



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 07:55 PM EDT

PDB ID : 7MIZ
EMDB ID : EMD-23869
Title : Atomic structure of cortical microtubule from *Toxoplasma gondii*
Authors : Wang, X.; Brown, A.; Sibley, L.D.; Zhang, R.
Deposited on : 2021-04-18
Resolution : 3.40 Å (reported)
Based on initial models : 6U42, 4FYU, 3JAS

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

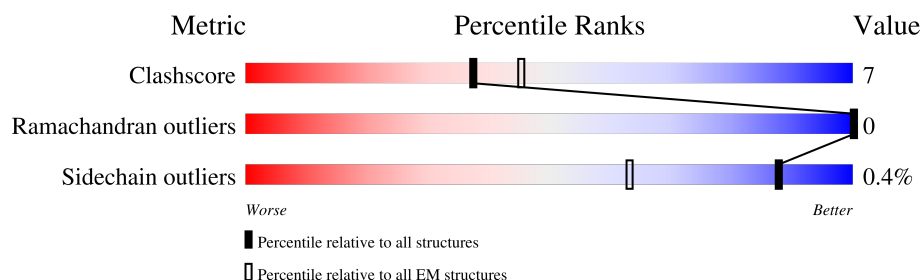
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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





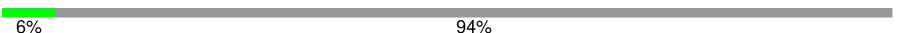












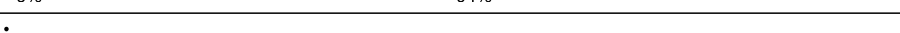
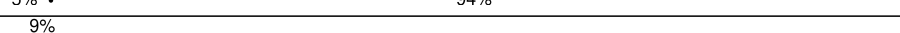








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	0	351	5% • 94%
1	1	351	5% • 94%
1	10	351	5% • 94%
1	11	351	6% 94%
1	12	351	5% • 94%
1	13	351	6% 94%
1	14	351	6% 94%
1	15	351	6% 94%


























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Mol	Chain	Length	Quality of chain
1	16	351	 6% • 94%
1	17	351	 6% • 94%
1	18	351	 6% • 94%
1	19	351	 6% • 94%
1	2	351	 6% • 94%
1	20	351	 6% • 94%
1	21	351	 6% • 94%
1	22	351	 5% • 94%
1	23	351	 5% • 94%
1	3	351	 6% • 94%
1	4	351	 6% • 94%
1	5	351	 6% • 94%
1	6	351	 6% • 94%
1	7	351	 5% • 94%
1	8	351	 6% • 94%
1	9	351	 5% • 94%
2	A0	453	 9% 76% 18% 6%
2	A2	453	 8% 75% 19% 6%
2	A4	453	 80% 14% • 6%
2	A6	453	 78% 17% 6%
2	A8	453	 76% 18% 6%
2	B0	453	 79% 15% 6%
2	B2	453	 80% 15% 6%
2	B4	453	 74% 20% 6%
2	B6	453	 77% 17% • 6%

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Mol	Chain	Length	Quality of chain
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	
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	











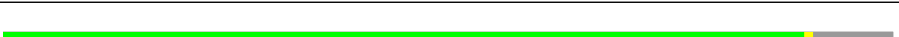


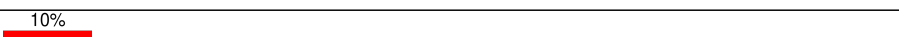
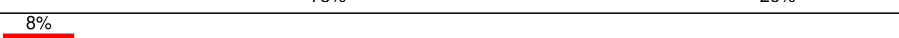
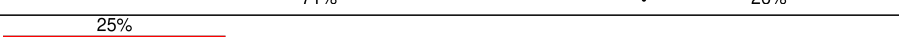

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Mol	Chain	Length	Quality of chain
3	B7	449	
3	B9	449	
3	C1	449	
3	C3	449	
3	C5	449	
3	C7	449	
3	C9	449	
3	D1	449	
3	D3	449	
3	D5	449	
3	D7	449	
3	D9	449	
3	E1	449	
3	E3	449	
3	E5	449	
3	E7	449	
3	E9	449	
3	F1	449	
4	a	220	
4	b	220	
4	c	220	
4	d	220	
4	e	220	
4	f	220	
4	g	220	

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Mol	Chain	Length	Quality of chain
4	h	220	 90% • 9%
4	i	220	 91% • 9%
4	j	220	 91% • 9%
4	m	220	 20% • 9%
4	n	220	 20% • 9%
4	o	220	 90% • 9%
4	p	220	 90% • 9%
4	q	220	 90% • 9%
4	r	220	 90% • 9%
4	s	220	 91% • 9%
4	t	220	 90% • 9%
4	u	220	 90% • 9%
4	v	220	 90% • 9%
5	k	189	 10% • 26%
5	l	189	 8% • 26%
5	w	189	 25% • 24%
5	x	189	 15% • 24%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 214754 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	0	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	1	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	2	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	3	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	4	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	5	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	6	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	7	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	8	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	9	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	10	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	11	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	12	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	13	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	14	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	15	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	16	22	Total	C	N	O	S	0	0
			174	114	28	31	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	17	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	18	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	19	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	20	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	21	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	22	20	Total	C	N	O	S	0	0
			160	105	26	28	1		
1	23	20	Total	C	N	O	S	0	0
			160	105	26	28	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	93	ARG	PRO	conflict	UNP A0A7J6K285
1	93	ARG	PRO	conflict	UNP A0A7J6K285
2	93	ARG	PRO	conflict	UNP A0A7J6K285
3	93	ARG	PRO	conflict	UNP A0A7J6K285
4	93	ARG	PRO	conflict	UNP A0A7J6K285
5	93	ARG	PRO	conflict	UNP A0A7J6K285
6	93	ARG	PRO	conflict	UNP A0A7J6K285
7	93	ARG	PRO	conflict	UNP A0A7J6K285
8	93	ARG	PRO	conflict	UNP A0A7J6K285
9	93	ARG	PRO	conflict	UNP A0A7J6K285
10	93	ARG	PRO	conflict	UNP A0A7J6K285
11	93	ARG	PRO	conflict	UNP A0A7J6K285
12	93	ARG	PRO	conflict	UNP A0A7J6K285
13	93	ARG	PRO	conflict	UNP A0A7J6K285
14	93	ARG	PRO	conflict	UNP A0A7J6K285
15	93	ARG	PRO	conflict	UNP A0A7J6K285
16	93	ARG	PRO	conflict	UNP A0A7J6K285
17	93	ARG	PRO	conflict	UNP A0A7J6K285
18	93	ARG	PRO	conflict	UNP A0A7J6K285
19	93	ARG	PRO	conflict	UNP A0A7J6K285
20	93	ARG	PRO	conflict	UNP A0A7J6K285
21	93	ARG	PRO	conflict	UNP A0A7J6K285
22	93	ARG	PRO	conflict	UNP A0A7J6K285
23	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	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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		
3	C3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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 PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	150	Total 1198	C 763	N 213	O 217	S 5	0	0
4	b	150	Total 1198	C 763	N 213	O 217	S 5	0	0
4	c	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	d	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	e	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	f	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	g	201	Total 1608	C 1021	N 283	O 297	S 7	0	0

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

- Molecule 5 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
5	l	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
5	w	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		
5	x	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		

There are 92 discrepancies between the modelled and reference sequences:

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

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

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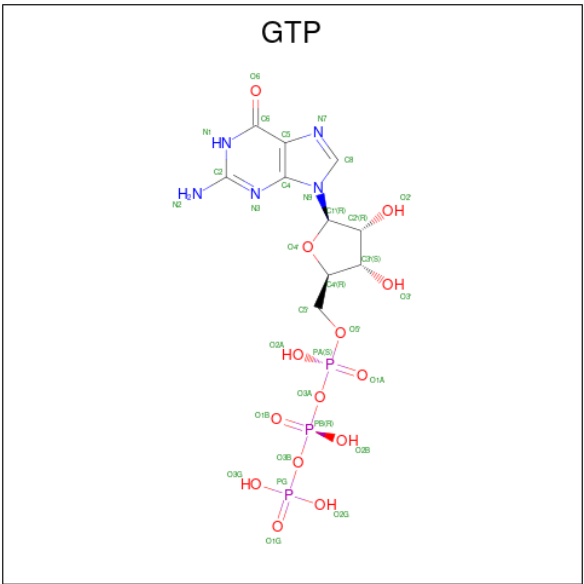
Chain	Residue	Modelled	Actual	Comment	Reference
l	187	GLN	-	insertion	UNP A0A7J6K232
l	188	ASN	-	insertion	UNP A0A7J6K232
l	189	VAL	-	insertion	UNP A0A7J6K232
w	167	SER	-	insertion	UNP A0A7J6K232
w	168	ALA	-	insertion	UNP A0A7J6K232
w	169	GLN	-	insertion	UNP A0A7J6K232
w	170	ARG	-	insertion	UNP A0A7J6K232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

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Chain	Residue	Modelled	Actual	Comment	Reference
x	183	LYS	-	insertion	UNP A0A7J6K232
x	184	ARG	-	insertion	UNP A0A7J6K232
x	185	LEU	-	insertion	UNP A0A7J6K232
x	186	PRO	-	insertion	UNP A0A7J6K232
x	187	GLN	-	insertion	UNP A0A7J6K232
x	188	ASN	-	insertion	UNP A0A7J6K232
x	189	VAL	-	insertion	UNP A0A7J6K232

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

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Mol	Chain	Residues	Atoms					AltConf
6	B4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	B6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	B8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

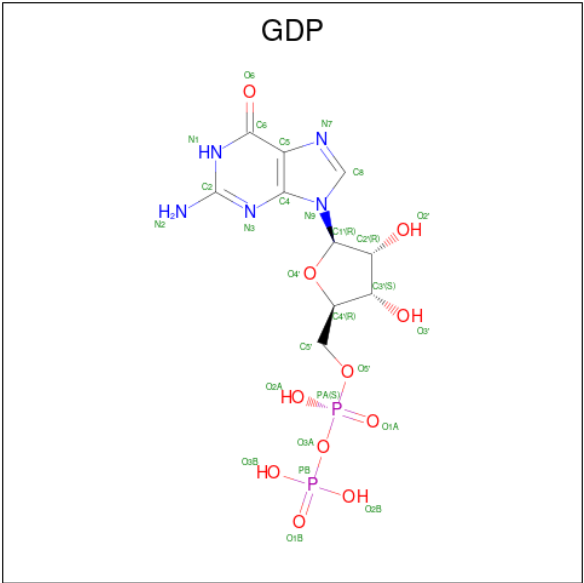
Mol	Chain	Residues	Atoms	AltConf
7	A0	1	Total Mg 1 1	0
7	A2	1	Total Mg 1 1	0
7	A4	1	Total Mg 1 1	0
7	A6	1	Total Mg 1 1	0
7	A8	1	Total Mg 1 1	0
7	B0	1	Total Mg 1 1	0
7	B2	1	Total Mg 1 1	0
7	B4	1	Total Mg 1 1	0
7	B6	1	Total Mg 1 1	0
7	B8	1	Total Mg 1 1	0
7	C0	1	Total Mg 1 1	0
7	C2	1	Total Mg 1 1	0
7	C4	1	Total Mg 1 1	0
7	C6	1	Total Mg 1 1	0
7	C8	1	Total Mg 1 1	0
7	D0	1	Total Mg 1 1	0
7	D2	1	Total Mg 1 1	0
7	D4	1	Total Mg 1 1	0
7	D6	1	Total Mg 1 1	0
7	D8	1	Total Mg 1 1	0
7	E0	1	Total Mg 1 1	0
7	E2	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
7	E4	1	Total	Mg	0
			1	1	
7	E6	1	Total	Mg	0
			1	1	
7	E8	1	Total	Mg	0
			1	1	
7	F0	1	Total	Mg	0
			1	1	

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

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Mol	Chain	Residues	Atoms					AltConf
8	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	B9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	F1	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 1: Microtubule associated protein SPM1

Chain 2: 6% 94%

MET	SER	GLY	GLN	ASN	SER	ASN	THR	PRO	LYS	LEU	PRO	SER	GLU	GLY	SER	ASP	TYR	GLY	TYR	PRO	GLN	LYS	GLN	PRO	TYR	LEU	PRO	LYS	GLU	GLN	ALA	ALA	CYS	CYS	LYS	GLY	ASN	ASP	ALA	TYR	LYS	GLY	ALA	SER	HIS	GLY	THR	VAL	GLN	PRO
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SER	HIS	PRO	GLU	GLU	ALA	GLN	LYS	TYR	ALA	ALA	GLY	ALA	ALA	ALA	GLY	GLY	GLU	THR	ILE	GLN	ARG	GLY	GLY	ARG	GLU	ARG	ASP	ARG	GLN	PRO	ALA	ALA	ALA	GLY	ASP	VAL	PRO	VAL	ALA	ALA	ARG	ARG	LEU	HIS	LEU	SER	SER	ASP	VAL	ASP	GLU	ALA	ALA	ALA	HIS	GLY	ARG	SER	SER	PRO	GLN	SER	ARG	HIS
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PRO	GLY	TYR	CYS	VAL	GLU	GLU	LEU	CYS	THR	GLY	MET	HIS	LYS	CYS	ILE	PRO	SER	ARG	ALA	PRO	PRO	PRO	PRO	THR	GLY	SER	THR	SER	GLN	TYR	ARG	GLU	GLN	PHE	VAL	PRO	PRO	LYS	PRO	PRO	LEU	PRO	PRO	PRO	THR	GLN	GLN	VAL	GLN	SER	THR	LEU	THR	PRO	PRO	PRO	PRO	PHE	GLU	ALA	GLN	GLN
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[illegible]

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

LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	TRP	TYR
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- Molecule 1: Microtubule associated protein SPM1

Chain 3: 6% 94%

MET	SER	GLY	GLY	ASN	ASN	THR	PRO	LYS	LEU	PRO	SER	GLU	GLY	SER	ASP	TYR	TYR	PRO	PRO	GLN	LYS	LYS	PRO	GLN	LYS	LEU	PRO	LYS	SER	GLU	GLN	ALA	ALA	CYS	CYS	LYS	GLY	GLY	ASN	ASP	ASP	ALA	ALA	TYR	LYS	VAL	THR	GLN	PHE
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SER	HIS	PRO	GLU	GLY	ALA	GLN	LYS	TYR	ALA	ALA	ALA	ALA	ALA	GLY	THR	ILE	GLN	ARG	GLY	ARG	GLY	ARG	VAL	ALA	ALA	ALA	ASP	ARG	GLN	PRO	ARG	ALA	ALA	ALA	GLY	ASP	VAL	PRO	PRO	ALA	ARG	ALA	ARG	ARG	LEU	HIS	LEU	SER	SER	ASP	VAL	ASP	GLU	ALA	ALA	HIS	GLY	ARG	GLN	SER	PRO	SER	SER	ARG	HIS
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PRO	GLY	TYR	CYS	VAL	GLU	GLU	LEU	CYS	THR	CYS	GLY	MET	HIS	LYS	CYS	ILE	PRO	SER	ARG	ALA	PRO	VAL	PRO	PHE	THR	GLY	SER	THR	GLN	TYR	ARG	GLN	GLU	PHE	VAL	PRO	PRO	LYS	PRO	LEU	PRO	PRO	PRO	THR	GLN	VAL	SER	GLN	VAL	THR	LEU	PRO	PRO	PHE	GLU	ALA
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SER	SER	TYR	ARG	THR	GLU	PHE	VAL	ALA	LYS	PRO	LEU	PRO	PRO	PRO	PRO	LYS	PHE	SER	GLU	VAL	LYS	LEU	PRO	PRO	THR	LEU	LEU	PRO	PHE	PHE	HIS	GLY	GLU	SER	SER	TYR	VAL	PRO	PRO	LYS	PRO	LEU	LEU	GLU	VAL	LYS	LEU	PRO	P237	P242
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R248	S249	E250	P258	PRO	VAL	GLN	THR	VAL	GLU	LYS	LEU	PRO	PRO	SER	SER	LEU	PRO	PHE	GLU	GLY	SER	THR	HIS	TYR	ARG	ASP	GLU	PHE	GLN	VAL	LYS	PRO	PRO	PRO	ALA	THR	LYS	LYS	VAL	THR	THR	LEU	ASP	ALA	THR	SER	TYR	ARG	PRO
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ASP	TYR	VAL	ALA	LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	TRP	TYR
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- Molecule 1: Microtubule associated protein SPM1

Chain 4: 6% 94%

MET	SER	GLY	GLY	ASN	ASN	THR	PRO	LYS	LEU	PRO	PRO	GLY	GLY	ASP	TYR	GLY	GLY	PRO	PRO	GLN	GLN	LYS	TYR	TYR	LEU	PRO	LYS	GLY	GLU	GLN	ALA	ALA	CYS	CYS	LYS	GLY	GLY	ASN	ASP	ALA	ALA	TYR	LYS	GLY	GLY	ALA	GLY	SER	HIS	GLY	THR	VAL	GLN	PRO
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SER	HIS	PRO	PRO	GLU	GLU	ALA	GLN	LYS	TYR	ALA	ALA	GLY	GLY	ALA	ALA	GLU	THR	ILE	GLN	ARG	GLY	ARG	GLU	ARG	VAL	ALA	ALA	ALA	ASP	ASP	GLN	PRO	ARG	ALA	ALA	GLY	ASP	VAL	VAL	PRO	PRO	ALA	ARG	ARG	LEU	HIS	LEU	SER	ASP	VAL	ASP	ALA	ALA	HIS	GLY	GLN	SER	PRO	SER	SER	ARG	HIS
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VAL	LYS	SER	ASN	PRO	ILE	CYS	PRO	GLU	SER	LYS	LEU	PRO	GLN	TYR	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	PRO	ASP	ASP	THR	GLN	GLN	TRP	TYR
E250	P258	PRO	VAL	GLN	THR	VAL	GLU	VAL	LYS	LEU	PRO	PRO	SER	GLY	GLY	THR	SER	GLN	ASP	PHE	GLU	GLN	ARG	THR	GLN	VAL	VAL	VAL	LYS	PRO	LEU	THR	ASP
SER	SER	TYR	ARG	THR	PHE	VAL	ALA	LYS	PRO	LEU	PRO	PRO	PRO	ALA	LYS	PHE	SER	GLU	VAL	LYS	LEU	PRO	THR	PRO	THR	VAL	ARG	THR	ASP	TYR	VAL	PRO	GLY
PRO	GLY	TYR	CYS	GLU	GLU	LEU	CYS	THR	CYS	GLY	GLY	NET	HIS	LYS	CYS	ILE	PRO	ARG	SER	PRO	THR	GLN	THR	SER	THR	GLY	GLY	THR	TYR	ARG	PRO	PRO	GLY

- Molecule 1: Microtubule associated protein SPM1

Chain 5:  6% 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 6:  6% 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 7: 5% • 94%

MET	SER	Gly	GLY	ASN	SER	THR	PRO	LYS	LEU	PRO	SER	GLU	GLY	SER	ASP	Tyr	TYR	PRO	PRO	GLN	LYS	GLN	LYS	LEU	PRO	LYS	GLU	GLN	ALA	ALA	CYS	CYS	LYS	GLY	GLY	ASN	ASP	ALA	ALA	TYR	LYS	VAL	THR	GLN	PHE
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SER	HIS	PRO	GLU	GLU	ALA	GLN	LYS	TYR	ALA	ALA	GLY	ALA	ALA	ALA	GLY	GLY	GLU	THR	ILE	GLN	ARG	GLY	GLU	ARG	GLU	ARG	ASP	ARG	GLN	PRO	ALA	ALA	ALA	GLY	ASP	VAL	PRO	ALA	ALA	ARG	ARG	LEU	HIS	LEU	SER	SER	ASP	VAL	ASP	GLU	ALA	ALA	ALA	HIS	ARG	GLY	GLN	SER	SER	SER	ARG	HIS
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PRO	GLY	TYR	CYS	VAL	GLU	GLU	LEU	CYS	THR	GLY	MET	HIS	LYS	CYS	ILE	PRO	SER	ARG	ALA	PRO	PRO	PRO	PRO	THR	GLY	SER	THR	SER	GLN	TYR	ARG	GLN	GLU	GLU	PHE	VAL	PRO	PRO	LYS	LEU	PRO	PRO	PRO	THR	GLN	GLN	VAL	GLN	SER	SER	GLN	VAL	THR	LEU	THR	PRO	PRO	PRO	SER	PRO	LEU	PRO	PRO	PHE	GLU	THR	ALA	GLN	GLN
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SER	SER	TYR	ARG	THR	GLU	PHE	VAL	ALA	ALA	PRO	PRO	PRO	PRO	ALA	ALA	PHE	SER	GLU	VAL	LYS	LYS	LEU	LEU	PRO	PRO	THR	PRO	PRO	THR	LEU	LEU	PRO	PHE	PHE	HIS	GLY	GLY	SER	SER	ALA	ALA	TYR	ARG	THR	ASP	TYR	VAL	VAL	LYS	PRO	PRO	LEU	LEU	GLU	GLU	VAL	VAL	LYS	LYS	LEU	LEU	PRO	PRO	9237	9244
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[illegible]

SER	ASP	TYR	VAL	ALA	LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	GLN	TRP	TYR
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- Molecule 1: Microtubule associated protein SPM1

Chain 8:  6% 94%

MET	SER	GLY	GLY	ASN	ASN	THR	PRO	LYS	LYS	LEU	PRO	PRO	SER	GLU	GLY	GLY	SER	ASP	TYR	TYR	TYR	PRO	PRO	GLN	LYS	LYS	LEU	PRO	LYS	SER	GLU	GLN	ALA	ALA	CYS	CYS	LYS	LYS	GLY	GLY	ASN	ASP	ALA	ALA	TYR	LYS	TYR	VAL	THR	GLN	PHE
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SER	HIS	PRO	HIS	GLU	GLY	ALA	ALA	GLN	LYS	TYR	ALA	ALA	GLY	GLY	ALA	ALA	GLU	THR	ILE	GLN	ARG	GLY	ARG	GLY	ARG	GLY	ASP	ASP	GLN	GLN	PRO	PRO	VAL	ASP	GLY	LEU	ARG	ARG	HIS	HIS	LEU	SER	SER	ASP	VAL	ASP	GLU	ALA	GLY	HIS	HIS	ARG	ARG	GLY	GLN	SER	SER	PRO	PRO	SER	SER	ARG	HIS
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PRO	GLY	TYR	CYS	VAL	GLU	GLU	LEU	CYS	THR	CYS	GLY	MET	HIS	LYS	CYS	CYS	ILE	PRO	SER	ARG	ALA	PRO	PRO	VAL	PHE	GLN	TYR	ARG	GLN	GLU	PHE	VAL	PRO	PRO	LYS	PRO	PRO	LEU	PRO	PRO	THR	GLN	VAL	SER	SER	GLN	VAL	THR	LEU	PRO	PRO	SER	LEU	PRO	PHE	GLU	PHE	ALA	THR
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SER	SER	TYR	ARG	THR	GLU	PHE	VAL	ALA	LYS	PRO	LEU	PRO	PRO	PRO	PRO	ALA	LYS	PHE	SER	GLU	VAL	LYS	LEU	PRO	PRO	THR	LEU	PHE	HIS	GLY	GLU	SER	ALA	TYR	ARG	THR	ASP	TYR	VAL	PRO	LYS	PRO	LEU	GLU	GLU	VAL	VAL	LYS	LEU	PRO	GLU	VAL	LYS	LEU	PRO	P237	T238
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[illegible]

TYR	VAL	ALA	LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	TRP	TYR
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- Molecule 1: Microtubule associated protein SPM1

Chain 9:  5% 94%

MET	SER	GLY	GLY	ASN	ASN	THR	PRO	LYS	LEU	PRO	SER	GLU	GLY	GLY	SER	ASP	TYR	GLY	TYR	PRO	GLN	LYS	PRO	GLN	LYS	TYR	LEU	PRO	LYS	SER	GLU	GLN	ALA	ALA	CYS	CYS	LYS	GLY	GLY	ASN	ASP	ALA	ALA	TYR	LYS	VAL	THR	GLN	PHE
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[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 10: 5% • 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 11:  6% 94%

[illegible]

SER	PRO	PRO	GLU	GLU	ALA	GLN	LYS	TYR	ALA	ALA	ALA	ALA	ALA	THR	THR	ILE	GLN	ARG	GLY	ARG	GLU	VAL	ALA	ALA	ASP	ARG	GLN	PRO	ARG	ALA	ALA	GLY	ASP	VAL	PRO	ALA	ARG	ARG	ARG	LEU	LEU	LEU	HIS	LEU	SER	SER	ASP	VAL	ASP	ASP	GLU	ALA	ALA	HIS	ARG	GLY	GLN	GLN	SER	PRO	SER	ARG	HIS
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[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 15:  6% 94%

[illegible]

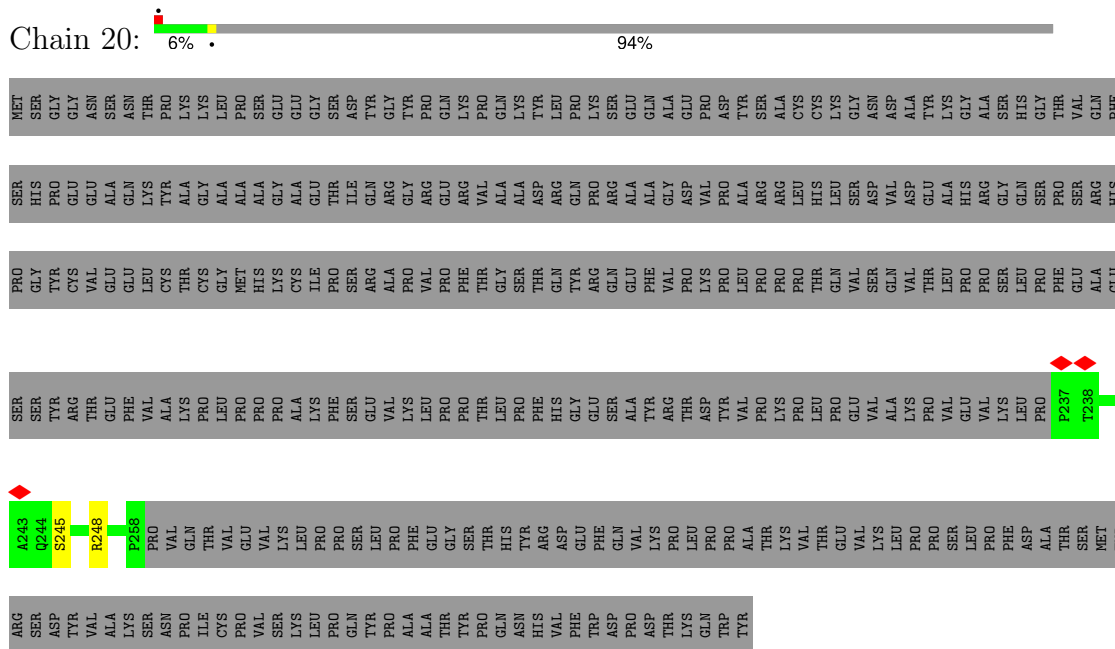
- Molecule 1: Microtubule associated protein SPM1

Chain 16: 6% • 94%

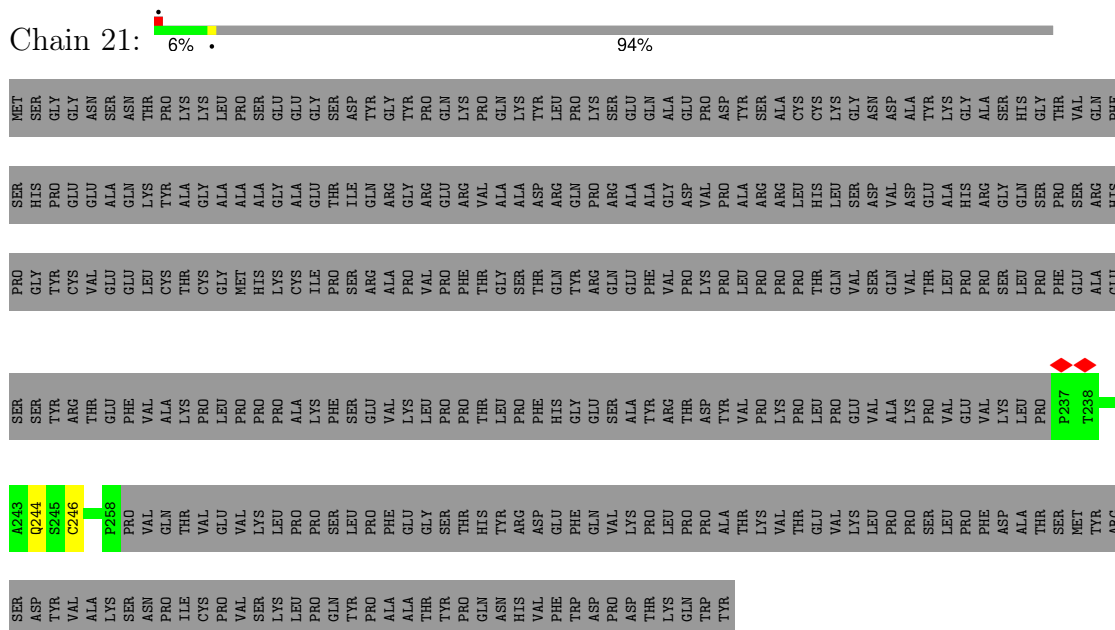
[illegible]

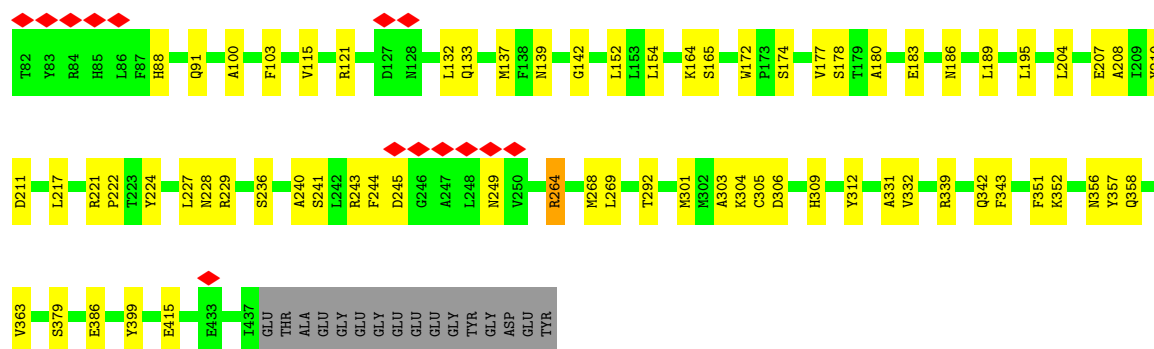
- Molecule 1: Microtubule associated protein SPM1

- Molecule 1: Microtubule associated protein SPM1

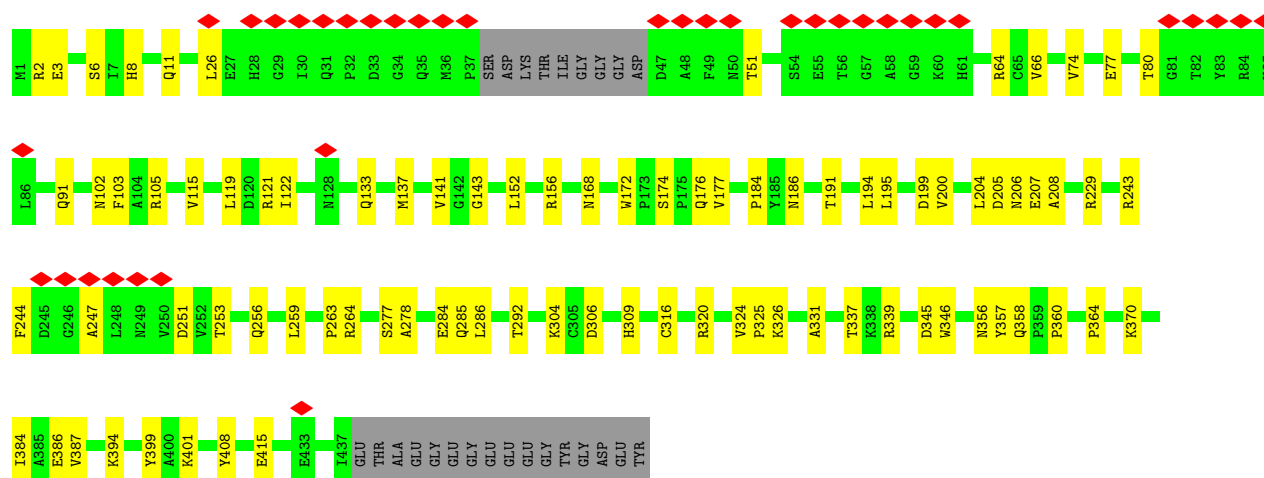
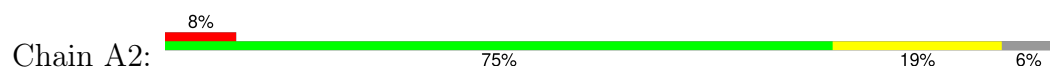


- Molecule 1: Microtubule associated protein SPM1

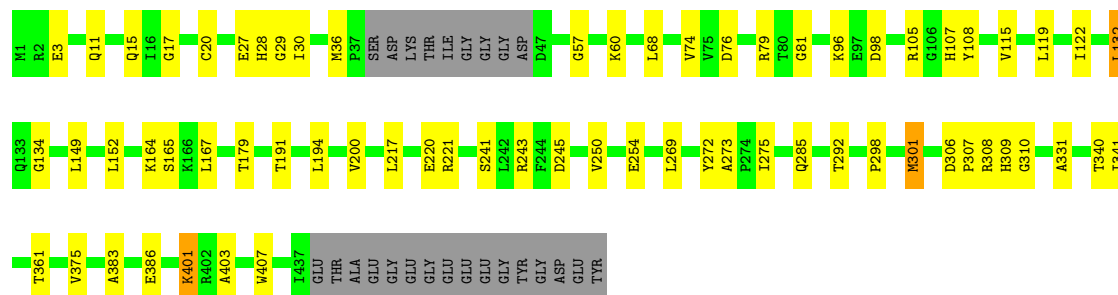
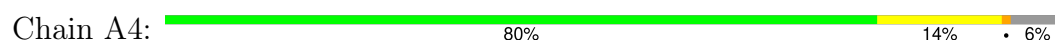




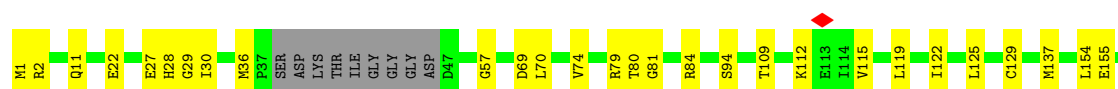
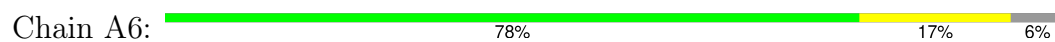
• Molecule 2: Tubulin alpha chain

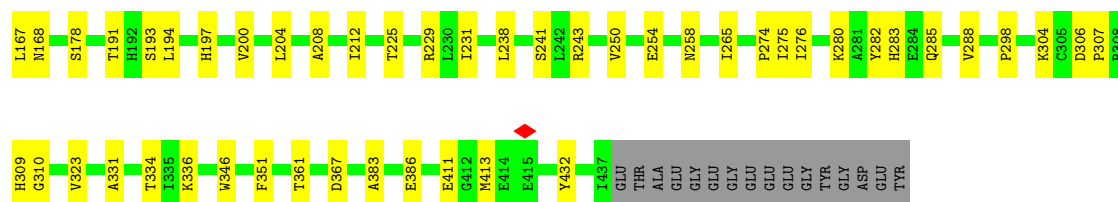


• Molecule 2: Tubulin alpha chain



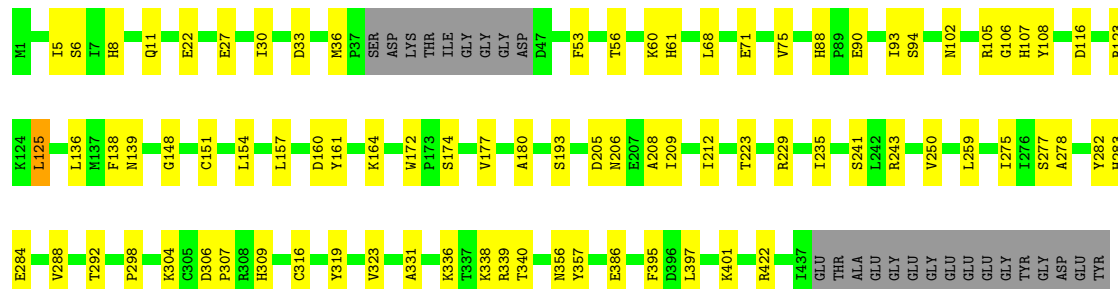
• Molecule 2: Tubulin alpha chain





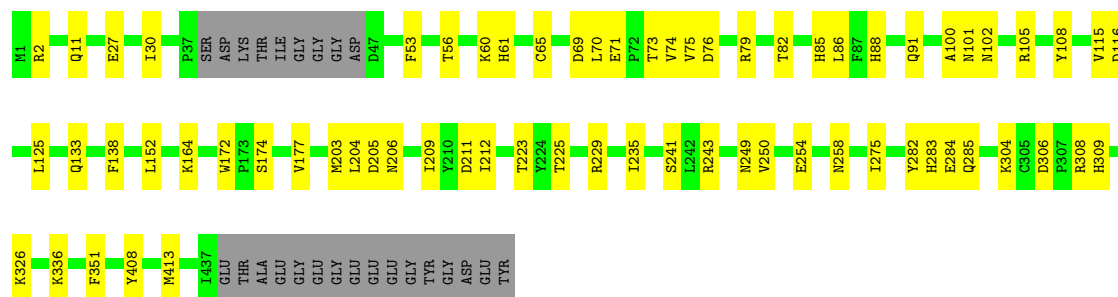
• Molecule 2: Tubulin alpha chain

Chain A8: 76% 18% 6%



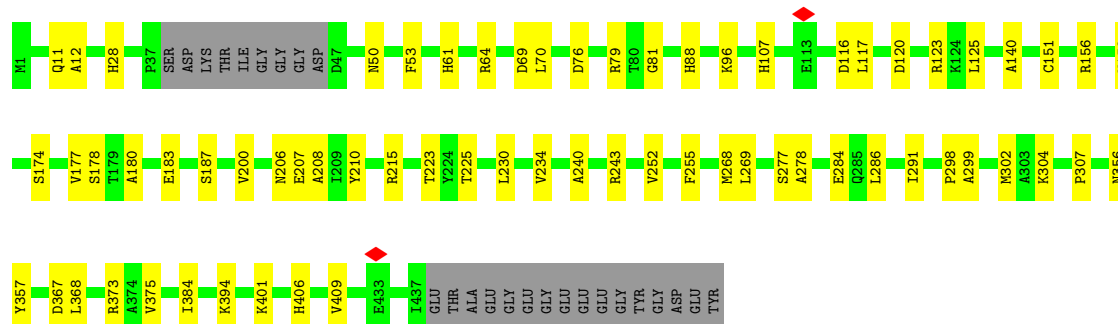
• Molecule 2: Tubulin alpha chain

Chain B0: 79% 15% 6%



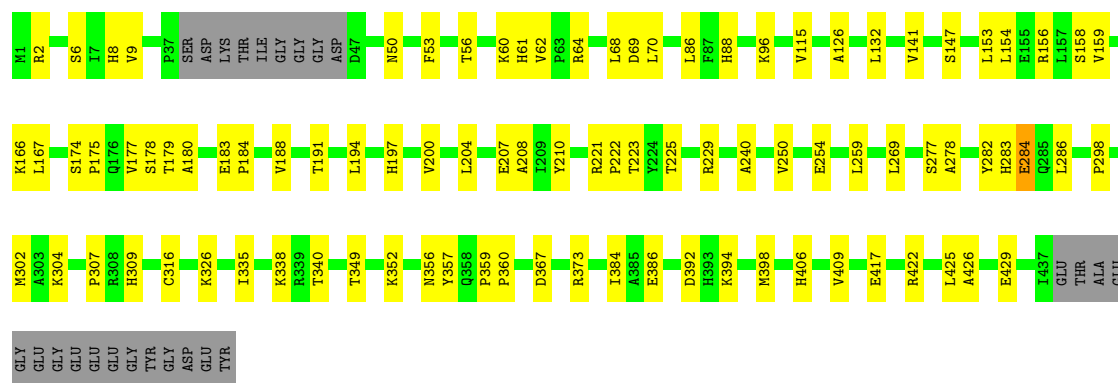
• Molecule 2: Tubulin alpha chain

Chain B2: 80% 15% 6%




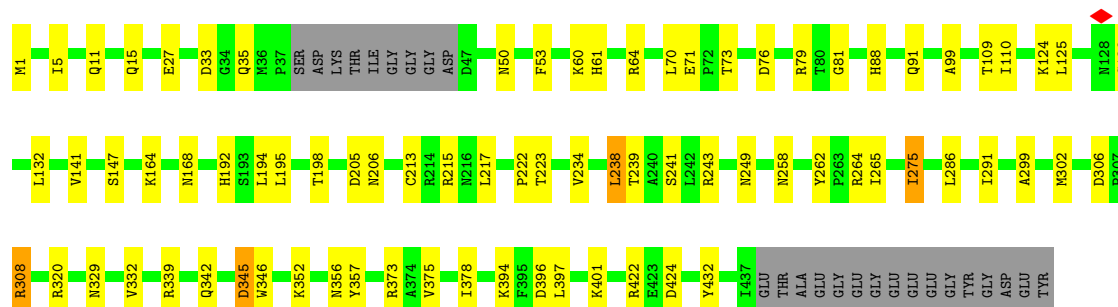
• Molecule 2: Tubulin alpha chain

Chain B4: 



