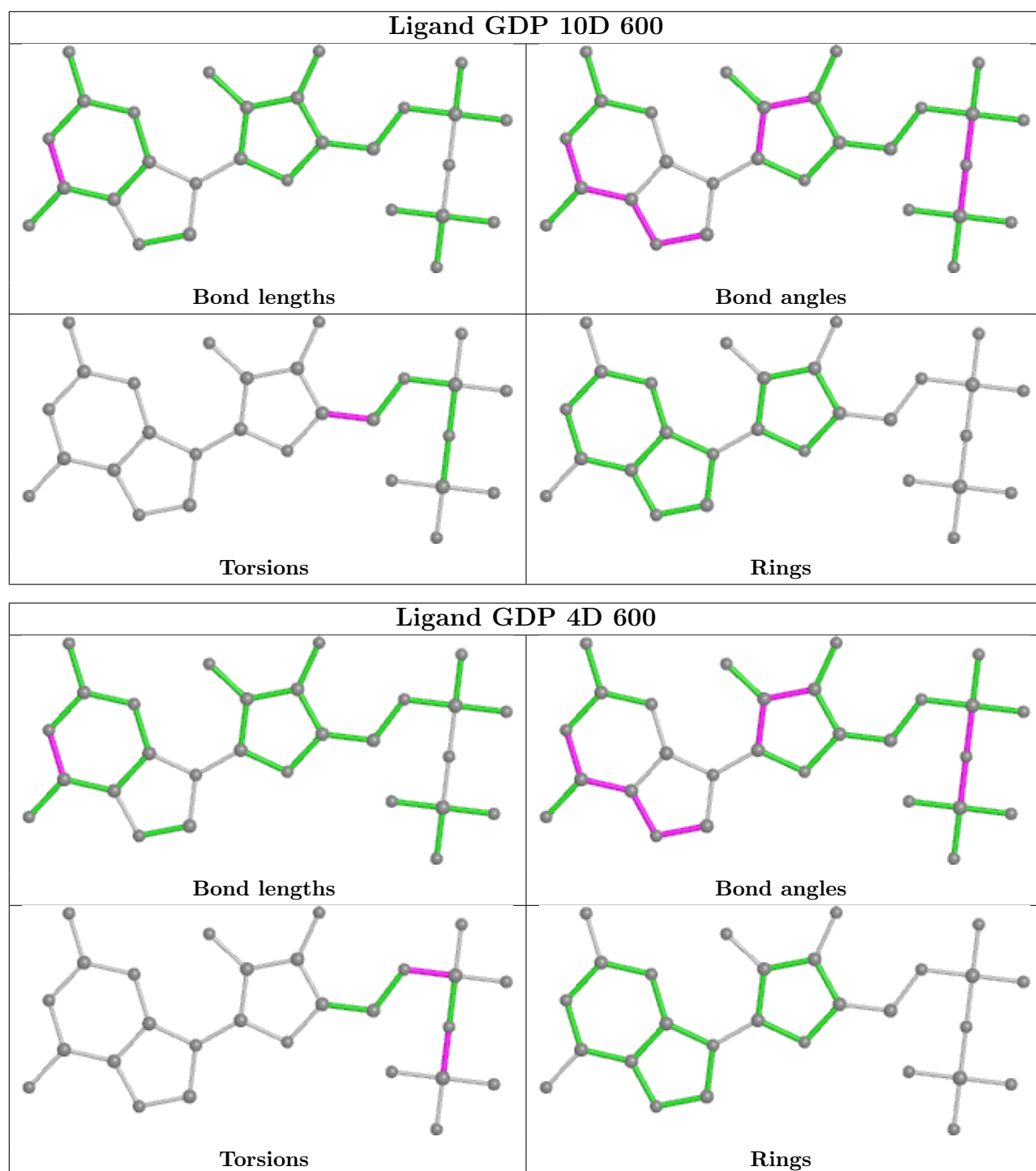


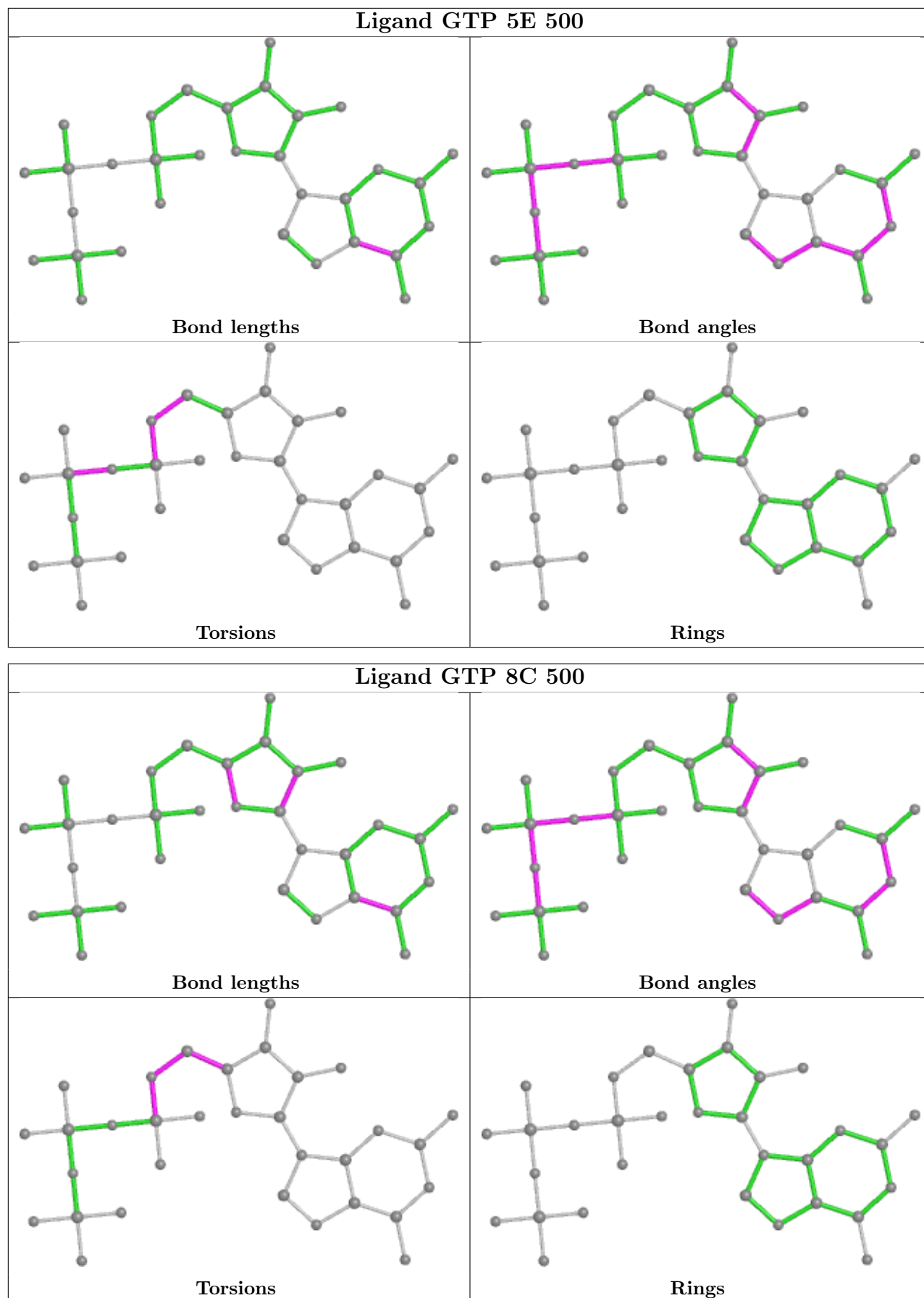


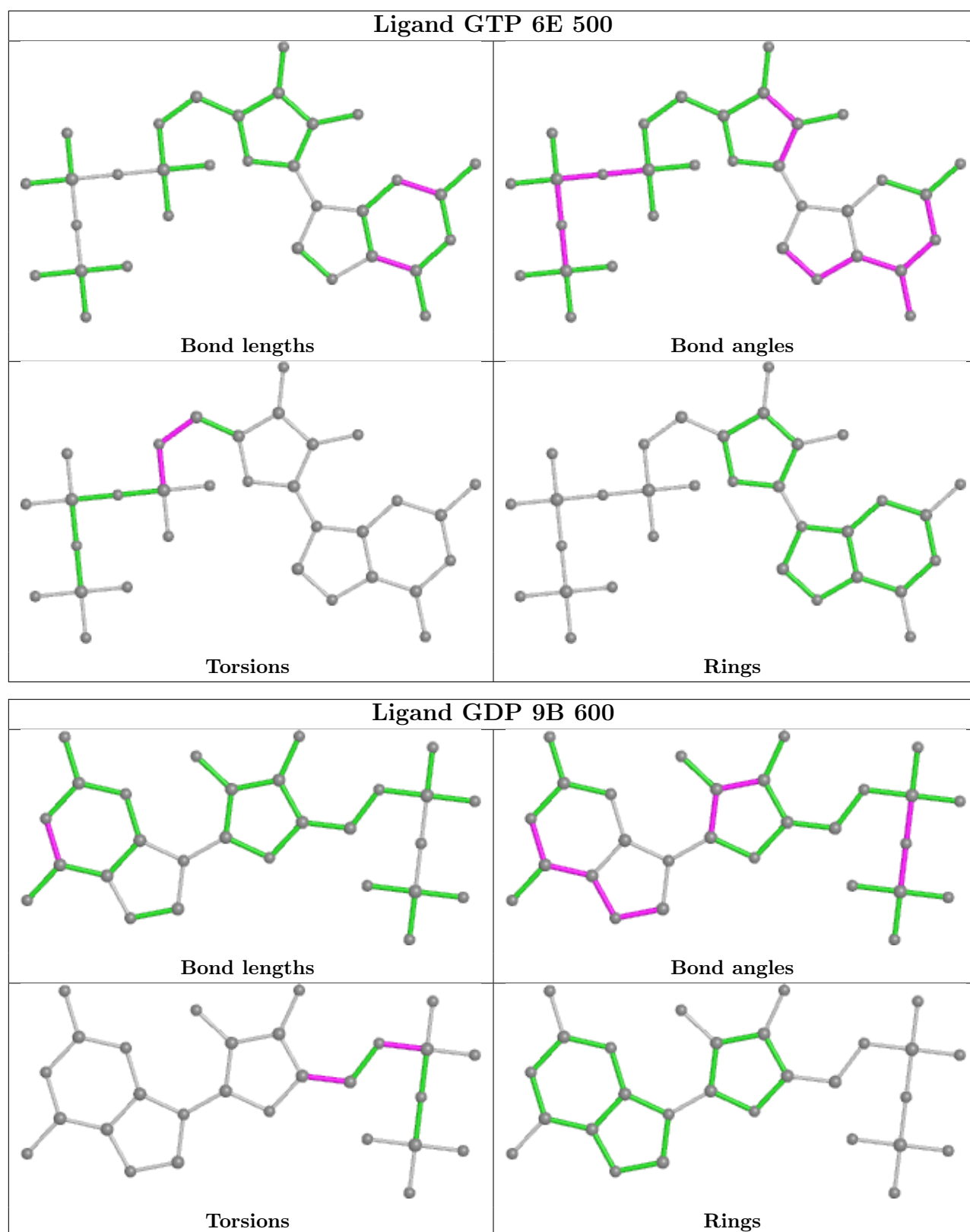


