



## wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 07:32 pm BST

PDB ID : 6TMG / pdb\_00006tmg  
EMDB ID : EMD-10520  
Title : Cryo-EM structure of Toxoplasma gondii mitochondrial ATP synthase dimer, membrane region model  
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.  
Deposited on : 2019-12-04  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

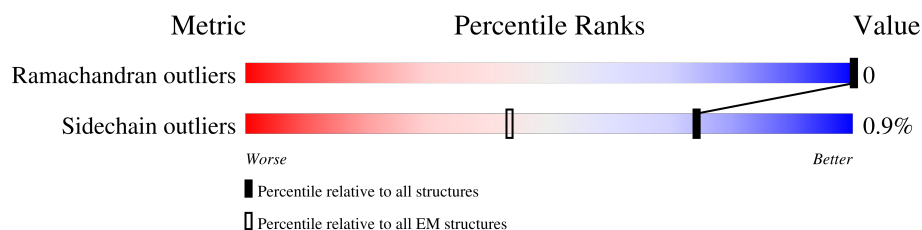
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 2.80 Å.

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



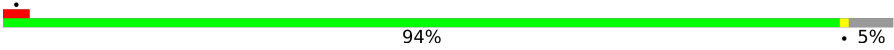




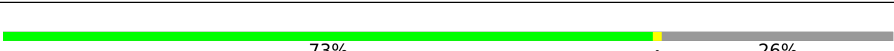
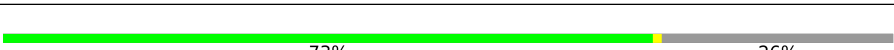

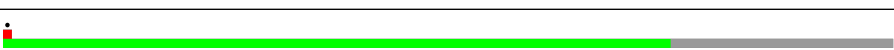

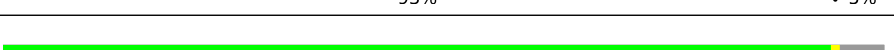
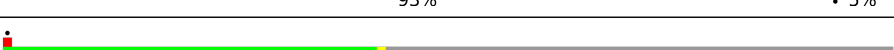

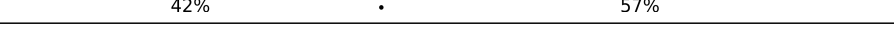
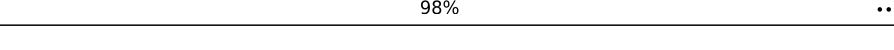
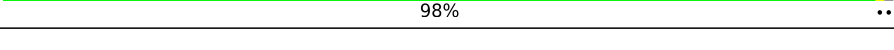





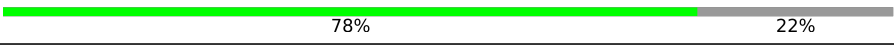
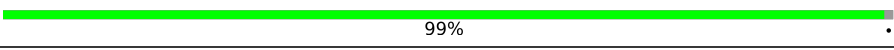
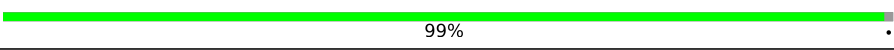
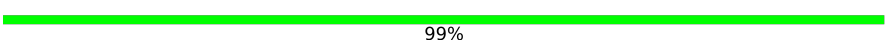
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	Q	134	<div> <div>7%</div> <div>96%</div> <div>..</div> </div>
1	q	134	<div> <div>6%</div> <div>96%</div> <div>..</div> </div>
2	I	236	<div> <div>38%</div> <div>62%</div> </div>
2	i	236	<div> <div>38%</div> <div>62%</div> </div>
3	T	133	<div> <div>69%</div> <div>31%</div> </div>
3	t	133	<div> <div>69%</div> <div>31%</div> </div>
4	G	252	<div> <div>44%</div> <div>56%</div> </div>
4	g	252	<div> <div>44%</div> <div>56%</div> </div>
5	O	157	<div> <div>94%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
5	o	157	
6	K	224	
6	k	224	
7	J	229	
7	j	229	
8	S	128	
8	s	128	
9	U	126	
9	u	126	
10	H	239	
10	h	239	
11	E	325	
11	e	325	
12	X	83	
12	x	83	
13	B	571	
13	b	571	
14	R	134	
14	r	134	
15	P	138	
15	p	138	
16	V	111	
16	v	111	
17	L	208	
17	l	208	

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Mol	Chain	Length	Quality of chain
18	C	398	
18	c	398	
19	D	310	
19	d	310	
20	M	205	
20	m	205	
21	N	166	
21	n	166	
22	F	267	
22	f	267	
23	W	106	
23	w	106	
24	A	536	
24	a	536	

## 2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 121066 atoms, of which 60518 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 ATPTG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		
1	Q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		

- Molecule 2 is a protein called ATPTG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	i	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	I	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		

- Molecule 3 is a protein called ATPTG14.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	t	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	T	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		

- Molecule 4 is a protein called ATPTG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	g	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		
4	G	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	51	VAL	PHE	conflict	UNP S7WD71

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Chain	Residue	Modelled	Actual	Comment	Reference
g	73	CYS	SER	conflict	UNP S7WD71
g	110	LYS	GLU	conflict	UNP S7WD71
g	233	THR	MET	conflict	UNP S7WD71
G	51	VAL	PHE	conflict	UNP S7WD71
G	73	CYS	SER	conflict	UNP S7WD71
G	110	LYS	GLU	conflict	UNP S7WD71
G	233	THR	MET	conflict	UNP S7WD71

- Molecule 5 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	o	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		
5	O	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		

- Molecule 6 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	K	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		

- Molecule 7 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	j	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	J	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		