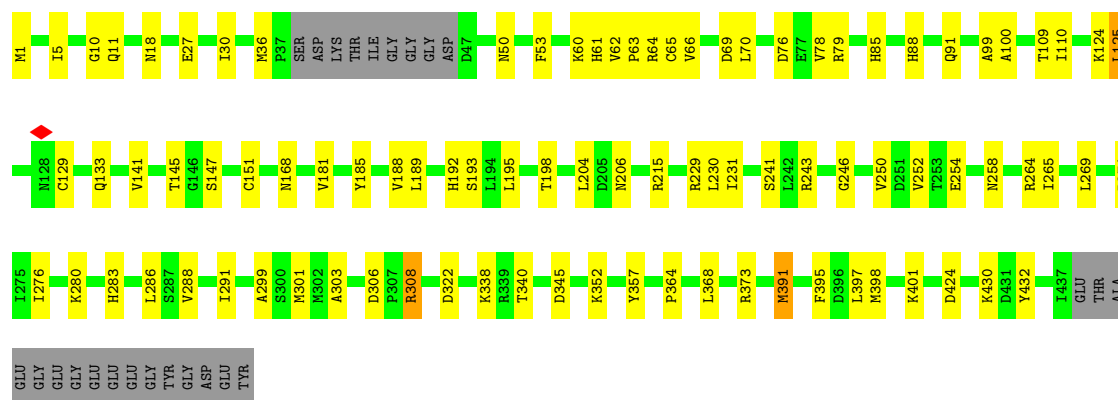
- Molecule 2: Tubulin alpha chain

Chain B6: 



- Molecule 2: Tubulin alpha chain

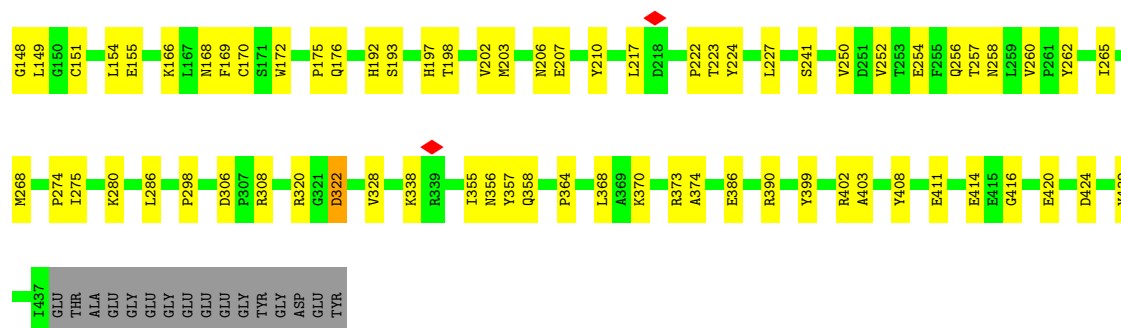
Chain B8: 



- Molecule 2: Tubulin alpha chain

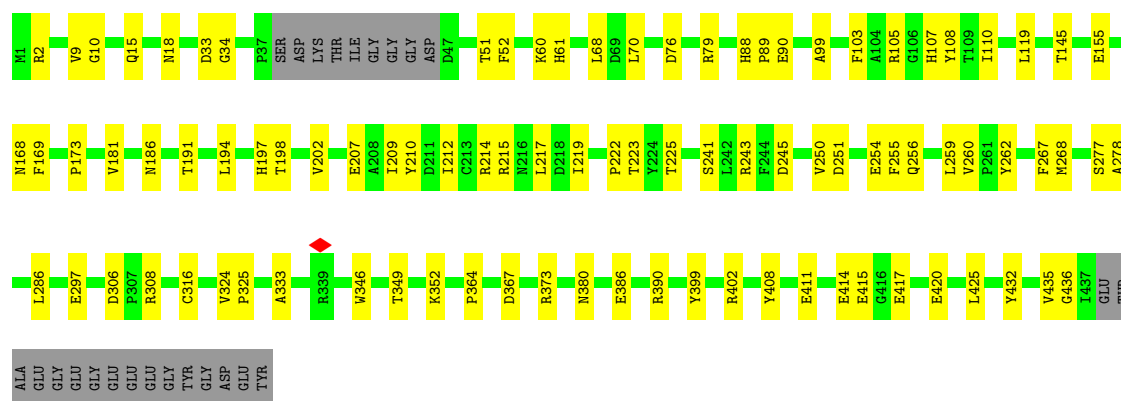
Chain C0: 





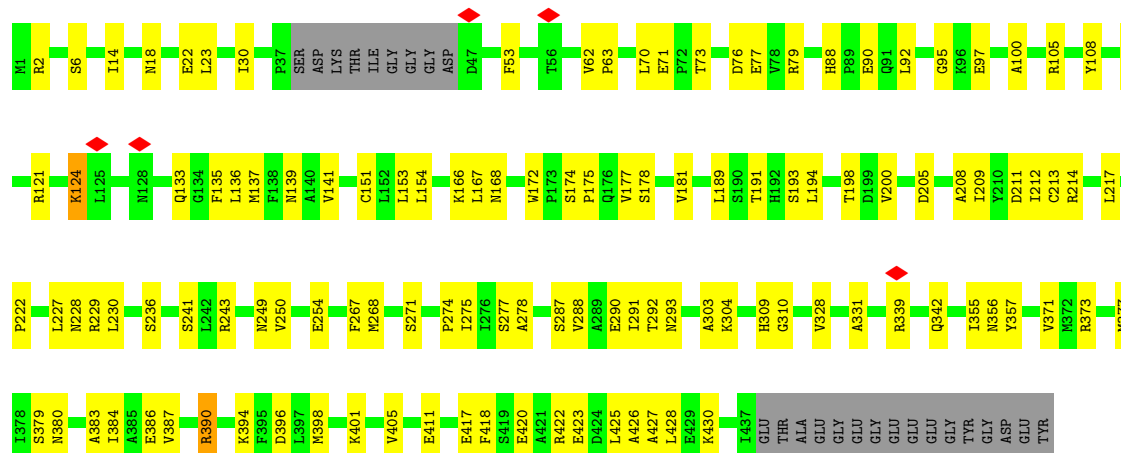
• Molecule 2: Tubulin alpha chain

Chain C2: 74% 20% 6%



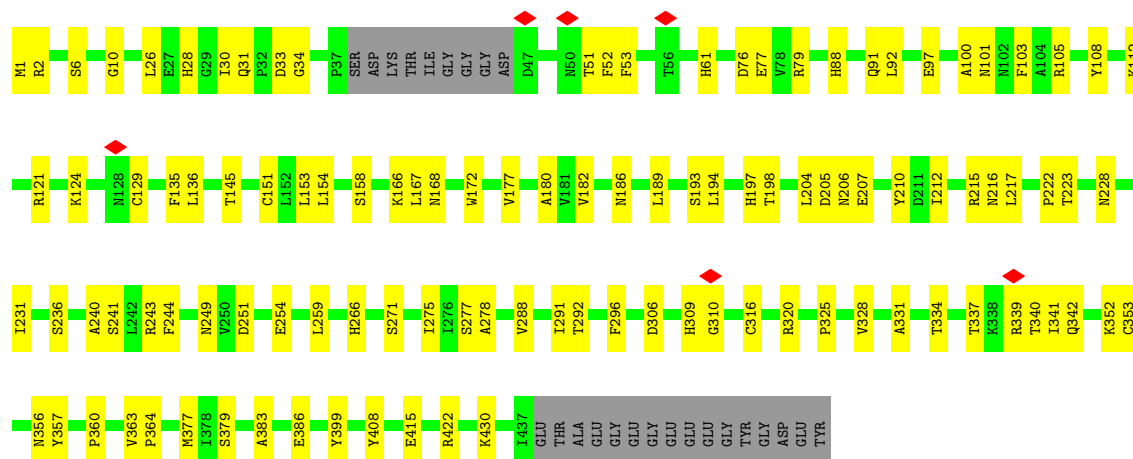
• Molecule 2: Tubulin alpha chain

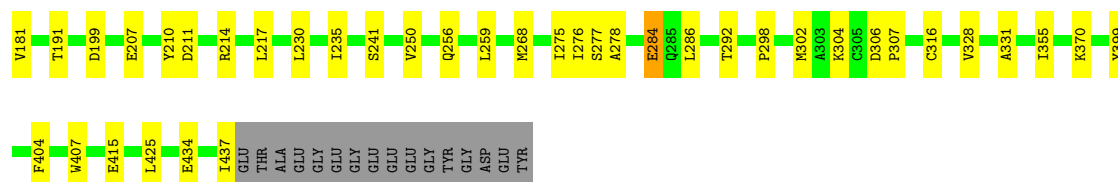
Chain C4: 68% 26% 6%



• Molecule 2: Tubulin alpha chain

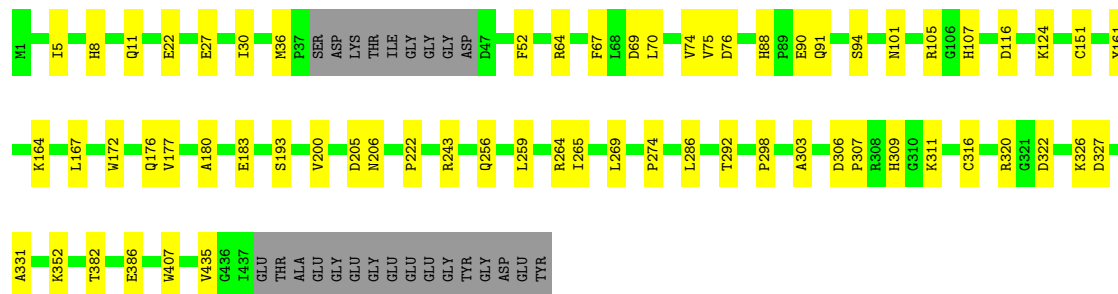
Chain C6: 70% 25% 6%





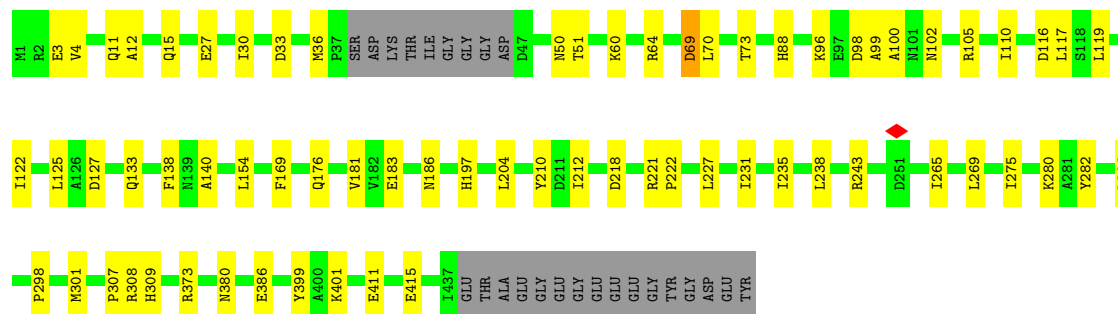
• Molecule 2: Tubulin alpha chain

Chain D4: 80% 14% 6%



• Molecule 2: Tubulin alpha chain

Chain D6: 79% 15% 6%



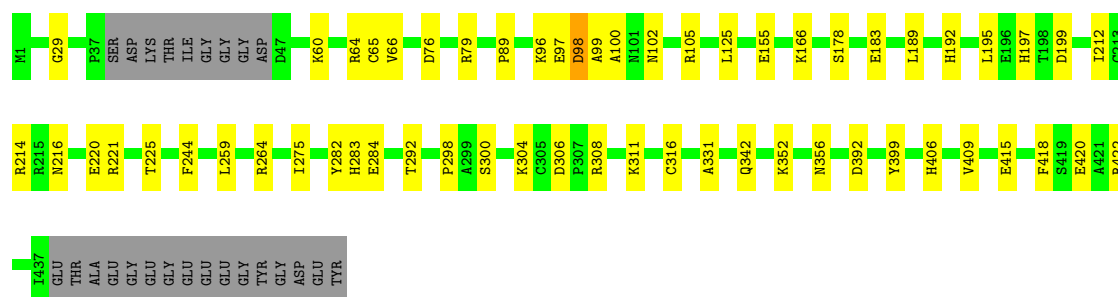
• Molecule 2: Tubulin alpha chain

Chain D8: 82% 13% 6%



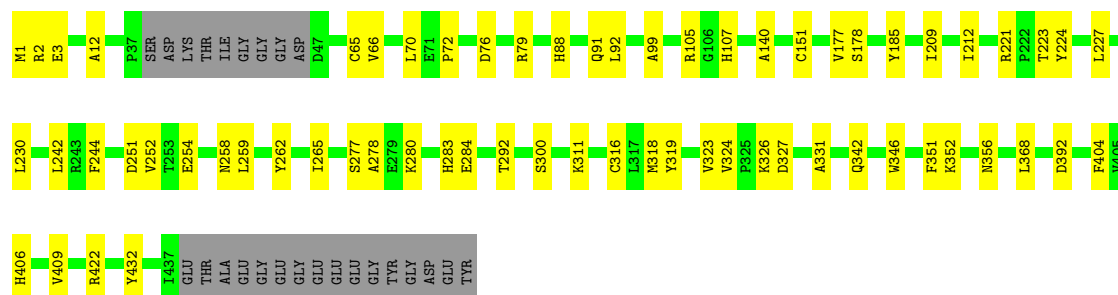
• Molecule 2: Tubulin alpha chain

Chain E0: 82% 13% 6%



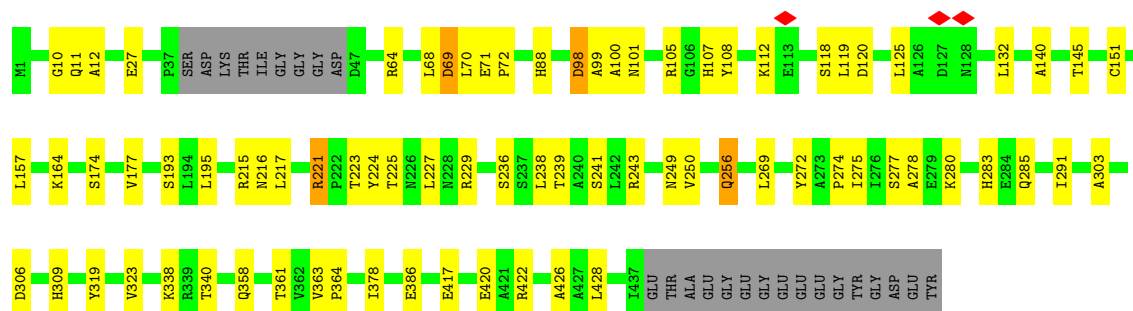
• Molecule 2: Tubulin alpha chain

Chain E2: 80% 14% 6%



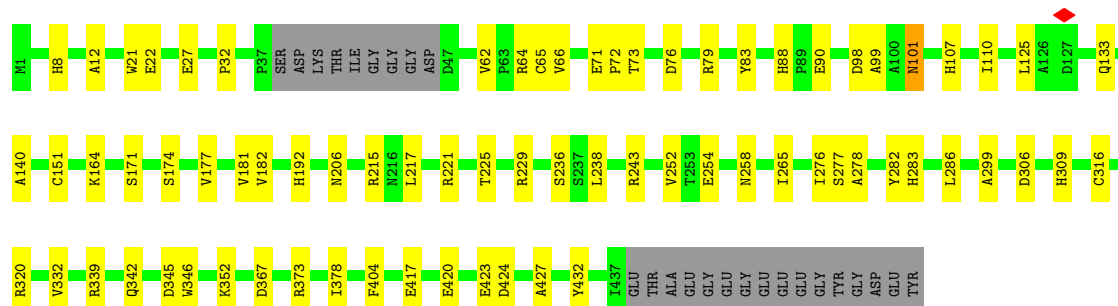
• Molecule 2: Tubulin alpha chain

Chain E4: 77% 16% 6%

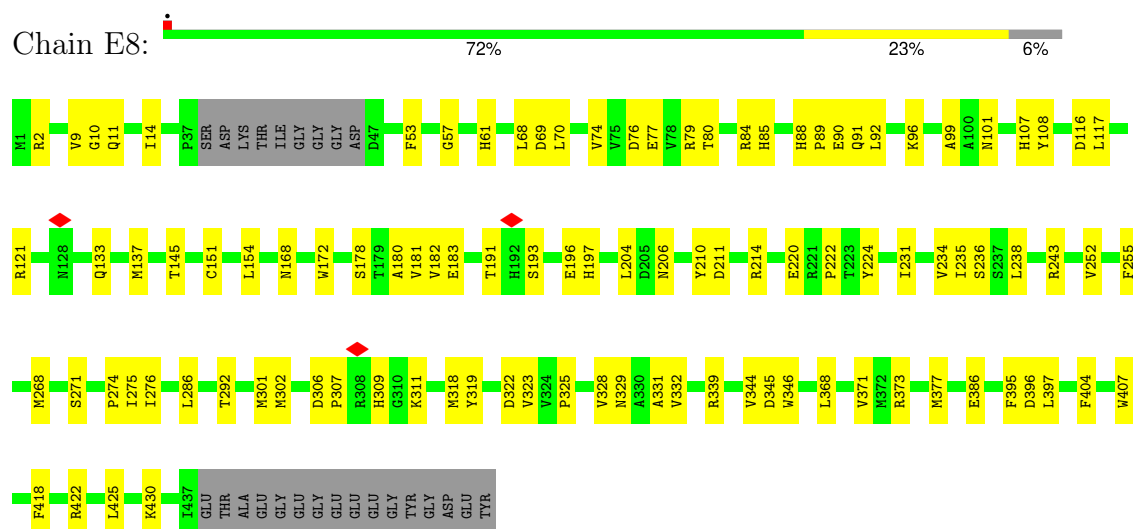


• Molecule 2: Tubulin alpha chain

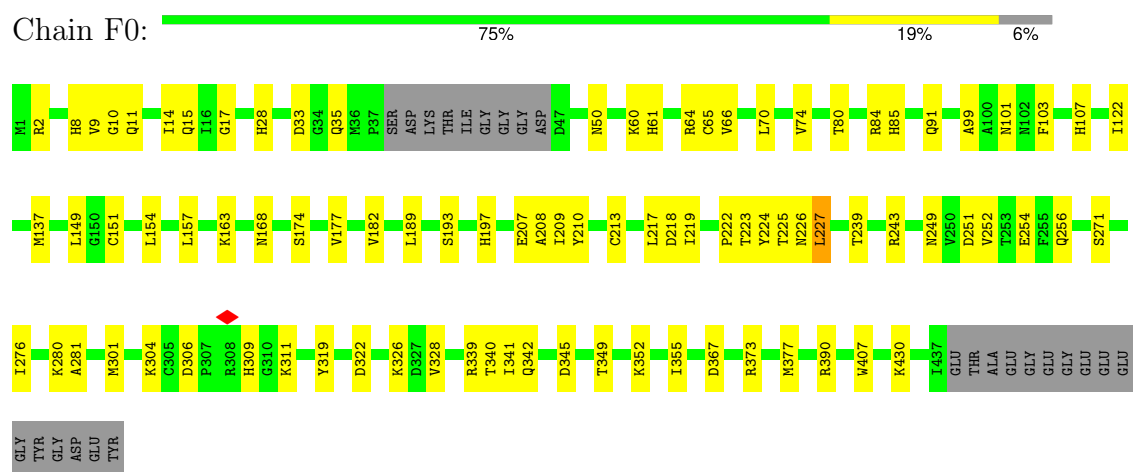
Chain E6: 78% 16% 6%



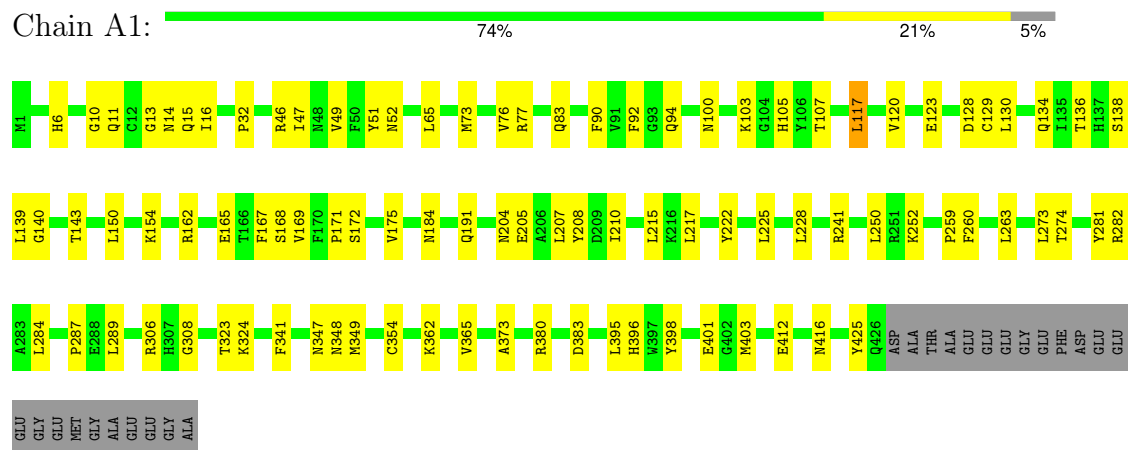
- Molecule 2: Tubulin alpha chain



- Molecule 2: Tubulin alpha chain



- Molecule 3: Tubulin beta chain



- Molecule 3: Tubulin beta chain

Response	Percentage
Yes, the U.S. is a democracy	76%
No, the U.S. is not a democracy	18%
Don't know	5%



Response	Percentage
U.S. should take action to protect the environment	76%
U.S. should not take action to protect the environment	19%
U.S. should not take action to protect the environment (unlabeled)	5%



Response	Percentage
Good	80%
Not good	15%
Don't know	5%




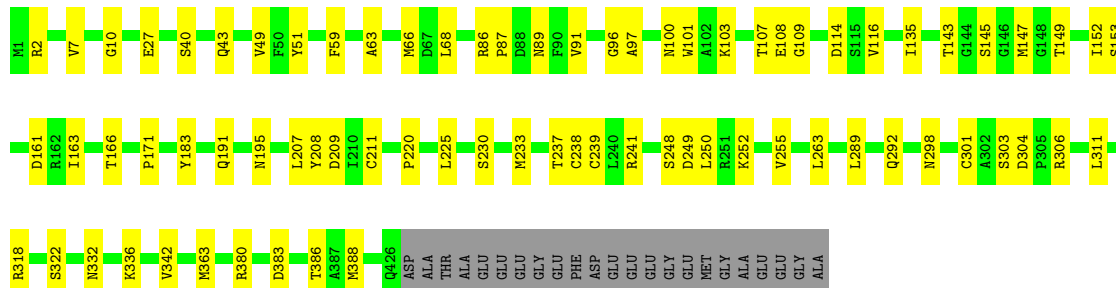
Category	Percentage
Very good	74%
Good	20%
Not good	5%




GLU
GLY
ALA

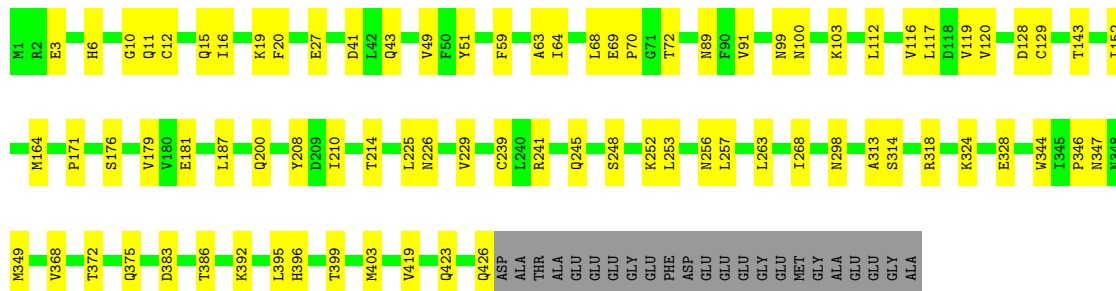
• Molecule 3: Tubulin beta chain

Chain B1:  78% 17% 5%




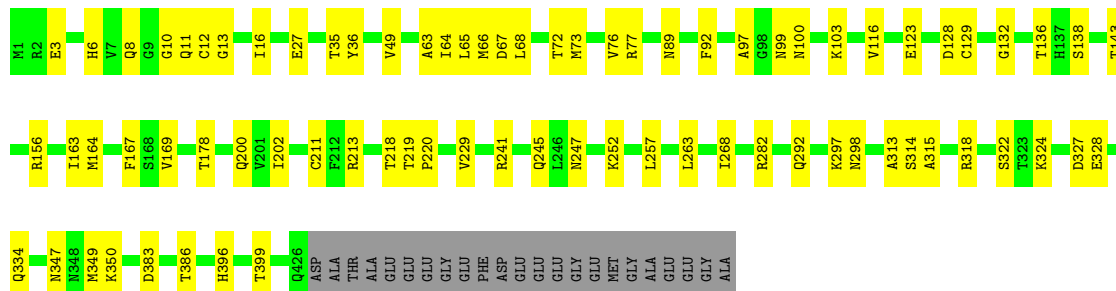
• Molecule 3: Tubulin beta chain

Chain B3:  77% 18% 5%




• Molecule 3: Tubulin beta chain

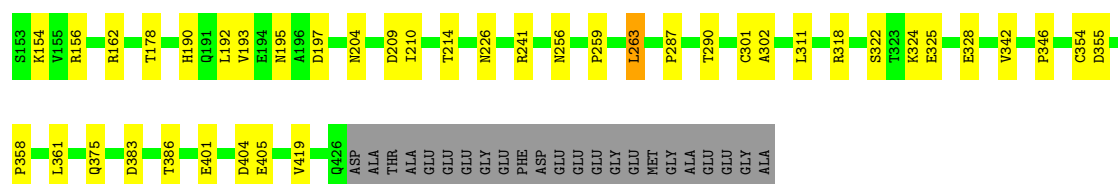
Chain B5:  78% 17% 5%



• Molecule 3: Tubulin beta chain

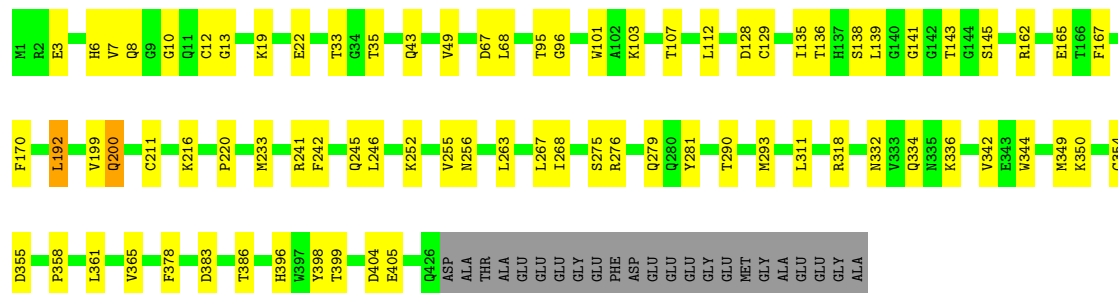
Chain B7:  78% 16% 5%





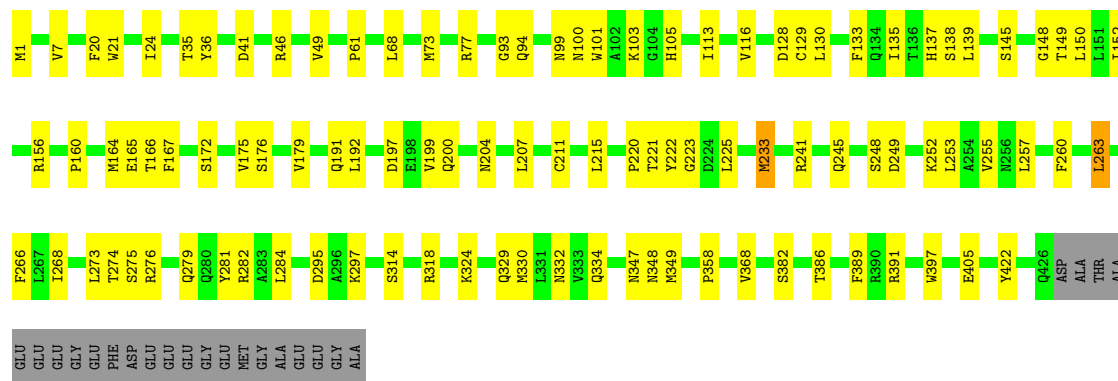
• Molecule 3: Tubulin beta chain

Chain B9: 77% 17% 5%



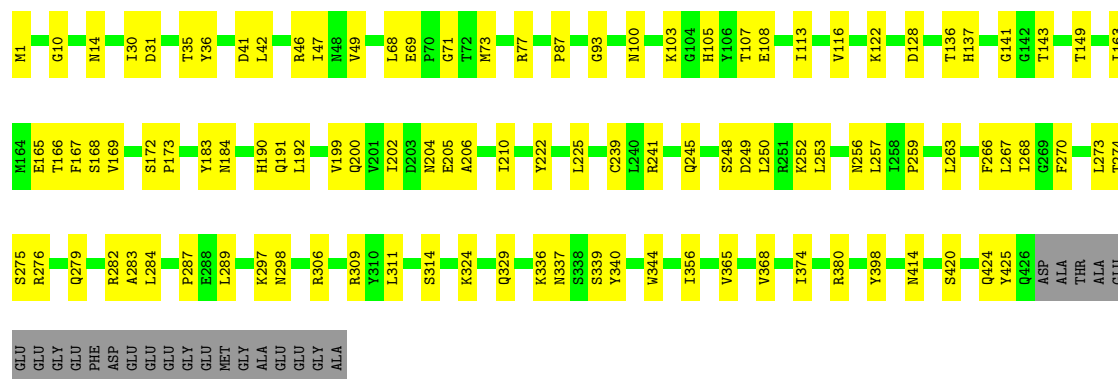
• Molecule 3: Tubulin beta chain

Chain C1: 72% 22% 5%

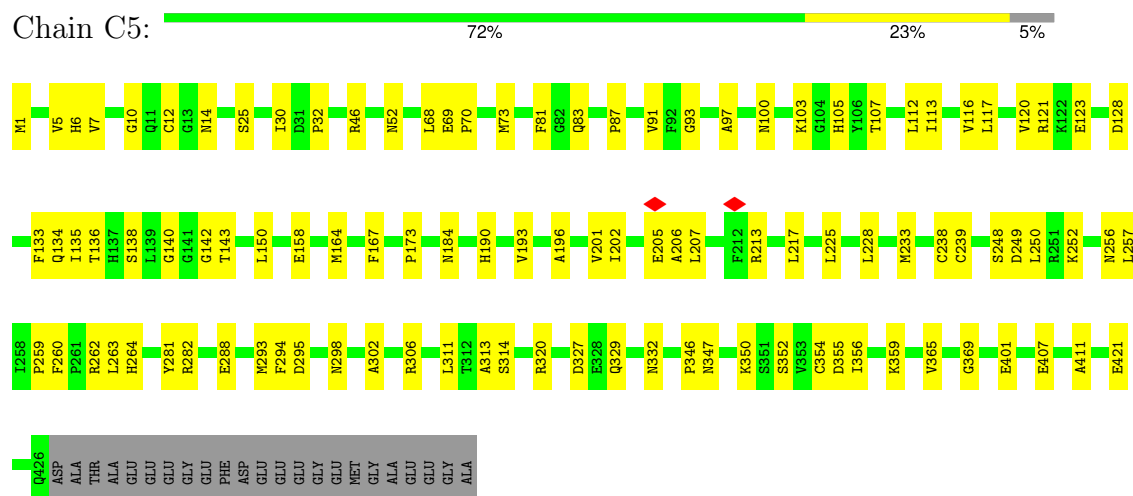


• Molecule 3: Tubulin beta chain

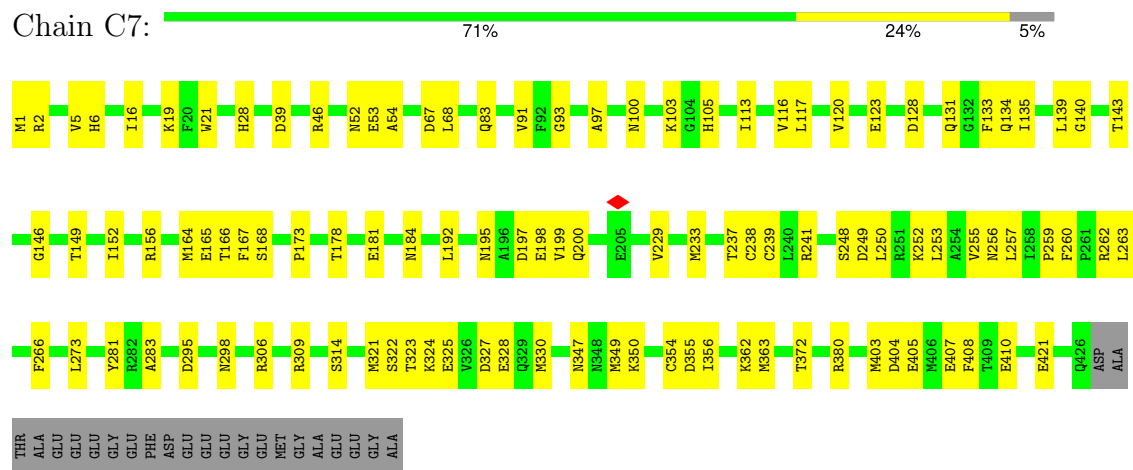
Chain C3: 72% 23% 5%



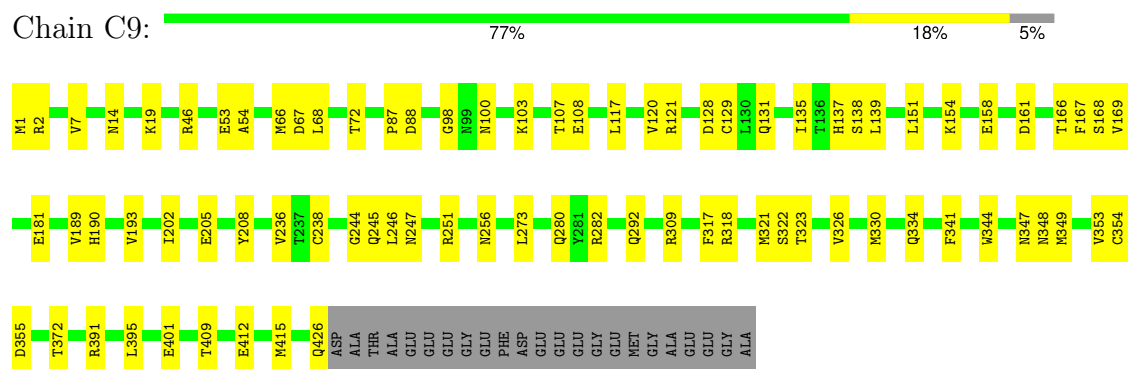
- Molecule 3: Tubulin beta chain



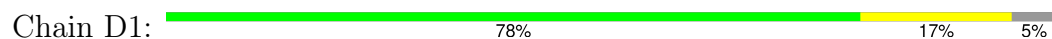
- Molecule 3: Tubulin beta chain

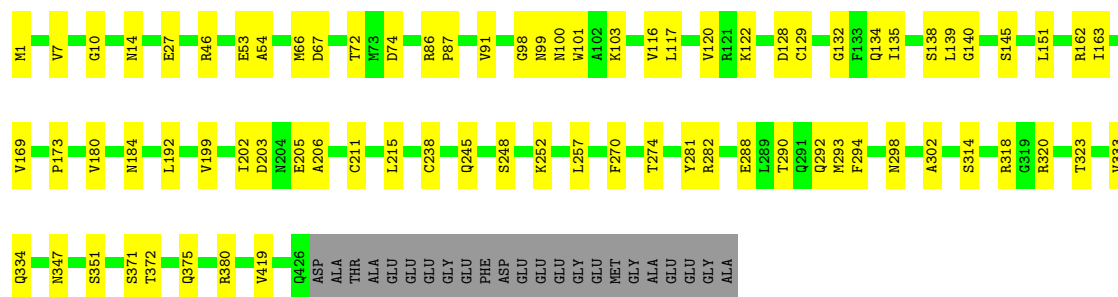


- Molecule 3: Tubulin beta chain



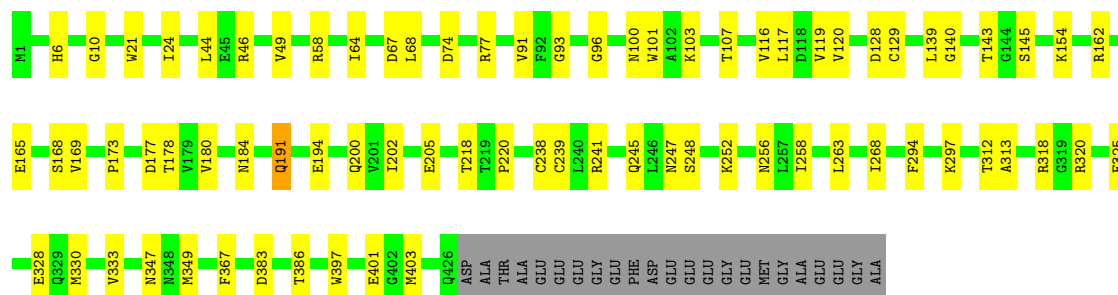
- Molecule 3: Tubulin beta chain





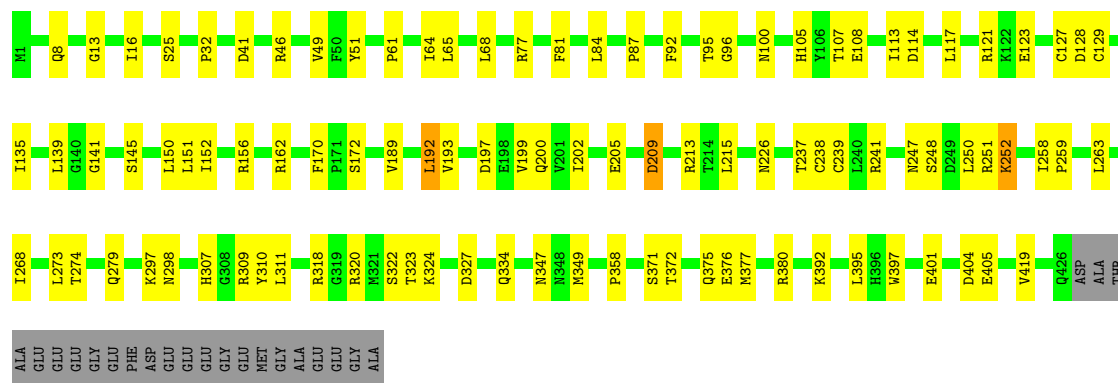
- Molecule 3: Tubulin beta chain

Chain D3: 78% 17% 5%



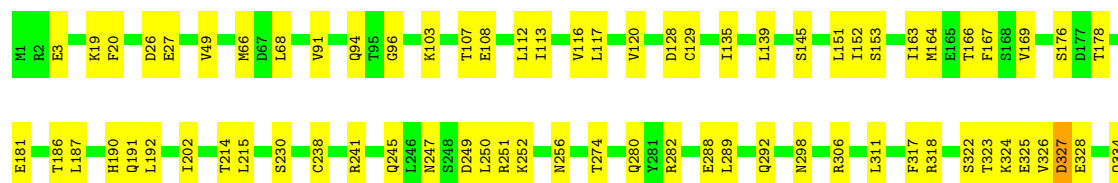
- Molecule 3: Tubulin beta chain

Chain D5: 73% 22% 5%



- Molecule 3: Tubulin beta chain

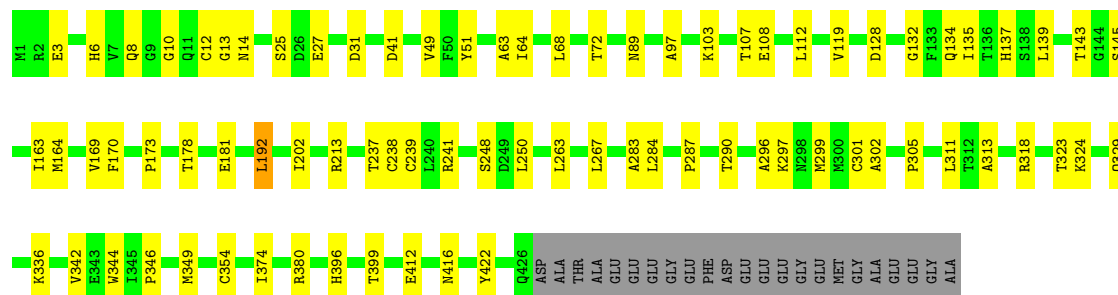
Chain D7: 75% 20% 5%





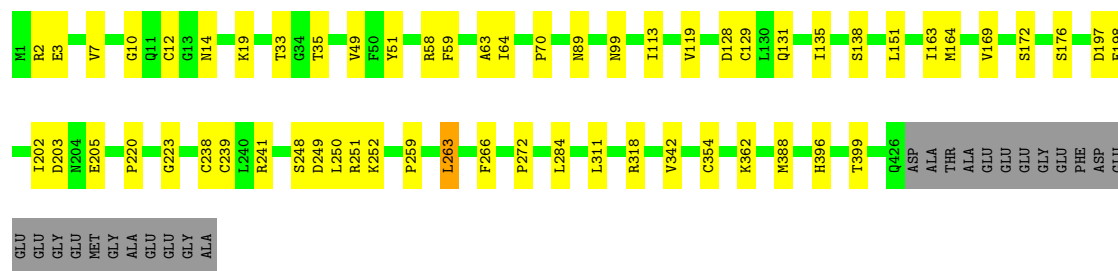
- Molecule 3: Tubulin beta chain

Chain D9:



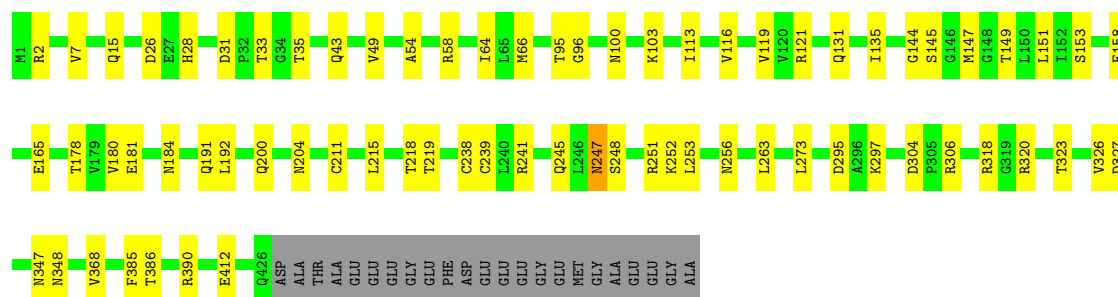
- Molecule 3: Tubulin beta chain

Chain E1:



- Molecule 3: Tubulin beta chain

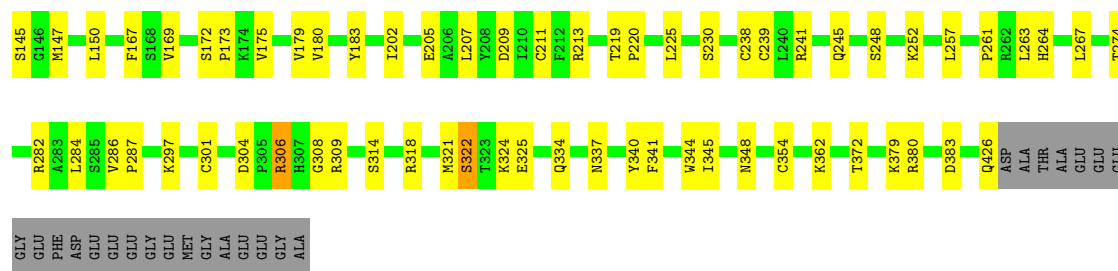
Chain E3:



- Molecule 3: Tubulin beta chain

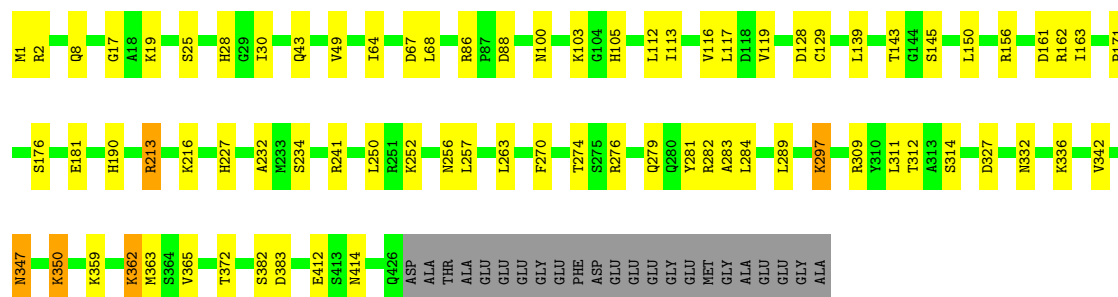
Chain E5:





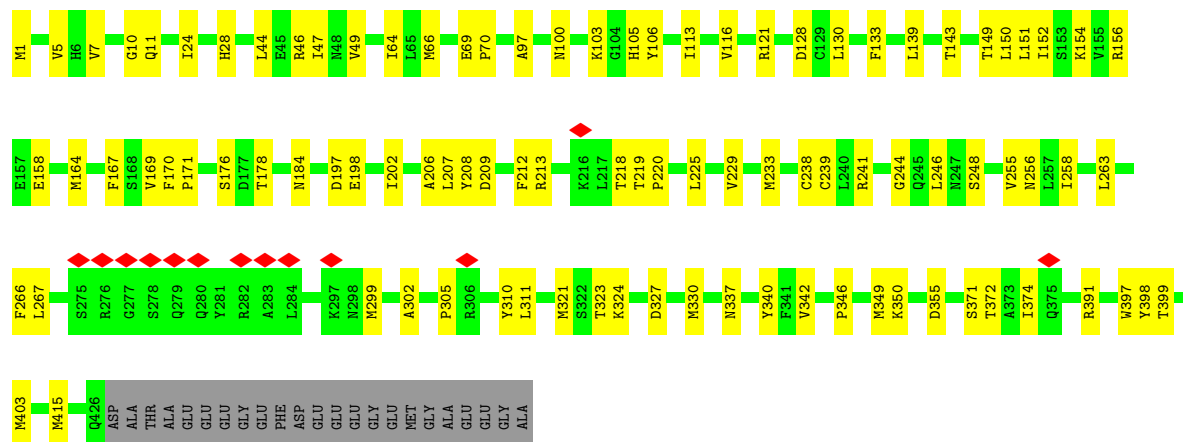
• Molecule 3: Tubulin beta chain

Chain E7: 78% 16% 5%



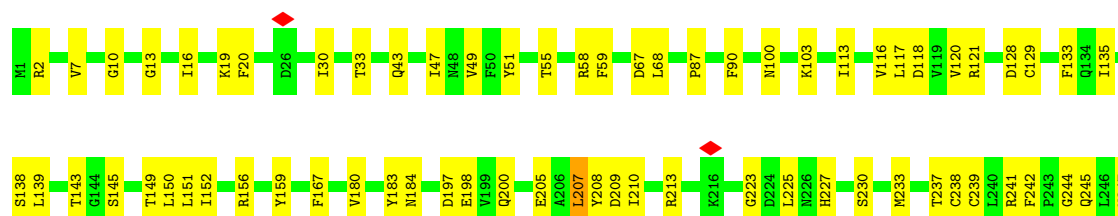
• Molecule 3: Tubulin beta chain

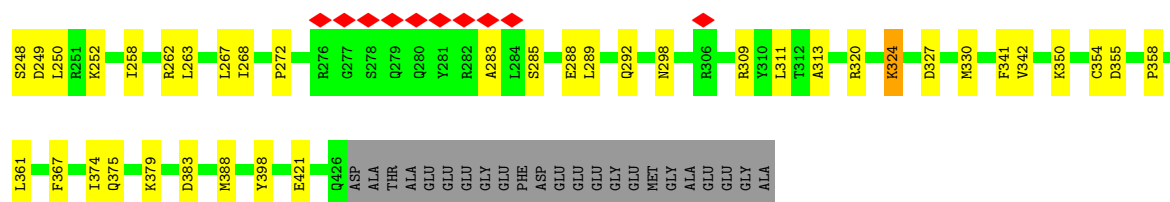
Chain E9: 73% 21% 5%



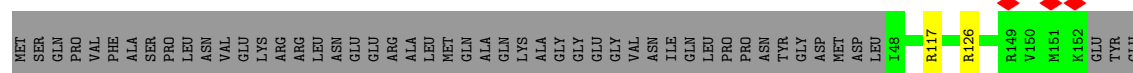
• Molecule 3: Tubulin beta chain

Chain F1: 71% 23% 5%

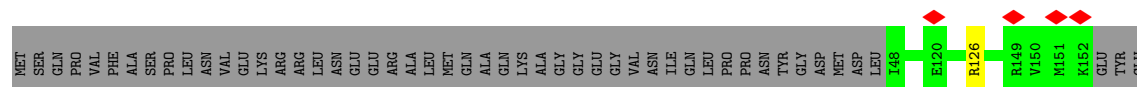




• Molecule 4: PDI family protein



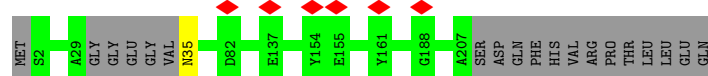
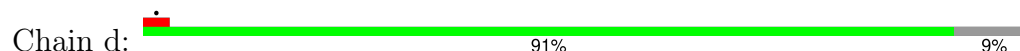
• Molecule 4: PDI family protein



• Molecule 4: PDI family protein



• Molecule 4: PDI family protein

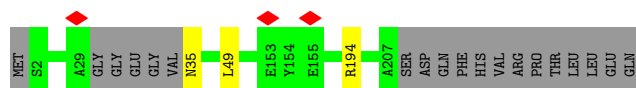


• Molecule 4: PDI family protein

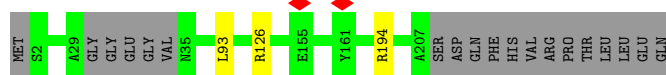




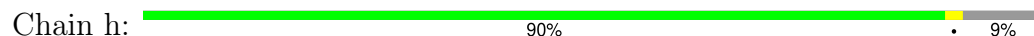
- Molecule 4: PDI family protein



- Molecule 4: PDI family protein



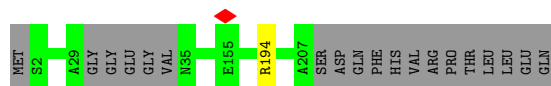
- Molecule 4: PDI family protein



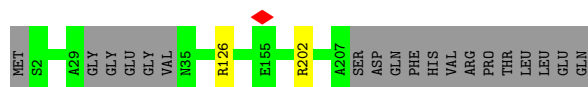
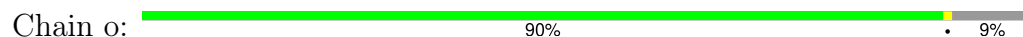
- Molecule 4: PDI family protein




- Molecule 4: PDI family protein



- Molecule 4: PDI family protein




- Molecule 4: PDI family protein

Chain p:  90% 9%




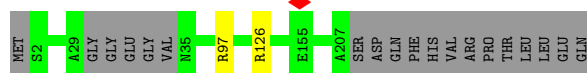
- Molecule 4: PDI family protein

Chain q:  90% 9%



- Molecule 4: PDI family protein

Chain r:  90% 9%




- Molecule 4: PDI family protein

Chain s:  91% 9%




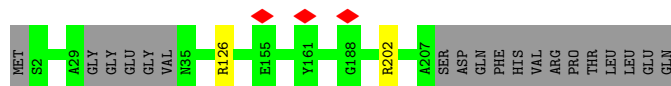
- Molecule 4: PDI family protein

Chain t:  90% 9%



- Molecule 4: PDI family protein

Chain u:  90% 9%

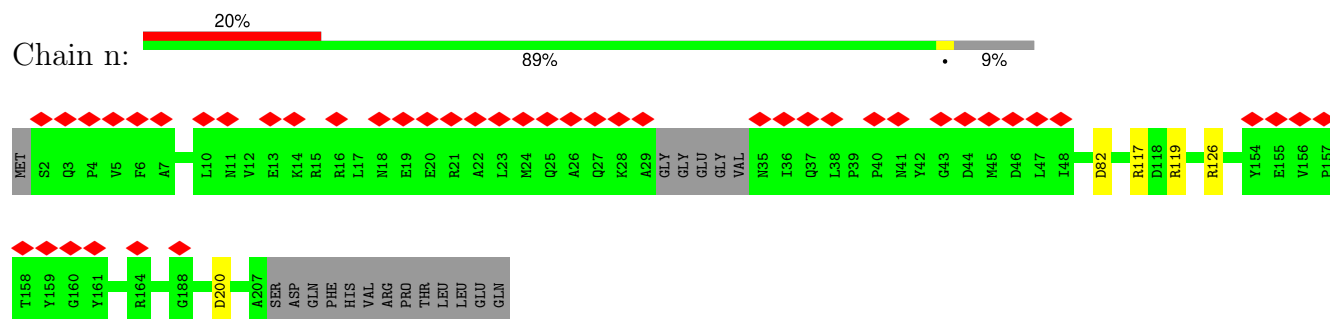


- Molecule 4: PDI family protein

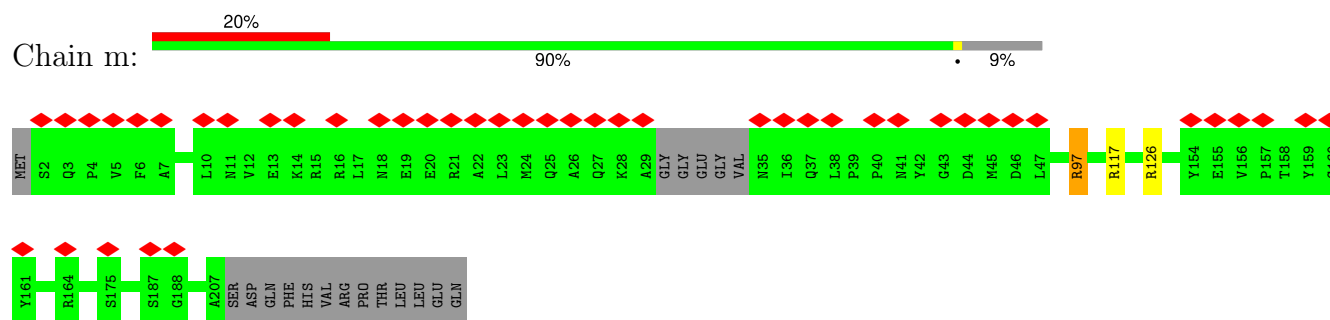
Chain v:  90% 9%



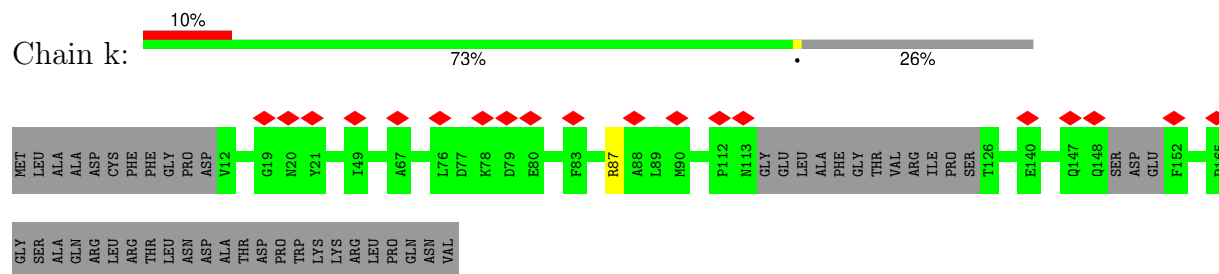
● Molecule 4: PDI family protein



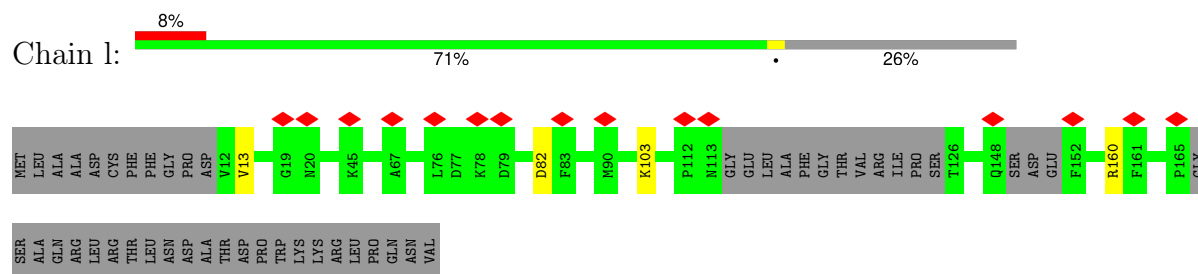
● Molecule 4: PDI family protein



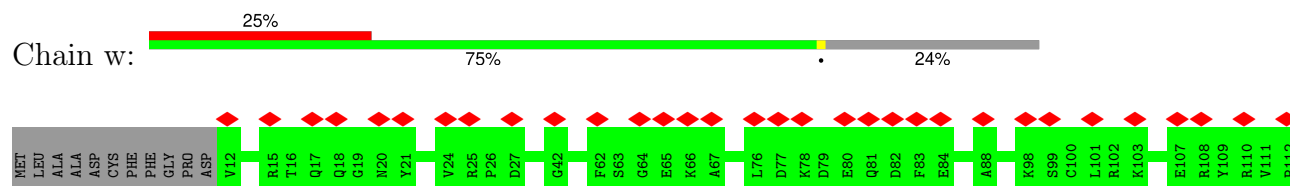
● Molecule 5: PDI family protein

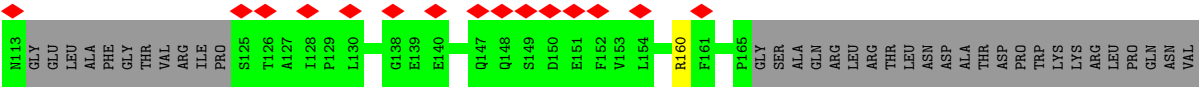


● Molecule 5: PDI family protein

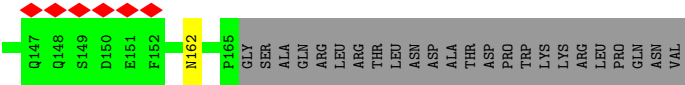
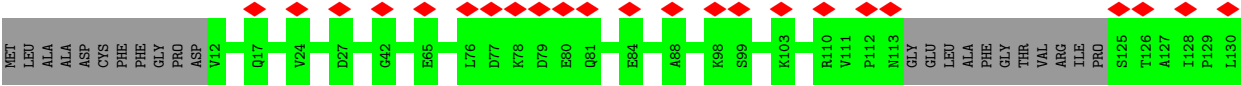


● Molecule 5: PDI family protein





• Molecule 5: PDI family protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	220139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF amplitude correction was performed as part of the 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.228	Depositor
Minimum map value	0.000	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.47	0/181	0.55	0/248
1	1	0.42	0/181	0.58	0/248
1	10	0.49	0/181	0.61	0/248
1	11	0.53	0/181	0.60	0/248
1	12	0.47	0/181	0.51	0/248
1	13	0.50	0/181	0.50	0/248
1	14	0.47	0/181	0.48	0/248
1	15	0.53	0/181	0.42	0/248
1	16	0.40	0/181	0.49	0/248
1	17	0.47	0/181	0.51	0/248
1	18	0.44	0/181	0.48	0/248
1	19	0.57	0/181	0.53	0/248
1	2	0.54	0/181	0.59	0/248
1	20	0.39	0/181	0.59	0/248
1	21	0.43	0/181	0.52	0/248
1	22	0.42	0/166	0.48	0/227
1	23	0.46	0/166	0.47	0/227
1	3	0.53	0/181	0.49	0/248
1	4	0.51	0/181	0.50	0/248
1	5	0.55	0/181	0.52	0/248
1	6	0.49	0/181	0.46	0/248
1	7	0.48	0/181	0.48	0/248
1	8	0.47	0/181	0.65	0/248
1	9	0.45	0/181	0.63	0/248
2	A0	0.42	0/3398	0.61	2/4606 (0.0%)
2	A2	0.39	0/3398	0.61	1/4606 (0.0%)
2	A4	0.53	0/3398	0.63	2/4606 (0.0%)
2	A6	0.48	0/3398	0.62	0/4606
2	A8	0.50	0/3398	0.60	2/4606 (0.0%)
2	B0	0.50	0/3398	0.62	4/4606 (0.1%)
2	B2	0.53	0/3398	0.62	1/4606 (0.0%)
2	B4	0.52	0/3398	0.63	2/4606 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	B6	0.53	0/3398	0.63	6/4606 (0.1%)
2	B8	0.55	0/3398	0.66	6/4606 (0.1%)
2	C0	0.44	0/3398	0.61	1/4606 (0.0%)
2	C2	0.45	0/3398	0.65	0/4606
2	C4	0.43	0/3398	0.65	4/4606 (0.1%)
2	C6	0.44	0/3398	0.68	3/4606 (0.1%)
2	C8	0.45	0/3398	0.60	1/4606 (0.0%)
2	D0	0.50	0/3398	0.61	0/4606
2	D2	0.45	0/3398	0.62	5/4606 (0.1%)
2	D4	0.52	0/3398	0.62	2/4606 (0.0%)
2	D6	0.42	0/3398	0.61	3/4606 (0.1%)
2	D8	0.52	0/3398	0.62	1/4606 (0.0%)
2	E0	0.37	0/3398	0.56	1/4606 (0.0%)
2	E2	0.44	0/3398	0.59	0/4606
2	E4	0.38	0/3398	0.65	6/4606 (0.1%)
2	E6	0.45	0/3398	0.58	0/4606
2	E8	0.39	0/3398	0.59	0/4606
2	F0	0.45	0/3398	0.60	2/4606 (0.0%)
3	A1	0.47	0/3404	0.66	6/4606 (0.1%)
3	A3	0.40	0/3404	0.62	3/4606 (0.1%)
3	A5	0.50	0/3404	0.65	2/4606 (0.0%)
3	A7	0.45	0/3404	0.61	3/4606 (0.1%)
3	A9	0.52	0/3404	0.68	6/4606 (0.1%)
3	B1	0.46	0/3404	0.65	3/4606 (0.1%)
3	B3	0.54	0/3404	0.62	2/4606 (0.0%)
3	B5	0.48	0/3404	0.61	1/4606 (0.0%)
3	B7	0.54	0/3404	0.63	3/4606 (0.1%)
3	B9	0.50	0/3404	0.63	3/4606 (0.1%)
3	C1	0.46	0/3404	0.66	3/4606 (0.1%)
3	C3	0.44	0/3404	0.68	3/4606 (0.1%)
3	C5	0.44	0/3404	0.65	1/4606 (0.0%)
3	C7	0.44	0/3404	0.63	2/4606 (0.0%)
3	C9	0.52	0/3404	0.64	2/4606 (0.0%)
3	D1	0.49	0/3404	0.64	1/4606 (0.0%)
3	D3	0.50	0/3404	0.63	2/4606 (0.0%)
3	D5	0.50	0/3404	0.66	6/4606 (0.1%)
3	D7	0.51	0/3404	0.65	4/4606 (0.1%)
3	D9	0.51	0/3404	0.64	4/4606 (0.1%)
3	E1	0.41	0/3404	0.58	2/4606 (0.0%)
3	E3	0.45	0/3404	0.62	5/4606 (0.1%)
3	E5	0.41	0/3404	0.64	3/4606 (0.1%)
3	E7	0.45	0/3404	0.61	3/4606 (0.1%)
3	E9	0.41	0/3404	0.64	4/4606 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	F1	0.45	0/3404	0.69	7/4606 (0.2%)
4	a	0.46	0/1225	0.62	0/1654
4	b	0.39	0/1225	0.55	0/1654
4	c	0.50	0/1645	0.64	0/2225
4	d	0.44	0/1645	0.65	0/2225
4	e	0.50	0/1645	0.63	0/2225
4	f	0.47	0/1645	0.61	1/2225 (0.0%)
4	g	0.50	0/1645	0.65	1/2225 (0.0%)
4	h	0.48	0/1645	0.58	0/2225
4	i	0.48	0/1645	0.66	0/2225
4	j	0.47	0/1645	0.67	1/2225 (0.0%)
4	m	0.41	0/1645	0.62	1/2225 (0.0%)
4	n	0.41	0/1645	0.66	3/2225 (0.1%)
4	o	0.49	0/1645	0.65	1/2225 (0.0%)
4	p	0.47	0/1645	0.64	1/2225 (0.0%)
4	q	0.45	0/1645	0.60	0/2225
4	r	0.49	0/1645	0.60	1/2225 (0.0%)
4	s	0.41	0/1645	0.61	0/2225
4	t	0.48	0/1645	0.62	0/2225
4	u	0.36	0/1645	0.57	1/2225 (0.0%)
4	v	0.45	0/1645	0.63	0/2225
5	k	0.37	0/1168	0.59	0/1578
5	l	0.37	0/1168	0.69	2/1578 (0.1%)
5	w	0.35	0/1201	0.55	0/1623
5	x	0.37	0/1201	0.54	0/1623
All	All	0.47	0/217964	0.63	152/295182 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A2	0	1
2	A4	0	2
2	A8	0	1
2	B4	0	1
2	B6	0	1
2	C8	0	1
2	D2	0	1
3	A1	0	1
3	B3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	B9	0	1
3	E5	0	2
5	1	0	1
All	All	0	14

There are no bond length outliers.

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C6	30	ILE	C-N-CA	10.74	148.56	121.70
3	A9	383	ASP	CB-CG-OD1	8.05	125.55	118.30
3	E9	130	LEU	CA-CB-CG	7.97	133.64	115.30
3	A9	73	MET	CG-SD-CE	-7.75	87.80	100.20
3	D5	41	ASP	CB-CG-OD1	7.71	125.24	118.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A1	191	GLN	Peptide
2	A2	401	LYS	Peptide
2	A4	254	GLU	Peptide
2	A4	401	LYS	Peptide
2	A8	401	LYS	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	0	174	0	171	3	0
1	1	174	0	171	5	0
1	10	174	0	171	3	0
1	11	174	0	171	1	0
1	12	174	0	171	3	0
1	13	174	0	171	1	0
1	14	174	0	171	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	15	174	0	171	1	0
1	16	174	0	171	2	0
1	17	174	0	171	2	0
1	18	174	0	171	1	0
1	19	174	0	171	2	0
1	2	174	0	171	1	0
1	20	174	0	171	2	0
1	21	174	0	171	3	0
1	22	160	0	156	3	0
1	23	160	0	156	3	0
1	3	174	0	171	2	0
1	4	174	0	171	2	0
1	5	174	0	171	2	0
1	6	174	0	171	1	0
1	7	174	0	171	3	0
1	8	174	0	171	1	0
1	9	174	0	171	2	0
2	A0	3325	0	3251	54	0
2	A2	3325	0	3252	54	0
2	A4	3325	0	3252	43	0
2	A6	3325	0	3252	48	0
2	A8	3325	0	3252	54	0
2	B0	3325	0	3252	47	0
2	B2	3325	0	3252	44	0
2	B4	3325	0	3252	62	0
2	B6	3325	0	3252	47	0
2	B8	3325	0	3252	61	0
2	C0	3325	0	3252	65	0
2	C2	3325	0	3252	69	0
2	C4	3325	0	3252	74	0
2	C6	3325	0	3251	69	0
2	C8	3325	0	3252	45	0
2	D0	3325	0	3252	38	0
2	D2	3325	0	3252	39	0
2	D4	3325	0	3252	41	0
2	D6	3325	0	3252	43	0
2	D8	3325	0	3252	38	0
2	E0	3325	0	3252	35	0
2	E2	3325	0	3252	45	0
2	E4	3325	0	3252	55	0
2	E6	3325	0	3252	50	0
2	E8	3325	0	3252	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F0	3325	0	3252	67	0
3	A1	3331	0	3207	58	0
3	A3	3331	0	3209	52	0
3	A5	3331	0	3207	53	0
3	A7	3331	0	3207	41	0
3	A9	3331	0	3207	58	0
3	B1	3331	0	3209	47	0
3	B3	3331	0	3207	50	0
3	B5	3331	0	3207	48	0
3	B7	3331	0	3209	47	0
3	B9	3331	0	3209	44	0
3	C1	3331	0	3209	72	0
3	C3	3331	0	3209	62	0
3	C5	3331	0	3209	65	0
3	C7	3331	0	3209	66	0
3	C9	3331	0	3209	59	0
3	D1	3331	0	3209	50	0
3	D3	3331	0	3207	56	0
3	D5	3331	0	3207	61	0
3	D7	3331	0	3207	63	0
3	D9	3331	0	3207	49	0
3	E1	3331	0	3207	39	0
3	E3	3331	0	3209	44	0
3	E5	3331	0	3207	60	0
3	E7	3331	0	3207	50	0
3	E9	3331	0	3206	68	0
3	F1	3331	0	3207	72	0
4	a	1198	0	1194	0	0
4	b	1198	0	1194	0	0
4	c	1608	0	1590	0	0
4	d	1608	0	1590	0	0
4	e	1608	0	1590	0	0
4	f	1608	0	1590	0	0
4	g	1608	0	1590	0	0
4	h	1608	0	1590	0	0
4	i	1608	0	1590	0	0
4	j	1608	0	1590	0	0
4	m	1608	0	1590	0	0
4	n	1608	0	1590	0	0
4	o	1608	0	1590	0	0
4	p	1608	0	1590	0	0
4	q	1608	0	1590	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	r	1608	0	1590	0	0
4	s	1608	0	1590	0	0
4	t	1608	0	1590	0	0
4	u	1608	0	1590	0	0
4	v	1608	0	1590	0	0
5	k	1140	0	1143	0	0
5	l	1140	0	1143	0	0
5	w	1172	0	1171	0	0
5	x	1172	0	1171	0	0
6	A0	32	0	12	2	0
6	A2	32	0	12	0	0
6	A4	32	0	12	0	0
6	A6	32	0	12	0	0
6	A8	32	0	12	1	0
6	B0	32	0	12	1	0
6	B2	32	0	12	1	0
6	B4	32	0	12	0	0
6	B6	32	0	12	2	0
6	B8	32	0	12	1	0
6	C0	32	0	12	2	0
6	C2	32	0	12	0	0
6	C4	32	0	12	1	0
6	C6	32	0	12	3	0
6	C8	32	0	12	1	0
6	D0	32	0	12	0	0
6	D2	32	0	12	0	0
6	D4	32	0	12	1	0
6	D6	32	0	12	0	0
6	D8	32	0	12	1	0
6	E0	32	0	12	0	0
6	E2	32	0	12	1	0
6	E4	32	0	12	0	0
6	E6	32	0	12	3	0
6	E8	32	0	12	2	0
6	F0	32	0	12	1	0
7	A0	1	0	0	0	0
7	A2	1	0	0	0	0
7	A4	1	0	0	0	0
7	A6	1	0	0	0	0
7	A8	1	0	0	0	0
7	B0	1	0	0	0	0
7	B2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B4	1	0	0	0	0
7	B6	1	0	0	0	0
7	B8	1	0	0	0	0
7	C0	1	0	0	0	0
7	C2	1	0	0	0	0
7	C4	1	0	0	0	0
7	C6	1	0	0	0	0
7	C8	1	0	0	0	0
7	D0	1	0	0	0	0
7	D2	1	0	0	0	0
7	D4	1	0	0	0	0
7	D6	1	0	0	0	0
7	D8	1	0	0	0	0
7	E0	1	0	0	0	0
7	E2	1	0	0	0	0
7	E4	1	0	0	0	0
7	E6	1	0	0	0	0
7	E8	1	0	0	0	0
7	F0	1	0	0	0	0
8	A1	28	0	12	2	0
8	A3	28	0	12	2	0
8	A5	28	0	12	0	0
8	A7	28	0	12	0	0
8	A9	28	0	12	1	0
8	B1	28	0	12	0	0
8	B3	28	0	12	1	0
8	B5	28	0	12	0	0
8	B7	28	0	12	1	0
8	B9	28	0	12	0	0
8	C1	28	0	12	1	0
8	C3	28	0	12	2	0
8	C5	28	0	12	1	0
8	C7	28	0	12	0	0
8	C9	28	0	12	0	0
8	D1	28	0	12	0	0
8	D3	28	0	12	0	0
8	D5	28	0	12	1	0
8	D7	28	0	12	0	0
8	D9	28	0	12	0	0
8	E1	28	0	12	0	0
8	E3	28	0	12	3	0
8	E5	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E7	28	0	12	0	0
8	E9	28	0	12	0	0
8	F1	28	0	12	1	0
All	All	214754	0	208287	2539	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 7.