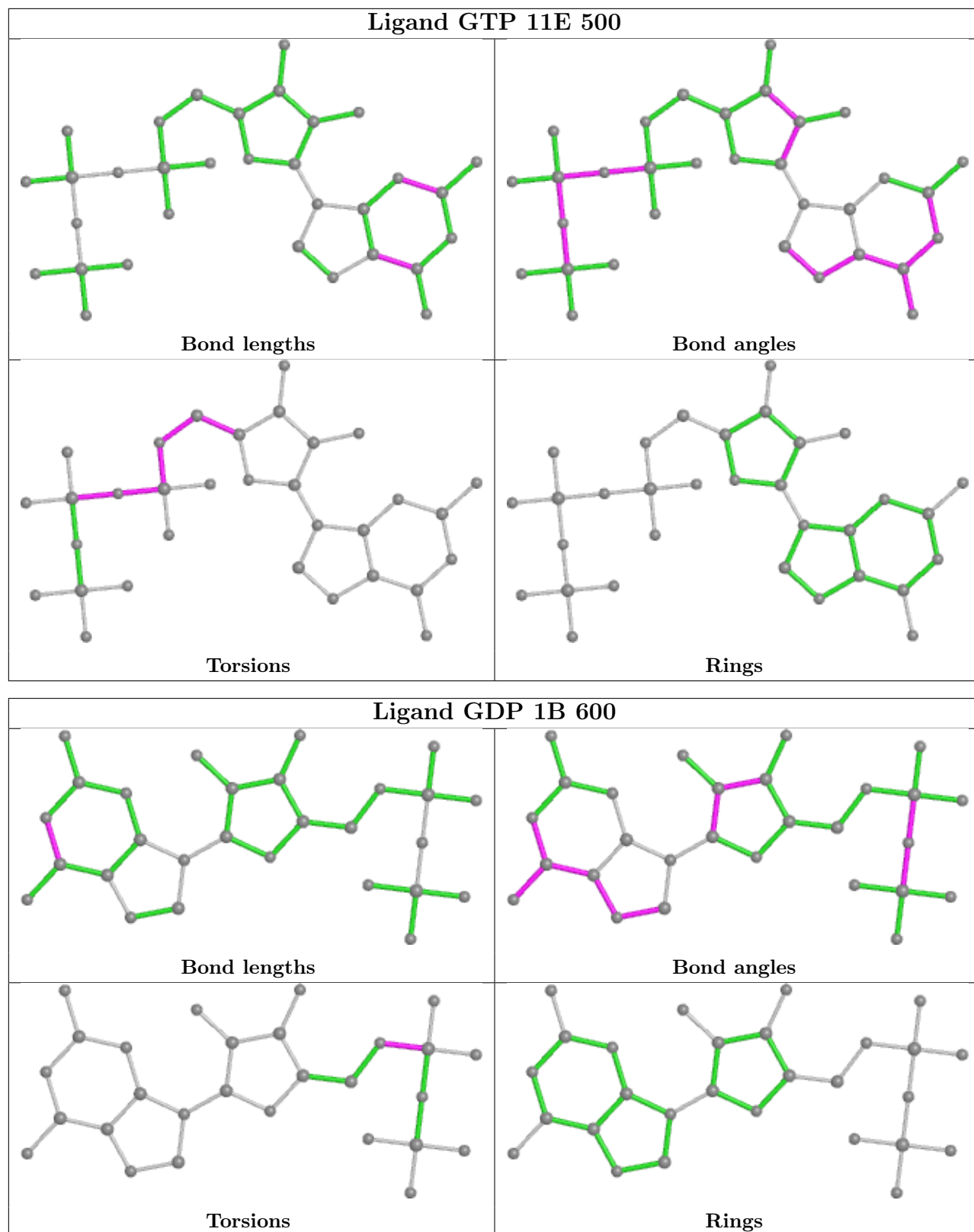


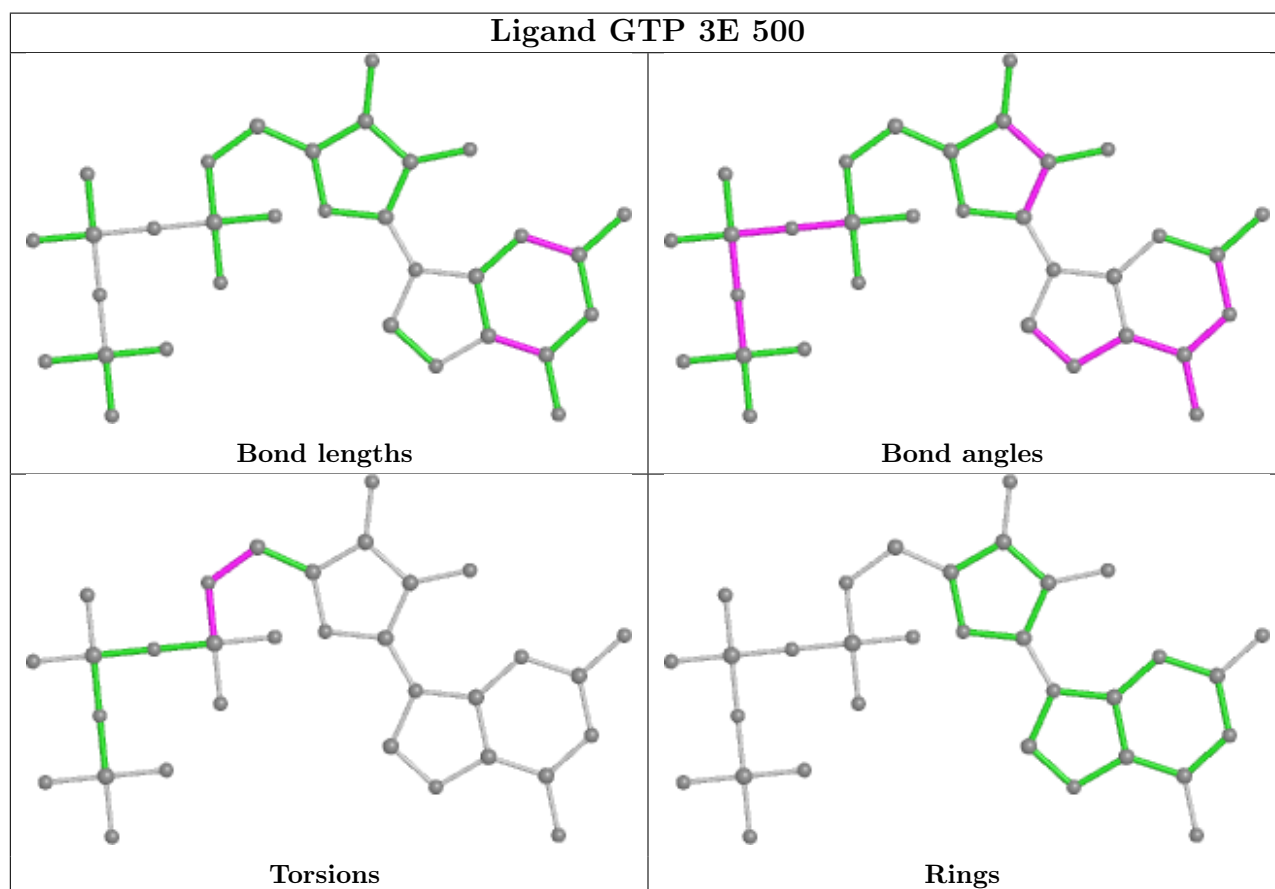
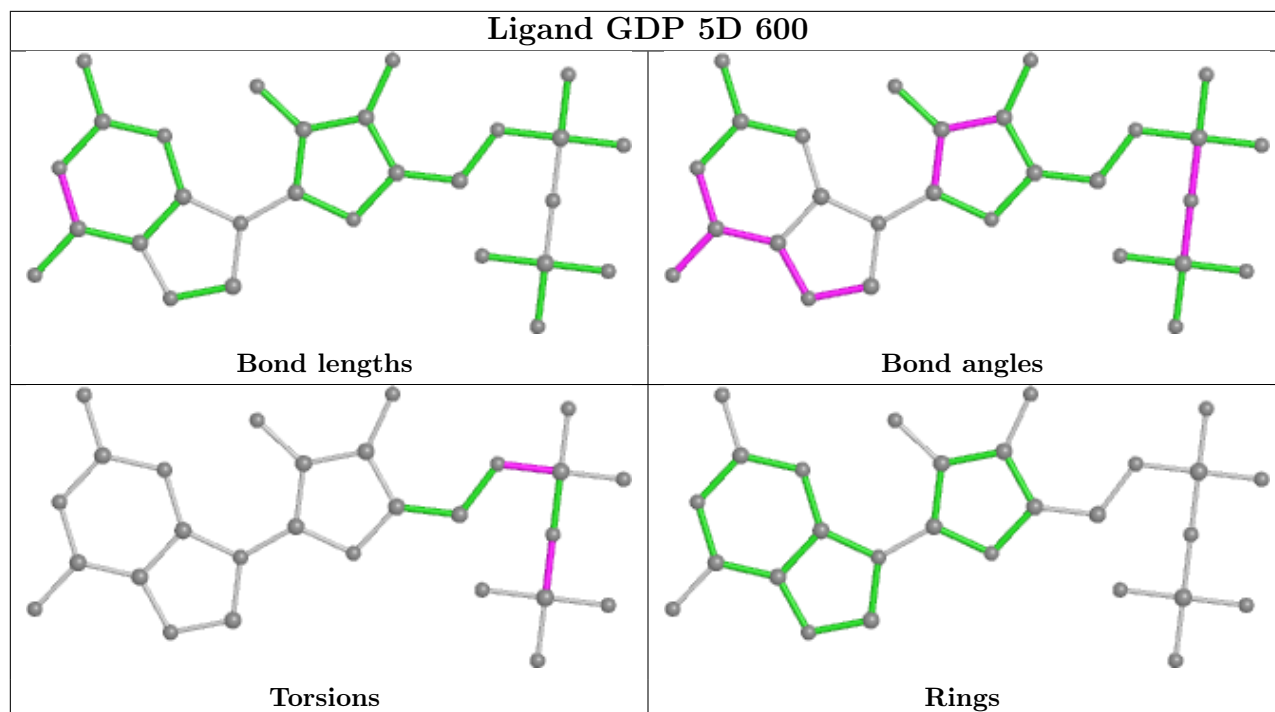