- Molecule 8 is a protein called ATPTG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	s	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	S	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		

- Molecule 9 is a protein called ATPTG15.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	u	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	U	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		

- Molecule 10 is a protein called ATPTG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	h	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	H	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	89	ASN	HIS	conflict	UNP A0A125YLR0
H	89	ASN	HIS	conflict	UNP A0A125YLR0

- Molecule 11 is a protein called ATPTG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	e	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	E	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	?	-	LYS	deletion	UNP A0A125YLR0
e	63	PRO	SER	conflict	UNP A0A125YLR0
e	99	LEU	PRO	conflict	UNP A0A125YLR0
e	312	ALA	THR	conflict	UNP A0A125YLR0
E	?	-	LYS	deletion	UNP A0A125YLR0
E	63	PRO	SER	conflict	UNP A0A125YLR0
E	99	LEU	PRO	conflict	UNP A0A125YLR0
E	312	ALA	THR	conflict	UNP A0A125YLR0

- Molecule 12 is a protein called ATPTG17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	x	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		
12	X	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	77	TRP	-	expression tag	UNP S7W180
x	78	MET	-	expression tag	UNP S7W180
x	79	PHE	-	expression tag	UNP S7W180
x	80	GLY	-	expression tag	UNP S7W180
x	81	ASN	-	expression tag	UNP S7W180
x	82	SER	-	expression tag	UNP S7W180
x	83	TYR	-	expression tag	UNP S7W180
X	77	TRP	-	expression tag	UNP S7W180
X	78	MET	-	expression tag	UNP S7W180
X	79	PHE	-	expression tag	UNP S7W180
X	80	GLY	-	expression tag	UNP S7W180
X	81	ASN	-	expression tag	UNP S7W180
X	82	SER	-	expression tag	UNP S7W180
X	83	TYR	-	expression tag	UNP S7W180

- Molecule 13 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	b	253	Total	C	H	N	O	S	0	0
			4157	1374	2056	328	390	9		
13	B	253	Total	C	H	N	O	S	0	0
			4157	1374	2056	328	390	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	50	LEU	SER	conflict	UNP S7V2T0
b	474	THR	ALA	conflict	UNP S7V2T0
B	50	LEU	SER	conflict	UNP S7V2T0
B	474	THR	ALA	conflict	UNP S7V2T0

- Molecule 14 is a protein called ATPTG12.



Mol	Chain	Residues	Atoms						AltConf	Trace
14	r	90	Total	C	H	N	O	S	0	0
			1485	470	750	128	133	4		
14	R	90	Total	C	H	N	O	S	0	0
			1485	470	750	128	133	4		

- Molecule 15 is a protein called ATPTG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	P	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		

- Molecule 16 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	v	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		
16	V	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	54	ALA	VAL	conflict	UNP S7UQT7
V	54	ALA	VAL	conflict	UNP S7UQT7

- Molecule 17 is a protein called ATPTG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	l	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	L	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		

- Molecule 18 is a protein called ATPTG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	c	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		
18	C	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		

- Molecule 19 is a protein called ATPTG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	d	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		
19	D	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		

- Molecule 20 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	m	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	M	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		

- Molecule 21 is a protein called ATPTG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	n	160	Total	C	H	N	O	S	0	0
			2451	774	1204	227	235	11		
21	N	160	Total	C	H	N	O	S	0	0
			2451	774	1204	227	235	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	140	SER	ALA	conflict	UNP A0A125YUZ2
N	140	SER	ALA	conflict	UNP A0A125YUZ2

- Molecule 22 is a protein called ATPTG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	f	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	F	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		

- Molecule 23 is a protein called ATPTG16.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	w	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		

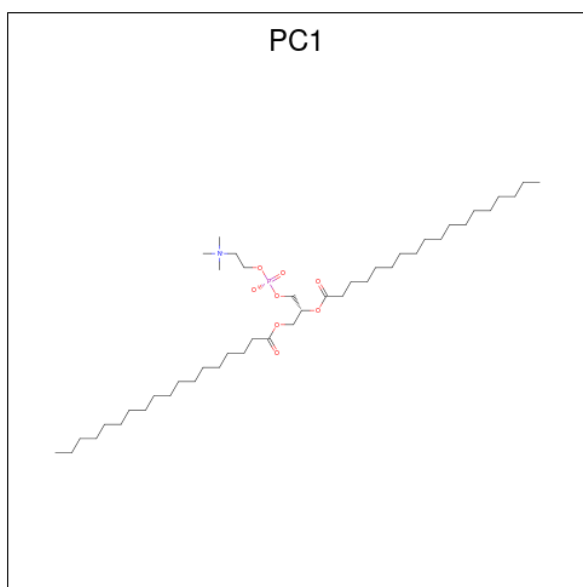
- Molecule 24 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	371	Total	C	H	N	O	S	0	0
			5895	1923	2873	523	558	18		
24	A	371	Total	C	H	N	O	S	0	0
			5895	1923	2873	523	558	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	351	THR	ALA	conflict	UNP S7V493
A	351	THR	ALA	conflict	UNP S7V493