The worst 5 of 2539 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:151:CYS:HG	2:D4:193:SER:HG	1.23	0.83
3:A9:248:SER:HA	3:A9:252:LYS:HG2	1.67	0.77
2:E2:88:HIS:HB3	2:E2:91:GLN:HG2	1.65	0.77
2:C6:6:SER:HA	2:C6:136:LEU:HB2	1.67	0.76
2:D0:142:GLY:HA3	2:D0:183:GLU:HG2	1.66	0.76

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	0	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	1	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	10	20/351 (6%)	16 (80%)	4 (20%)	0	100	100
1	11	20/351 (6%)	17 (85%)	3 (15%)	0	100	100
1	12	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	13	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	14	20/351 (6%)	19 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	15	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	16	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	17	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	18	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	19	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	2	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	20	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	21	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	22	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	23	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	3	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	4	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	5	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	6	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	7	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	8	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	9	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
2	A0	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	A2	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	A4	424/453 (94%)	398 (94%)	26 (6%)	0	100	100
2	A6	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	A8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	B0	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
2	B2	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
2	B4	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	B6	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	B8	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	C0	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	C2	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	C4	424/453 (94%)	385 (91%)	39 (9%)	0	100	100
2	C6	424/453 (94%)	396 (93%)	28 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C8	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	D0	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	D2	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	D4	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	D6	424/453 (94%)	410 (97%)	14 (3%)	0	100	100
2	D8	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
2	E0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E2	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	E4	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	E6	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E8	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	F0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
3	A1	424/449 (94%)	391 (92%)	33 (8%)	0	100	100
3	A3	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
3	A5	424/449 (94%)	388 (92%)	36 (8%)	0	100	100
3	A7	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	A9	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
3	B1	424/449 (94%)	400 (94%)	24 (6%)	0	100	100
3	B3	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	B5	424/449 (94%)	400 (94%)	24 (6%)	0	100	100
3	B7	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	B9	424/449 (94%)	405 (96%)	19 (4%)	0	100	100
3	C1	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	C3	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	C5	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	C7	424/449 (94%)	394 (93%)	30 (7%)	0	100	100
3	C9	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
3	D1	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	D3	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
3	D5	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	D7	424/449 (94%)	401 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D9	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	E1	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
3	E3	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	E5	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	E7	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	E9	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
3	F1	424/449 (94%)	388 (92%)	36 (8%)	0	100	100
4	a	146/220 (66%)	136 (93%)	10 (7%)	0	100	100
4	b	146/220 (66%)	135 (92%)	11 (8%)	0	100	100
4	c	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	d	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
4	e	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	f	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	g	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	h	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	i	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	j	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	m	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	n	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	o	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
4	p	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	q	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	r	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	s	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	t	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	u	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
4	v	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
5	k	133/189 (70%)	128 (96%)	5 (4%)	0	100	100
5	l	133/189 (70%)	128 (96%)	5 (4%)	0	100	100
5	w	139/189 (74%)	134 (96%)	5 (4%)	0	100	100
5	x	139/189 (74%)	129 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	26906/37032 (73%)	25394 (94%)	1512 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	20/305 (7%)	20 (100%)	0	100	100
1	1	20/305 (7%)	20 (100%)	0	100	100
1	10	20/305 (7%)	20 (100%)	0	100	100
1	11	20/305 (7%)	20 (100%)	0	100	100
1	12	20/305 (7%)	20 (100%)	0	100	100
1	13	20/305 (7%)	20 (100%)	0	100	100
1	14	20/305 (7%)	20 (100%)	0	100	100
1	15	20/305 (7%)	20 (100%)	0	100	100
1	16	20/305 (7%)	20 (100%)	0	100	100
1	17	20/305 (7%)	20 (100%)	0	100	100
1	18	20/305 (7%)	20 (100%)	0	100	100
1	19	20/305 (7%)	20 (100%)	0	100	100
1	2	20/305 (7%)	20 (100%)	0	100	100
1	20	20/305 (7%)	20 (100%)	0	100	100
1	21	20/305 (7%)	20 (100%)	0	100	100
1	22	18/305 (6%)	18 (100%)	0	100	100
1	23	18/305 (6%)	18 (100%)	0	100	100
1	3	20/305 (7%)	20 (100%)	0	100	100
1	4	20/305 (7%)	20 (100%)	0	100	100
1	5	20/305 (7%)	20 (100%)	0	100	100
1	6	20/305 (7%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	20/305 (7%)	20 (100%)	0	100	100
1	8	20/305 (7%)	20 (100%)	0	100	100
1	9	20/305 (7%)	20 (100%)	0	100	100
2	A0	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	A2	359/379 (95%)	359 (100%)	0	100	100
2	A4	359/379 (95%)	357 (99%)	2 (1%)	84	90
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%)	91	95
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%)	358 (100%)	1 (0%)	91	95
2	B8	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	C0	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	C2	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	C4	359/379 (95%)	355 (99%)	4 (1%)	70	81
2	C6	359/379 (95%)	357 (99%)	2 (1%)	84	90
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%)	358 (100%)	1 (0%)	91	95
2	D4	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	D6	359/379 (95%)	359 (100%)	0	100	100
2	D8	359/379 (95%)	359 (100%)	0	100	100
2	E0	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	E2	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	E4	359/379 (95%)	357 (99%)	2 (1%)	84	90
2	E6	359/379 (95%)	357 (99%)	2 (1%)	84	90
2	E8	359/379 (95%)	358 (100%)	1 (0%)	91	95
2	F0	359/379 (95%)	358 (100%)	1 (0%)	91	95
3	A1	364/381 (96%)	362 (100%)	2 (0%)	86	91
3	A3	364/381 (96%)	360 (99%)	4 (1%)	70	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A5	364/381 (96%)	364 (100%)	0	100	100
3	A7	364/381 (96%)	363 (100%)	1 (0%)	91	95
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%)	362 (100%)	2 (0%)	86	91
3	B5	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	B7	364/381 (96%)	362 (100%)	2 (0%)	86	91
3	B9	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	C1	364/381 (96%)	364 (100%)	0	100	100
3	C3	364/381 (96%)	362 (100%)	2 (0%)	86	91
3	C5	364/381 (96%)	362 (100%)	2 (0%)	86	91
3	C7	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	C9	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	D1	364/381 (96%)	362 (100%)	2 (0%)	86	91
3	D3	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	D5	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	D7	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	D9	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	E1	364/381 (96%)	364 (100%)	0	100	100
3	E3	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	E5	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	E7	364/381 (96%)	360 (99%)	4 (1%)	70	81
3	E9	364/381 (96%)	363 (100%)	1 (0%)	91	95
3	F1	364/381 (96%)	364 (100%)	0	100	100
4	a	130/190 (68%)	128 (98%)	2 (2%)	60	76
4	b	130/190 (68%)	129 (99%)	1 (1%)	79	87
4	c	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	d	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	e	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	f	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	g	174/190 (92%)	172 (99%)	2 (1%)	70	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	h	174/190 (92%)	170 (98%)	4 (2%)	45	67
4	i	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	j	174/190 (92%)	174 (100%)	0	100	100
4	m	174/190 (92%)	171 (98%)	3 (2%)	56	74
4	n	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	o	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	p	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	q	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	r	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	s	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	t	174/190 (92%)	172 (99%)	2 (1%)	70	81
4	u	174/190 (92%)	173 (99%)	1 (1%)	84	90
4	v	174/190 (92%)	171 (98%)	3 (2%)	56	74
5	k	122/164 (74%)	121 (99%)	1 (1%)	79	87
5	l	122/164 (74%)	121 (99%)	1 (1%)	79	87
5	w	127/164 (77%)	126 (99%)	1 (1%)	79	87
5	x	127/164 (77%)	126 (99%)	1 (1%)	79	87
All	All	23164/31536 (74%)	23071 (100%)	93 (0%)	88	93

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	a	126	ARG
4	i	117	ARG
4	c	126	ARG
4	g	126	ARG
4	p	126	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
4	t	11	ASN
4	t	181	GLN
3	C7	347	ASN
3	C7	134	GLN

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Mol	Chain	Res	Type
4	u	181	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
6	GTP	E4	501	7	29,34,34	1.24	1 (3%)	35,54,54	1.30	4 (11%)
6	GTP	D0	501	7	29,34,34	1.34	3 (10%)	35,54,54	1.36	4 (11%)
6	GTP	B6	501	7	29,34,34	1.36	3 (10%)	35,54,54	1.38	4 (11%)
6	GTP	B0	501	7	29,34,34	1.27	2 (6%)	35,54,54	1.36	4 (11%)
6	GTP	E6	501	7	29,34,34	1.27	3 (10%)	35,54,54	1.31	4 (11%)
6	GTP	A6	501	7	29,34,34	1.32	3 (10%)	35,54,54	1.33	4 (11%)
8	GDP	A5	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.08	2 (6%)
8	GDP	E7	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.21	3 (10%)
8	GDP	E9	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
8	GDP	A1	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.22	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GTP	E2	501	7	29,34,34	1.33	3 (10%)	35,54,54	1.34	4 (11%)
8	GDP	C9	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.20	3 (10%)
8	GDP	B7	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	2 (6%)
6	GTP	A4	501	7	29,34,34	1.37	3 (10%)	35,54,54	1.34	4 (11%)
6	GTP	A8	501	7	29,34,34	1.30	2 (6%)	35,54,54	1.40	4 (11%)
8	GDP	C7	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	2 (6%)
6	GTP	A2	501	7	29,34,34	1.26	2 (6%)	35,54,54	1.30	4 (11%)
6	GTP	B2	501	7	29,34,34	1.35	3 (10%)	35,54,54	1.39	5 (14%)
8	GDP	A9	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.19	5 (16%)
8	GDP	B3	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.17	2 (6%)
8	GDP	B5	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.07	2 (6%)
6	GTP	C0	501	7	29,34,34	1.30	3 (10%)	35,54,54	1.33	4 (11%)
8	GDP	D5	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
8	GDP	E3	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.14	2 (6%)
6	GTP	D8	501	7	29,34,34	1.30	2 (6%)	35,54,54	1.33	4 (11%)
6	GTP	D2	501	7	29,34,34	1.30	2 (6%)	35,54,54	1.36	4 (11%)
6	GTP	C2	501	7	29,34,34	1.28	2 (6%)	35,54,54	1.31	3 (8%)
8	GDP	E1	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.17	2 (6%)
8	GDP	C3	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.23	3 (10%)
8	GDP	D1	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.14	3 (10%)
8	GDP	F1	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	3 (10%)
8	GDP	C5	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.30	5 (16%)
8	GDP	D7	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.08	2 (6%)
8	GDP	E5	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	4 (13%)
6	GTP	B4	501	7	29,34,34	1.38	3 (10%)	35,54,54	1.33	5 (14%)
6	GTP	F0	501	7	29,34,34	1.28	3 (10%)	35,54,54	1.31	4 (11%)
6	GTP	C6	501	7	29,34,34	1.30	2 (6%)	35,54,54	1.38	5 (14%)
6	GTP	E8	501	7	29,34,34	1.25	3 (10%)	35,54,54	1.36	4 (11%)
8	GDP	A3	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.18	2 (6%)
8	GDP	B1	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
6	GTP	C4	501	7	29,34,34	1.33	2 (6%)	35,54,54	1.32	5 (14%)
6	GTP	B8	501	7	29,34,34	1.35	3 (10%)	35,54,54	1.36	4 (11%)
6	GTP	D4	501	7	29,34,34	1.36	2 (6%)	35,54,54	1.45	5 (14%)
6	GTP	E0	501	7	29,34,34	1.26	2 (6%)	35,54,54	1.33	4 (11%)
6	GTP	A0	501	7	29,34,34	1.29	3 (10%)	35,54,54	1.33	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GTP	D6	501	7	29,34,34	1.21	2 (6%)	35,54,54	1.39	4 (11%)
8	GDP	A7	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.15	3 (10%)
8	GDP	D3	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.17	2 (6%)
8	GDP	B9	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	2 (6%)
8	GDP	D9	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.15	2 (6%)
8	GDP	C1	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.15	2 (6%)
6	GTP	C8	501	7	29,34,34	1.33	3 (10%)	35,54,54	1.33	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GTP	E4	501	7	-	6/18/38/38	0/3/3/3
6	GTP	D0	501	7	-	3/18/38/38	0/3/3/3
6	GTP	B6	501	7	-	6/18/38/38	0/3/3/3
6	GTP	B0	501	7	-	7/18/38/38	0/3/3/3
6	GTP	E6	501	7	-	5/18/38/38	0/3/3/3
6	GTP	A6	501	7	-	6/18/38/38	0/3/3/3
8	GDP	A5	501	-	-	3/12/32/32	0/3/3/3
8	GDP	E7	501	-	-	3/12/32/32	0/3/3/3
8	GDP	E9	501	-	-	4/12/32/32	0/3/3/3
8	GDP	A1	501	-	-	6/12/32/32	0/3/3/3
6	GTP	E2	501	7	-	4/18/38/38	0/3/3/3
8	GDP	C9	501	-	-	3/12/32/32	0/3/3/3
8	GDP	B7	501	-	-	3/12/32/32	0/3/3/3
6	GTP	A4	501	7	-	4/18/38/38	0/3/3/3
6	GTP	A8	501	7	-	4/18/38/38	0/3/3/3
8	GDP	C7	501	-	-	1/12/32/32	0/3/3/3
6	GTP	A2	501	7	-	7/18/38/38	0/3/3/3
6	GTP	B2	501	7	-	6/18/38/38	0/3/3/3
8	GDP	A9	501	-	-	5/12/32/32	0/3/3/3
8	GDP	B3	501	-	-	4/12/32/32	0/3/3/3
8	GDP	B5	501	-	-	2/12/32/32	0/3/3/3
6	GTP	C0	501	7	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D5	501	-	-	6/12/32/32	0/3/3/3
8	GDP	E3	501	-	-	0/12/32/32	0/3/3/3
6	GTP	D8	501	7	-	5/18/38/38	0/3/3/3
6	GTP	D2	501	7	-	7/18/38/38	0/3/3/3
6	GTP	C2	501	7	-	3/18/38/38	0/3/3/3
8	GDP	E1	501	-	-	2/12/32/32	0/3/3/3
8	GDP	C3	501	-	-	4/12/32/32	0/3/3/3
8	GDP	D1	501	-	-	3/12/32/32	0/3/3/3
8	GDP	F1	501	-	-	4/12/32/32	0/3/3/3
8	GDP	C5	501	-	-	6/12/32/32	0/3/3/3
8	GDP	D7	501	-	-	4/12/32/32	0/3/3/3
8	GDP	E5	501	-	-	3/12/32/32	0/3/3/3
6	GTP	B4	501	7	-	4/18/38/38	0/3/3/3
6	GTP	F0	501	7	-	7/18/38/38	0/3/3/3
6	GTP	C6	501	7	-	4/18/38/38	0/3/3/3
6	GTP	E8	501	7	-	6/18/38/38	0/3/3/3
8	GDP	A3	501	-	-	2/12/32/32	0/3/3/3
8	GDP	B1	501	-	-	5/12/32/32	0/3/3/3
6	GTP	C4	501	7	-	5/18/38/38	0/3/3/3
6	GTP	B8	501	7	-	6/18/38/38	0/3/3/3
6	GTP	D4	501	7	-	4/18/38/38	0/3/3/3
6	GTP	E0	501	7	-	2/18/38/38	0/3/3/3
6	GTP	A0	501	7	-	8/18/38/38	0/3/3/3
6	GTP	D6	501	7	-	7/18/38/38	0/3/3/3
8	GDP	A7	501	-	-	4/12/32/32	0/3/3/3
8	GDP	D3	501	-	-	4/12/32/32	0/3/3/3
8	GDP	B9	501	-	-	3/12/32/32	0/3/3/3
8	GDP	D9	501	-	-	5/12/32/32	0/3/3/3
8	GDP	C1	501	-	-	5/12/32/32	0/3/3/3
6	GTP	C8	501	7	-	3/18/38/38	0/3/3/3

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A4	501	GTP	C5-C6	-5.28	1.37	1.47
6	D4	501	GTP	C5-C6	-5.21	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B4	501	GTP	C5-C6	-5.08	1.37	1.47
6	A6	501	GTP	C5-C6	-5.07	1.37	1.47
6	C8	501	GTP	C5-C6	-5.07	1.37	1.47

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E8	501	GTP	C8-N7-C5	3.81	109.04	102.55
6	C2	501	GTP	C8-N7-C5	3.76	108.96	102.55
6	D8	501	GTP	C8-N7-C5	3.76	108.96	102.55
6	A0	501	GTP	C8-N7-C5	3.75	108.93	102.55
6	B6	501	GTP	C8-N7-C5	3.74	108.91	102.55

There are no chirality outliers.

5 of 231 torsion outliers are listed below:

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

There are no ring outliers.

27 monomers are involved in 40 short contacts:

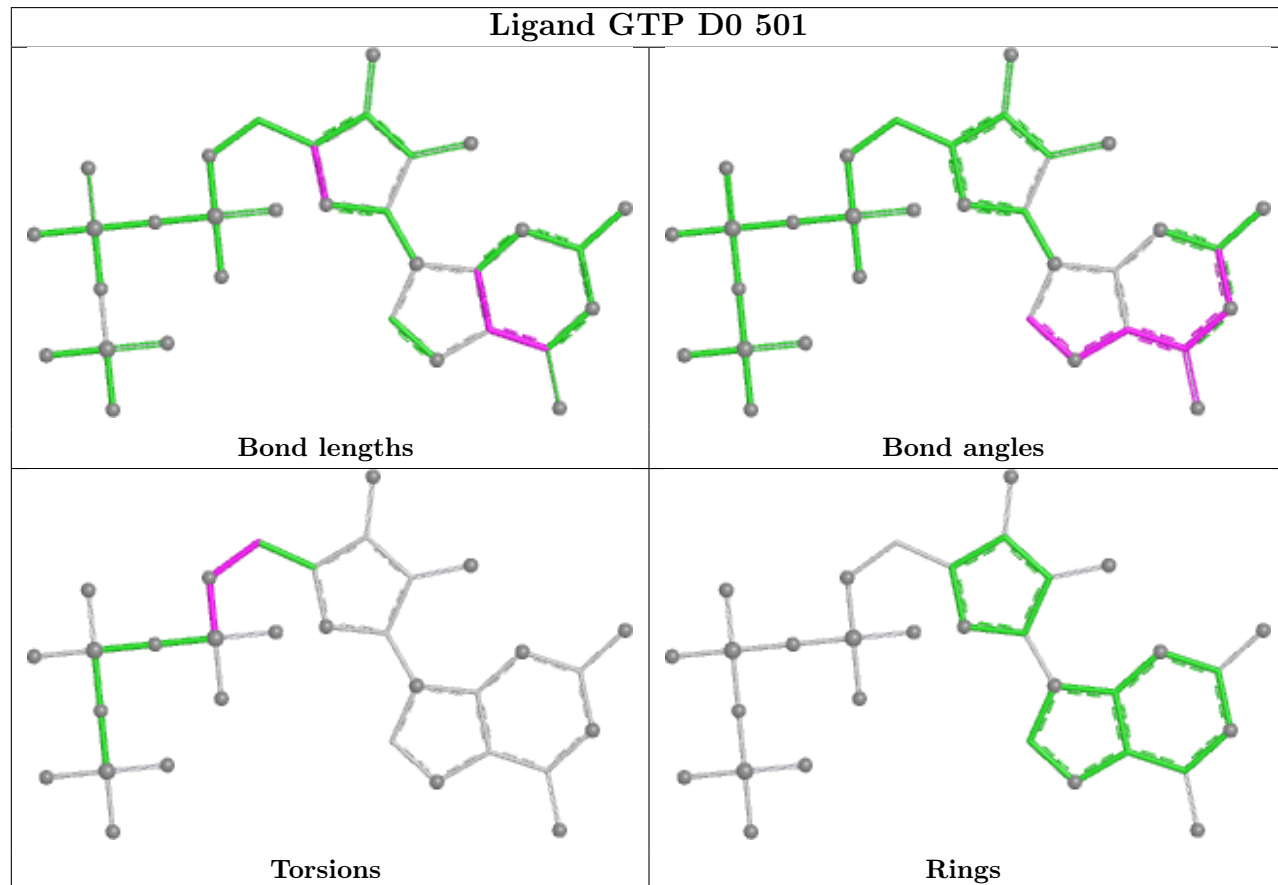
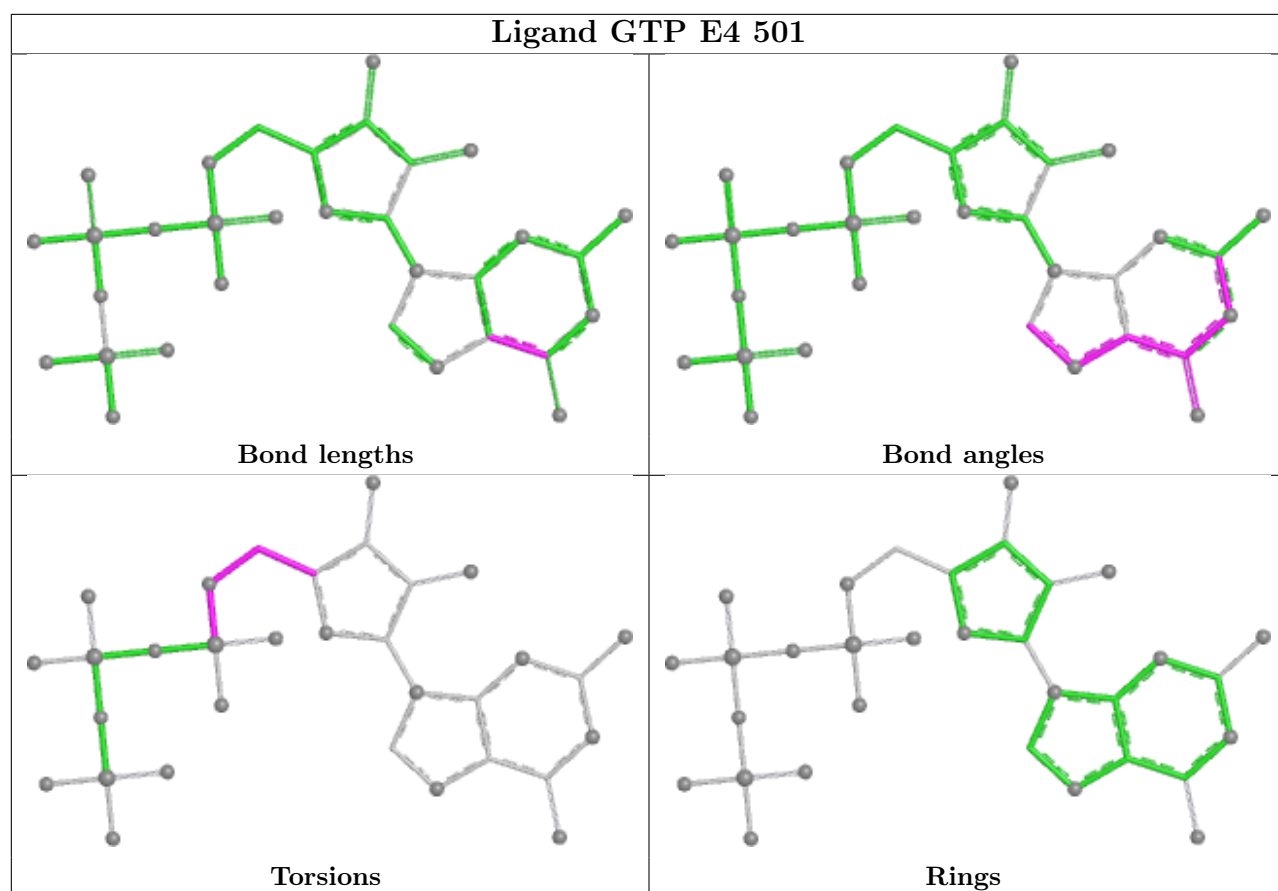
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B6	501	GTP	2	0
6	B0	501	GTP	1	0
6	E6	501	GTP	3	0
8	A1	501	GDP	2	0
6	E2	501	GTP	1	0
8	B7	501	GDP	1	0
6	A8	501	GTP	1	0
6	B2	501	GTP	1	0
8	A9	501	GDP	1	0
8	B3	501	GDP	1	0
6	C0	501	GTP	2	0
8	D5	501	GDP	1	0
8	E3	501	GDP	3	0
6	D8	501	GTP	1	0

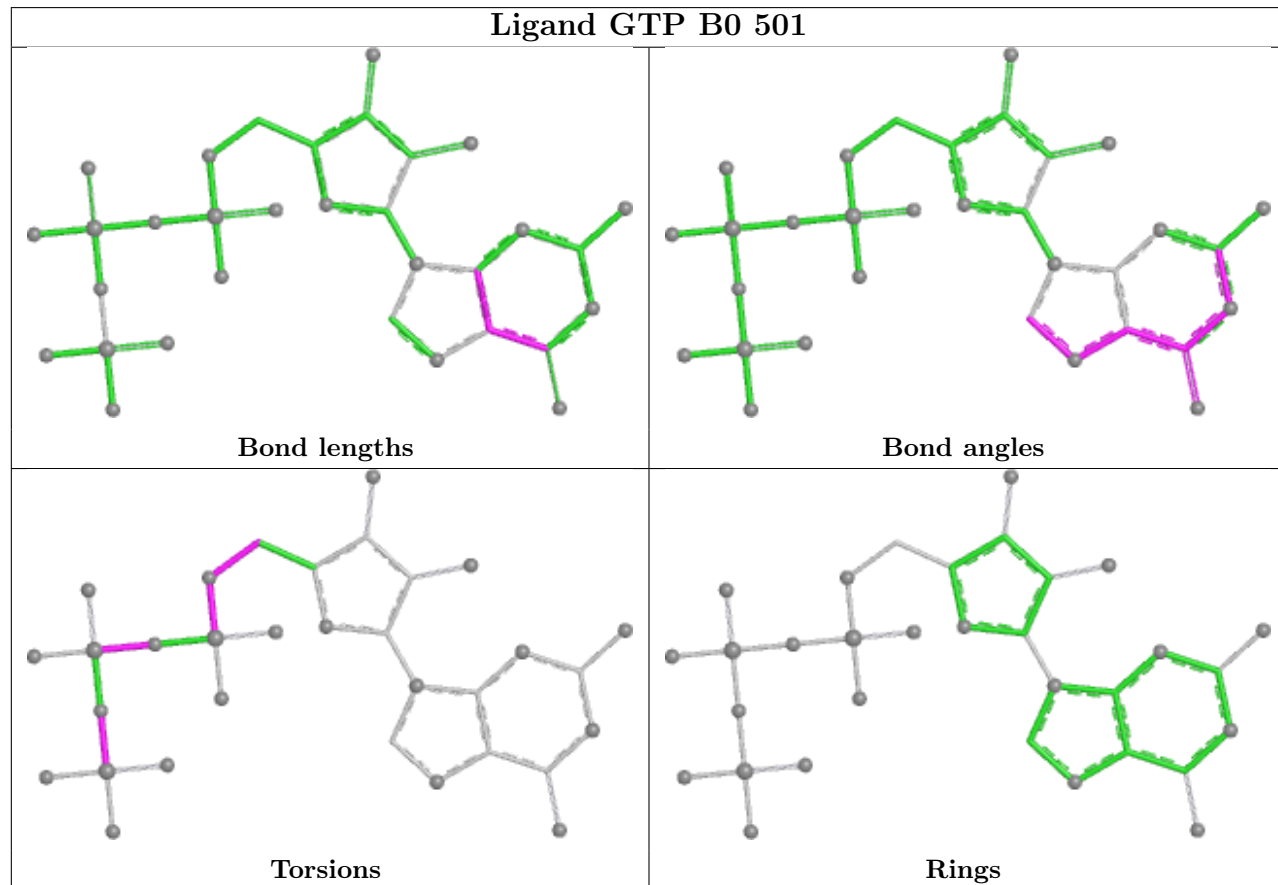
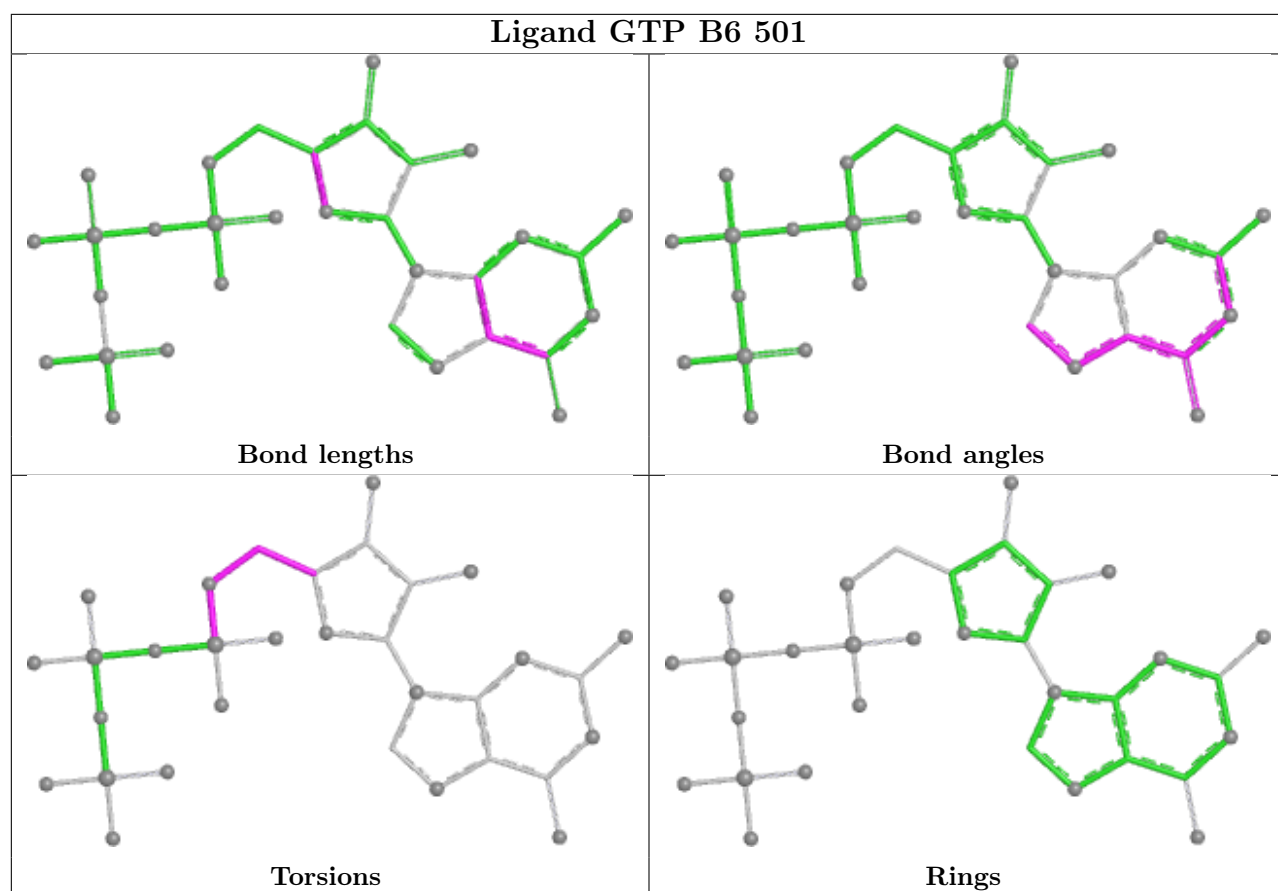
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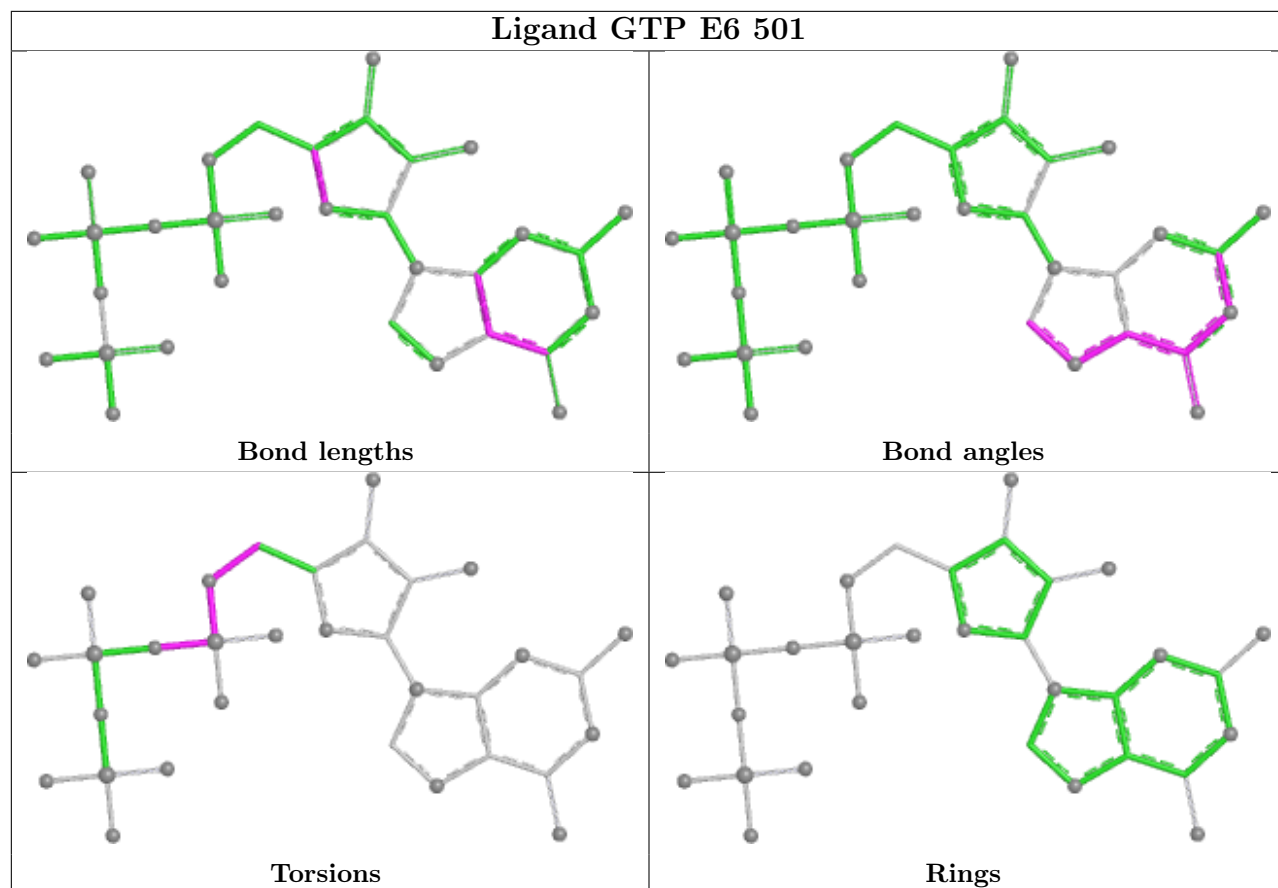
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C3	501	GDP	2	0
8	F1	501	GDP	1	0
8	C5	501	GDP	1	0
6	F0	501	GTP	1	0
6	C6	501	GTP	3	0
6	E8	501	GTP	2	0
8	A3	501	GDP	2	0
6	C4	501	GTP	1	0
6	B8	501	GTP	1	0
6	D4	501	GTP	1	0
6	A0	501	GTP	2	0
8	C1	501	GDP	1	0
6	C8	501	GTP	1	0

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

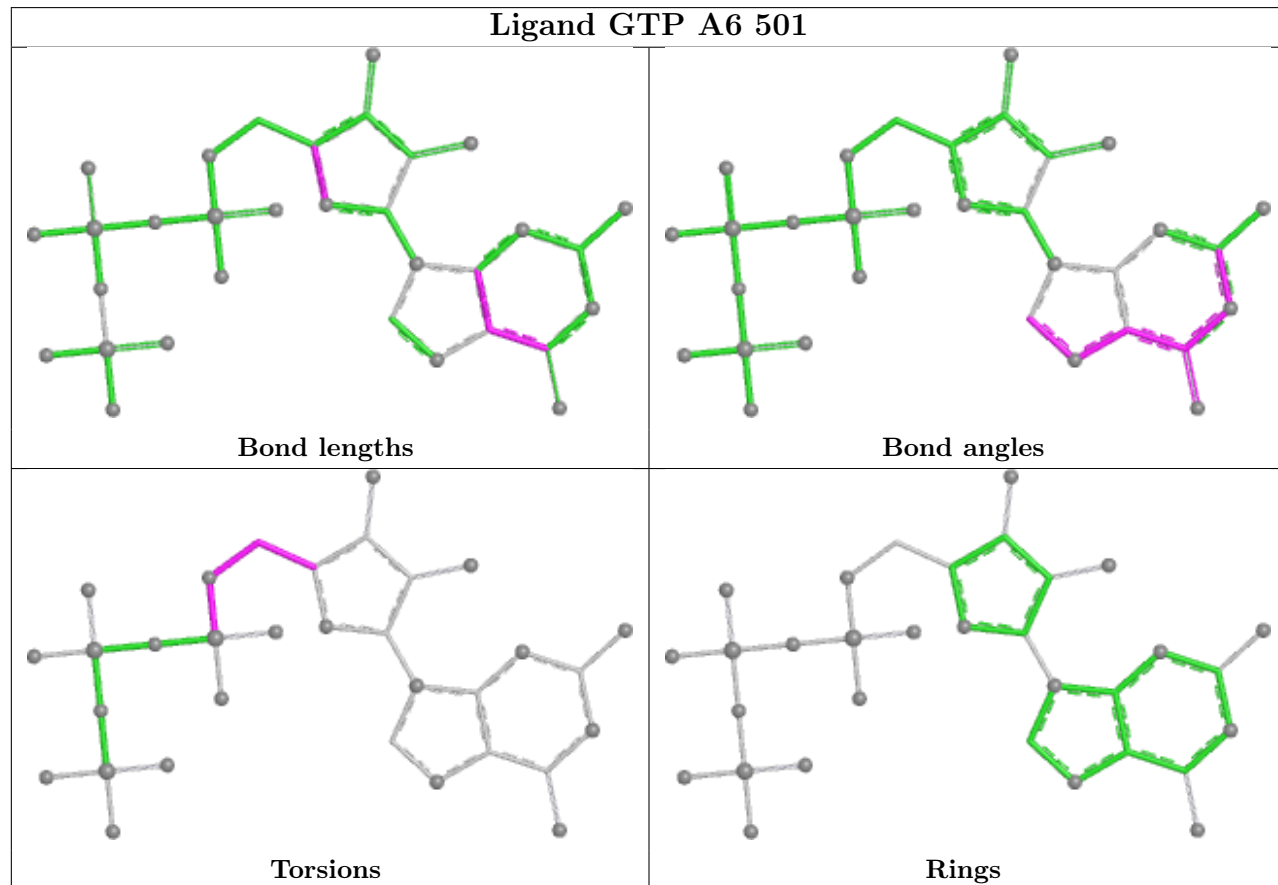


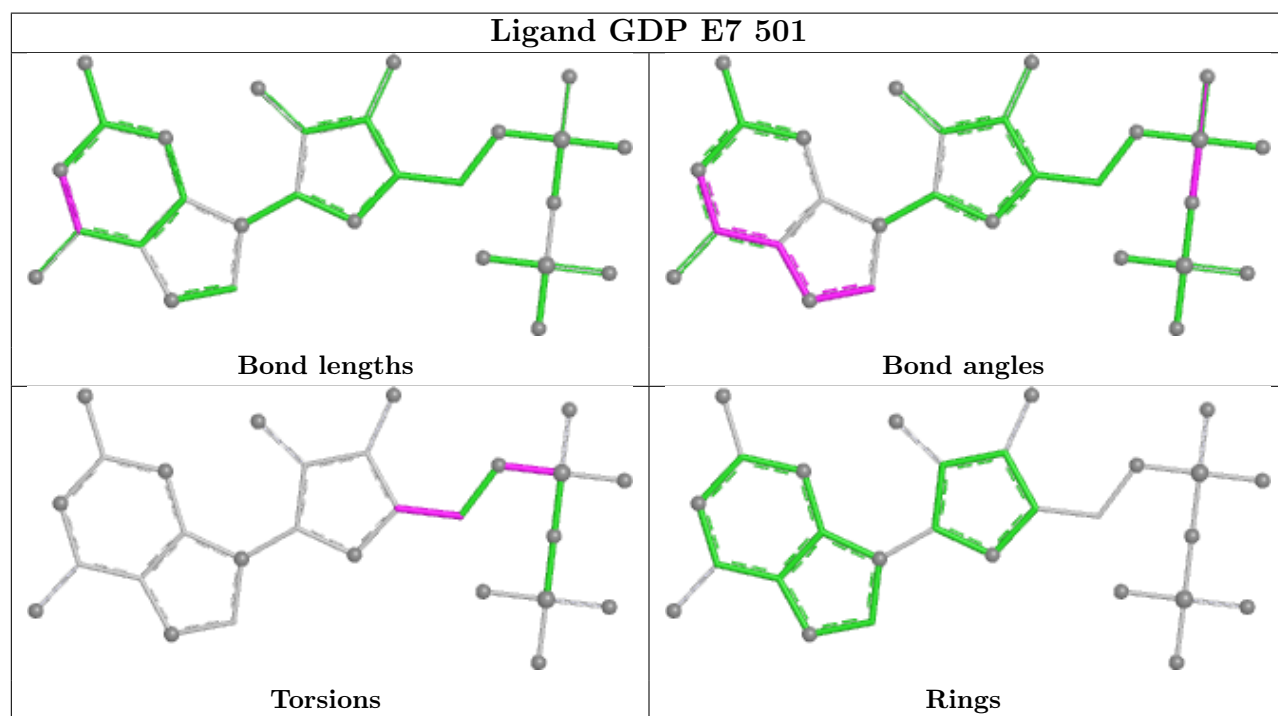
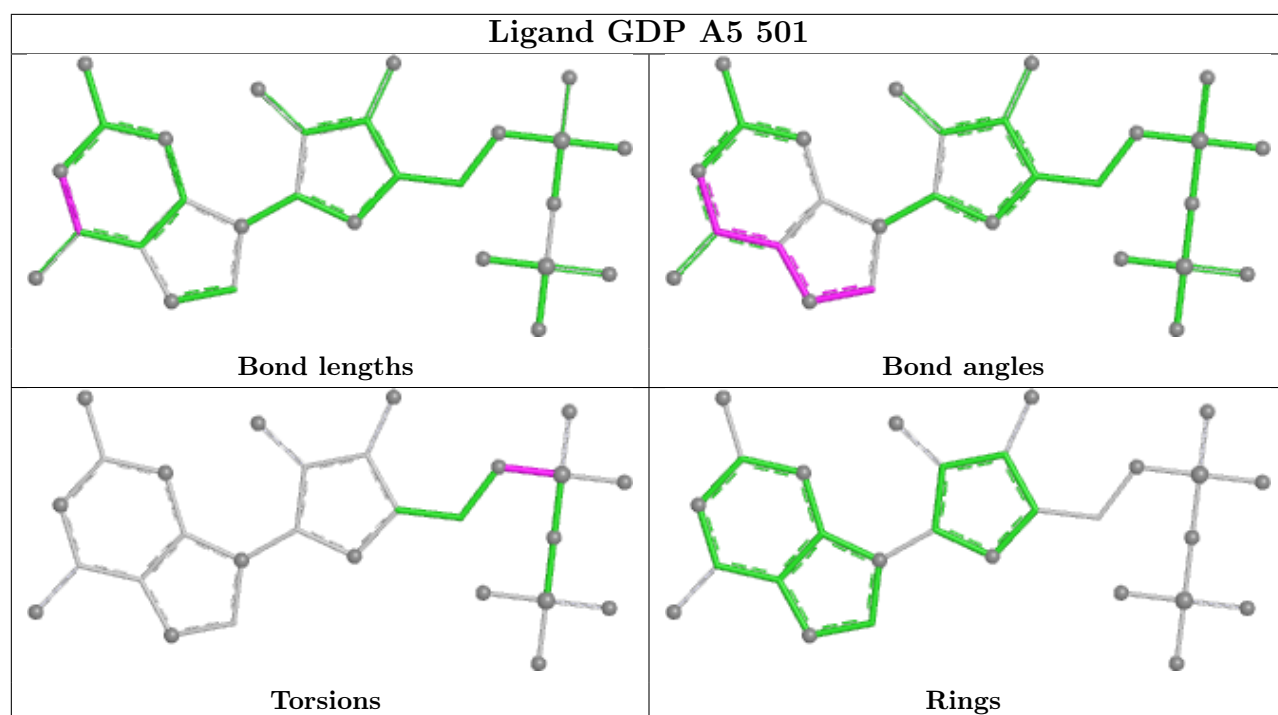