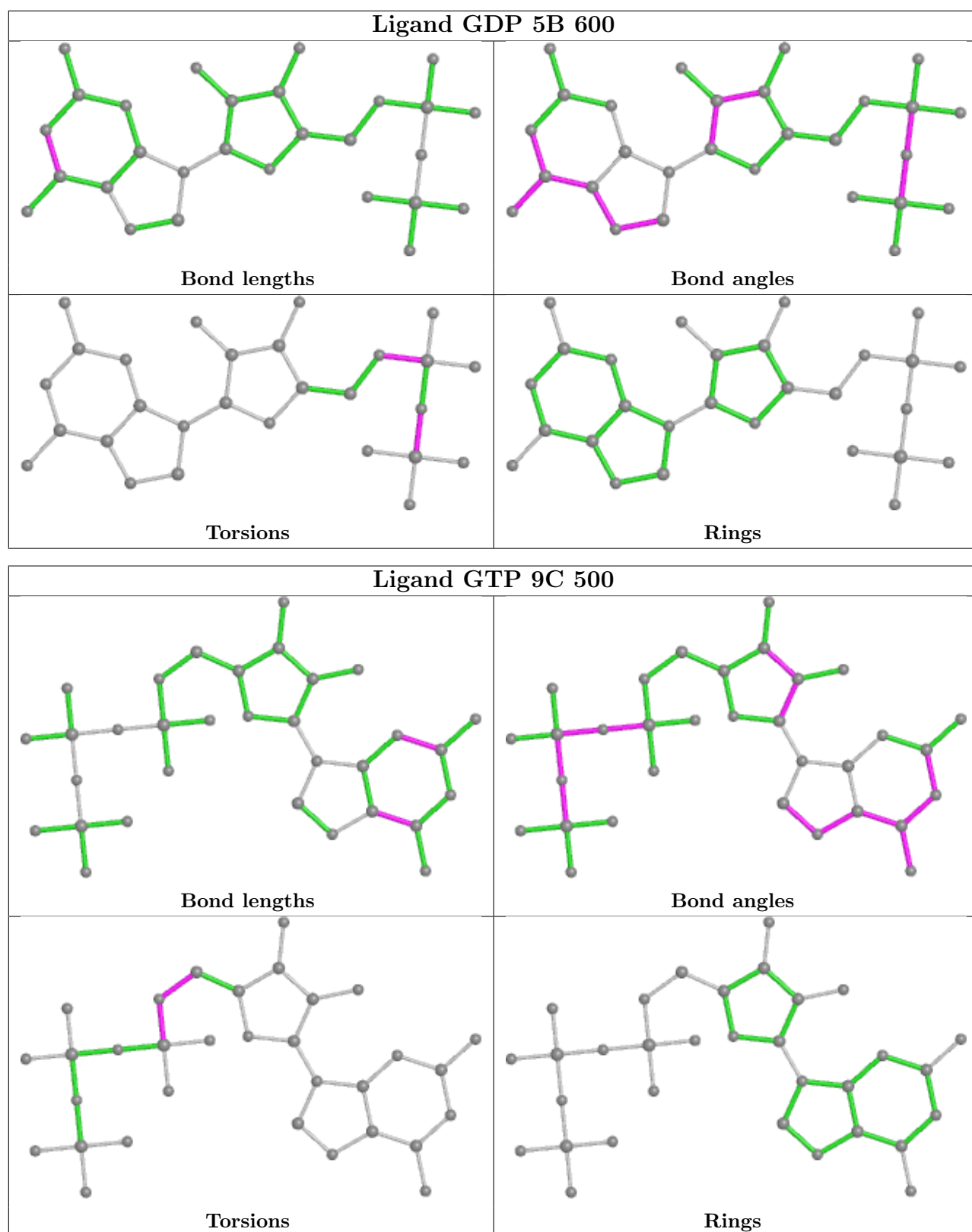


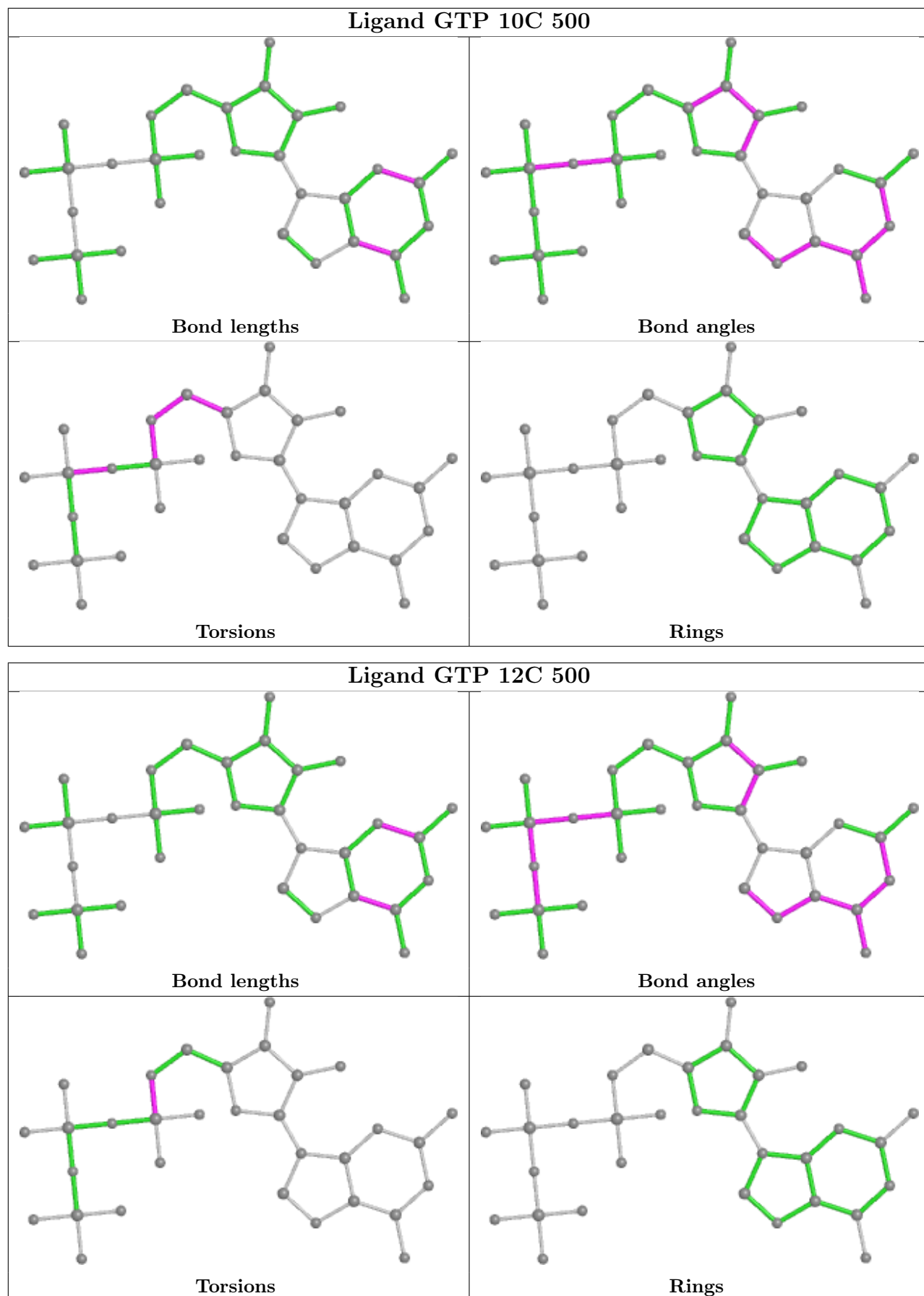




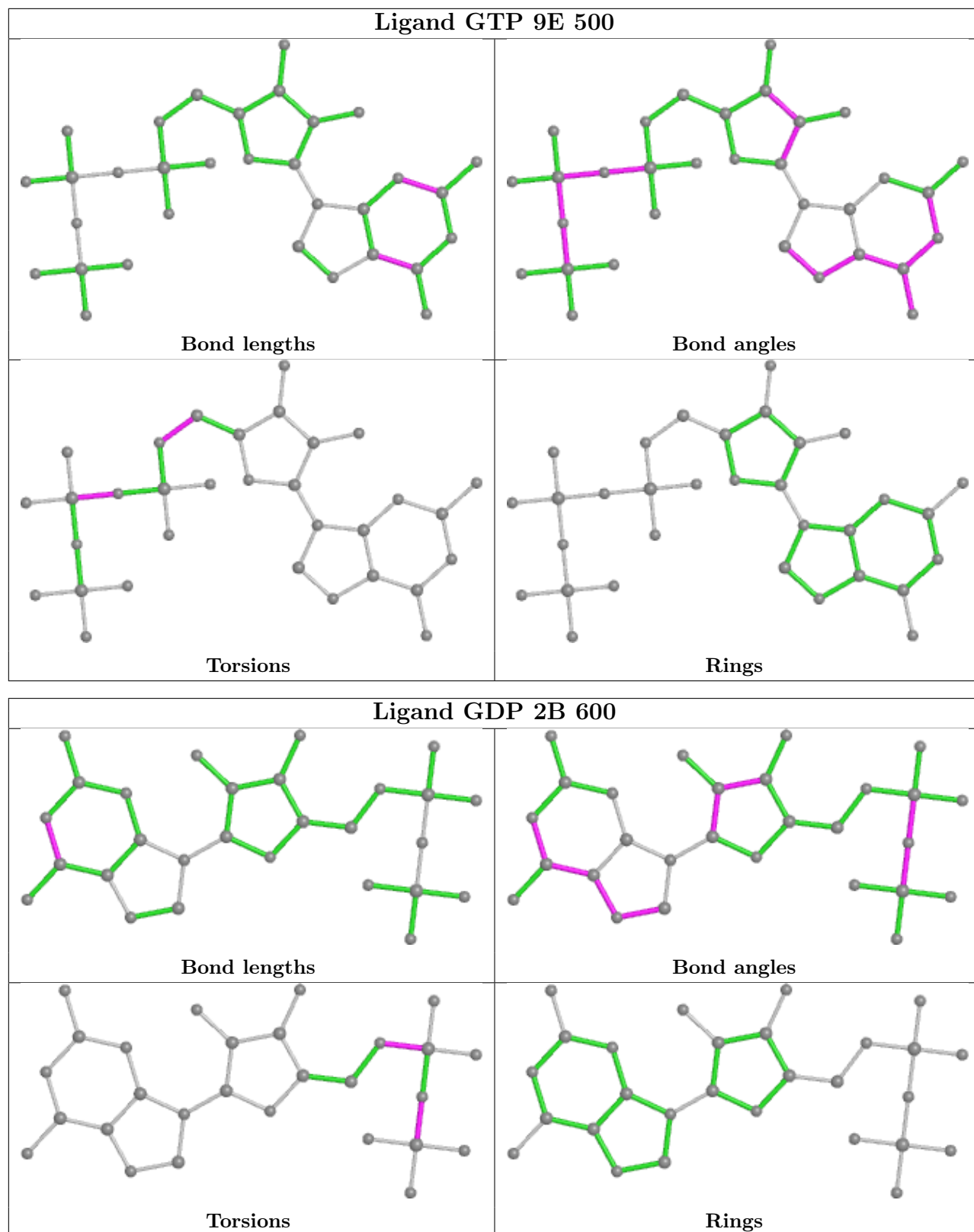


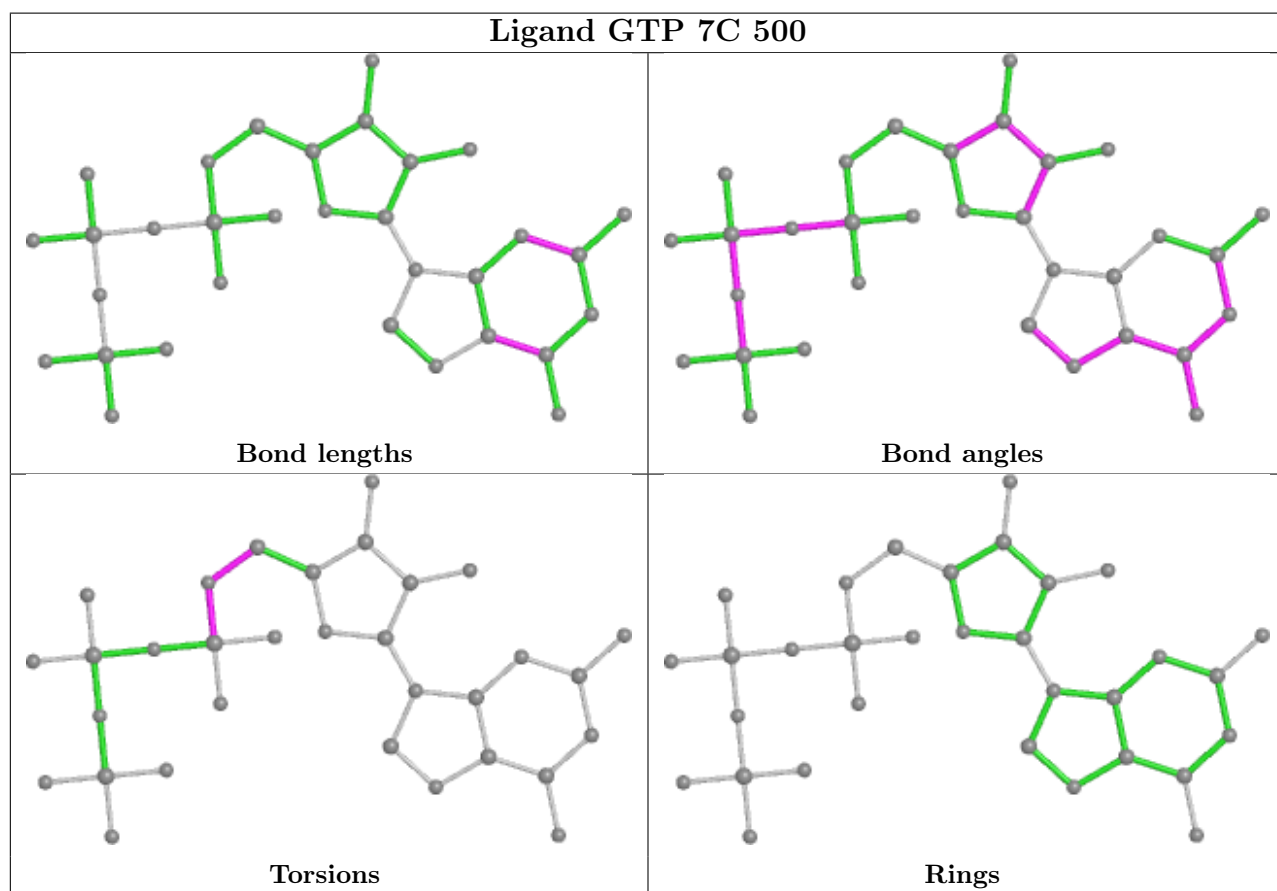
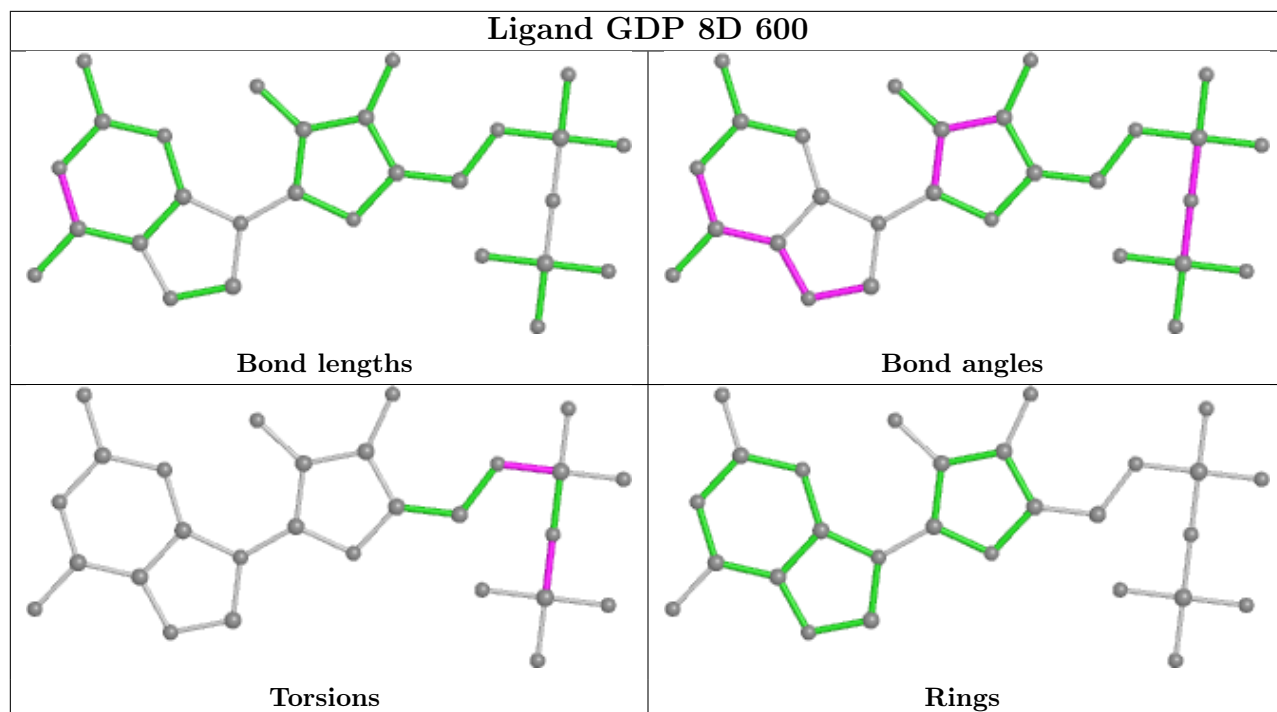