- Molecule 25 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



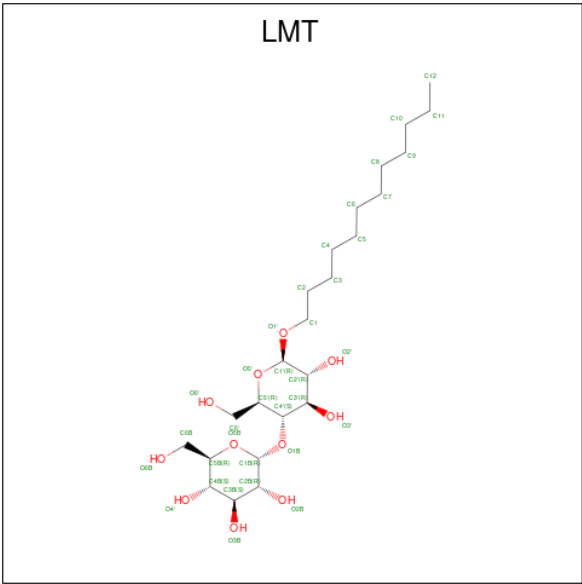
Mol	Chain	Residues	Atoms						AltConf
25	o	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
25	o	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
25	v	1	Total	C	H	N	O	P
			142	44	88	1	8	1
25	O	1	Total	C	H	N	O	P
			142	44	88	1	8	1
25	O	1	Total	C	H	N	O	P
			142	44	88	1	8	1
25	V	1	Total	C	H	N	O	P
			142	44	88	1	8	1

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



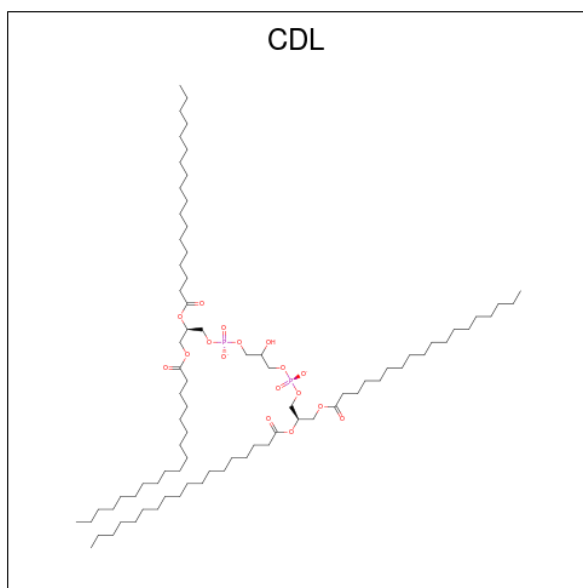
Mol	Chain	Residues	Atoms				AltConf
26	o	1	Total	C	H	O	0
			81	24	46	11	
26	h	1	Total	C	H	O	0
			81	24	46	11	
26	x	1	Total	C	H	O	0
			81	24	46	11	
26	c	1	Total	C	H	O	0
			81	24	46	11	
26	c	1	Total	C	H	O	0
			81	24	46	11	
26	d	1	Total	C	H	O	0
			81	24	46	11	
26	d	1	Total	C	H	O	0
			81	24	46	11	

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Mol	Chain	Residues	Atoms				AltConf
26	O	1	Total	C	H	O	0
			81	24	46	11	
26	H	1	Total	C	H	O	0
			81	24	46	11	
26	X	1	Total	C	H	O	0
			81	24	46	11	
26	C	1	Total	C	H	O	0
			81	24	46	11	
26	C	1	Total	C	H	O	0
			81	24	46	11	
26	D	1	Total	C	H	O	0
			81	24	46	11	
26	D	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 27 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



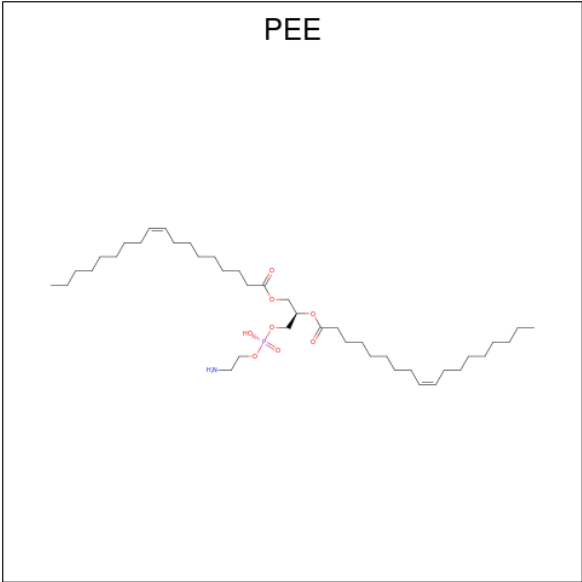
Mol	Chain	Residues	Atoms					AltConf
27	o	1	Total	C	H	O	P	0
			256	81	156	17	2	
27	u	1	Total	C	H	O	P	0
			256	81	156	17	2	
27	h	1	Total	C	H	O	P	0
			256	81	156	17	2	
27	e	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 256	C 81	H 156	O 17	P 2	0
27	v	1	Total 256	C 81	H 156	O 17	P 2	0
27	c	1	Total 256	C 81	H 156	O 17	P 2	0
27	d	1	Total 256	C 81	H 156	O 17	P 2	0
27	O	1	Total 256	C 81	H 156	O 17	P 2	0
27	U	1	Total 256	C 81	H 156	O 17	P 2	0
27	H	1	Total 256	C 81	H 156	O 17	P 2	0
27	E	1	Total 256	C 81	H 156	O 17	P 2	0
27	B	1	Total 256	C 81	H 156	O 17	P 2	0
27	B	1	Total 256	C 81	H 156	O 17	P 2	0
27	V	1	Total 256	C 81	H 156	O 17	P 2	0
27	V	1	Total 256	C 81	H 156	O 17	P 2	0
27	C	1	Total 256	C 81	H 156	O 17	P 2	0
27	D	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 28 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).