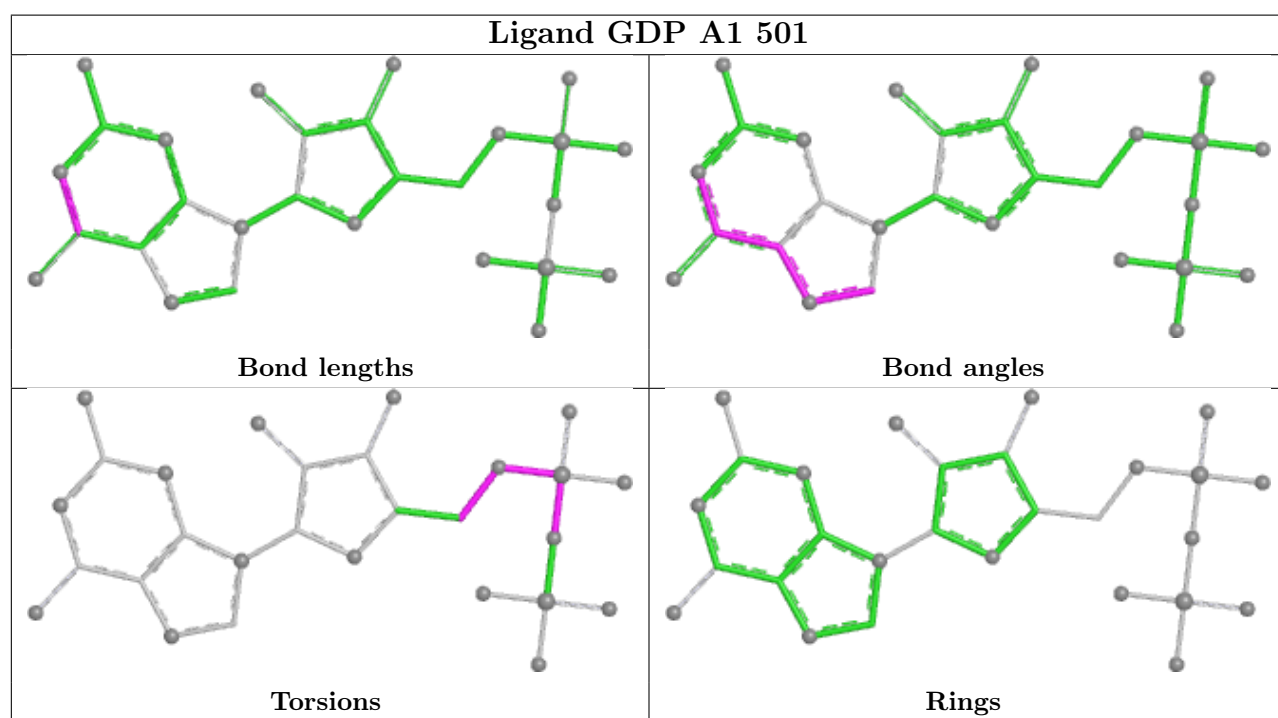
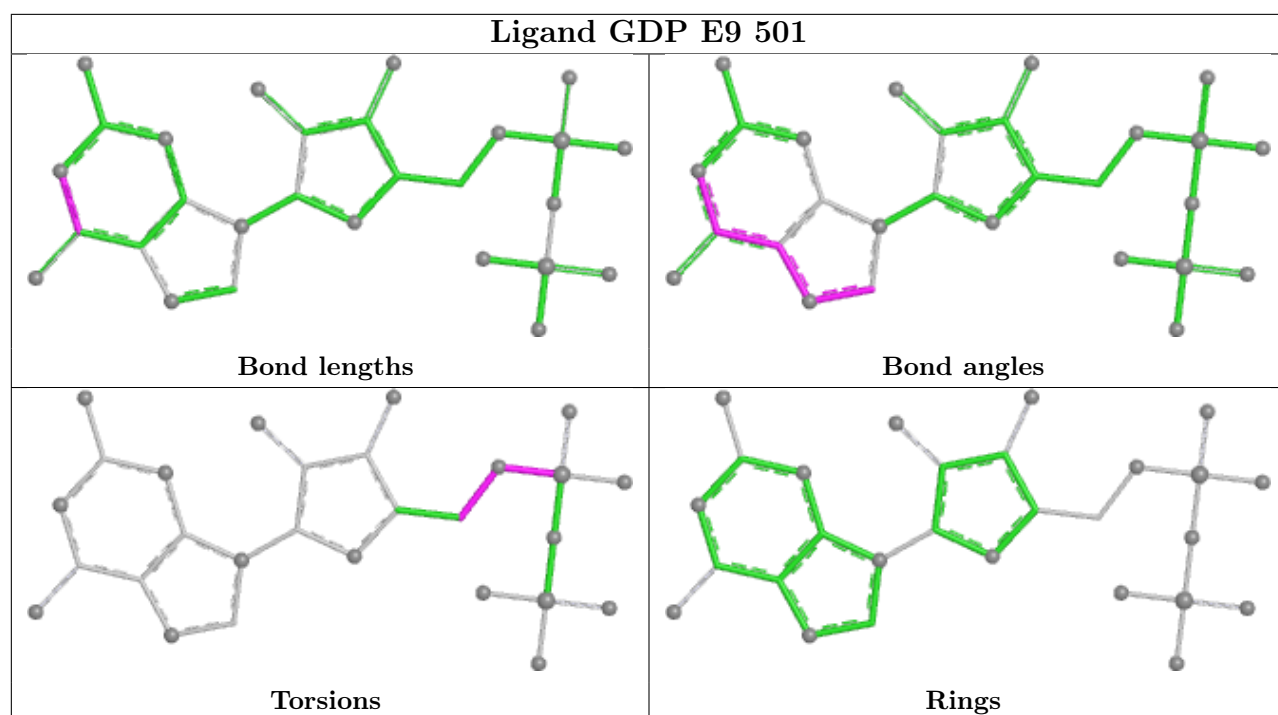
Ligand GTP E6 501

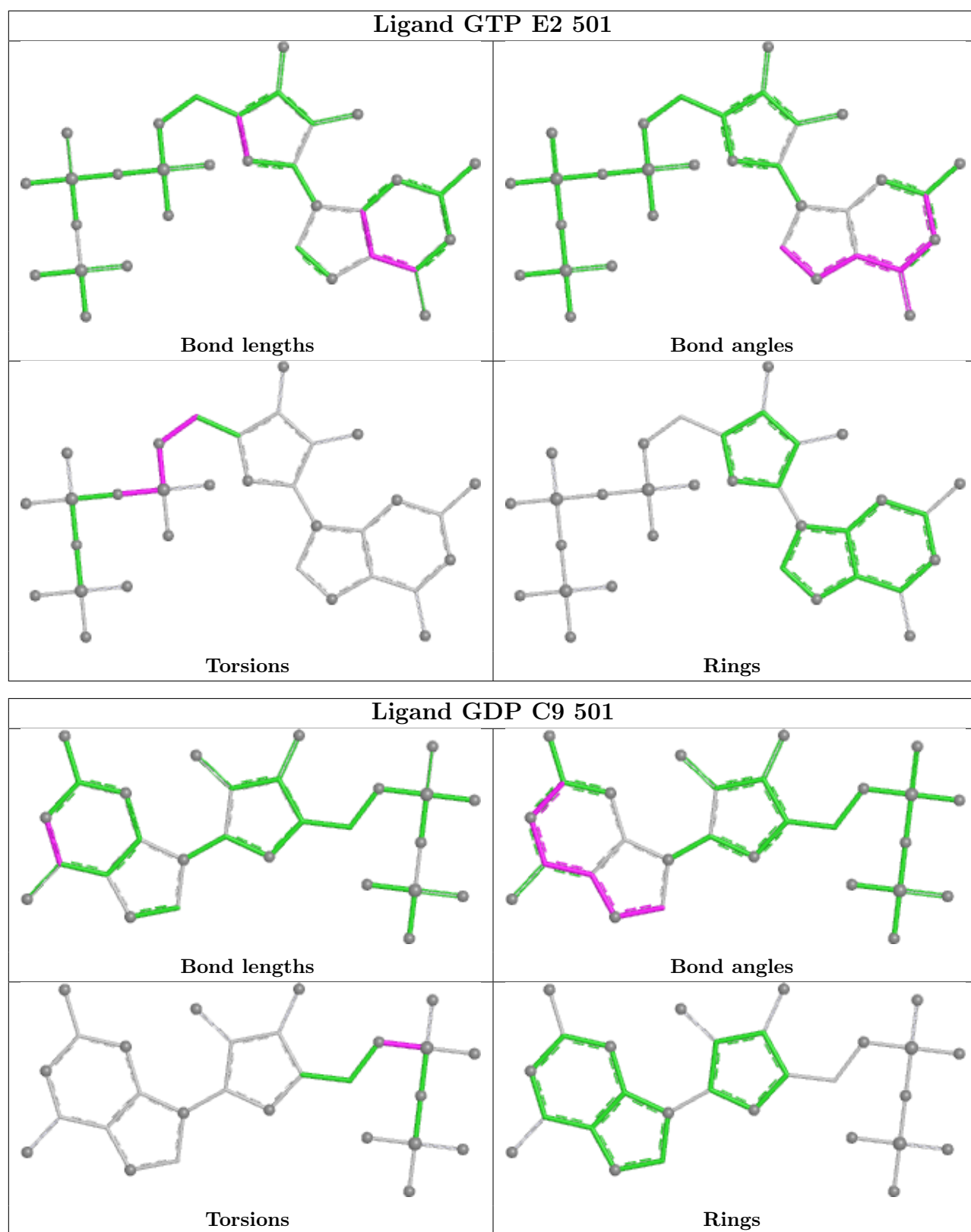


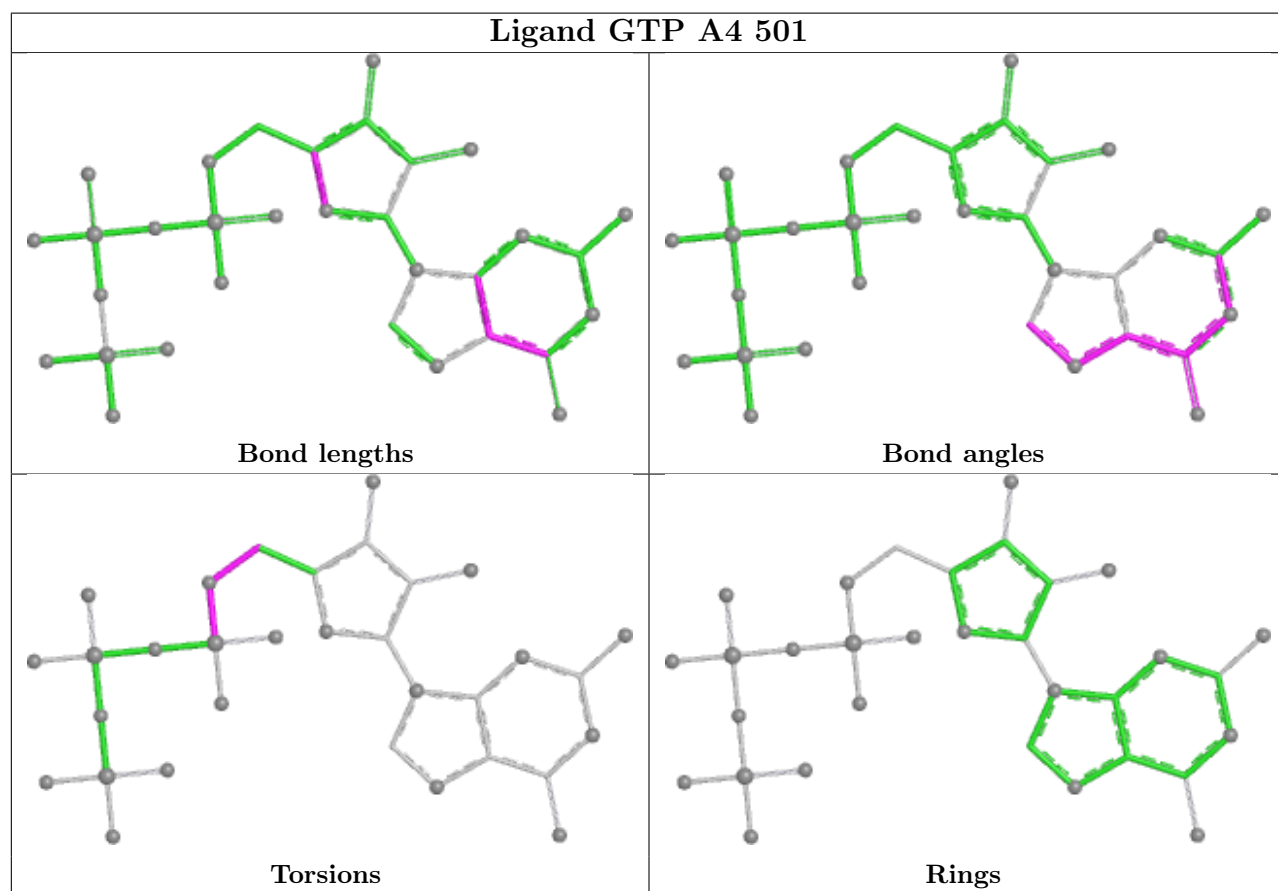
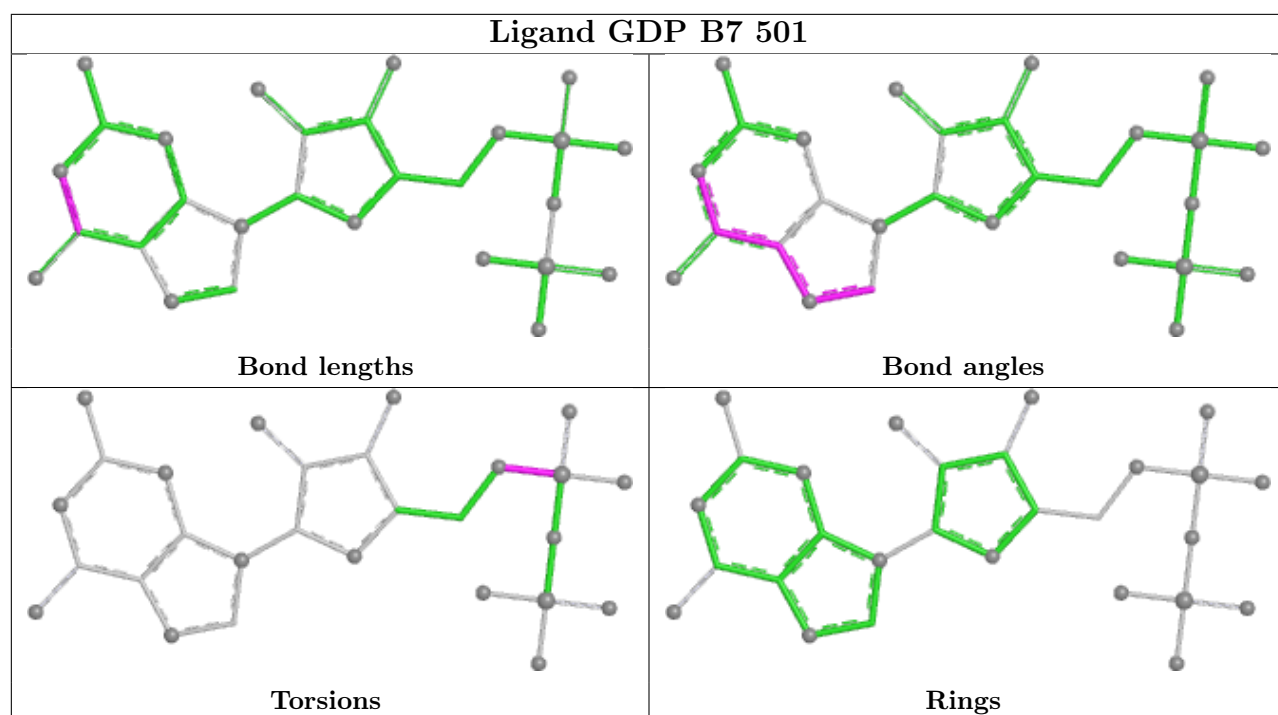
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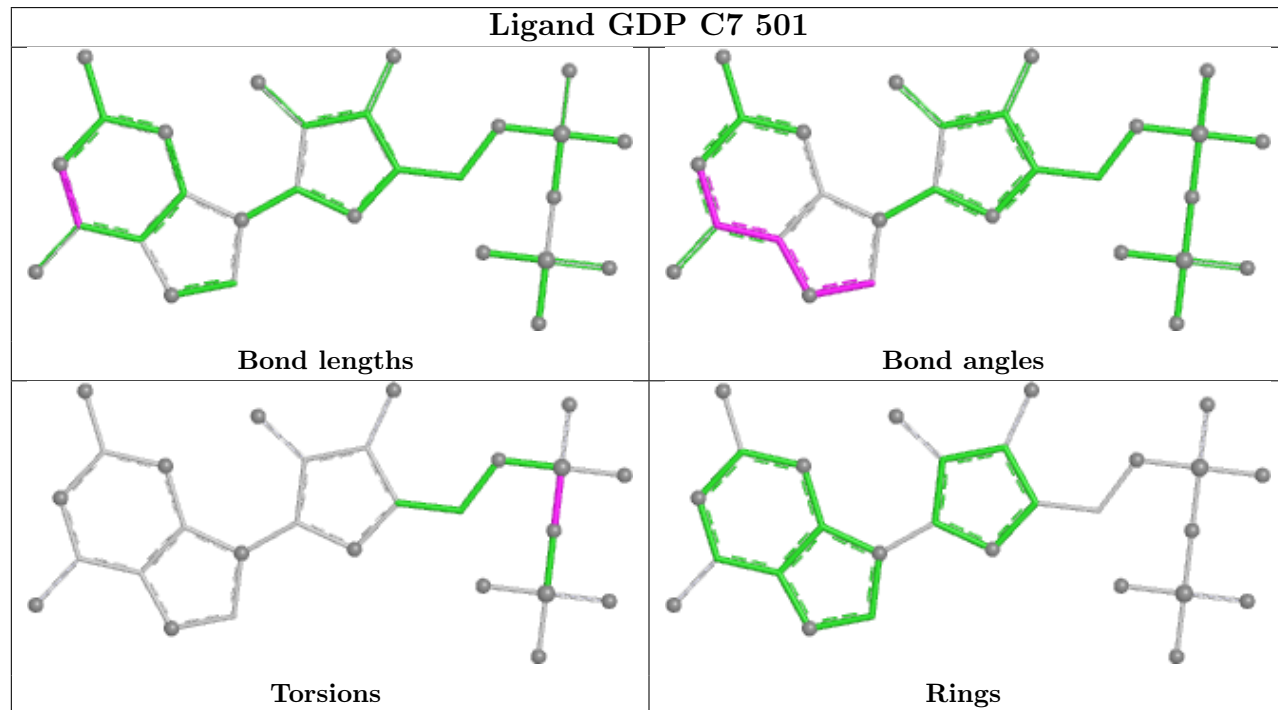
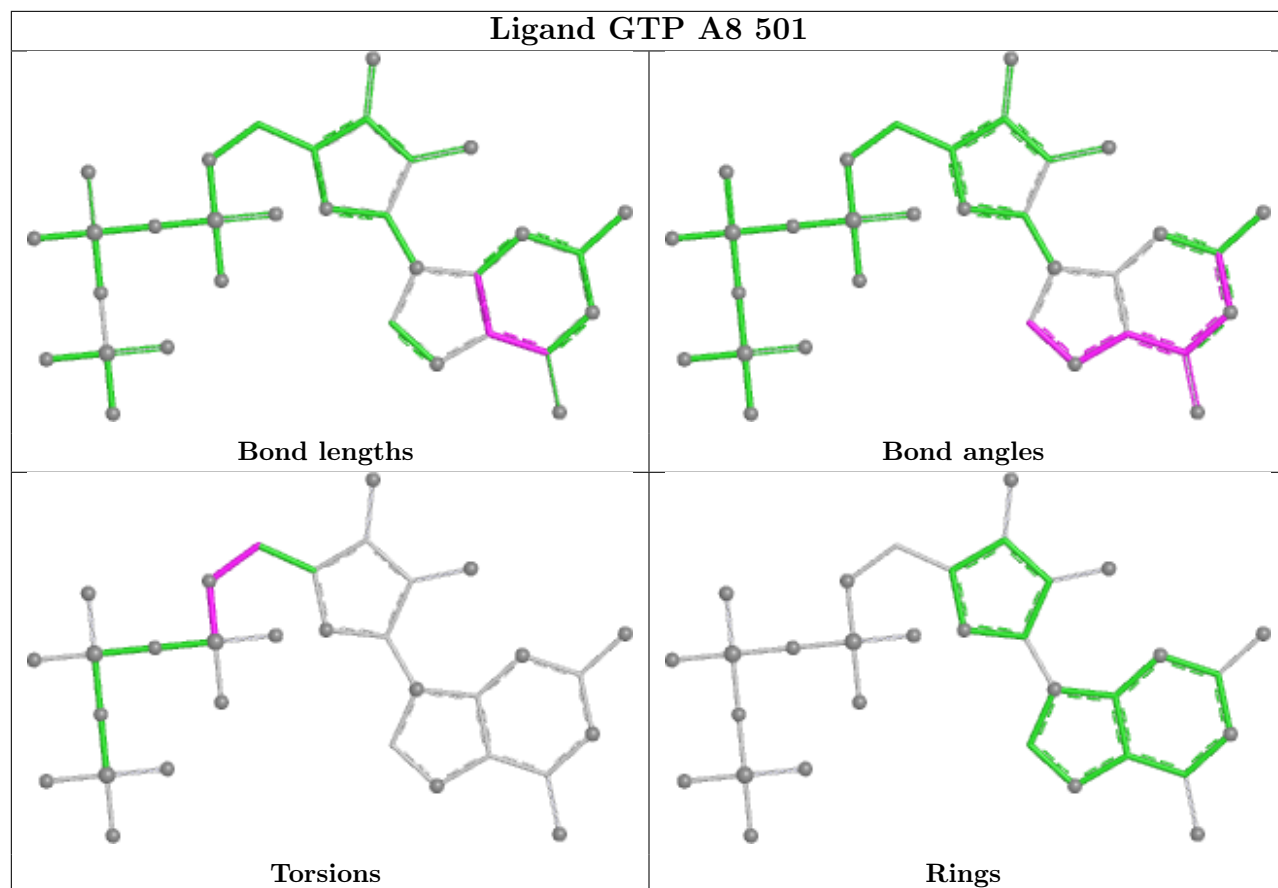




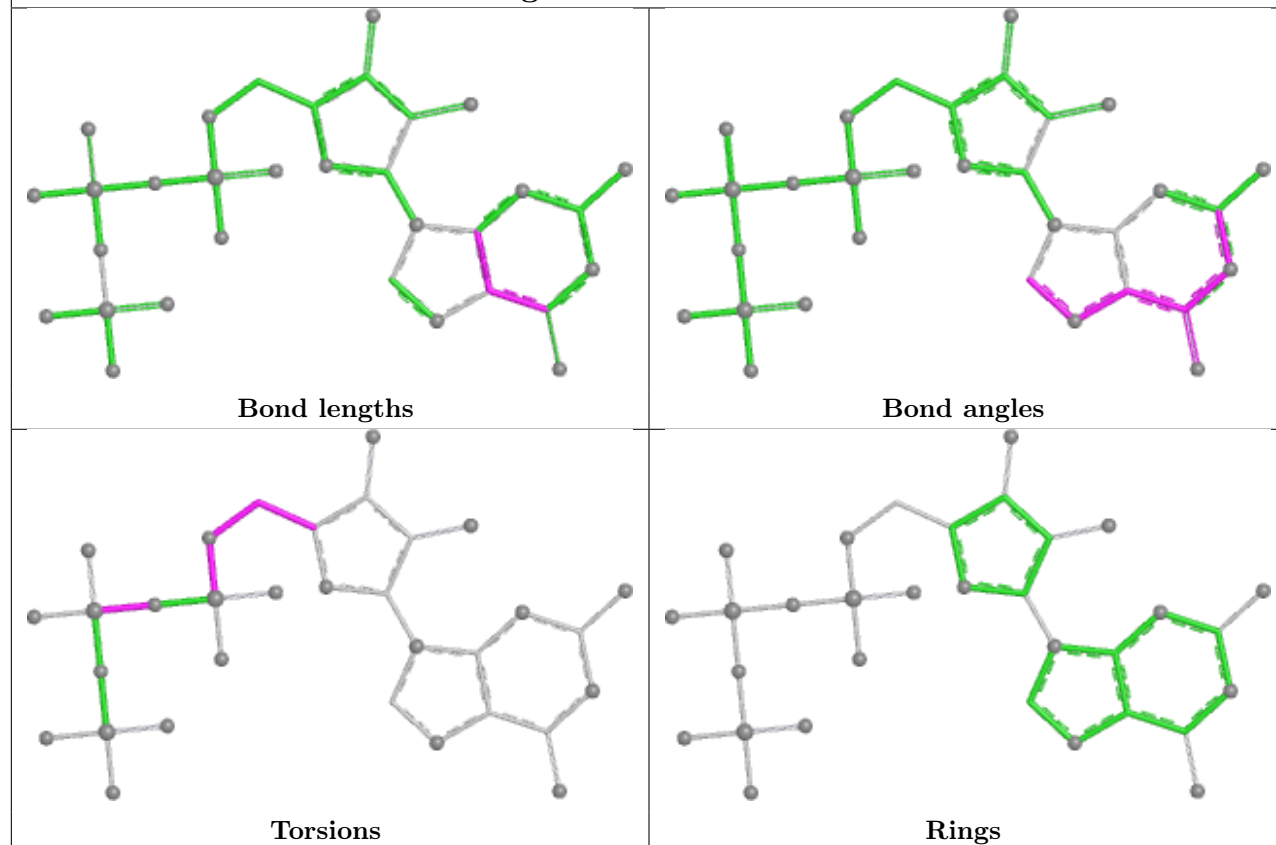




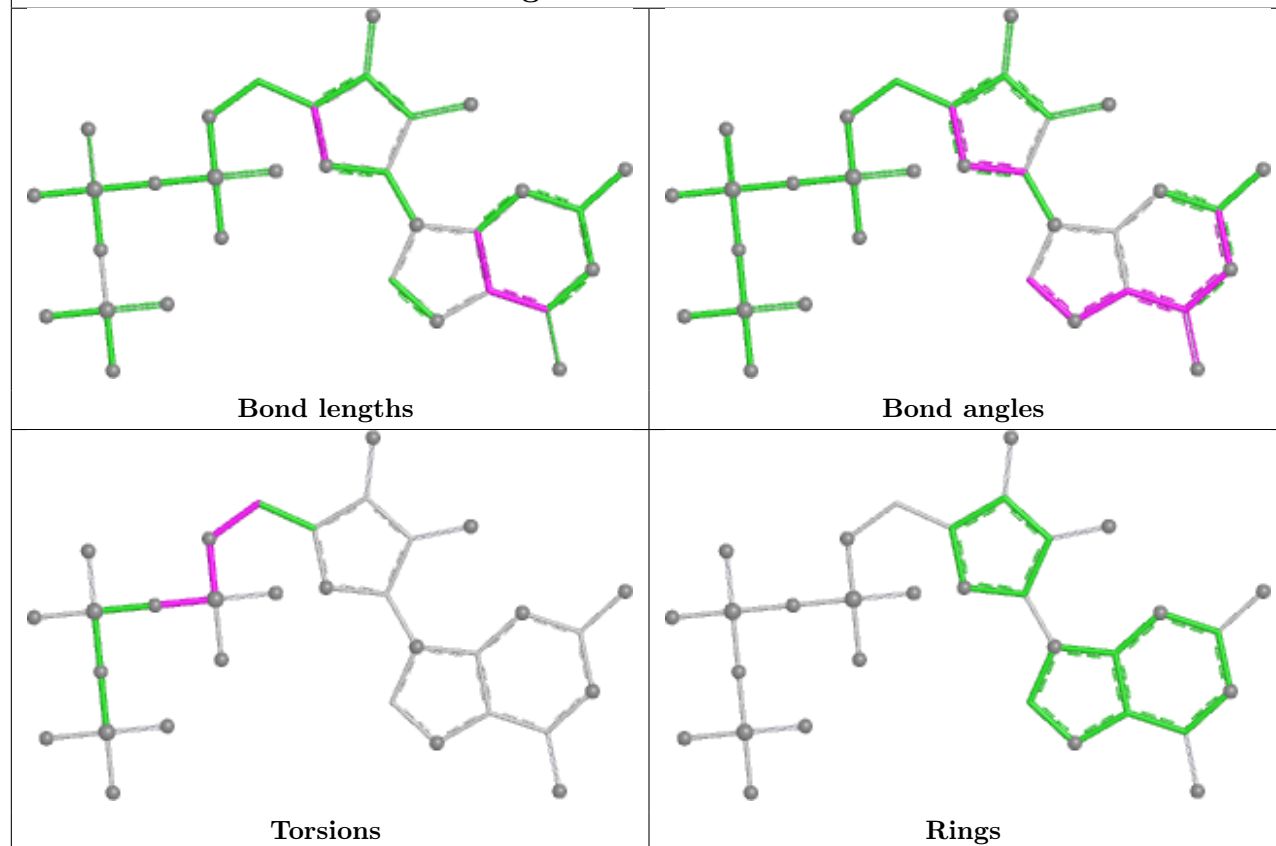


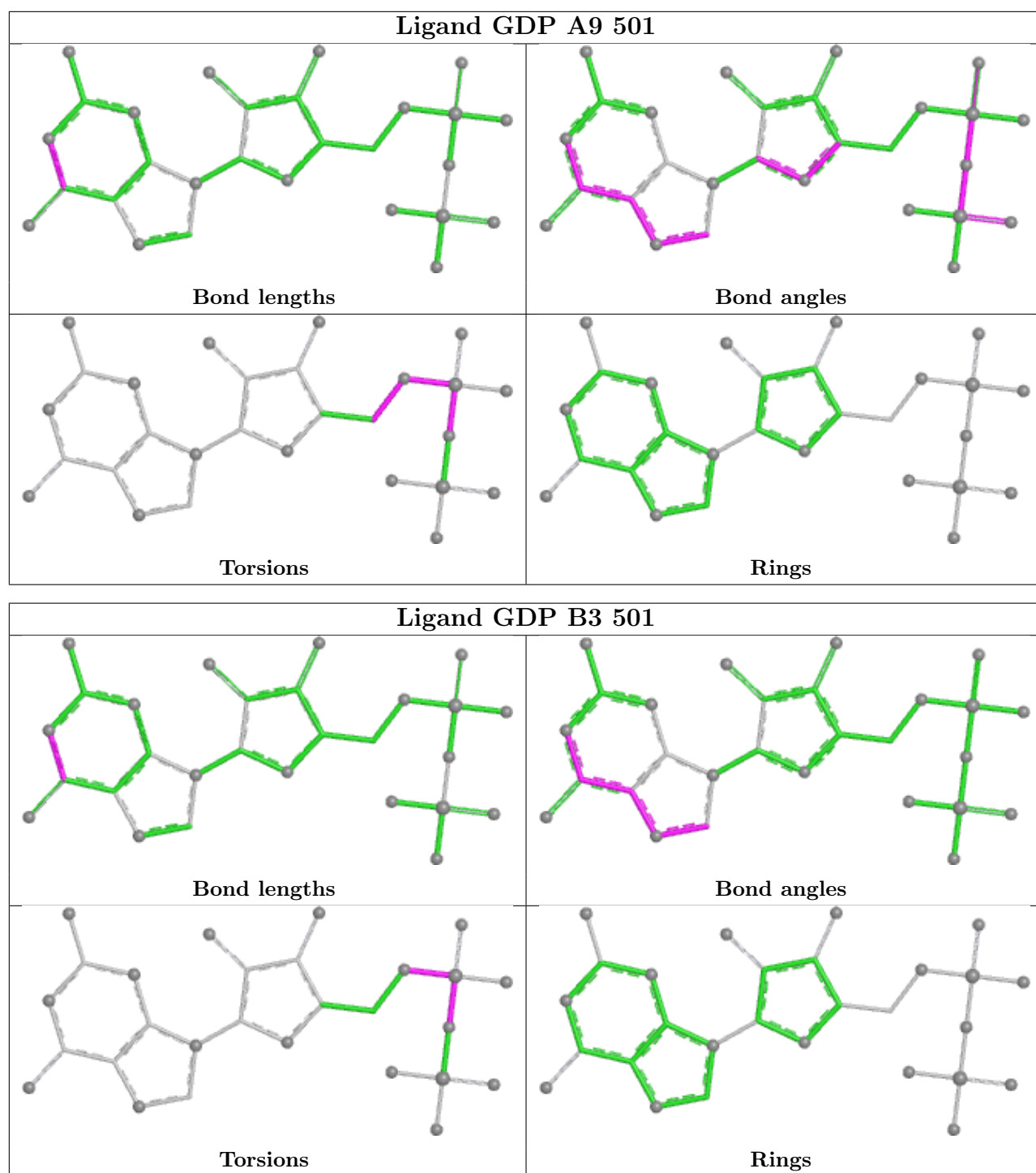


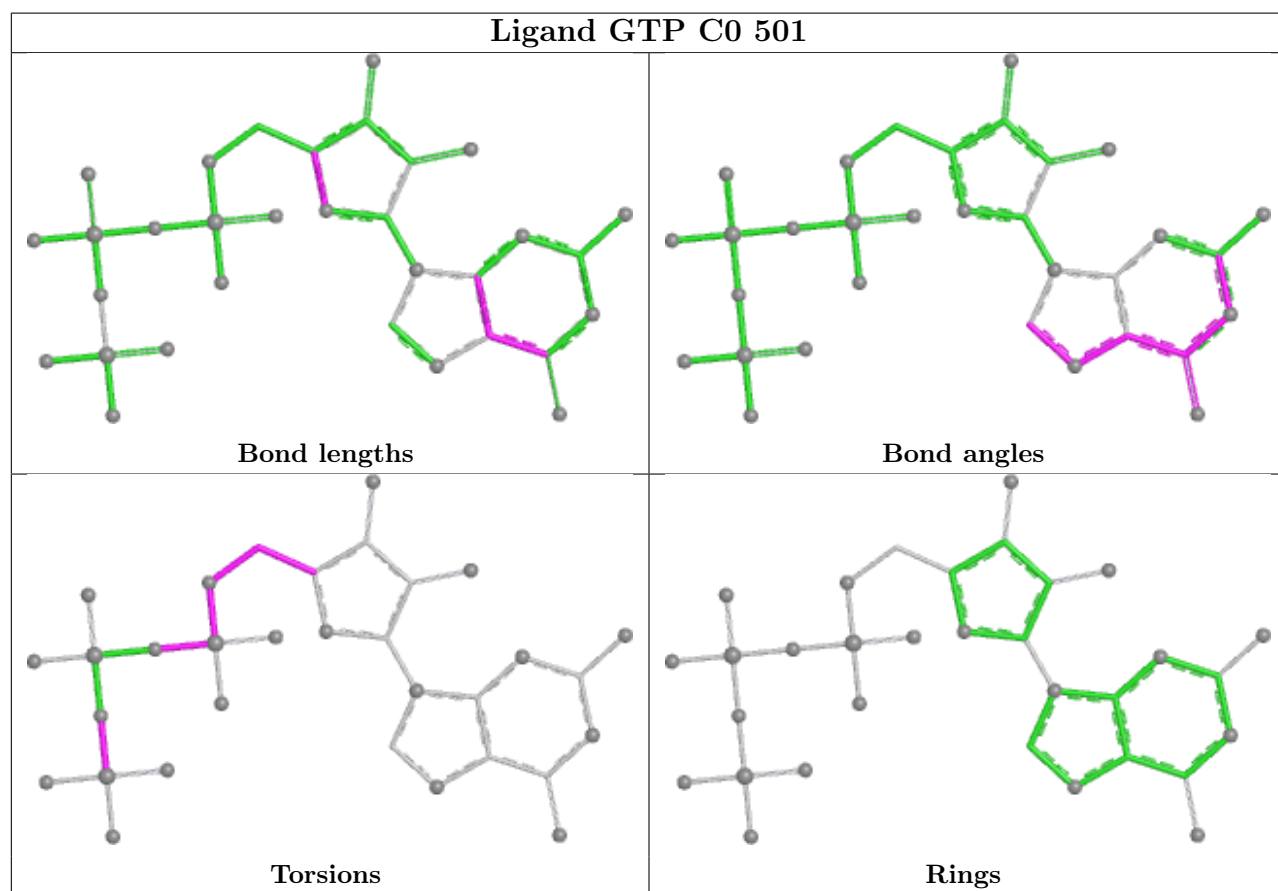
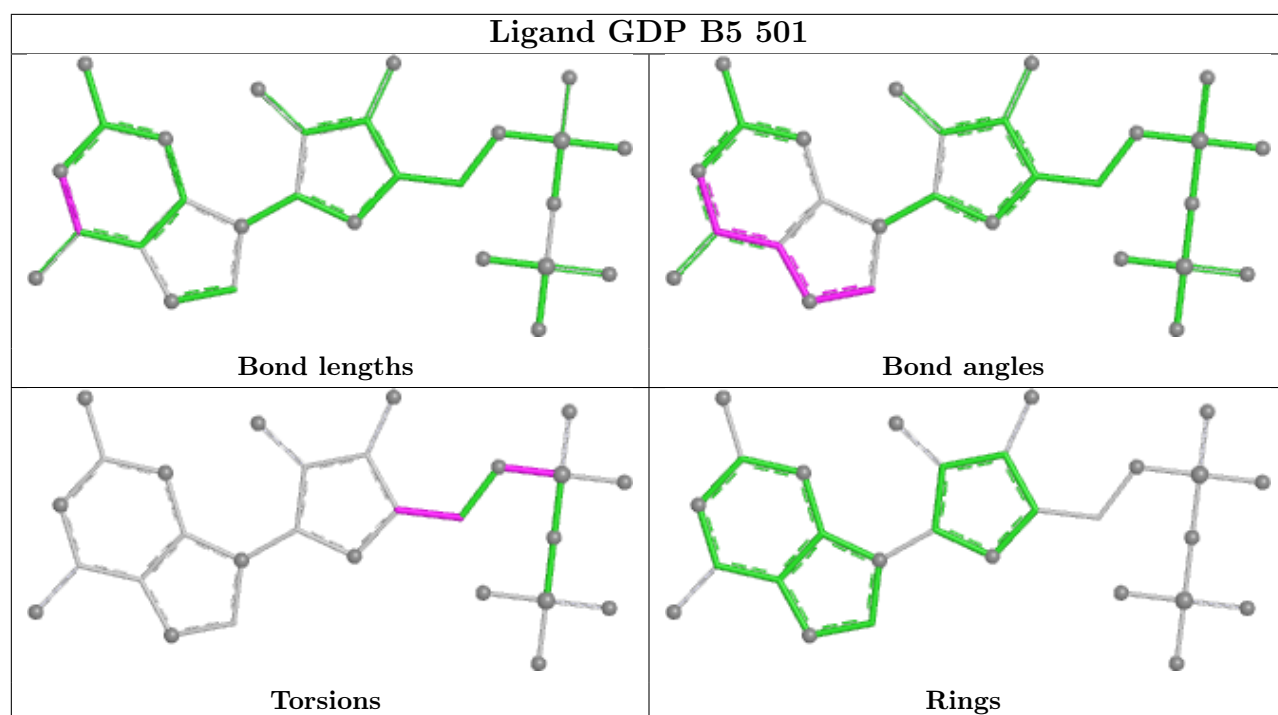
Ligand GTP A2 501

