



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:48 PM UTC

PDB ID : 9YA2 / pdb_00009ya2
EMDB ID : EMD-72718
Title : Cryo-EM structure of intraconoidal microtubule 1 (ICMT1) from *Toxoplasma gondii* (8-nm repeat)
Authors : Zeng, J.; Zhang, R.
Deposited on : 2025-09-15
Resolution : 3.34 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

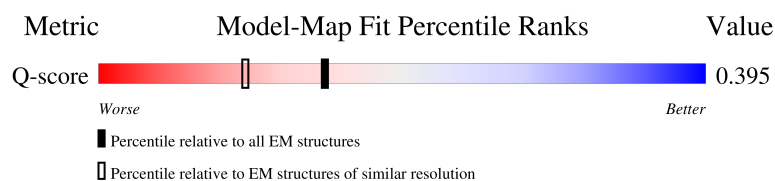
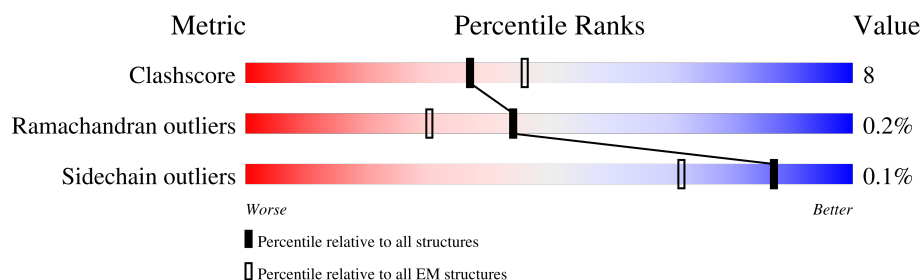
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.34 Å.

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



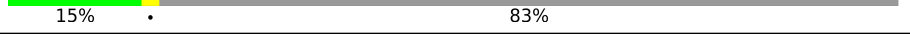
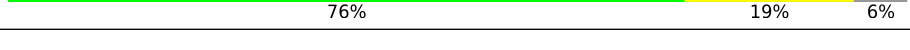
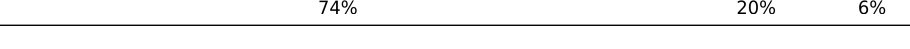
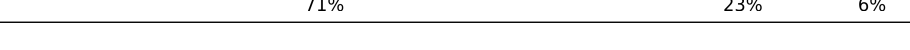
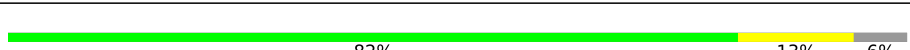
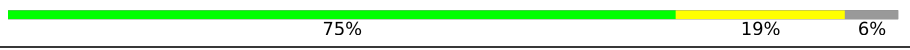
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14446 (2.84 - 3.84)

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

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	
1	C	351	
1	D	351	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	351	
1	F	351	
1	G	351	
1	H	351	
1	I	351	
1	J	351	
1	K	351	
2	A0	453	
2	A2	453	
2	A4	453	
2	A6	453	
2	A8	453	
2	B0	453	
2	B2	453	
2	B4	453	
2	B6	453	
2	B8	453	
2	C0	453	
2	C2	453	
2	C4	453	
2	C6	453	
2	C8	453	
2	D0	453	
2	D2	453	
2	D4	453	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D6	453	
2	D8	453	
2	E0	453	
2	E2	453	
2	E4	453	
2	E6	453	
2	E8	453	
2	F0	453	
3	A1	449	
3	A3	449	
3	A5	449	
3	A7	449	
3	A9	449	
3	B1	449	
3	B3	449	
3	B5	449	
3	B7	449	
3	B9	449	
3	C1	449	
3	C3	449	
3	C5	449	
3	C7	449	
3	C9	449	
3	D1	449	
3	D3	449	

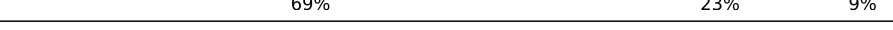
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D5	449	
3	D7	449	
3	D9	449	
3	E1	449	
3	E3	449	
3	E5	449	
3	E7	449	
3	E9	449	
3	F1	449	
4	L	1678	
4	M	1678	
4	N	1678	
4	Q	1678	
4	V	1678	
4	W	1678	
5	O	583	
5	P	583	
6	R	336	
6	S	336	
6	T	336	
6	U	336	
7	a	220	
7	b	220	
7	c	220	
7	d	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	e	220	
7	f	220	
7	g	220	
7	h	220	
7	i	220	
7	j	220	
7	m	220	
7	n	220	
7	o	220	
7	p	220	
7	q	220	
7	r	220	
7	s	220	
7	t	220	
7	u	220	
7	v	220	
7	w	220	
7	x	220	
8	k	189	
8	l	189	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 231266 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 Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	59	Total	C	N	O	S	0	0
			464	306	74	83	1		
1	B	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	C	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	D	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	E	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	F	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	G	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	H	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	I	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	J	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
1	K	60	Total	C	N	O	S	0	0
			471	311	75	84	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ARG	PRO	conflict	UNP A0A7J6K285
B	93	ARG	PRO	conflict	UNP A0A7J6K285
C	93	ARG	PRO	conflict	UNP A0A7J6K285
D	93	ARG	PRO	conflict	UNP A0A7J6K285
E	93	ARG	PRO	conflict	UNP A0A7J6K285
F	93	ARG	PRO	conflict	UNP A0A7J6K285
G	93	ARG	PRO	conflict	UNP A0A7J6K285
H	93	ARG	PRO	conflict	UNP A0A7J6K285

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	93	ARG	PRO	conflict	UNP A0A7J6K285
J	93	ARG	PRO	conflict	UNP A0A7J6K285
K	93	ARG	PRO	conflict	UNP A0A7J6K285

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	A2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	A4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	A6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	A8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	D0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	D2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	D4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	F0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	C5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	C7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	C9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	F1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

- Molecule 4 is a protein called ICMAP2, TGME49_224700.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	162	Total 1334	C 868	N 226	O 231	S 9	0	0
4	M	162	Total 1334	C 868	N 226	O 231	S 9	0	0
4	N	162	Total 1334	C 868	N 226	O 231	S 9	0	0
4	Q	162	Total 1334	C 868	N 226	O 231	S 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	162	Total	C	N	O	S	0	0
			1334	868	226	231	9		
4	W	162	Total	C	N	O	S	0	0
			1334	868	226	231	9		

- Molecule 5 is a protein called TLAP3 (apical cap protein AC5), TGME49_235380.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	219	Total	C	N	O	S	0	0
			1736	1078	328	328	2		
5	P	219	Total	C	N	O	S	0	0
			1736	1078	328	328	2		

- Molecule 6 is a protein called TLAP4 (thioredoxin-like associated protein), TGME49_201760.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	113	Total	C	N	O	S	0	0
			954	592	182	179	1		
6	S	22	Total	C	N	O	S	0	0
			182	112	38	31	1		
6	T	113	Total	C	N	O	S	0	0
			954	592	182	179	1		
6	U	91	Total	C	N	O		0	0
			772	480	144	148			

- Molecule 7 is a protein called TRXL1, TGME49_232410.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	161	Total	C	N	O	S	0	0
			1289	824	224	236	5		
7	b	161	Total	C	N	O	S	0	0
			1289	824	224	236	5		
7	c	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	d	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	e	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	f	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	g	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	i	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	j	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	m	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	n	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	o	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	p	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	q	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	r	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	s	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	t	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	u	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	v	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	w	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
7	x	201	Total 1608	C 1021	N 283	O 297	S 7	0	0

- Molecule 8 is a protein called TRXL2, TGME49_225790.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	145	Total 1187	C 770	N 209	O 203	S 5	0	0
8	l	145	Total 1187	C 770	N 209	O 203	S 5	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	167	SER	-	expression tag	UNP A0A7J6K232

Continued on next page...

Continued from previous page...

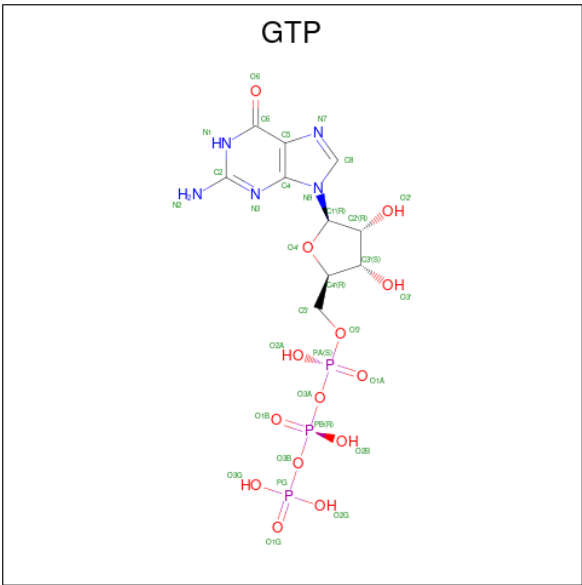
Chain	Residue	Modelled	Actual	Comment	Reference
k	168	ALA	-	expression tag	UNP A0A7J6K232
k	169	GLN	-	expression tag	UNP A0A7J6K232
k	170	ARG	-	expression tag	UNP A0A7J6K232
k	171	LEU	-	expression tag	UNP A0A7J6K232
k	172	ARG	-	expression tag	UNP A0A7J6K232
k	173	THR	-	expression tag	UNP A0A7J6K232
k	174	LEU	-	expression tag	UNP A0A7J6K232
k	175	ASN	-	expression tag	UNP A0A7J6K232
k	176	ASP	-	expression tag	UNP A0A7J6K232
k	177	ALA	-	expression tag	UNP A0A7J6K232
k	178	THR	-	expression tag	UNP A0A7J6K232
k	179	ASP	-	expression tag	UNP A0A7J6K232
k	180	PRO	-	expression tag	UNP A0A7J6K232
k	181	TRP	-	expression tag	UNP A0A7J6K232
k	182	LYS	-	expression tag	UNP A0A7J6K232
k	183	LYS	-	expression tag	UNP A0A7J6K232
k	184	ARG	-	expression tag	UNP A0A7J6K232
k	185	LEU	-	expression tag	UNP A0A7J6K232
k	186	PRO	-	expression tag	UNP A0A7J6K232
k	187	GLN	-	expression tag	UNP A0A7J6K232
k	188	ASN	-	expression tag	UNP A0A7J6K232
k	189	VAL	-	expression tag	UNP A0A7J6K232
l	167	SER	-	expression tag	UNP A0A7J6K232
l	168	ALA	-	expression tag	UNP A0A7J6K232
l	169	GLN	-	expression tag	UNP A0A7J6K232
l	170	ARG	-	expression tag	UNP A0A7J6K232
l	171	LEU	-	expression tag	UNP A0A7J6K232
l	172	ARG	-	expression tag	UNP A0A7J6K232
l	173	THR	-	expression tag	UNP A0A7J6K232
l	174	LEU	-	expression tag	UNP A0A7J6K232
l	175	ASN	-	expression tag	UNP A0A7J6K232
l	176	ASP	-	expression tag	UNP A0A7J6K232
l	177	ALA	-	expression tag	UNP A0A7J6K232
l	178	THR	-	expression tag	UNP A0A7J6K232
l	179	ASP	-	expression tag	UNP A0A7J6K232
l	180	PRO	-	expression tag	UNP A0A7J6K232
l	181	TRP	-	expression tag	UNP A0A7J6K232
l	182	LYS	-	expression tag	UNP A0A7J6K232
l	183	LYS	-	expression tag	UNP A0A7J6K232
l	184	ARG	-	expression tag	UNP A0A7J6K232
l	185	LEU	-	expression tag	UNP A0A7J6K232
l	186	PRO	-	expression tag	UNP A0A7J6K232

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1	187	GLN	-	expression tag	UNP A0A7J6K232
1	188	ASN	-	expression tag	UNP A0A7J6K232
1	189	VAL	-	expression tag	UNP A0A7J6K232

- Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B6	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	B8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C3	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A0	1	Total	Mg	0
			1	1	
10	A2	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

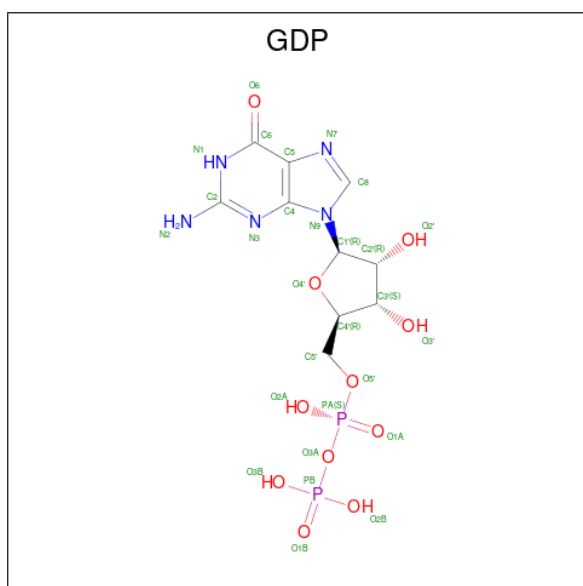
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	A5	1	1	1	0
10	A7	1	1	1	0
10	A8	1	1	1	0
10	B0	1	1	1	0
10	B2	1	1	1	0
10	B4	1	1	1	0
10	B6	1	1	1	0
10	B8	1	1	1	0
10	C0	1	1	1	0
10	C2	1	1	1	0
10	C4	1	1	1	0
10	C6	1	1	1	0
10	C8	1	1	1	0
10	D0	1	1	1	0
10	D2	1	1	1	0
10	D4	1	1	1	0
10	D6	1	1	1	0
10	D8	1	1	1	0
10	E1	1	1	1	0
10	E2	1	1	1	0
10	E4	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
10	E6	1	Total	Mg	0
			1	1	
10	E9	1	Total	Mg	0
			1	1	
10	F0	1	Total	Mg	0
			1	1	

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

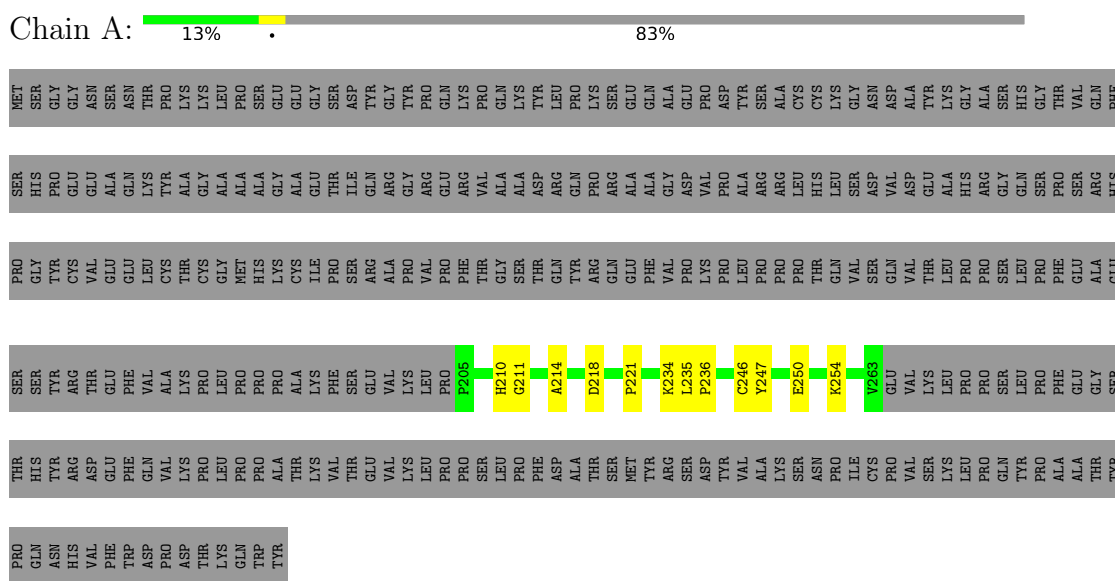
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
11	B7	1	Total 28	C 10	N 5	O 11	P 2	0
11	B9	1	Total 28	C 10	N 5	O 11	P 2	0
11	C1	1	Total 28	C 10	N 5	O 11	P 2	0
11	C3	1	Total 28	C 10	N 5	O 11	P 2	0
11	C5	1	Total 28	C 10	N 5	O 11	P 2	0
11	C7	1	Total 28	C 10	N 5	O 11	P 2	0
11	C9	1	Total 28	C 10	N 5	O 11	P 2	0
11	D1	1	Total 28	C 10	N 5	O 11	P 2	0
11	D3	1	Total 28	C 10	N 5	O 11	P 2	0
11	D5	1	Total 28	C 10	N 5	O 11	P 2	0
11	D7	1	Total 28	C 10	N 5	O 11	P 2	0
11	D9	1	Total 28	C 10	N 5	O 11	P 2	0
11	E1	1	Total 28	C 10	N 5	O 11	P 2	0
11	E3	1	Total 28	C 10	N 5	O 11	P 2	0
11	E5	1	Total 28	C 10	N 5	O 11	P 2	0
11	E7	1	Total 28	C 10	N 5	O 11	P 2	0
11	E9	1	Total 28	C 10	N 5	O 11	P 2	0
11	F1	1	Total 28	C 10	N 5	O 11	P 2	0

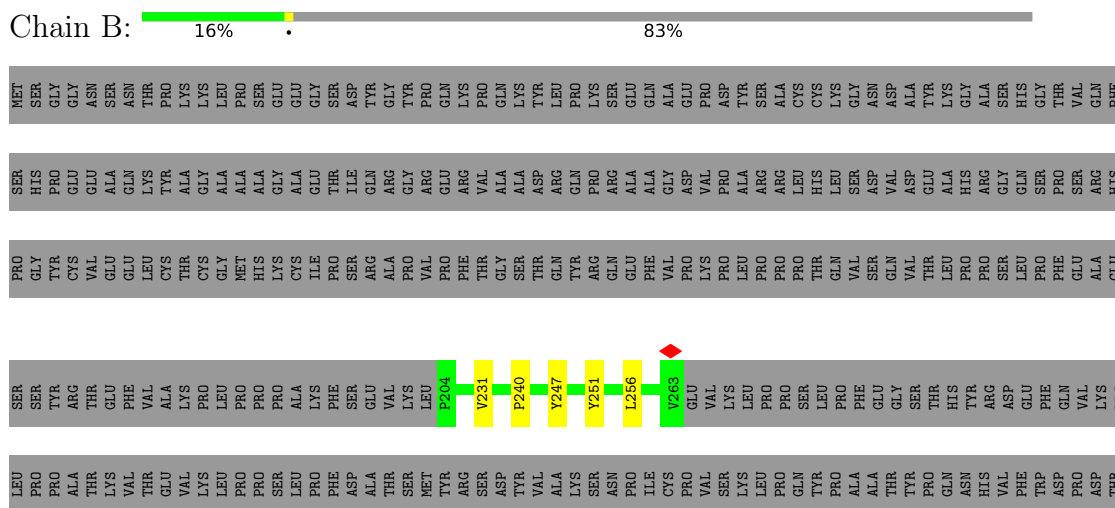
3 Residue-property plots

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

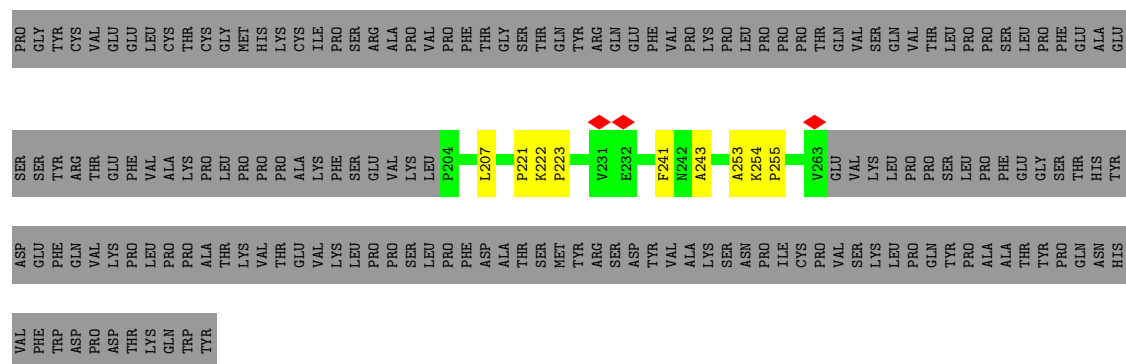
- Molecule 1: Microtubule associated protein SPM1



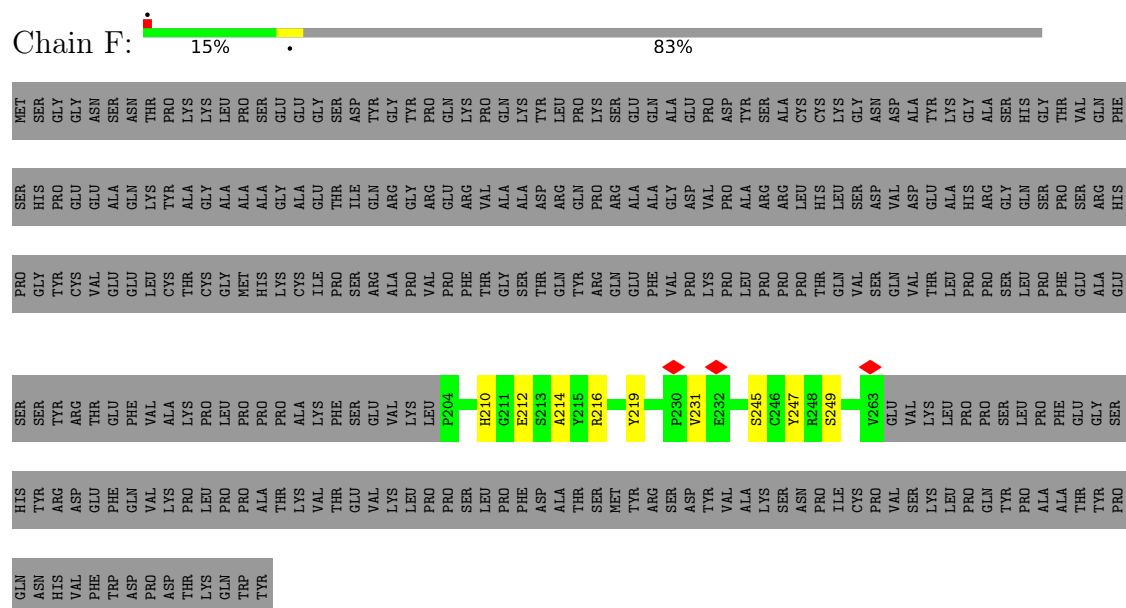
- Molecule 1: Microtubule associated protein SPM1



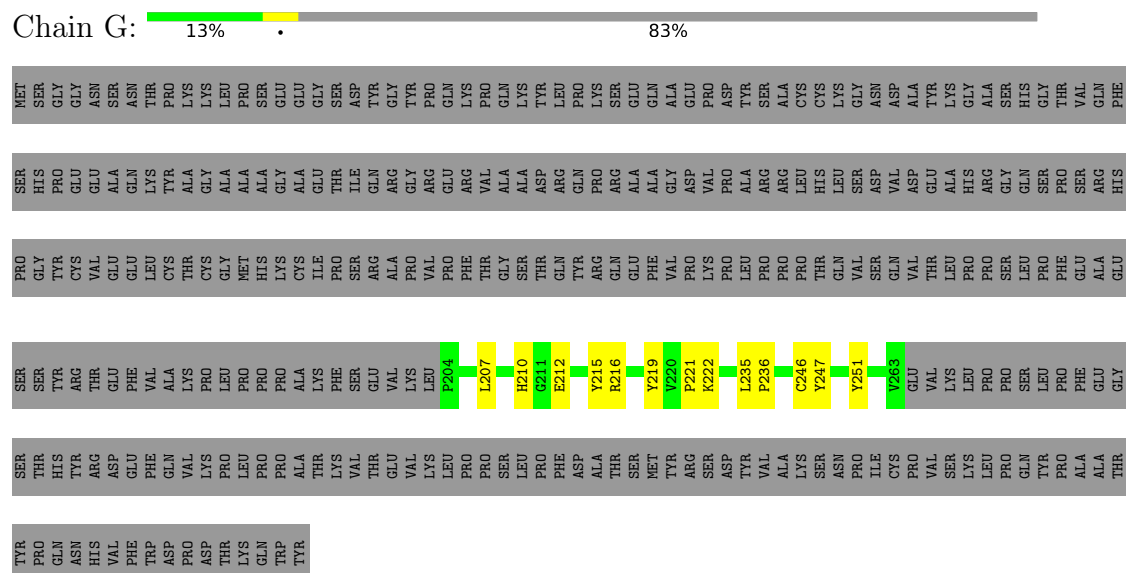
[illegible]



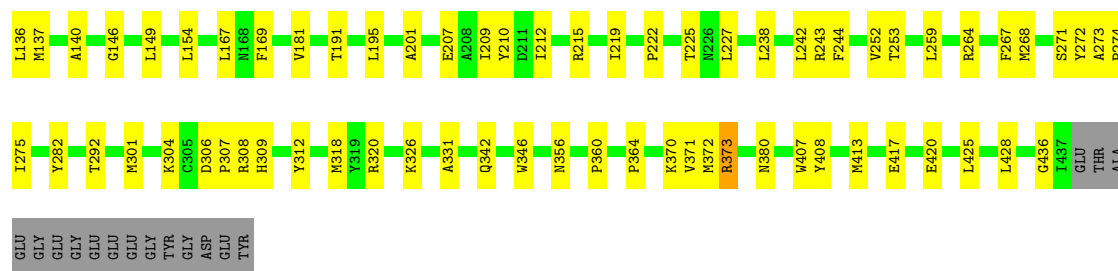
- Molecule 1: Microtubule associated protein SPM1



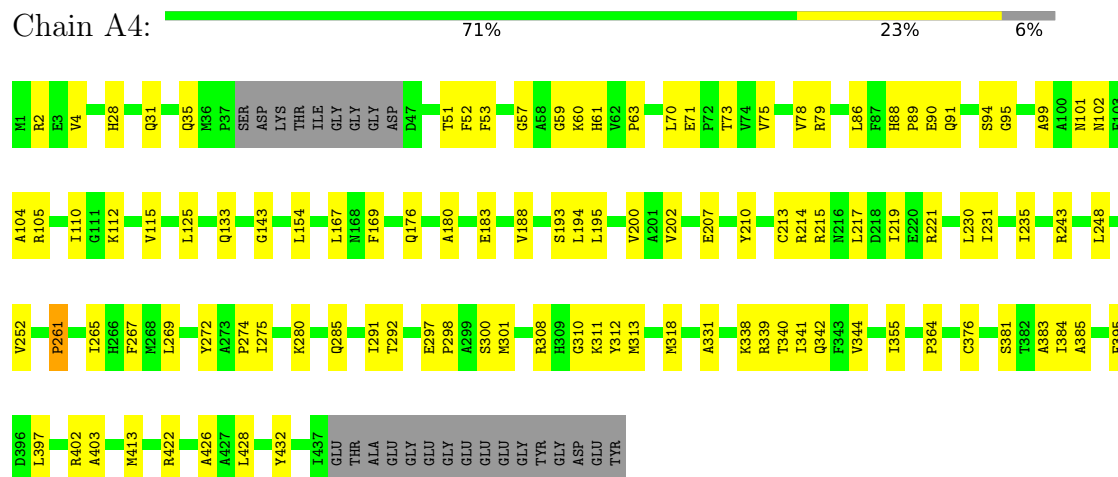
- Molecule 1: Microtubule associated protein SPM1



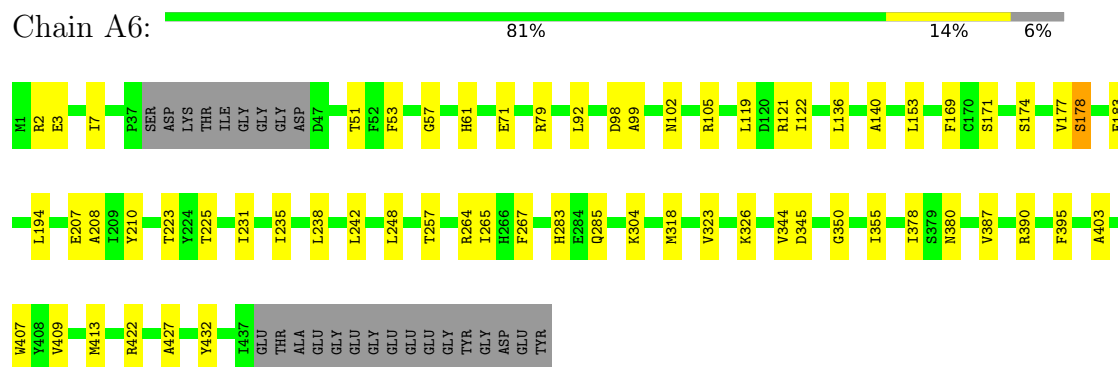
[illegible]