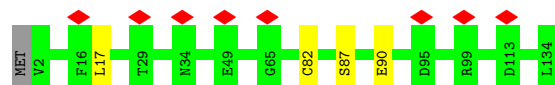


Mol	Chain	Residues	Atoms						AltConf
28	j	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	j	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	c	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	C	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

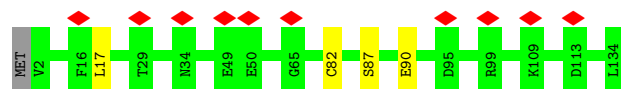
### 3 Residue-property plots [i](#)

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

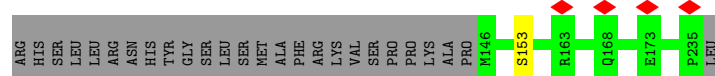
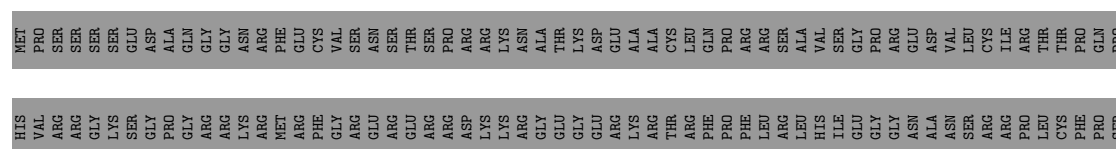
- Molecule 1: ATPTG11



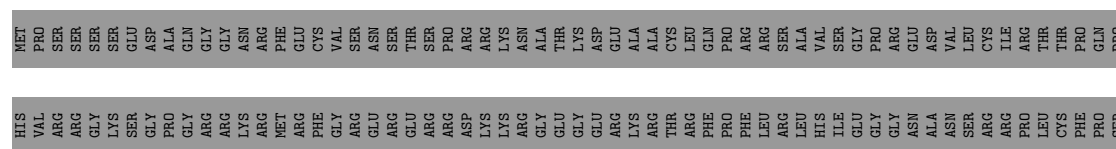
- Molecule 1: ATPTG11



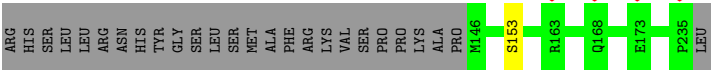
- Molecule 2: ATPTG7



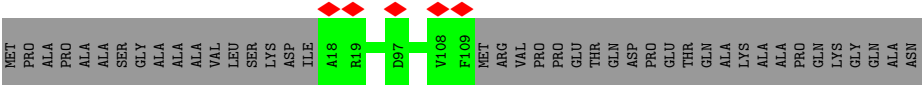
- Molecule 2: ATPTG7



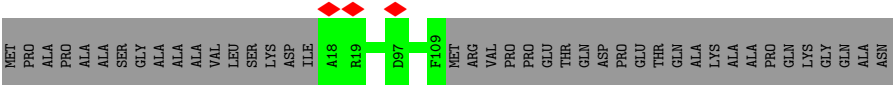




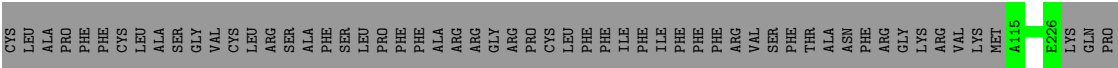
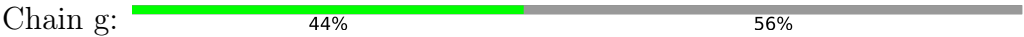
• Molecule 3: ATPTG14



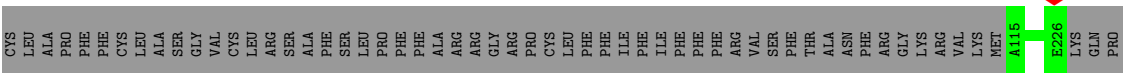
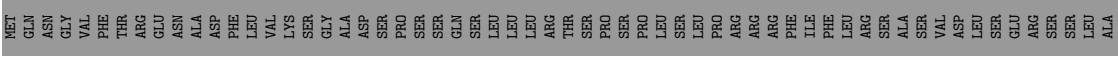
• Molecule 3: ATPTG14



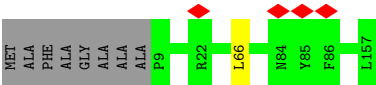
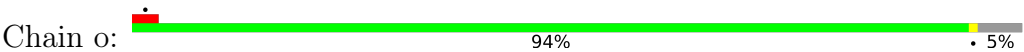
• Molecule 4: ATPTG5