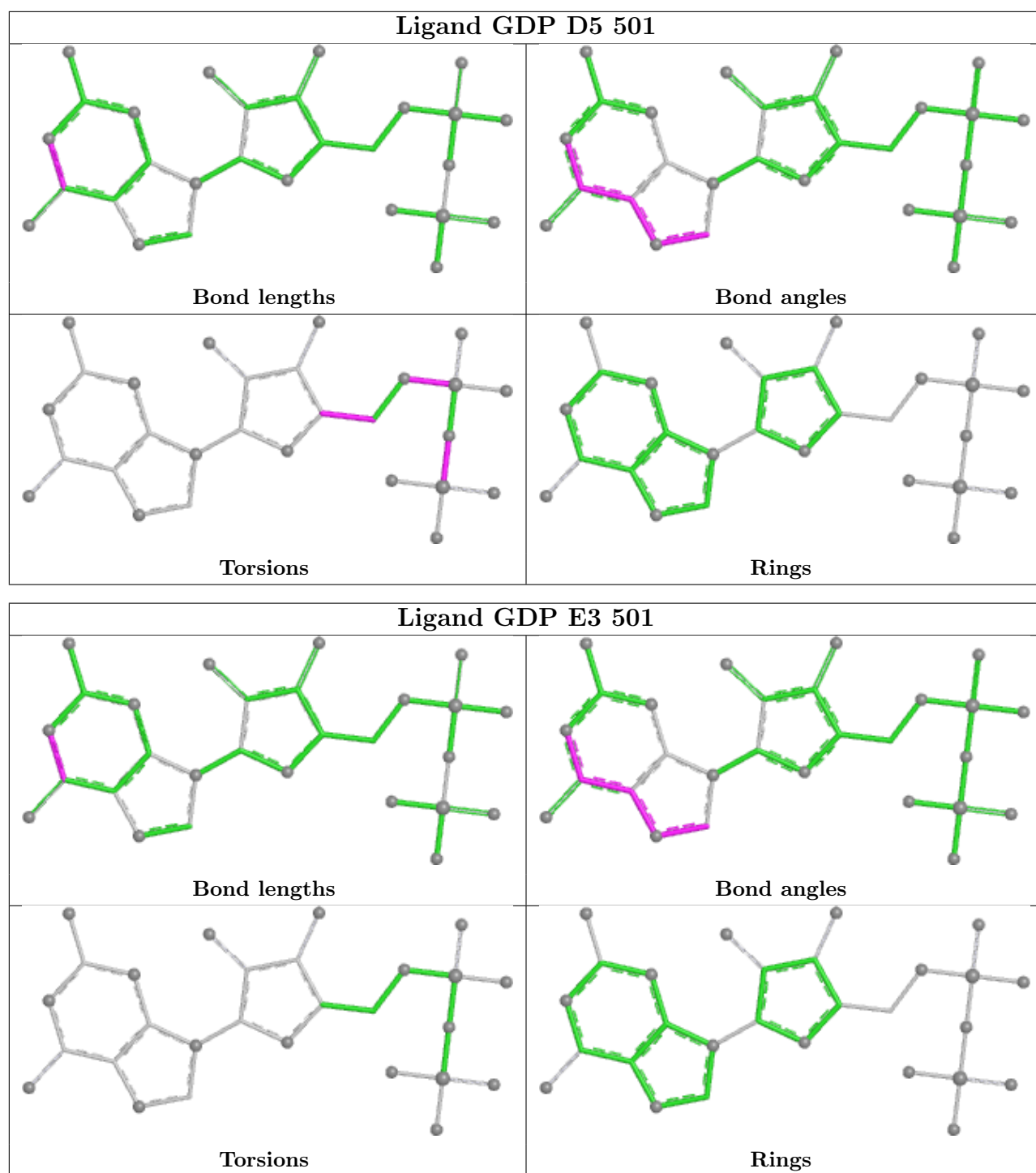


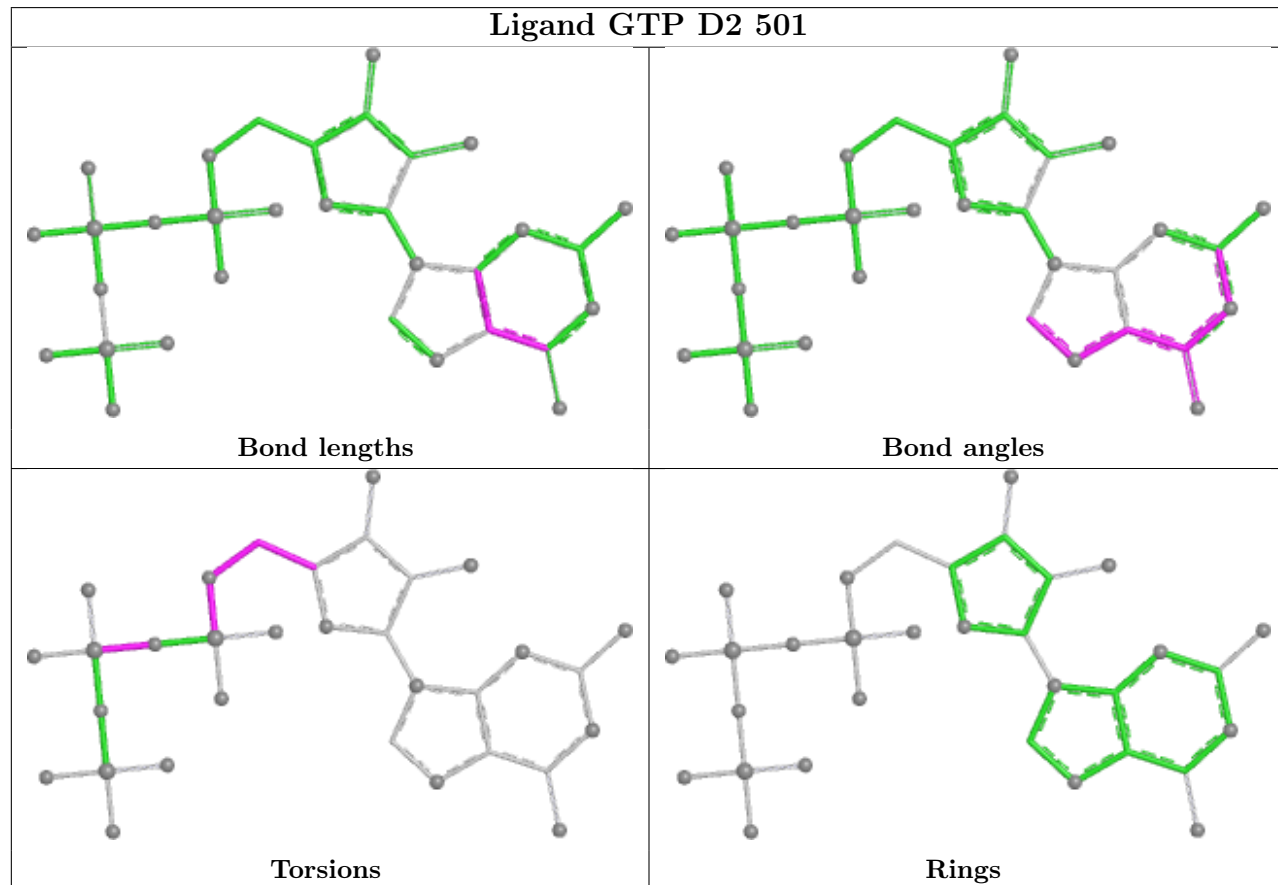
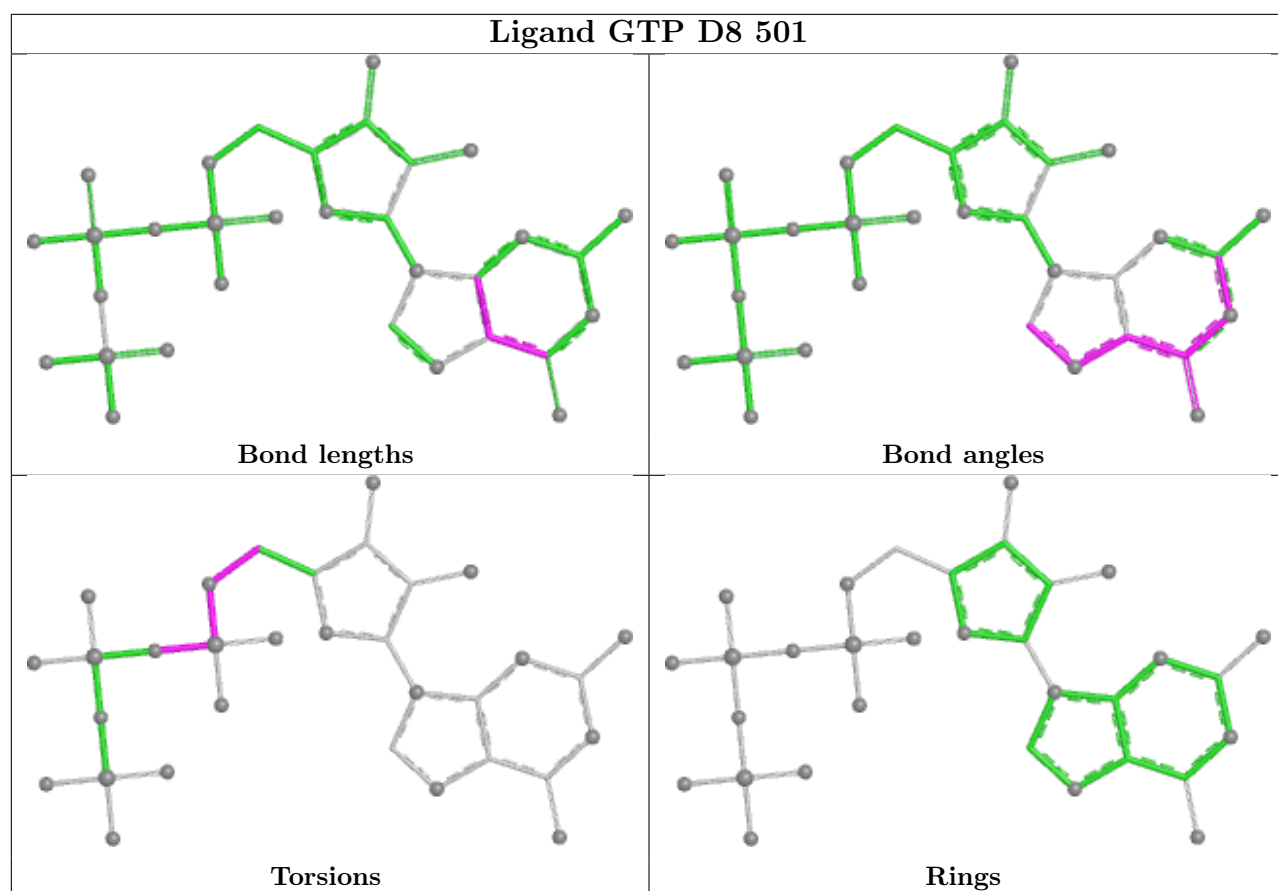
Ligand GTP B2 501

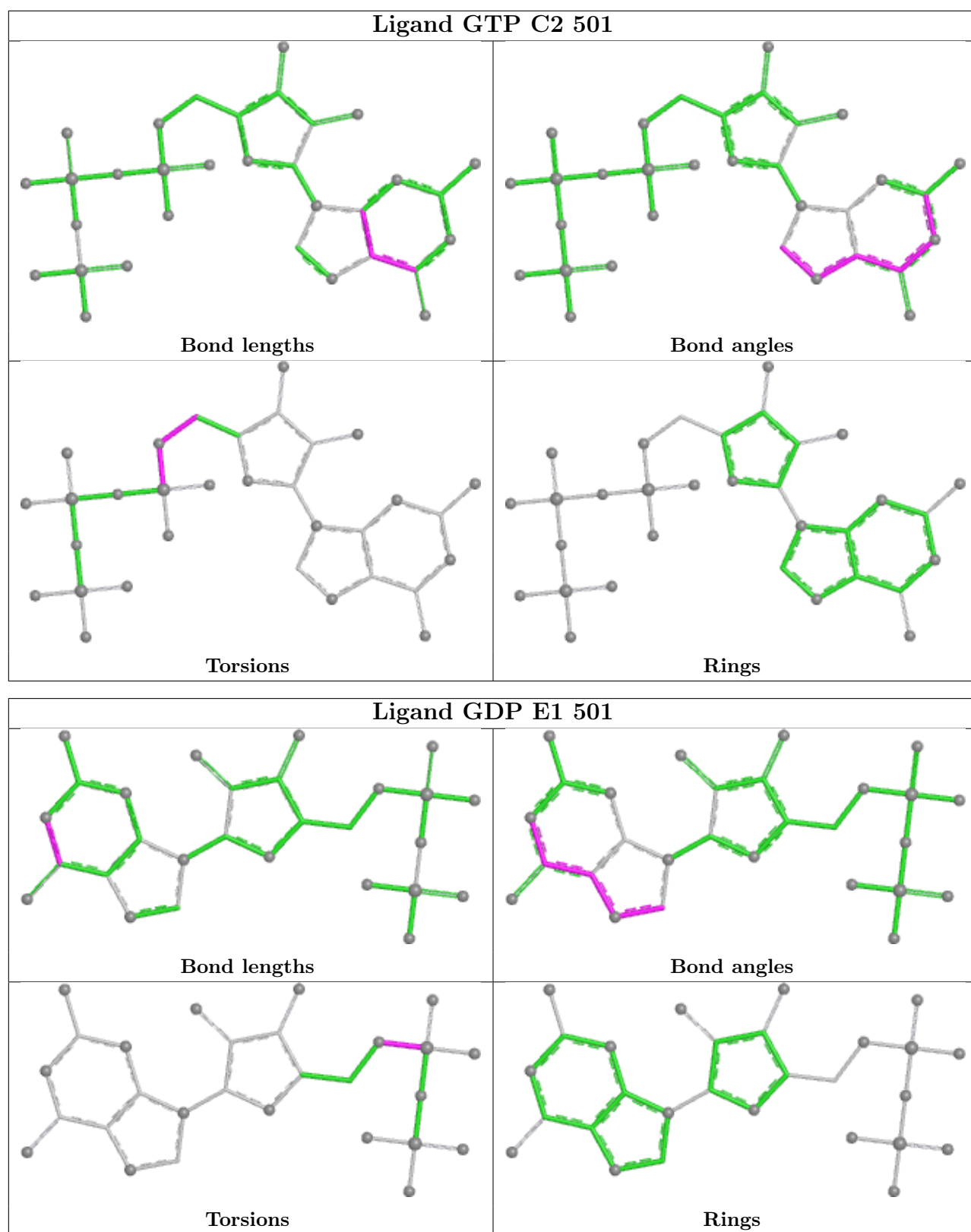


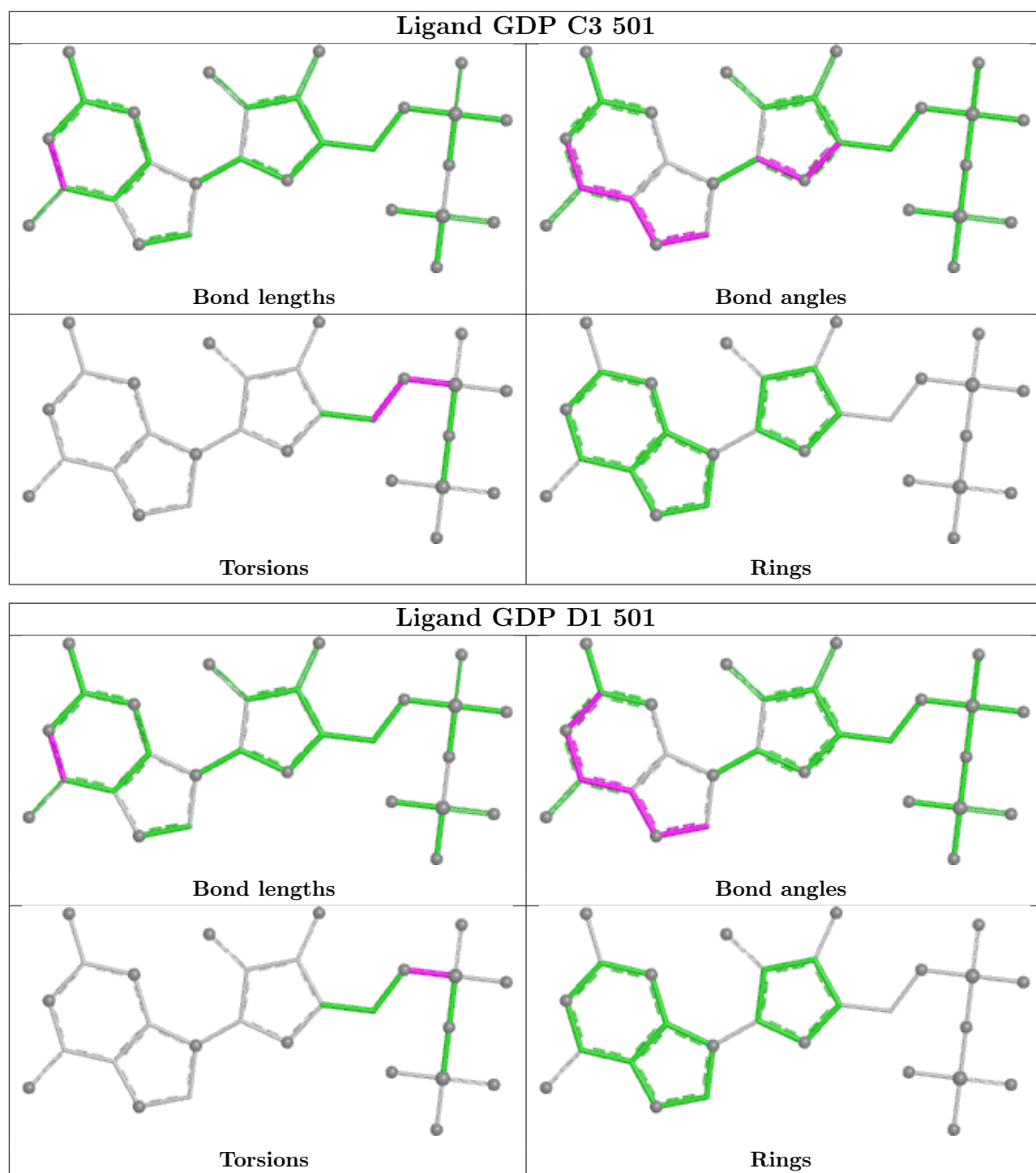


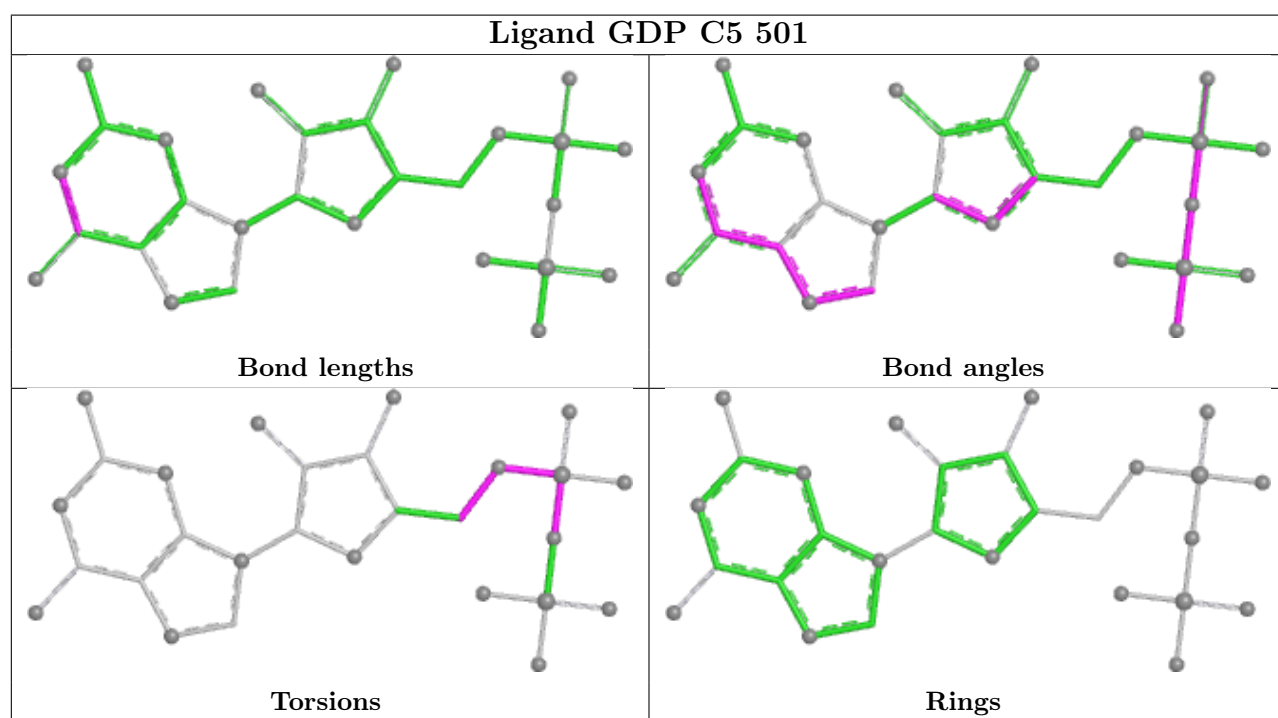
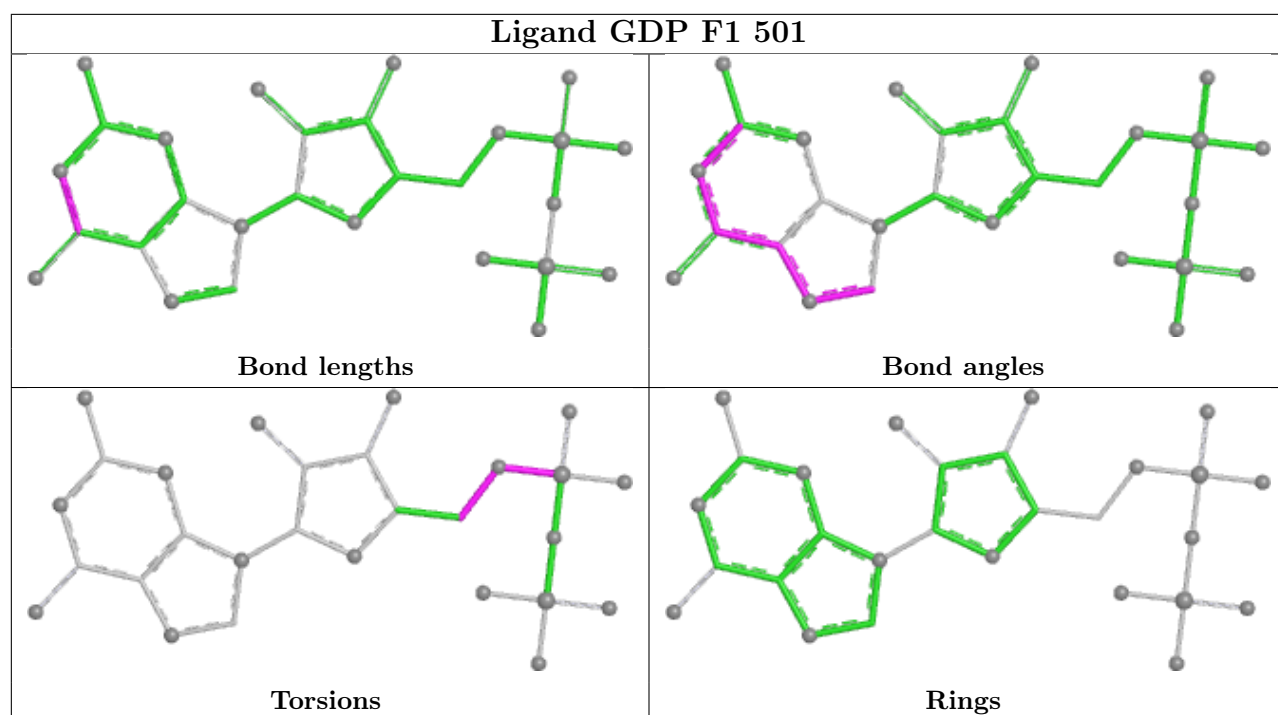


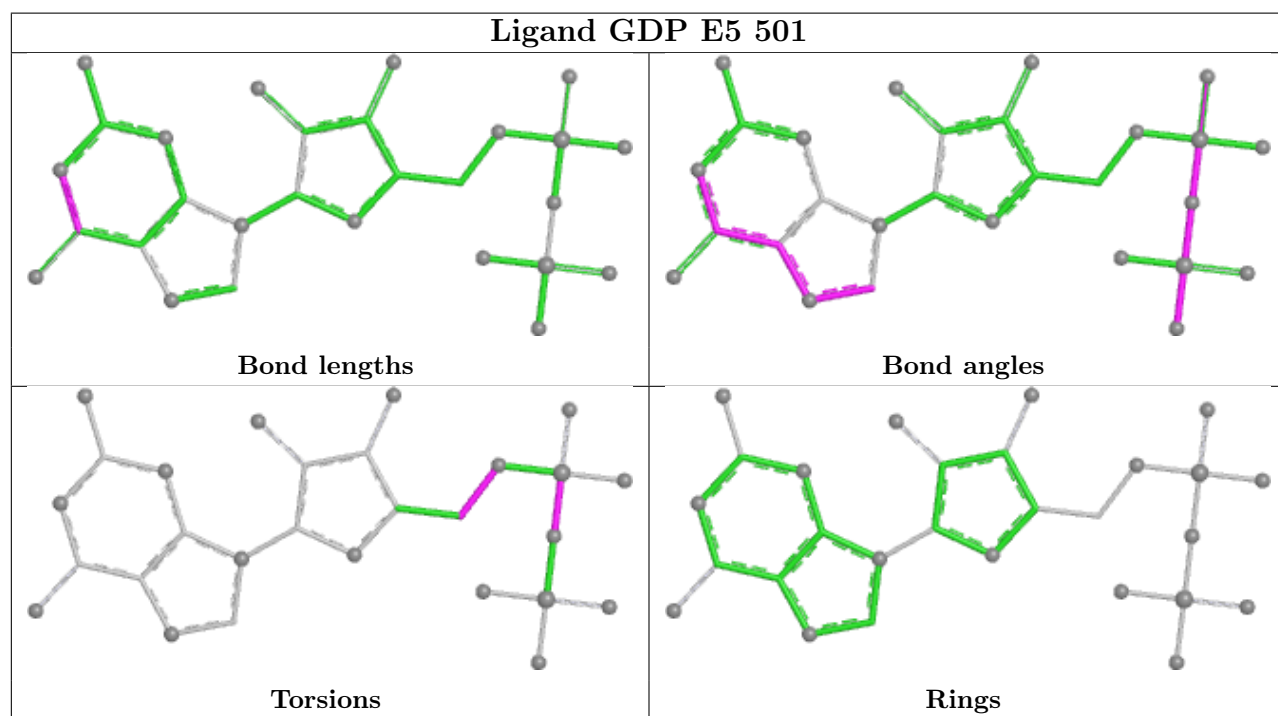
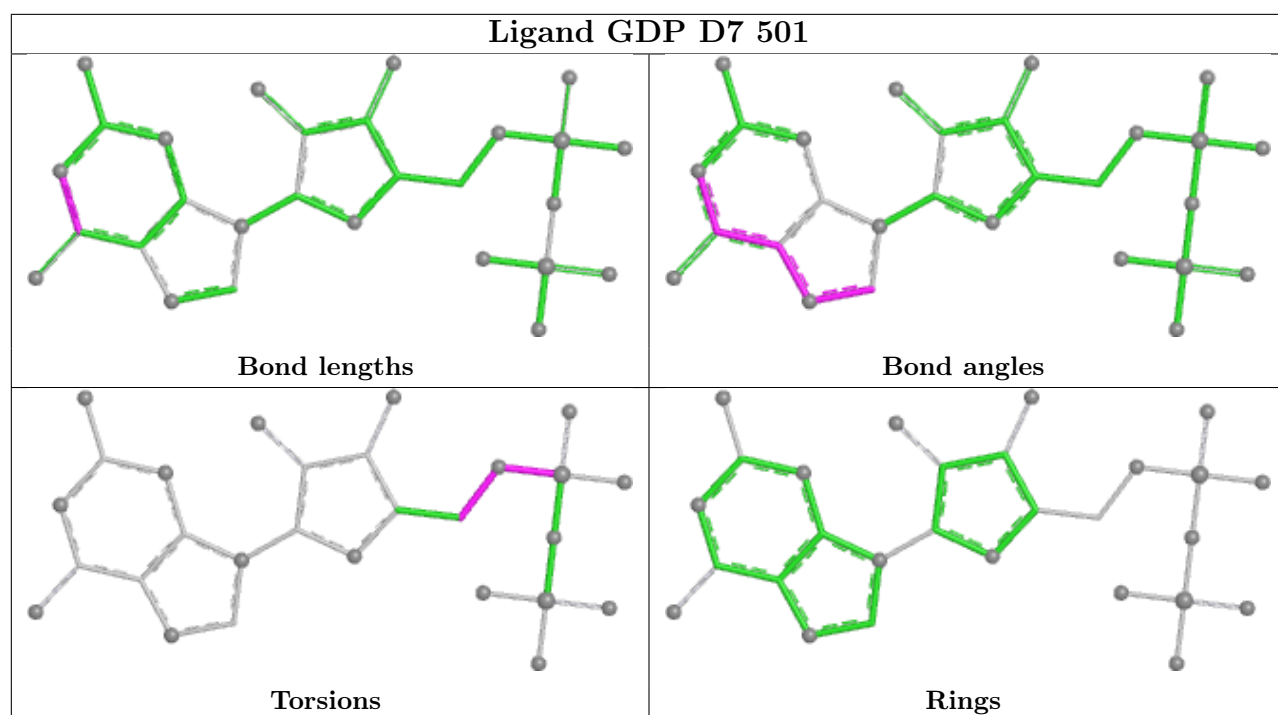