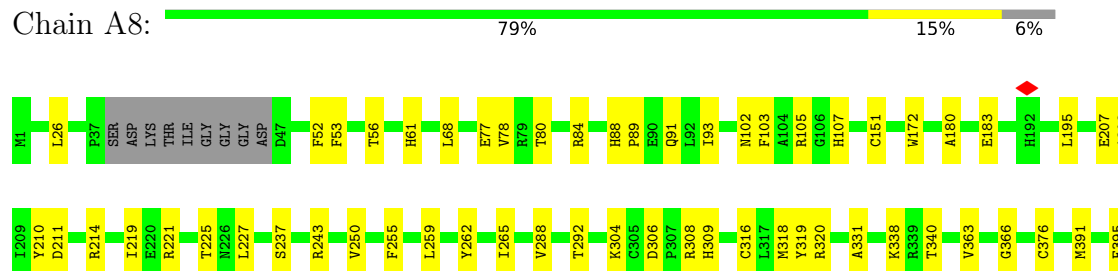
• Molecule 2: Tubulin alpha chain



• Molecule 2: Tubulin alpha chain



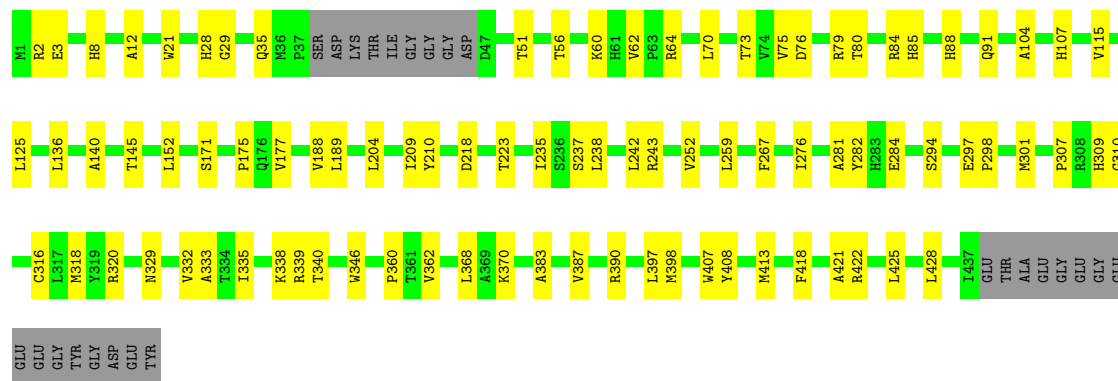
• Molecule 2: Tubulin alpha chain





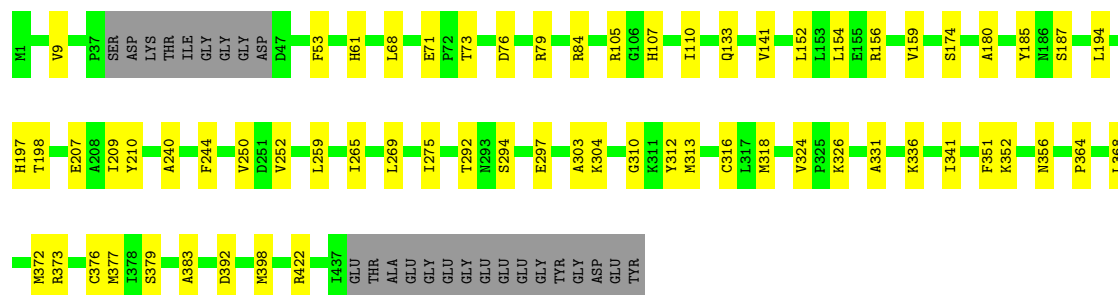
• Molecule 2: Tubulin alpha chain

Chain B0: 75% 19% 6%



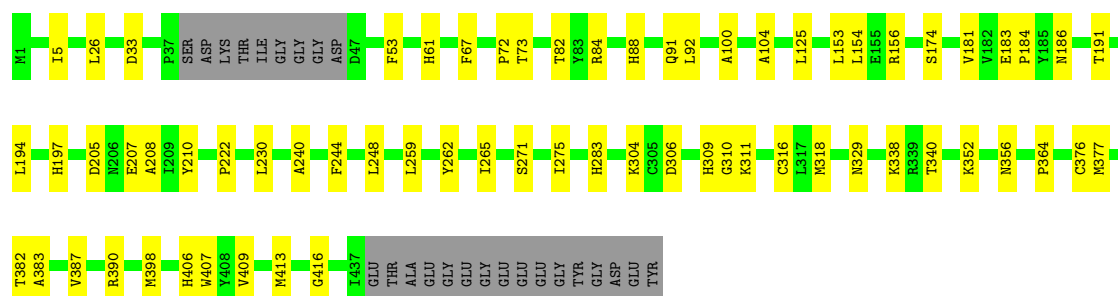
• Molecule 2: Tubulin alpha chain

Chain B2: 80% 14% 6%



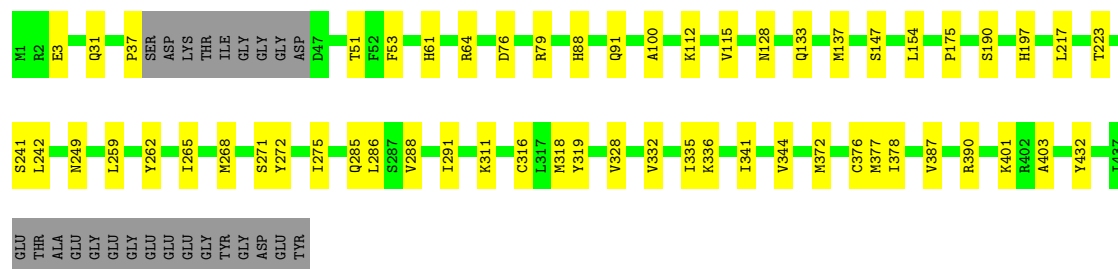
• Molecule 2: Tubulin alpha chain

Chain B4: 80% 15% 6%



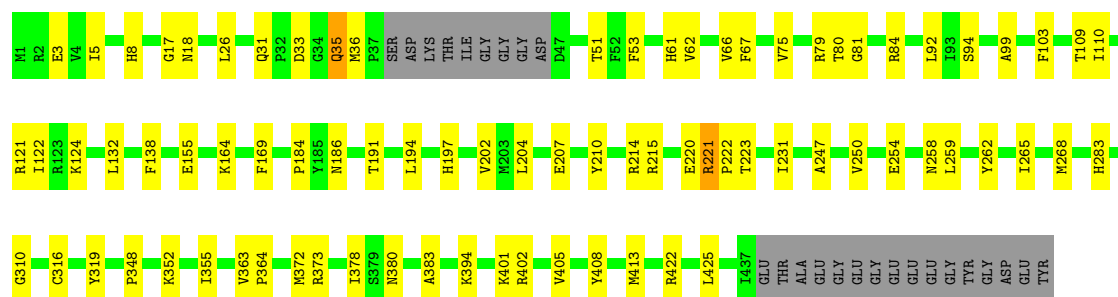
• Molecule 2: Tubulin alpha chain

Chain B6: 82% 13% 6%



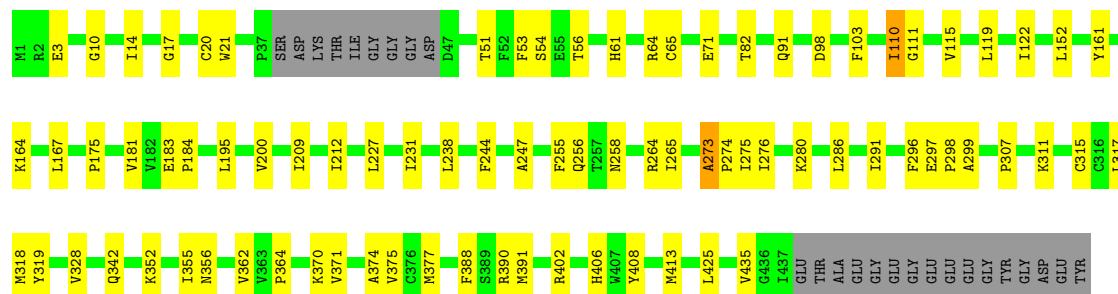
- Molecule 2: Tubulin alpha chain

Chain B8: 77% 17% 6%



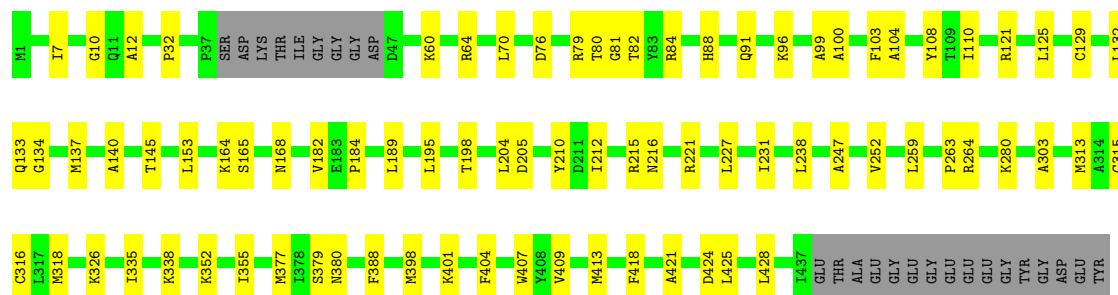
- Molecule 2: Tubulin alpha chain

Chain C0: 76% 18% 6%



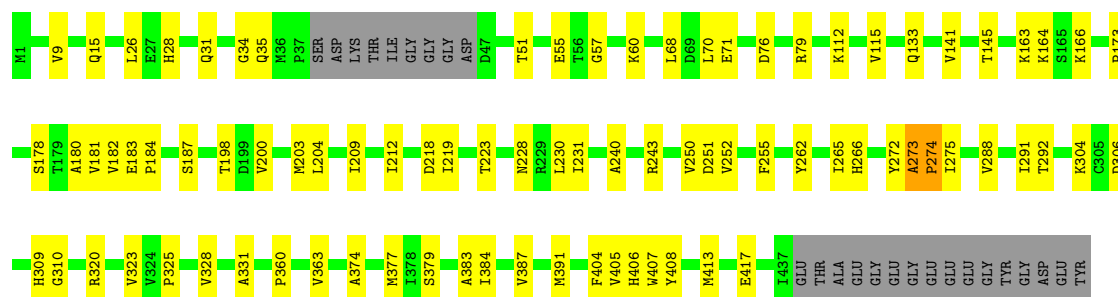
- Molecule 2: Tubulin alpha chain

Chain C2: 77% 18% 6%



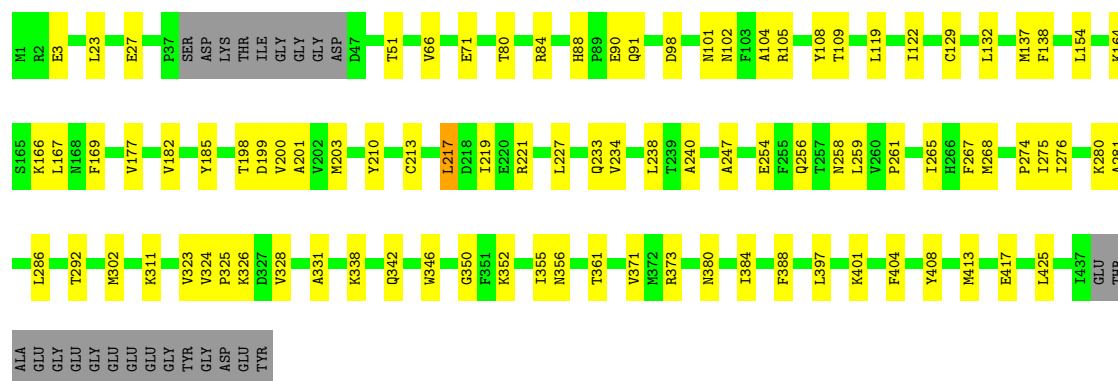
- Molecule 2: Tubulin alpha chain

Chain C4:  76% 18% 6%



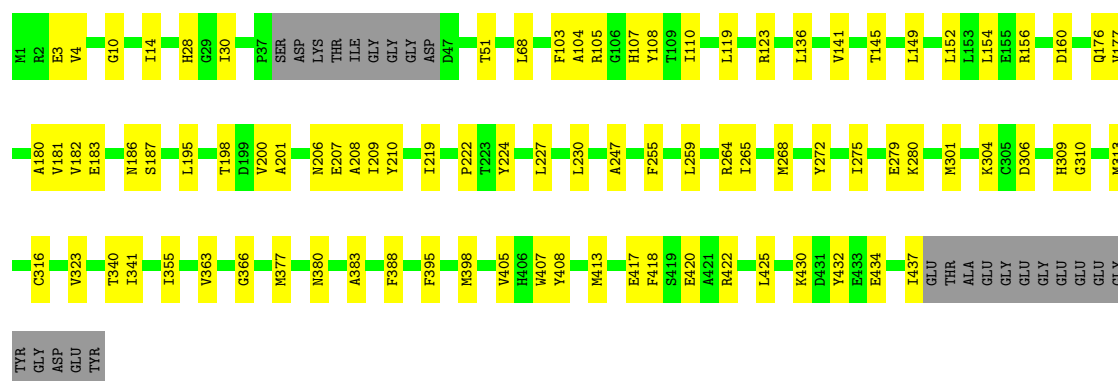
• Molecule 2: Tubulin alpha chain

Chain C6:  74% 20% 6%



• Molecule 2: Tubulin alpha chain

Chain C8:  75% 19% 6%



• Molecule 2: Tubulin alpha chain

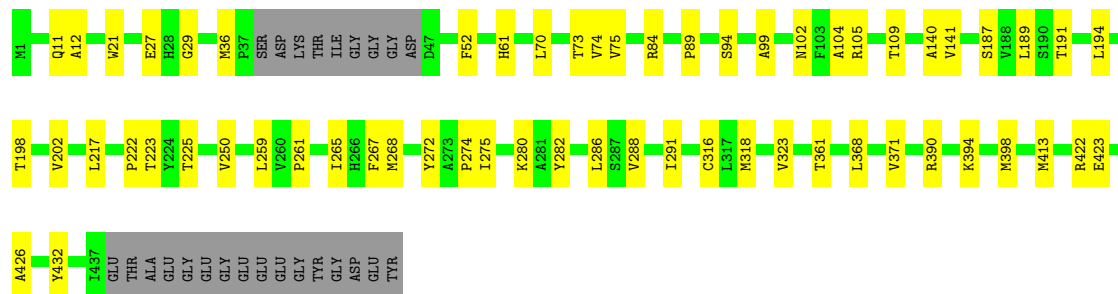
Chain D0:  76% 19% 6%





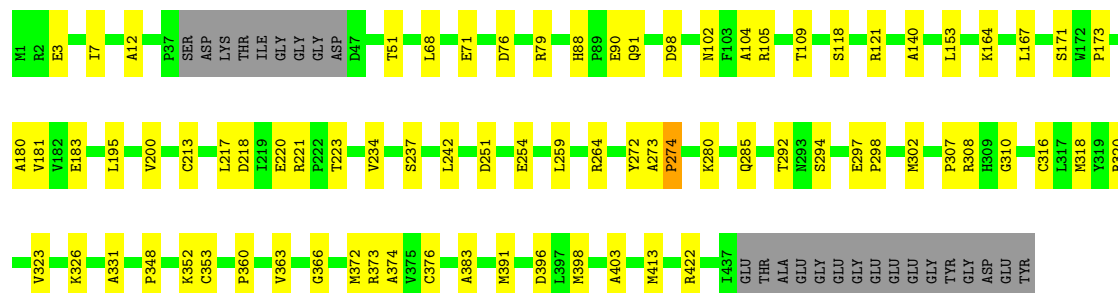
• Molecule 2: Tubulin alpha chain

Chain D2: 81% 13% 6%



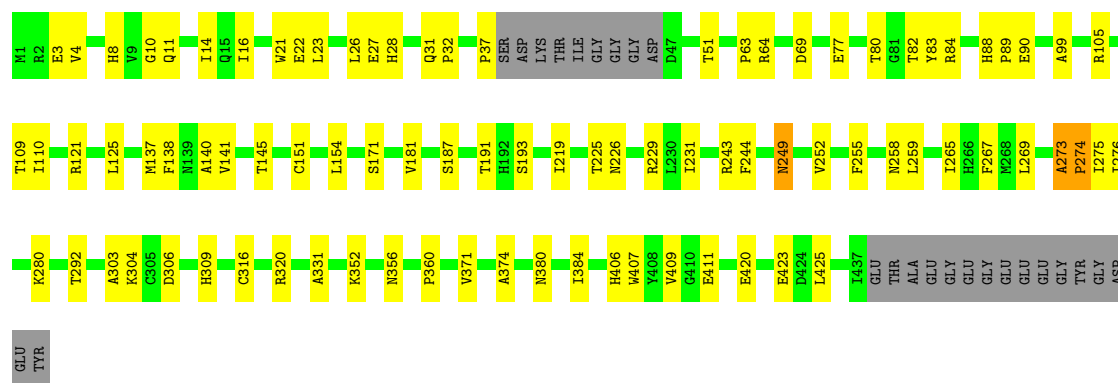
• Molecule 2: Tubulin alpha chain

Chain D4: 77% 17% 6%



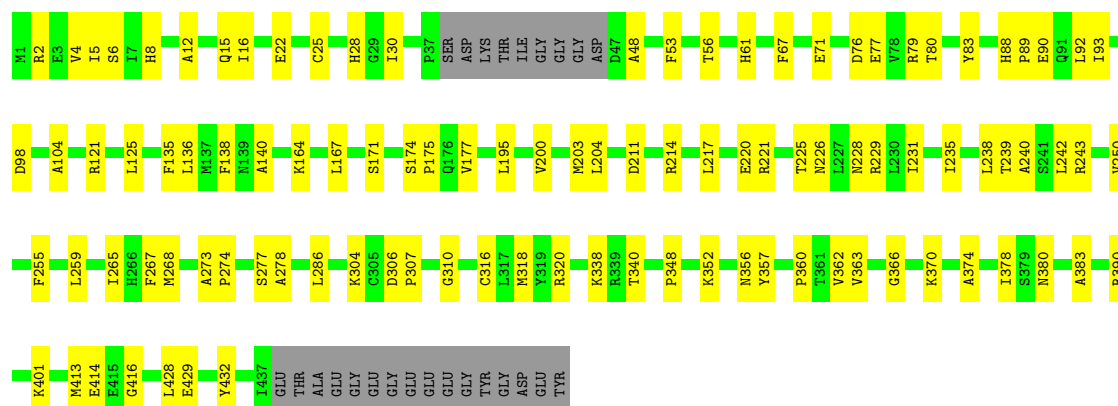
• Molecule 2: Tubulin alpha chain

Chain D6: 75% 19% 6%



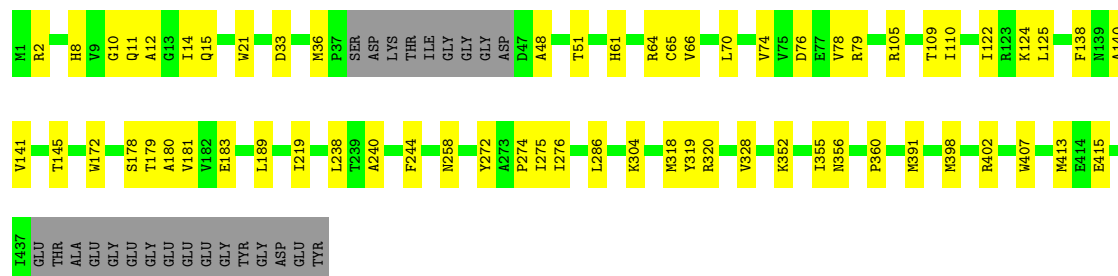
• Molecule 2: Tubulin alpha chain

Chain D8:  72% 23% 6%



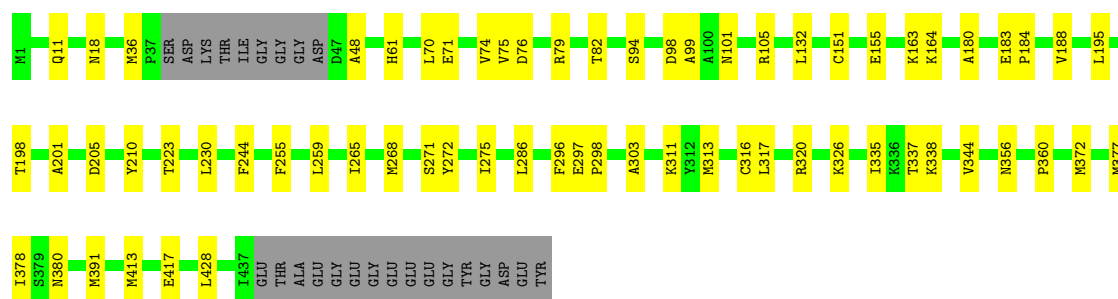
• Molecule 2: Tubulin alpha chain

Chain E0:  81% 14% 6%



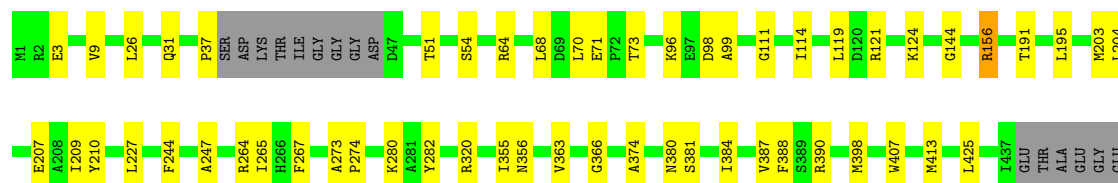
• Molecule 2: Tubulin alpha chain

Chain E2:  80% 15% 6%



• Molecule 2: Tubulin alpha chain

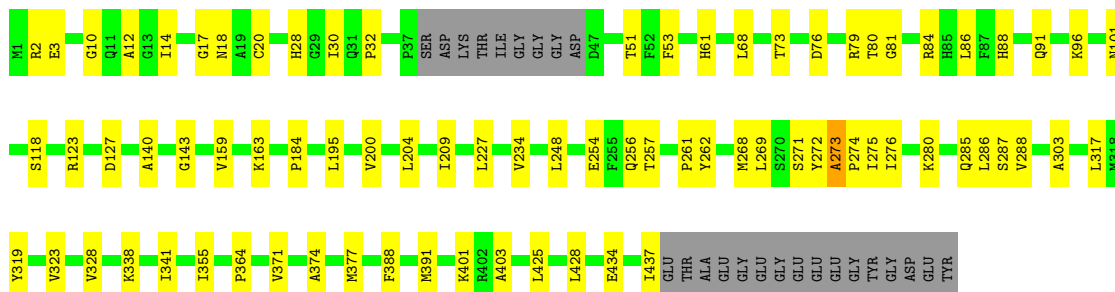
Chain E4:  82% 12% 6%



GLY
GLU
GLU
GLU
GLY
TYR
GLY
ASP
GLU
TYR

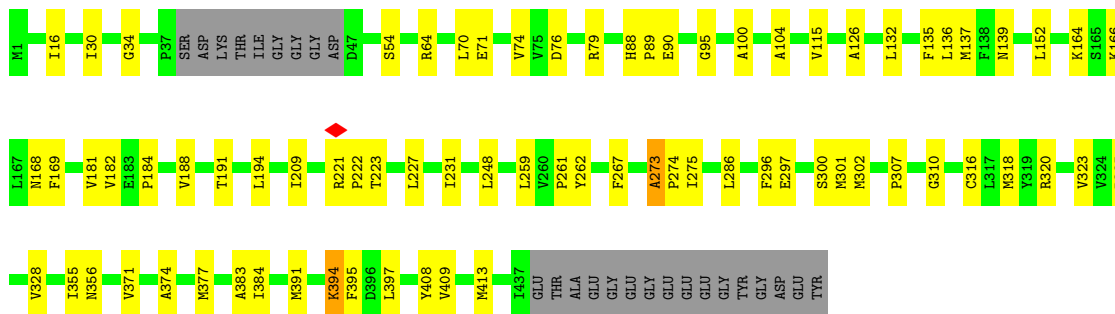
• Molecule 2: Tubulin alpha chain

Chain E6: 77% 17% 6%



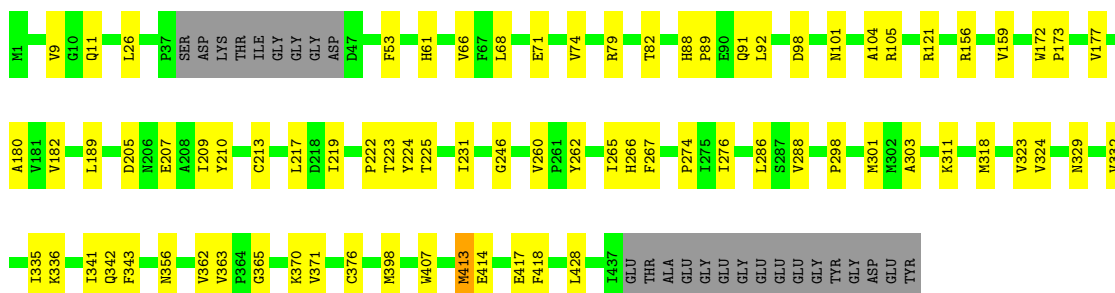
• Molecule 2: Tubulin alpha chain

Chain E8: 78% 16% 6%



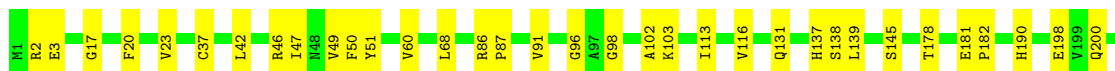
• Molecule 2: Tubulin alpha chain

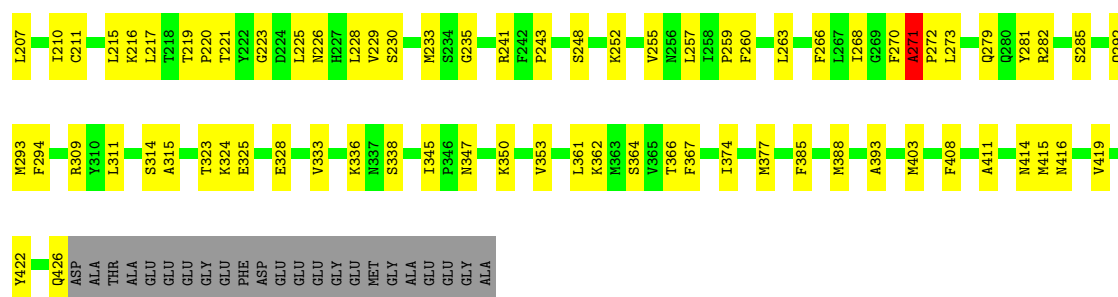
Chain F0: 77% 17% 6%



• Molecule 3: Tubulin beta chain

Chain A1: 71% 24% 5%





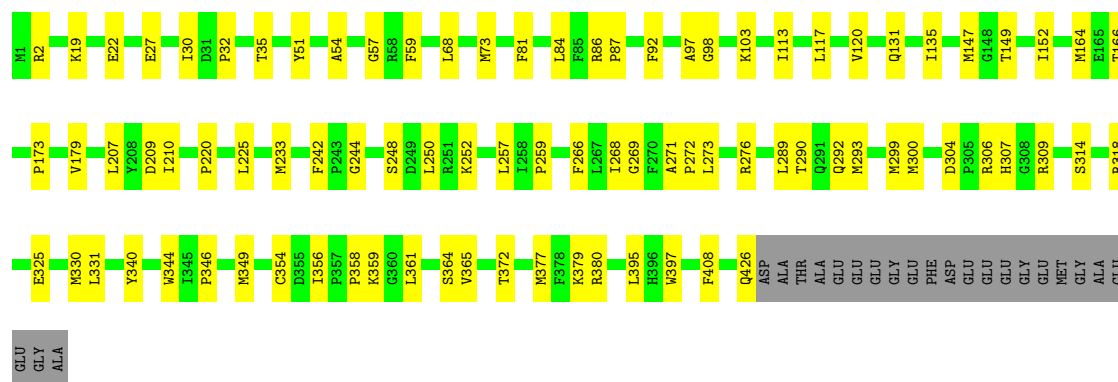
• Molecule 3: Tubulin beta chain

Chain A3: 72% 22% 5%



• Molecule 3: Tubulin beta chain

Chain A5: 76% 19% 5%



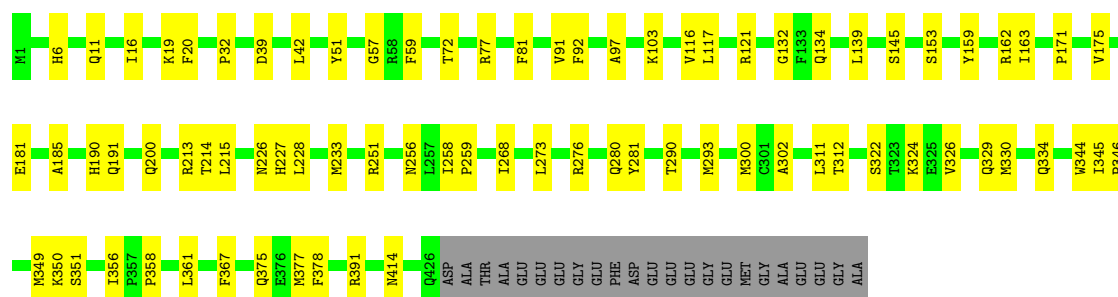
• Molecule 3: Tubulin beta chain

Chain A7: 82% 13% 5%

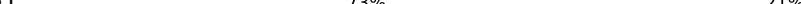


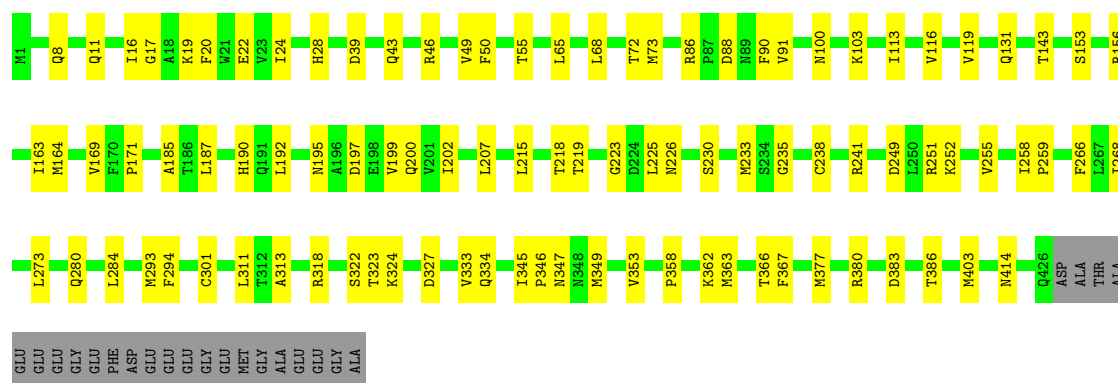
- Molecule 3: Tubulin beta chain

Chain A9:  77% 18% 5%



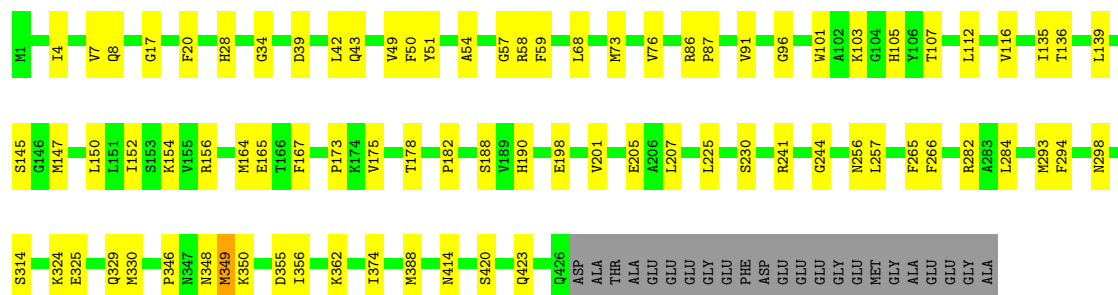
- Molecule 3: Tubulin beta chain

Chain B1:  73% 21% 5%

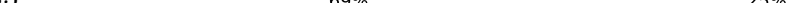


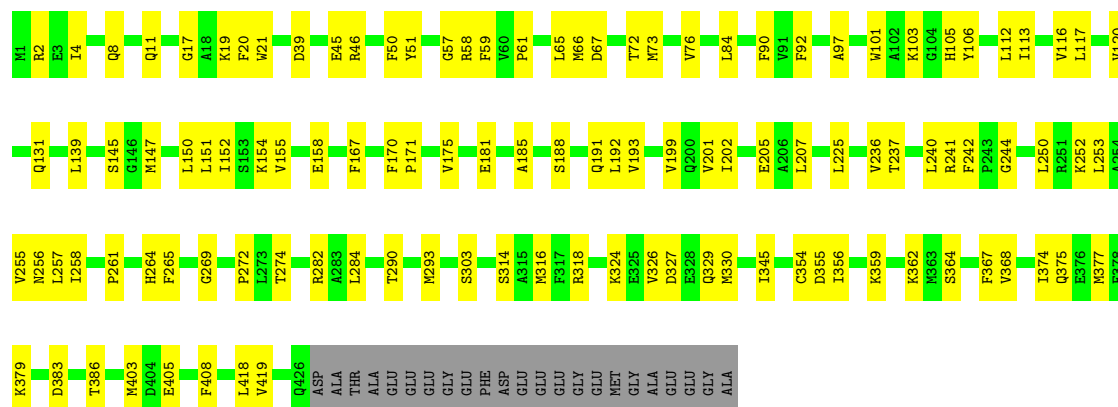
- Molecule 3: Tubulin beta chain

Chain B3:  77% 18% 5%



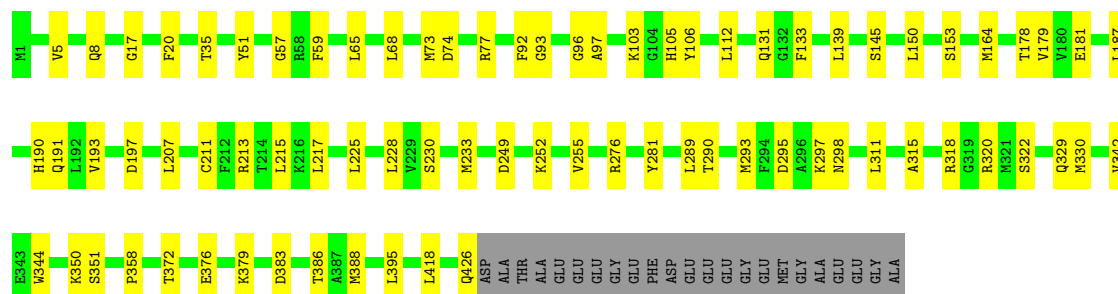
- Molecule 3: Tubulin beta chain

Chain B5:  69% 25% 5%



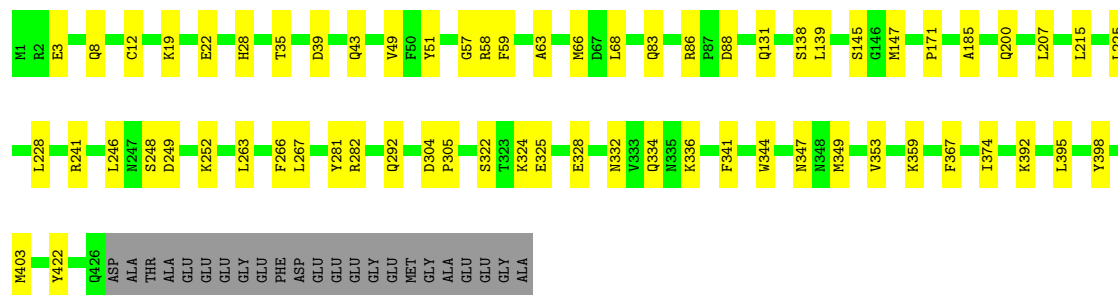
- Molecule 3: Tubulin beta chain

Chain B7: 78% 17% 5%



- Molecule 3: Tubulin beta chain

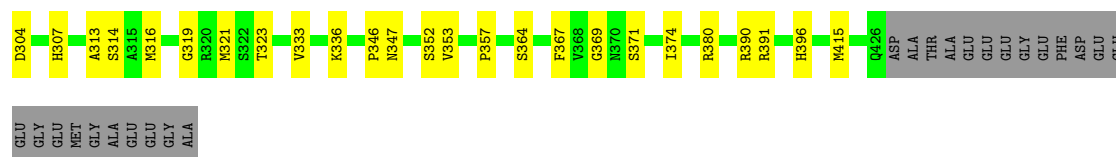
Chain B9: 80% 14% 5%



- Molecule 3: Tubulin beta chain

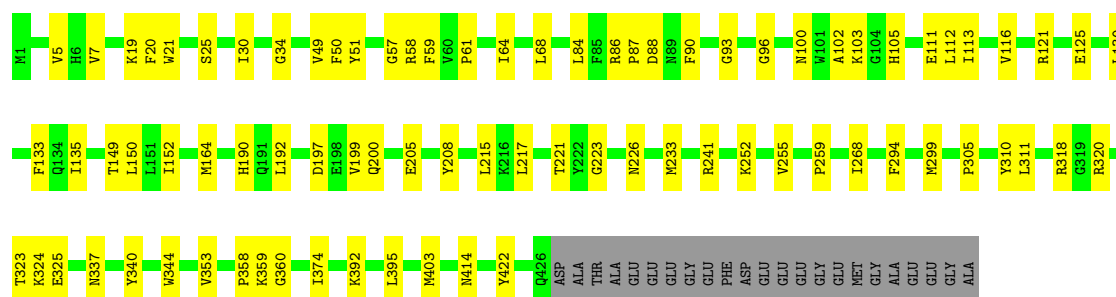
Chain C1: 74% 20% 5%





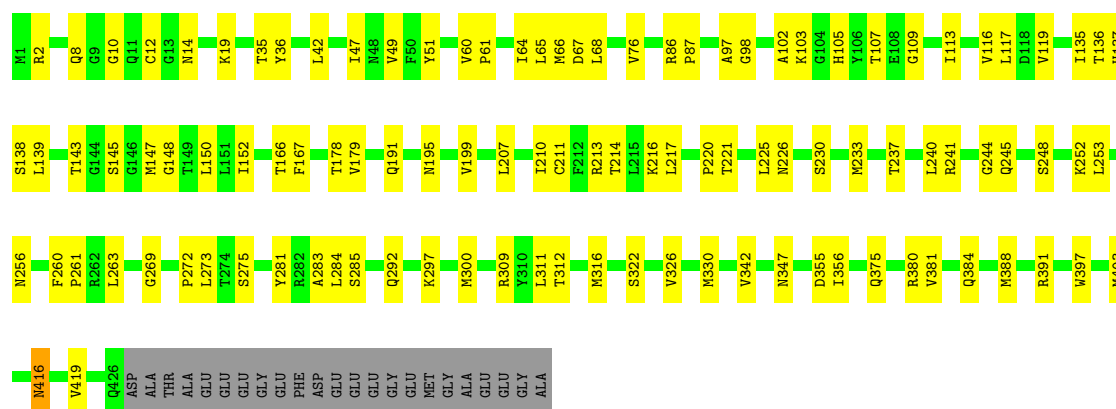
- Molecule 3: Tubulin beta chain

Chain C3: 77% 18% 5%



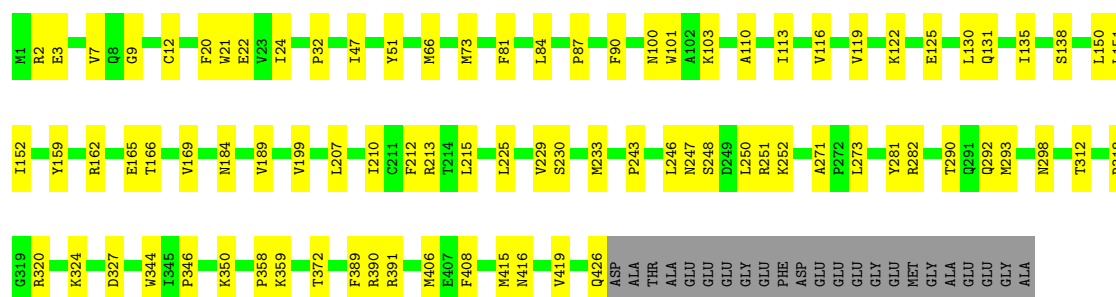
- Molecule 3: Tubulin beta chain

Chain C5: 71% 24% 5%



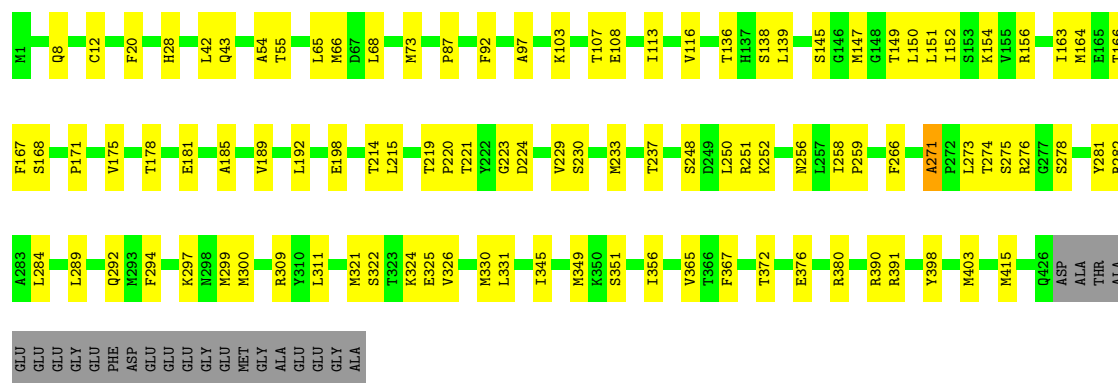
- Molecule 3: Tubulin beta chain

Chain C7: 76% 19% 5%



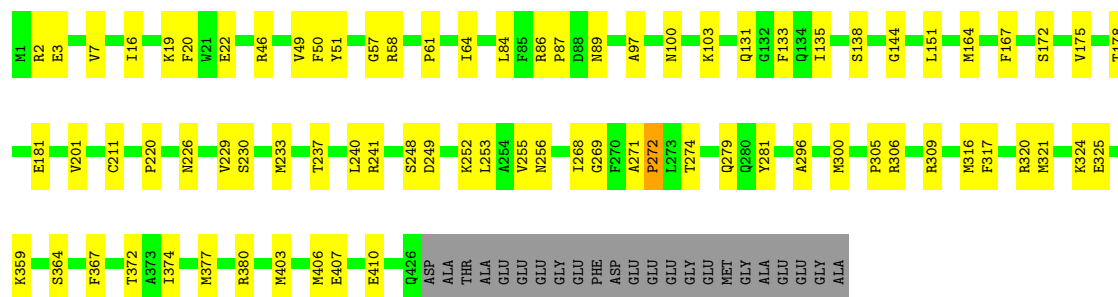
- Molecule 3: Tubulin beta chain

Chain C9:  72% 22% 5%



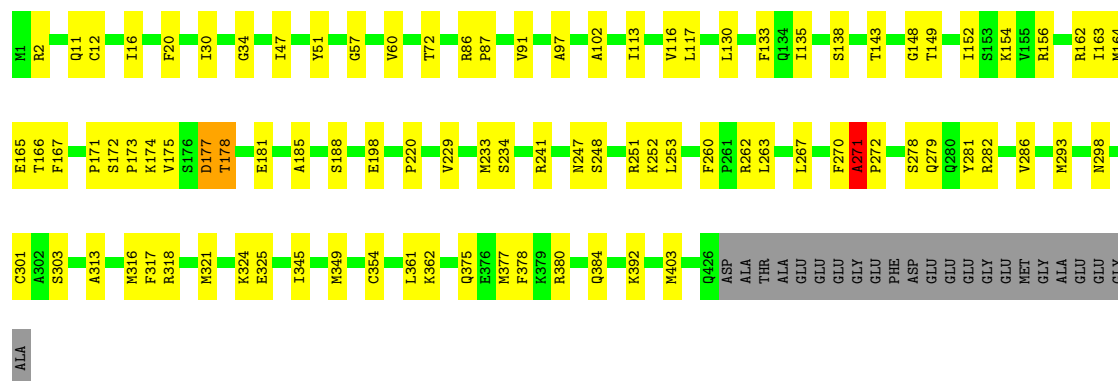
• Molecule 3: Tubulin beta chain

Chain D1:  77% 17% 5%



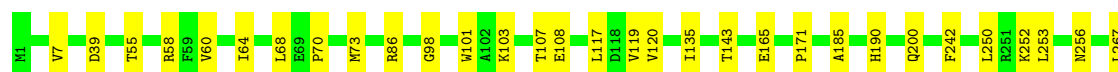
• Molecule 3: Tubulin beta chain

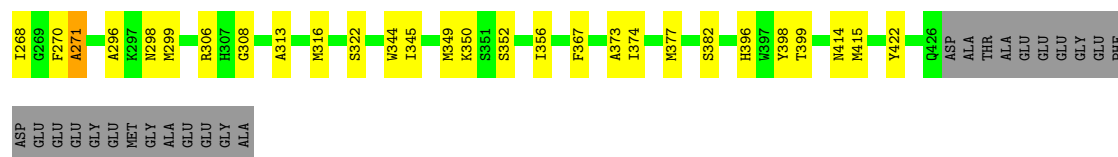
Chain D3:  74% 20% 5%



• Molecule 3: Tubulin beta chain

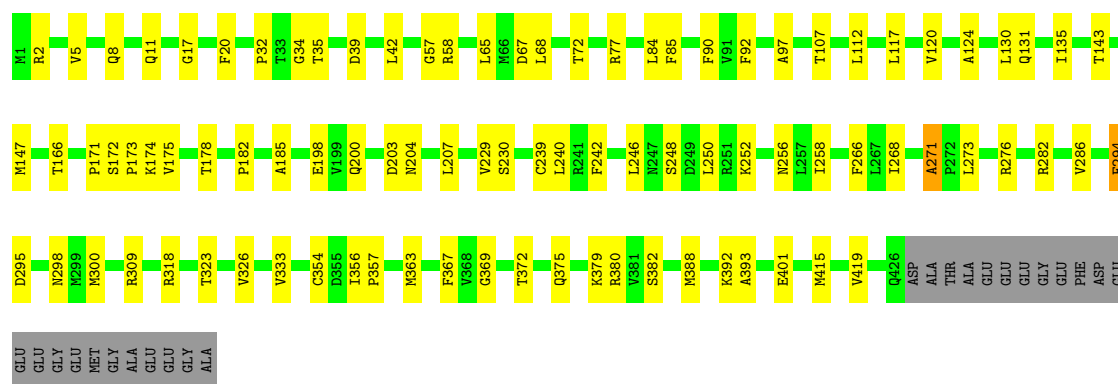
Chain D5:  82% 13% 5%





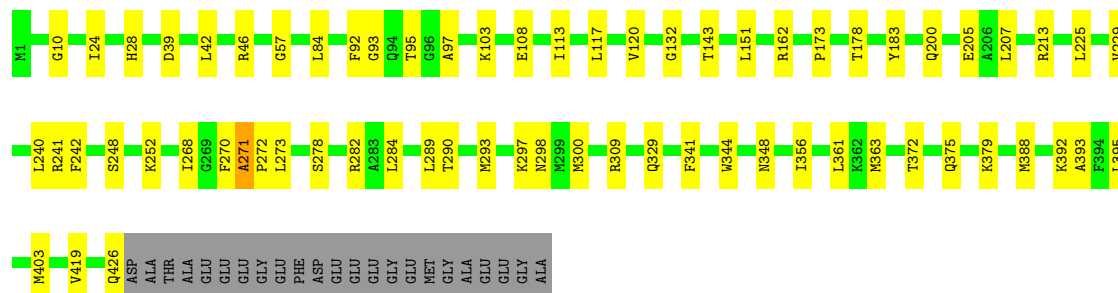
- Molecule 3: Tubulin beta chain

Chain D7: 75% 20% 5%



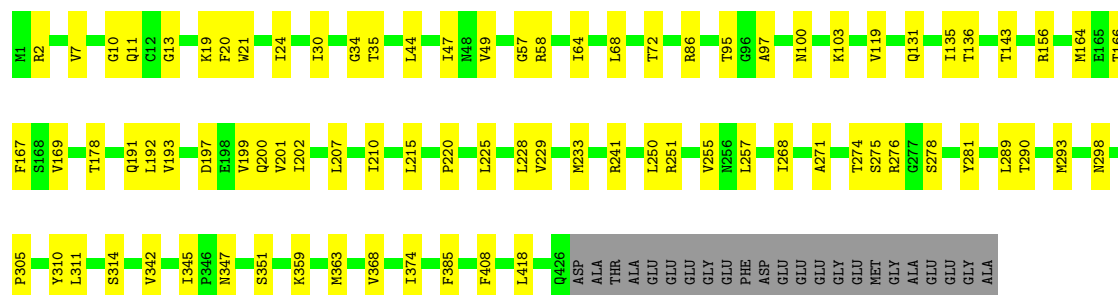
- Molecule 3: Tubulin beta chain

Chain D9: 80% 15% 5%



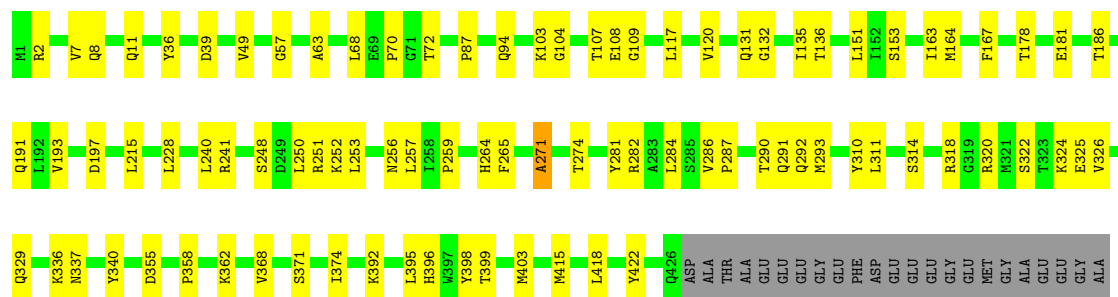
- Molecule 3: Tubulin beta chain

Chain E1: 76% 18% 5%

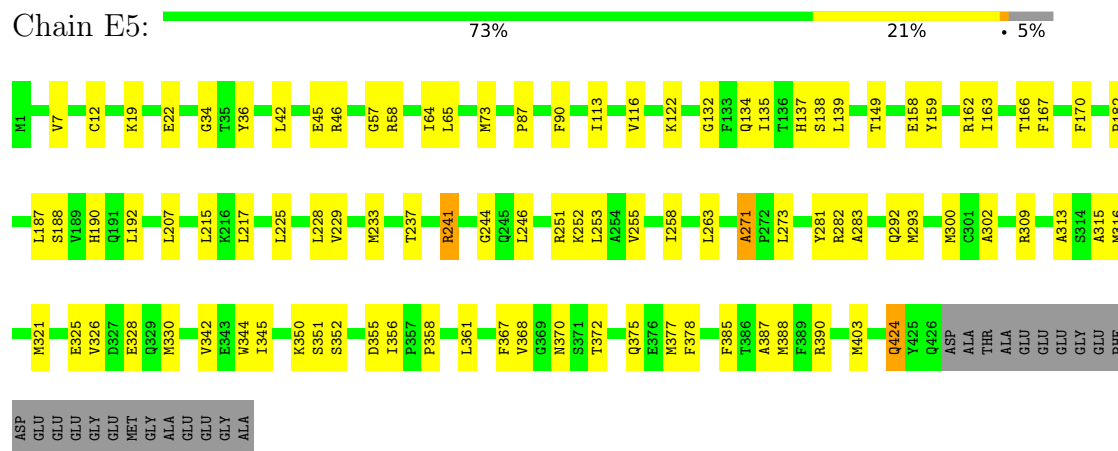


- Molecule 3: Tubulin beta chain

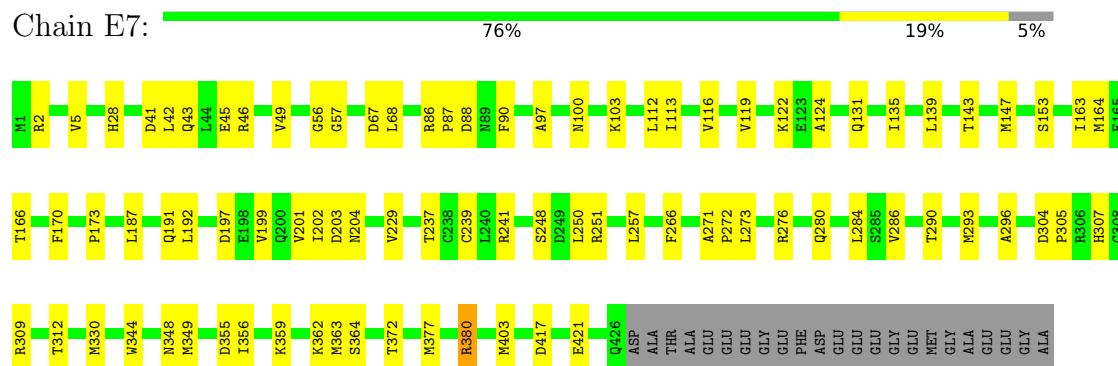
Chain E3: 75% 20% 5%



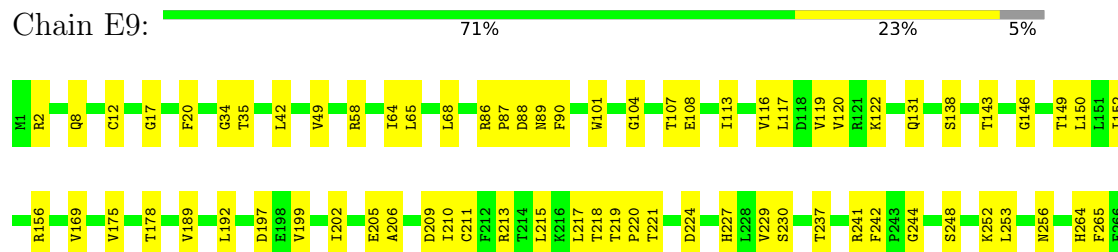
• Molecule 3: Tubulin beta chain



• Molecule 3: Tubulin beta chain



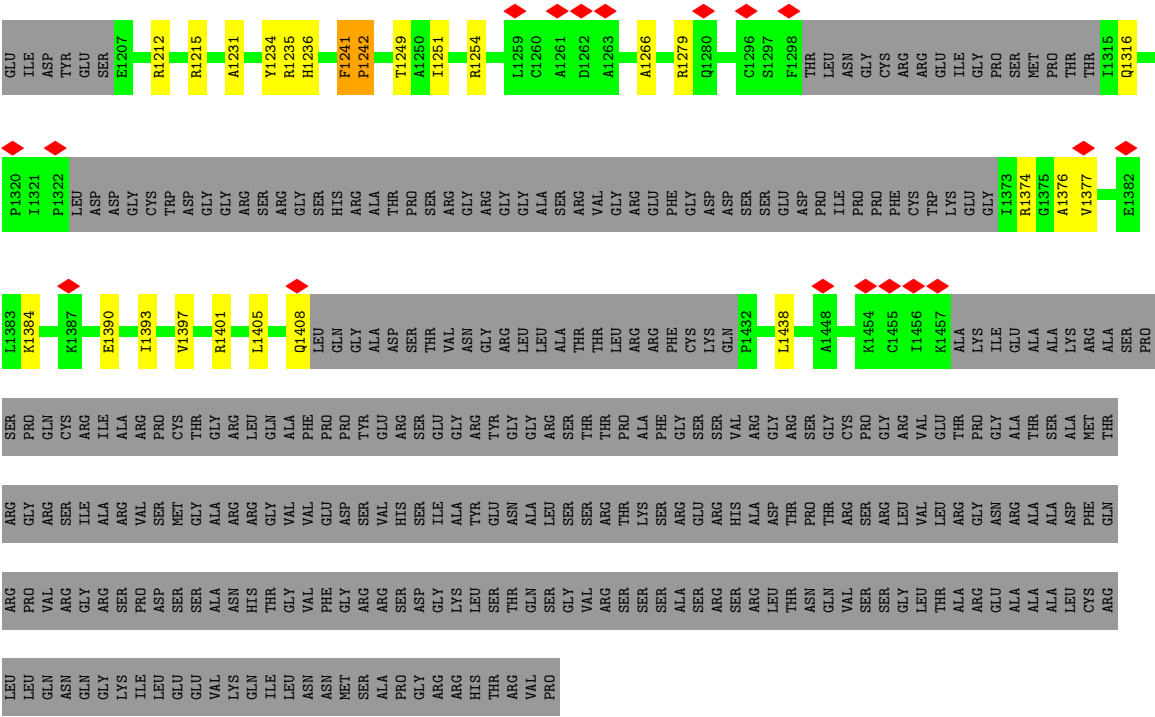
• Molecule 3: Tubulin beta chain



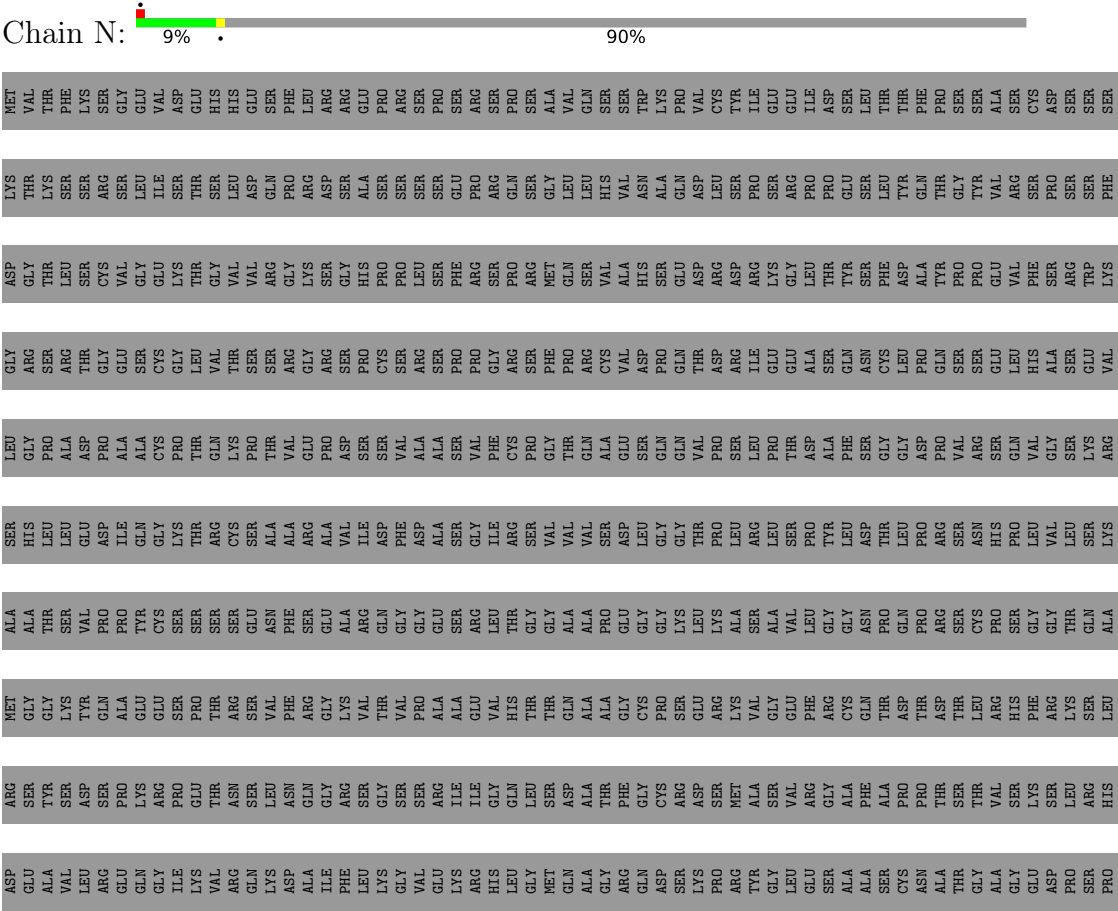
- Molecule 4: ICMAP2, TGME49 224700







● Molecule 4: ICMAP2, TGME49_224700



● Molecule 4: ICMAP2, TGME49 224700



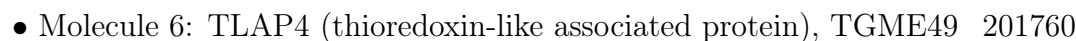
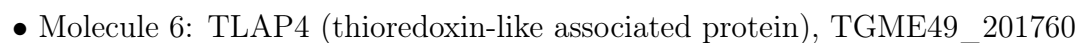