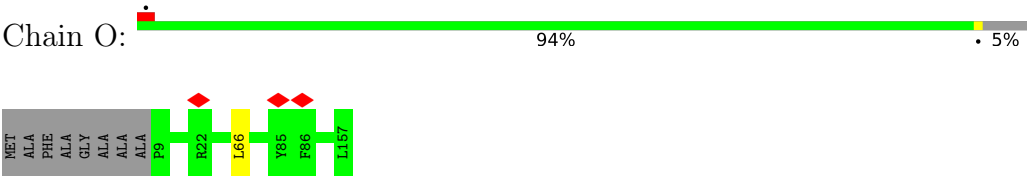
• Molecule 4: ATPTG5



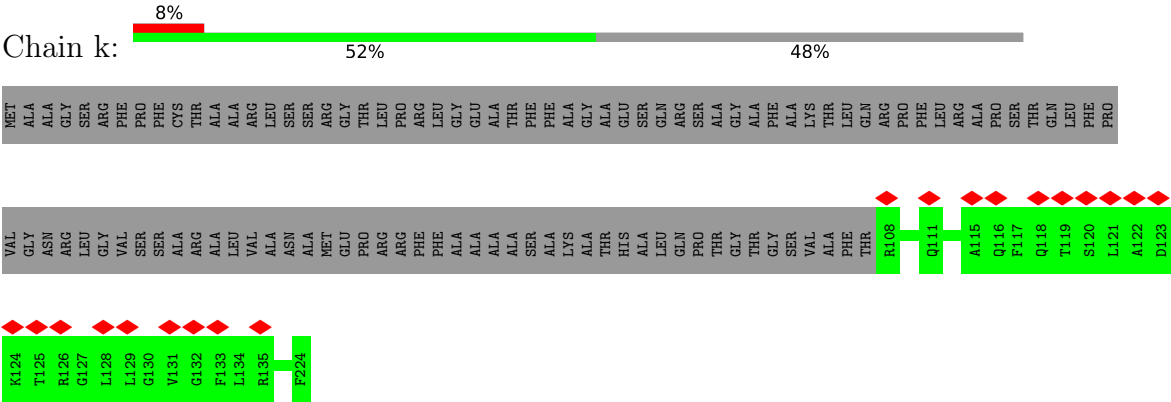
• Molecule 5: subunit k



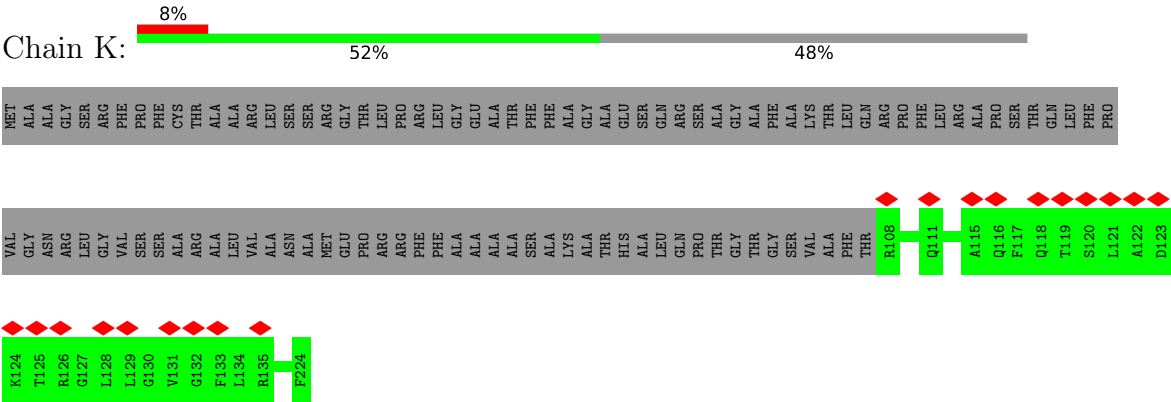
• Molecule 5: subunit k



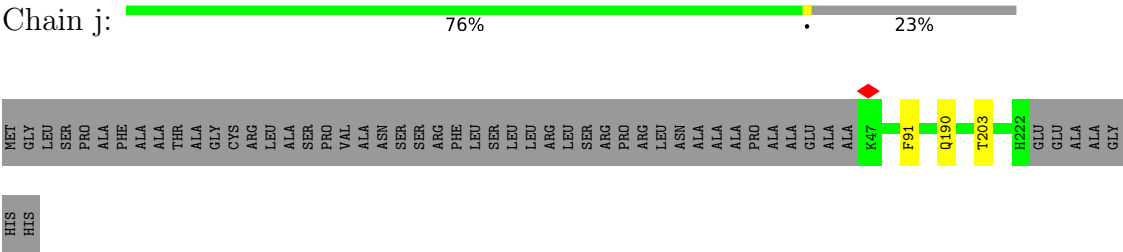
• Molecule 6: subunit a



• Molecule 6: subunit a

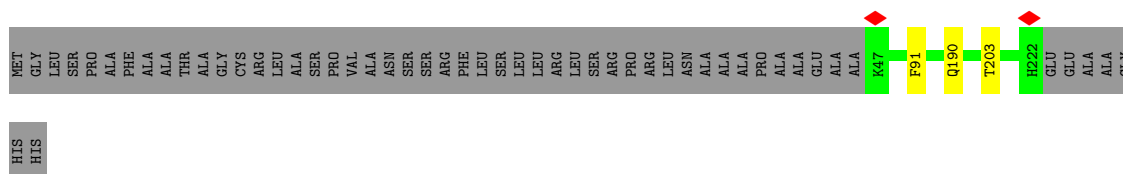


• Molecule 7: subunit i/j



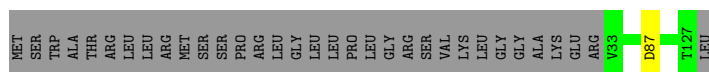
• Molecule 7: subunit i/j





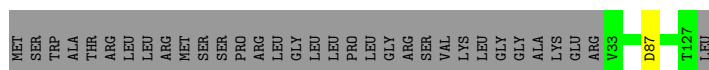
• Molecule 8: ATPTG13

Chain s: 73% 26%



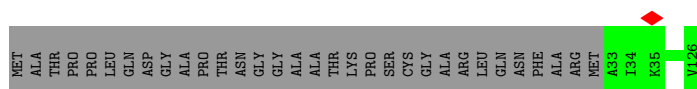
• Molecule 8: ATPTG13

Chain S: 73% 26%