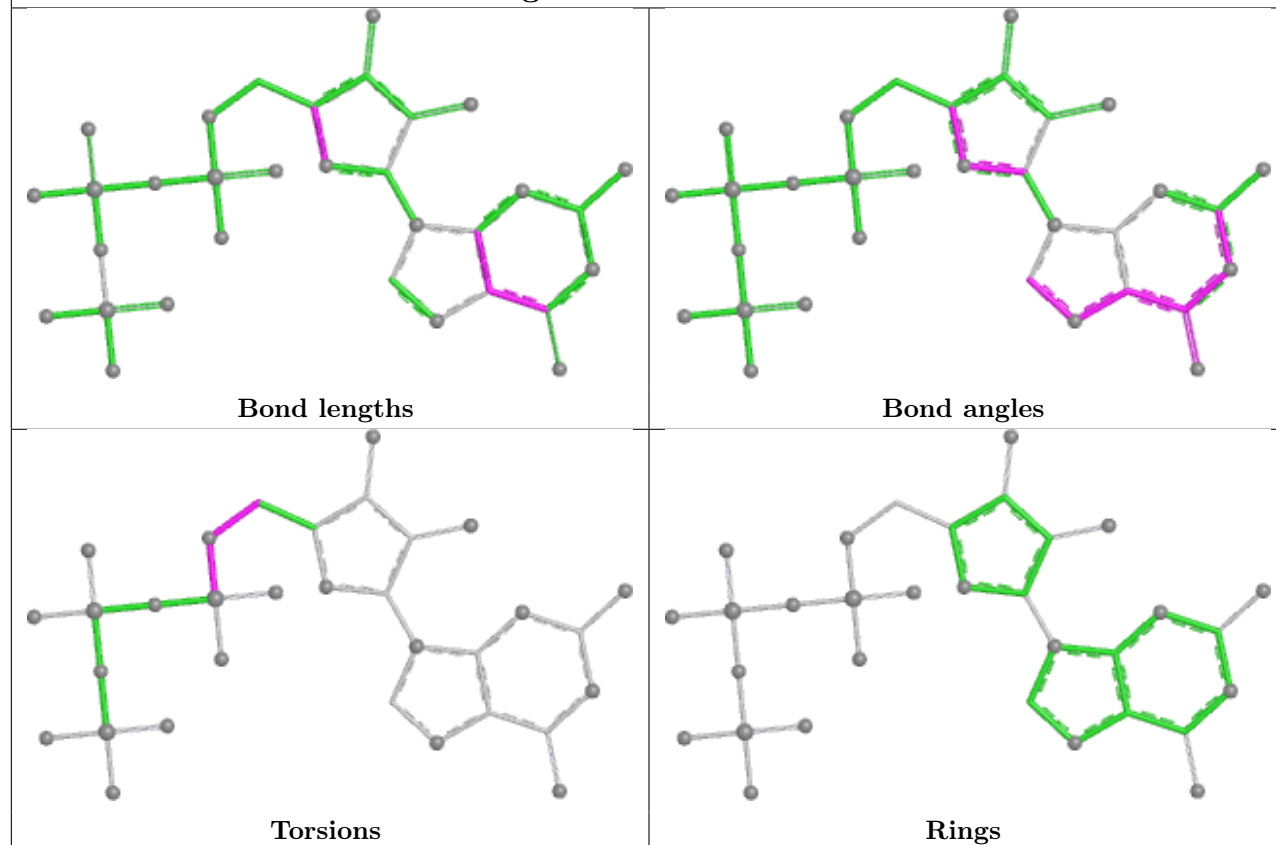




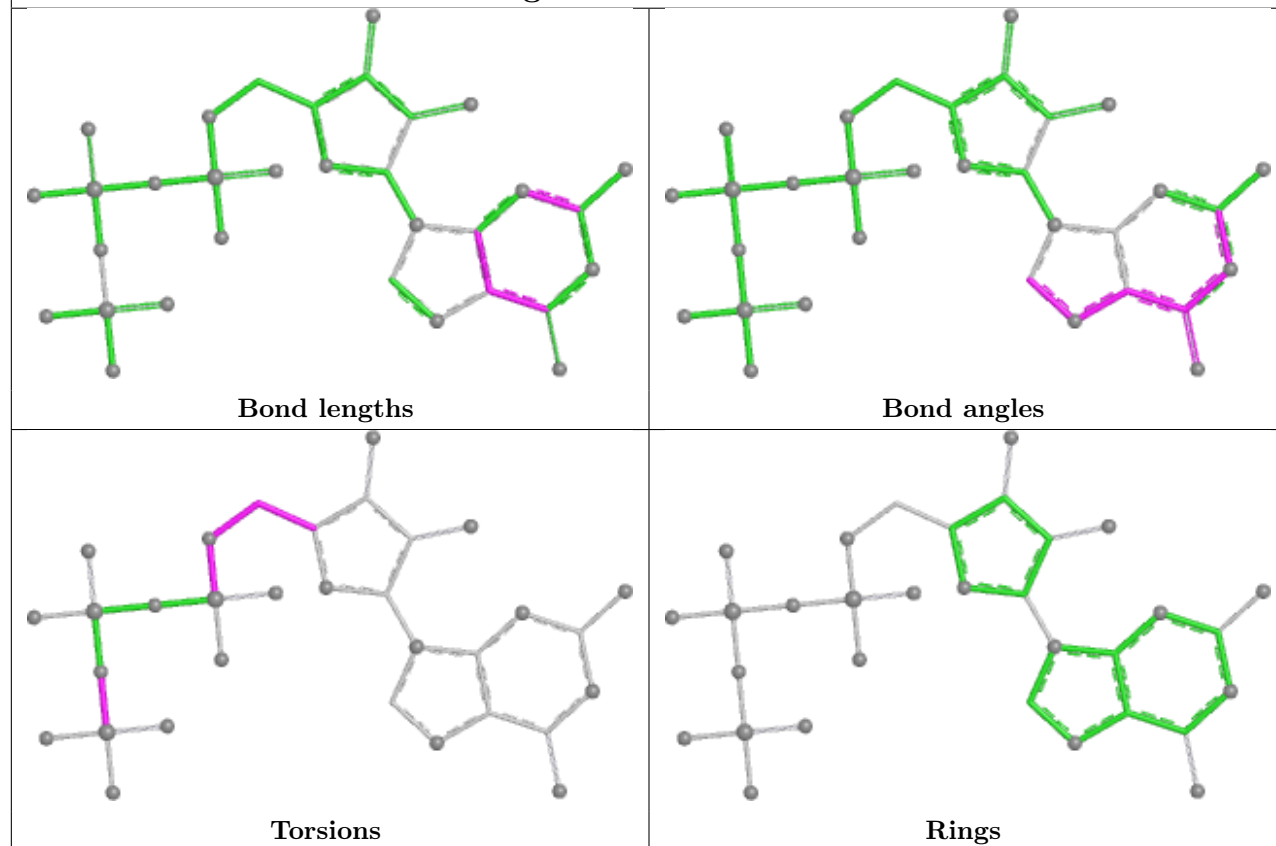




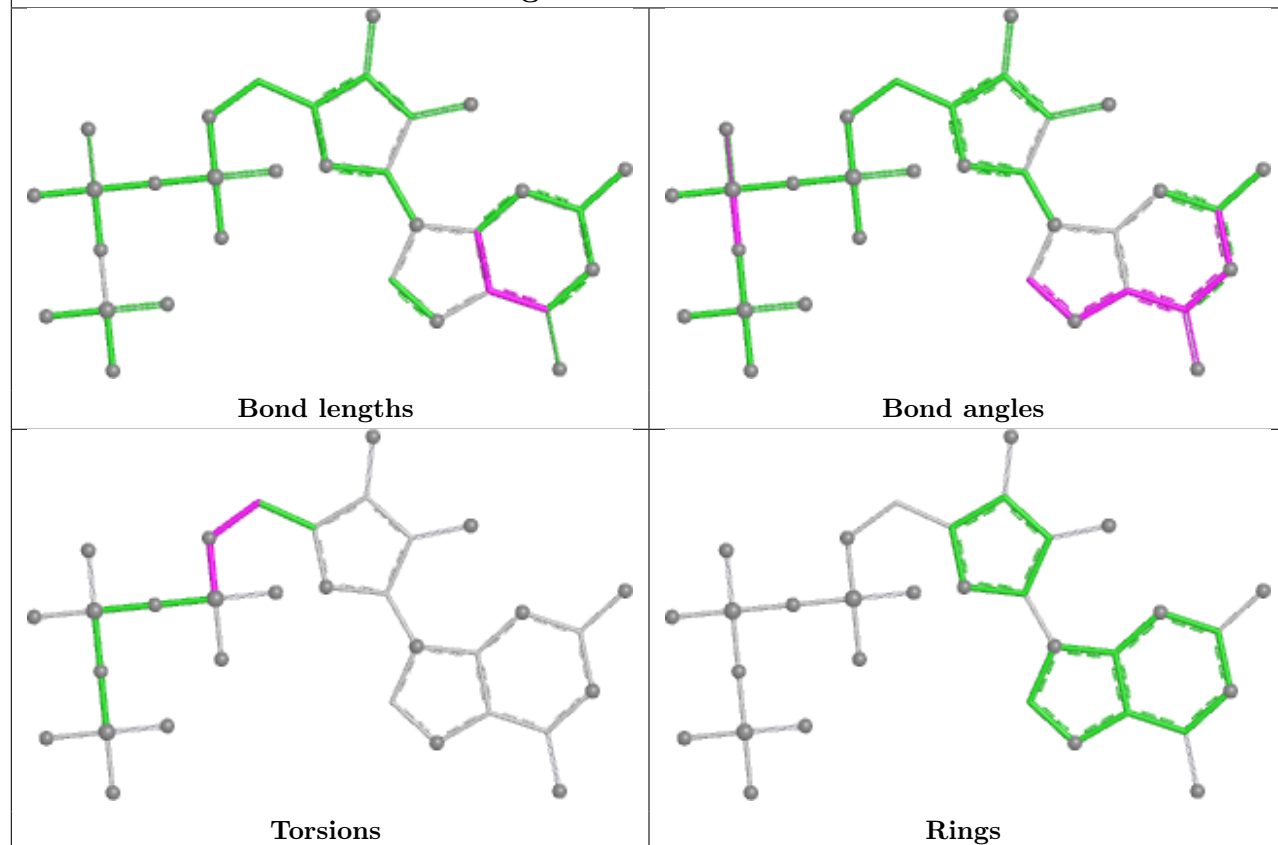
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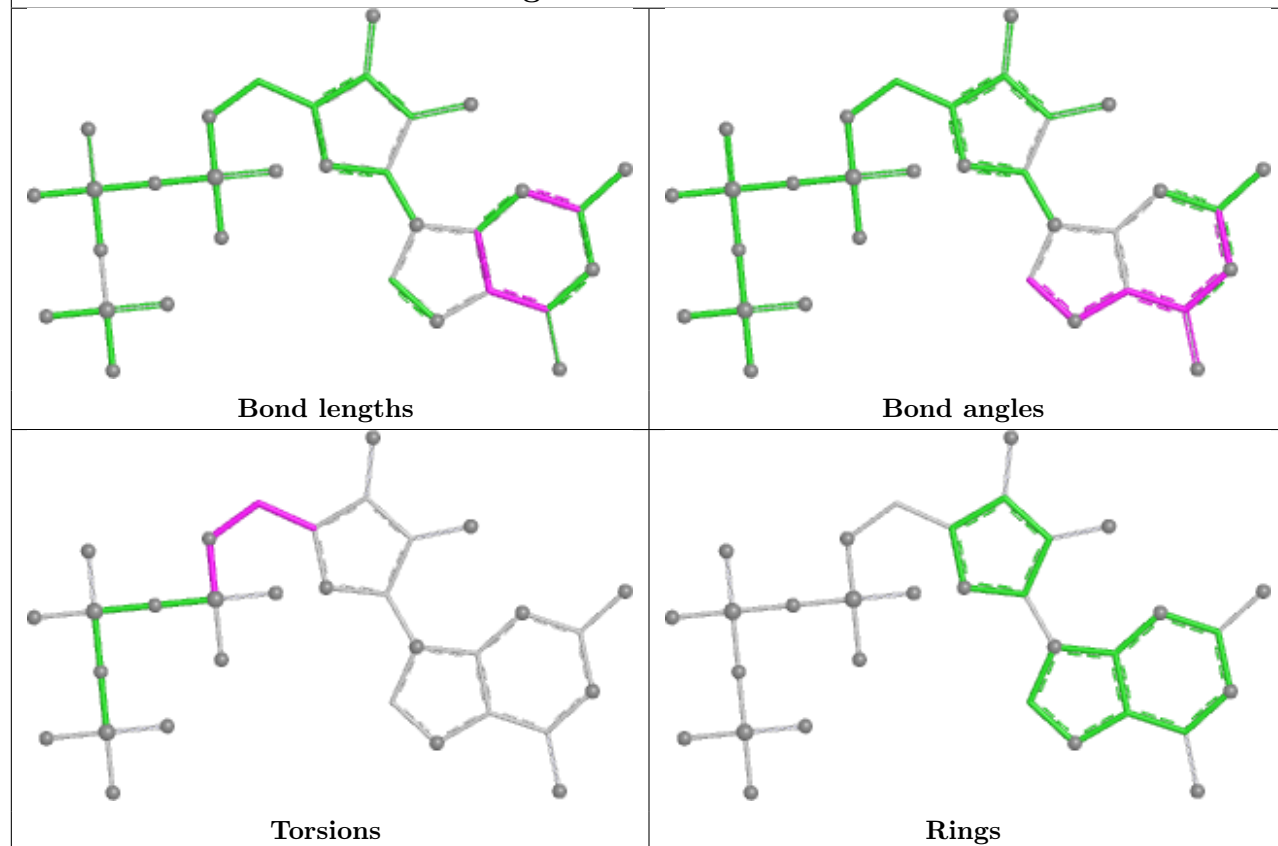
Ligand GTP F0 501

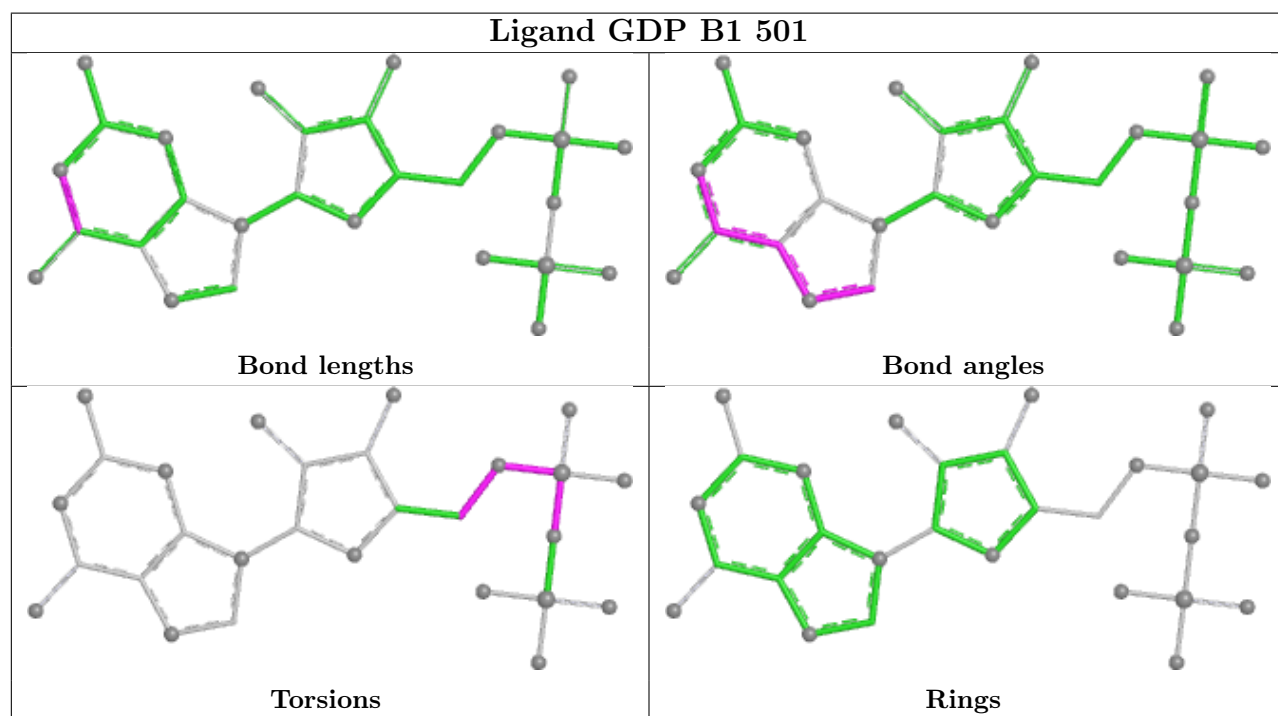
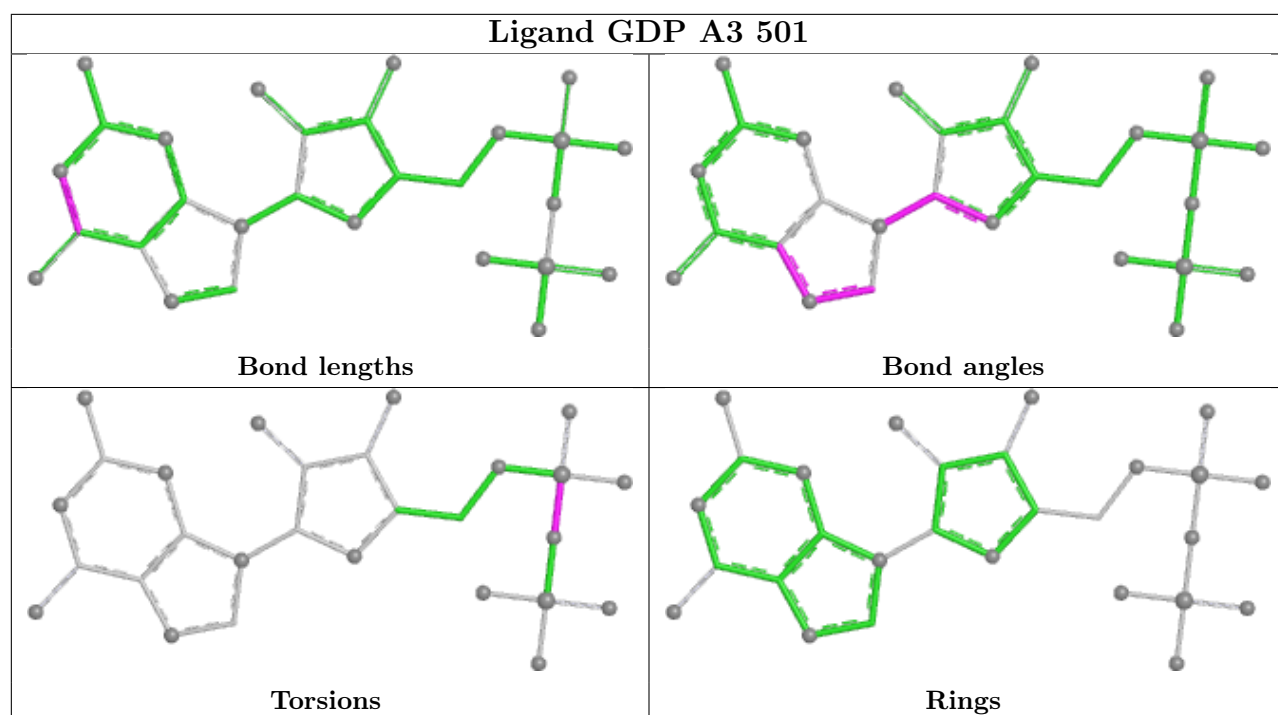


Ligand GTP C6 501

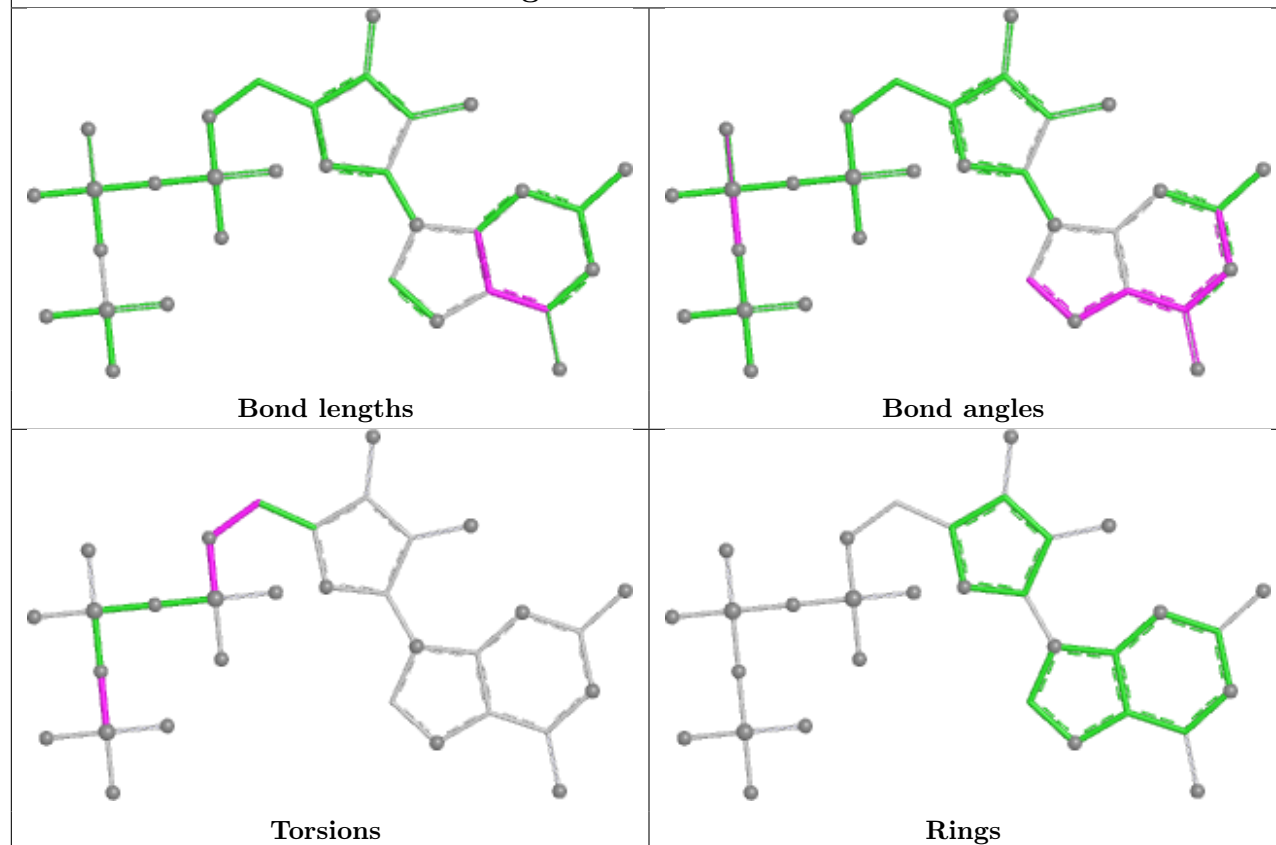


Ligand GTP E8 501

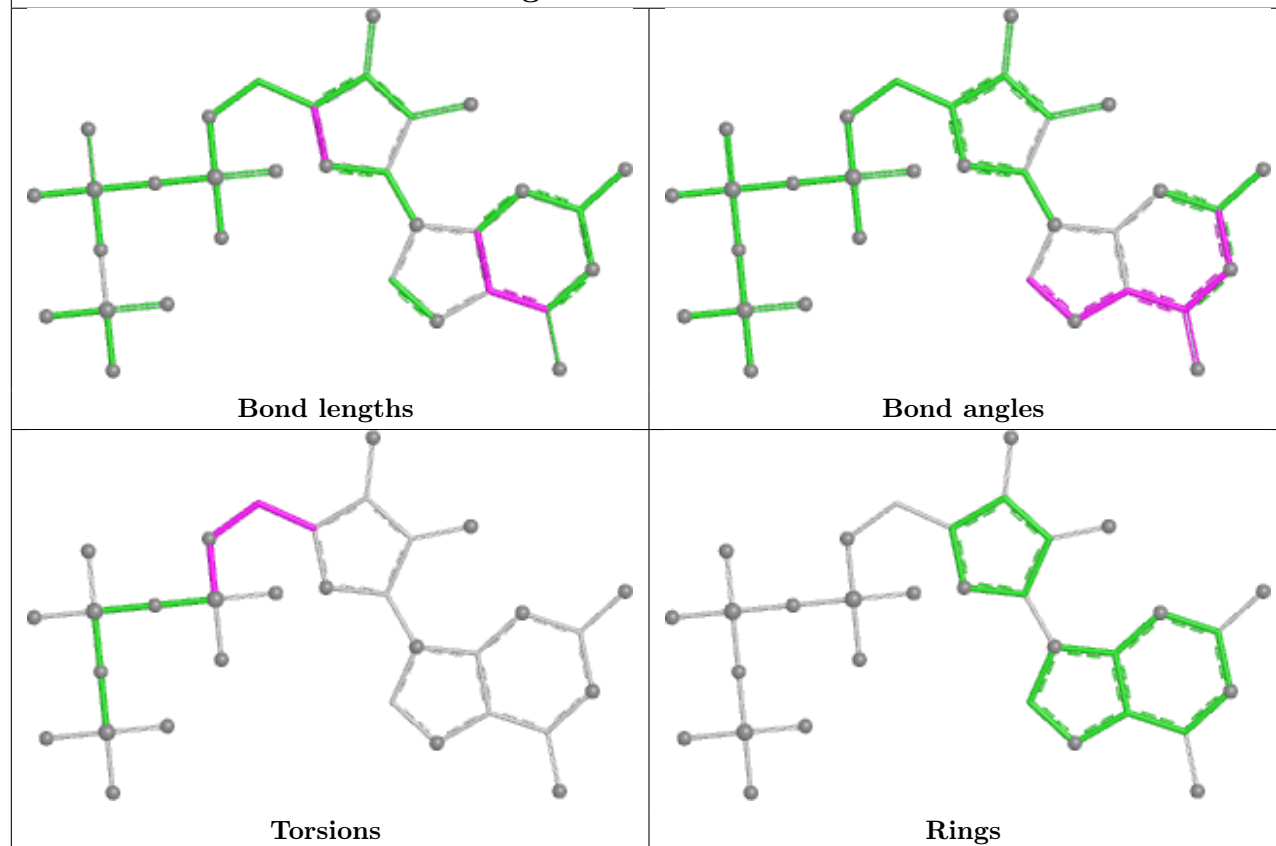




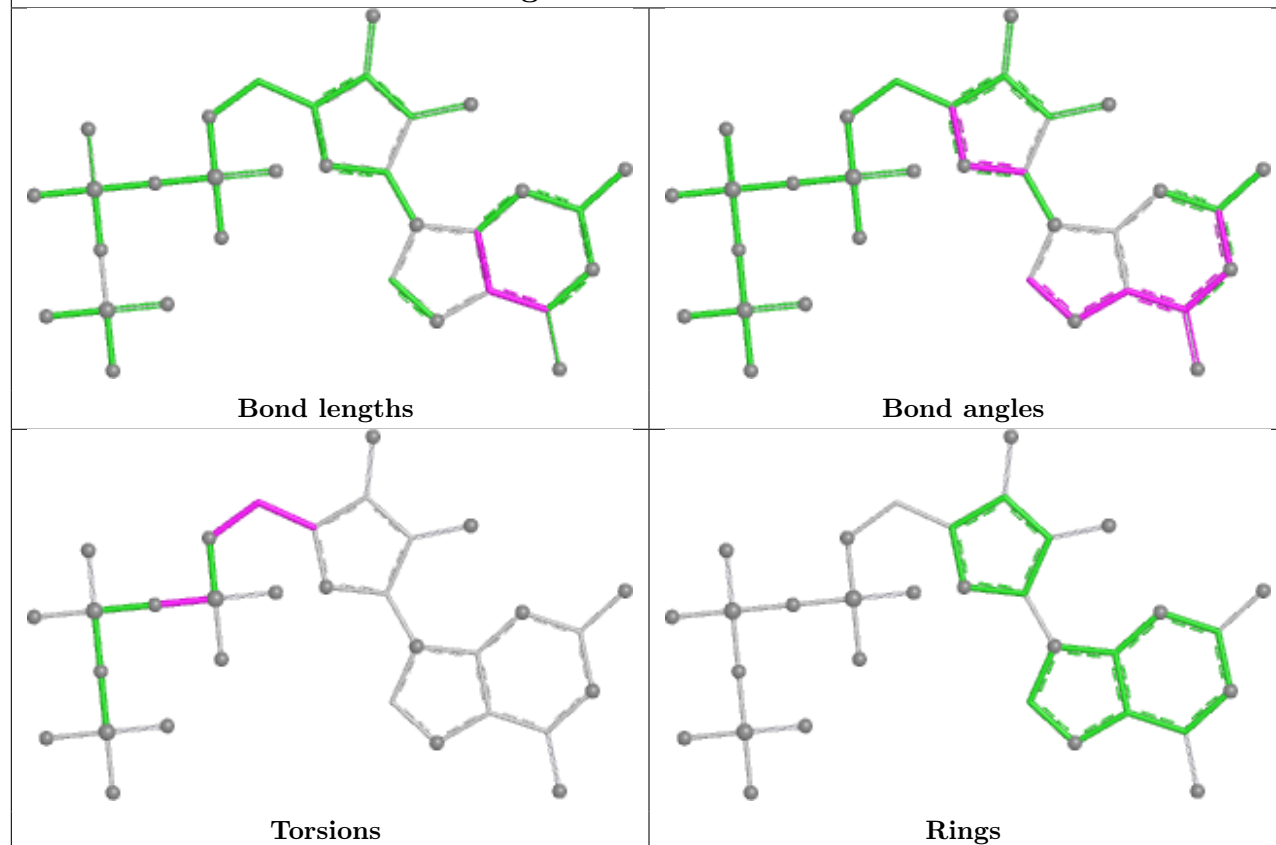
Ligand GTP C4 501



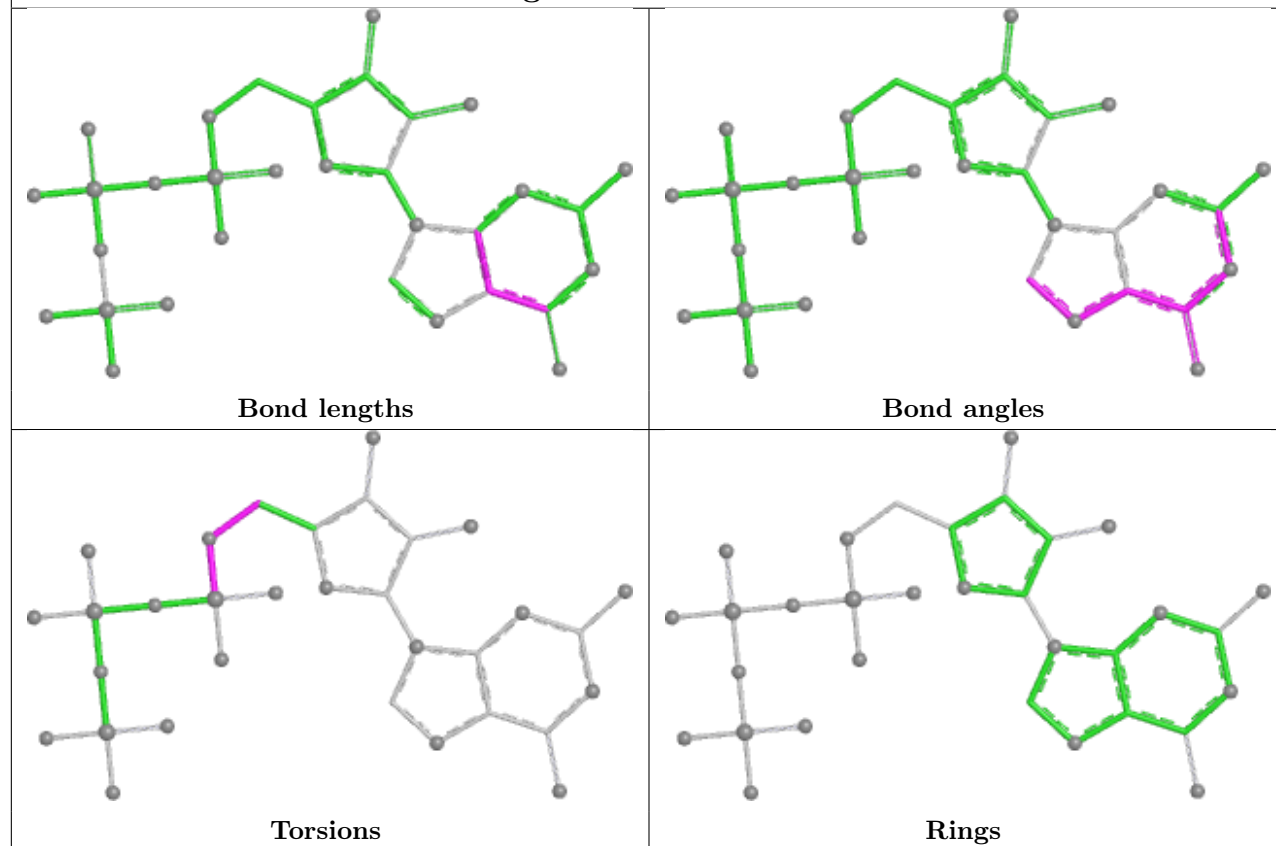
Ligand GTP B8 501



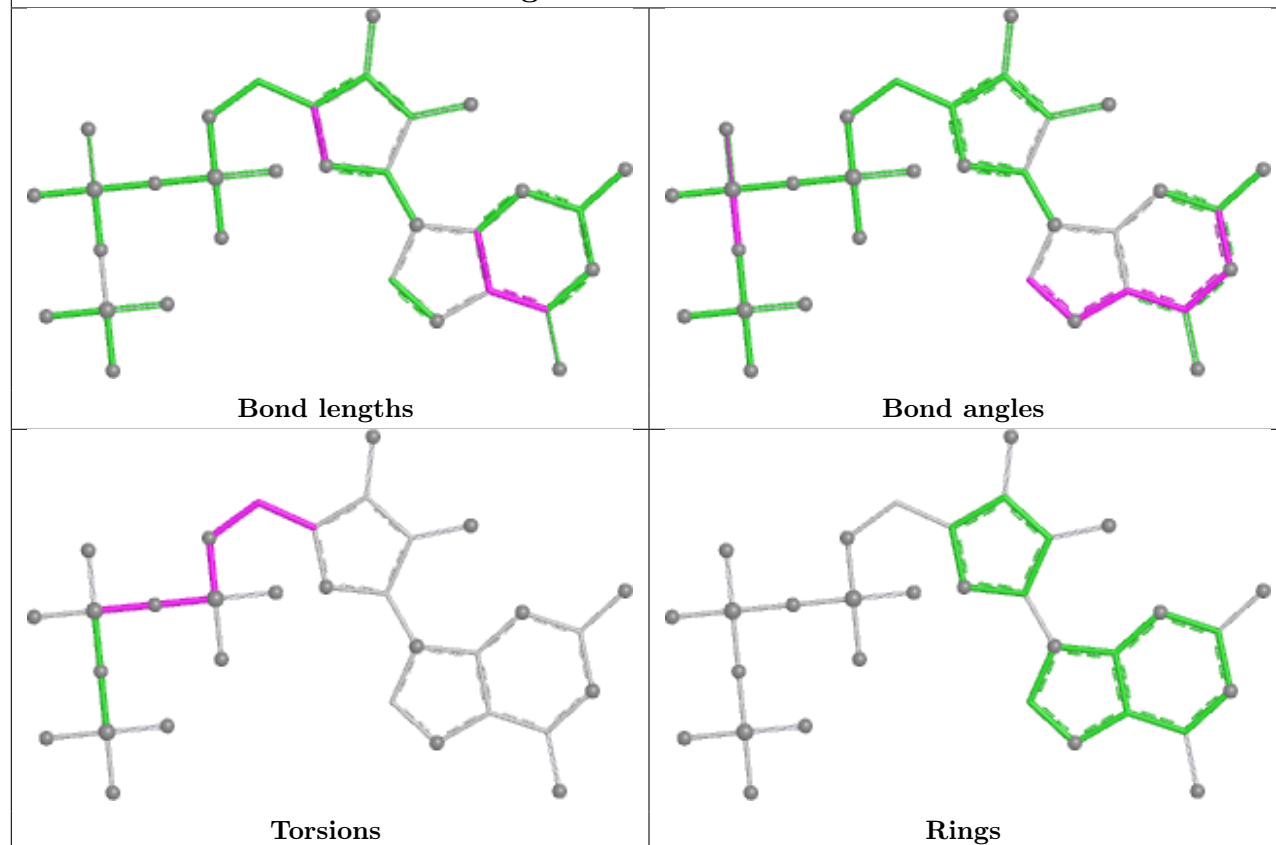
Ligand GTP D4 501



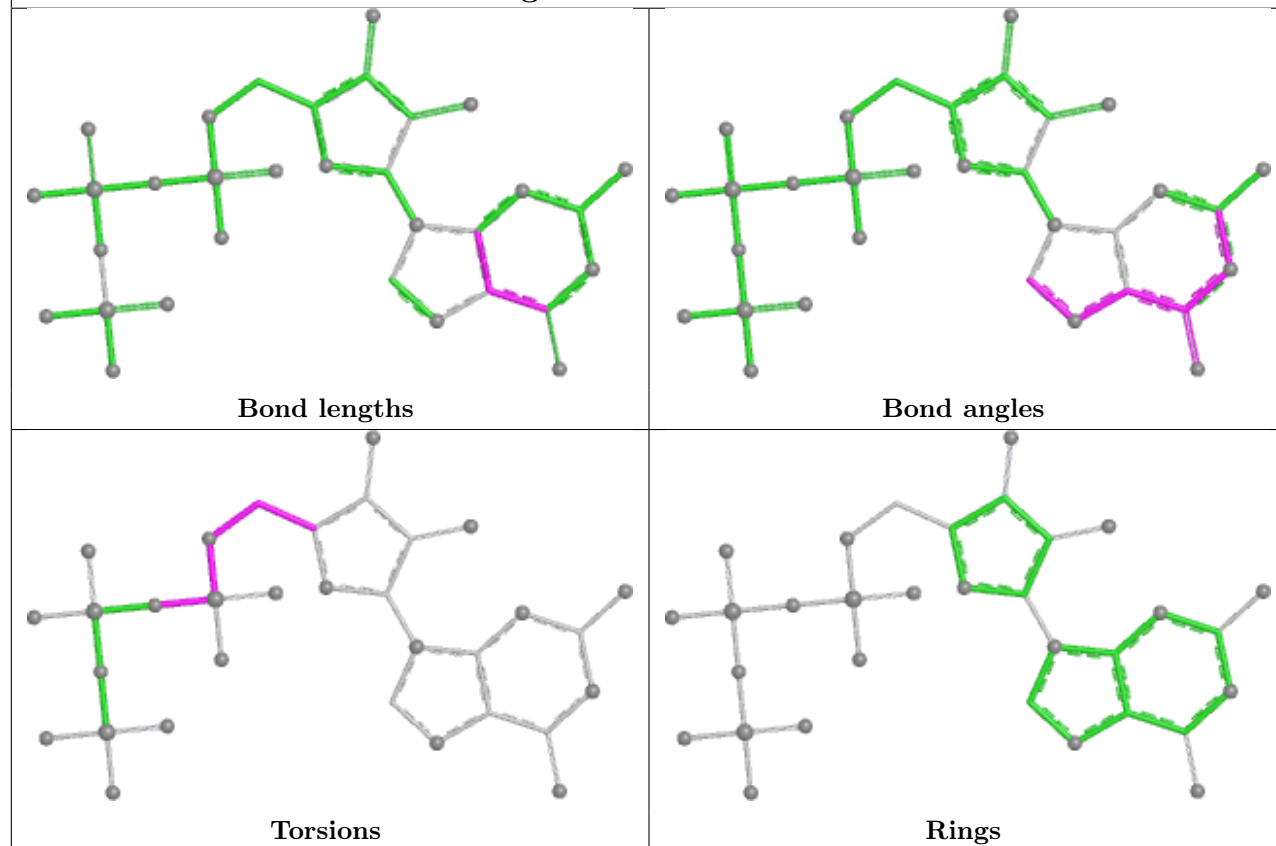
Ligand GTP E0 501

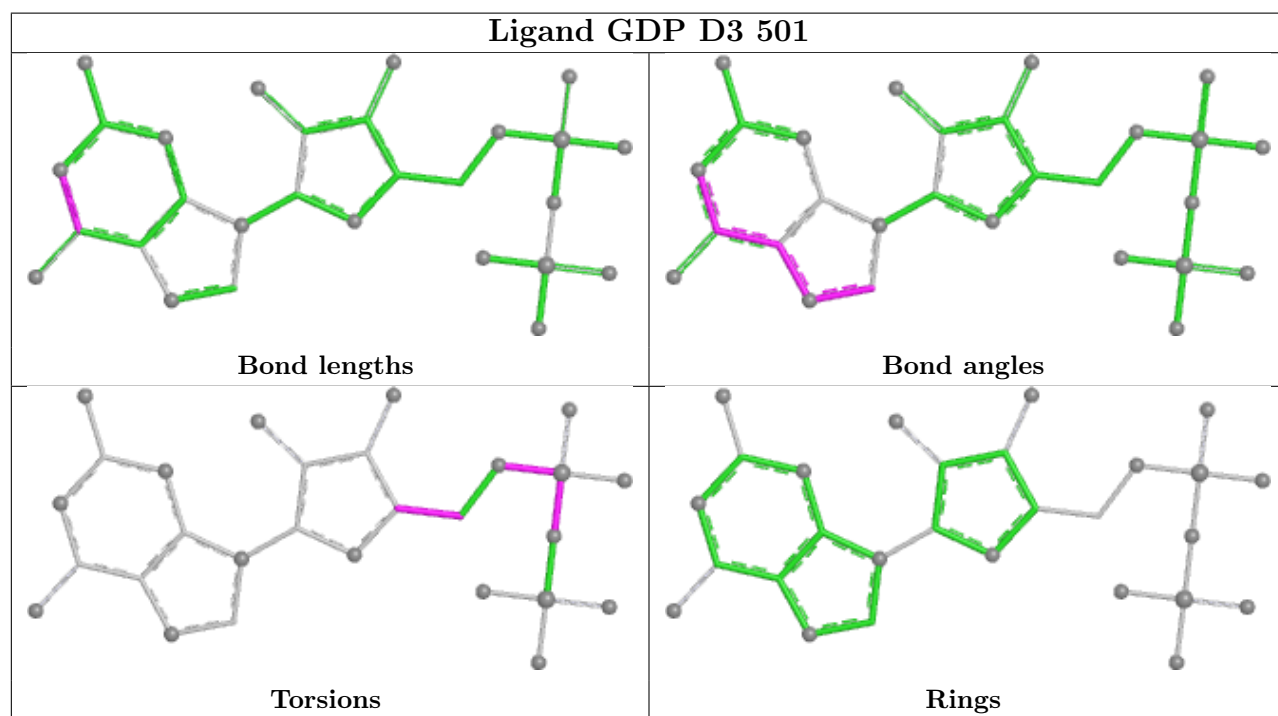
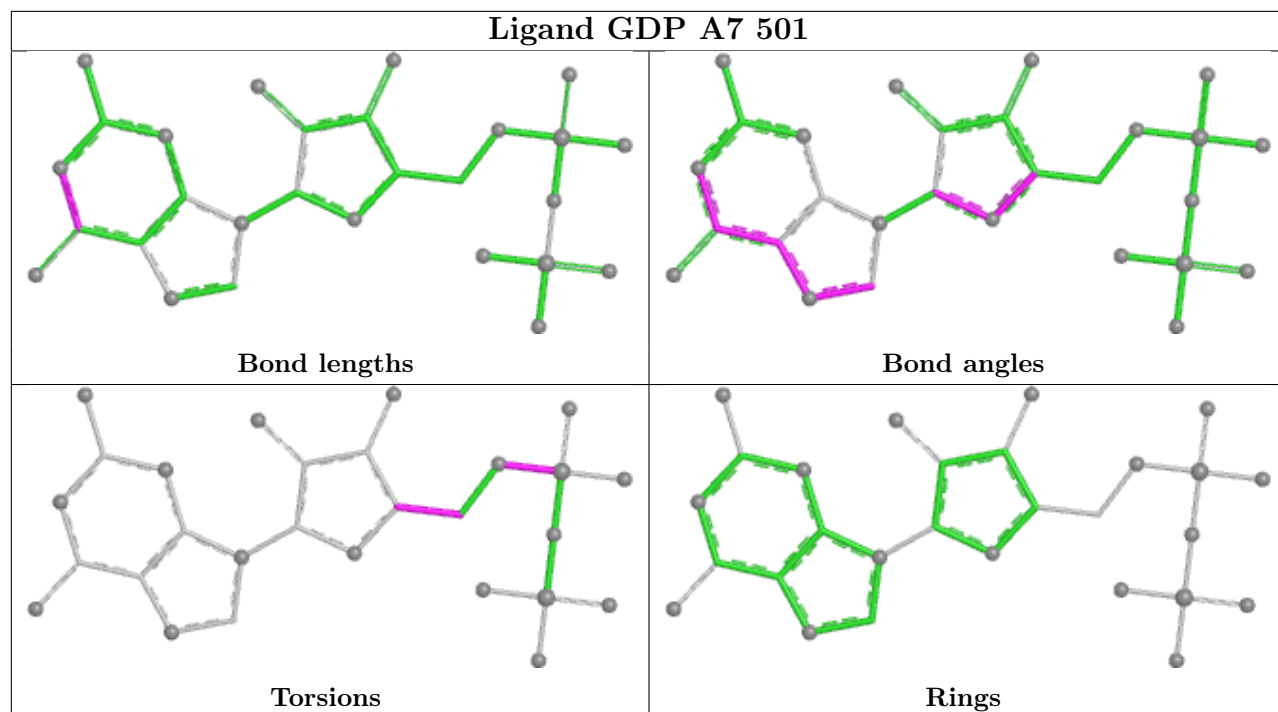