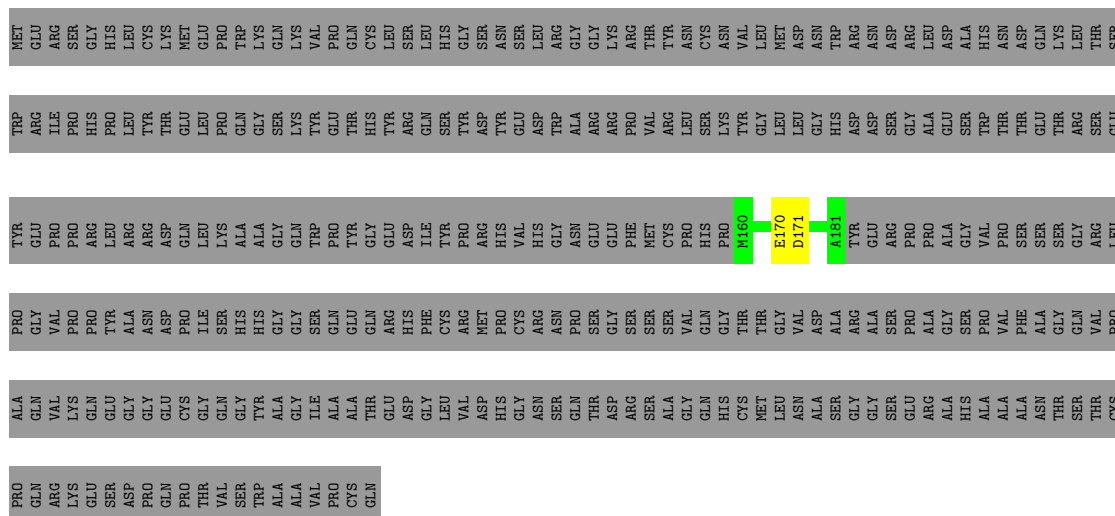


● Molecule 4: ICMAP2, TGME49 224700

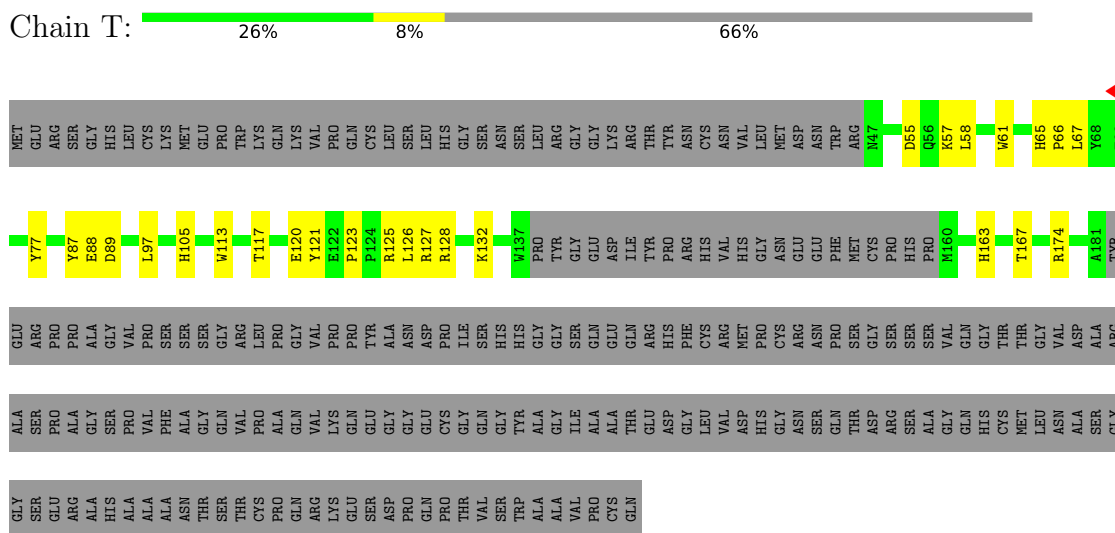




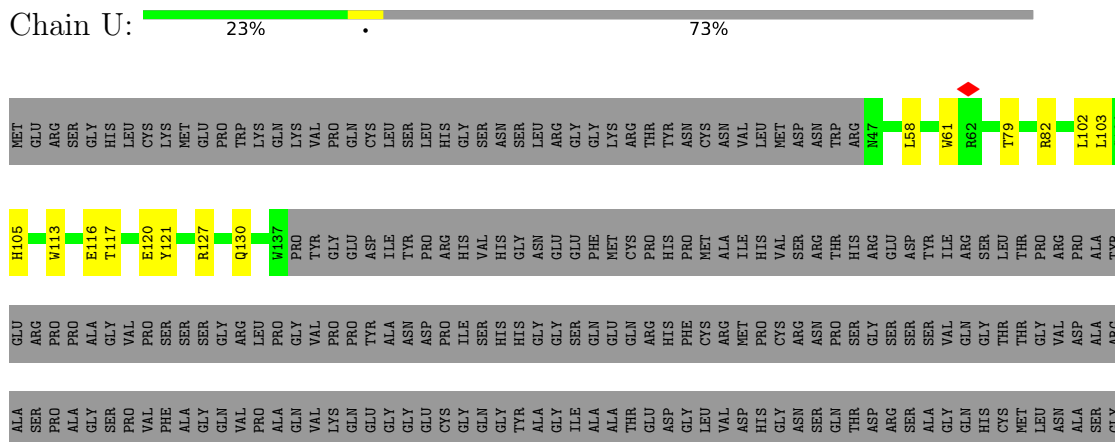




- Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49_201760



- Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49_201760



GLY SER GLN ARG ALA HIS ALA ALA THR SER THR CYS PRO GLN ARG LYS LYS GLU SER ASP PRO GLN LEU MET PRO THR VAL THR VAL

• Molecule 7: TRXL1, TGME49_232410

Chain a: 55% 18% 27%

MET SER GLN PRO VAL PHE ALA SER PRO LEU ASN VAL GLU LYS ARG ARG LEU ASN GLU SER ASP PRO GLN LEU MET PRO THR VAL THR VAL
D82 P83 K84 A104 F112 L115 E123 R126 A127 H128 R129 P130 M131 L132 S133 I134 L140 T141 A142 I143 L144 K145 R146 K152 E153 Y154 R164 P168 S169 V170 I171 V172 I173 G174 R178 E179 A180 Q181 F182 L183 R202 A207 SER ASP GLN PHE HIS
VAL ARG PRO THR LEU LEU GLN

• Molecule 7: TRXL1, TGME49_232410

Chain b: 57% 16% 27%

MET SER GLN PRO VAL PHE ALA SER PRO LEU ASN VAL GLU LYS ARG ARG LEU ASN GLU SER ASP PRO GLN LEU MET PRO THR VAL THR VAL
Y86 R97 N100 E101 Q106 I111 L115 R149 K152 E153 Y154 E155 T158 Y159 G162 S163 R164 V170 I171 V172 R178 E179 A180 L183 P184 L189 R194 L197 R198 Y199 D200 W201 A207 SER ASP GLN PHE HIS VAL ARG PRO THR LEU LEU
GLN

• Molecule 7: TRXL1, TGME49_232410

Chain c: 68% 23% 9%

MET S2 P9 N11 V12 E13 K14 R15 E19 A29 GLY GLY GLU VAL N35 N36 Q37 L47 F50 G53 S54 L55 V62 I63 P64 H67 L68 K71 S72 V73 A74 L75 A78 P83 K84 C85 P90 R97 E101 I108 E109 F112
V113 S114 L115 L132 S133 I134 L140 T141 I143 L144 K145 R146 H147 K152 P157 T158 Y159 L183 P184 I185 C186 L189 E190 M45 E191 L196 L197 A207 SER ASP GLN PHE HIS VAL ARG PRO THR LEU LEU GLN

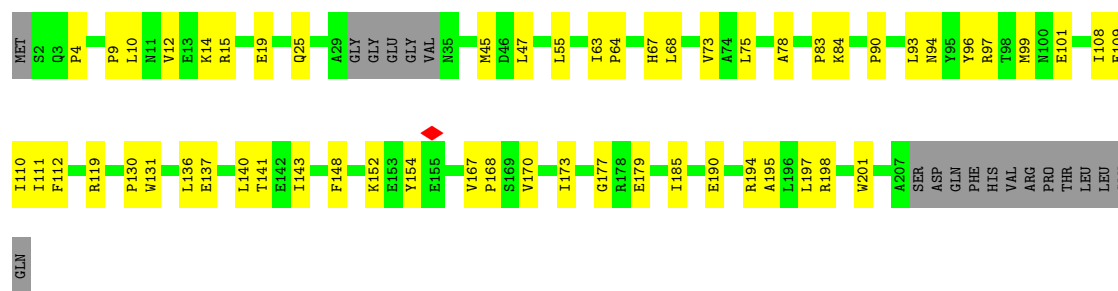
• Molecule 7: TRXL1, TGME49_232410

Chain d: 70% 22% 9%

MET S2 Q3 P4 V5 P9 L10 N11 V12 R15 M18 E19 A26 A29 GLY GLY GLU VAL N35 I36 Y42 M45 L55 P64 H67 S72 L75 P90 R97 M100 E101 I108 I111 L115 F122 I134 D135 L136
L140 T141 I143 L144 K145 R146 H147 R149 K152 F153 Y154 Y161 V170 I171 V172 E179 A180 Q181 F182 L183 P184 I185 E191 L196 A207 SER ASP GLN PHE HIS VAL ARG PRO THR LEU LEU GLN

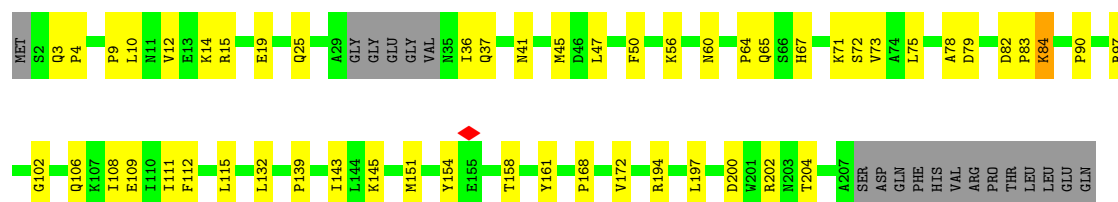
• Molecule 7: TRXL1, TGME49_232410

Chain e:  66% 25% 9%



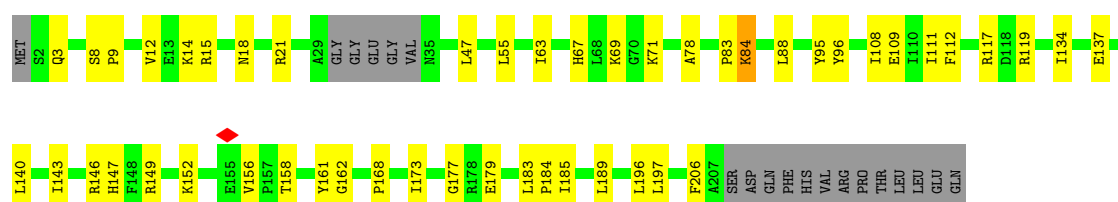
- Molecule 7: TRXL1, TGME49_232410

Chain f:  67% 24% 9%



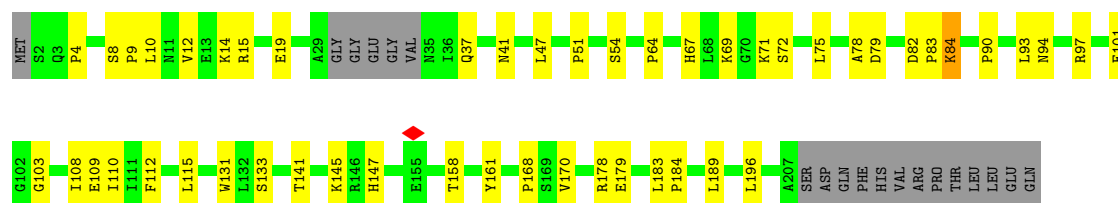
- Molecule 7: TRXL1, TGME49_232410

Chain g:  69% 22% 9%



- Molecule 7: TRXL1, TGME49_232410

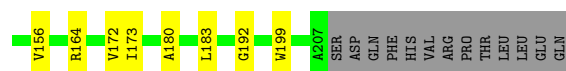
Chain h:  69% 22% 9%



- Molecule 7: TRXL1, TGME49_232410

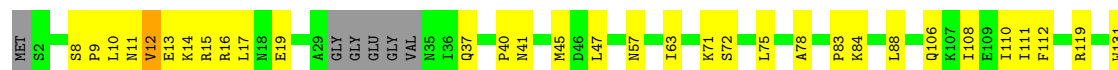
Chain i:  74% 18% 9%





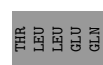
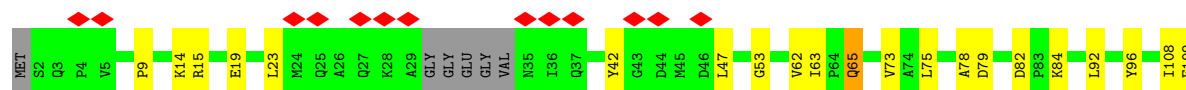
- Molecule 7: TRXL1, TGME49_232410

Chain j: 70% 21% 9%



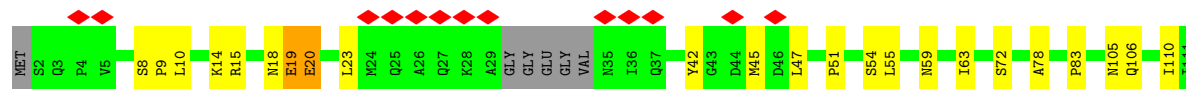
- Molecule 7: TRXL1, TGME49_232410

Chain m: 6% 68% 23% 9%



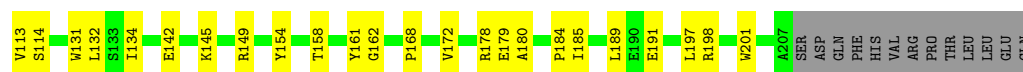
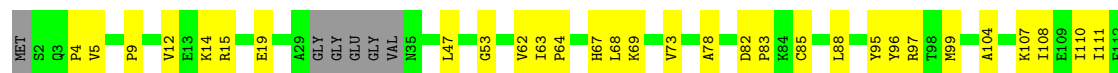
- Molecule 7: TRXL1, TGME49_232410

Chain n: 6% 70% 20% 9%



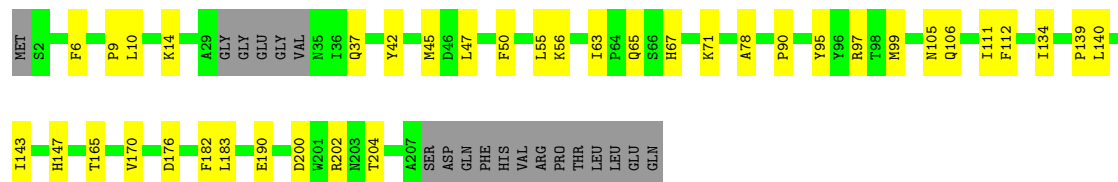
- Molecule 7: TRXL1, TGME49_232410

Chain o: 67% 25% 9%



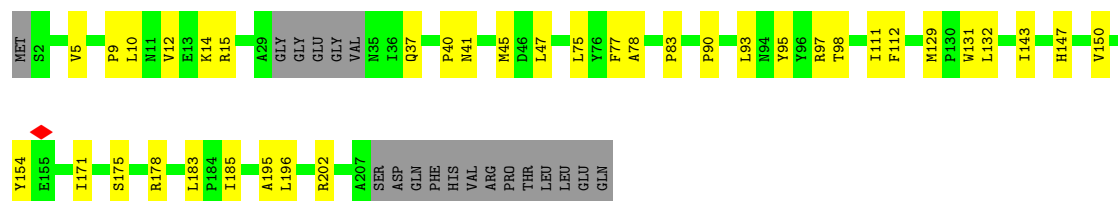
- Molecule 7: TRXL1, TGME49_232410

Chain p:  74% 17% 9%



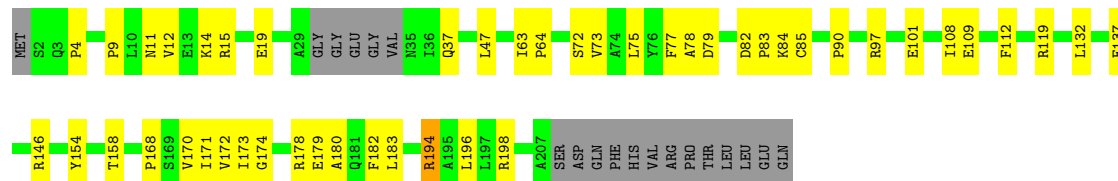
• Molecule 7: TRXL1, TGME49_232410

Chain q:  75% 17% 9%



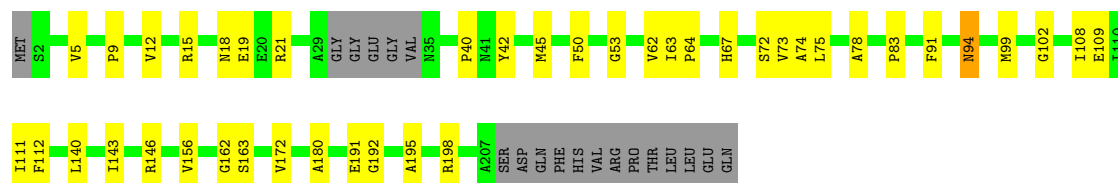
• Molecule 7: TRXL1, TGME49_232410

Chain r:  70% 21% 9%



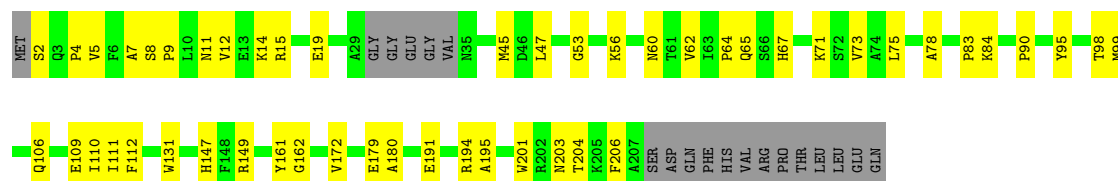
• Molecule 7: TRXL1, TGME49_232410

Chain s:  72% 19% 9%



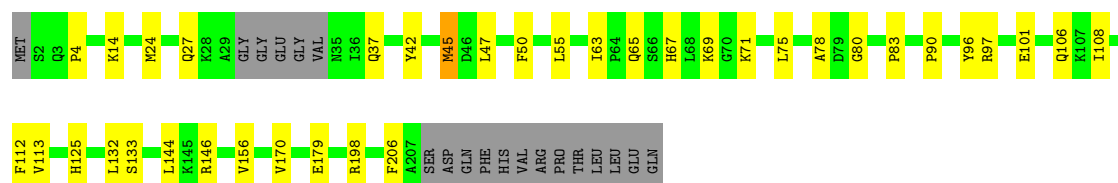
• Molecule 7: TRXL1, TGME49_232410

Chain t:  69% 23% 9%



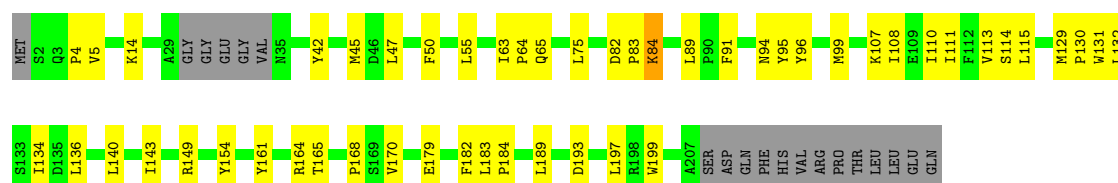
- Molecule 7: TRXL1, TGME49_232410

Chain u: 



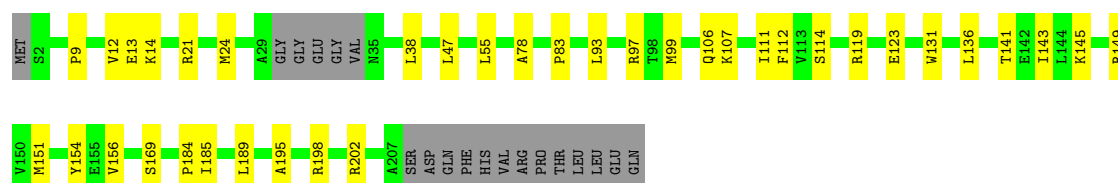
- Molecule 7: TRXL1, TGME49_232410

Chain v: 



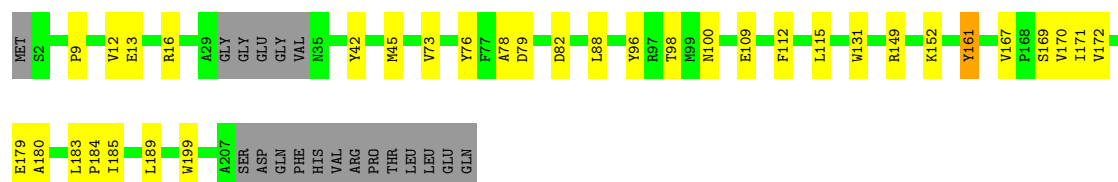
- Molecule 7: TRXL1, TGME49_232410

Chain w: 



- Molecule 7: TRXL1, TGME49_232410

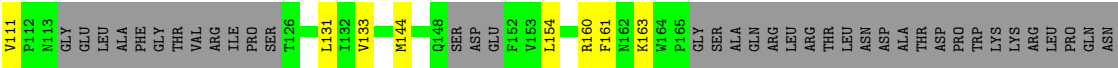
Chain x: 



- Molecule 8: TRXL2, TGME49_225790

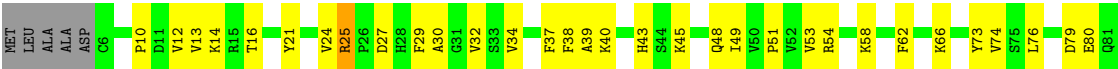
Chain k: 





VAL

• Molecule 8: TRXL2, TGME49_225790



PRO
TRP
LYS
LYS
ARG
LEU
PRO
GLN
ASN
VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57592	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.205	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/483	0.60	0/667
1	B	0.23	0/491	0.60	0/679
1	C	0.27	0/491	0.86	2/679 (0.3%)
1	D	0.31	0/491	0.90	1/679 (0.1%)
1	E	0.28	0/491	0.61	0/679
1	F	0.25	0/491	0.59	0/679
1	G	0.24	0/491	0.55	0/679
1	H	0.29	0/491	0.65	0/679
1	I	0.29	0/491	0.67	0/679
1	J	0.24	0/491	0.60	0/679
1	K	0.24	0/491	0.60	0/679
2	A0	0.25	0/3398	0.61	4/4606 (0.1%)
2	A2	0.26	0/3398	0.64	0/4606
2	A4	0.26	0/3398	0.66	0/4606
2	A6	0.26	0/3398	0.64	2/4606 (0.0%)
2	A8	0.24	0/3398	0.53	0/4606
2	B0	0.22	0/3398	0.54	0/4606
2	B2	0.23	0/3398	0.52	1/4606 (0.0%)
2	B4	0.22	0/3398	0.52	0/4606
2	B6	0.23	0/3398	0.51	0/4606
2	B8	0.27	1/3398 (0.0%)	0.54	1/4606 (0.0%)
2	C0	0.22	0/3398	0.57	0/4606
2	C2	0.26	0/3398	0.63	2/4606 (0.0%)
2	C4	0.24	0/3398	0.66	1/4606 (0.0%)
2	C6	0.26	0/3398	0.63	2/4606 (0.0%)
2	C8	0.25	0/3398	0.58	0/4606
2	D0	0.26	0/3398	0.60	1/4606 (0.0%)
2	D2	0.25	0/3398	0.58	0/4606
2	D4	0.27	0/3398	0.62	0/4606
2	D6	0.26	0/3398	0.58	0/4606
2	D8	0.27	0/3398	0.61	0/4606
2	E0	0.22	0/3398	0.54	0/4606

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	E2	0.25	0/3398	0.61	0/4606
2	E4	0.23	0/3398	0.60	1/4606 (0.0%)
2	E6	0.24	0/3398	0.61	2/4606 (0.0%)
2	E8	0.24	0/3398	0.59	3/4606 (0.1%)
2	F0	0.25	0/3398	0.59	1/4606 (0.0%)
3	A1	0.27	0/3404	0.70	5/4606 (0.1%)
3	A3	0.24	0/3404	0.62	1/4606 (0.0%)
3	A5	0.25	0/3404	0.65	4/4606 (0.1%)
3	A7	0.21	0/3404	0.54	2/4606 (0.0%)
3	A9	0.23	0/3404	0.56	0/4606
3	B1	0.23	0/3404	0.59	0/4606
3	B3	0.25	0/3404	0.62	4/4606 (0.1%)
3	B5	0.26	0/3404	0.63	0/4606
3	B7	0.25	0/3404	0.60	0/4606
3	B9	0.23	0/3404	0.59	0/4606
3	C1	0.27	0/3404	0.68	0/4606
3	C3	0.24	0/3404	0.63	1/4606 (0.0%)
3	C5	0.26	0/3404	0.68	2/4606 (0.0%)
3	C7	0.24	0/3404	0.63	1/4606 (0.0%)
3	C9	0.27	0/3404	0.64	0/4606
3	D1	0.25	0/3404	0.62	0/4606
3	D3	0.26	0/3404	0.62	5/4606 (0.1%)
3	D5	0.24	0/3404	0.61	3/4606 (0.1%)
3	D7	0.24	0/3404	0.60	1/4606 (0.0%)
3	D9	0.26	0/3404	0.64	2/4606 (0.0%)
3	E1	0.26	0/3404	0.64	1/4606 (0.0%)
3	E3	0.24	0/3404	0.58	0/4606
3	E5	0.26	1/3404 (0.0%)	0.60	0/4606
3	E7	0.26	0/3404	0.63	1/4606 (0.0%)
3	E9	0.24	0/3404	0.63	4/4606 (0.1%)
3	F1	0.25	0/3404	0.69	2/4606 (0.0%)
4	L	0.23	0/1364	0.68	0/1841
4	M	0.23	0/1364	0.68	0/1841
4	N	0.22	0/1364	0.64	0/1841
4	Q	0.24	0/1364	0.69	0/1841
4	V	0.27	0/1364	0.67	0/1841
4	W	0.23	0/1364	0.66	0/1841
5	O	0.28	0/1768	0.81	5/2392 (0.2%)
5	P	0.30	0/1768	0.82	0/2392
6	R	0.32	0/982	0.78	1/1332 (0.1%)
6	S	0.26	0/186	0.67	0/251
6	T	0.31	0/982	0.79	0/1332
6	U	0.27	0/796	0.67	0/1081

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	a	0.30	0/1321	0.79	2/1788 (0.1%)
7	b	0.28	0/1321	0.71	1/1788 (0.1%)
7	c	0.27	0/1645	0.69	2/2225 (0.1%)
7	d	0.26	0/1645	0.63	1/2225 (0.0%)
7	e	0.26	0/1645	0.61	0/2225
7	f	0.29	0/1645	0.71	1/2225 (0.0%)
7	g	0.32	0/1645	0.63	1/2225 (0.0%)
7	h	0.28	0/1645	0.66	1/2225 (0.0%)
7	i	0.27	0/1645	0.68	2/2225 (0.1%)
7	j	0.28	0/1645	0.71	4/2225 (0.2%)
7	m	0.26	0/1645	0.64	1/2225 (0.0%)
7	n	0.28	0/1645	0.70	4/2225 (0.2%)
7	o	0.26	0/1645	0.60	0/2225
7	p	0.29	0/1645	0.65	0/2225
7	q	0.25	0/1645	0.56	0/2225
7	r	0.27	0/1645	0.64	1/2225 (0.0%)
7	s	0.27	0/1645	0.65	2/2225 (0.1%)
7	t	0.26	0/1645	0.62	1/2225 (0.0%)
7	u	0.28	0/1645	0.69	1/2225 (0.0%)
7	v	0.27	0/1645	0.63	1/2225 (0.0%)
7	w	0.24	0/1645	0.61	0/2225
7	x	0.27	0/1645	0.63	0/2225
8	k	0.26	0/1218	0.64	0/1646
8	l	0.33	0/1218	0.88	0/1646
All	All	0.25	2/234889 (0.0%)	0.63	95/318163 (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
1	D	0	2
2	A2	0	1
2	A6	0	1
2	B0	0	1
2	C0	0	1
2	C4	0	2
2	C8	0	1
2	D2	0	1
2	D4	0	2
2	D6	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D8	0	1
2	E4	0	2
2	E6	0	1
2	E8	0	2
3	A1	0	2
3	A3	0	1
3	A5	0	1
3	B3	0	1
3	C1	0	1
3	C5	0	2
3	C7	0	1
3	C9	0	1
3	D1	0	1
3	D3	0	1
3	D5	0	2
3	D7	0	2
3	D9	0	1
3	E1	0	1
3	E3	0	1
3	E5	0	3
3	E7	0	2
3	E9	0	1
3	F1	0	2
4	L	0	1
4	M	0	1
4	N	0	1
4	Q	0	1
4	V	0	1
4	W	0	1
5	P	0	3
6	R	0	2
6	T	0	1
7	a	0	1
7	b	0	1
7	p	0	1
7	x	0	1
8	l	0	2
All	All	0	64

All (2) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B8	35	GLN	C-N	5.96	1.42	1.33
3	E5	241	ARG	C-N	-5.21	1.26	1.33

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ALA	CA-C-N	9.24	154.31	121.59
1	C	253	ALA	C-N-CA	9.24	154.31	121.59
3	B3	349	MET	CB-CG-SD	-9.05	85.56	112.70
5	O	498	THR	CA-C-N	8.80	138.34	121.54
5	O	498	THR	C-N-CA	8.80	138.34	121.54

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A1	137	HIS	Peptide
3	A1	271	ALA	Peptide
2	A2	373	ARG	Sidechain
3	A3	200	GLN	Peptide
3	A5	271	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	464	0	469	10	0
1	B	471	0	476	4	0
1	C	471	0	475	12	0
1	D	471	0	476	19	0
1	E	471	0	476	9	0
1	F	471	0	476	7	0
1	G	471	0	476	10	0
1	H	471	0	476	9	0
1	I	471	0	476	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	471	0	476	12	0
1	K	471	0	476	5	0
2	A0	3325	0	3252	58	0
2	A2	3325	0	3252	66	0
2	A4	3325	0	3252	68	0
2	A6	3325	0	3252	45	0
2	A8	3325	0	3251	49	0
2	B0	3325	0	3252	61	0
2	B2	3325	0	3252	40	0
2	B4	3325	0	3252	46	0
2	B6	3325	0	3252	36	0
2	B8	3325	0	3251	59	0
2	C0	3325	0	3252	53	0
2	C2	3325	0	3252	54	0
2	C4	3325	0	3252	52	0
2	C6	3325	0	3252	64	0
2	C8	3325	0	3252	61	0
2	D0	3325	0	3252	54	0
2	D2	3325	0	3252	40	0
2	D4	3325	0	3252	53	0
2	D6	3325	0	3252	63	0
2	D8	3325	0	3252	66	0
2	E0	3325	0	3252	42	0
2	E2	3325	0	3252	42	0
2	E4	3325	0	3252	35	0
2	E6	3325	0	3252	47	0
2	E8	3325	0	3252	43	0
2	F0	3325	0	3252	52	0
3	A1	3331	0	3207	77	0
3	A3	3331	0	3209	74	0
3	A5	3331	0	3207	59	0
3	A7	3331	0	3207	37	0
3	A9	3331	0	3207	55	0
3	B1	3331	0	3209	65	0
3	B3	3331	0	3207	55	0
3	B5	3331	0	3207	75	0
3	B7	3331	0	3209	53	0
3	B9	3331	0	3209	40	0
3	C1	3331	0	3209	60	0
3	C3	3331	0	3207	52	0
3	C5	3331	0	3209	73	0
3	C7	3331	0	3209	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C9	3331	0	3209	73	0
3	D1	3331	0	3209	54	0
3	D3	3331	0	3207	65	0
3	D5	3331	0	3207	33	0
3	D7	3331	0	3207	57	0
3	D9	3331	0	3207	39	0
3	E1	3331	0	3207	53	0
3	E3	3331	0	3209	59	0
3	E5	3331	0	3207	59	0
3	E7	3331	0	3207	57	0
3	E9	3331	0	3206	70	0
3	F1	3331	0	3207	63	0
4	L	1334	0	1345	15	0
4	M	1334	0	1345	17	0
4	N	1334	0	1345	11	0
4	Q	1334	0	1345	15	0
4	V	1334	0	1345	17	0
4	W	1334	0	1345	18	0
5	O	1736	0	1725	22	0
5	P	1736	0	1725	45	0
6	R	954	0	899	23	0
6	S	182	0	183	1	0
6	T	954	0	899	21	0
6	U	772	0	716	14	0
7	a	1289	0	1274	29	0
7	b	1289	0	1274	31	0
7	c	1608	0	1590	36	0
7	d	1608	0	1590	35	0
7	e	1608	0	1590	42	0
7	f	1608	0	1590	39	0
7	g	1608	0	1590	32	0
7	h	1608	0	1590	40	0
7	i	1608	0	1590	26	0
7	j	1608	0	1590	29	0
7	m	1608	0	1590	35	0
7	n	1608	0	1590	35	0
7	o	1608	0	1590	38	0
7	p	1608	0	1590	28	0
7	q	1608	0	1590	27	0
7	r	1608	0	1590	32	0
7	s	1608	0	1590	31	0
7	t	1608	0	1590	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	u	1608	0	1590	26	0
7	v	1608	0	1590	34	0
7	w	1608	0	1590	26	0
7	x	1608	0	1590	20	0
8	k	1187	0	1180	26	0
8	l	1187	0	1180	29	0
9	A0	32	0	12	0	0
9	A2	32	0	12	0	0
9	A4	32	0	12	0	0
9	A6	32	0	12	0	0
9	A8	32	0	12	0	0
9	B0	32	0	12	0	0
9	B2	32	0	12	0	0
9	B4	32	0	12	0	0
9	B6	32	0	12	0	0
9	B8	32	0	12	0	0
9	C0	32	0	12	0	0
9	C3	32	0	12	0	0
9	C4	32	0	12	0	0
9	C6	32	0	12	0	0
9	C8	32	0	12	0	0
9	D0	32	0	12	0	0
9	D2	32	0	12	0	0
9	D4	32	0	12	0	0
9	D6	32	0	12	0	0
9	D8	32	0	12	0	0
9	E0	32	0	12	0	0
9	E2	32	0	12	0	0
9	E4	32	0	12	1	0
9	E6	32	0	12	0	0
9	E8	32	0	12	0	0
9	F0	32	0	12	0	0
10	A0	1	0	0	0	0
10	A2	1	0	0	0	0
10	A5	1	0	0	0	0
10	A7	1	0	0	0	0
10	A8	1	0	0	0	0
10	B0	1	0	0	0	0
10	B2	1	0	0	0	0
10	B4	1	0	0	0	0
10	B6	1	0	0	0	0
10	B8	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C0	1	0	0	0	0
10	C2	1	0	0	0	0
10	C4	1	0	0	0	0
10	C6	1	0	0	0	0
10	C8	1	0	0	0	0
10	D0	1	0	0	0	0
10	D2	1	0	0	0	0
10	D4	1	0	0	0	0
10	D6	1	0	0	0	0
10	D8	1	0	0	0	0
10	E1	1	0	0	0	0
10	E2	1	0	0	0	0
10	E4	1	0	0	0	0
10	E6	1	0	0	0	0
10	E9	1	0	0	0	0
10	F0	1	0	0	0	0
11	A1	28	0	12	1	0
11	A3	28	0	12	0	0
11	A5	28	0	12	0	0
11	A7	28	0	12	0	0
11	A9	28	0	12	0	0
11	B1	28	0	12	0	0
11	B3	28	0	12	1	0
11	B5	28	0	12	0	0
11	B7	28	0	12	0	0
11	B9	28	0	12	0	0
11	C1	28	0	12	0	0
11	C3	28	0	12	0	0
11	C5	28	0	12	0	0
11	C7	28	0	12	0	0
11	C9	28	0	12	0	0
11	D1	28	0	12	0	0
11	D3	28	0	12	0	0
11	D5	28	0	12	0	0
11	D7	28	0	12	0	0
11	D9	28	0	12	0	0
11	E1	28	0	12	0	0
11	E3	28	0	12	0	0
11	E5	28	0	12	2	0
11	E7	28	0	12	1	0
11	E9	28	0	12	0	0
11	F1	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	231266	0	224728	3480	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 8.

The worst 5 of 3480 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)
3:A3:258:ILE:HD12	3:A3:264:HIS:HB3	1.57	0.86
1:D:245:SER:O	1:D:249:SER:HB3	1.77	0.84
2:B4:407:TRP:HE1	3:B5:258:ILE:HG23	1.42	0.83
3:D3:130:LEU:HB3	3:D3:162:ARG:HE	1.46	0.80
7:h:12:VAL:HG12	7:h:15:ARG:HH21	1.45	0.80

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	A	57/351 (16%)	45 (79%)	12 (21%)	0	100	100
1	B	58/351 (16%)	52 (90%)	6 (10%)	0	100	100
1	C	58/351 (16%)	53 (91%)	5 (9%)	0	100	100
1	D	58/351 (16%)	50 (86%)	8 (14%)	0	100	100
1	E	58/351 (16%)	53 (91%)	5 (9%)	0	100	100
1	F	58/351 (16%)	52 (90%)	6 (10%)	0	100	100
1	G	58/351 (16%)	52 (90%)	6 (10%)	0	100	100
1	H	58/351 (16%)	53 (91%)	5 (9%)	0	100	100
1	I	58/351 (16%)	54 (93%)	4 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	58/351 (16%)	49 (84%)	9 (16%)	0	100	100
1	K	58/351 (16%)	54 (93%)	4 (7%)	0	100	100
2	A0	424/453 (94%)	391 (92%)	33 (8%)	0	100	100
2	A2	424/453 (94%)	391 (92%)	32 (8%)	1 (0%)	43	71
2	A4	424/453 (94%)	387 (91%)	35 (8%)	2 (0%)	24	55
2	A6	424/453 (94%)	379 (89%)	45 (11%)	0	100	100
2	A8	424/453 (94%)	413 (97%)	11 (3%)	0	100	100
2	B0	424/453 (94%)	413 (97%)	11 (3%)	0	100	100
2	B2	424/453 (94%)	415 (98%)	9 (2%)	0	100	100
2	B4	424/453 (94%)	410 (97%)	14 (3%)	0	100	100
2	B6	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
2	B8	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	C0	424/453 (94%)	391 (92%)	32 (8%)	1 (0%)	43	71
2	C2	424/453 (94%)	381 (90%)	42 (10%)	1 (0%)	43	71
2	C4	424/453 (94%)	383 (90%)	38 (9%)	3 (1%)	18	49
2	C6	424/453 (94%)	384 (91%)	39 (9%)	1 (0%)	43	71
2	C8	424/453 (94%)	392 (92%)	32 (8%)	0	100	100
2	D0	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
2	D2	424/453 (94%)	379 (89%)	44 (10%)	1 (0%)	43	71
2	D4	424/453 (94%)	390 (92%)	33 (8%)	1 (0%)	43	71
2	D6	424/453 (94%)	395 (93%)	28 (7%)	1 (0%)	43	71
2	D8	424/453 (94%)	383 (90%)	40 (9%)	1 (0%)	43	71
2	E0	424/453 (94%)	398 (94%)	26 (6%)	0	100	100
2	E2	424/453 (94%)	390 (92%)	33 (8%)	1 (0%)	43	71
2	E4	424/453 (94%)	385 (91%)	39 (9%)	0	100	100
2	E6	424/453 (94%)	381 (90%)	41 (10%)	2 (0%)	24	55
2	E8	424/453 (94%)	384 (91%)	39 (9%)	1 (0%)	43	71
2	F0	424/453 (94%)	410 (97%)	14 (3%)	0	100	100
3	A1	424/449 (94%)	384 (91%)	39 (9%)	1 (0%)	43	71
3	A3	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	A5	424/449 (94%)	386 (91%)	38 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A7	424/449 (94%)	405 (96%)	19 (4%)	0	100	100
3	A9	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
3	B1	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	B3	424/449 (94%)	405 (96%)	19 (4%)	0	100	100
3	B5	424/449 (94%)	404 (95%)	20 (5%)	0	100	100
3	B7	424/449 (94%)	405 (96%)	19 (4%)	0	100	100
3	B9	424/449 (94%)	404 (95%)	20 (5%)	0	100	100
3	C1	424/449 (94%)	391 (92%)	32 (8%)	1 (0%)	43	71
3	C3	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	C5	424/449 (94%)	384 (91%)	40 (9%)	0	100	100
3	C7	424/449 (94%)	383 (90%)	40 (9%)	1 (0%)	43	71
3	C9	424/449 (94%)	382 (90%)	42 (10%)	0	100	100
3	D1	424/449 (94%)	381 (90%)	42 (10%)	1 (0%)	43	71
3	D3	424/449 (94%)	380 (90%)	43 (10%)	1 (0%)	43	71
3	D5	424/449 (94%)	382 (90%)	40 (9%)	2 (0%)	24	55
3	D7	424/449 (94%)	386 (91%)	36 (8%)	2 (0%)	24	55
3	D9	424/449 (94%)	383 (90%)	40 (9%)	1 (0%)	43	71
3	E1	424/449 (94%)	382 (90%)	40 (9%)	2 (0%)	24	55
3	E3	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	E5	424/449 (94%)	376 (89%)	48 (11%)	0	100	100
3	E7	424/449 (94%)	384 (91%)	39 (9%)	1 (0%)	43	71
3	E9	424/449 (94%)	388 (92%)	33 (8%)	3 (1%)	18	49
3	F1	424/449 (94%)	380 (90%)	41 (10%)	3 (1%)	18	49
4	L	154/1678 (9%)	150 (97%)	3 (2%)	1 (1%)	21	51
4	M	154/1678 (9%)	152 (99%)	1 (1%)	1 (1%)	21	51
4	N	154/1678 (9%)	151 (98%)	2 (1%)	1 (1%)	21	51
4	Q	154/1678 (9%)	148 (96%)	5 (3%)	1 (1%)	21	51
4	V	154/1678 (9%)	150 (97%)	3 (2%)	1 (1%)	21	51
4	W	154/1678 (9%)	148 (96%)	5 (3%)	1 (1%)	21	51
5	O	209/583 (36%)	174 (83%)	32 (15%)	3 (1%)	9	34
5	P	209/583 (36%)	160 (77%)	42 (20%)	7 (3%)	3	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	R	109/336 (32%)	85 (78%)	24 (22%)	0	100	100
6	S	20/336 (6%)	17 (85%)	3 (15%)	0	100	100
6	T	109/336 (32%)	85 (78%)	24 (22%)	0	100	100
6	U	89/336 (26%)	73 (82%)	16 (18%)	0	100	100
7	a	159/220 (72%)	138 (87%)	21 (13%)	0	100	100
7	b	159/220 (72%)	137 (86%)	22 (14%)	0	100	100
7	c	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	d	197/220 (90%)	182 (92%)	15 (8%)	0	100	100
7	e	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
7	f	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
7	g	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	h	197/220 (90%)	189 (96%)	8 (4%)	0	100	100
7	i	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
7	j	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	m	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
7	n	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
7	o	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	p	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	q	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	r	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	s	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	t	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
7	u	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
7	v	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	w	197/220 (90%)	179 (91%)	18 (9%)	0	100	100
7	x	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
8	k	139/189 (74%)	133 (96%)	6 (4%)	0	100	100
8	l	139/189 (74%)	122 (88%)	17 (12%)	0	100	100
All	All	28890/45109 (64%)	26676 (92%)	2162 (8%)	52 (0%)	44	71