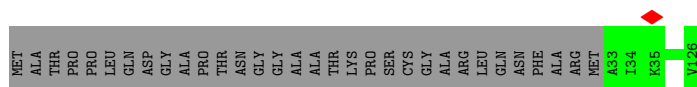
• Molecule 9: ATPTG15

Chain u: 75% 25%



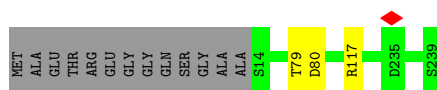
• Molecule 9: ATPTG15

Chain U: 75% 25%



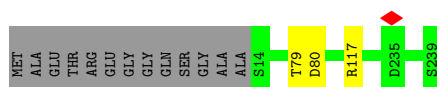
• Molecule 10: ATPTG6

Chain h: 93% 5%

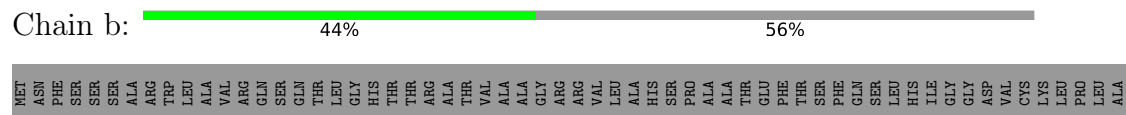
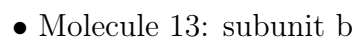
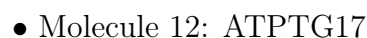
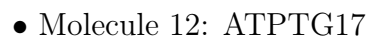
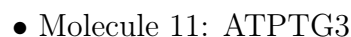


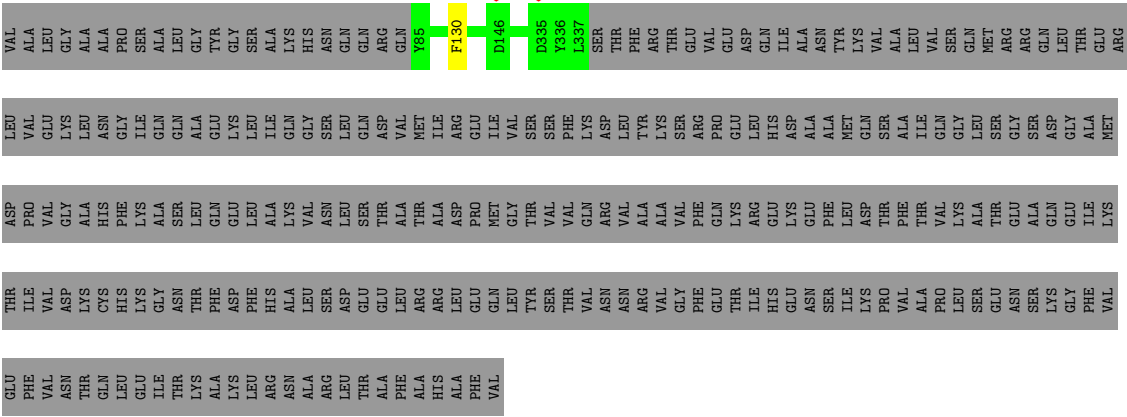
• Molecule 10: ATPTG6

Chain H: 93% 5%

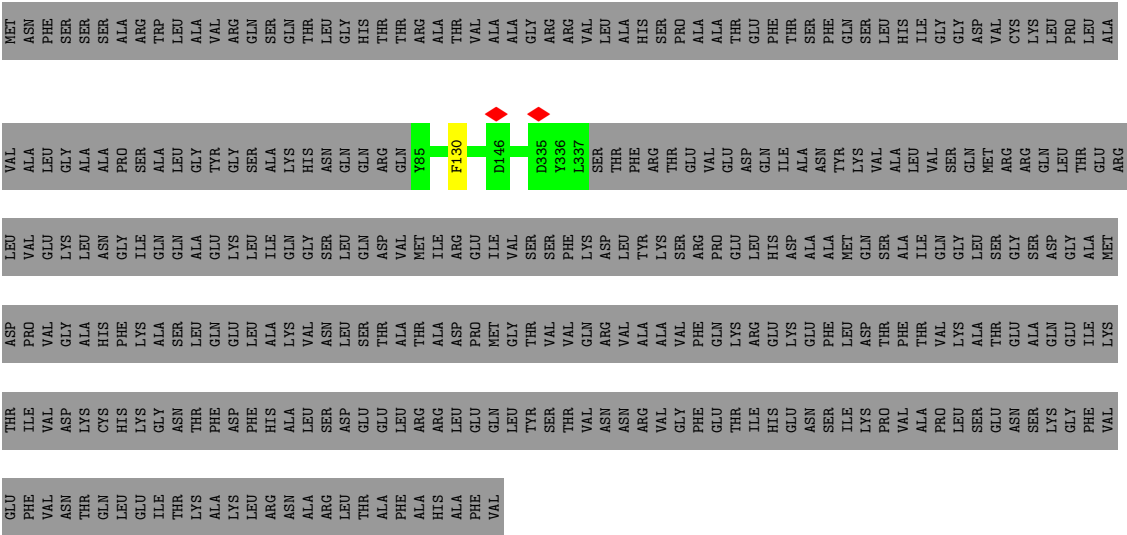
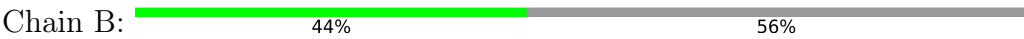