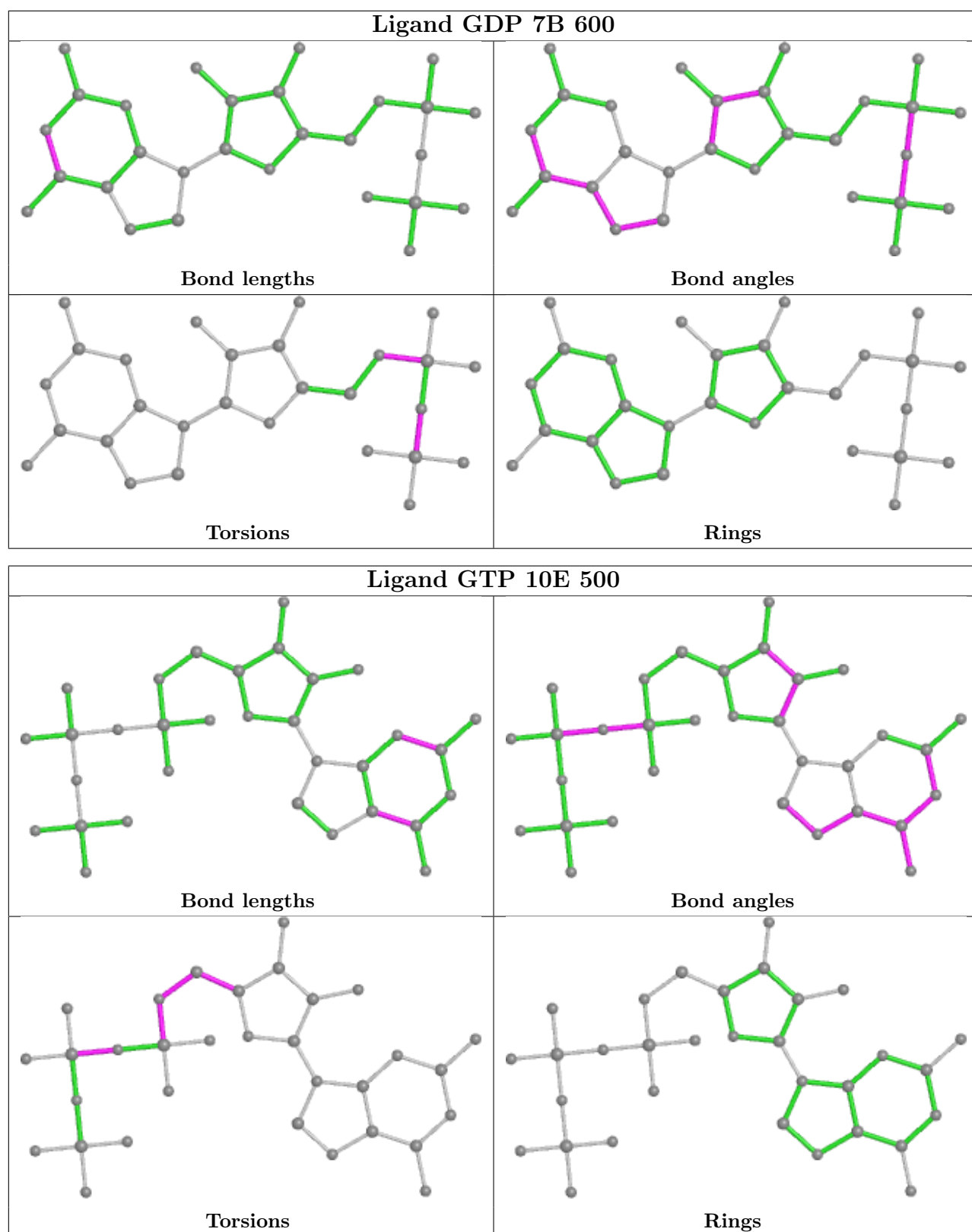


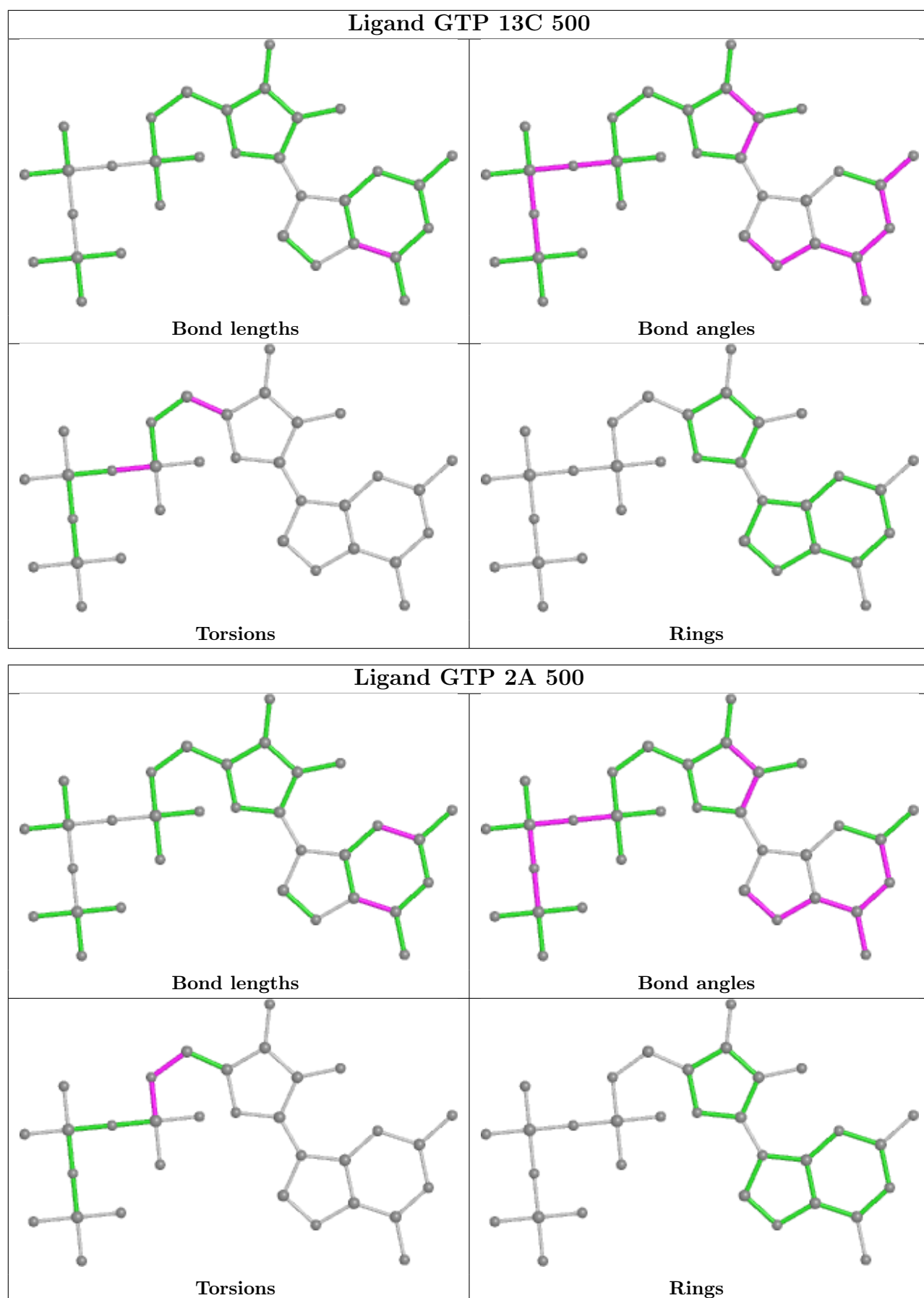


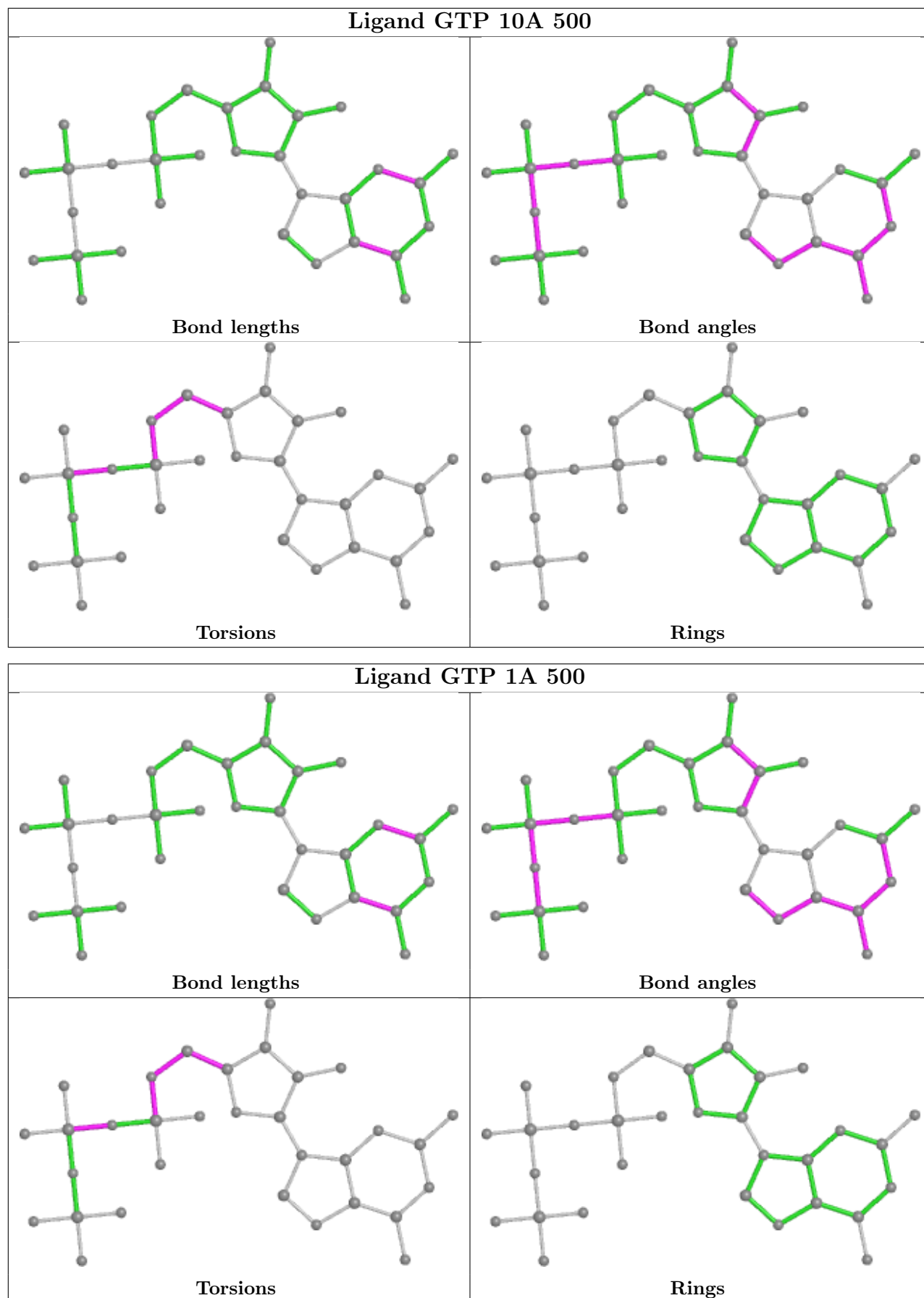


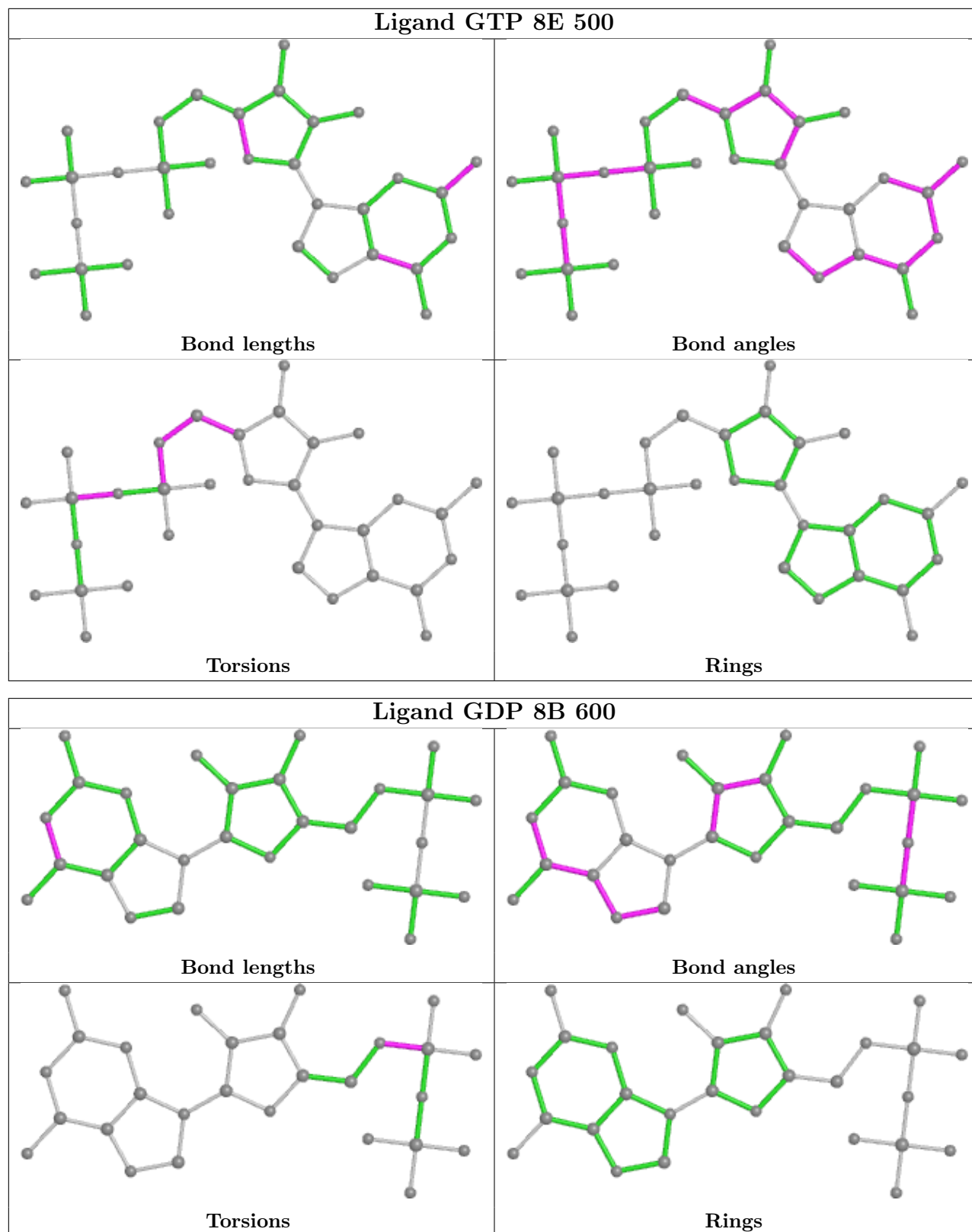


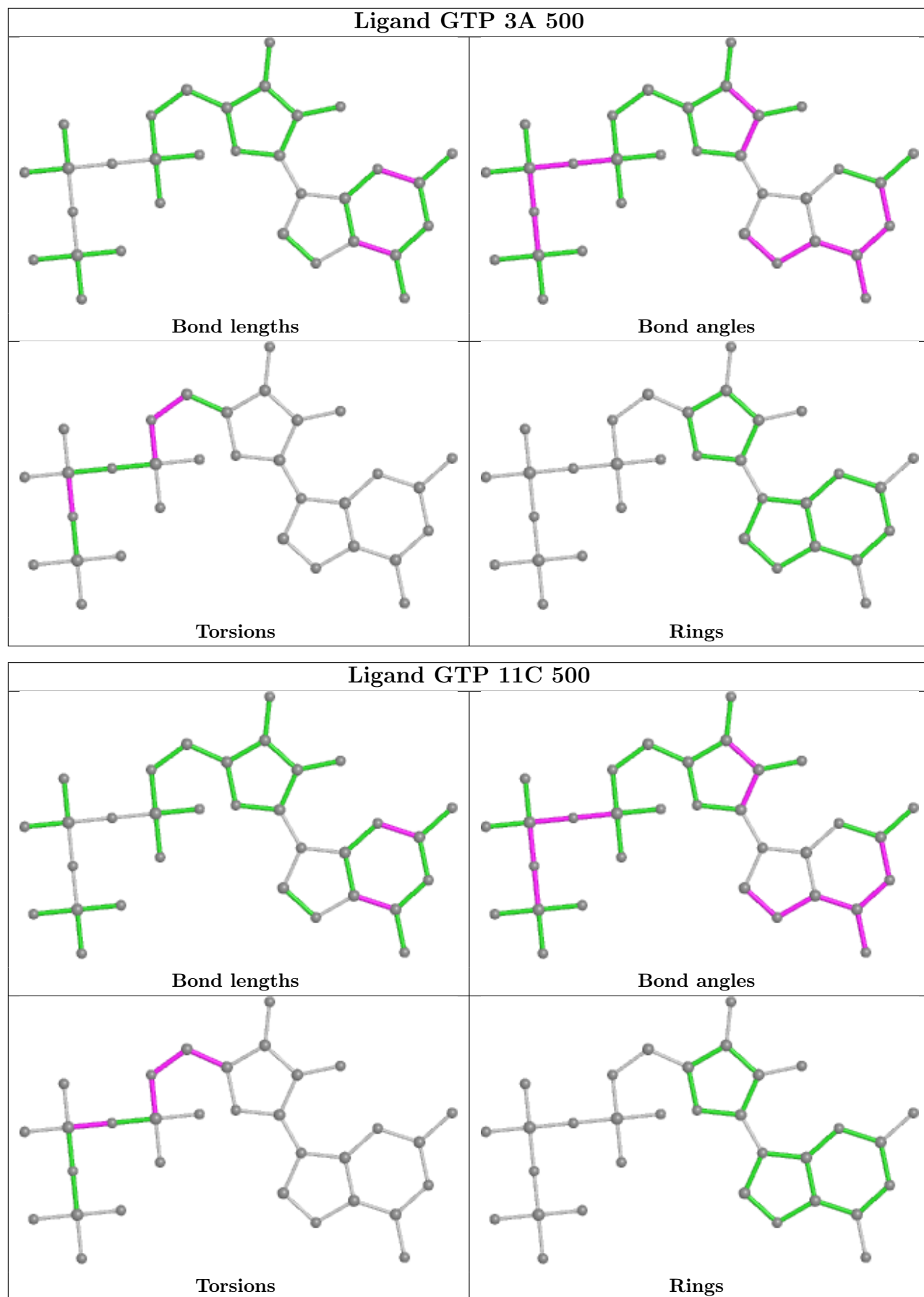