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C4	219	ILE
3	C7	125	GLU
3	D3	178	THR
3	D7	178	THR
3	E1	95	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	54/305 (18%)	54 (100%)	0	100	100
1	B	55/305 (18%)	55 (100%)	0	100	100
1	C	55/305 (18%)	55 (100%)	0	100	100
1	D	55/305 (18%)	55 (100%)	0	100	100
1	E	55/305 (18%)	55 (100%)	0	100	100
1	F	55/305 (18%)	55 (100%)	0	100	100
1	G	55/305 (18%)	55 (100%)	0	100	100
1	H	55/305 (18%)	55 (100%)	0	100	100
1	I	55/305 (18%)	55 (100%)	0	100	100
1	J	55/305 (18%)	55 (100%)	0	100	100
1	K	55/305 (18%)	55 (100%)	0	100	100
2	A0	359/379 (95%)	359 (100%)	0	100	100
2	A2	359/379 (95%)	359 (100%)	0	100	100
2	A4	359/379 (95%)	359 (100%)	0	100	100
2	A6	359/379 (95%)	359 (100%)	0	100	100
2	A8	359/379 (95%)	359 (100%)	0	100	100
2	B0	359/379 (95%)	358 (100%)	1 (0%)	86	85
2	B2	359/379 (95%)	359 (100%)	0	100	100
2	B4	359/379 (95%)	359 (100%)	0	100	100
2	B6	359/379 (95%)	359 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B8	359/379 (95%)	359 (100%)	0	100	100
2	C0	359/379 (95%)	359 (100%)	0	100	100
2	C2	359/379 (95%)	359 (100%)	0	100	100
2	C4	359/379 (95%)	359 (100%)	0	100	100
2	C6	359/379 (95%)	359 (100%)	0	100	100
2	C8	359/379 (95%)	359 (100%)	0	100	100
2	D0	359/379 (95%)	359 (100%)	0	100	100
2	D2	359/379 (95%)	359 (100%)	0	100	100
2	D4	359/379 (95%)	359 (100%)	0	100	100
2	D6	359/379 (95%)	358 (100%)	1 (0%)	86	85
2	D8	359/379 (95%)	359 (100%)	0	100	100
2	E0	359/379 (95%)	359 (100%)	0	100	100
2	E2	359/379 (95%)	359 (100%)	0	100	100
2	E4	359/379 (95%)	359 (100%)	0	100	100
2	E6	359/379 (95%)	359 (100%)	0	100	100
2	E8	359/379 (95%)	359 (100%)	0	100	100
2	F0	359/379 (95%)	359 (100%)	0	100	100
3	A1	364/381 (96%)	364 (100%)	0	100	100
3	A3	364/381 (96%)	364 (100%)	0	100	100
3	A5	364/381 (96%)	364 (100%)	0	100	100
3	A7	364/381 (96%)	364 (100%)	0	100	100
3	A9	364/381 (96%)	364 (100%)	0	100	100
3	B1	364/381 (96%)	364 (100%)	0	100	100
3	B3	364/381 (96%)	364 (100%)	0	100	100
3	B5	364/381 (96%)	364 (100%)	0	100	100
3	B7	364/381 (96%)	364 (100%)	0	100	100
3	B9	364/381 (96%)	363 (100%)	1 (0%)	86	85
3	C1	364/381 (96%)	364 (100%)	0	100	100
3	C3	364/381 (96%)	364 (100%)	0	100	100
3	C5	364/381 (96%)	363 (100%)	1 (0%)	86	85
3	C7	364/381 (96%)	364 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C9	364/381 (96%)	364 (100%)	0	100	100
3	D1	364/381 (96%)	364 (100%)	0	100	100
3	D3	364/381 (96%)	364 (100%)	0	100	100
3	D5	364/381 (96%)	364 (100%)	0	100	100
3	D7	364/381 (96%)	364 (100%)	0	100	100
3	D9	364/381 (96%)	364 (100%)	0	100	100
3	E1	364/381 (96%)	363 (100%)	1 (0%)	86	85
3	E3	364/381 (96%)	364 (100%)	0	100	100
3	E5	364/381 (96%)	363 (100%)	1 (0%)	86	85
3	E7	364/381 (96%)	364 (100%)	0	100	100
3	E9	364/381 (96%)	364 (100%)	0	100	100
3	F1	364/381 (96%)	363 (100%)	1 (0%)	86	85
4	L	143/1401 (10%)	143 (100%)	0	100	100
4	M	143/1401 (10%)	143 (100%)	0	100	100
4	N	143/1401 (10%)	143 (100%)	0	100	100
4	Q	143/1401 (10%)	143 (100%)	0	100	100
4	V	143/1401 (10%)	143 (100%)	0	100	100
4	W	143/1401 (10%)	143 (100%)	0	100	100
5	O	193/502 (38%)	193 (100%)	0	100	100
5	P	193/502 (38%)	193 (100%)	0	100	100
6	R	101/280 (36%)	101 (100%)	0	100	100
6	S	20/280 (7%)	20 (100%)	0	100	100
6	T	101/280 (36%)	101 (100%)	0	100	100
6	U	81/280 (29%)	81 (100%)	0	100	100
7	a	139/190 (73%)	139 (100%)	0	100	100
7	b	139/190 (73%)	139 (100%)	0	100	100
7	c	174/190 (92%)	173 (99%)	1 (1%)	78	81
7	d	174/190 (92%)	174 (100%)	0	100	100
7	e	174/190 (92%)	173 (99%)	1 (1%)	78	81
7	f	174/190 (92%)	173 (99%)	1 (1%)	78	81
7	g	174/190 (92%)	174 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	174/190 (92%)	174 (100%)	0	100	100
7	i	174/190 (92%)	174 (100%)	0	100	100
7	j	174/190 (92%)	173 (99%)	1 (1%)	78	81
7	m	174/190 (92%)	173 (99%)	1 (1%)	78	81
7	n	174/190 (92%)	174 (100%)	0	100	100
7	o	174/190 (92%)	174 (100%)	0	100	100
7	p	174/190 (92%)	174 (100%)	0	100	100
7	q	174/190 (92%)	174 (100%)	0	100	100
7	r	174/190 (92%)	174 (100%)	0	100	100
7	s	174/190 (92%)	173 (99%)	1 (1%)	78	81
7	t	174/190 (92%)	174 (100%)	0	100	100
7	u	174/190 (92%)	173 (99%)	1 (1%)	78	81
7	v	174/190 (92%)	174 (100%)	0	100	100
7	w	174/190 (92%)	173 (99%)	1 (1%)	78	81
7	x	174/190 (92%)	174 (100%)	0	100	100
8	k	127/164 (77%)	127 (100%)	0	100	100
8	l	127/164 (77%)	127 (100%)	0	100	100
All	All	24961/38153 (65%)	24946 (100%)	15 (0%)	87	89

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	c	37	GLN
7	u	37	GLN
7	e	25	GLN
7	w	106	GLN
7	m	65	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 336 such sidechains are listed below:

Mol	Chain	Res	Type
3	E3	245	GLN
4	V	1280	GLN
2	E4	216	ASN
2	E8	356	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	f	125	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 26 are monoatomic - leaving 52 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$
9	GTP	A2	501	-	33,34,34	0.89	1 (3%)	50,54,54	1.58	8 (16%)
9	GTP	B0	501	10	33,34,34	0.90	1 (3%)	50,54,54	1.59	10 (20%)
9	GTP	C3	501	10	33,34,34	0.91	2 (6%)	50,54,54	1.59	9 (18%)
9	GTP	D8	501	10	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
11	GDP	C9	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.73	6 (13%)
9	GTP	E8	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.62	10 (20%)
11	GDP	C3	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
11	GDP	A5	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.72	6 (13%)
9	GTP	D0	501	10	33,34,34	0.90	2 (6%)	50,54,54	1.59	9 (18%)
11	GDP	E5	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	GDP	D7	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
11	GDP	F1	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	6 (13%)
9	GTP	B4	501	-	33,34,34	0.88	0	50,54,54	1.59	8 (16%)
11	GDP	E1	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
11	GDP	B5	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
11	GDP	D9	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
11	GDP	D3	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	8 (17%)
11	GDP	E3	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.72	6 (13%)
11	GDP	E7	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.81	7 (15%)
11	GDP	A1	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
9	GTP	C4	501	10	33,34,34	0.90	1 (3%)	50,54,54	1.63	9 (18%)
11	GDP	D5	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.81	7 (15%)
9	GTP	D2	501	10	33,34,34	0.89	1 (3%)	50,54,54	1.63	9 (18%)
9	GTP	E2	501	10	33,34,34	0.92	2 (6%)	50,54,54	1.68	9 (18%)
9	GTP	E4	501	10	33,34,34	0.92	1 (3%)	50,54,54	1.63	10 (20%)
11	GDP	D1	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
11	GDP	C5	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
9	GTP	B8	501	10	33,34,34	0.92	1 (3%)	50,54,54	1.64	8 (16%)
11	GDP	B3	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
9	GTP	D4	501	10	33,34,34	0.90	1 (3%)	50,54,54	1.52	10 (20%)
9	GTP	F0	501	10	33,34,34	0.90	1 (3%)	50,54,54	1.68	11 (22%)
11	GDP	A9	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	8 (17%)
9	GTP	A0	501	10	33,34,34	0.89	1 (3%)	50,54,54	1.62	9 (18%)
9	GTP	D6	501	10	33,34,34	0.95	0	50,54,54	1.57	8 (16%)
9	GTP	A4	501	10	33,34,34	0.88	0	50,54,54	1.59	8 (16%)
9	GTP	C6	501	10	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
9	GTP	C0	501	10	33,34,34	0.90	1 (3%)	50,54,54	1.55	9 (18%)
11	GDP	C1	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.74	7 (15%)
9	GTP	B6	501	10	33,34,34	0.88	1 (3%)	50,54,54	1.55	8 (16%)
9	GTP	E6	501	10	33,34,34	0.98	2 (6%)	50,54,54	1.64	11 (22%)
11	GDP	C7	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.73	7 (15%)
11	GDP	A7	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
9	GTP	B2	501	-	33,34,34	0.88	0	50,54,54	1.60	8 (16%)
11	GDP	E9	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
9	GTP	A6	501	10	33,34,34	0.94	1 (3%)	50,54,54	1.64	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	GDP	B9	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.83	7 (15%)
11	GDP	B1	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.88	7 (15%)
9	GTP	C8	501	10	33,34,34	0.91	1 (3%)	50,54,54	1.60	8 (16%)
11	GDP	B7	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	6 (13%)
9	GTP	A8	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.62	11 (22%)
11	GDP	A3	501	-	29,30,30	1.24	4 (13%)	45,47,47	1.81	9 (20%)
9	GTP	E0	501	10	33,34,34	0.93	1 (3%)	50,54,54	1.64	11 (22%)

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
9	GTP	A2	501	-	-	6/22/38/38	0/3/3/3
9	GTP	B0	501	10	-	7/22/38/38	0/3/3/3
9	GTP	C3	501	10	-	7/22/38/38	0/3/3/3
9	GTP	D8	501	10	-	4/22/38/38	0/3/3/3
11	GDP	C9	501	-	-	3/16/32/32	0/3/3/3
9	GTP	E8	501	-	-	6/22/38/38	0/3/3/3
11	GDP	C3	502	-	-	3/16/32/32	0/3/3/3
11	GDP	A5	502	-	-	1/16/32/32	0/3/3/3
9	GTP	D0	501	10	-	6/22/38/38	0/3/3/3
11	GDP	E5	501	-	-	4/16/32/32	0/3/3/3
11	GDP	D7	501	-	-	4/16/32/32	0/3/3/3
11	GDP	F1	501	-	-	2/16/32/32	0/3/3/3
9	GTP	B4	501	-	-	5/22/38/38	0/3/3/3
11	GDP	E1	502	-	-	2/16/32/32	0/3/3/3
11	GDP	B5	501	-	-	2/16/32/32	0/3/3/3
11	GDP	D9	501	-	-	6/16/32/32	0/3/3/3
11	GDP	D3	501	-	-	5/16/32/32	0/3/3/3
11	GDP	E3	501	-	-	0/16/32/32	0/3/3/3
11	GDP	E7	501	-	-	8/16/32/32	0/3/3/3
11	GDP	A1	501	-	-	2/16/32/32	0/3/3/3
9	GTP	C4	501	10	-	7/22/38/38	0/3/3/3
11	GDP	D5	501	-	-	3/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GTP	D2	501	10	-	1/22/38/38	0/3/3/3
9	GTP	E2	501	10	-	7/22/38/38	0/3/3/3
9	GTP	E4	501	10	-	8/22/38/38	0/3/3/3
11	GDP	D1	501	-	-	3/16/32/32	0/3/3/3
11	GDP	C5	501	-	-	4/16/32/32	0/3/3/3
9	GTP	B8	501	10	-	9/22/38/38	0/3/3/3
11	GDP	B3	501	-	-	3/16/32/32	0/3/3/3
9	GTP	D4	501	10	-	7/22/38/38	0/3/3/3
9	GTP	F0	501	10	-	10/22/38/38	0/3/3/3
11	GDP	A9	501	-	-	5/16/32/32	0/3/3/3
9	GTP	A0	501	10	-	9/22/38/38	0/3/3/3
9	GTP	D6	501	10	-	4/22/38/38	0/3/3/3
9	GTP	A4	501	10	-	6/22/38/38	0/3/3/3
9	GTP	C6	501	10	-	3/22/38/38	0/3/3/3
9	GTP	C0	501	10	-	2/22/38/38	0/3/3/3
11	GDP	C1	501	-	-	4/16/32/32	0/3/3/3
9	GTP	B6	501	10	-	6/22/38/38	0/3/3/3
9	GTP	E6	501	10	-	6/22/38/38	0/3/3/3
11	GDP	C7	501	-	-	4/16/32/32	0/3/3/3
11	GDP	A7	502	-	-	3/16/32/32	0/3/3/3
9	GTP	B2	501	-	-	8/22/38/38	0/3/3/3
11	GDP	E9	502	-	-	4/16/32/32	0/3/3/3
9	GTP	A6	501	10	-	5/22/38/38	0/3/3/3
11	GDP	B9	501	-	-	3/16/32/32	0/3/3/3
11	GDP	B1	501	-	-	3/16/32/32	0/3/3/3
9	GTP	C8	501	10	-	6/22/38/38	0/3/3/3
11	GDP	B7	501	-	-	2/16/32/32	0/3/3/3
9	GTP	A8	501	-	-	5/22/38/38	0/3/3/3
11	GDP	A3	501	-	-	11/16/32/32	0/3/3/3
9	GTP	E0	501	10	-	9/22/38/38	0/3/3/3

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A3	501	GDP	C5-C4	3.14	1.47	1.38
11	C5	501	GDP	C5-C4	3.10	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E7	501	GDP	C5-C4	3.08	1.47	1.38
11	C1	501	GDP	C5-C4	3.05	1.47	1.38
11	F1	501	GDP	C5-C4	3.04	1.47	1.38

The worst 5 of 416 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B1	501	GDP	C5-C4-N3	-6.45	118.12	128.39
11	E7	501	GDP	C5-C4-N3	-6.43	118.15	128.39
11	B9	501	GDP	C5-C4-N3	-6.42	118.17	128.39
11	D5	501	GDP	C5-C4-N3	-6.32	118.32	128.39
11	C5	501	GDP	C5-C4-N3	-6.25	118.44	128.39

There are no chirality outliers.

5 of 253 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A0	501	GTP	C5'-O5'-PA-O3A
9	A0	501	GTP	C5'-O5'-PA-O1A
9	A0	501	GTP	C5'-O5'-PA-O2A
9	A2	501	GTP	C5'-O5'-PA-O3A
9	A2	501	GTP	C5'-O5'-PA-O1A

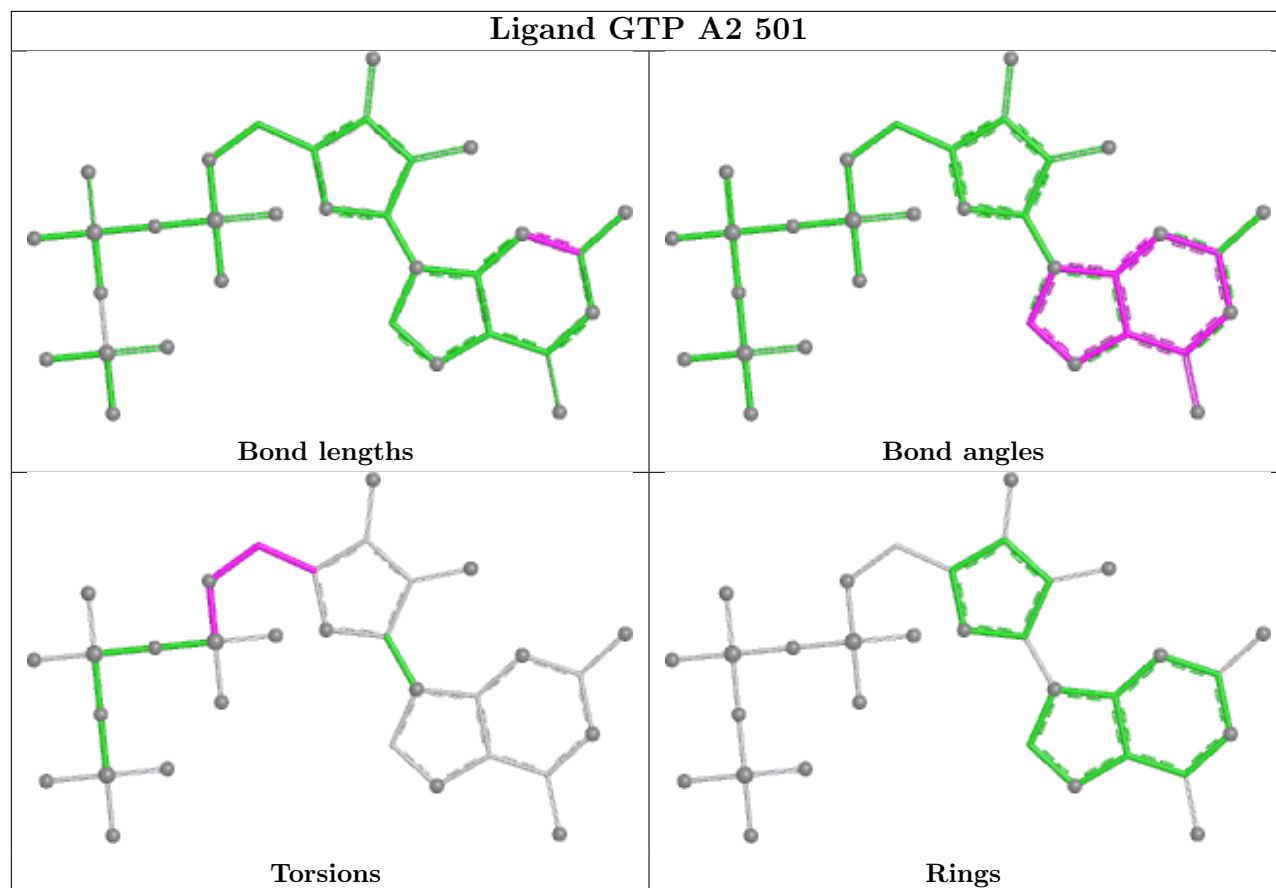
There are no ring outliers.

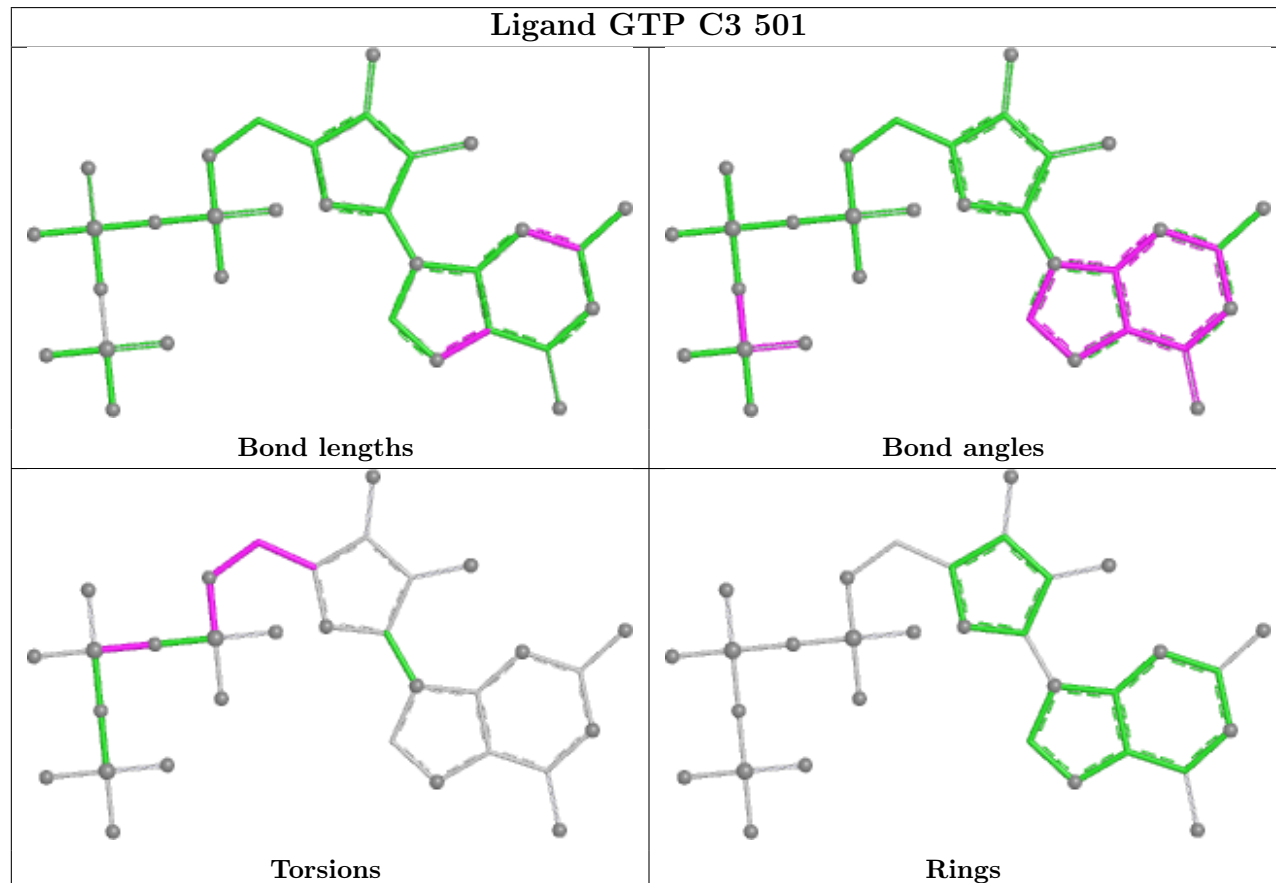
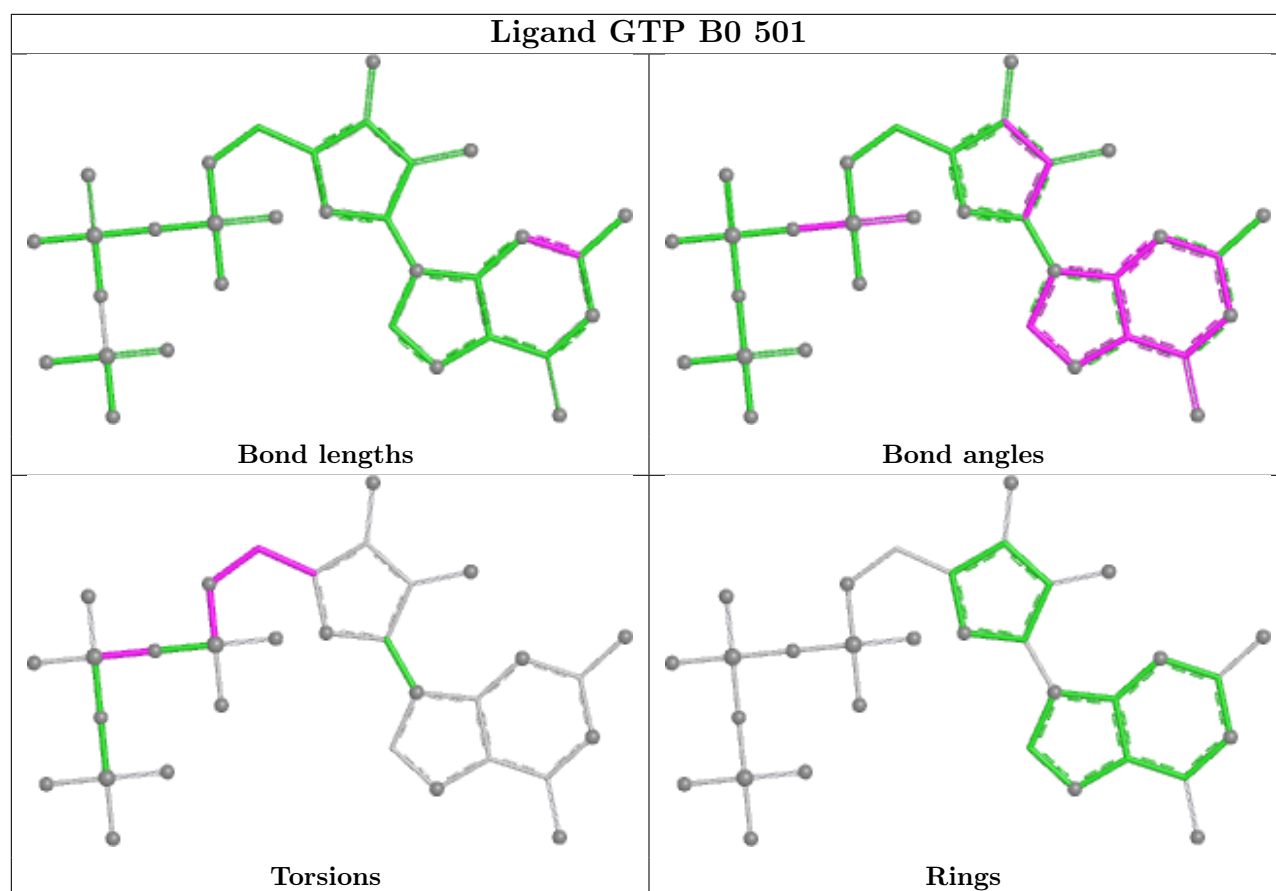
5 monomers are involved in 6 short contacts:

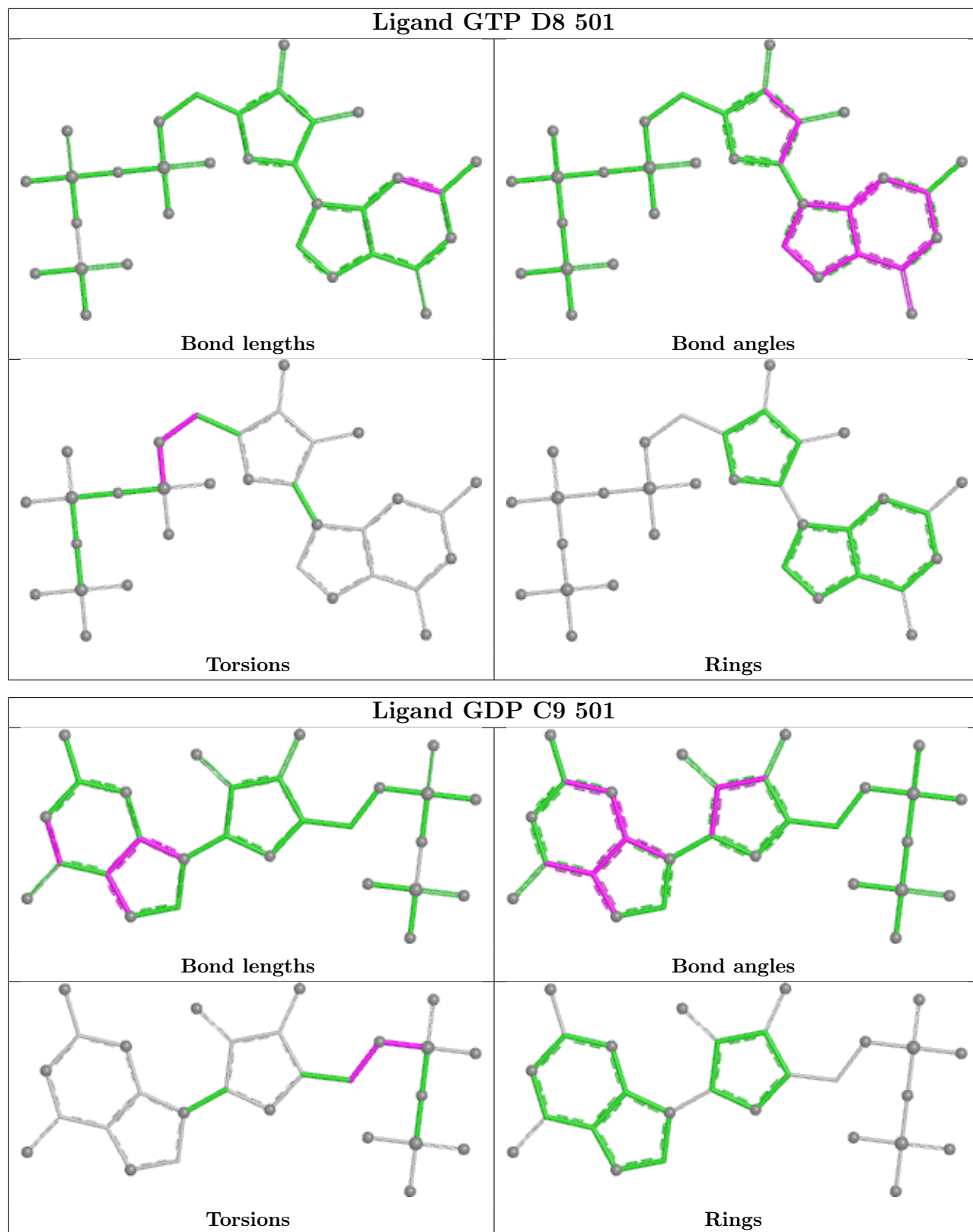
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E5	501	GDP	2	0
11	E7	501	GDP	1	0
11	A1	501	GDP	1	0
9	E4	501	GTP	1	0
11	B3	501	GDP	1	0

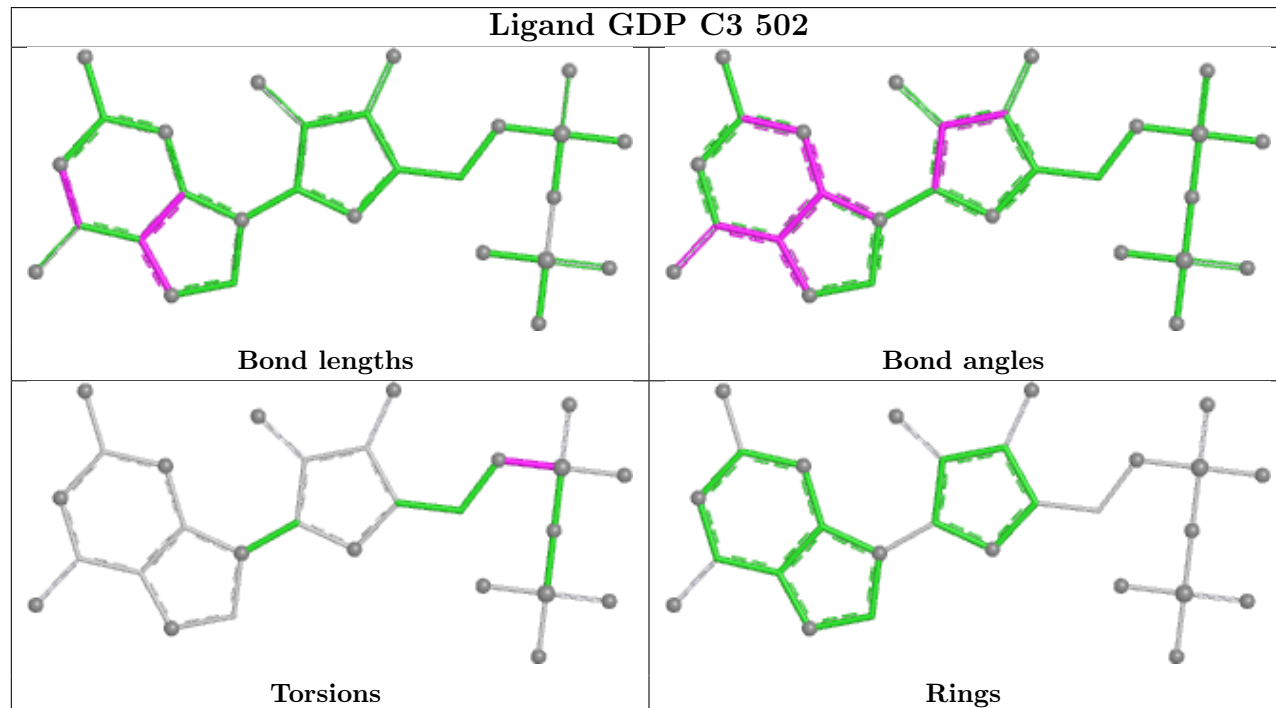
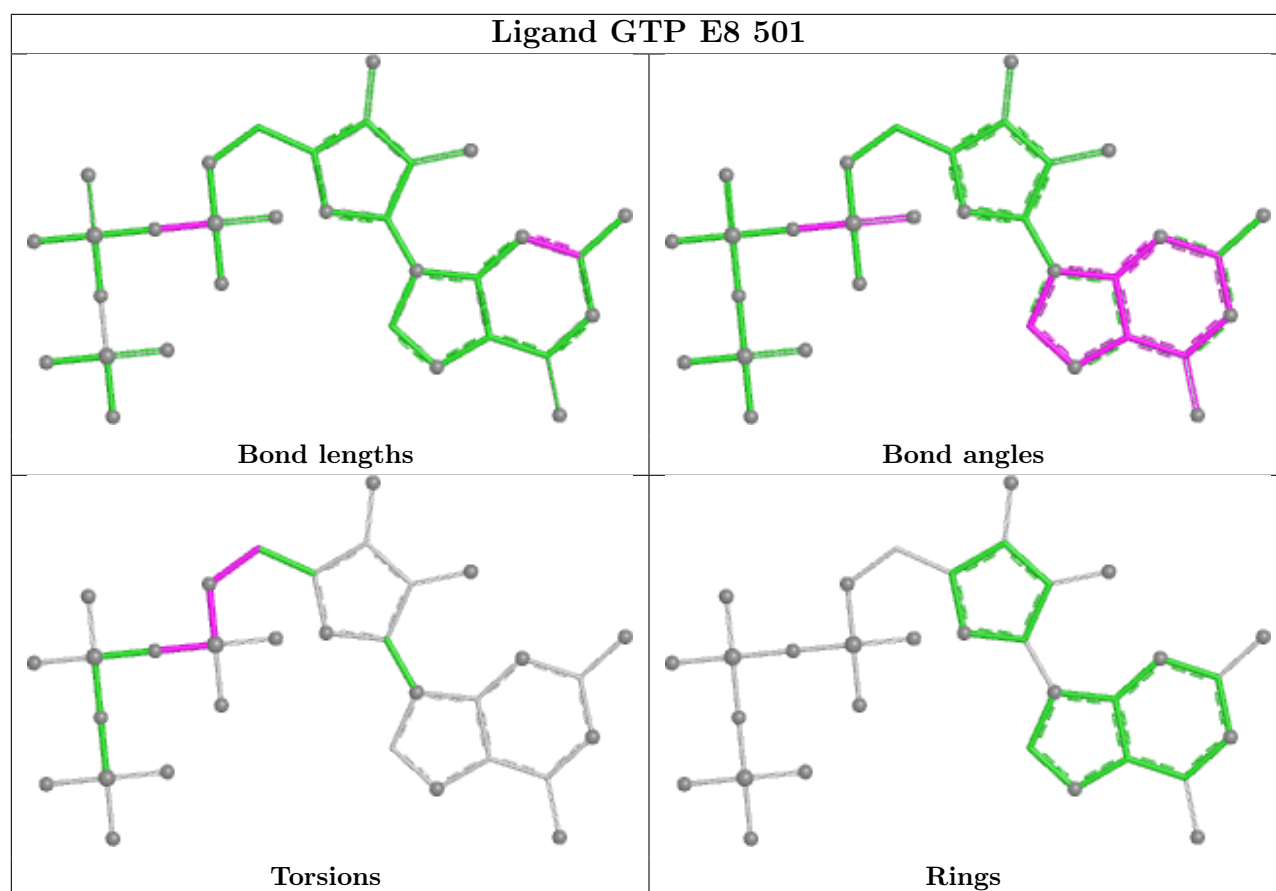
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

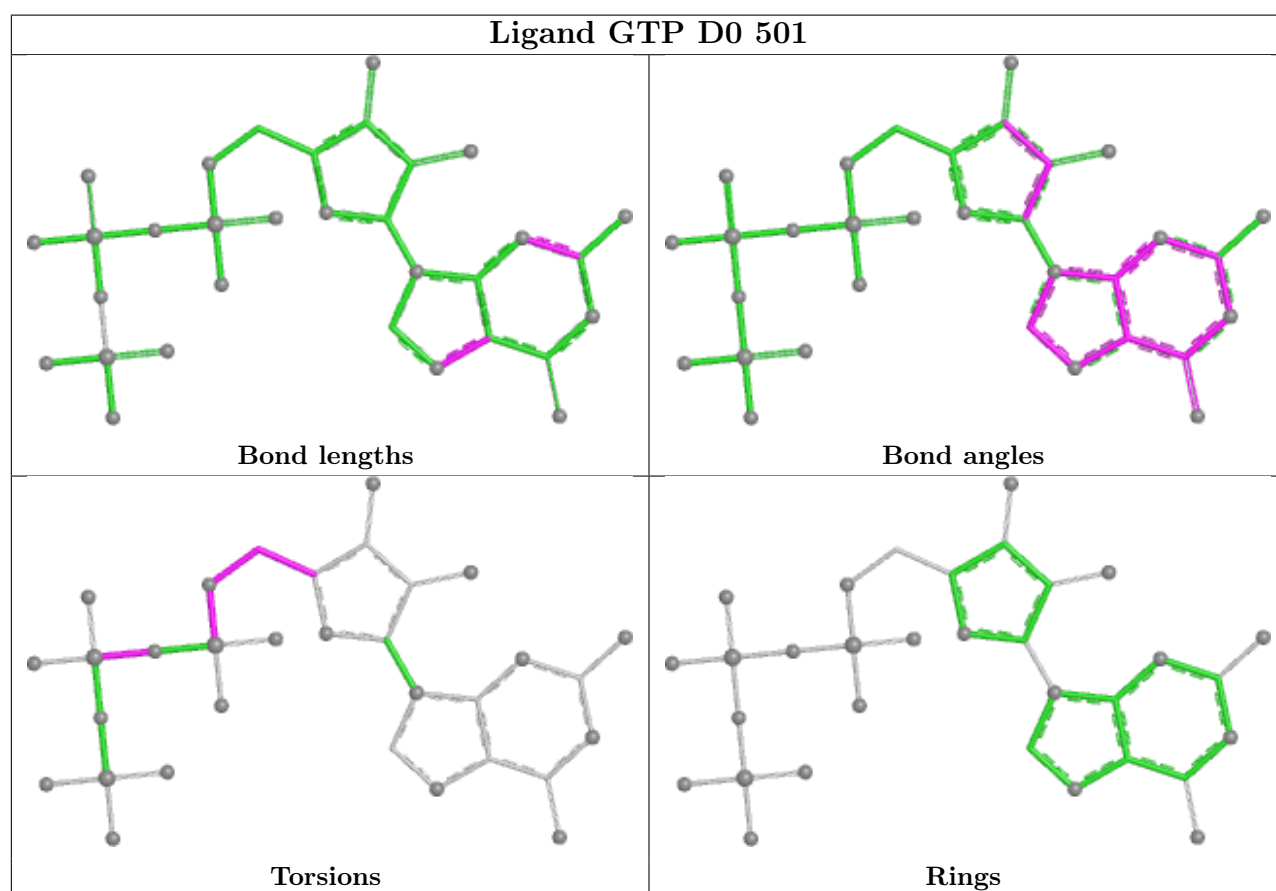
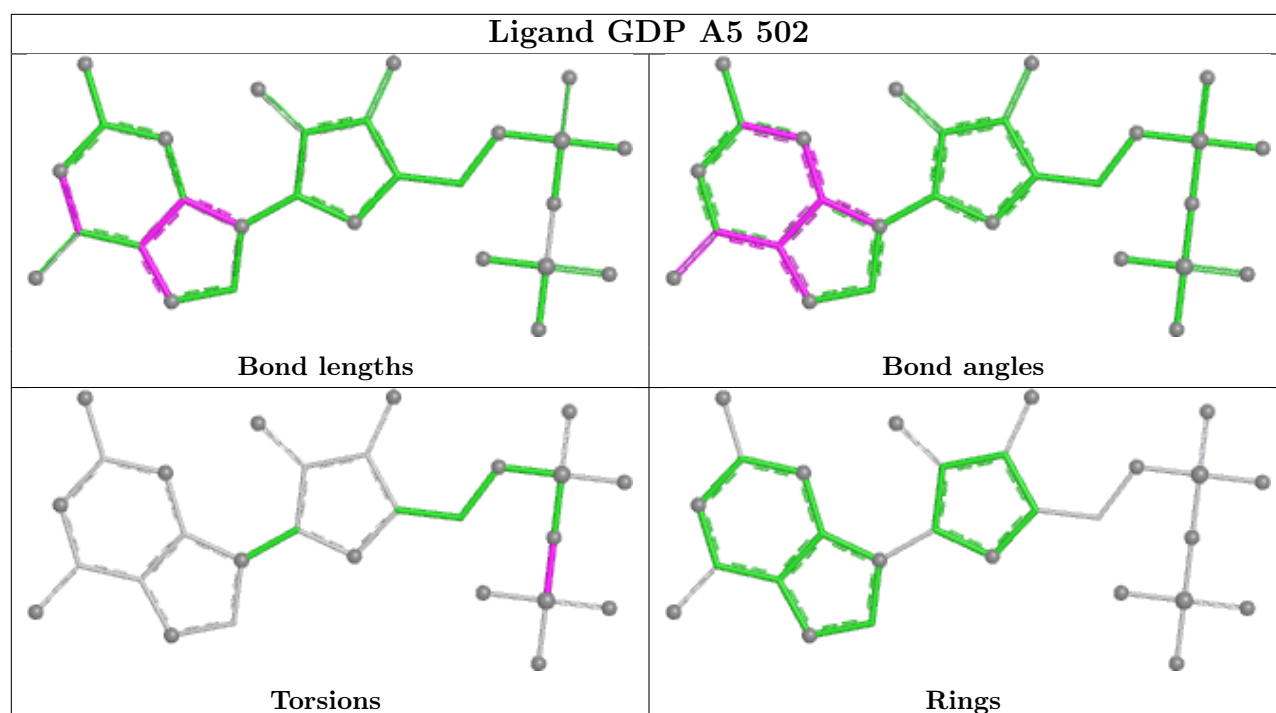
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