• Molecule 11: ATPTG3

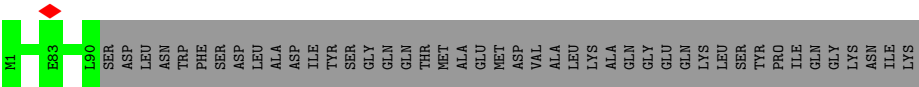




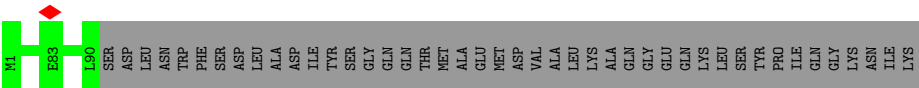
● Molecule 13: subunit b




● Molecule 14: ATPTG12



● Molecule 14: ATPTG12




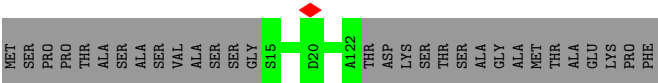
● Molecule 15: ATPTG10

Chain p:  78% 22%



• Molecule 15: ATPTG10

Chain P:  78% 22%



• Molecule 16: subunit f

Chain v:  99%



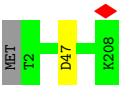
• Molecule 16: subunit f

Chain V:  99%



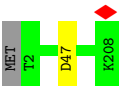
• Molecule 17: ATPTG8

Chain l:  99%



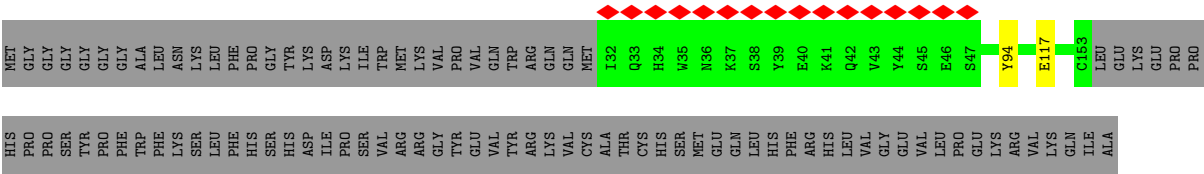
• Molecule 17: ATPTG8

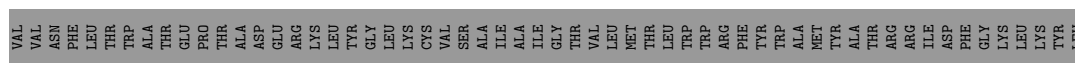
Chain L:  99%



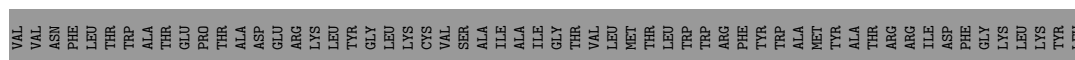
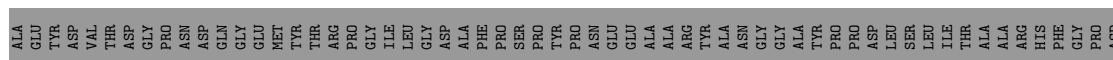
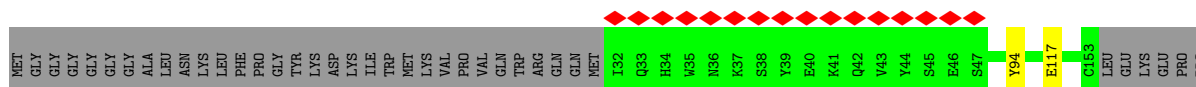
• Molecule 18: ATPTG1

Chain c:  30% 69%

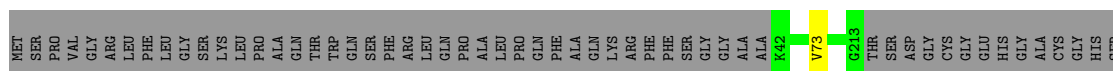
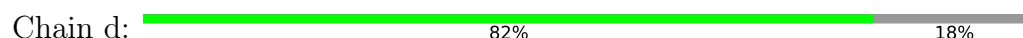




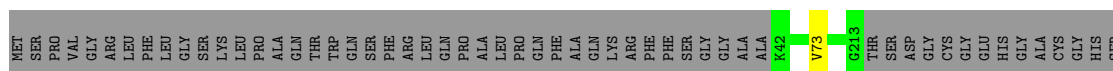
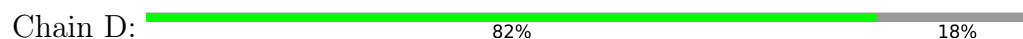
- Molecule 18: ATPTG1



- Molecule 19: ATPG2



- Molecule 19: ATPTG2



- Molecule 20: subunit 8



MET	ASN	ALA	THR	PHE	PHE	GLY	ARG	LEU	THR	PRO	ALA	ALA	ALA	ALA	ALA	ALA	ARG	ARG	VAL	ALA	VAL	SER	PHE	PHE	GLY	ARG	ARG	ALA	ARG	SER	SER	ALA	ALA	GLY	PHE	GLY	THR	PRO	GLN	HIS	ARG	VAL	ALA	ALA	LEU	ARG	PRO	PRO	PRO	SER	GLN	ARG	PRO	PRO	ALA	ALA	GLU	ARG	ALA	ALA	HIS	ASN	LEU	ALA	LYS	SER	SER	GLN	THR	LEU	ARG	SER	VAL
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LYS	ALA	HIS	GLY	ARG	GLN	SER	GLY	LYS	LYS	GLU	ALA	GLN	SER	THR	ARG	GLU	SER	VAL	ALA	GLY	ARG	ARG	GLY	PHE	ALA	ARG	ALA	ALA	VAL	VAL	GLY	GLY	ALA	ALA	THR	THR	GLY	CYS	MET	LEU	VAL	ALA	ALA	ALA	A96	D103	Q191	ASP	ALA	ALA	PRO	THR	LYS	THR	GLY	SER	THR	SER	ALA	ALA	LYS	LYS
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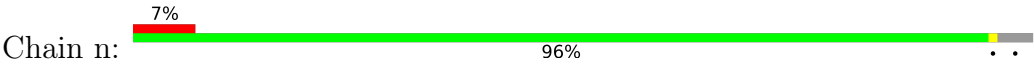
● Molecule 20: subunit 8