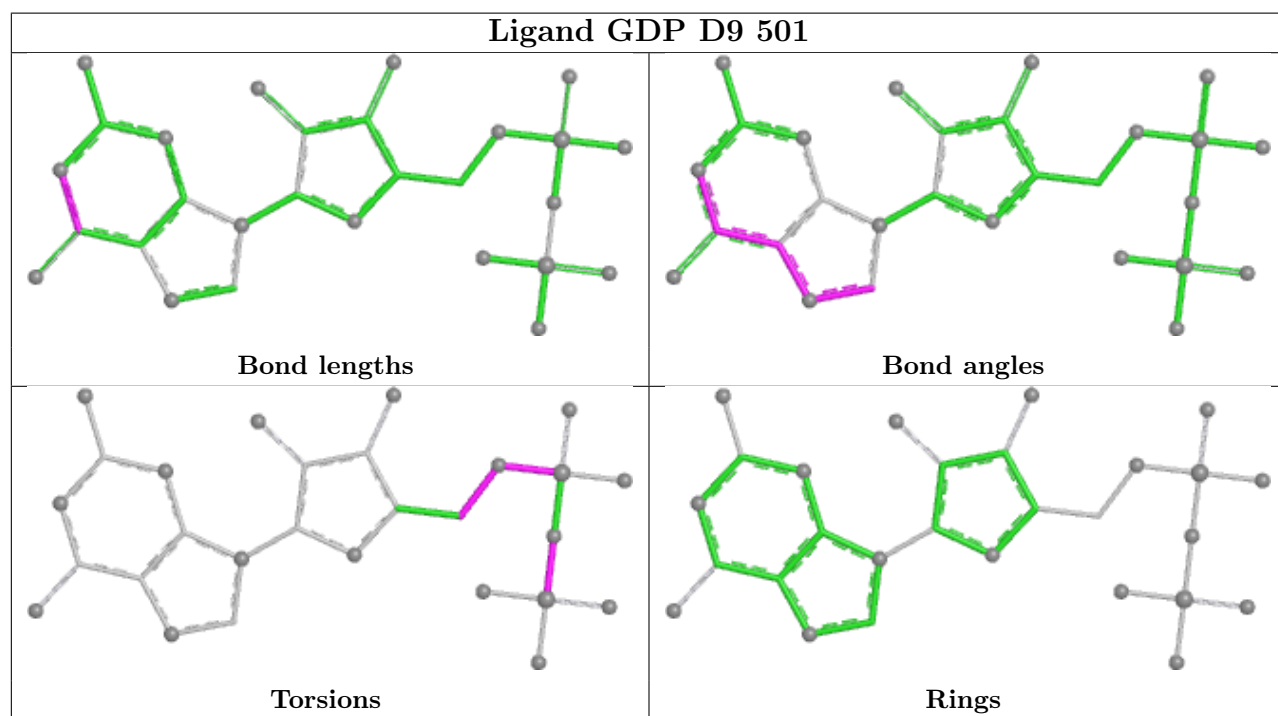
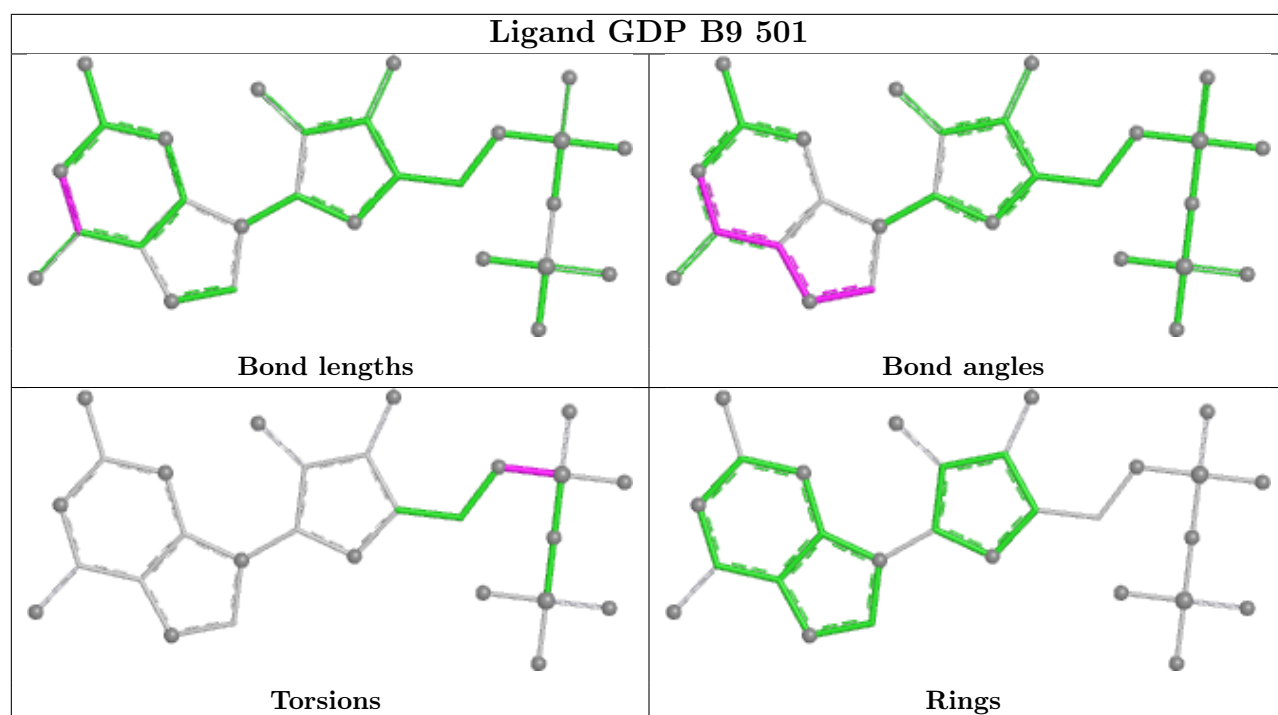
Ligand GTP A0 501

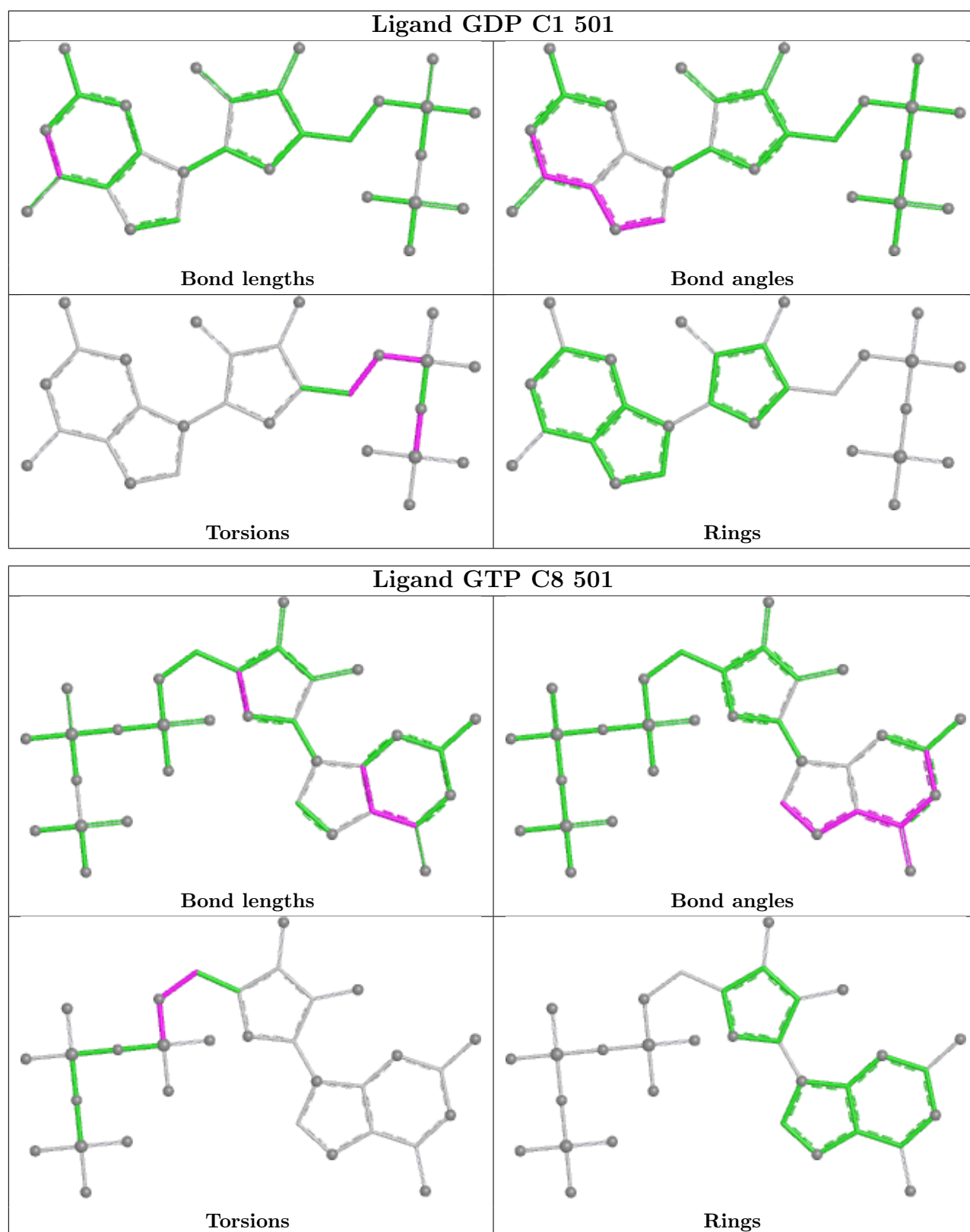


Ligand GTP D6 501









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

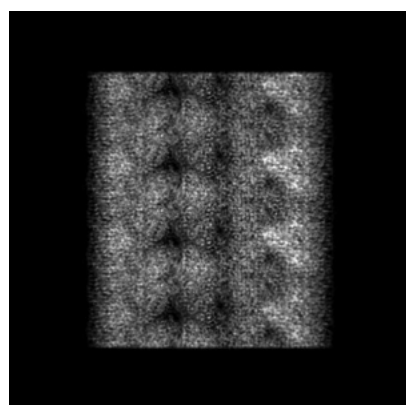
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23869. These allow visual inspection of the internal detail of the map and identification of artifacts.

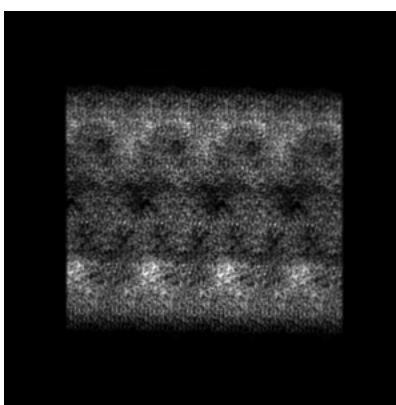
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

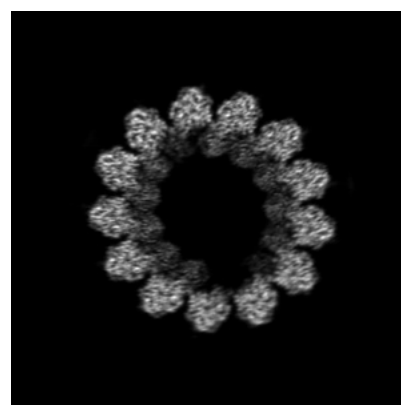
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 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](#)

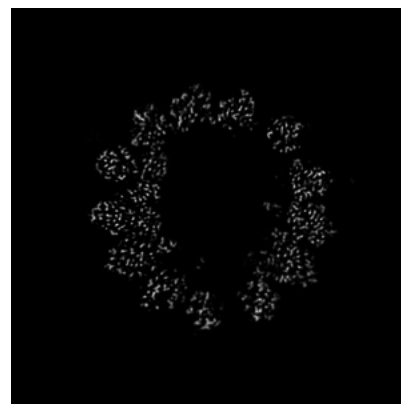
6.3.1 Primary map



X Index: 121



Y Index: 287

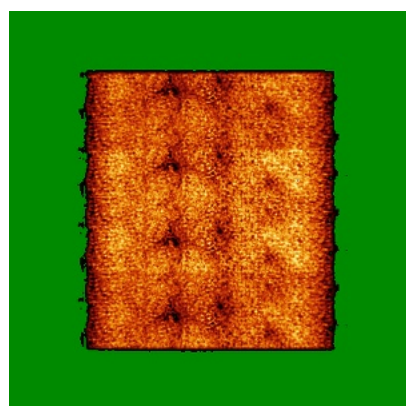


Z Index: 146

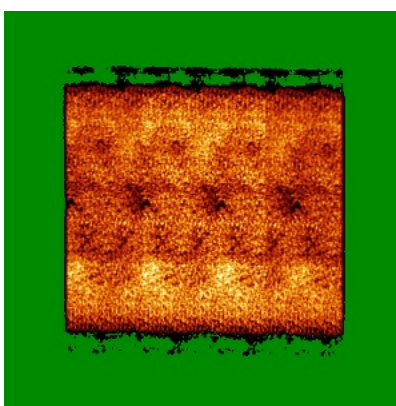
The images above show the largest variance slices of the map in three orthogonal directions.

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

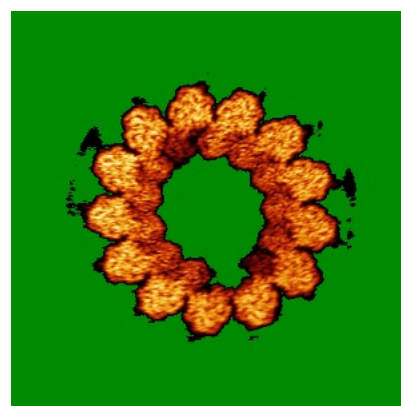
6.4.1 Primary map



X



Y

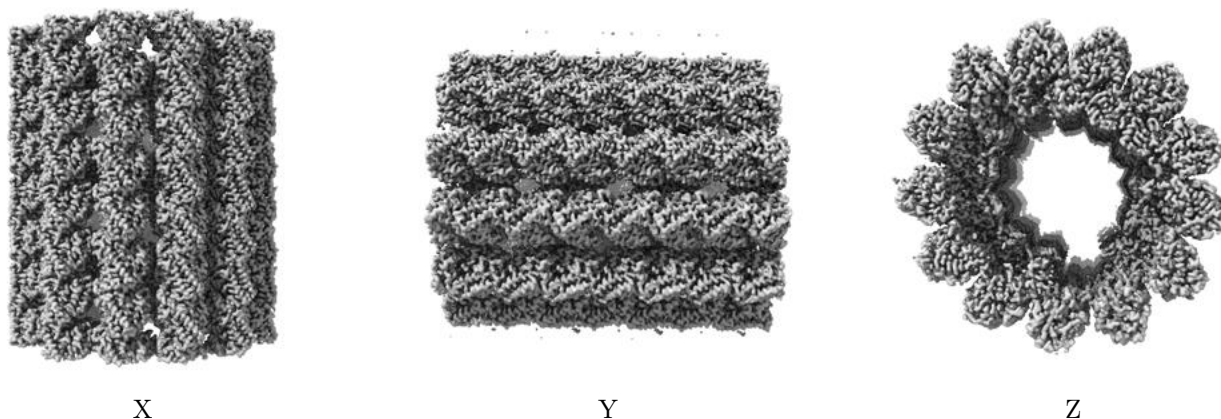


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

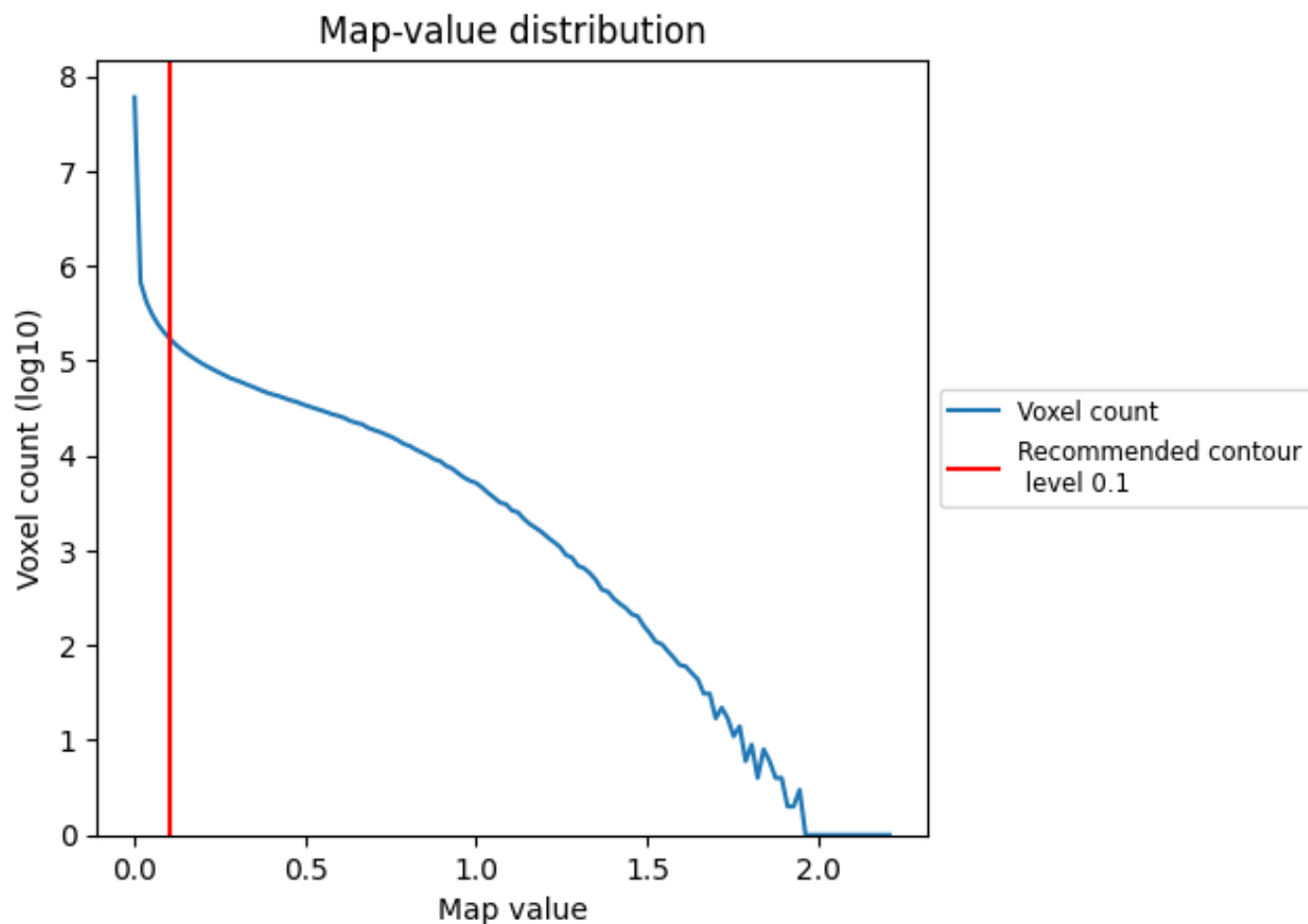
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

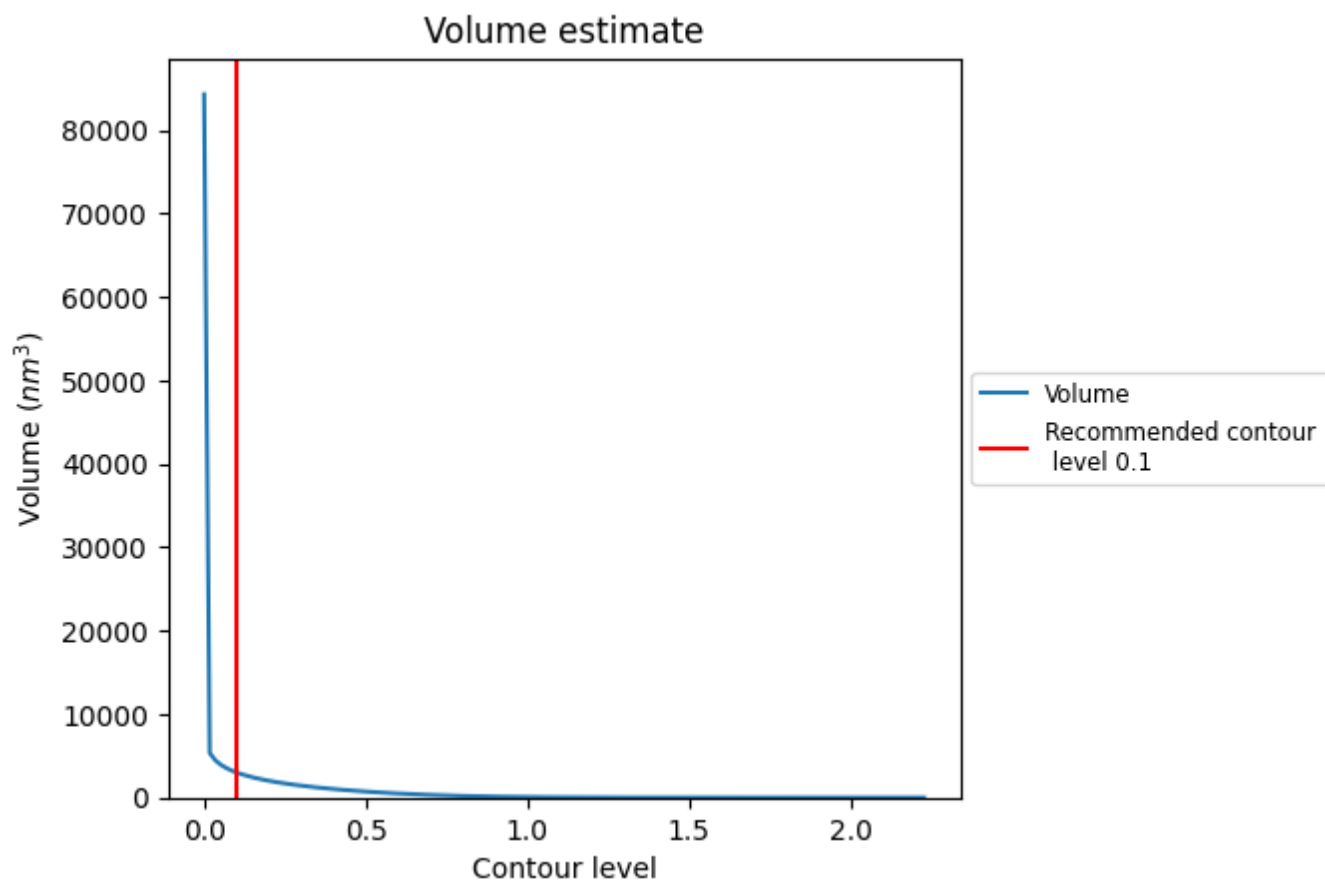
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

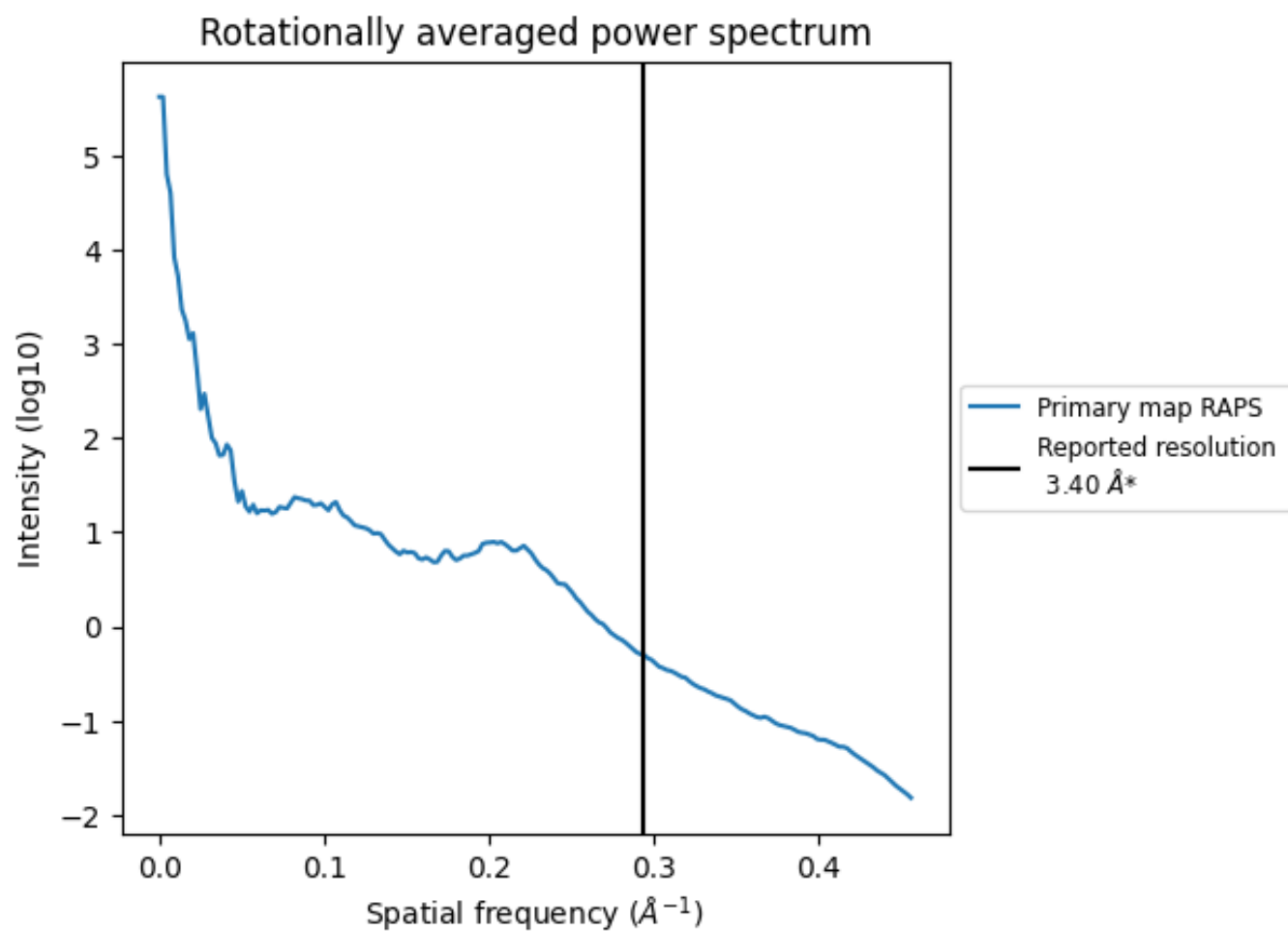
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3014 nm^3 ; this corresponds to an approximate mass of 2723 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 0.294 Å⁻¹

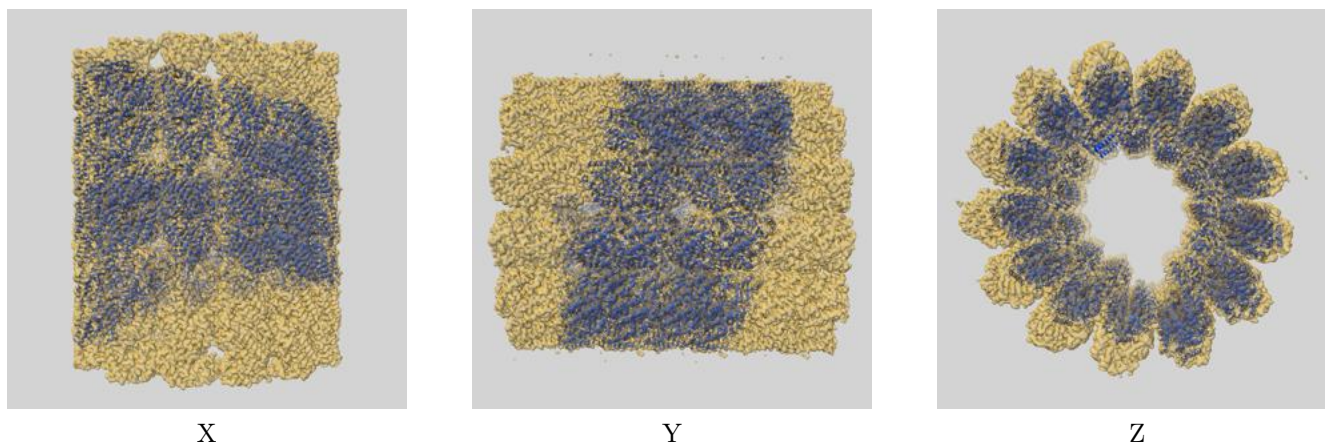
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

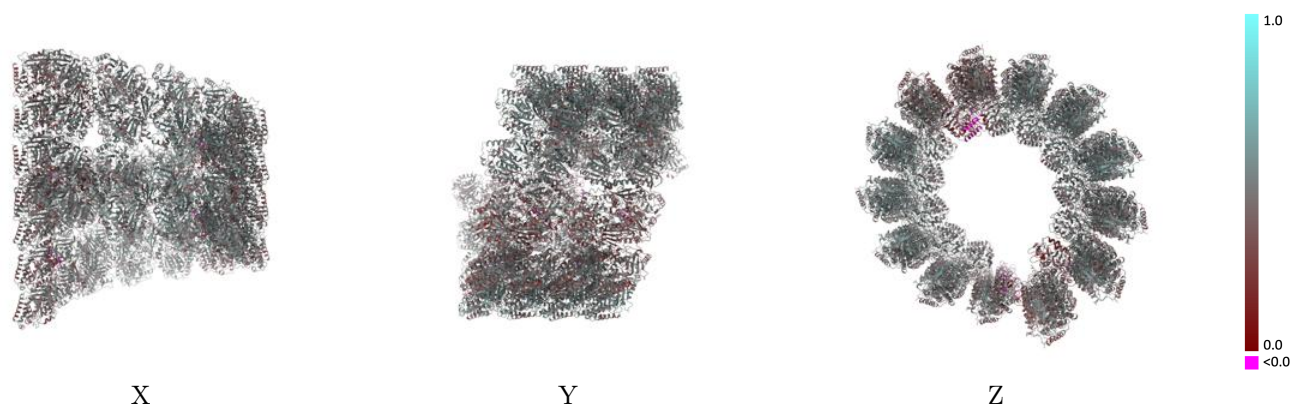
This section contains information regarding the fit between EMDB map EMD-23869 and PDB model 7MIZ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



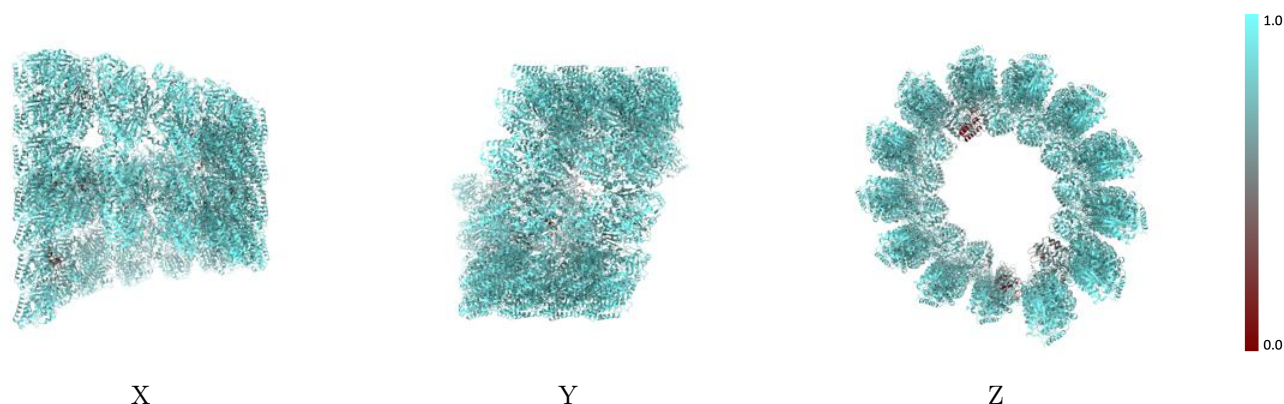
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



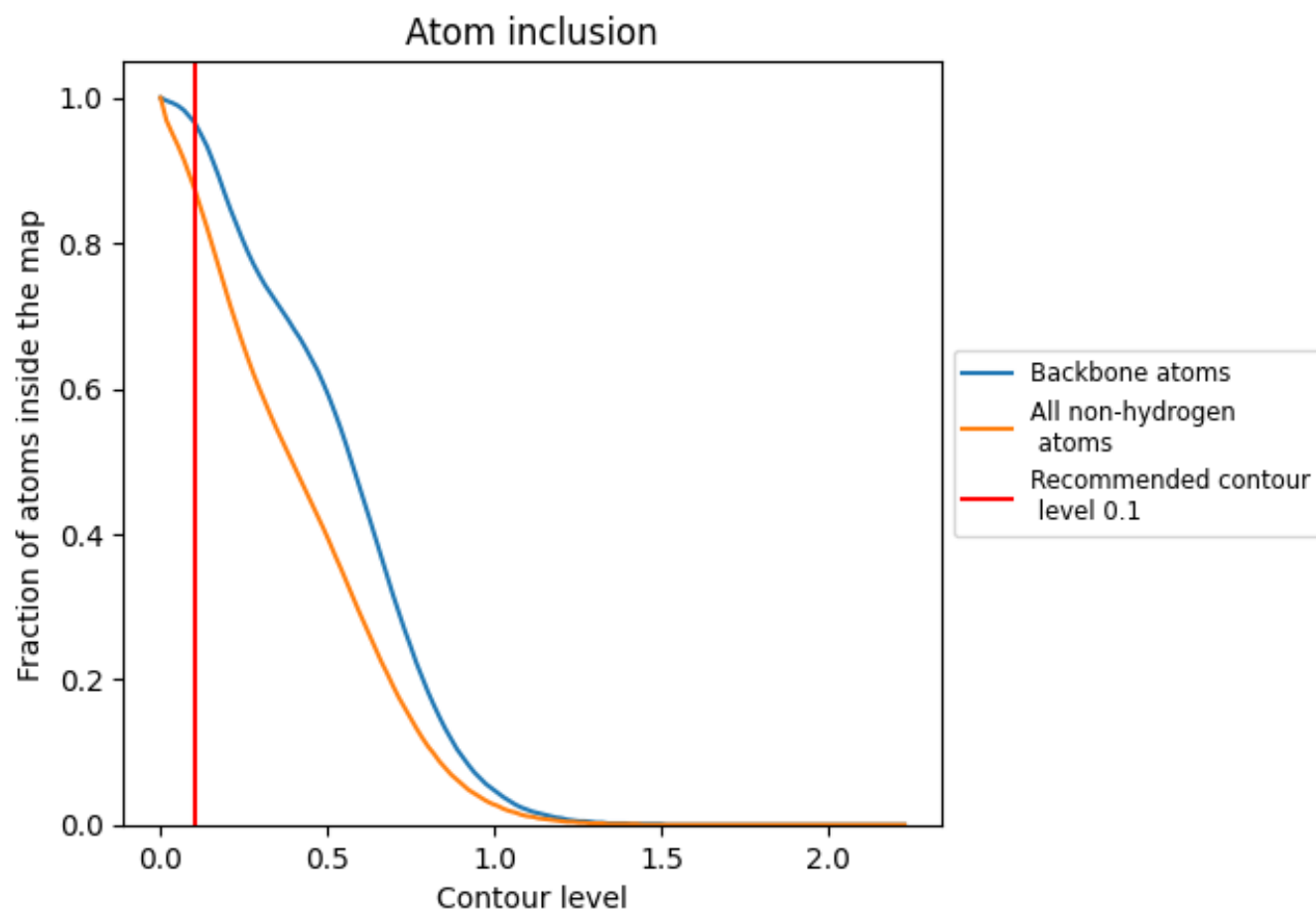
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 88% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.4600
0	 0.8650	 0.4810
1	 0.8350	 0.4680
10	 0.9060	 0.4870
11	 0.9060	 0.4880
12	 0.8820	 0.4790
13	 0.8760	 0.4810
14	 0.8710	 0.4930
15	 0.8530	 0.4860
16	 0.8650	 0.4610
17	 0.8820	 0.4620
18	 0.9350	 0.4860
19	 0.9410	 0.4850
2	 0.8350	 0.4640
20	 0.6940	 0.4110
21	 0.7350	 0.4290
22	 0.5900	 0.3640
23	 0.6150	 0.3760
3	 0.8410	 0.4650
4	 0.8240	 0.4800
5	 0.8410	 0.4860
6	 0.8590	 0.4920
7	 0.8590	 0.4880
8	 0.8240	 0.4230
9	 0.8290	 0.4280
A0	 0.7810	 0.3990
A1	 0.8960	 0.4390
A2	 0.7860	 0.3920
A3	 0.8560	 0.4180
A4	 0.8830	 0.4680
A5	 0.9020	 0.4770
A6	 0.8920	 0.4680
A7	 0.8820	 0.4700
A8	 0.9040	 0.4900
A9	 0.8970	 0.4830



















































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Chain	Atom inclusion	Q-score
B0	 0.8950	 0.4860
B1	 0.8860	 0.4820
B2	 0.9100	 0.5040
B3	 0.8940	 0.5030
B4	 0.9090	 0.5030
B5	 0.8870	 0.4990
B6	 0.9100	 0.4990
B7	 0.8980	 0.5050
B8	 0.9170	 0.5000
B9	 0.9050	 0.4990
C0	 0.8770	 0.4160
C1	 0.8490	 0.4190
C2	 0.8820	 0.4190
C3	 0.8550	 0.4150
C4	 0.8620	 0.4020
C5	 0.8630	 0.4040
C6	 0.8560	 0.4050
C7	 0.8680	 0.4040
C8	 0.8970	 0.4740
C9	 0.9070	 0.4830
D0	 0.8860	 0.4810
D1	 0.9190	 0.4890
D2	 0.8970	 0.4870
D3	 0.9200	 0.5010
D4	 0.8800	 0.4960
D5	 0.9220	 0.5020
D6	 0.9080	 0.4910
D7	 0.9230	 0.4990
D8	 0.8990	 0.5050
D9	 0.9200	 0.5020
E0	 0.8960	 0.4680
E1	 0.9110	 0.4820
E2	 0.9100	 0.4810
E3	 0.9150	 0.4910
E4	 0.9000	 0.4530
E5	 0.9080	 0.4680
E6	 0.9180	 0.4730
E7	 0.9060	 0.4790
E8	 0.8710	 0.4230
E9	 0.8510	 0.4190
F0	 0.8990	 0.4420
F1	 0.8530	 0.4330

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Chain	Atom inclusion	Q-score
a	 0.7830	 0.4260
b	 0.7790	 0.4120
c	 0.8410	 0.4650
d	 0.8490	 0.4550
e	 0.8780	 0.4830
f	 0.8900	 0.4800
g	 0.8840	 0.4870
h	 0.8810	 0.4840
i	 0.8820	 0.4470
j	 0.8820	 0.4450
k	 0.6920	 0.2870
l	 0.6830	 0.2870
m	 0.6830	 0.3280
n	 0.6800	 0.3290
o	 0.8890	 0.4830
p	 0.8850	 0.4830
q	 0.8950	 0.4800
r	 0.8940	 0.4950
s	 0.8990	 0.4730
t	 0.8970	 0.4920
u	 0.8750	 0.4490
v	 0.8770	 0.4640
w	 0.5560	 0.2960
x	 0.6150	 0.3200