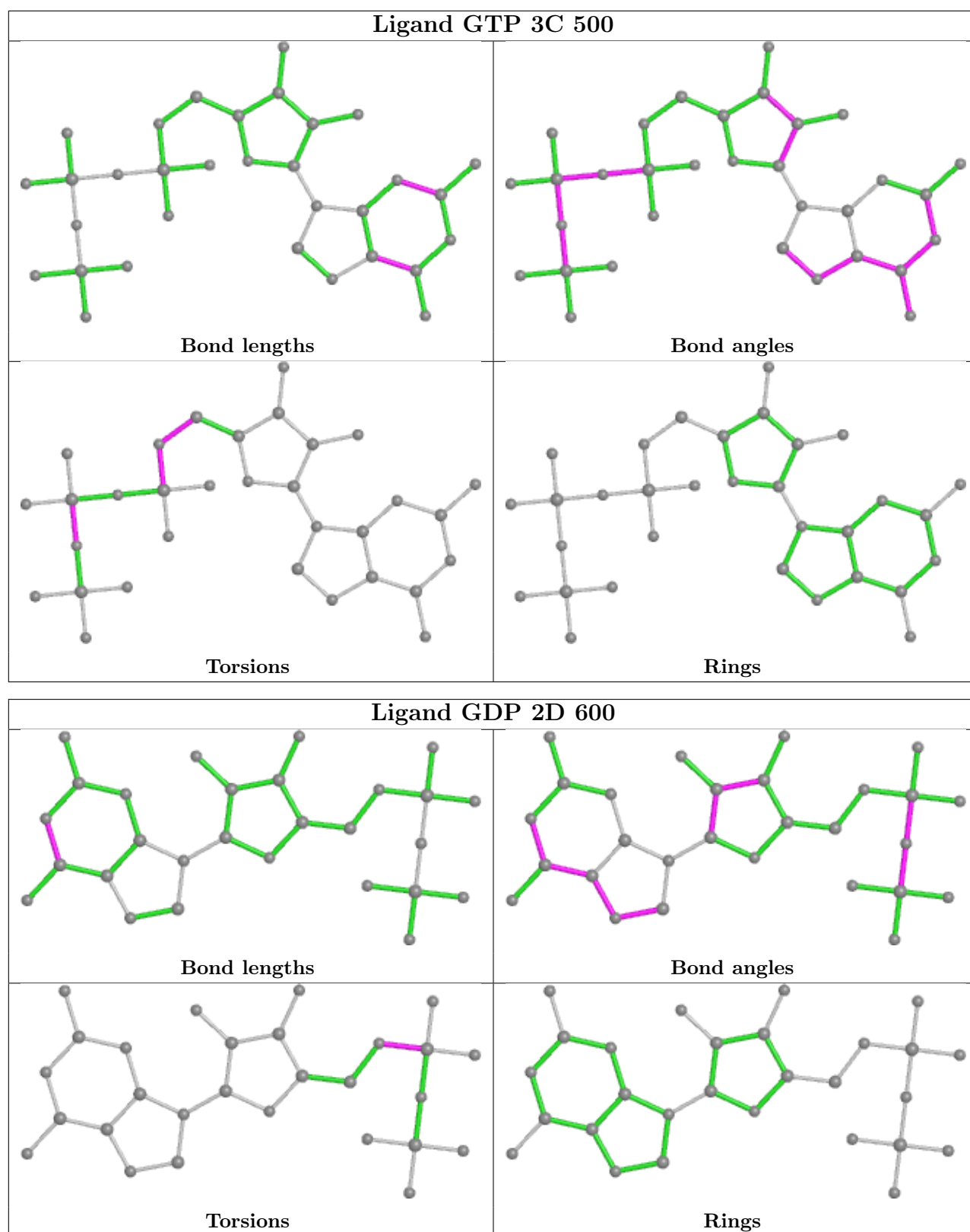




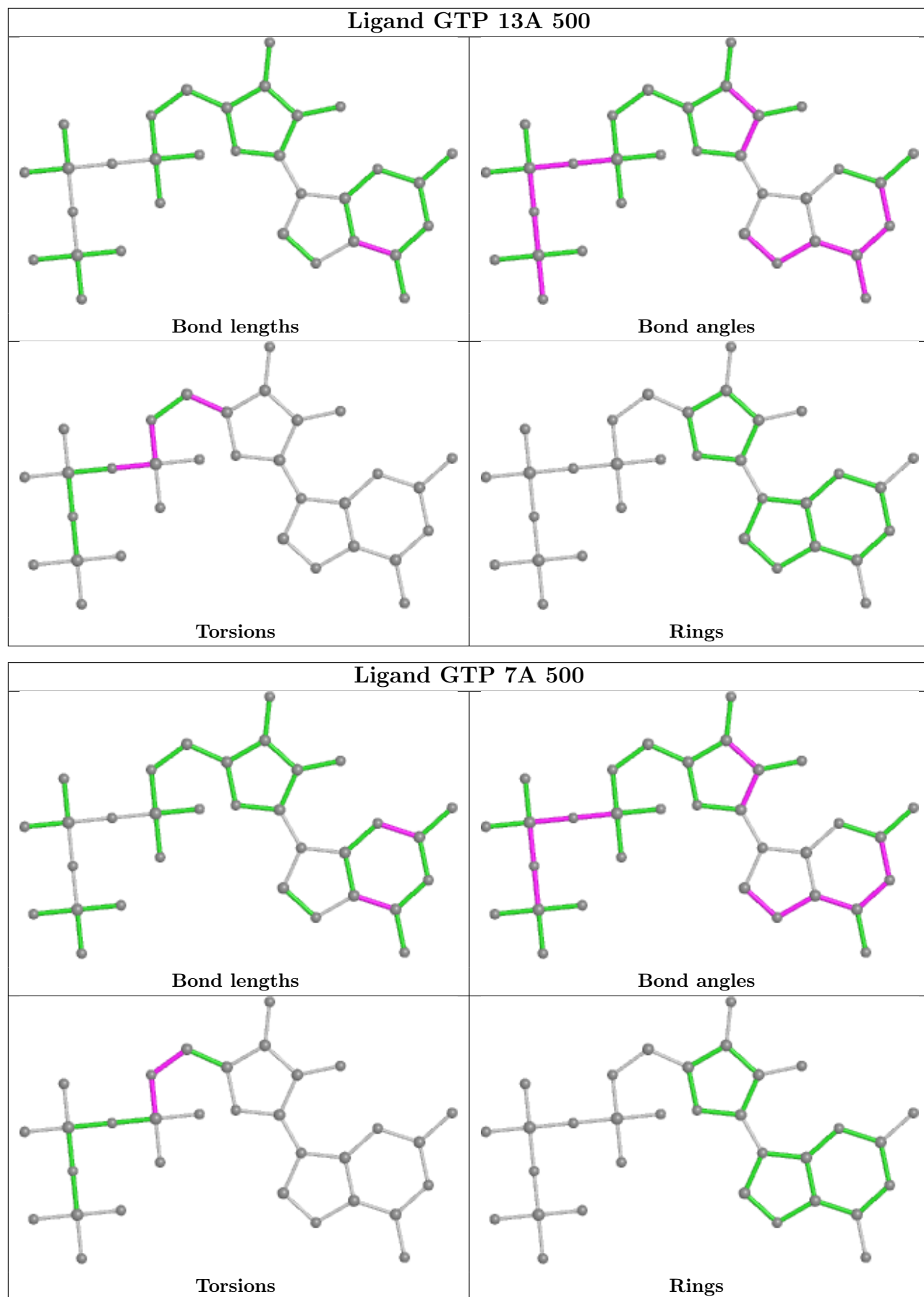


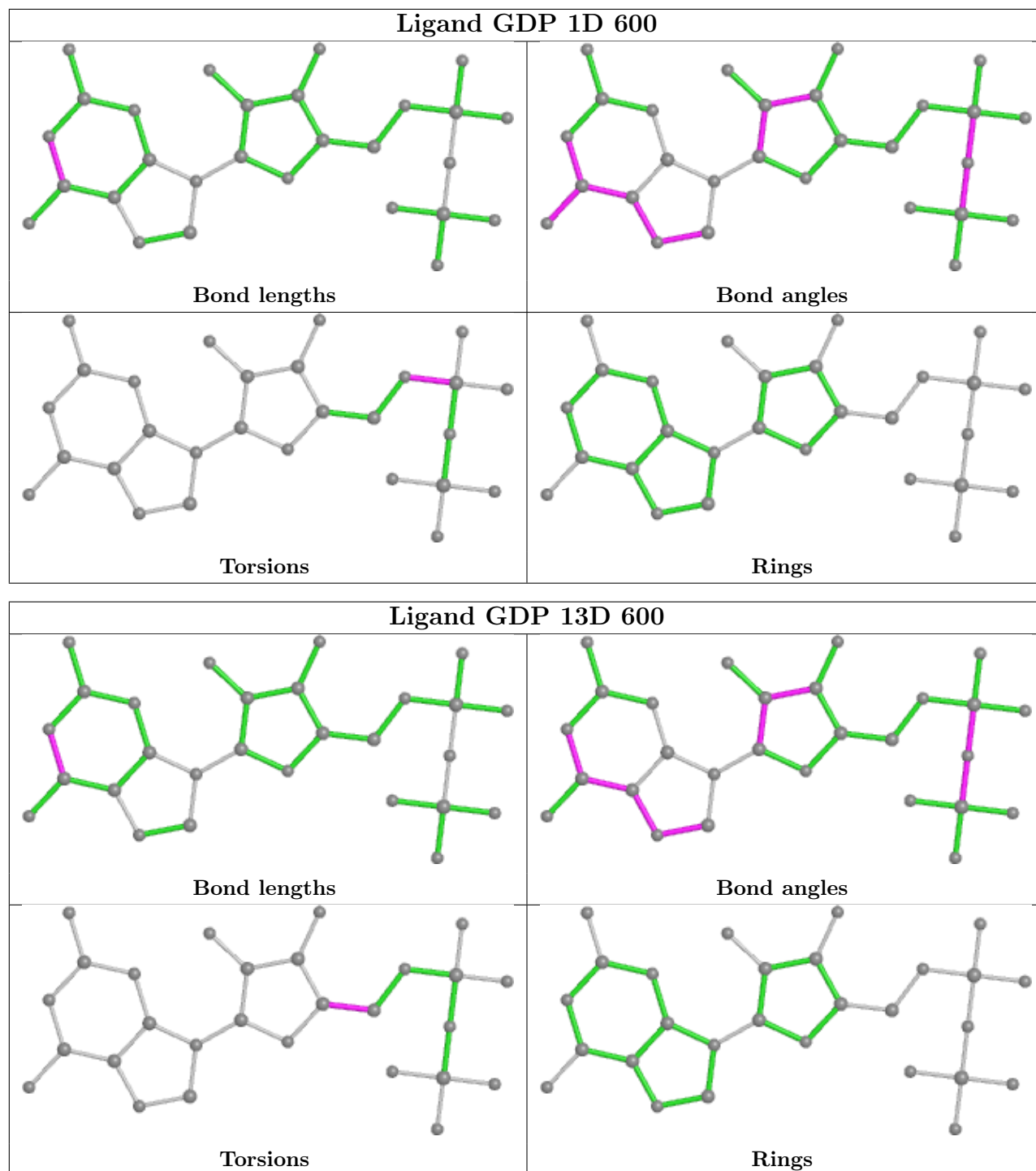


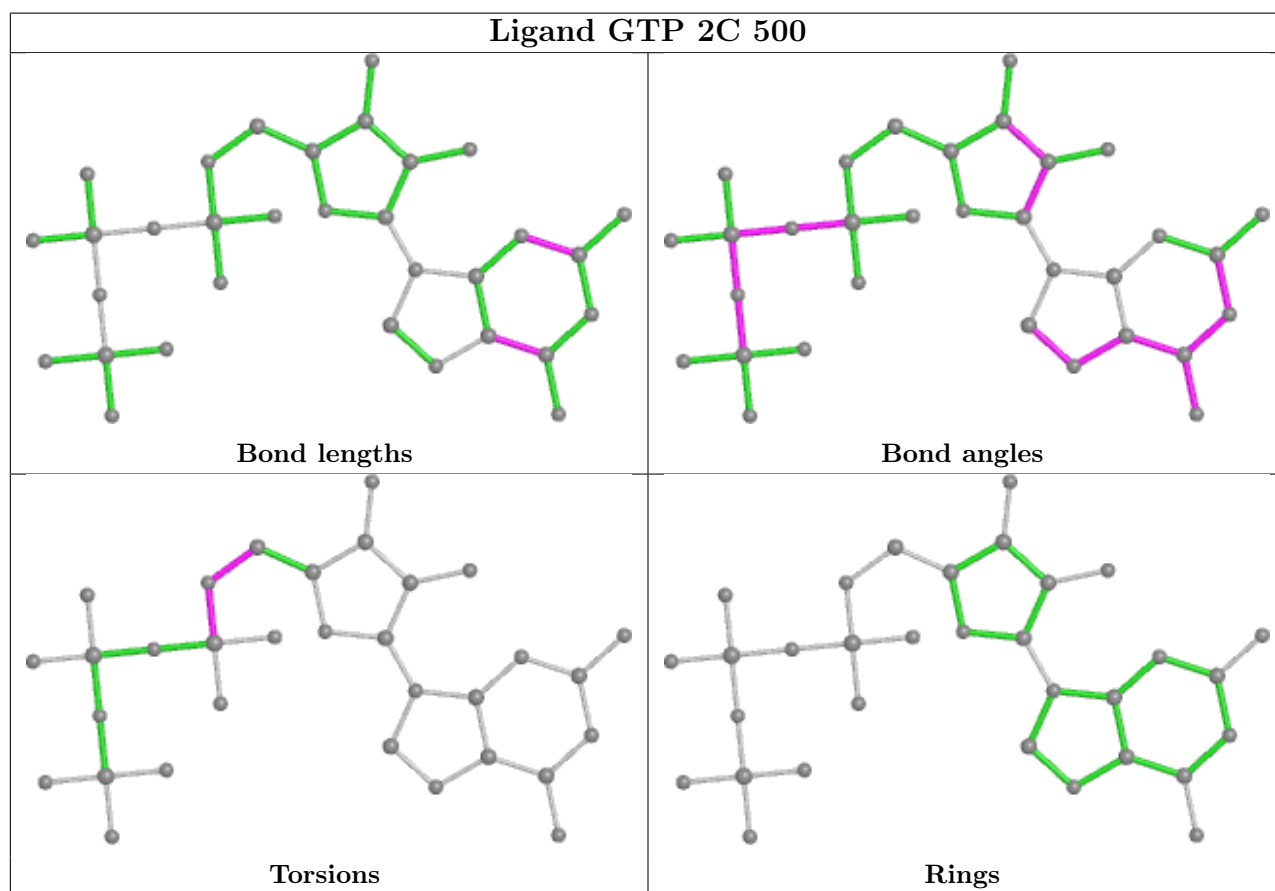
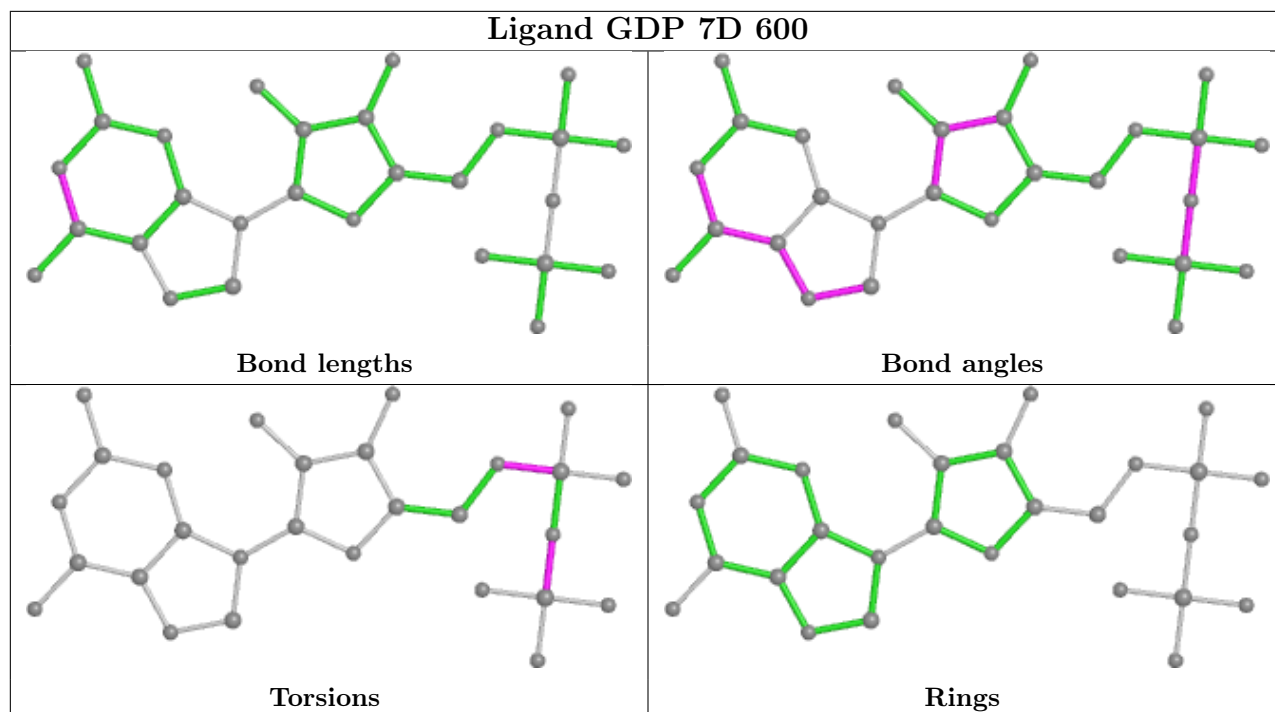