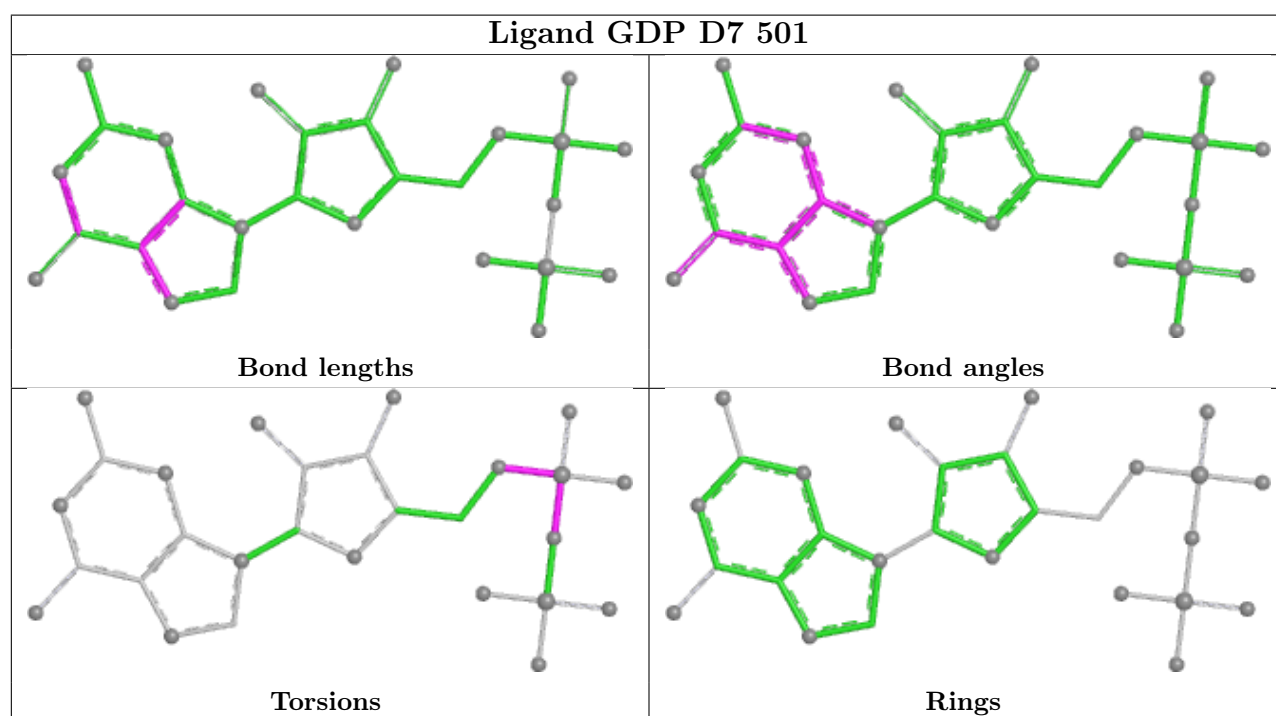
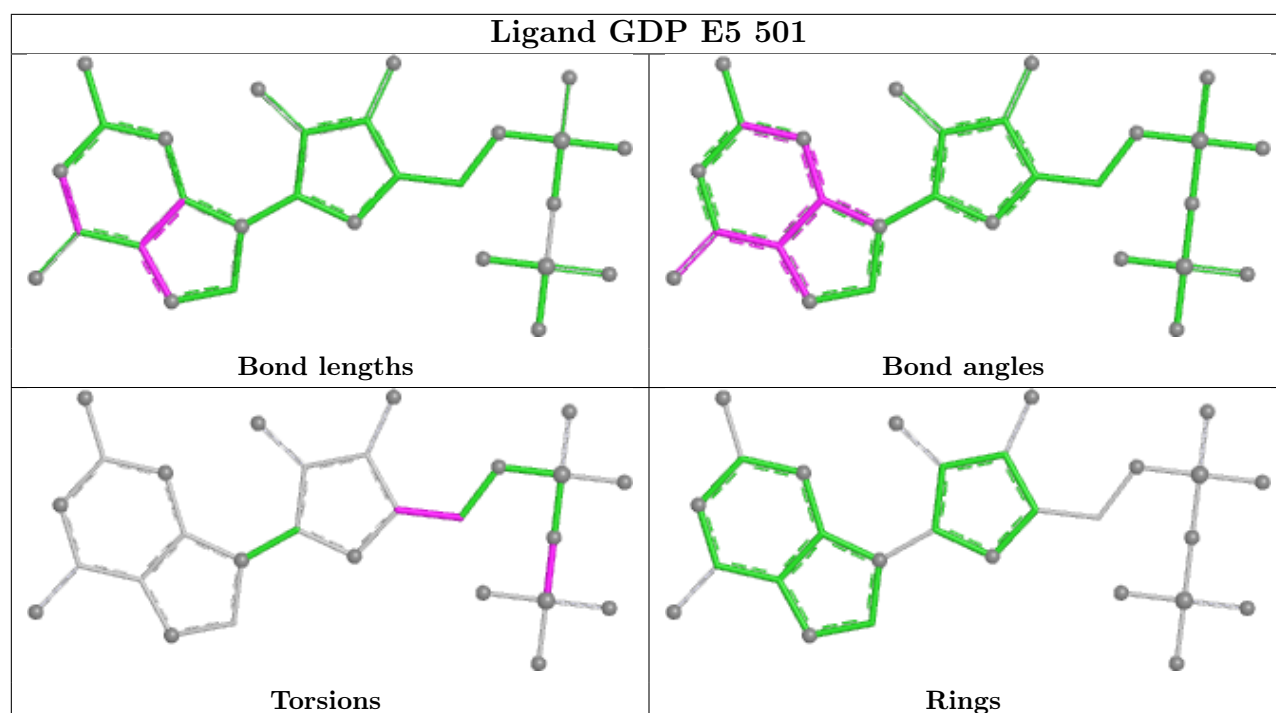


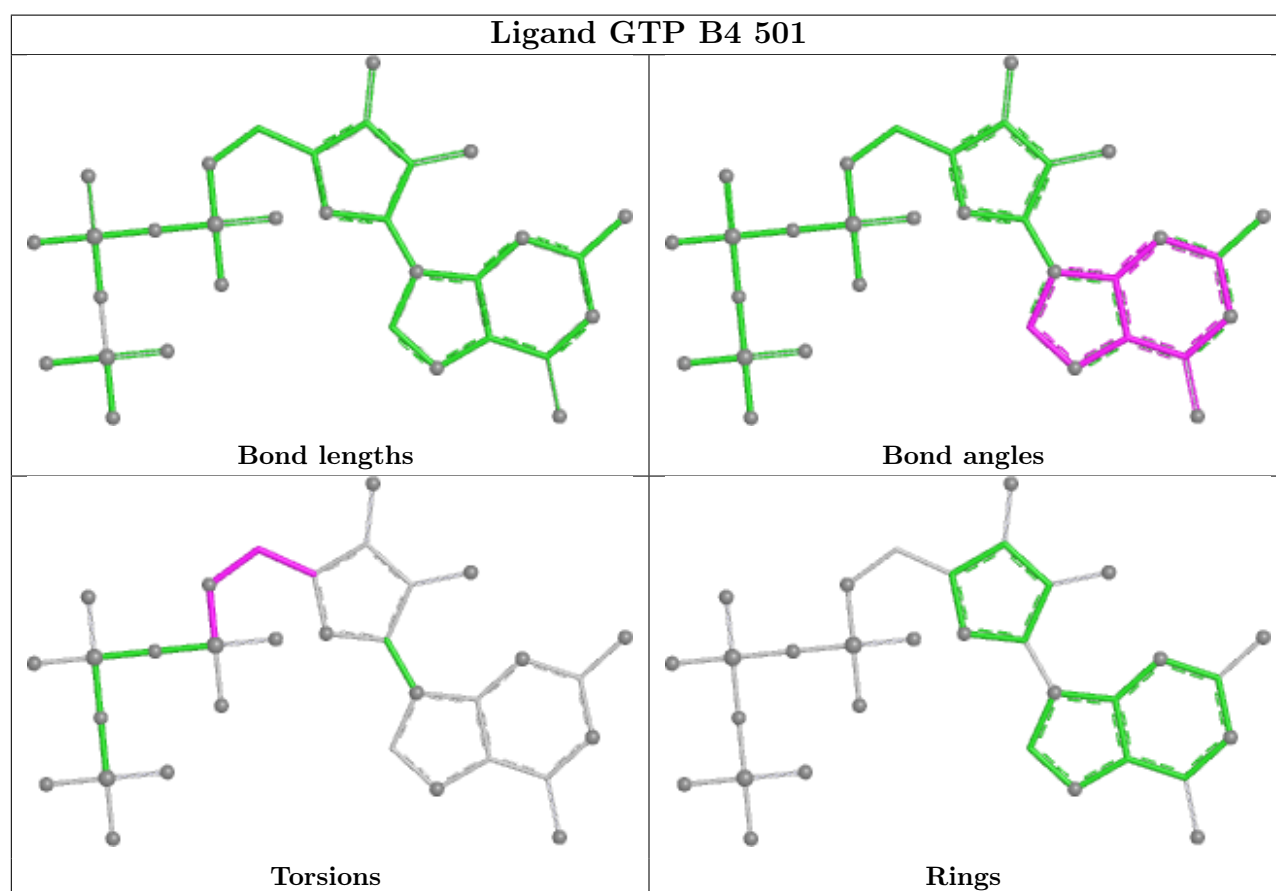
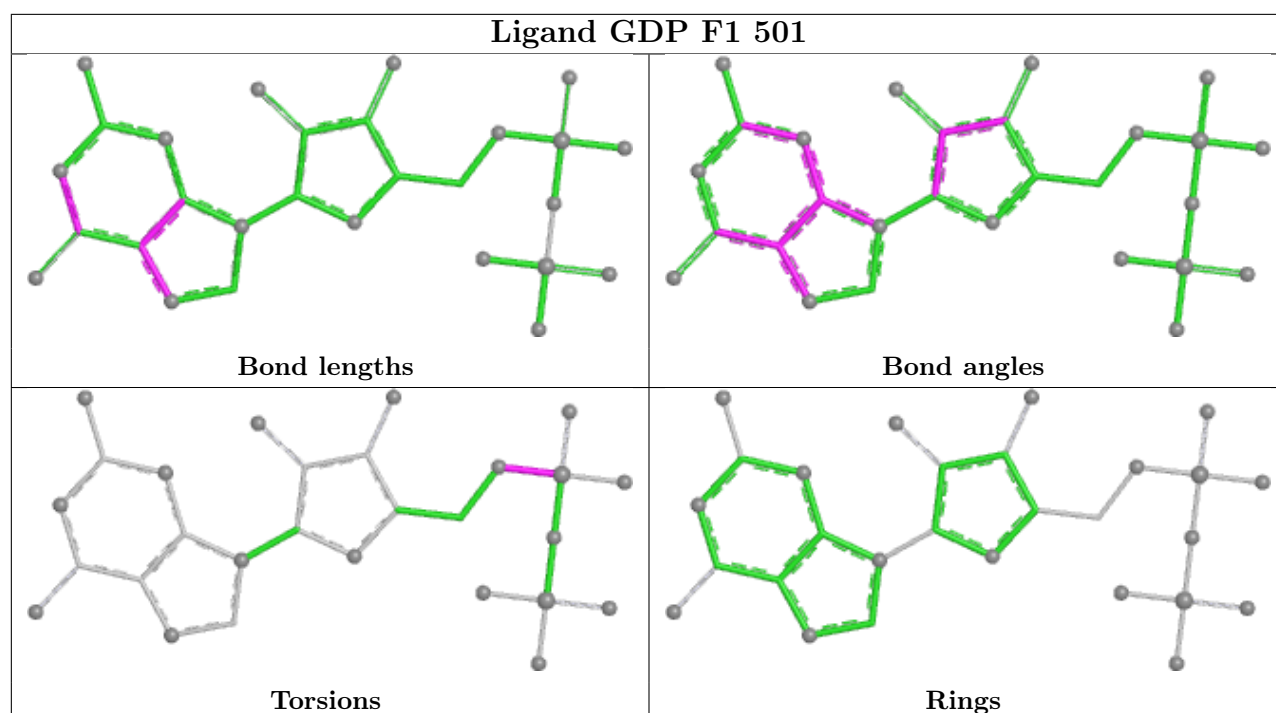


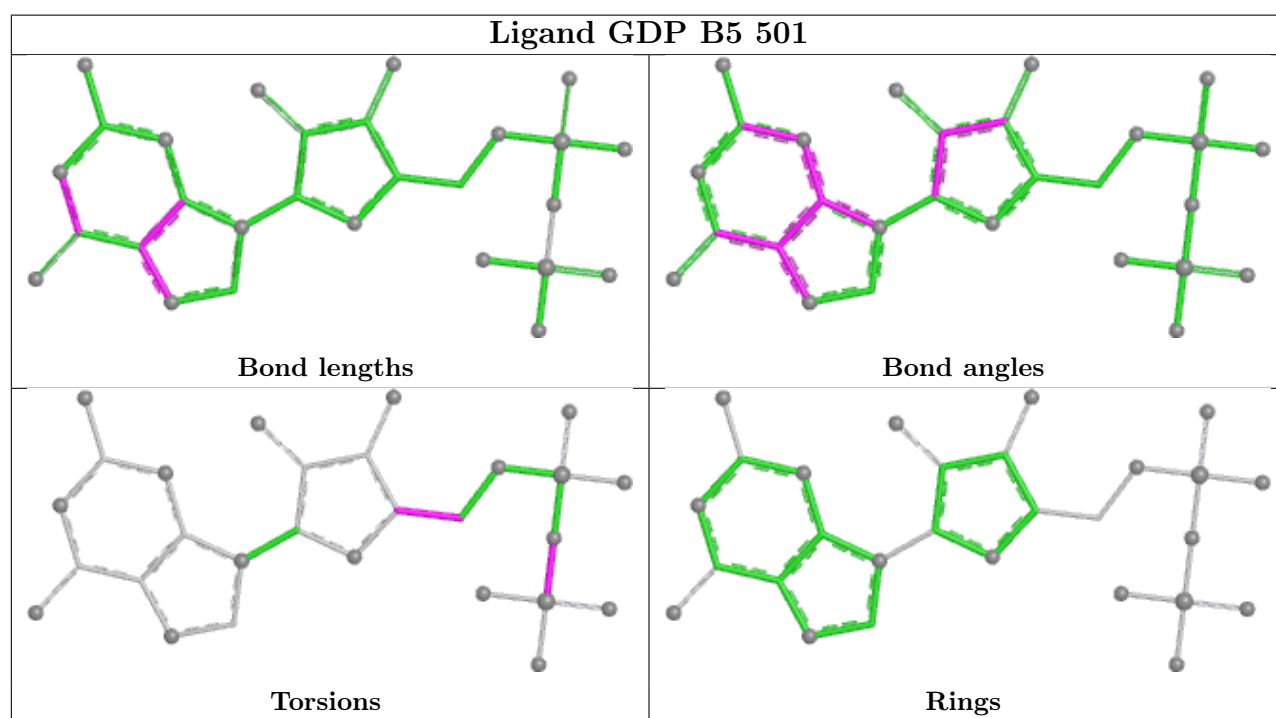
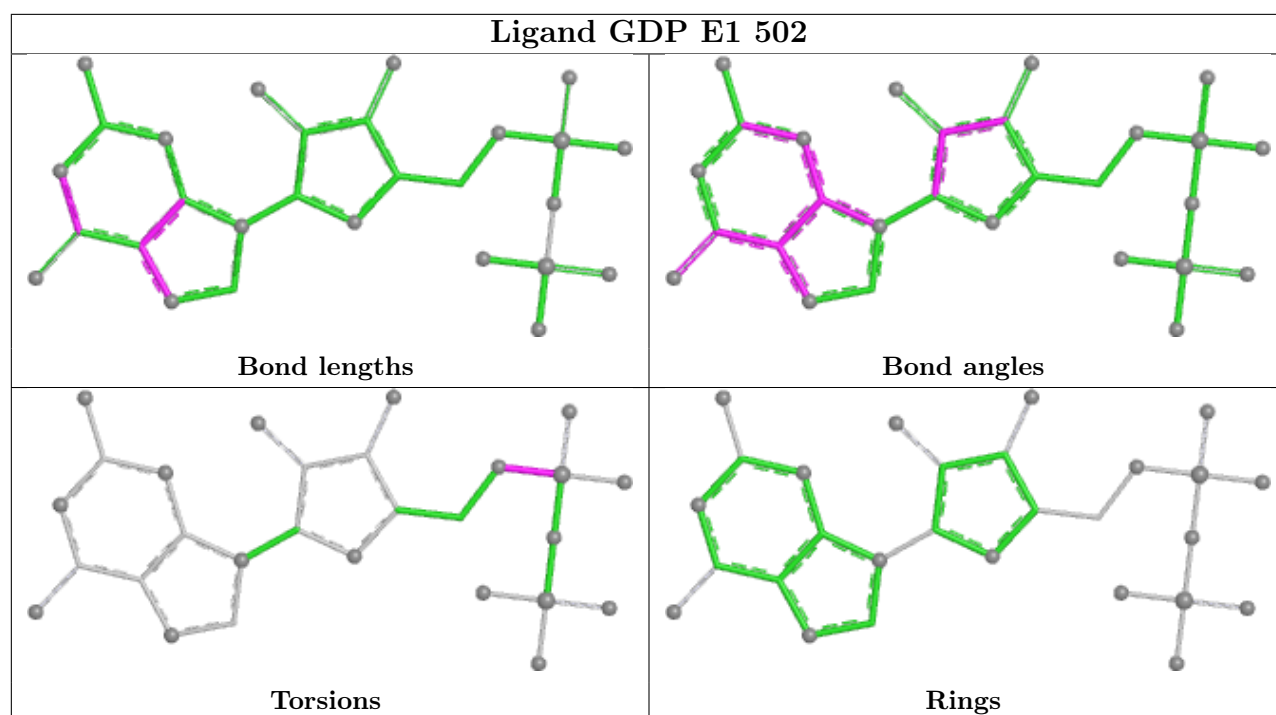


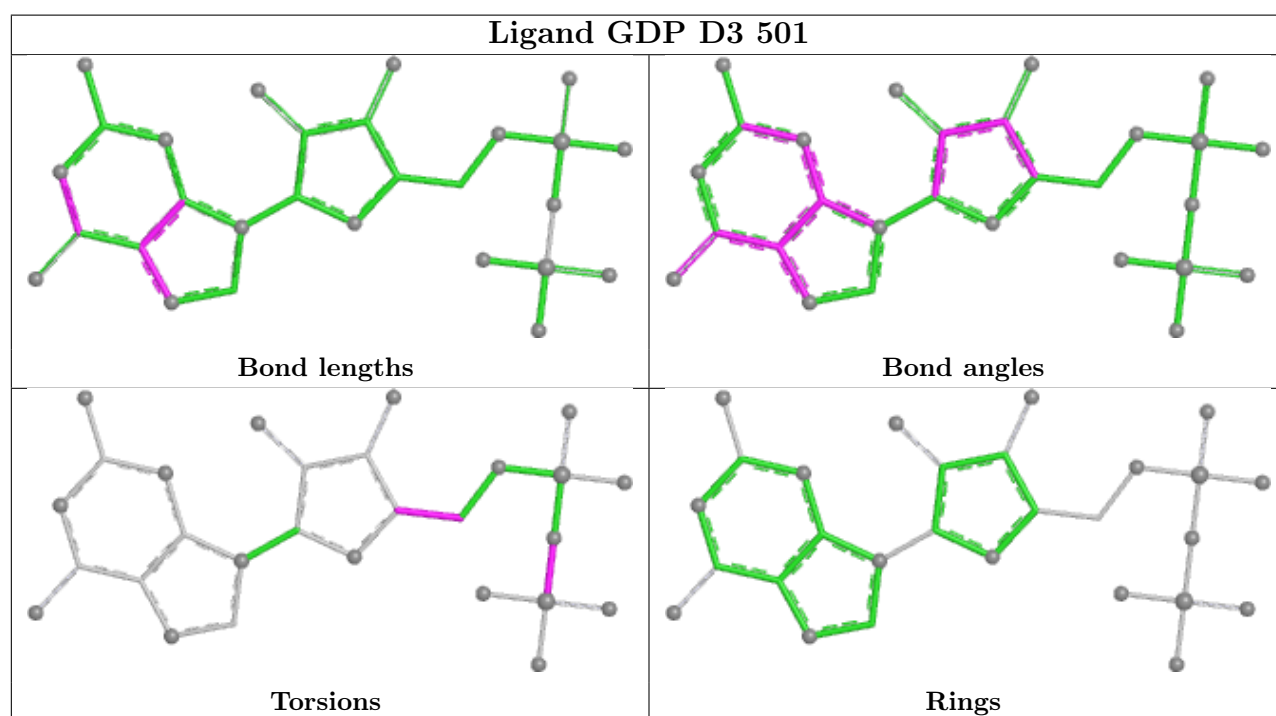
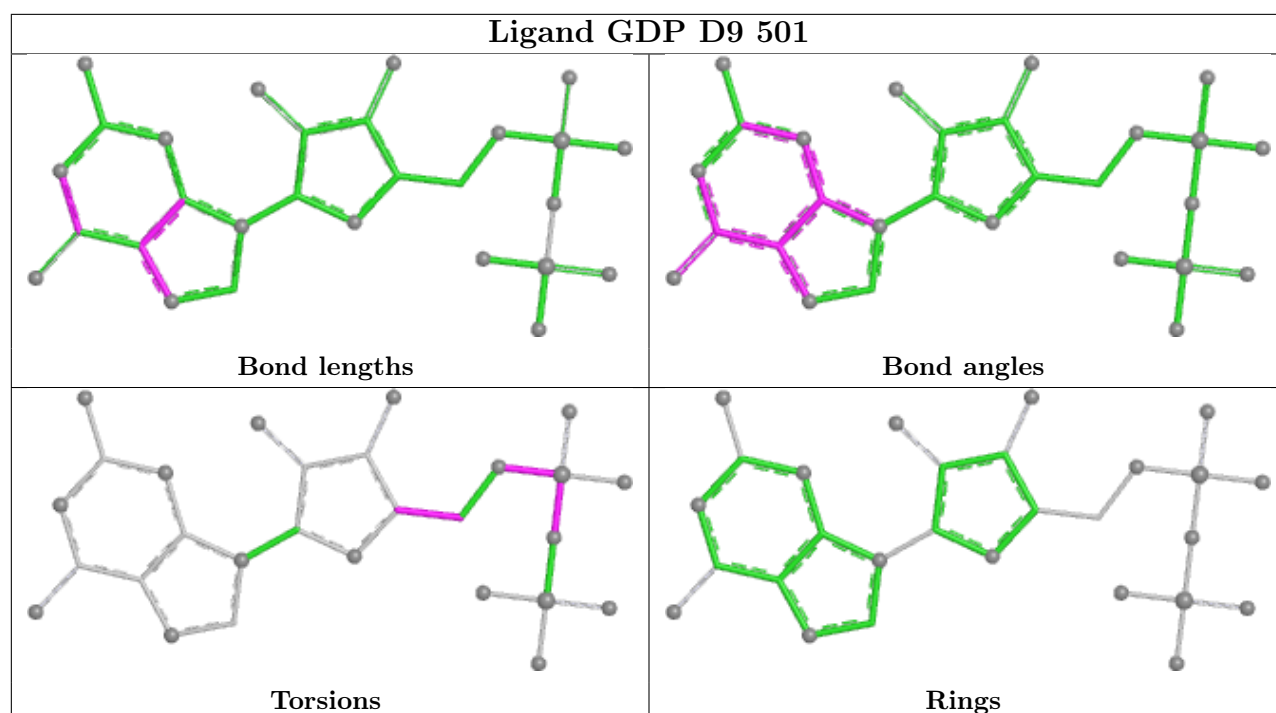


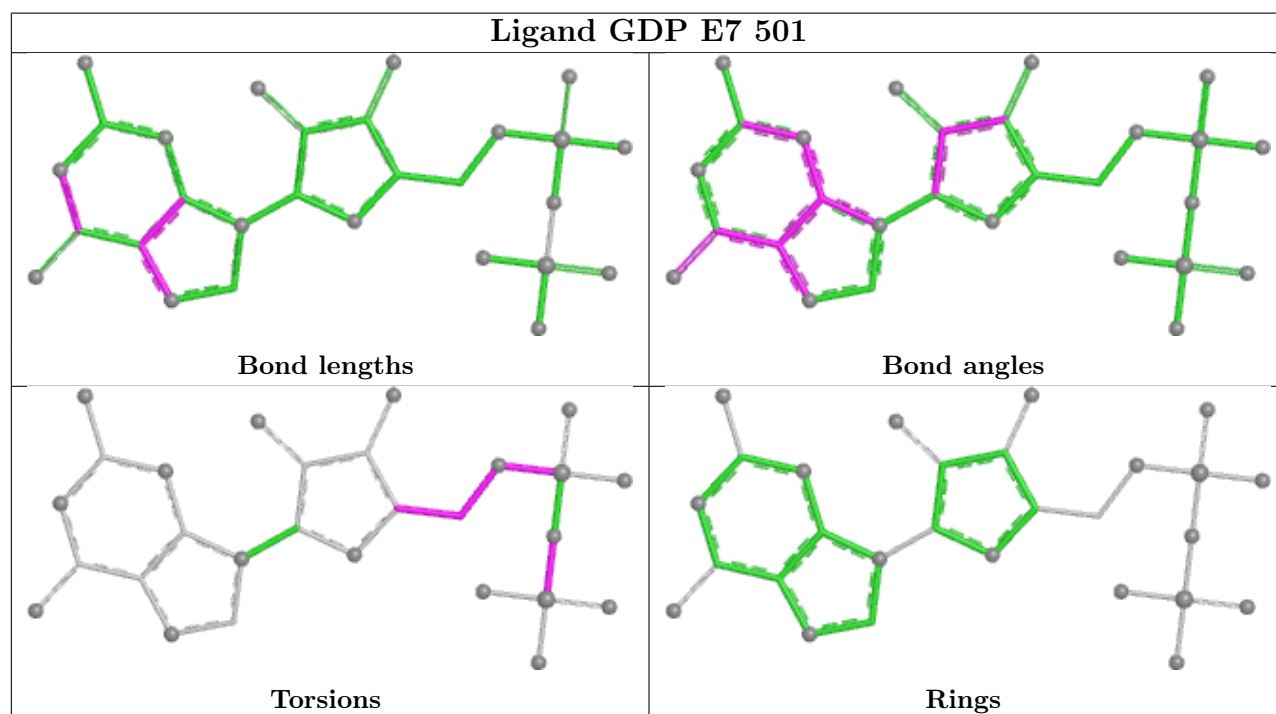
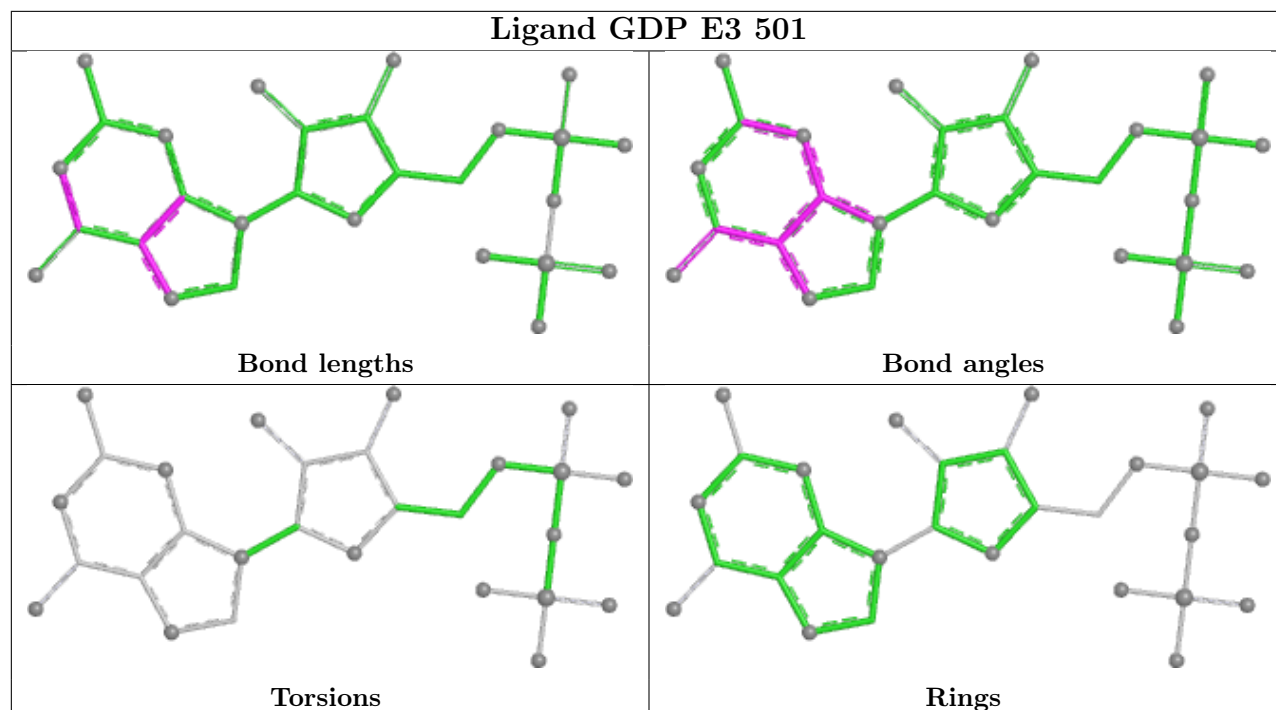


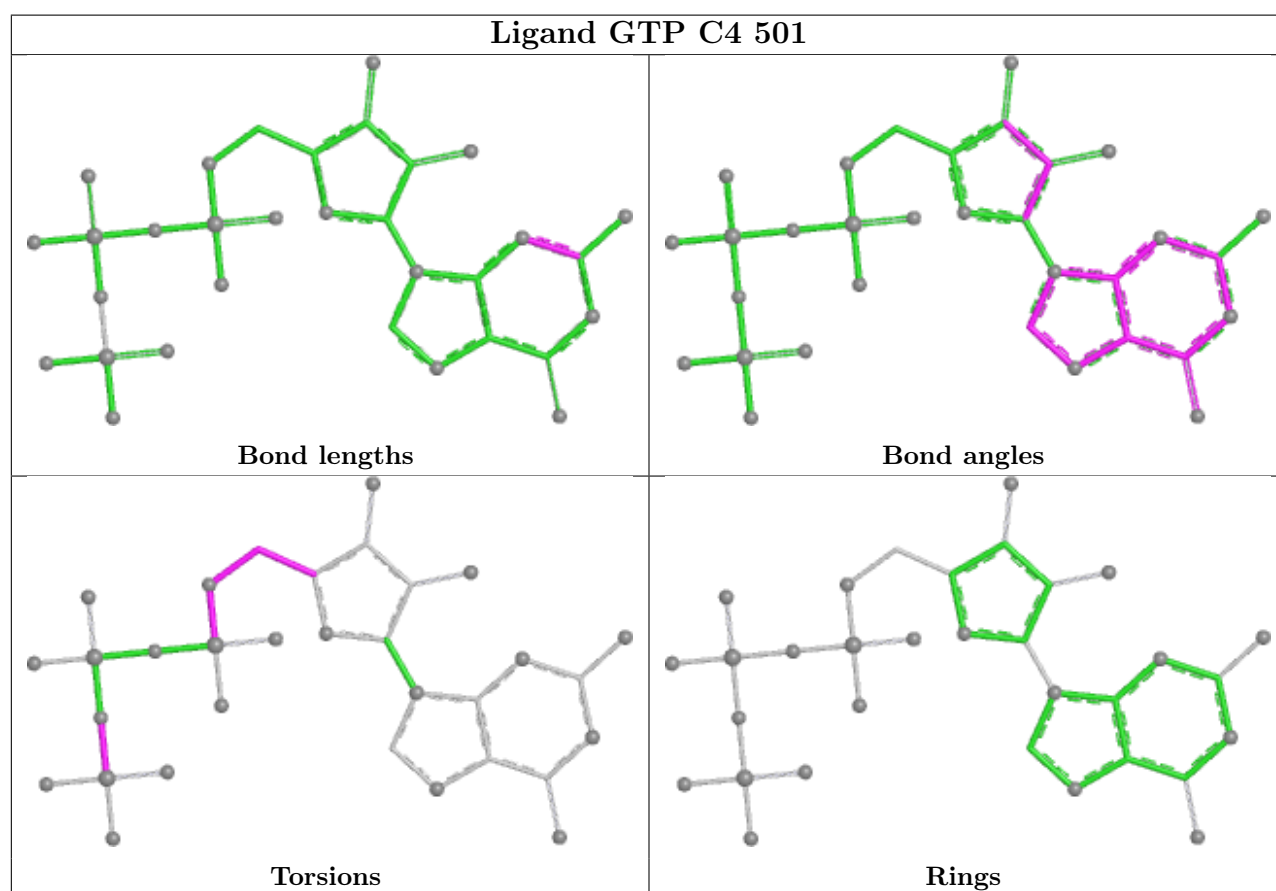
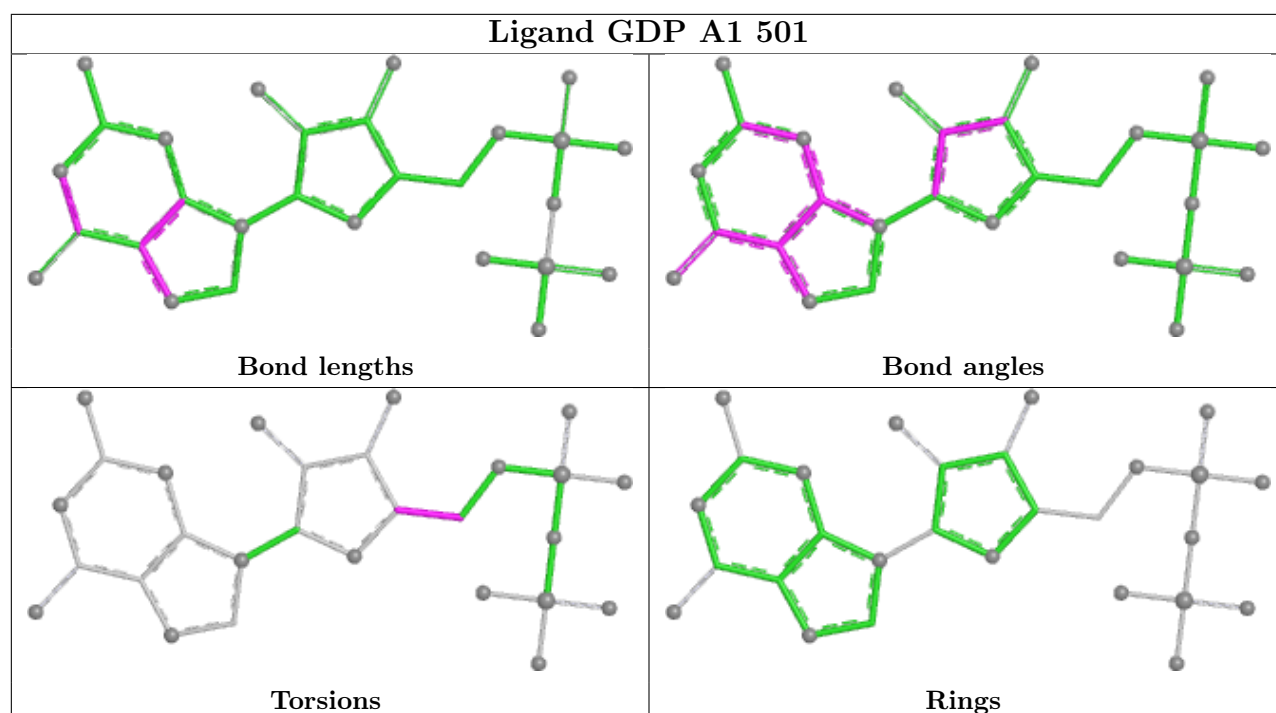


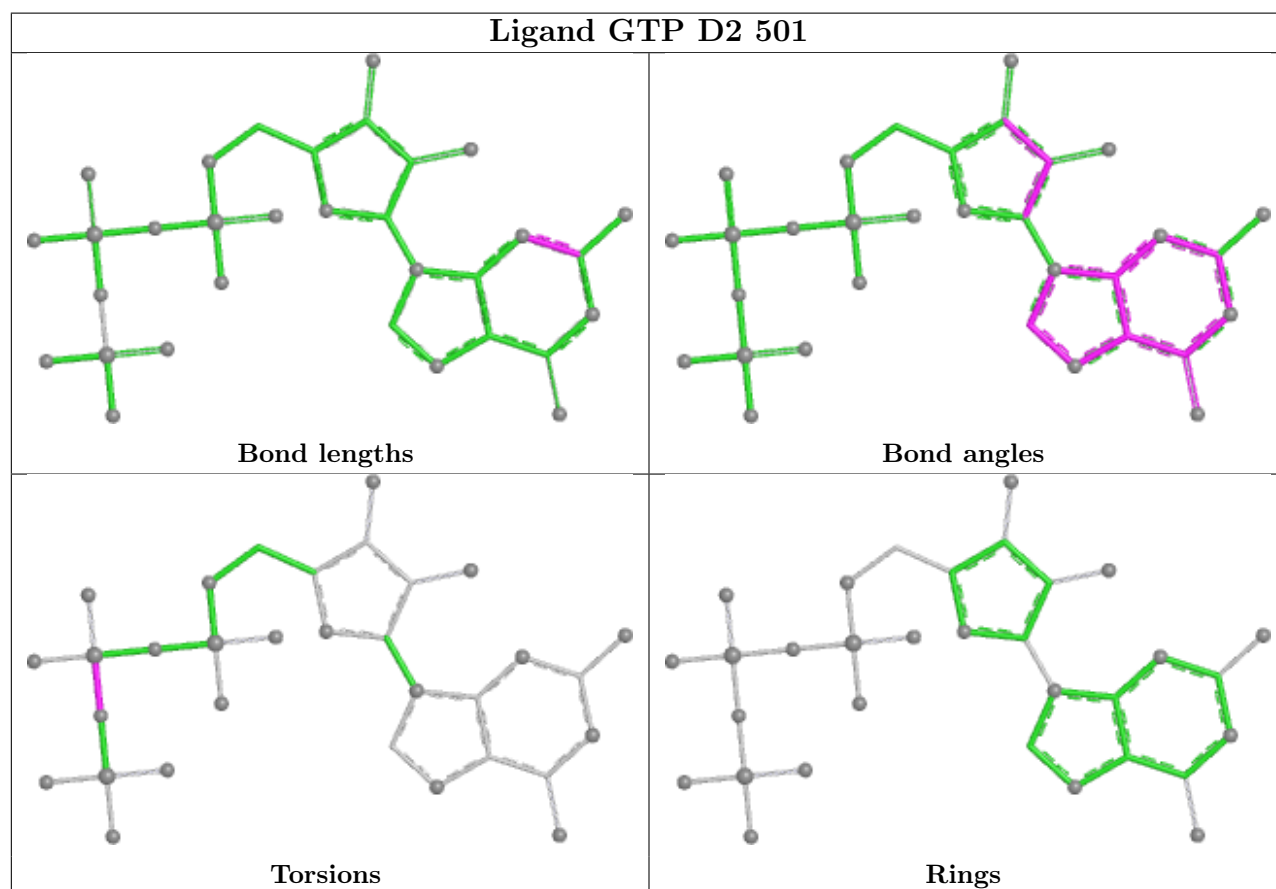
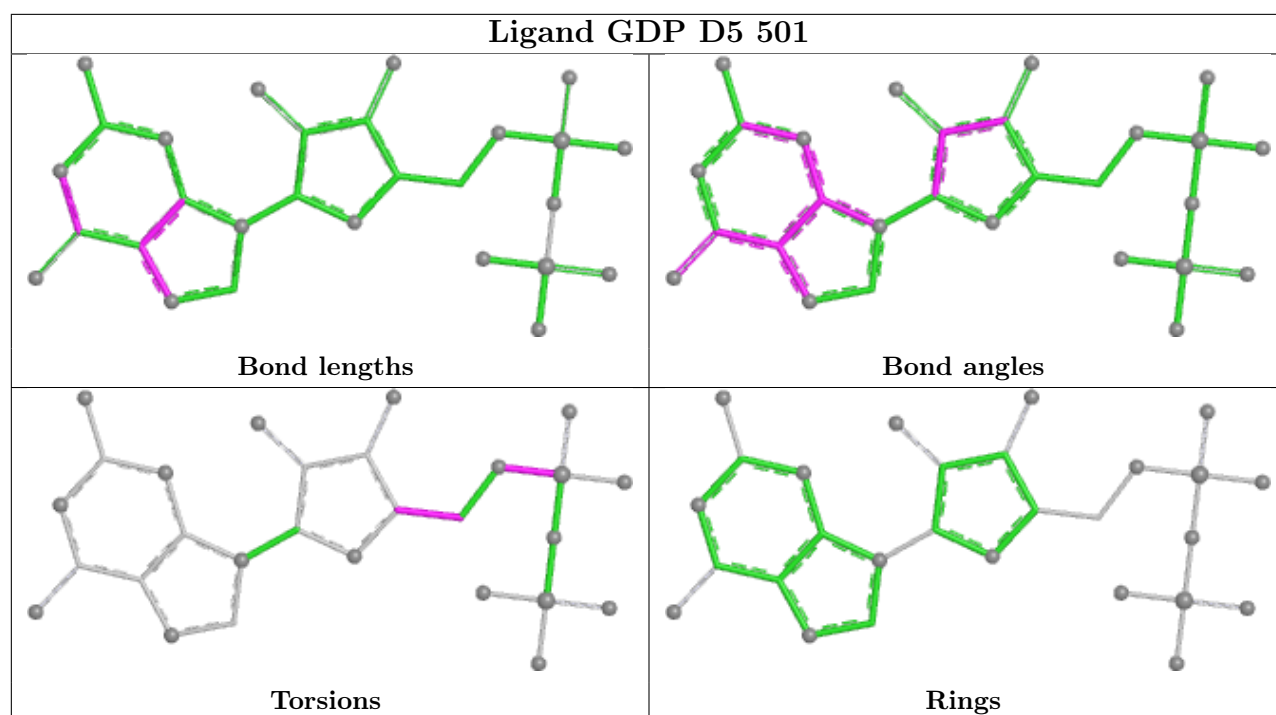


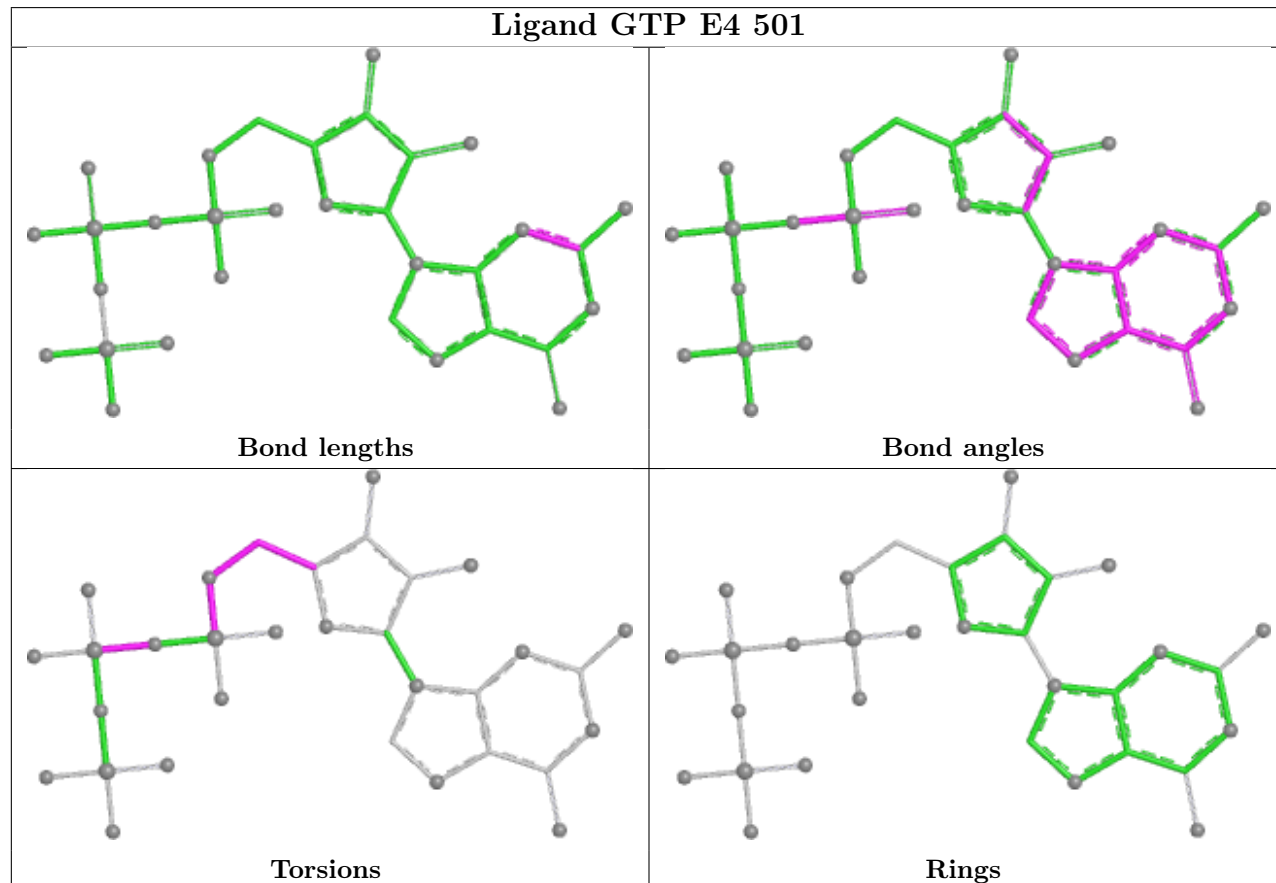
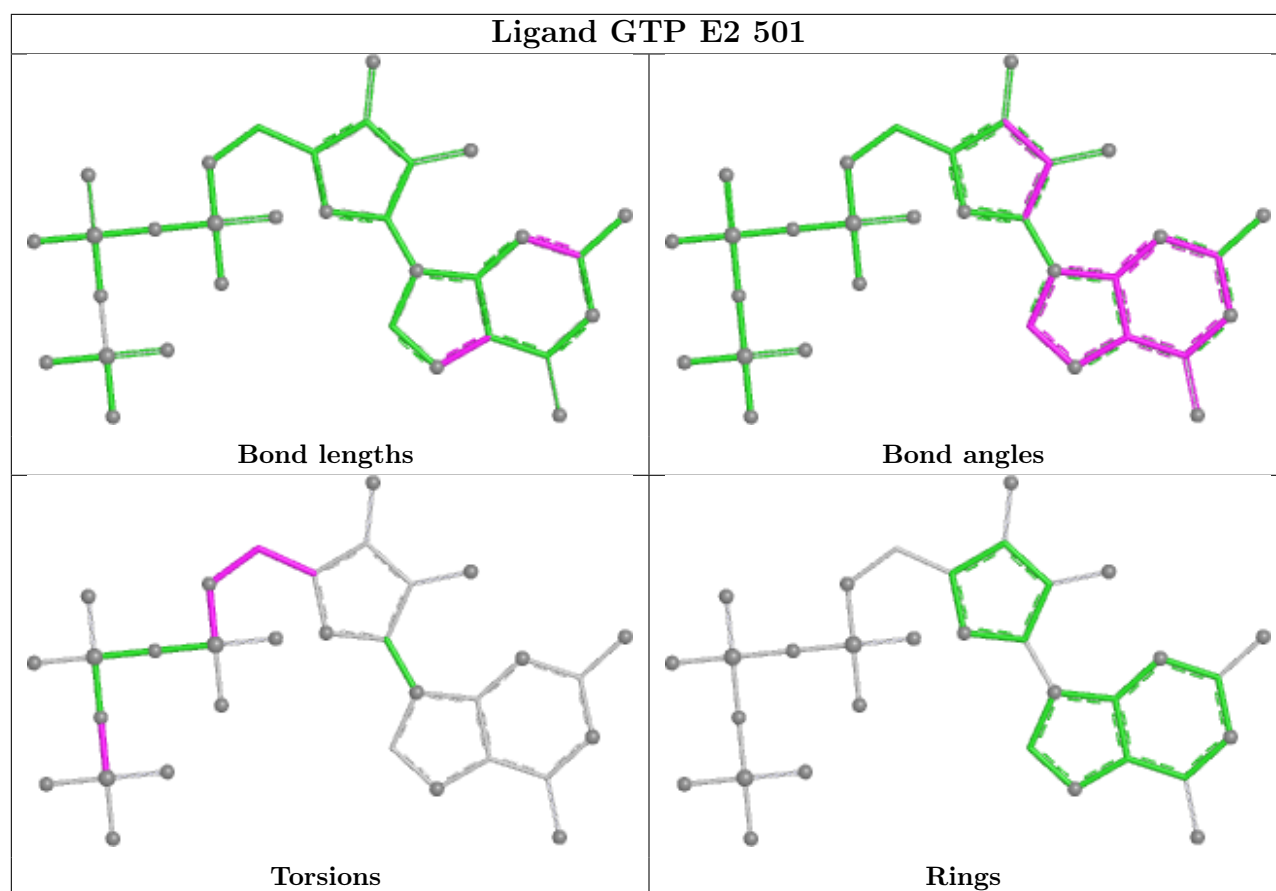