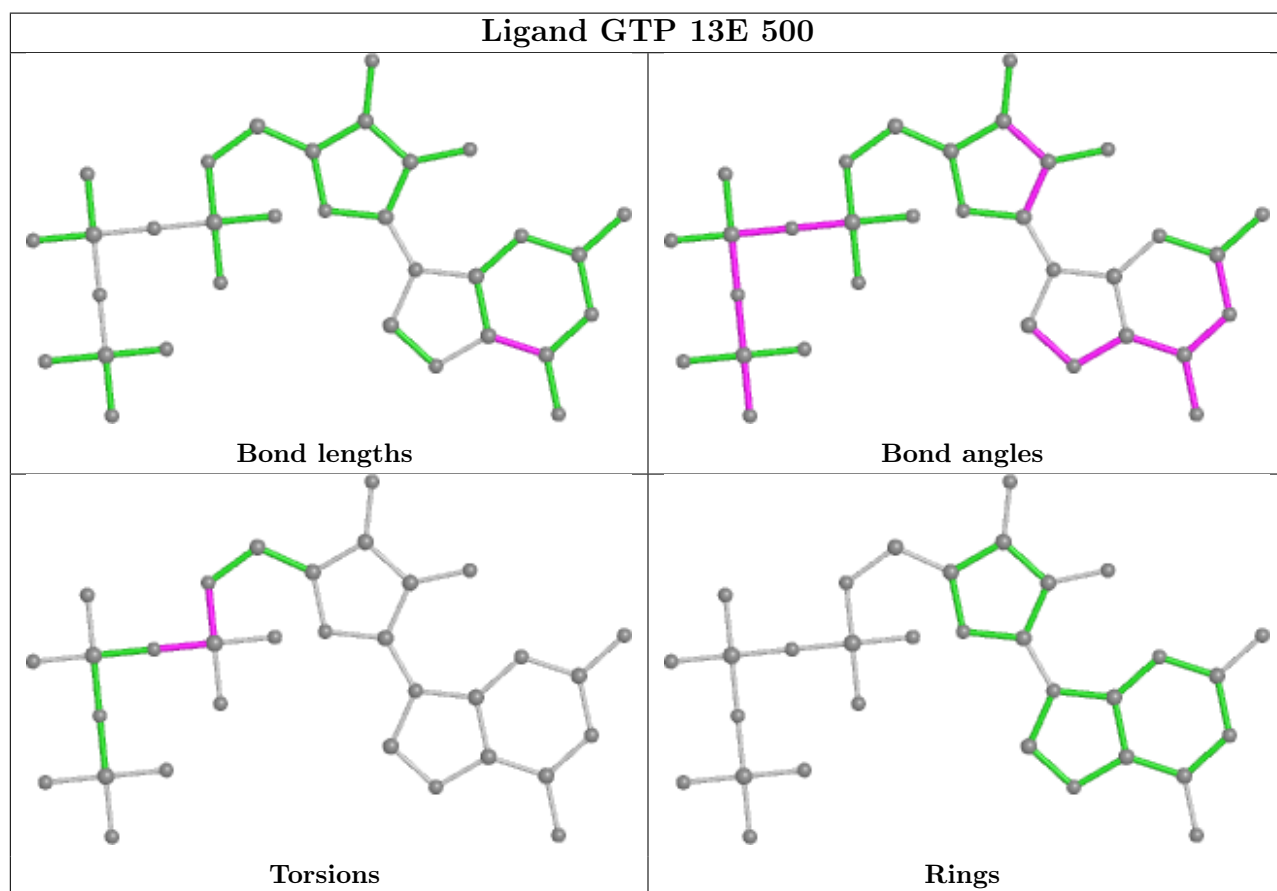
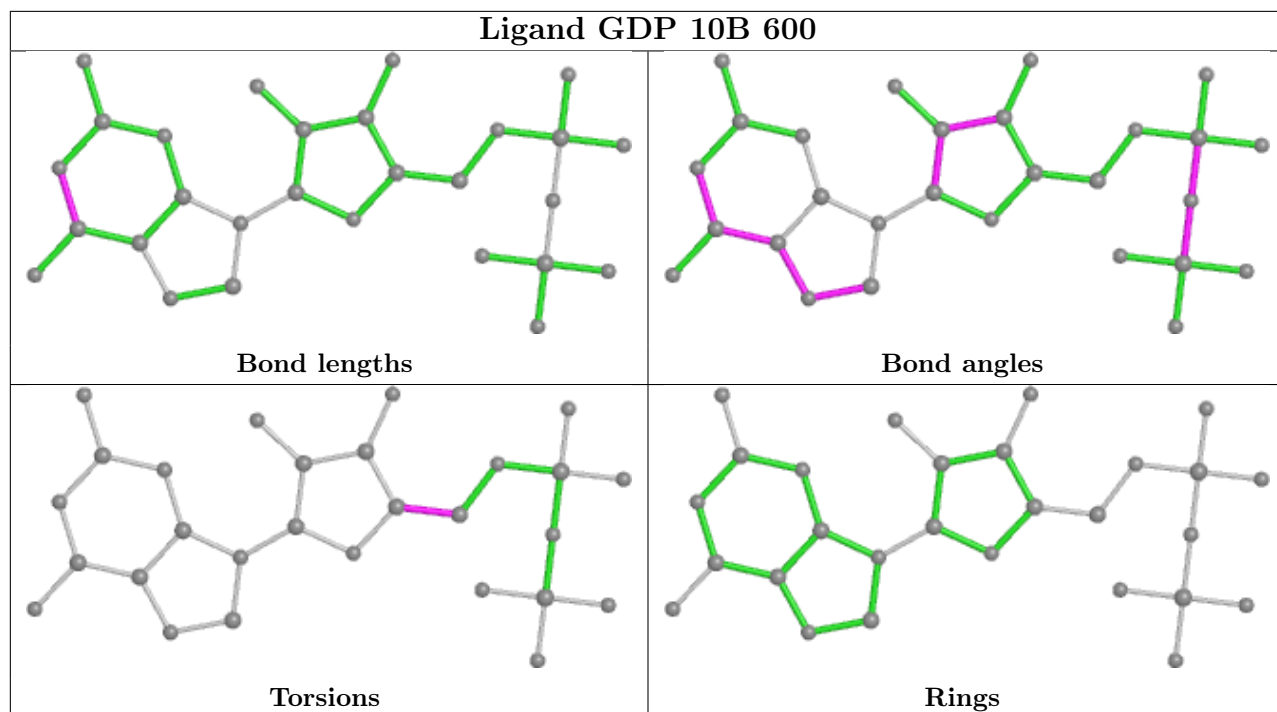


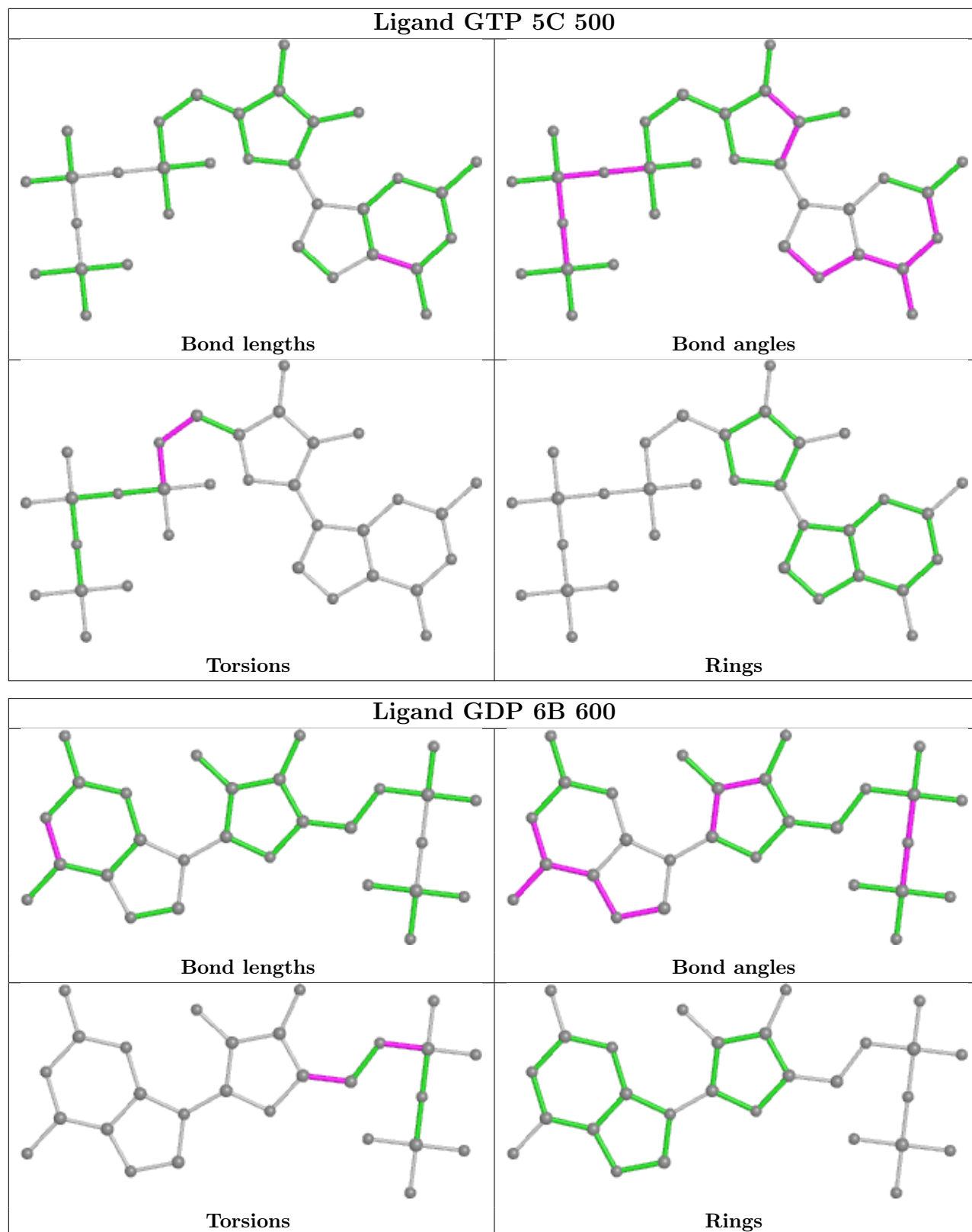


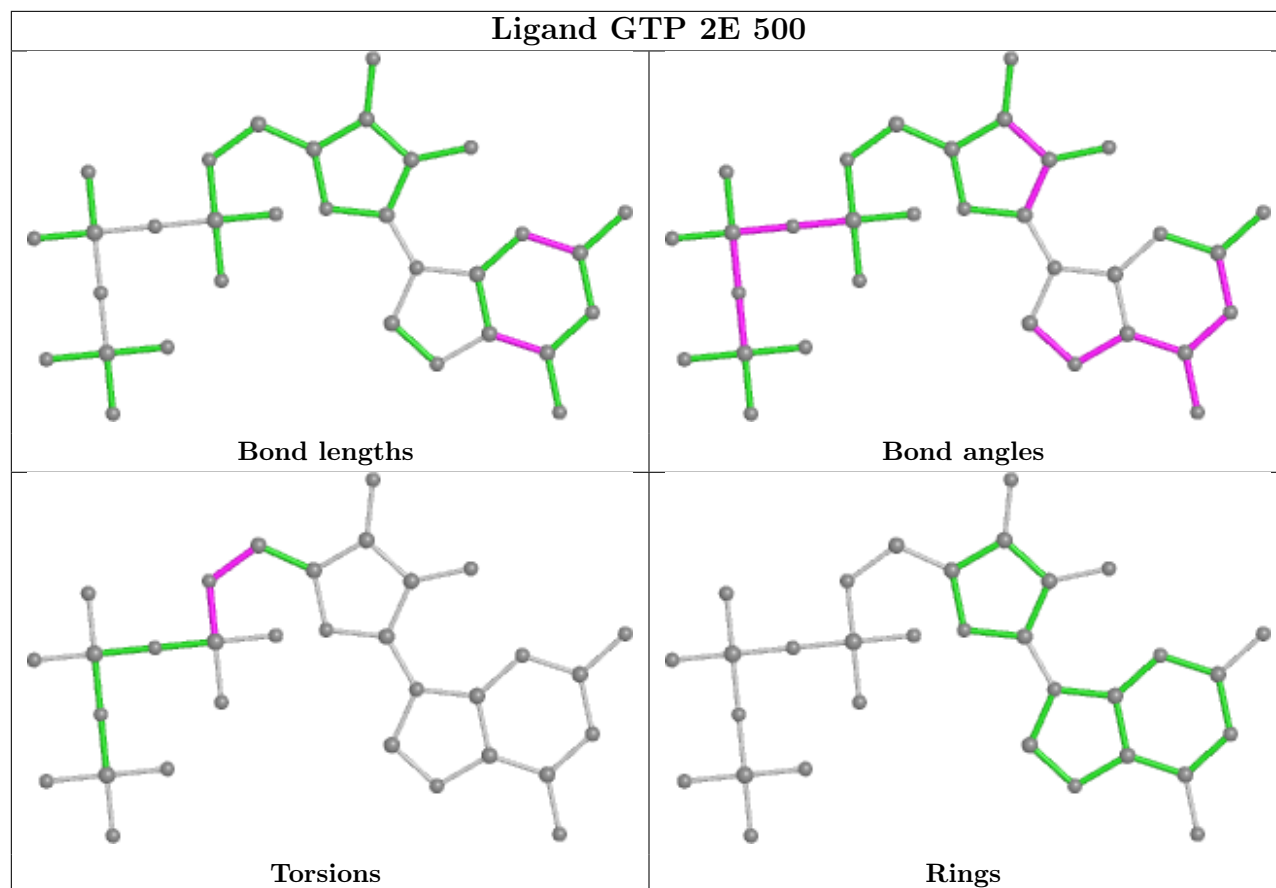












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

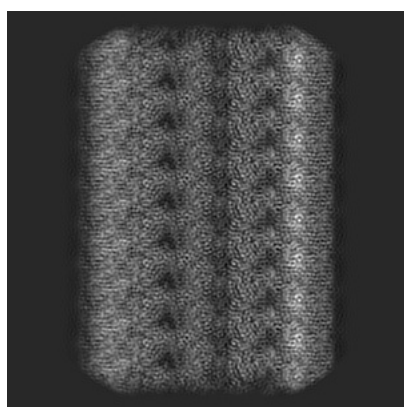
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14150. These allow visual inspection of the internal detail of the map and identification of artifacts.

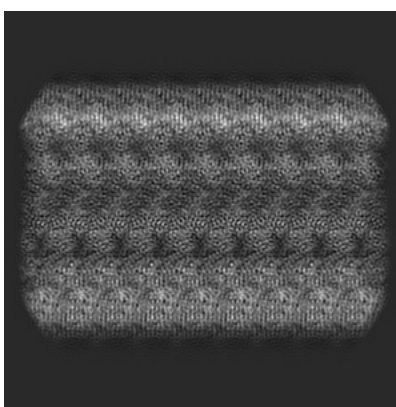
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

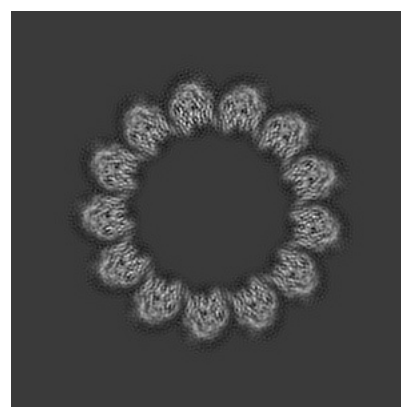
#### 6.1.1 Primary map



X



Y

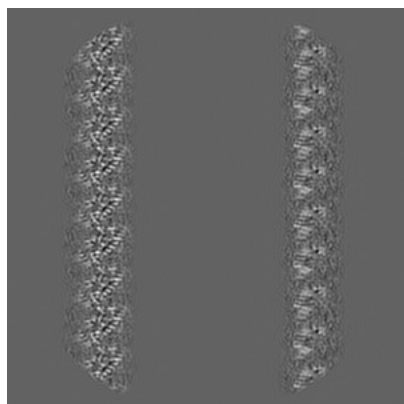


Z

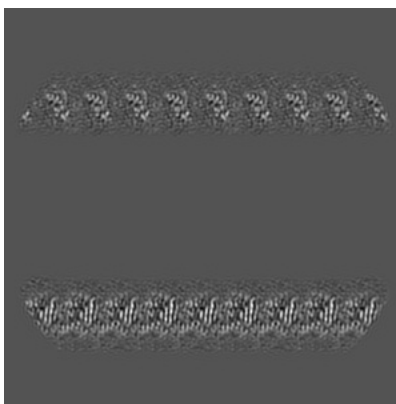
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

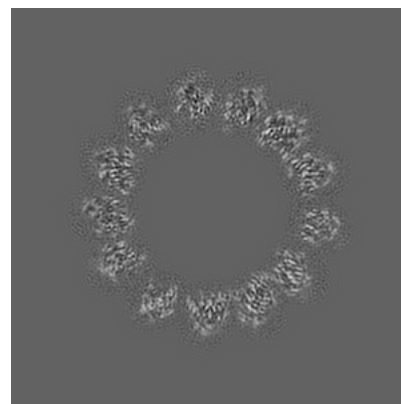
#### 6.2.1 Primary map



X Index: 196



Y Index: 196

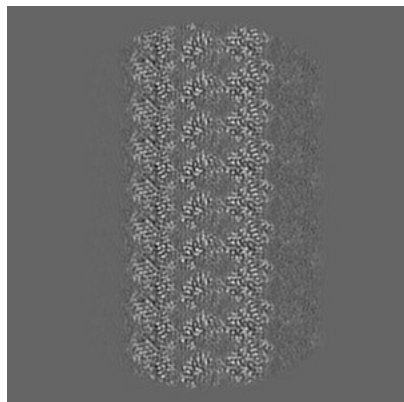


Z Index: 196

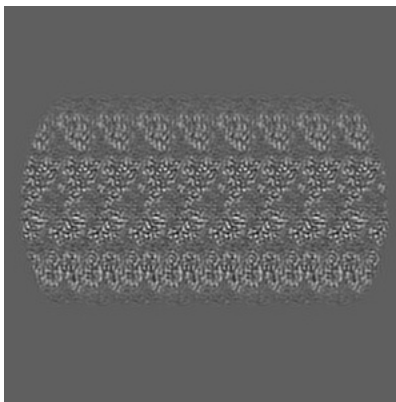
The images above show central slices of the map in three orthogonal directions.