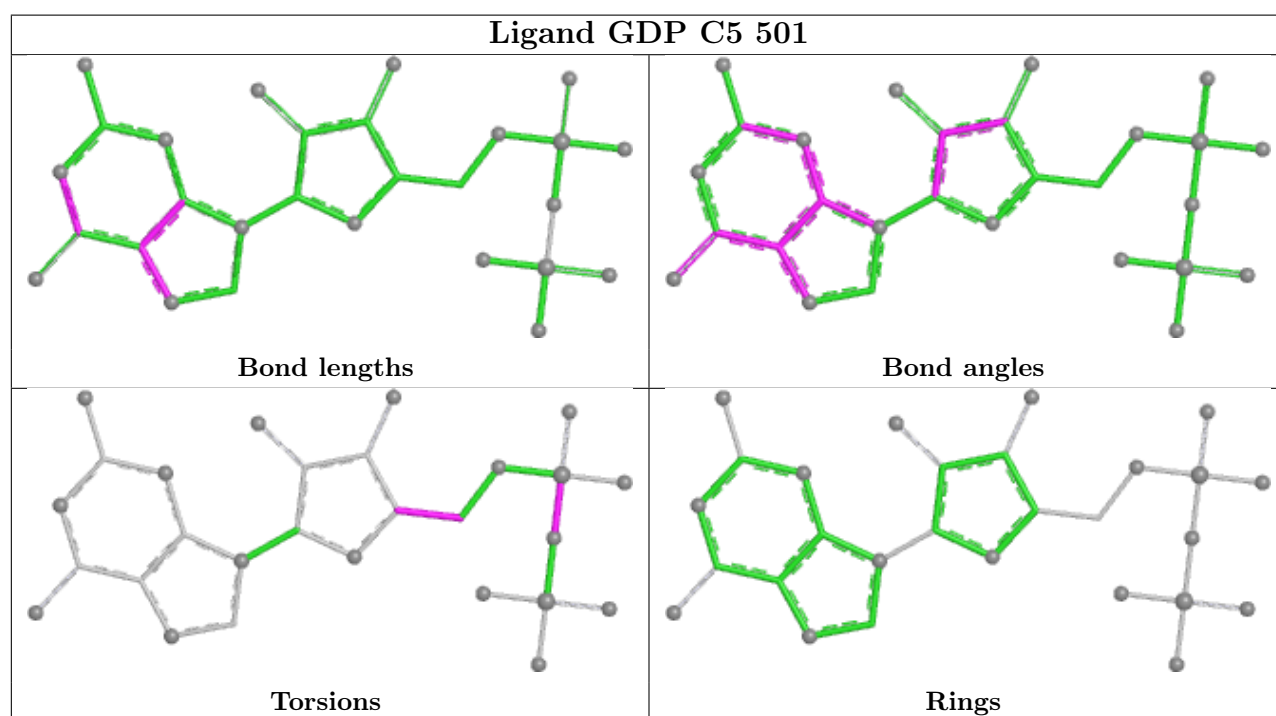
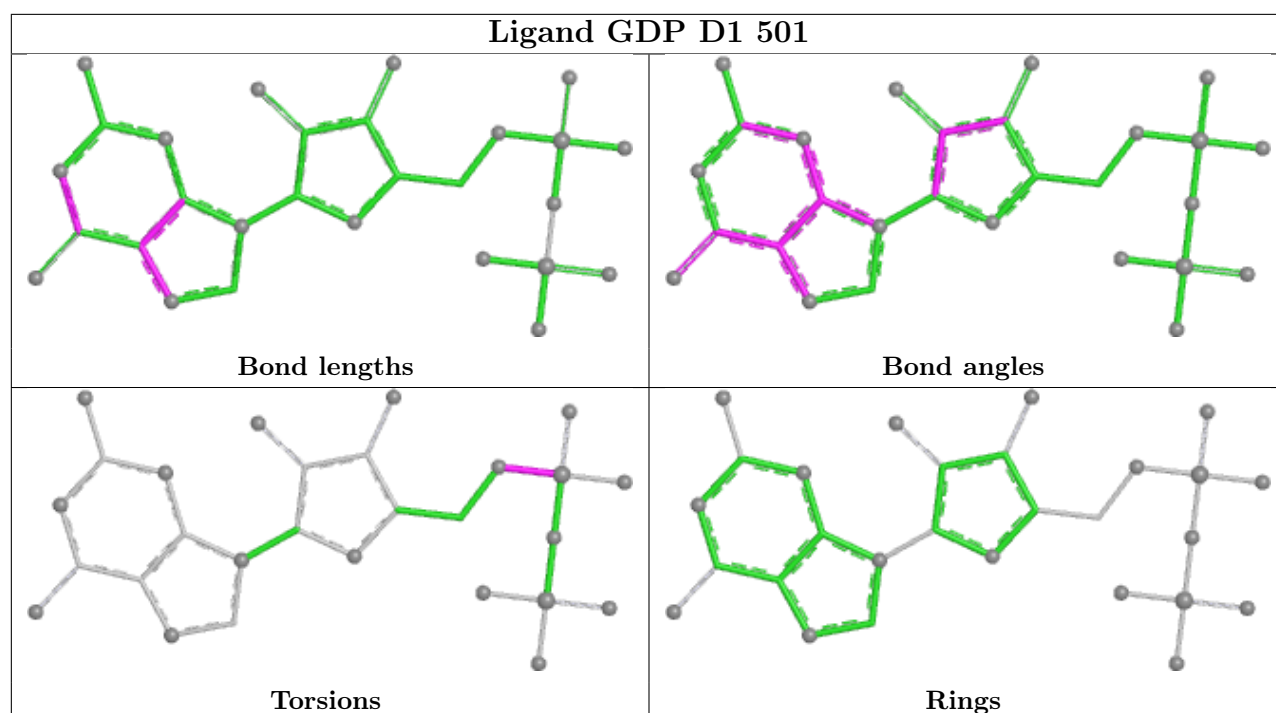


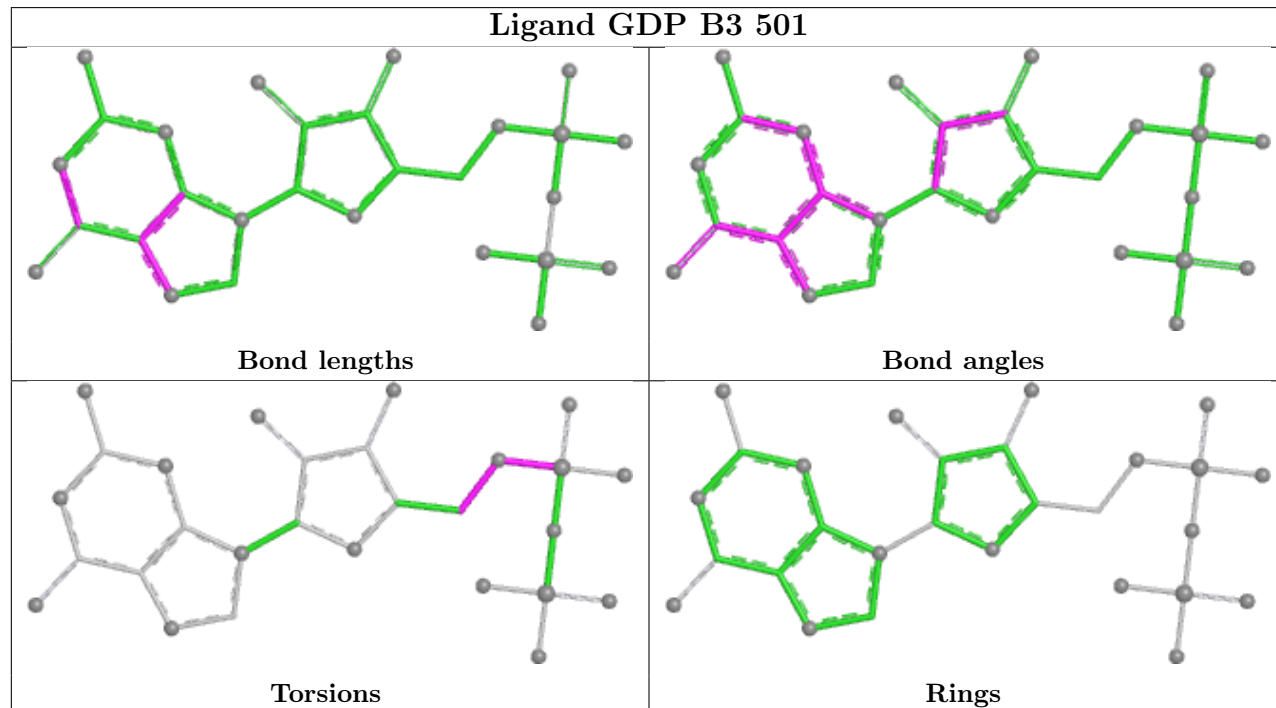
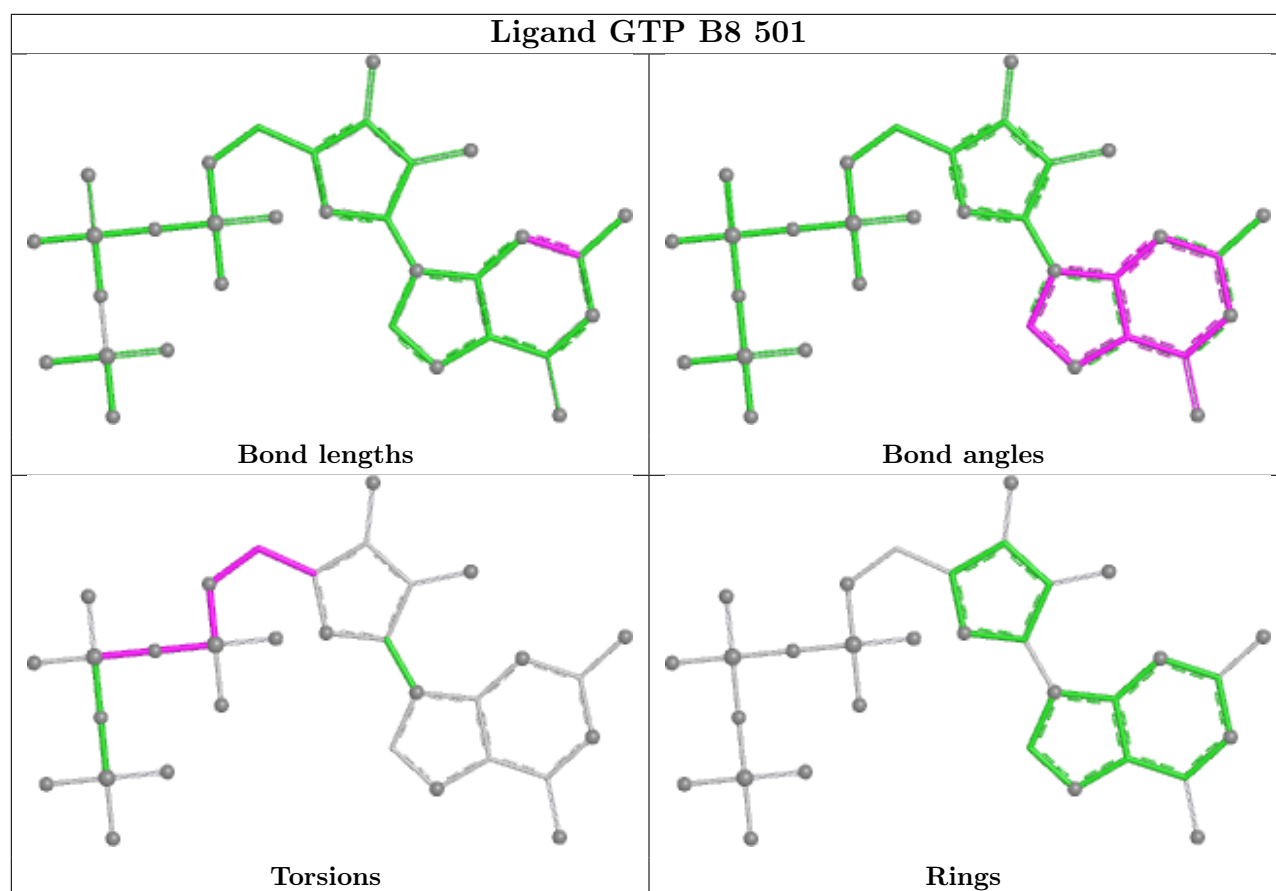


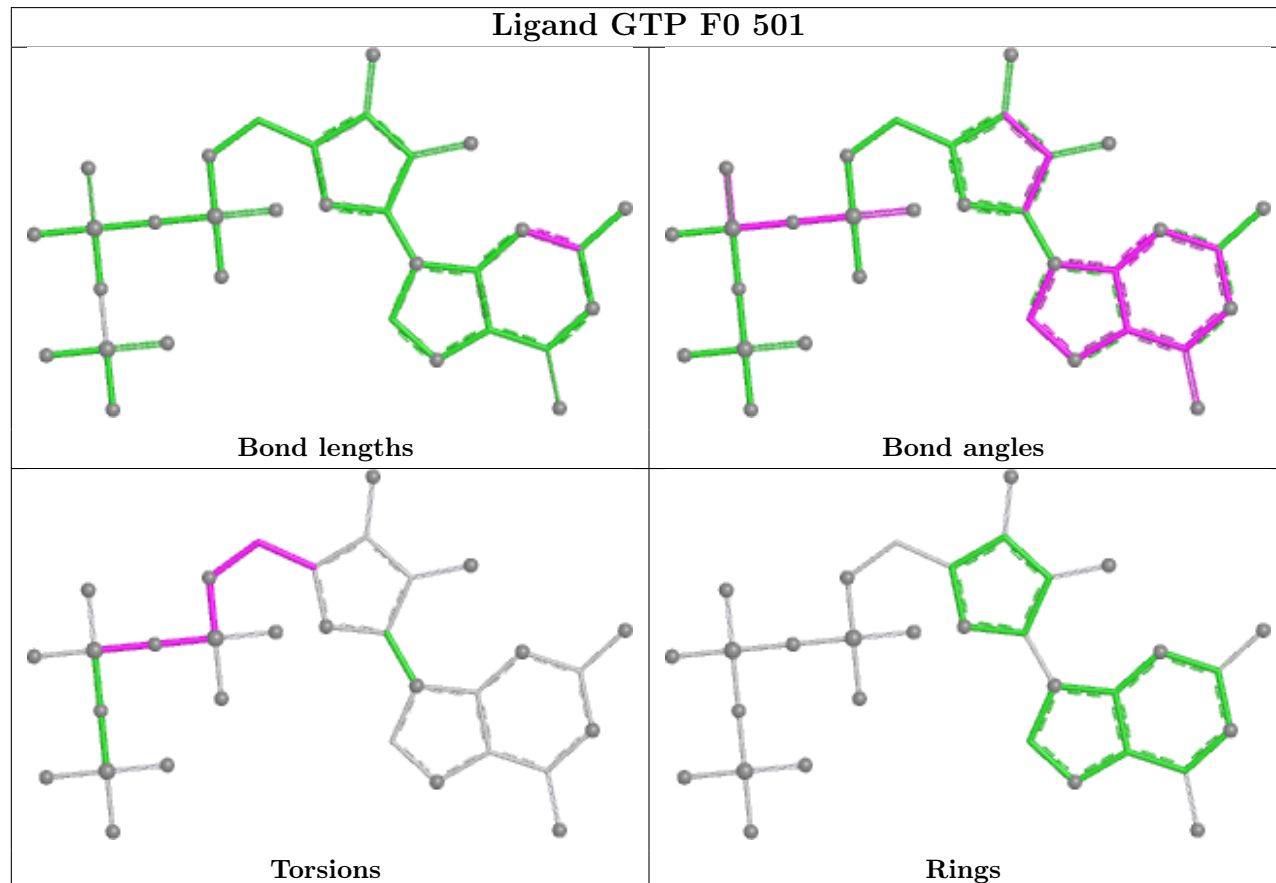
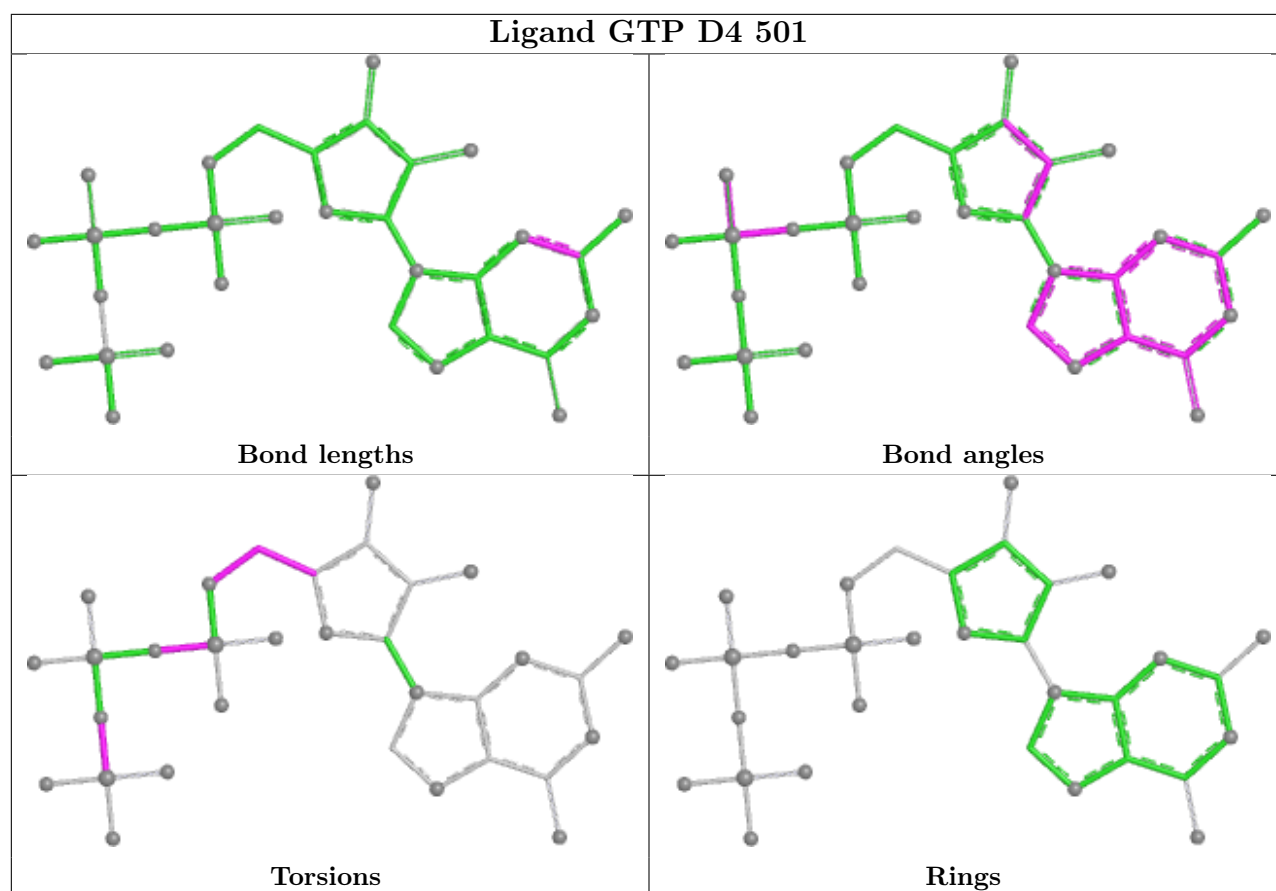


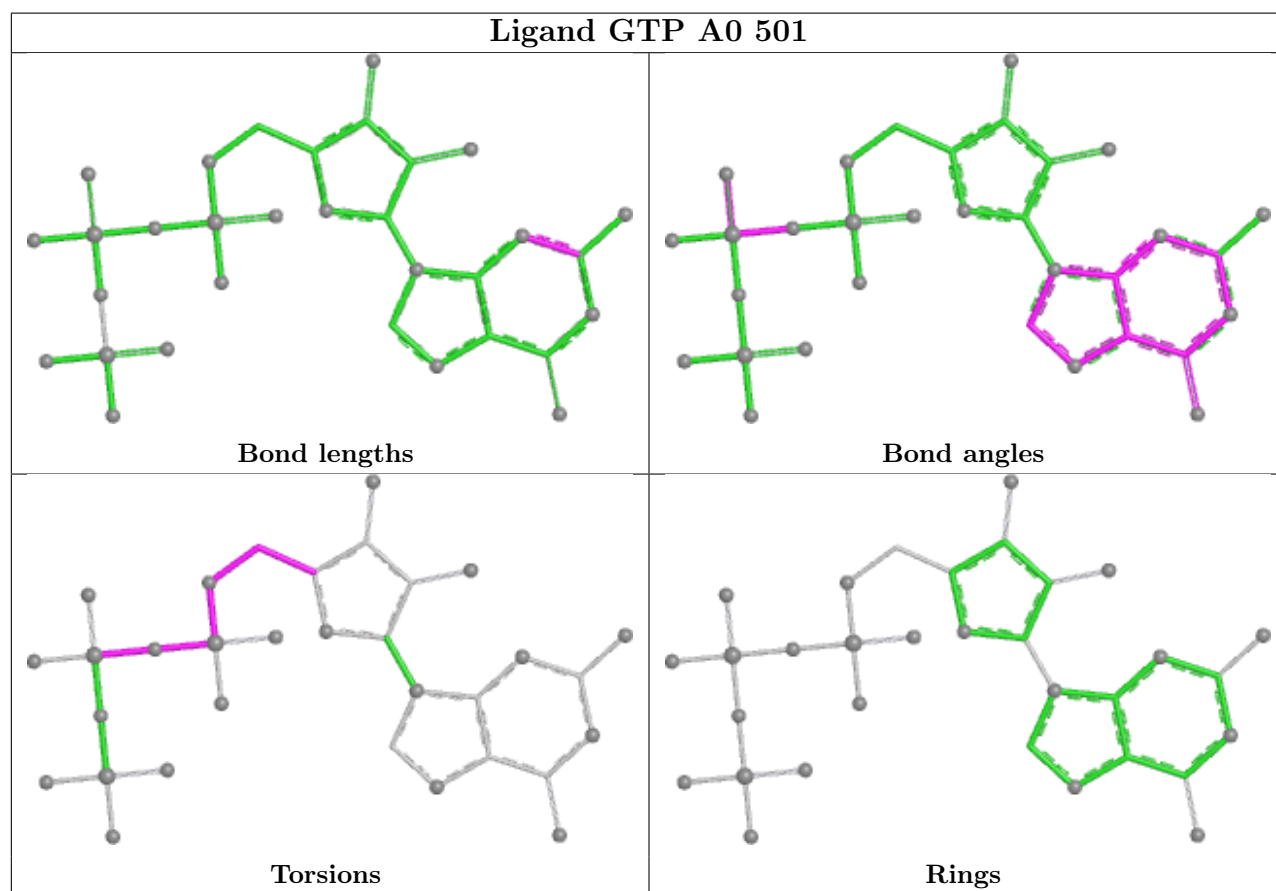
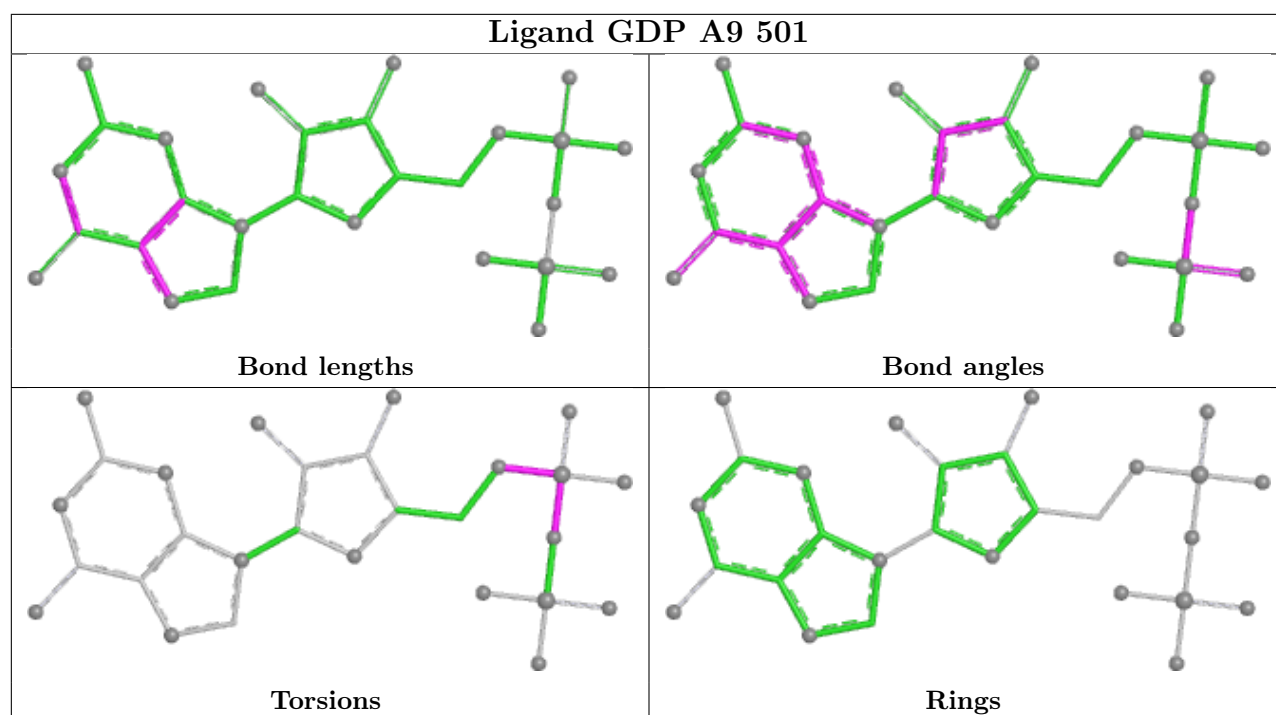




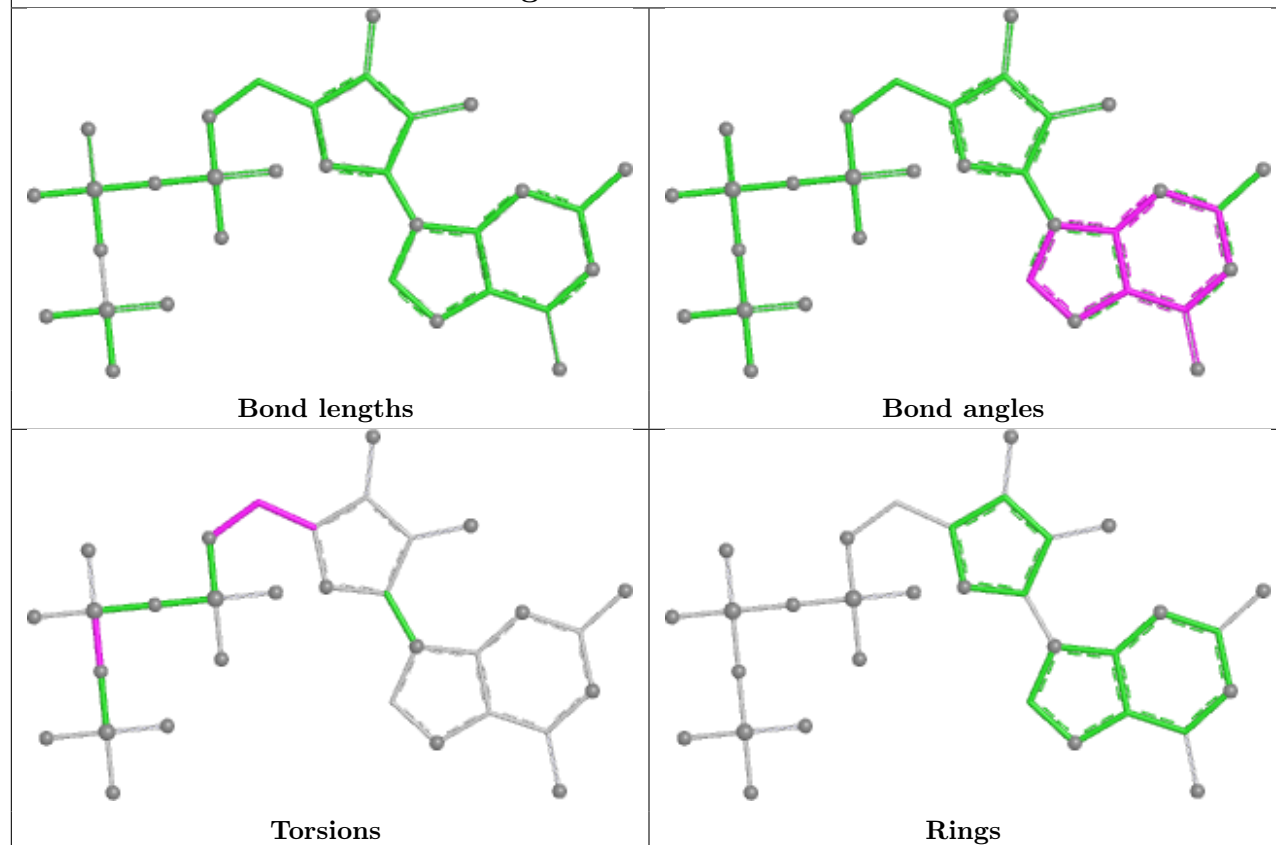




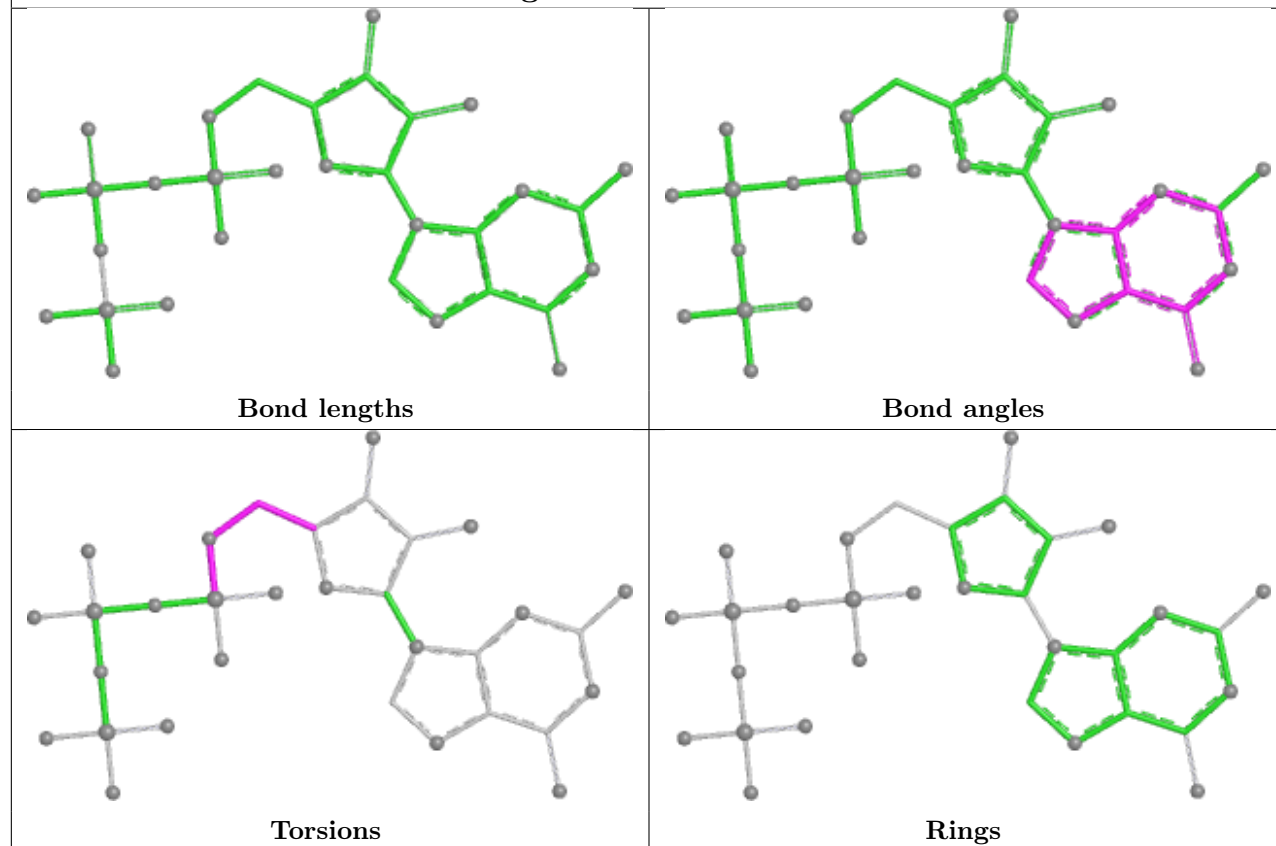




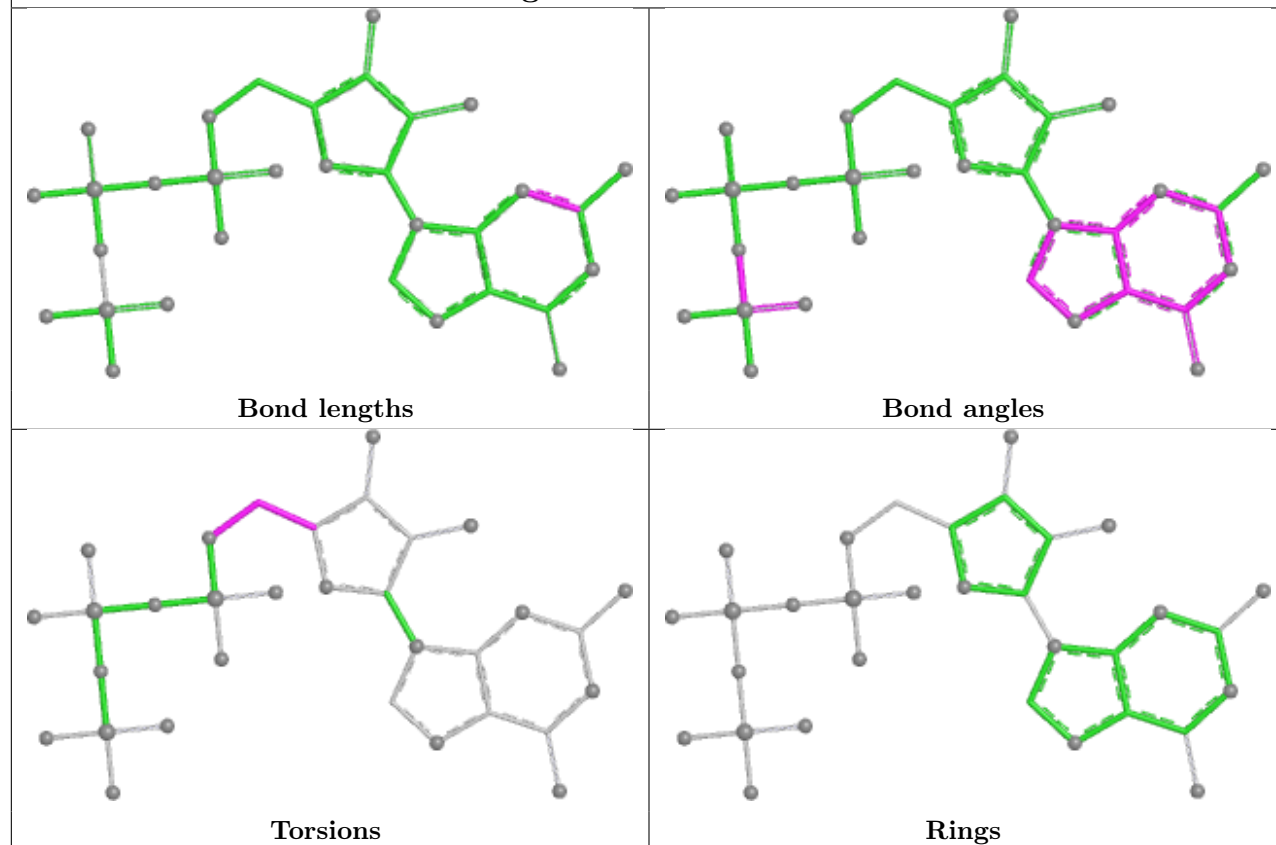
Ligand GTP D6 501



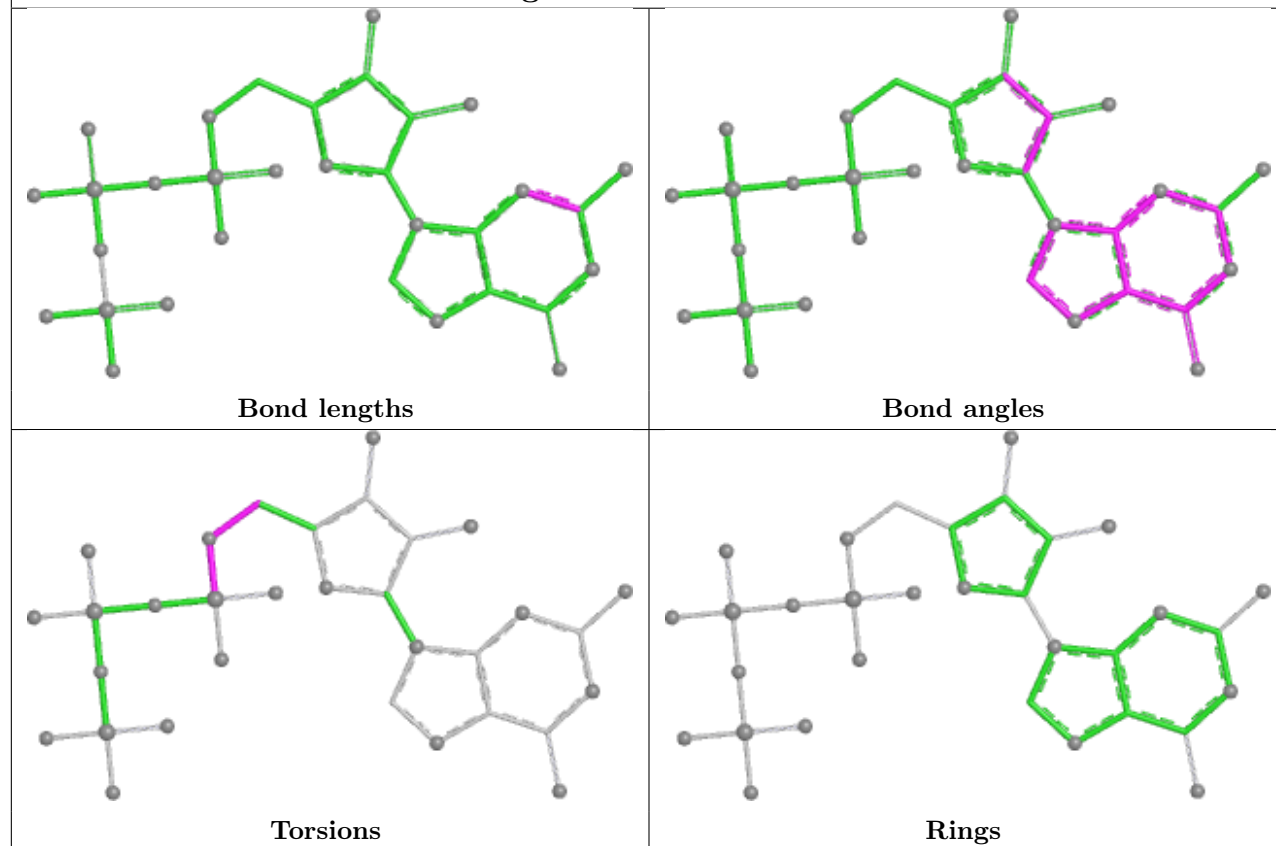
Ligand GTP A4 501

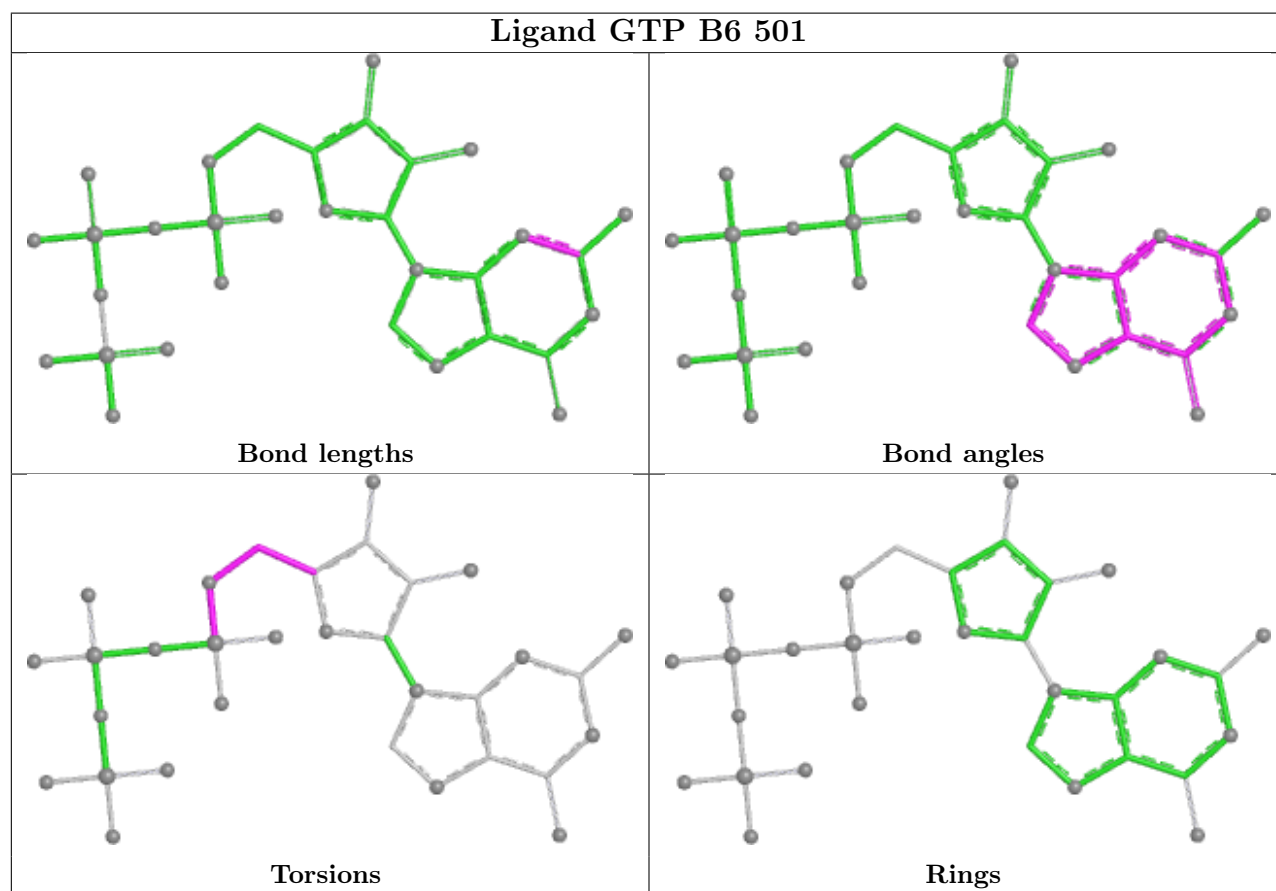
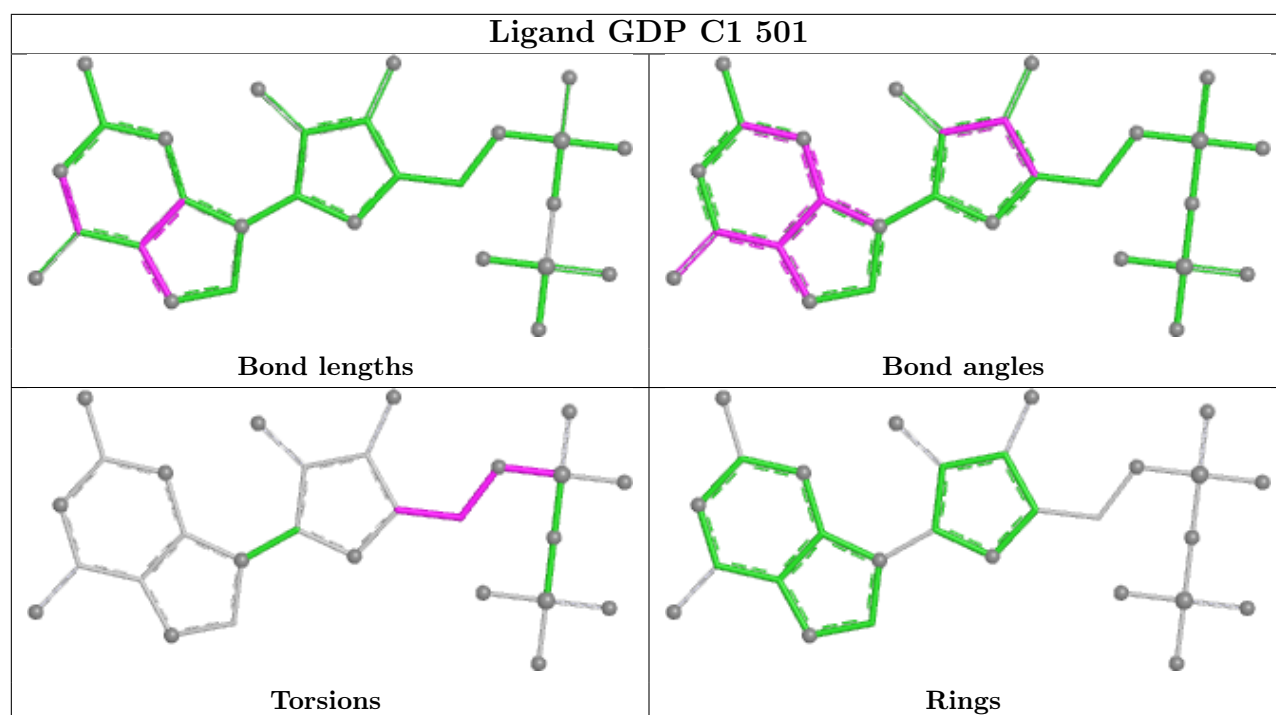