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

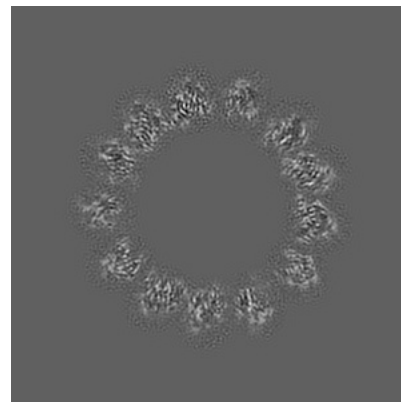
### 6.3.1 Primary map



X Index: 107



Y Index: 284

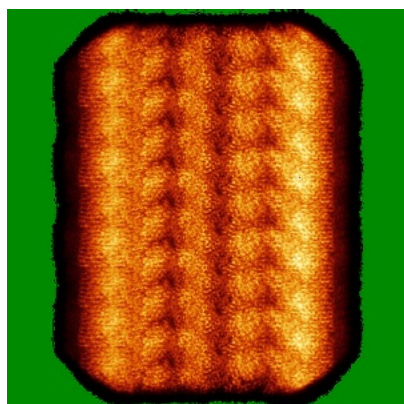


Z Index: 170

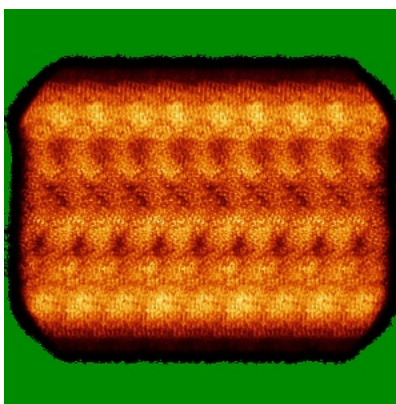
The images above show the largest variance slices of the map in three orthogonal directions.

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

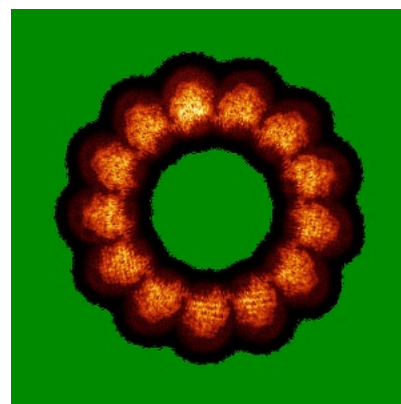
### 6.4.1 Primary map



X



Y



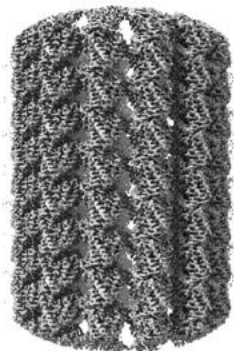
Z

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

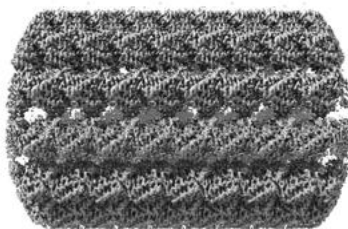


## 6.5 Orthogonal surface views [i](#)

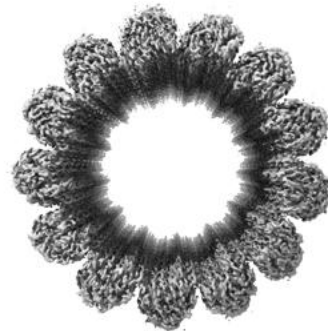
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.582. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

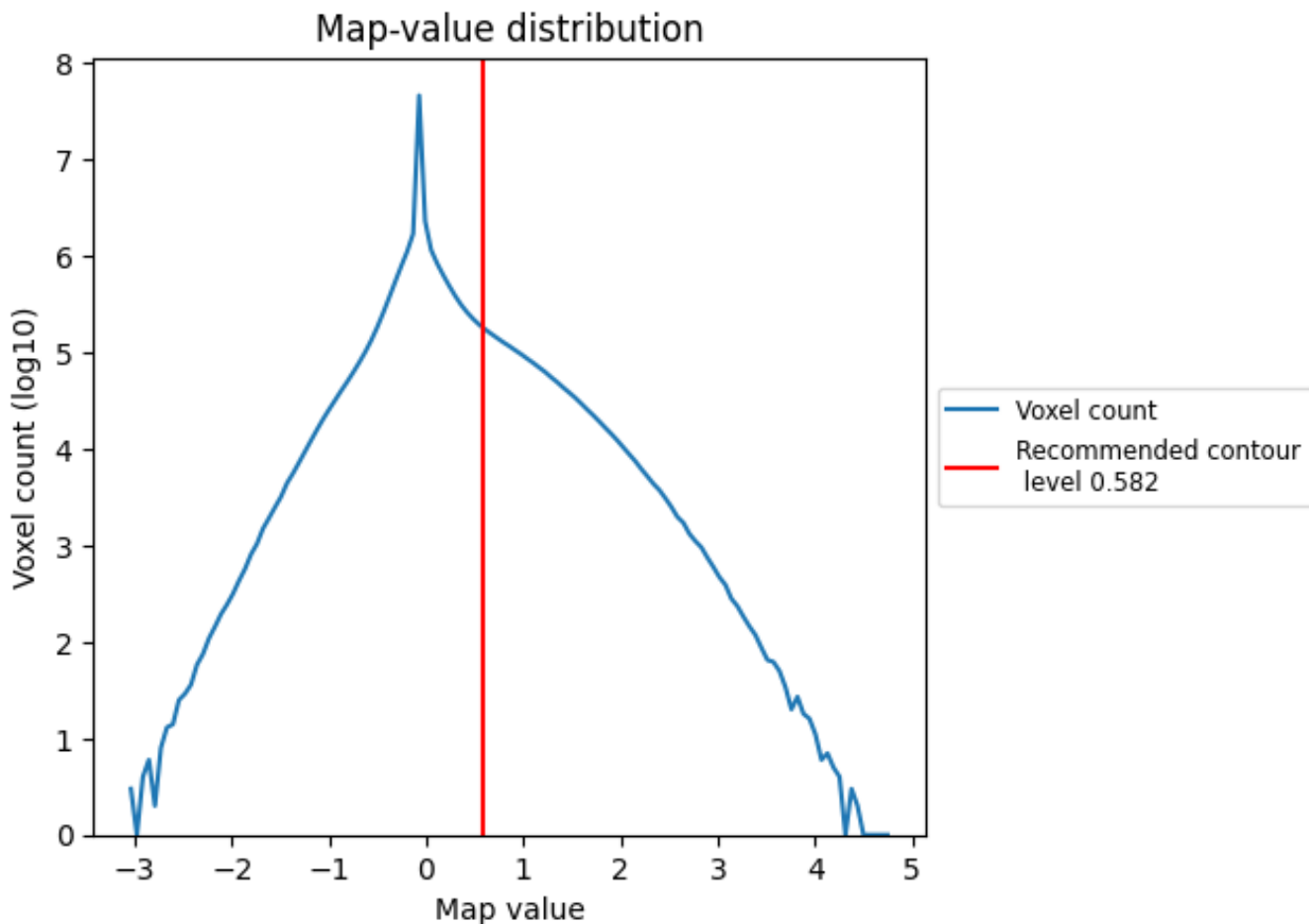
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

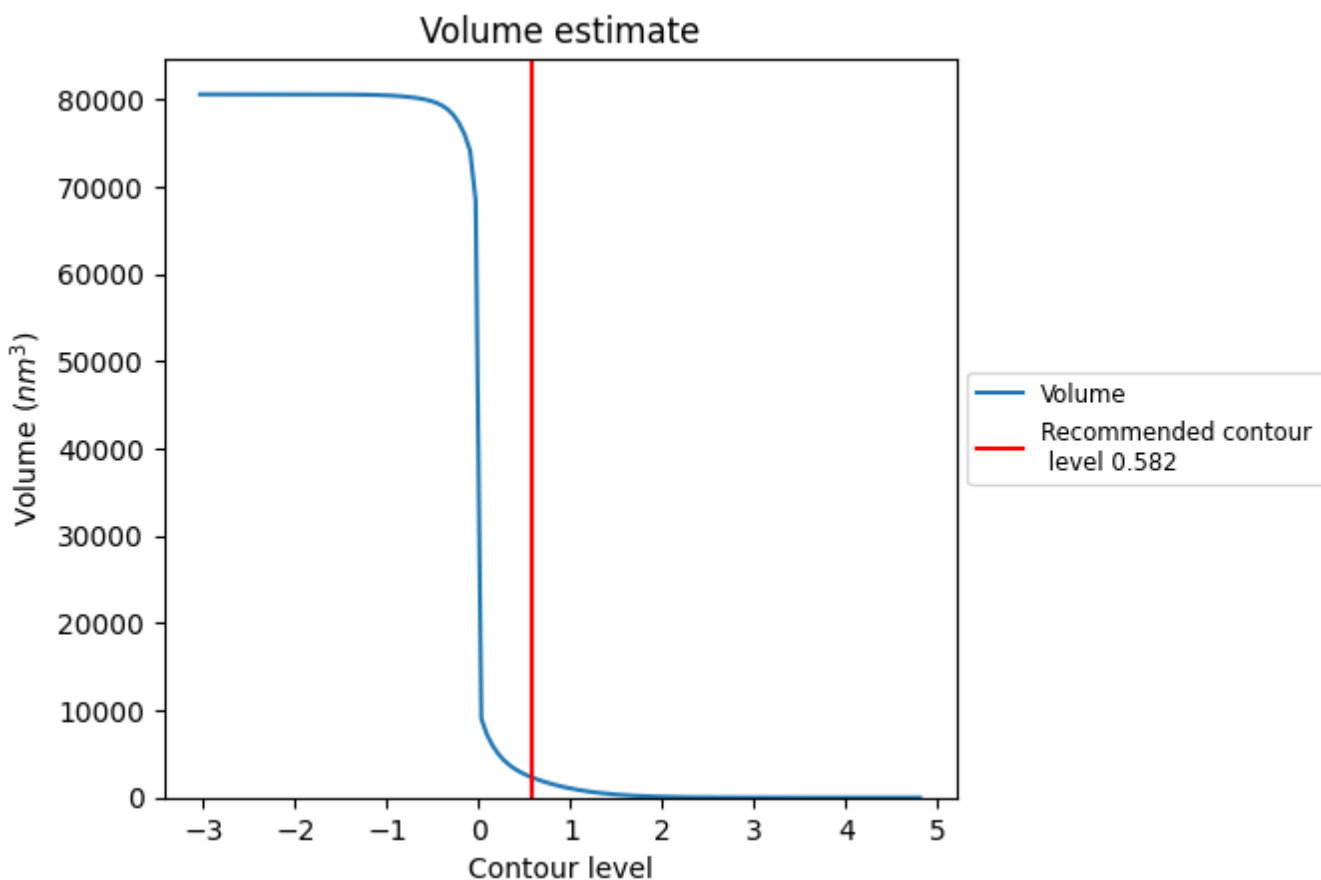
This section contains the results of statistical analysis of the map.

### 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.

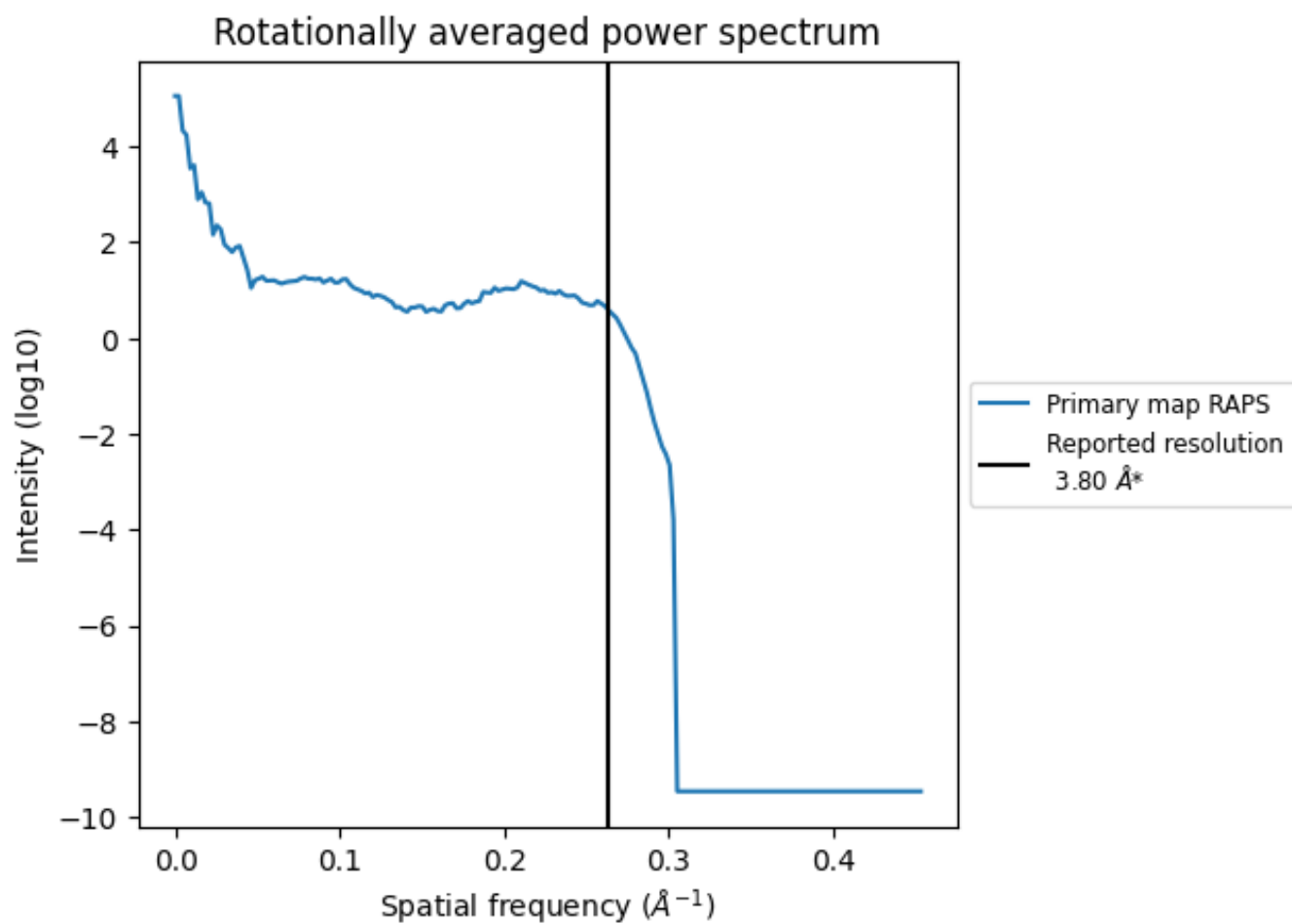
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2293 nm<sup>3</sup>; this corresponds to an approximate mass of 2072 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](#)

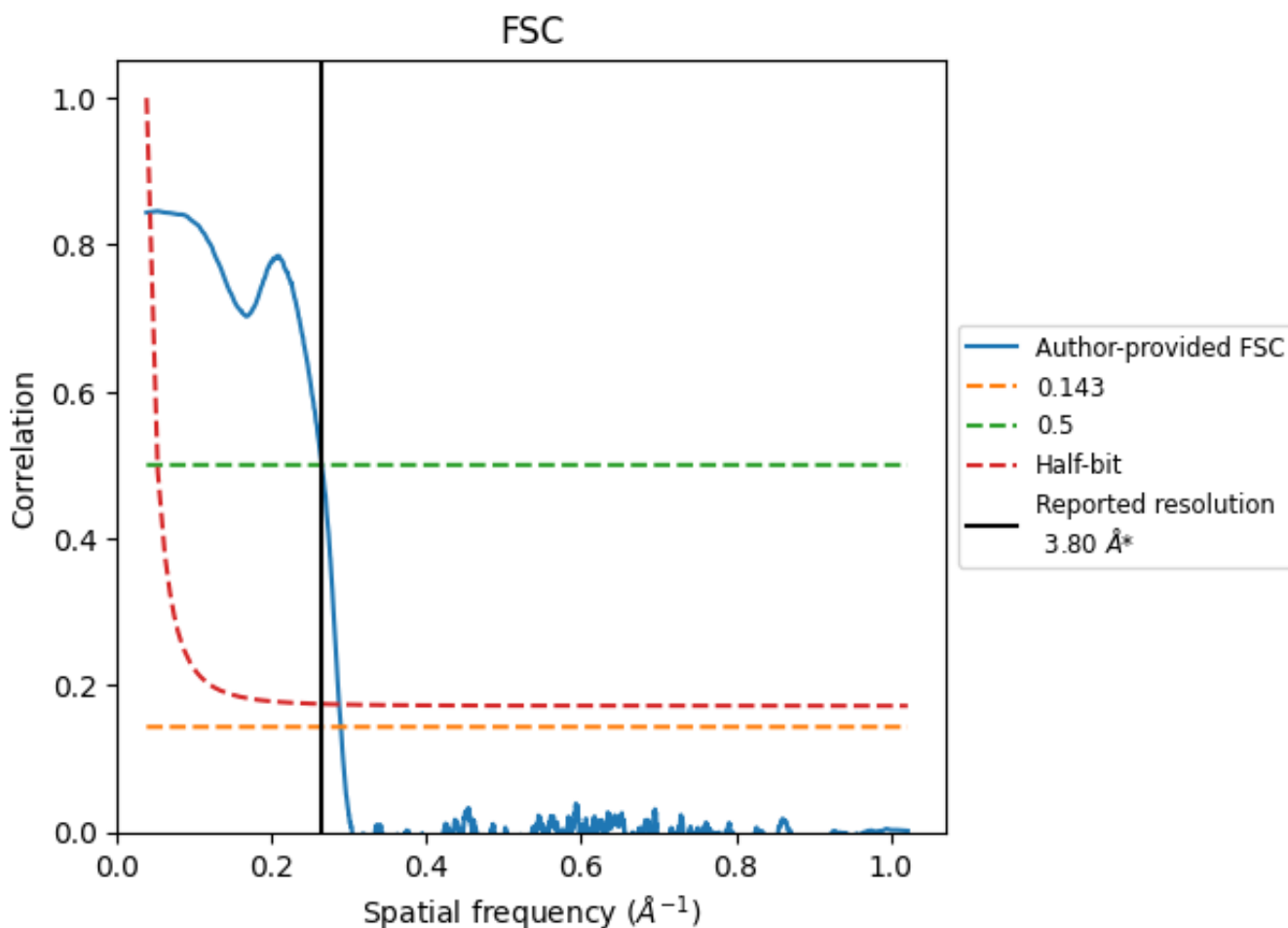


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

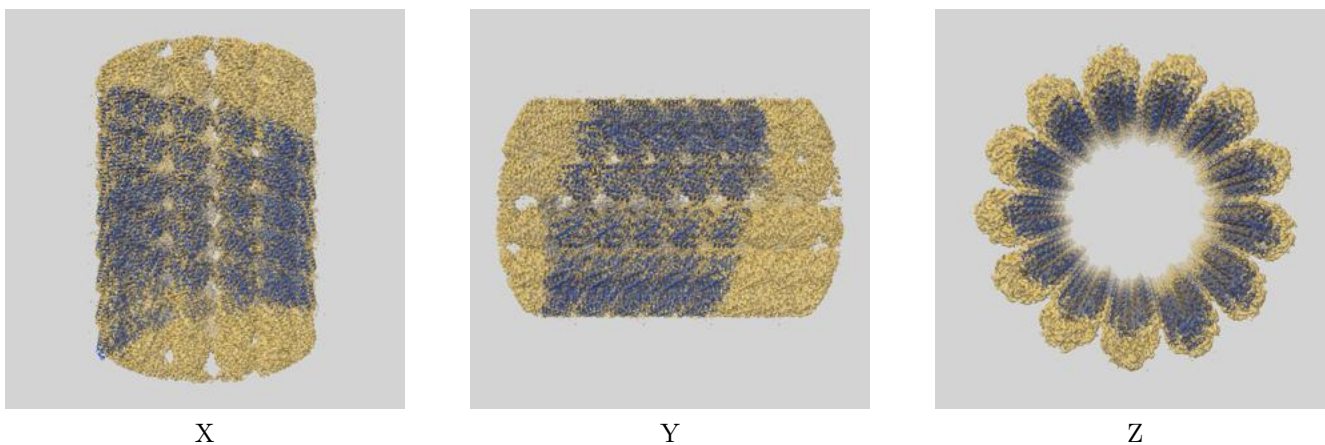
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.80	-
Author-provided FSC curve	3.46	3.78	3.48
Unmasked-calculated*	-	-	-

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

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

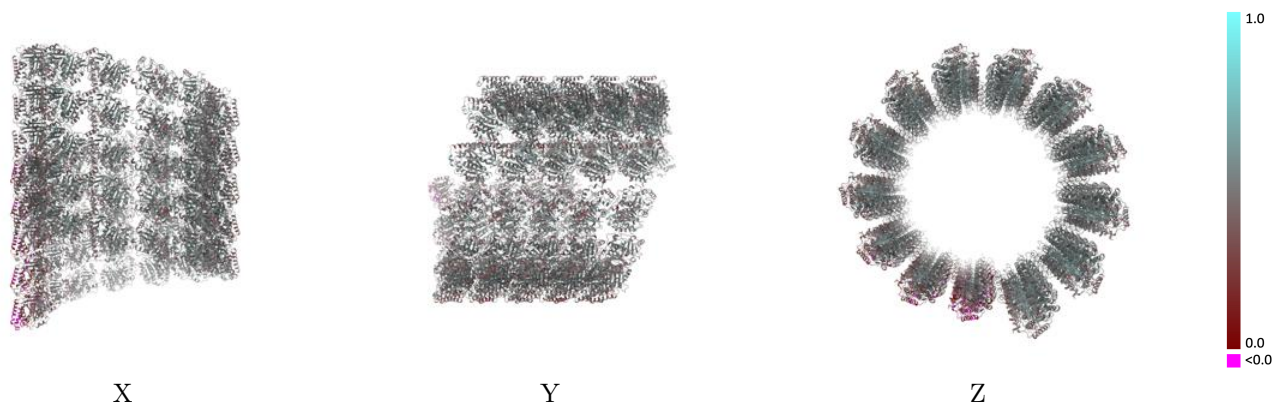
This section contains information regarding the fit between EMDB map EMD-14150 and PDB model 7QUP. Per-residue inclusion information can be found in section 3 on page 52.

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



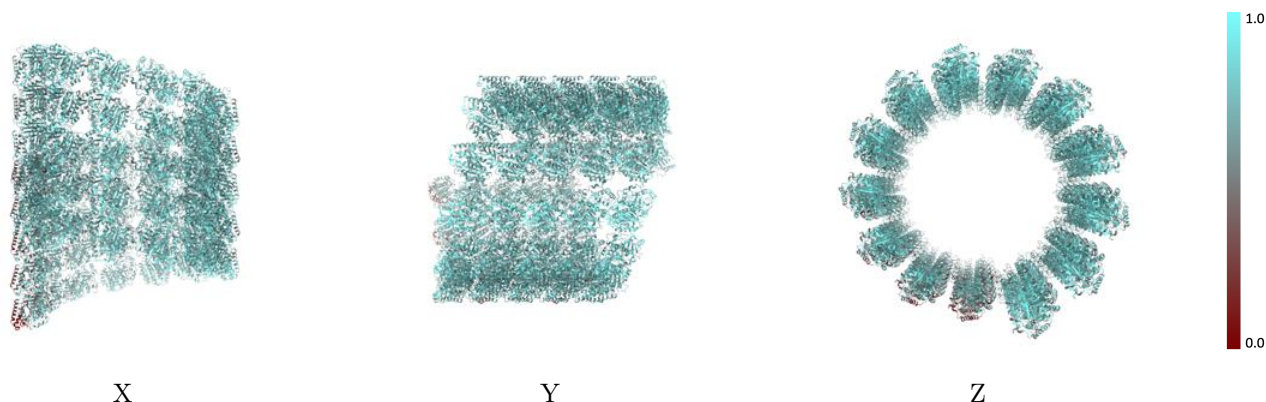
The images above show the 3D surface view of the map at the recommended contour level 0.582 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

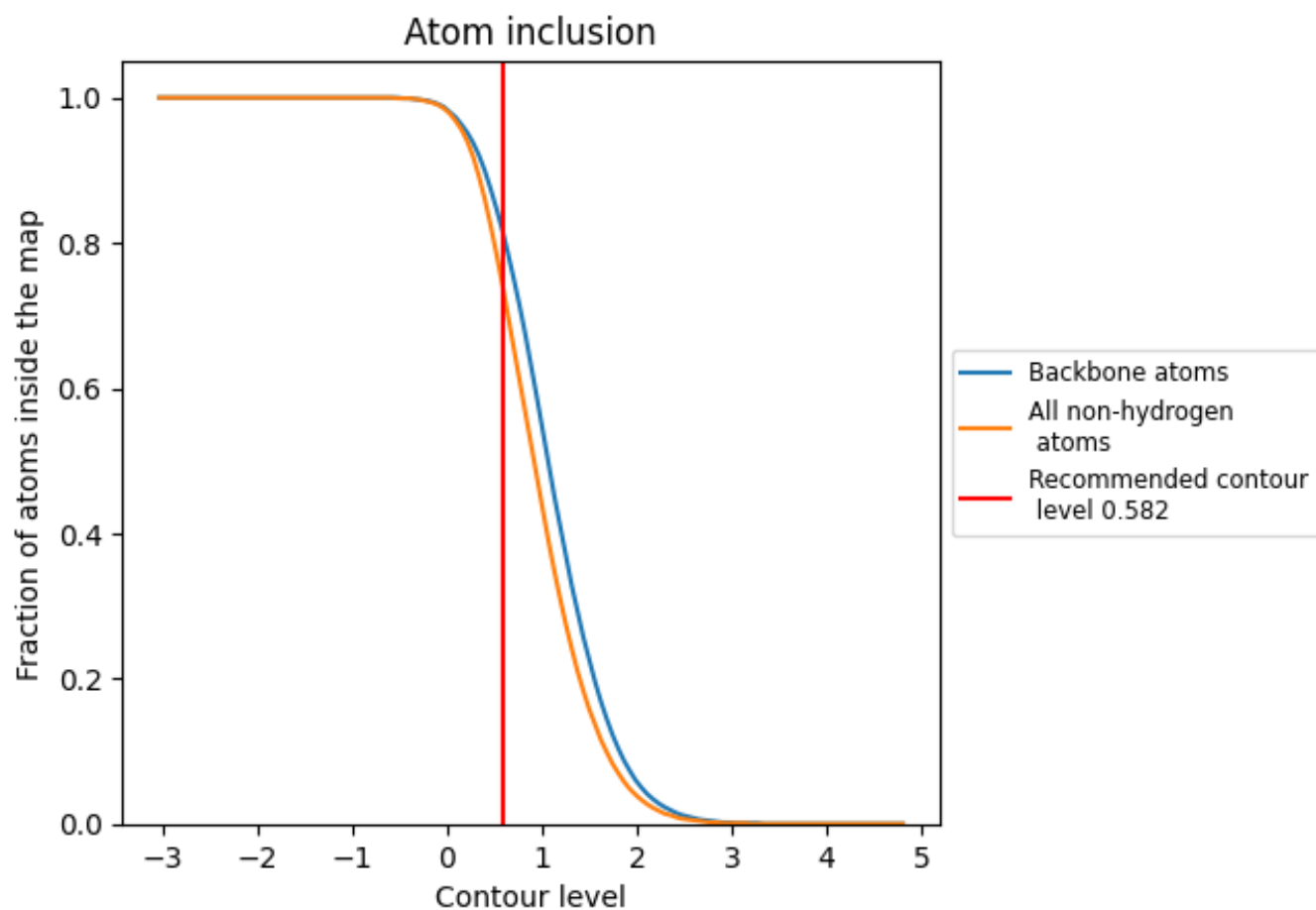
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.582).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.582) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7420	 0.4600
10A	 0.7530	 0.4610
10B	 0.7390	 0.4610
10C	 0.7560	 0.4650
10D	 0.7350	 0.4620
10E	 0.7380	 0.4570
11A	 0.7340	 0.4390
11B	 0.7330	 0.4460
11C	 0.7340	 0.4400
11D	 0.7290	 0.4440
11E	 0.7190	 0.4350
12A	 0.6760	 0.4040
12B	 0.6910	 0.4180
12C	 0.6850	 0.4120
12D	 0.6960	 0.4210
12E	 0.6300	 0.3960
13A	 0.5920	 0.3290
13B	 0.6470	 0.3510
13C	 0.6100	 0.3460
13D	 0.6310	 0.3470
13E	 0.5120	 0.3050
1A	 0.7350	 0.4760
1B	 0.7070	 0.4690
1C	 0.7450	 0.4760
1D	 0.7130	 0.4710
1E	 0.7470	 0.4780
2A	 0.7520	 0.4880
2B	 0.7340	 0.4870
2C	 0.7620	 0.4920
2D	 0.7370	 0.4870
2E	 0.7580	 0.4890
3A	 0.7630	 0.4840
3B	 0.7560	 0.4840
3C	 0.7680	 0.4870
3D	 0.7550	 0.4820



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Chain	Atom inclusion	Q-score
3E	 0.7570	 0.4860
4A	 0.7600	 0.4830
4B	 0.7640	 0.4870
4C	 0.7680	 0.4890
4D	 0.7660	 0.4880
4E	 0.7660	 0.4870
5A	 0.7660	 0.4810
5B	 0.7760	 0.4840
5C	 0.7610	 0.4830
5D	 0.7740	 0.4850
5E	 0.7600	 0.4820
6A	 0.7690	 0.4780
6B	 0.7740	 0.4830
6C	 0.7760	 0.4790
6D	 0.7760	 0.4840
6E	 0.7660	 0.4800
7A	 0.8250	 0.4870
7B	 0.8200	 0.4890
7C	 0.8190	 0.4880
7D	 0.8190	 0.4880
7E	 0.8210	 0.4860
8A	 0.7800	 0.4750
8B	 0.7650	 0.4770
8C	 0.7770	 0.4740
8D	 0.7620	 0.4760
8E	 0.7720	 0.4730
9A	 0.7680	 0.4710
9B	 0.7530	 0.4730
9C	 0.7700	 0.4740
9D	 0.7500	 0.4730
9E	 0.7600	 0.4700