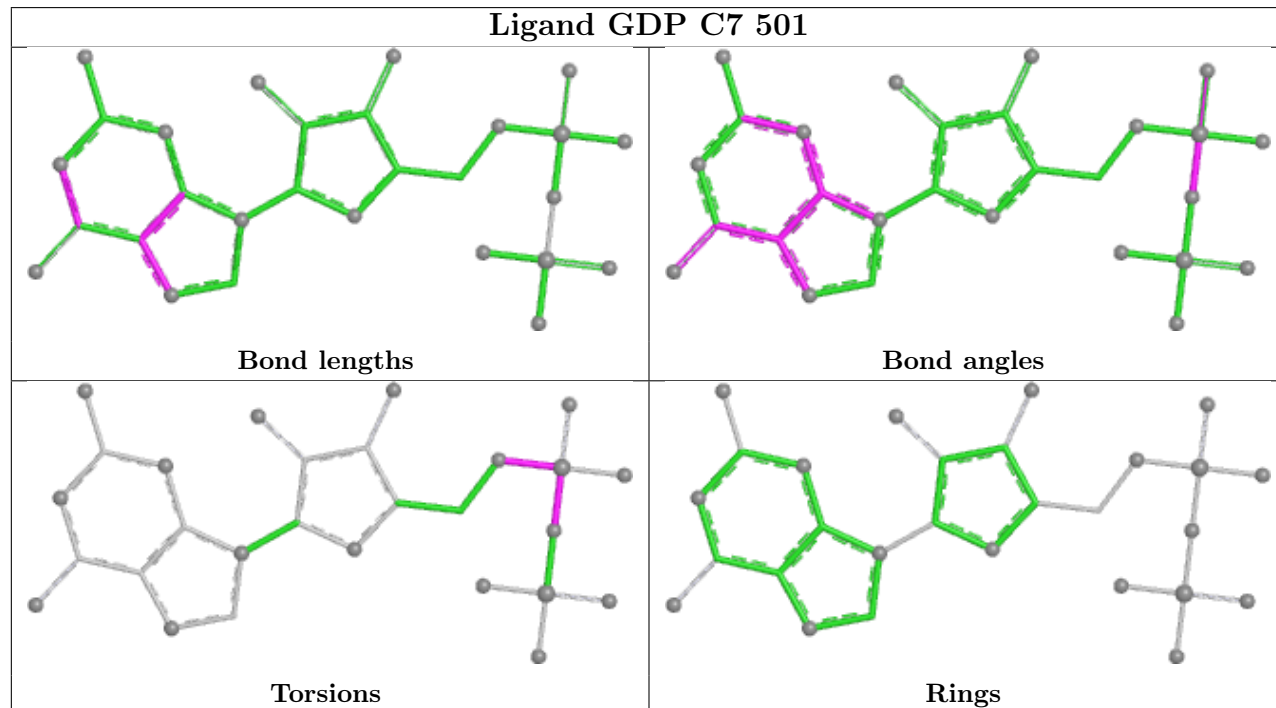
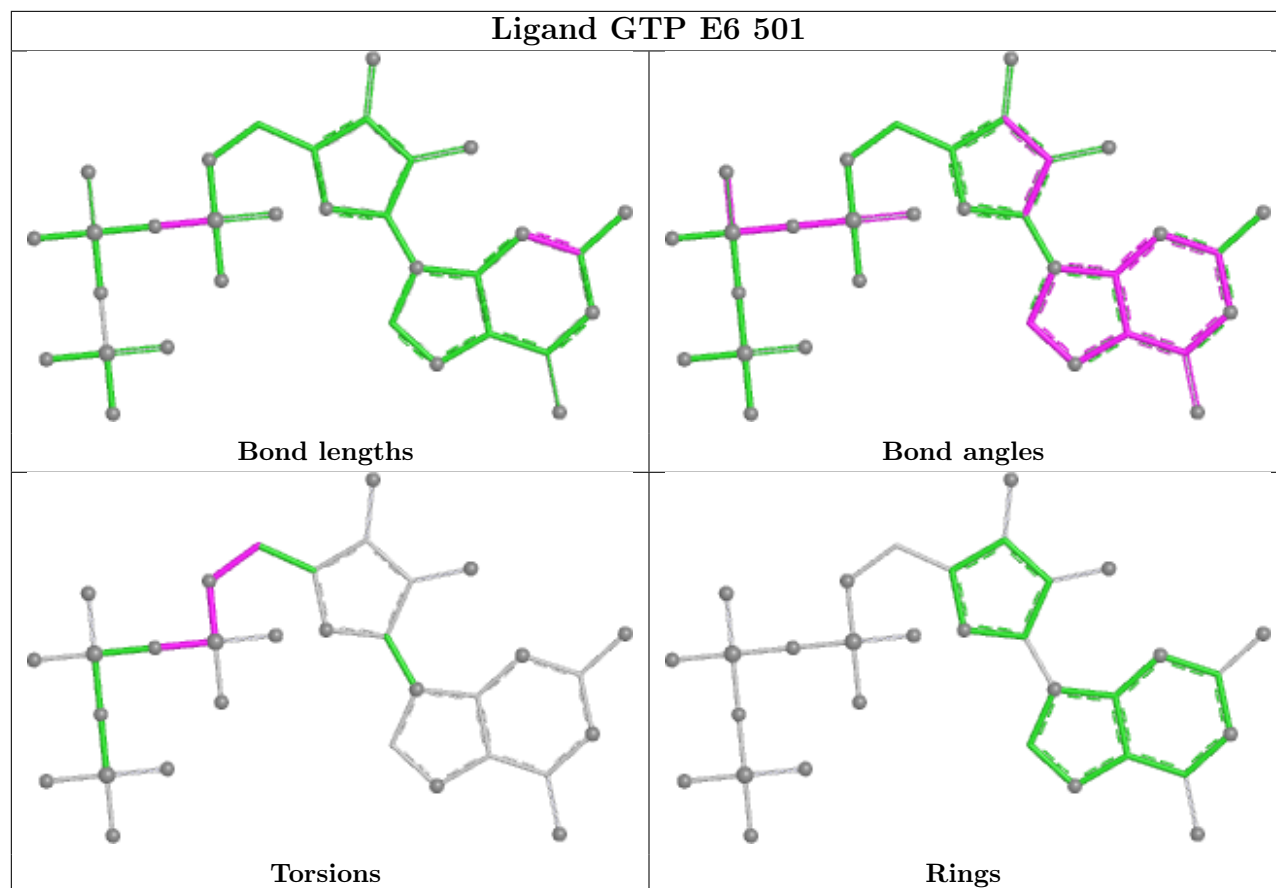
Ligand GTP C6 501

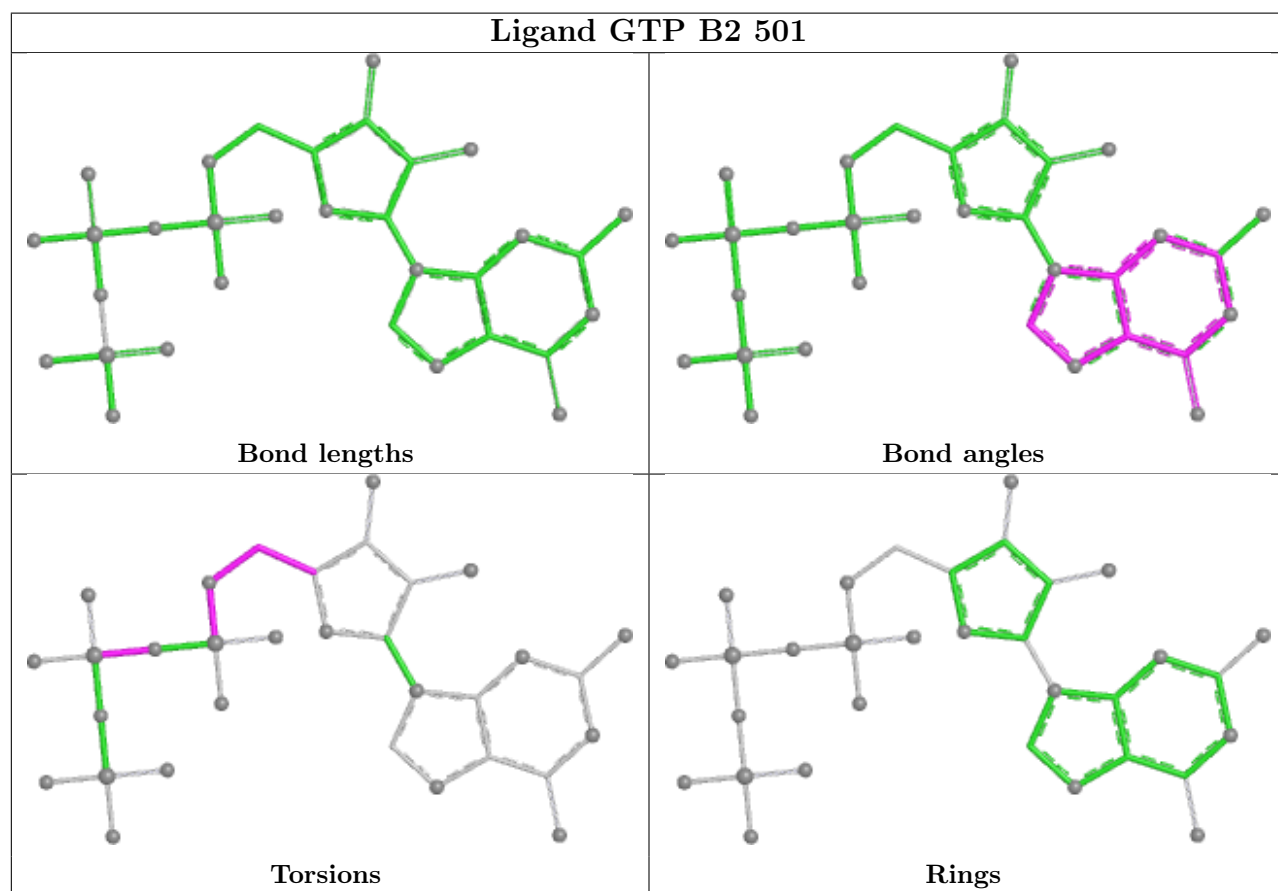
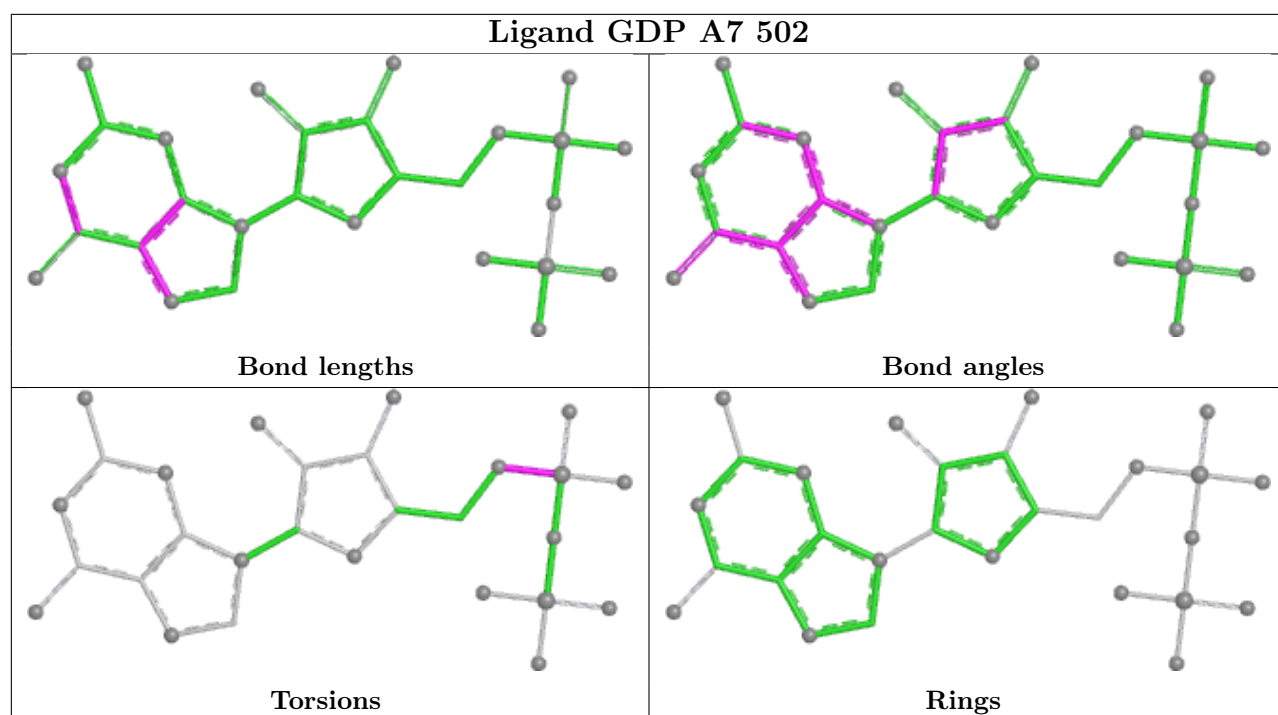


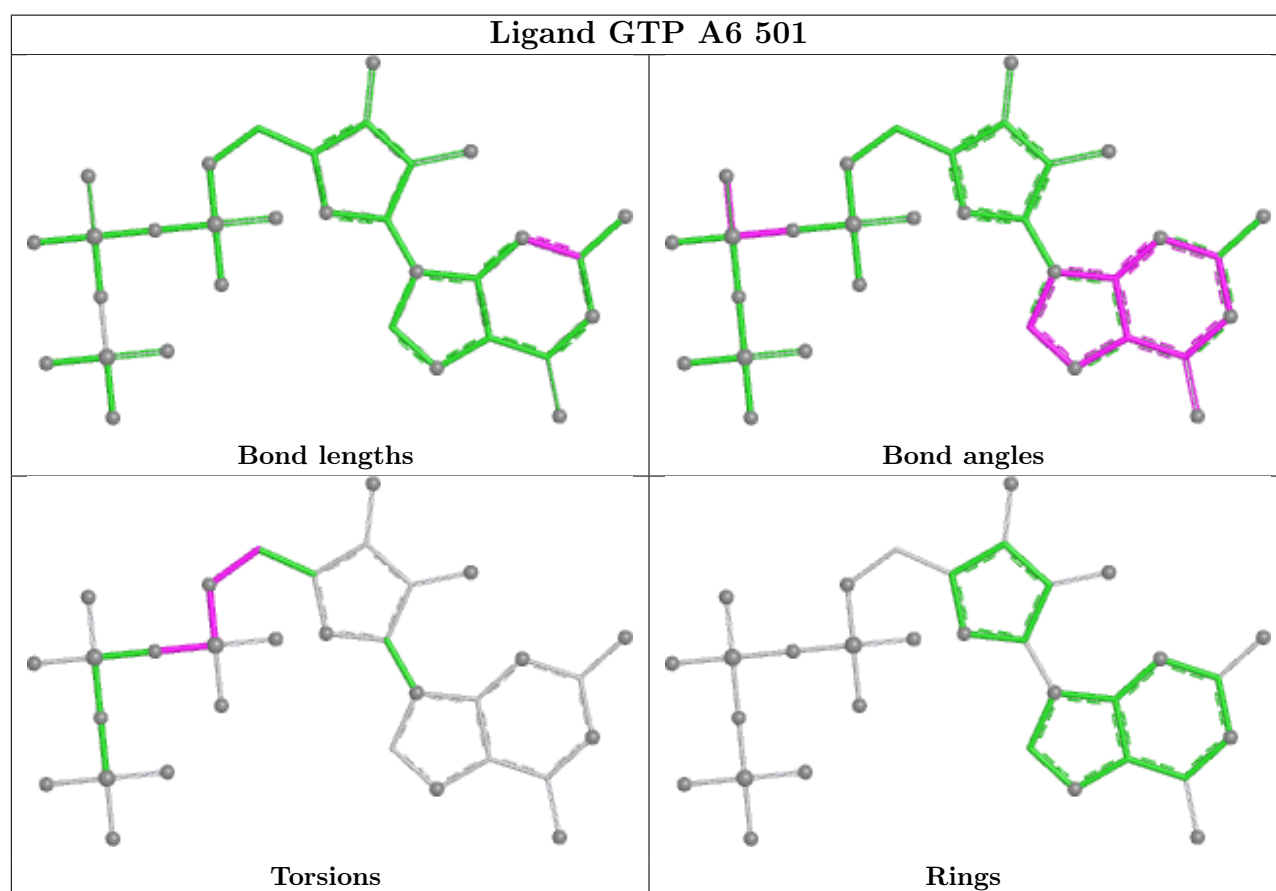
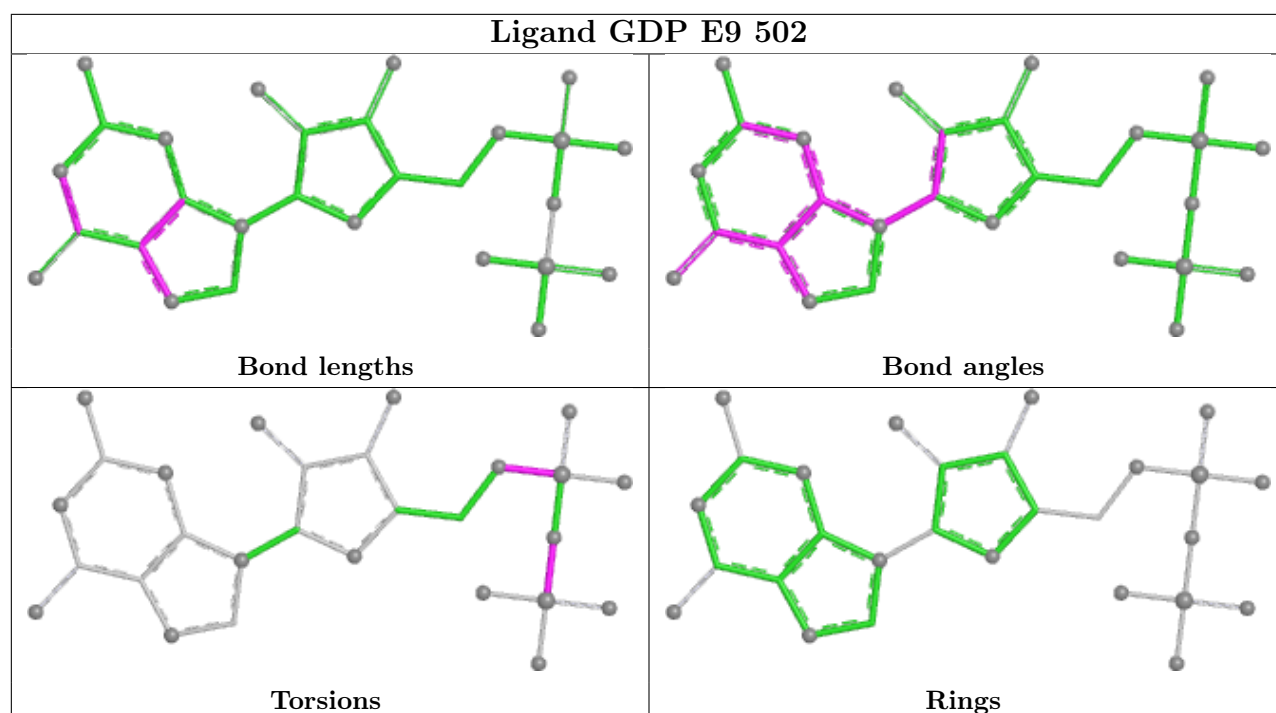
Ligand GTP C0 501

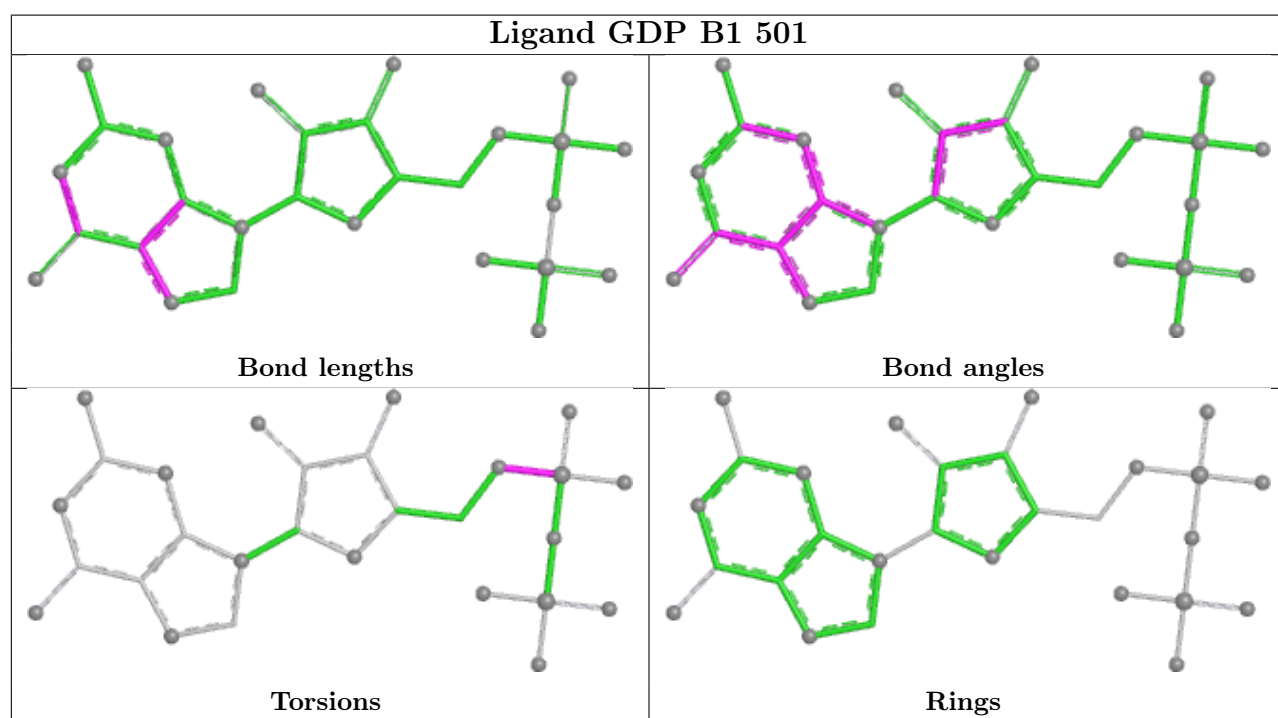
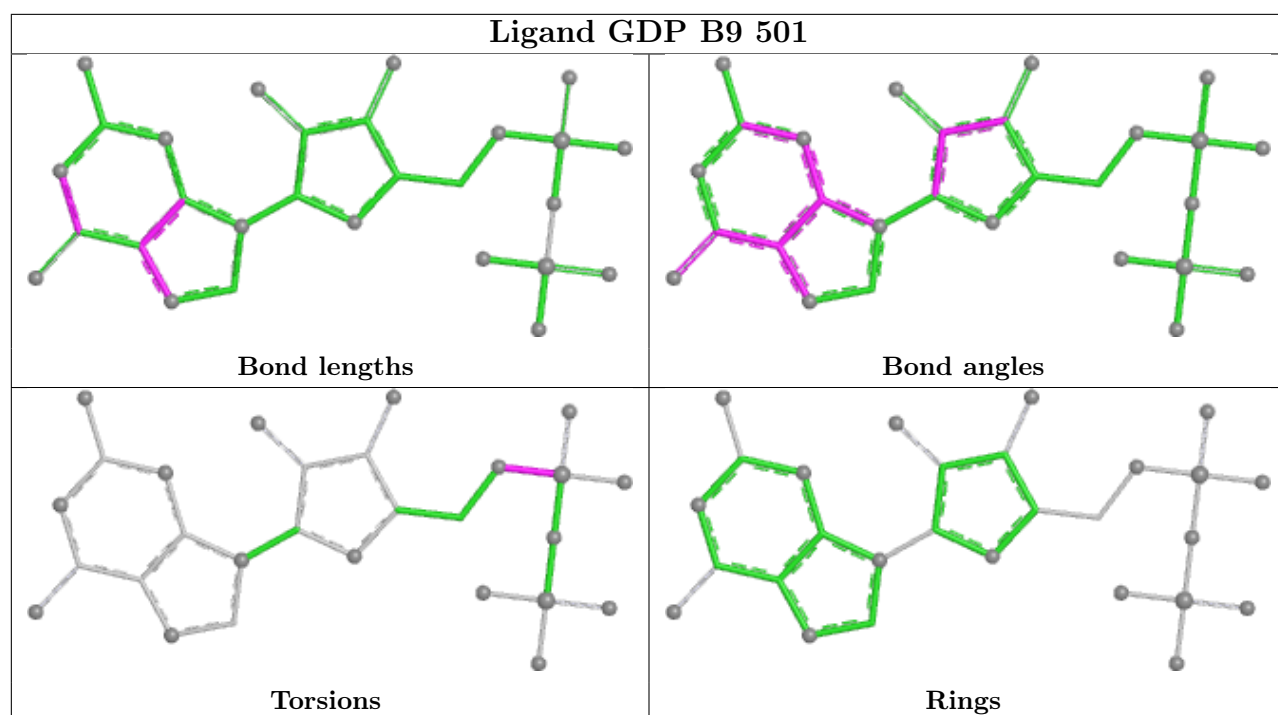


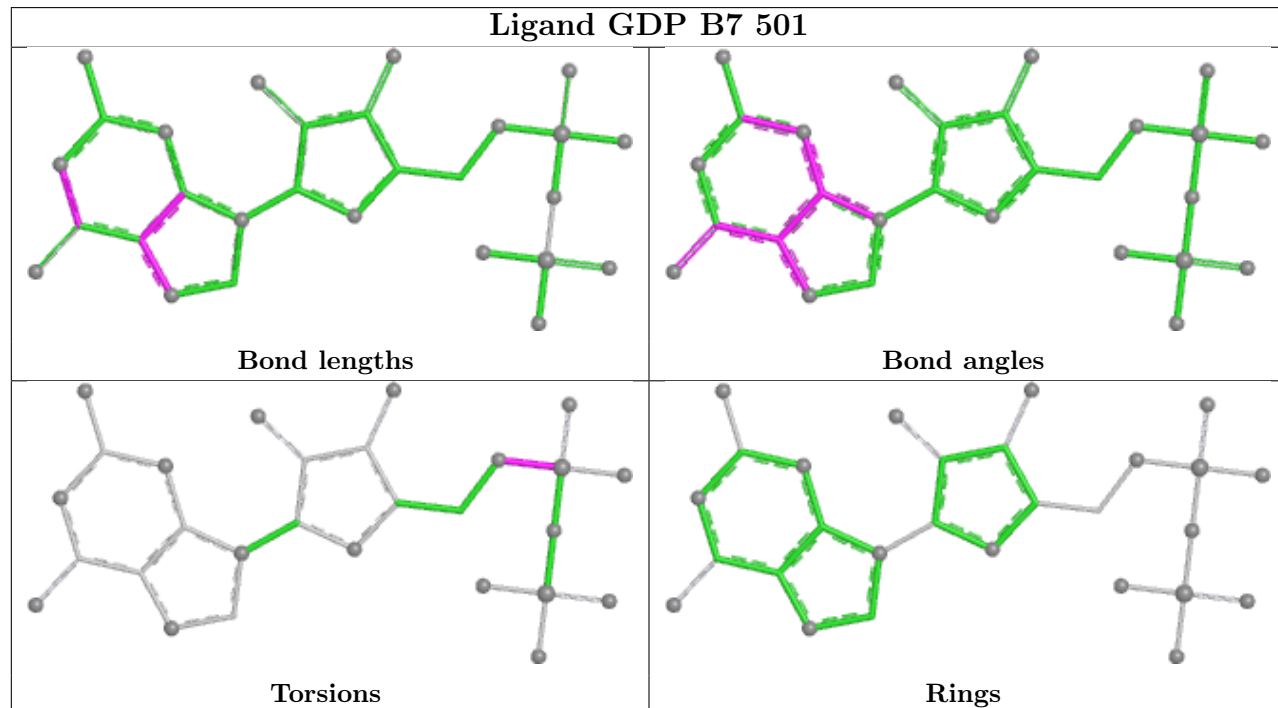
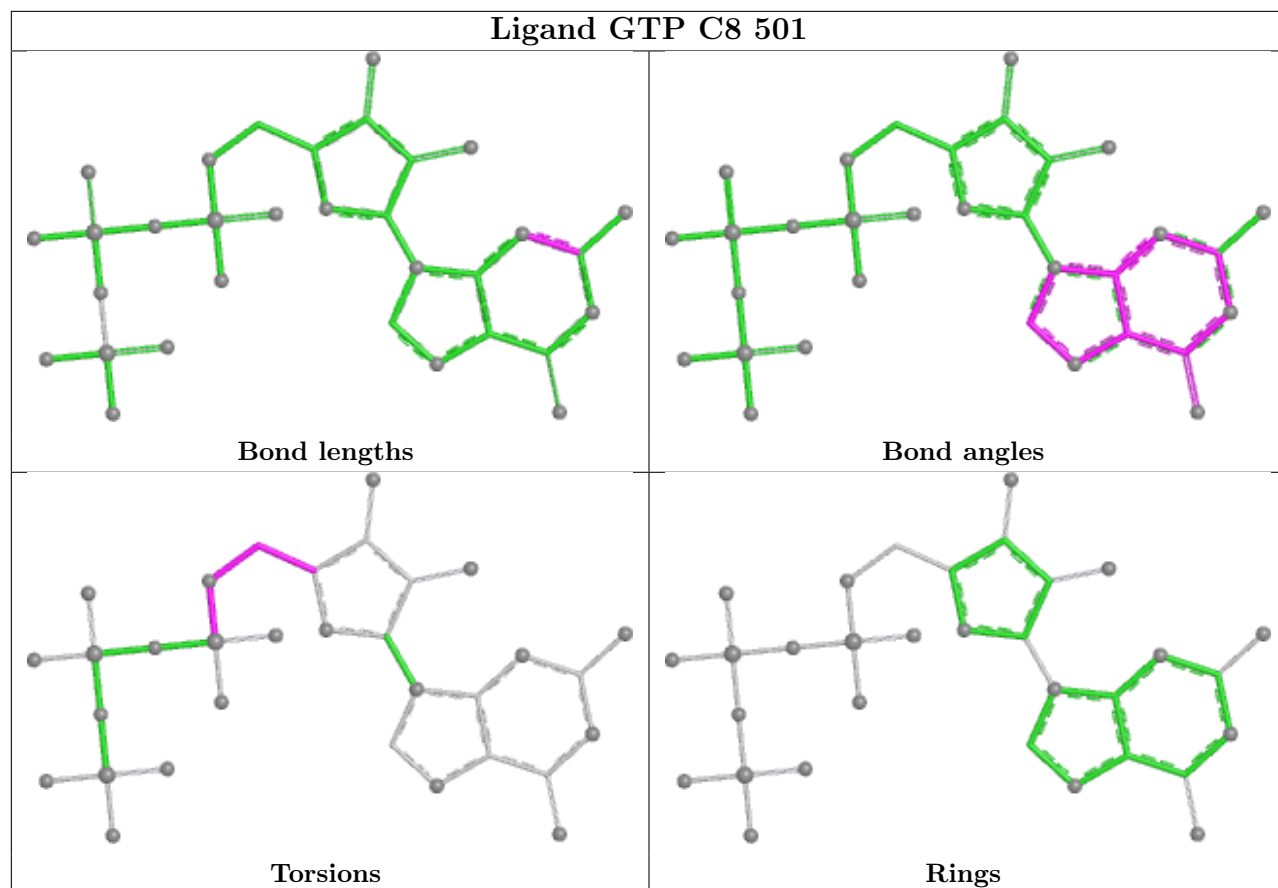


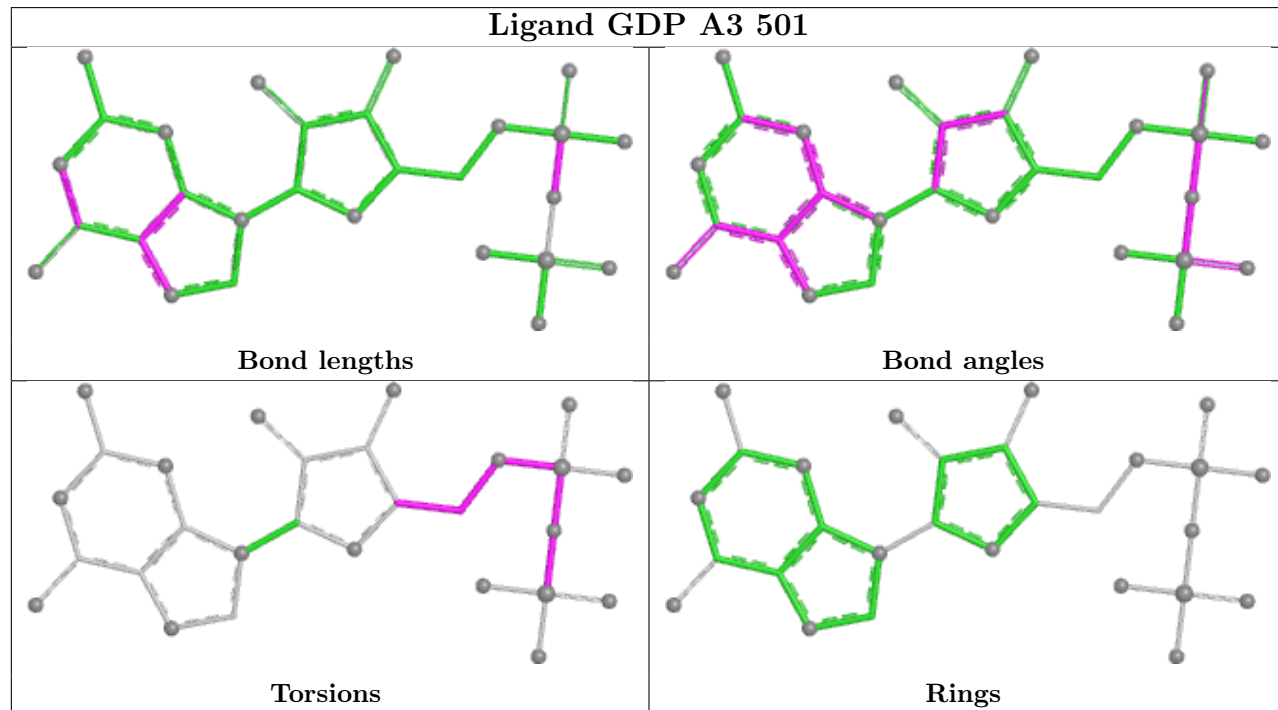
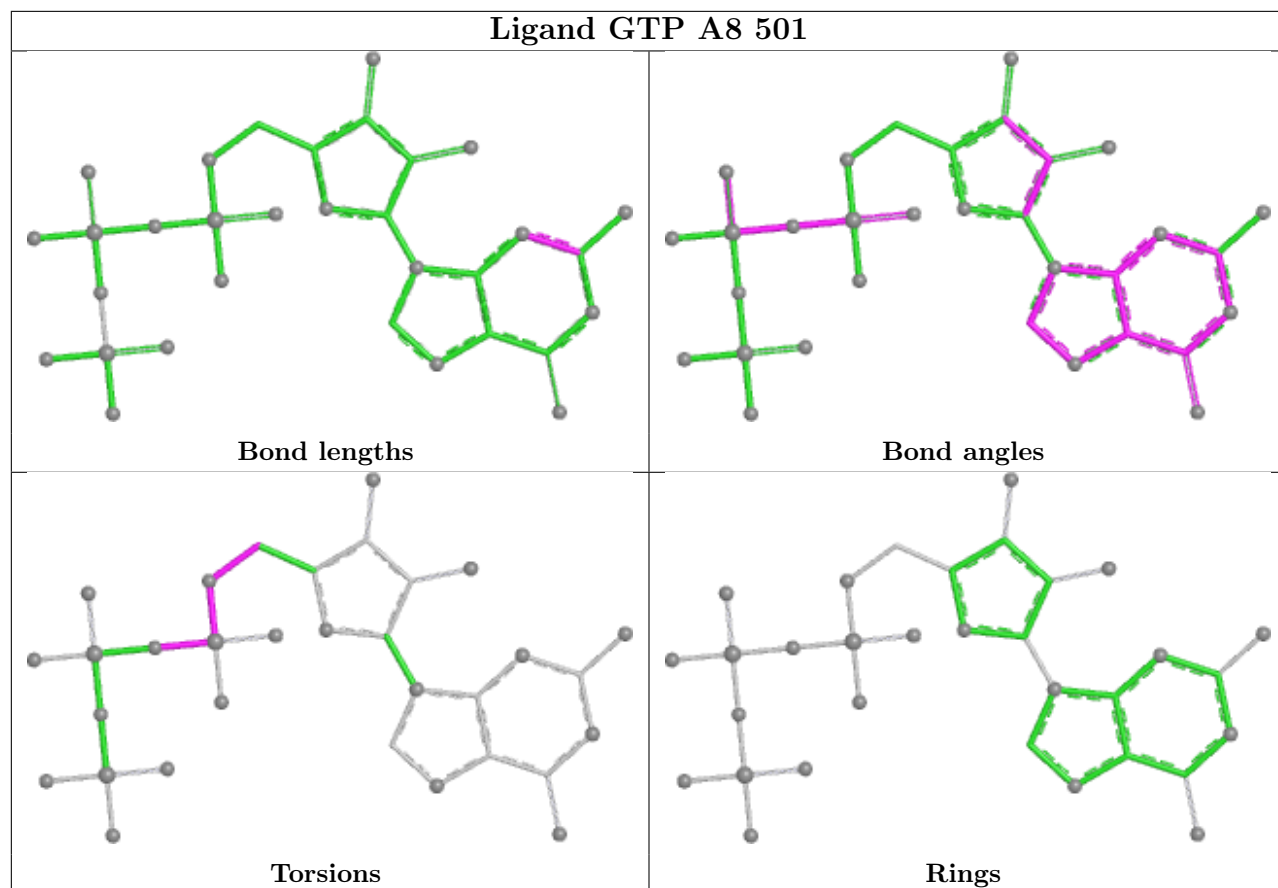


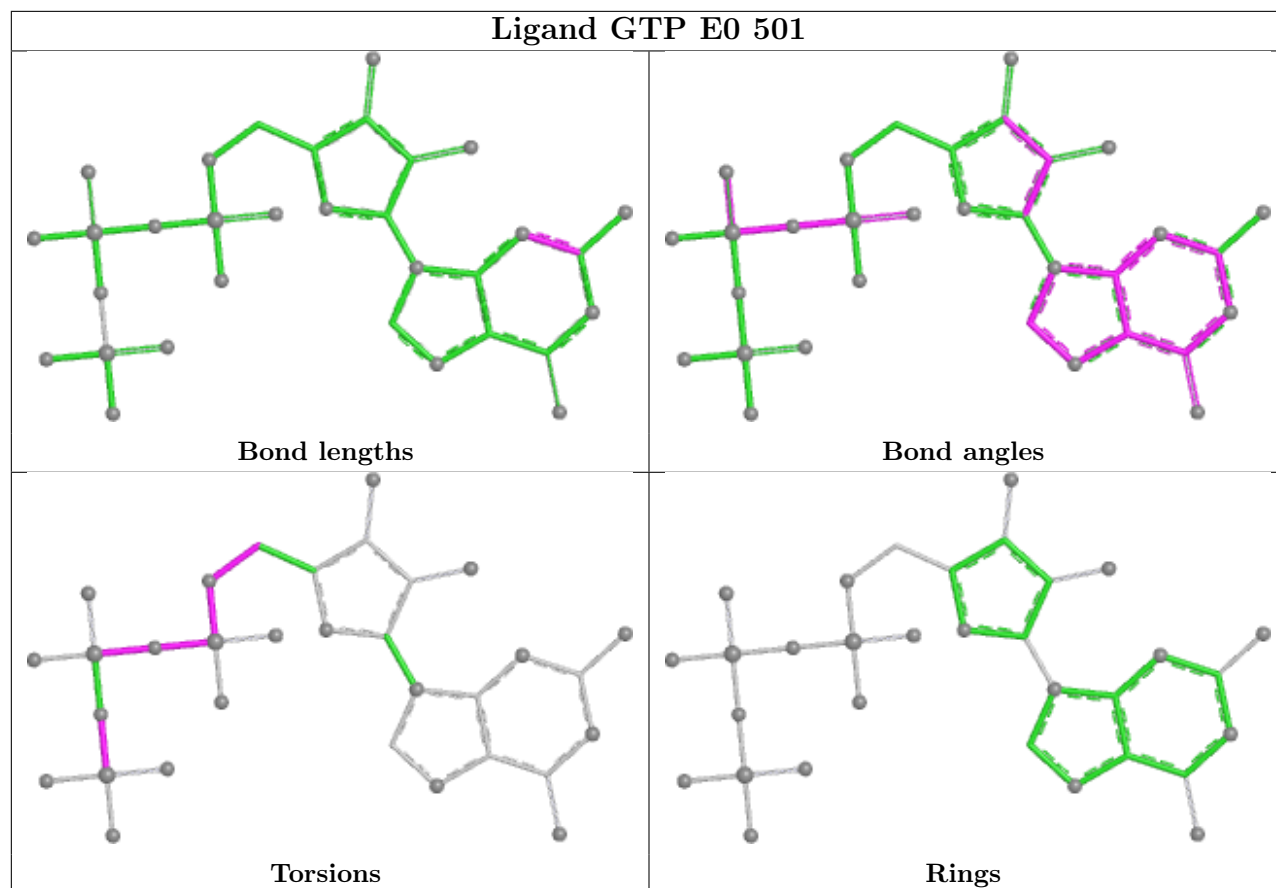












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

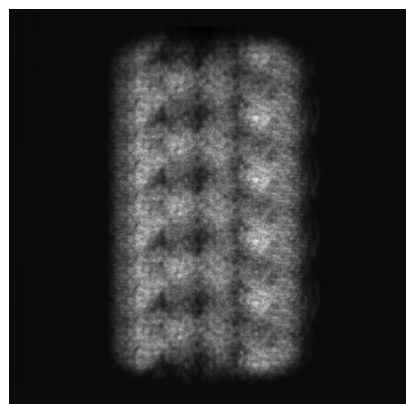
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72718. These allow visual inspection of the internal detail of the map and identification of artifacts.

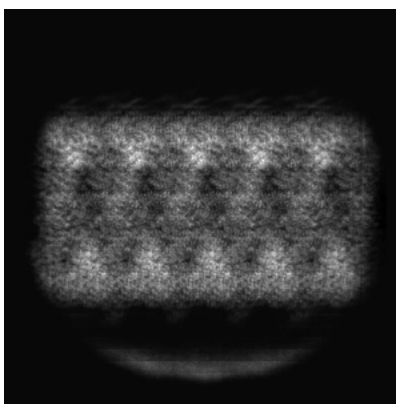
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

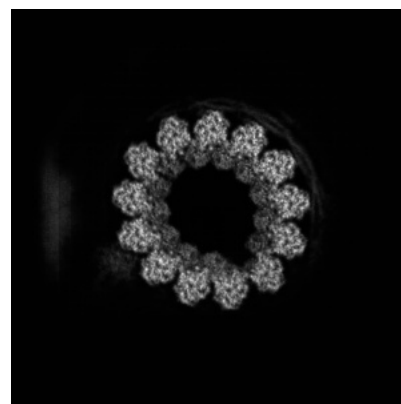
6.1.1 Primary map



X

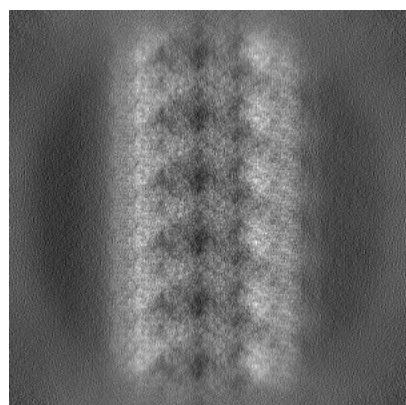


Y

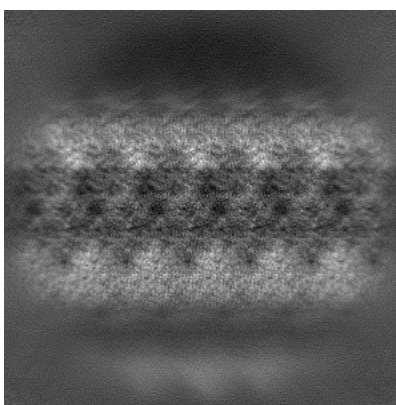


Z

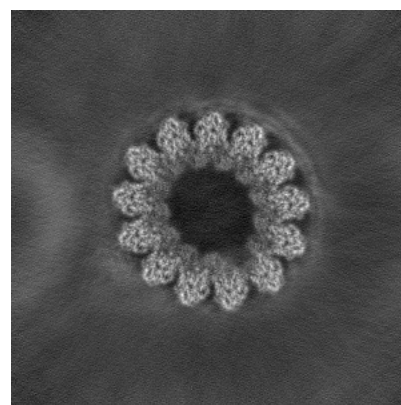
6.1.2 Raw map



X



Y

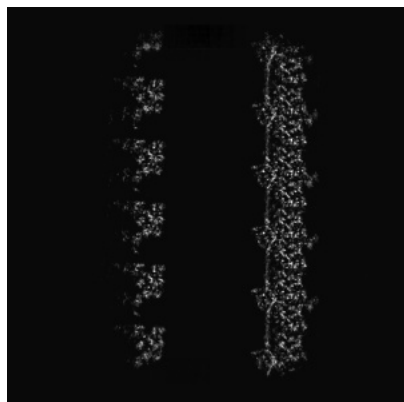


Z

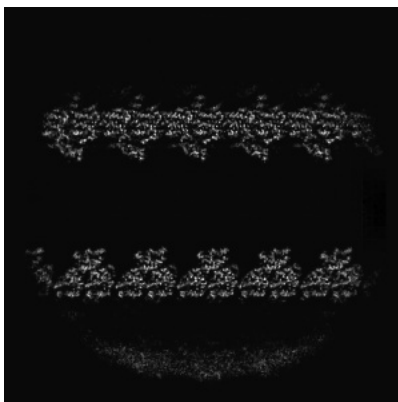
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

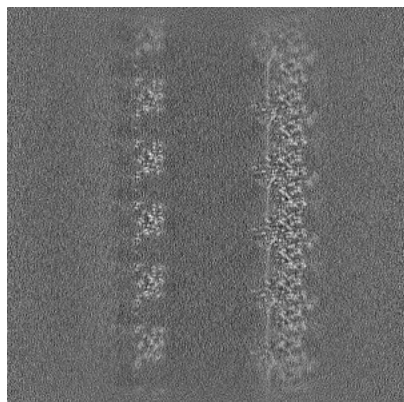


Y Index: 200

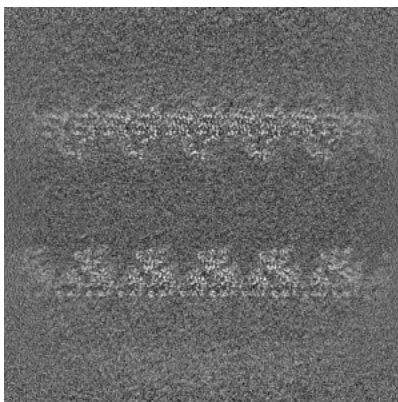


Z Index: 200

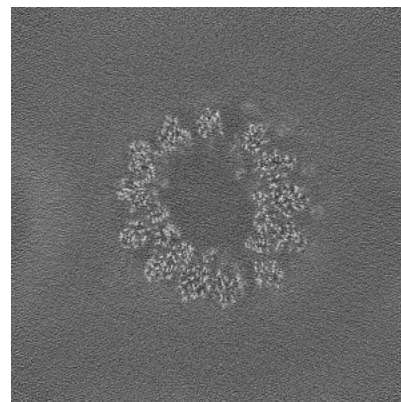
6.2.2 Raw map



X Index: 200



Y Index: 200

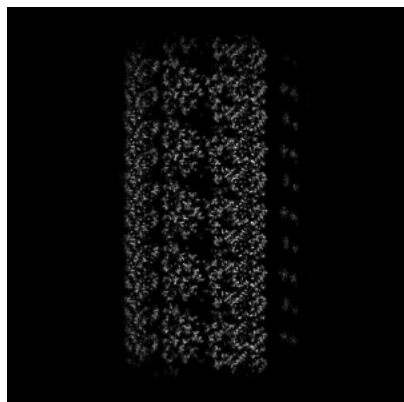


Z Index: 200

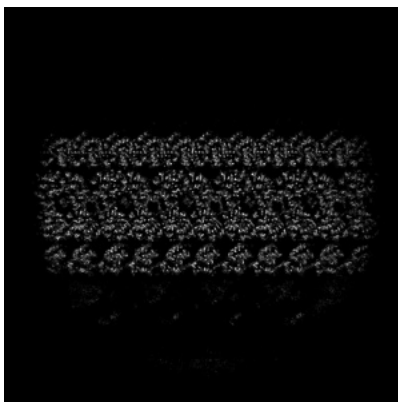
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

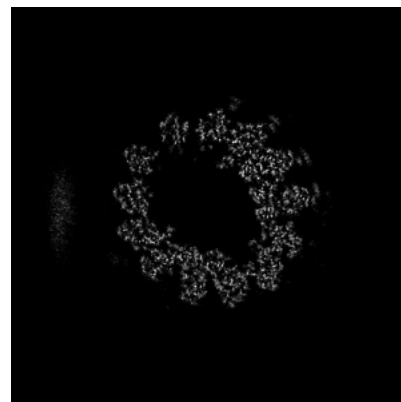
6.3.1 Primary map



X Index: 265

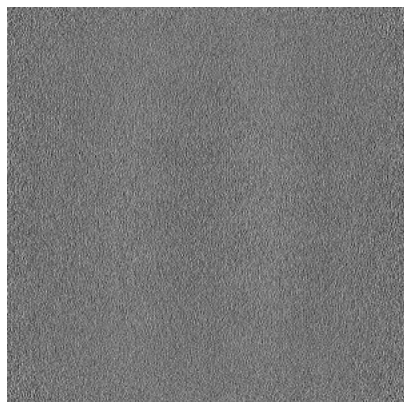


Y Index: 129

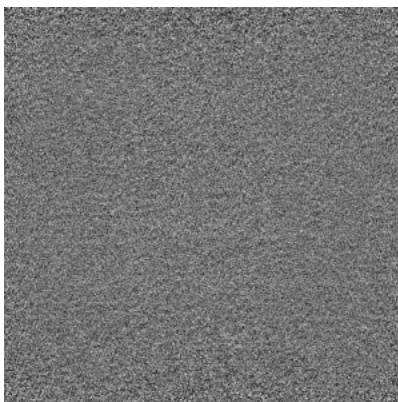


Z Index: 126

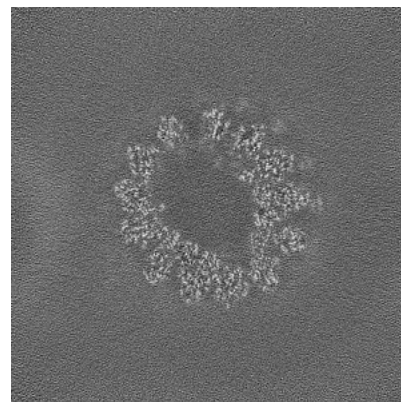
6.3.2 Raw map



X Index: 0



Y Index: 1

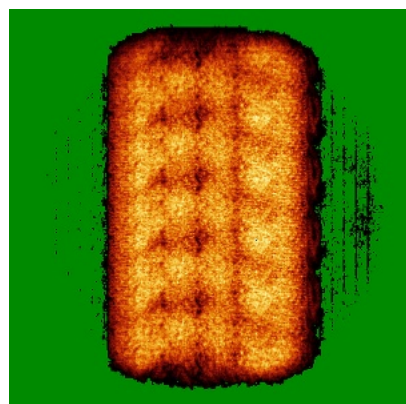


Z Index: 194

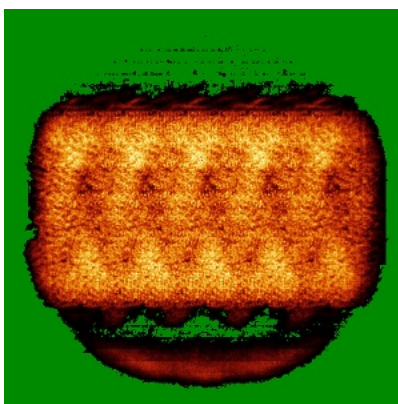
The images above show the largest variance slices of the map in three orthogonal directions.

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

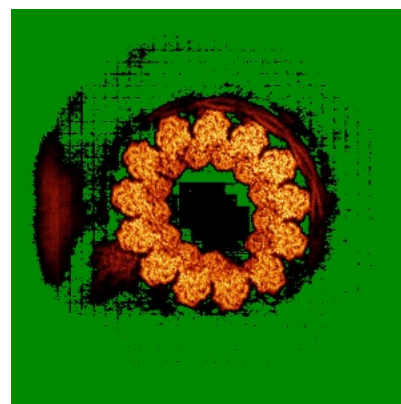
6.4.1 Primary map



X

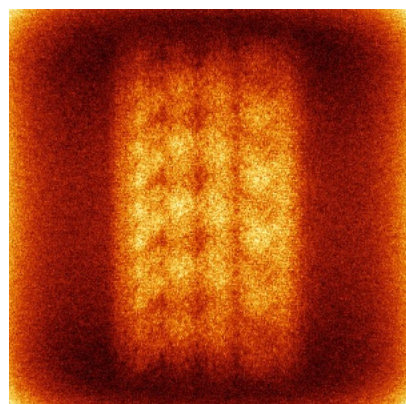


Y

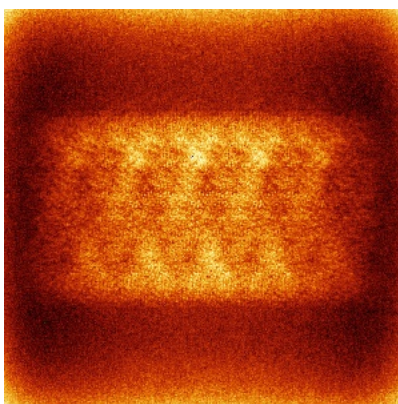


Z

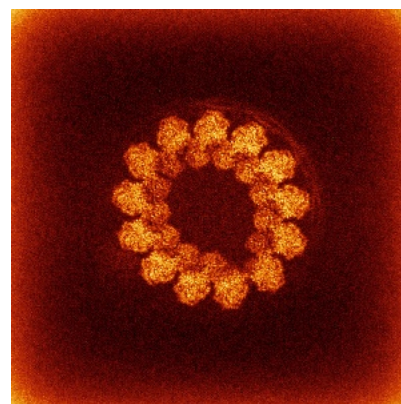
6.4.2 Raw map



X



Y

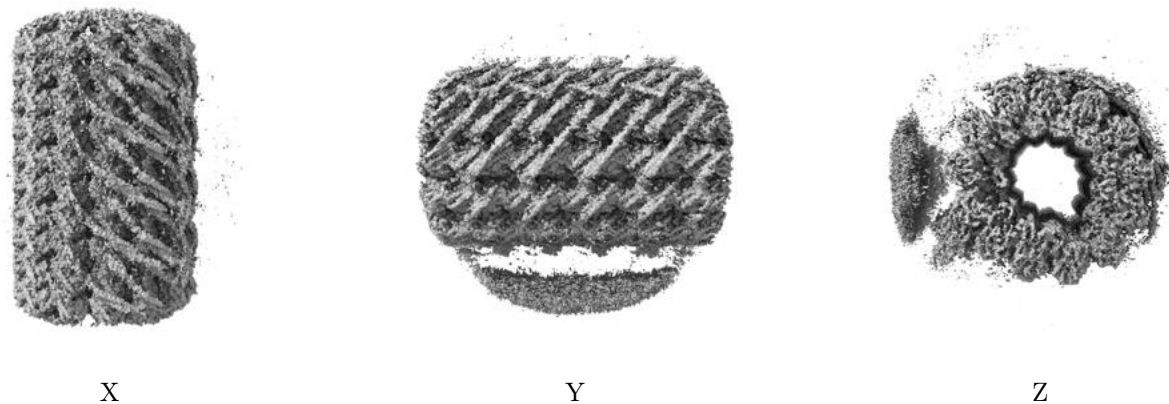


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

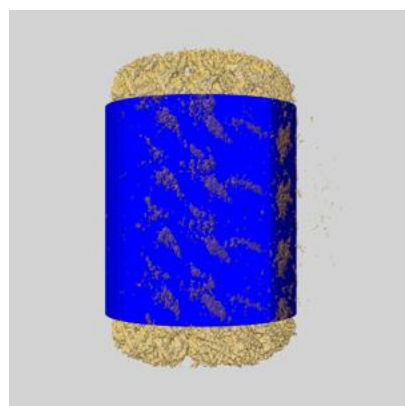
6.6 Mask visualisation [i](#)

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

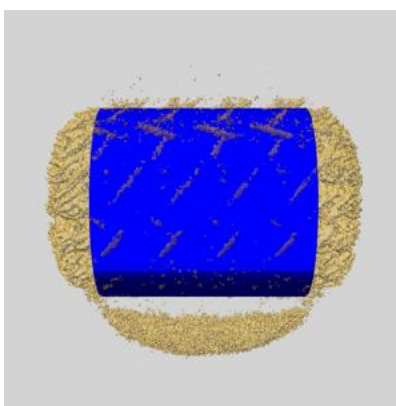
A mask typically either:

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

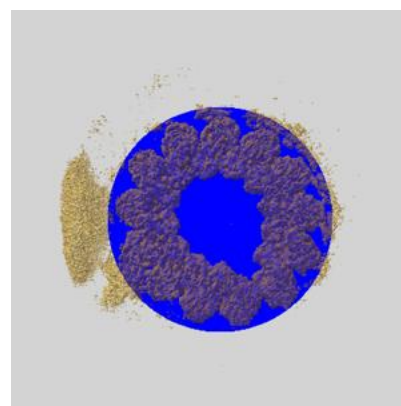
6.6.1 emd_72718_msk_1.map [i](#)



X



Y

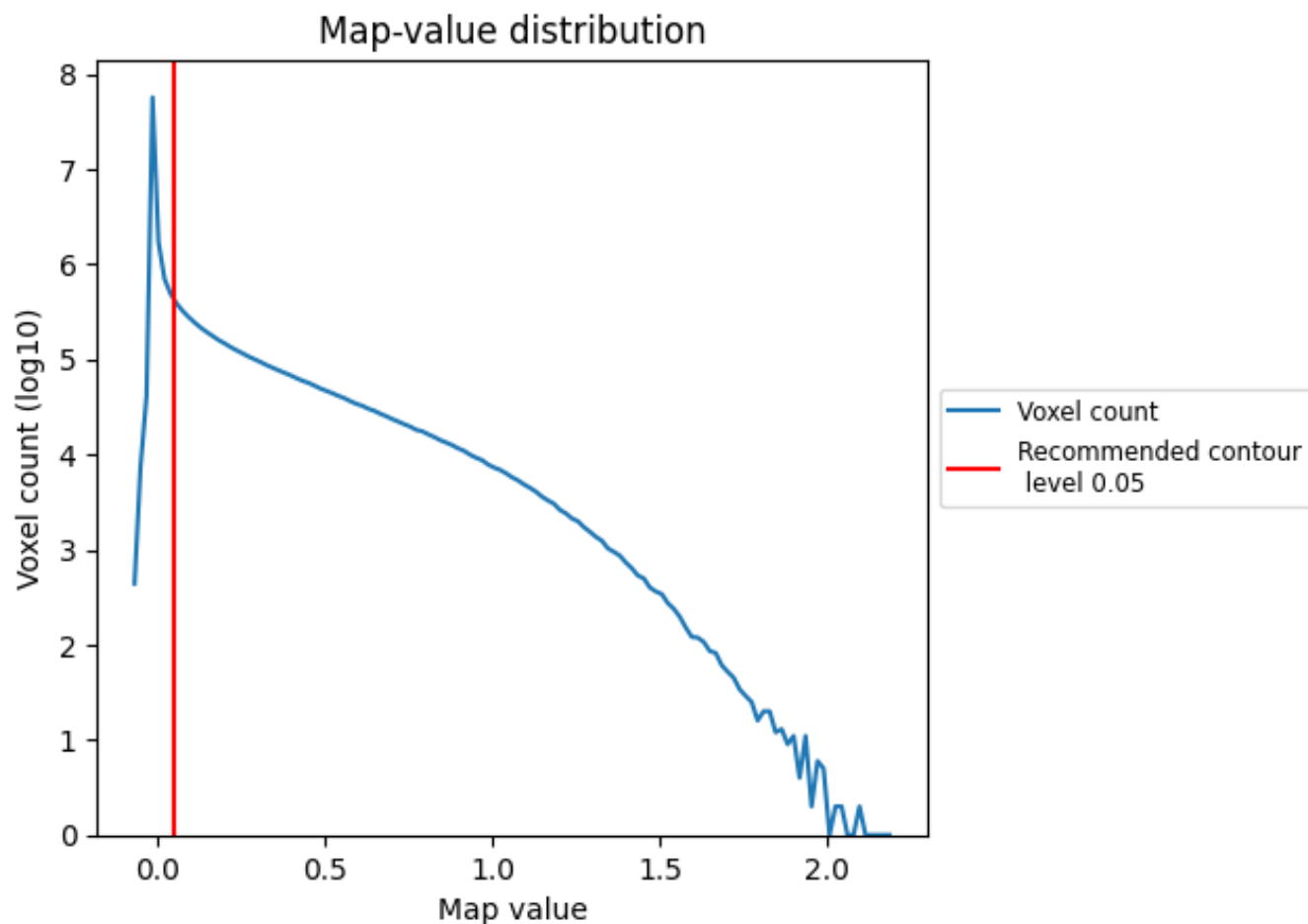


Z

7 Map analysis [i](#)

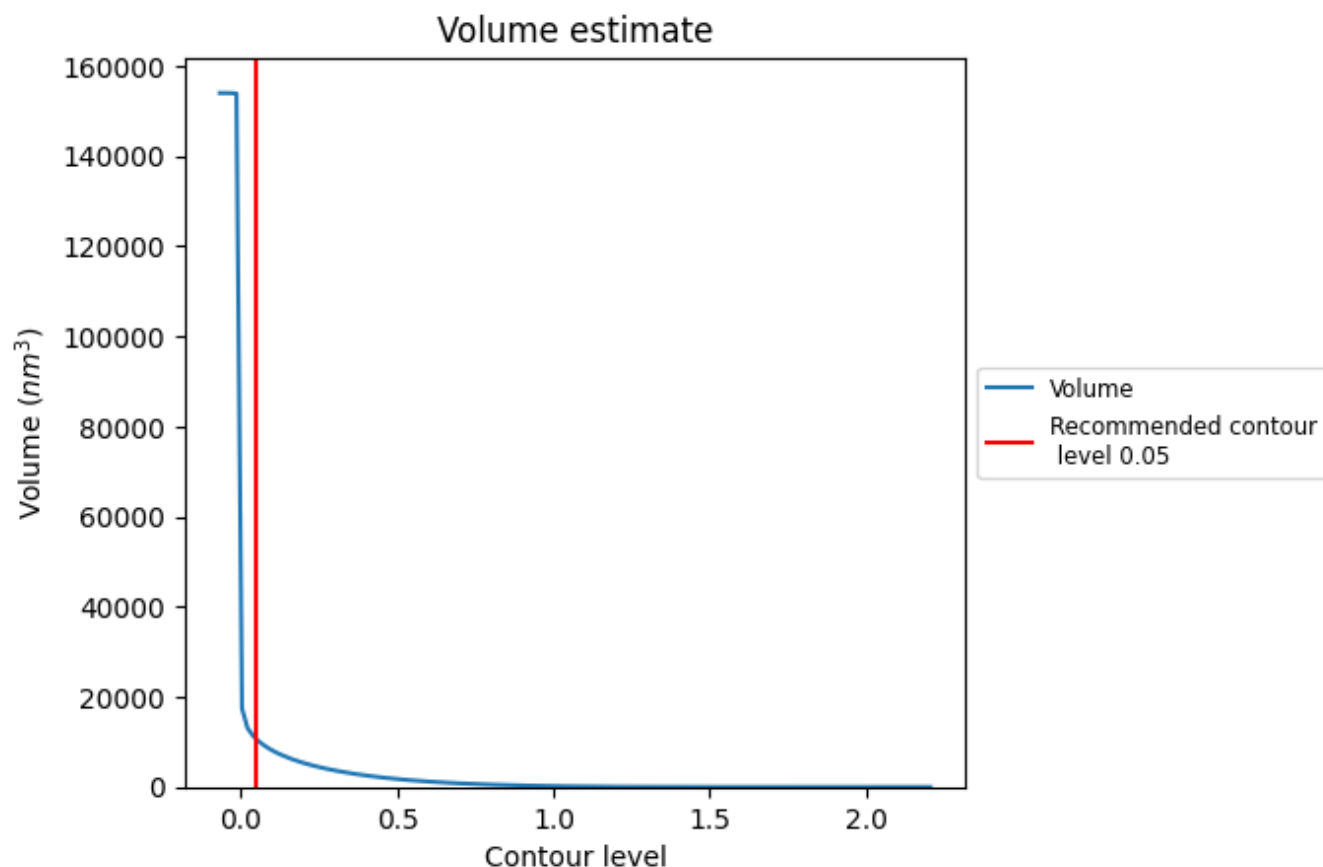
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

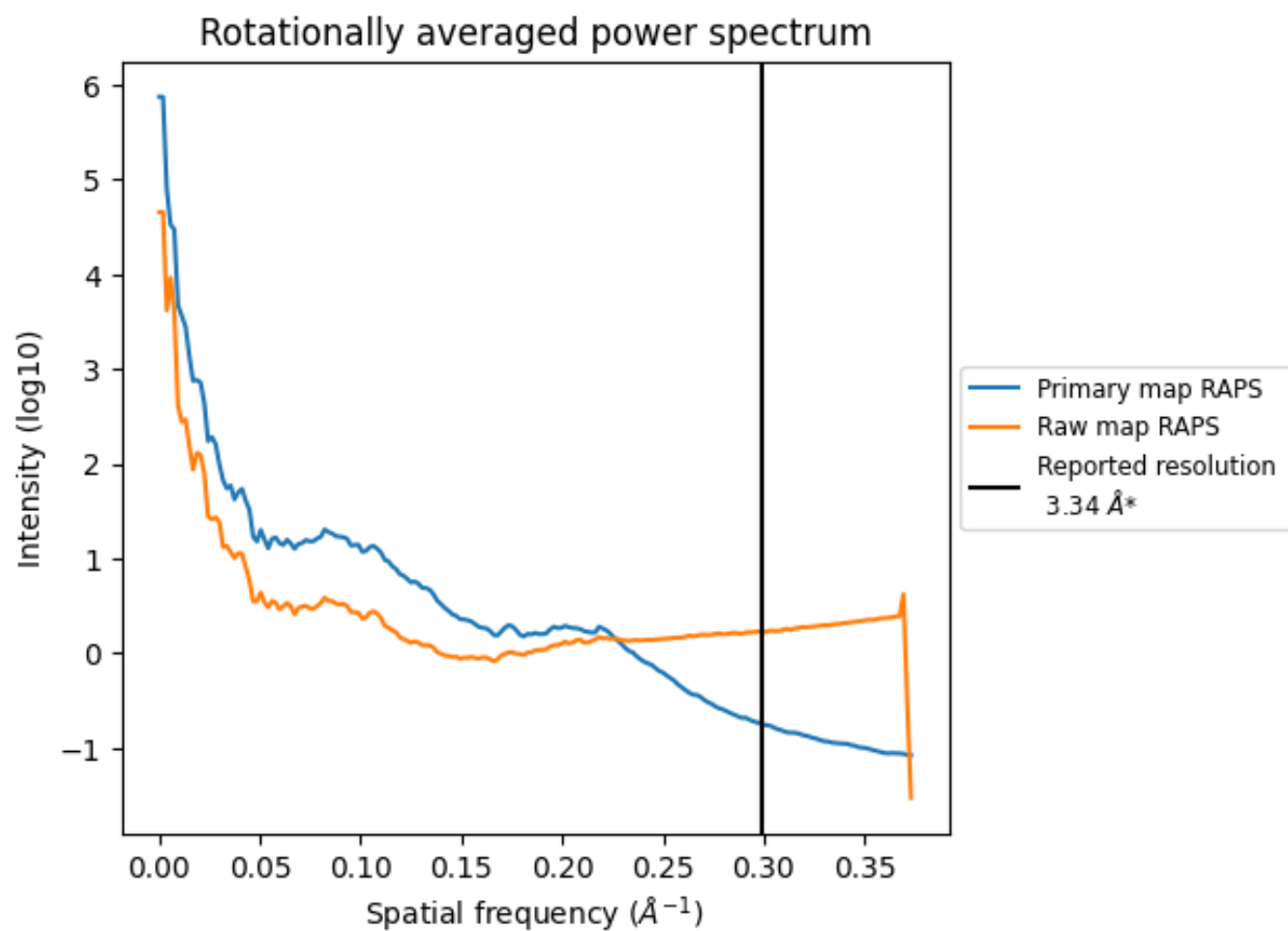
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10584 nm³; this corresponds to an approximate mass of 9561 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

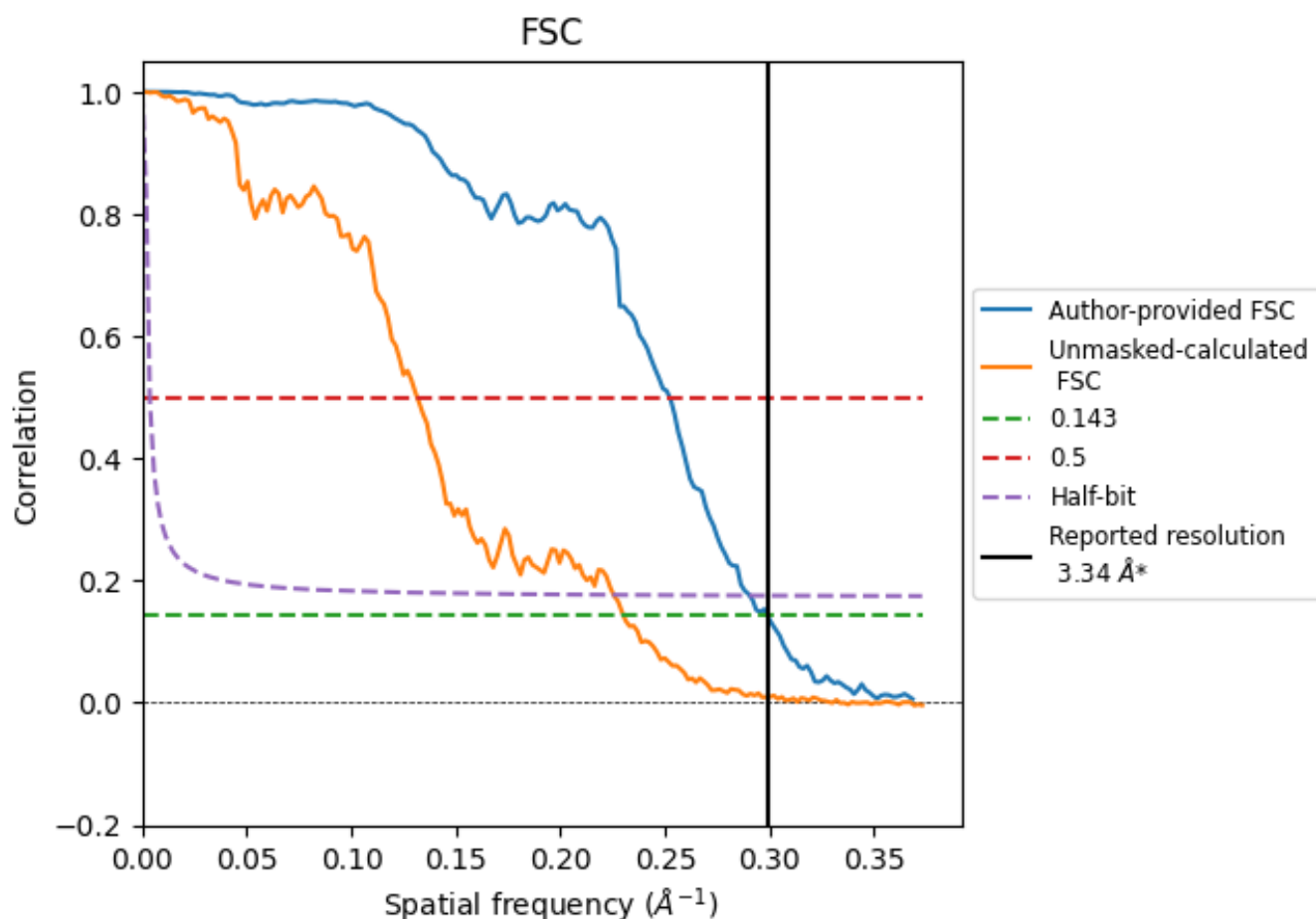


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

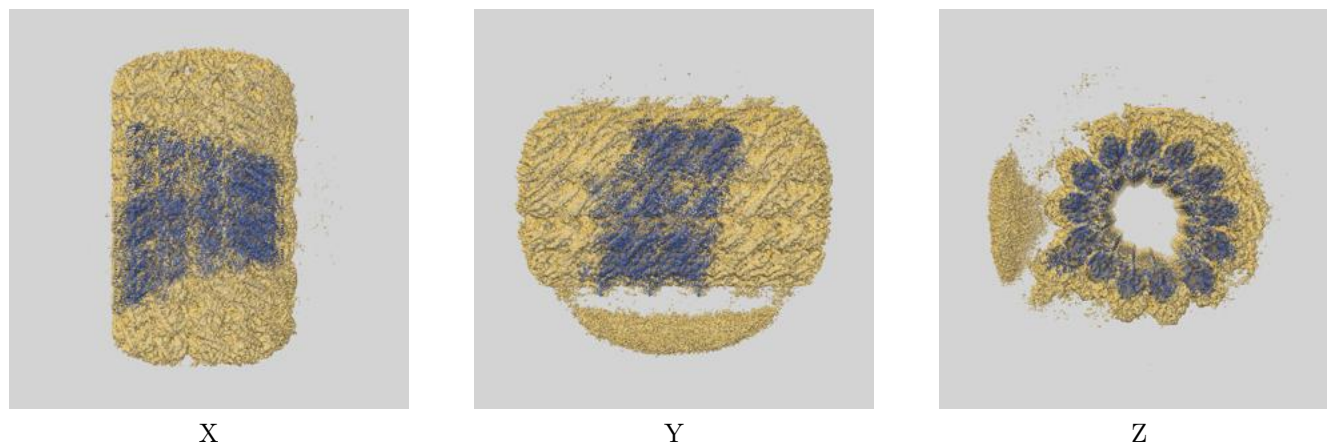
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.96	3.44
Unmasked-calculated*	4.34	7.60	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.34 by more than 10 %

9 Map-model fit [i](#)

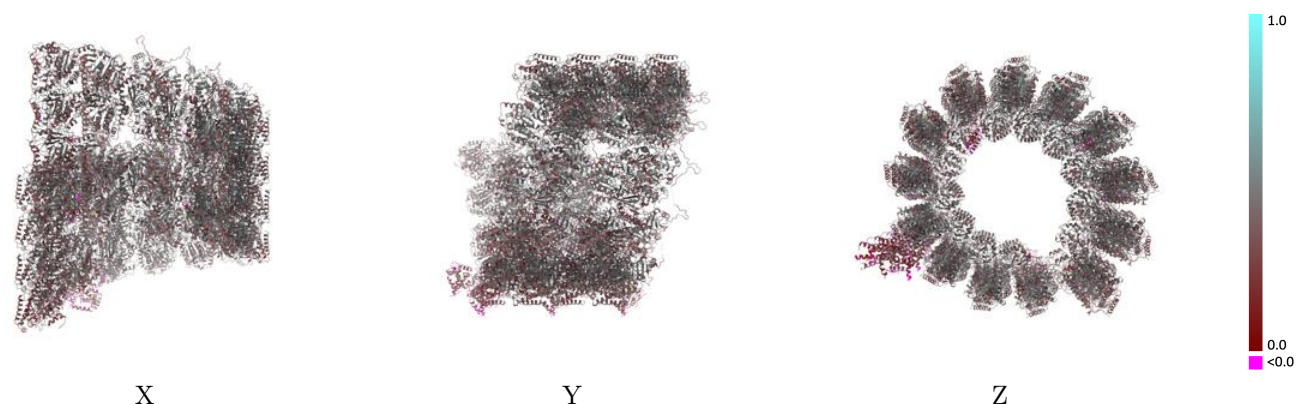
This section contains information regarding the fit between EMDB map EMD-72718 and PDB model 9YA2. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



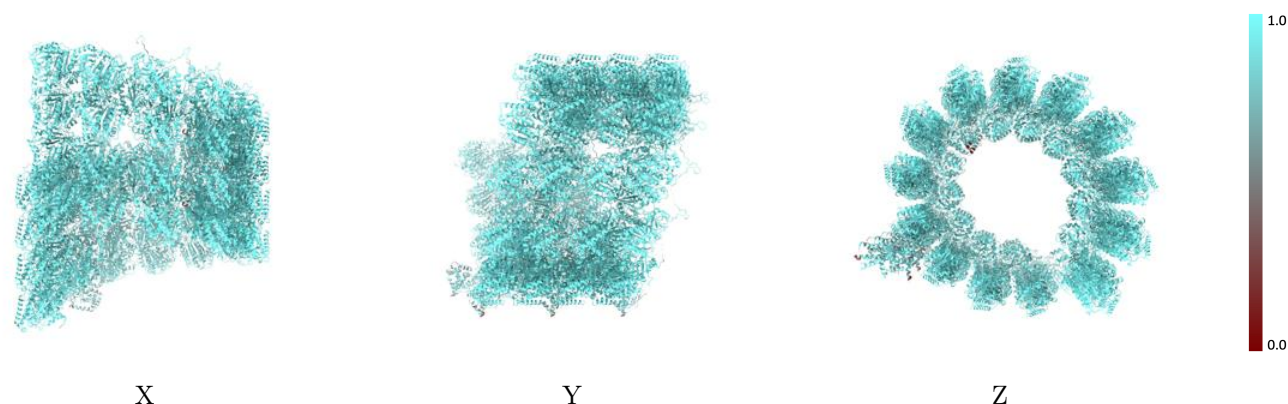
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



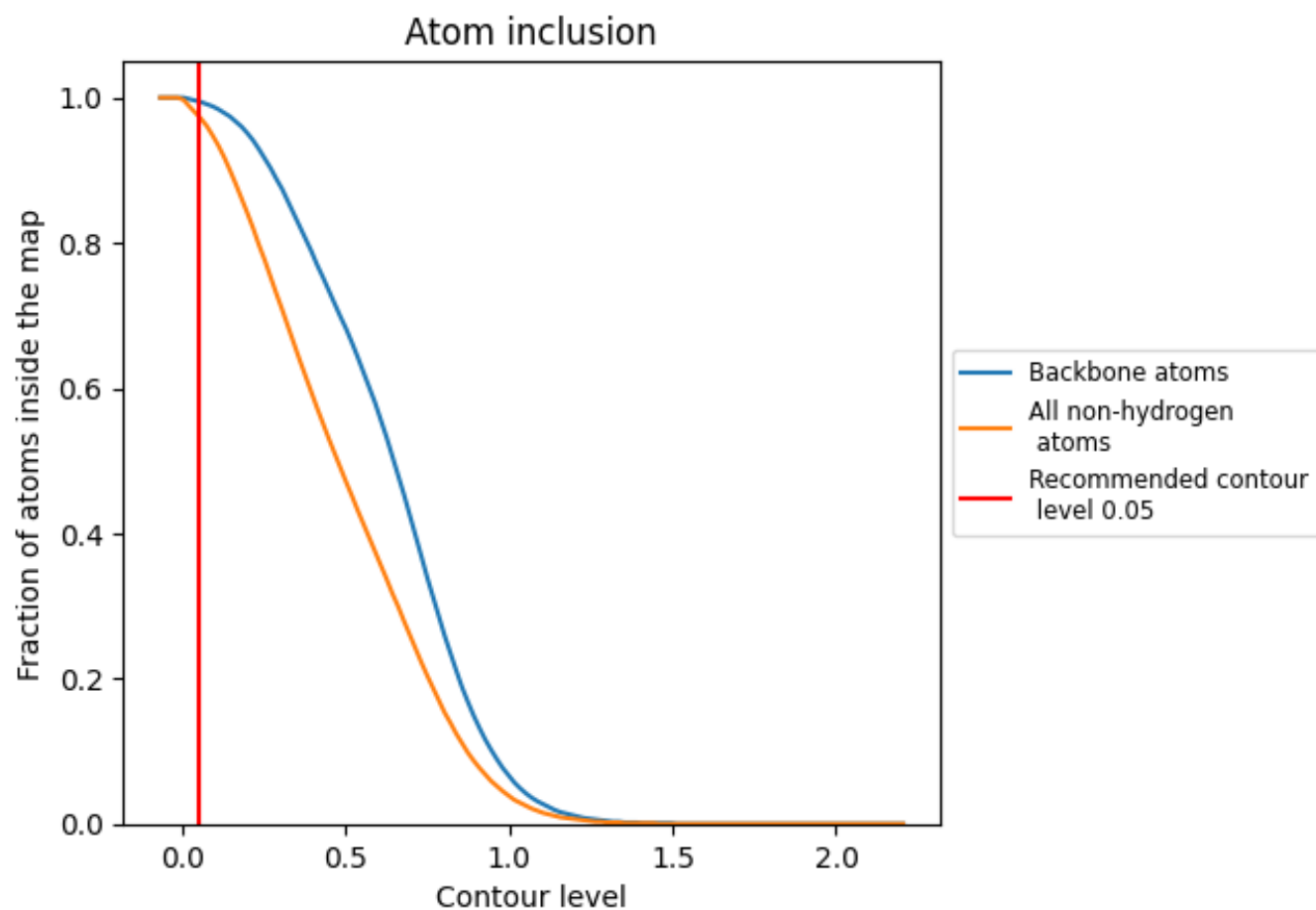
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.3950
A	 0.9580	 0.3710
A0	 0.9900	 0.4020
A1	 0.9850	 0.3950
A2	 0.9910	 0.3960
A3	 0.9710	 0.3350
A4	 0.9910	 0.4120
A5	 0.9890	 0.4100
A6	 0.9890	 0.4060
A7	 0.9810	 0.3730
A8	 0.9830	 0.4030
A9	 0.9880	 0.4070
B	 0.9420	 0.3870
B0	 0.9860	 0.4020
B1	 0.9860	 0.3890
B2	 0.9890	 0.4080
B3	 0.9860	 0.4130
B4	 0.9860	 0.4090
B5	 0.9840	 0.3900
B6	 0.9870	 0.4070
B7	 0.9850	 0.4110
B8	 0.9840	 0.4030
B9	 0.9840	 0.3960
C	 0.9160	 0.3690
C0	 0.9900	 0.4160
C1	 0.9830	 0.3990
C2	 0.9850	 0.4010
C3	 0.9800	 0.3760
C4	 0.9850	 0.4030
C5	 0.9830	 0.4080
C6	 0.9860	 0.3990
C7	 0.9830	 0.3920
C8	 0.9890	 0.4340
C9	 0.9860	 0.4330
D	 0.8810	 0.1270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
D0	 0.9900	 0.4380
D1	 0.9880	 0.4310
D2	 0.9910	 0.4360
D3	 0.9890	 0.4410
D4	 0.9910	 0.4340
D5	 0.9900	 0.4430
D6	 0.9910	 0.4340
D7	 0.9890	 0.4390
D8	 0.9900	 0.4290
D9	 0.9890	 0.4330
E	 0.9160	 0.3410
E0	 0.9920	 0.4210
E1	 0.9940	 0.4240
E2	 0.9910	 0.4240
E3	 0.9920	 0.4280
E4	 0.9880	 0.4020
E5	 0.9900	 0.4200
E6	 0.9940	 0.4230
E7	 0.9900	 0.4180
E8	 0.9830	 0.3910
E9	 0.9870	 0.4100
F	 0.9140	 0.3570
F0	 0.9840	 0.3850
F1	 0.9910	 0.4070
G	 0.9290	 0.3540
H	 0.9460	 0.3580
I	 0.8660	 0.3380
J	 0.9610	 0.3750
K	 0.9570	 0.3820
L	 0.7910	 0.2090
M	 0.7520	 0.1490
N	 0.7980	 0.1980
O	 0.9200	 0.3270
P	 0.9100	 0.3050
Q	 0.7850	 0.1870
R	 0.9170	 0.3060
S	 0.9420	 0.3510
T	 0.9240	 0.3170
U	 0.9260	 0.3230
V	 0.7790	 0.1570
W	 0.8070	 0.1890
a	 0.9850	 0.3830

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9780	 0.3730
c	 0.9780	 0.4050
d	 0.9790	 0.3920
e	 0.9800	 0.4010
f	 0.9830	 0.3910
g	 0.9830	 0.3980
h	 0.9780	 0.3990
i	 0.9750	 0.3920
j	 0.9760	 0.3830
k	 0.9410	 0.3150
l	 0.9630	 0.3320
m	 0.8950	 0.3390
n	 0.8940	 0.3260
o	 0.9810	 0.4180
p	 0.9820	 0.4260
q	 0.9750	 0.4330
r	 0.9830	 0.4250
s	 0.9800	 0.4260
t	 0.9830	 0.4300
u	 0.9800	 0.4010
v	 0.9780	 0.4110
w	 0.9730	 0.3850
x	 0.9590	 0.3910