MET	THR	THR	PHE	ASP	LEU	THR	PRO	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ARG	ARG	GLU	SER	VAL	ALA	VAL	SER	PHE	PHE	GLY	ARG	ARG	ALA	SER	SER	ALA	VAL	GLY	SER	GLY	PHE	THR	GLN	HIS	ARG	VAL	LEU	VAL	ALA	ALA	LEU	ARG	PRO	PRO	PRO	SER	GLN	ARG	PRO	PRO	ALA	GLU	ARG	LYS	THR	GLY	ALA	ASN	HIS	THR	SER	ALA	LYS	LYS	SER	SER	GLN	THR	LEU	ARG	SER	VAL
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LYS	ALA	HIS	GLY	ARG	GLN	SER	GLY	LYS	LYS	GLU	ALA	GLN	SER	THR	ARG	GLU	SER	VAL	ALA	GLY	ARG	ARG	GLY	PHE	ALA	ARG	ALA	ALA	VAL	VAL	GLY	GLY	ALA	ALA	THR	THR	GLY	CYS	MET	LEU	VAL	ALA	ALA	ALA	A96	D103	Q191	ASP	ALA	ALA	PRO	THR	LYS	THR	GLY	SER	THR	SER	ALA	ALA	LYS	LYS
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● Molecule 21: ATPTG9



MET	SER	GLY	ASP	SER	VAL	A7	P8	H9	Q10	R11	D38	R82	S96	S97	P98	S99	S100	R136	A166
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● Molecule 21: ATPTG9



MET	SER	GLY	ASP	SER	VAL	A7	P8	H9	Q10	R11	D38	R82	S96	S97	P98	S99	S100	R136	A166
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● Molecule 22: ATPTG4



MET	ALA	LEU	ASN	ARG	VAL	PRO	SER	ARG	VAL	LEU	PRO	PHE	ALA	VAL	SER	GLY	TYR	VAL	HIS	PRO	ARG	ASN	ALA	CYS	ARG	LEU	PRO	ALA	ALA	ALA	VAL	SER	SER	VAL	VAL	PRO	SER	SER	SER	VAL	VAL	ALA	PHE	SER	SER	ARG	THR	ASN	PHE	LEU	SER	ARG	SER	SER	ALA	VAL	MET	SER
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HIS	PRO	CYS	ALA	ALA	THR	ALA	ARG	HIS	PHE	S71	S101	A102	SER	SER	GLY	ILE	ALA	ALA	SER	GLY	THR	ASN	A112	L113	K114	S163	D200	S209	A267
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● Molecule 22: ATPTG4



MET	ALA	LEU	ASN	ARG	VAL	PRO	SER	ARG	VAL	LEU	PRO	PHE	ALA	VAL	SER	GLY	TYR	VAL	HIS	PRO	ARG	ASN	ALA	CYS	ARG	LEU	PRO	ALA	ALA	ALA	VAL	SER	SER	VAL	VAL	PRO	SER	SER	SER	VAL	VAL	ALA	PHE	SER	SER	ARG	THR	ASN	PHE	LEU	SER	ARG	SER	SER	ALA	VAL	MET	SER
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HIS	PRO	CYS	ALA	ALA	THR	ALA	ARG	HIS	PHE	S71	SER	A102	SER	SER	GLY	ILE	ALA	ALA	SER	GLY	THR	ASN	A112	L113	K114	S163	S209	A267
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	101505	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, CDL, LMT, PEE

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	Q	0.28	0/1103	0.41	0/1496
1	q	0.28	0/1103	0.41	0/1496
2	I	0.29	0/719	0.41	0/962
2	i	0.29	0/719	0.41	0/962
3	T	0.28	0/741	0.43	0/1007
3	t	0.28	0/741	0.43	0/1007
4	G	0.29	0/896	0.41	0/1216
4	g	0.29	0/896	0.41	0/1216
5	O	0.33	0/1250	0.43	0/1682
5	o	0.33	0/1250	0.43	0/1682
6	K	0.32	0/981	0.38	0/1321
6	k	0.32	0/981	0.39	0/1321
7	J	0.36	0/1573	0.42	0/2137
7	j	0.36	0/1573	0.42	0/2137
8	S	0.32	0/826	0.41	0/1119
8	s	0.32	0/826	0.41	0/1119
9	U	0.34	0/770	0.41	0/1040
9	u	0.34	0/770	0.41	0/1040
10	H	0.33	0/1902	0.41	0/2575
10	h	0.33	0/1902	0.41	0/2575
11	E	0.34	0/1154	0.42	0/1572
11	e	0.34	0/1154	0.42	0/1572
12	X	0.29	0/678	0.40	0/923
12	x	0.29	0/678	0.40	0/923
13	B	0.33	0/2159	0.40	0/2920
13	b	0.33	0/2159	0.41	0/2920
14	R	0.31	0/750	0.42	0/1008
14	r	0.31	0/750	0.42	0/1008
15	P	0.30	0/888	0.37	0/1202
15	p	0.30	0/888	0.37	0/1202
16	V	0.34	0/944	0.41	0/1280
16	v	0.34	0/944	0.41	0/1280

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	L	0.31	0/1651	0.41	0/2227
17	l	0.31	0/1651	0.41	0/2227
18	C	0.33	0/1057	0.40	0/1428
18	c	0.33	0/1057	0.40	0/1428
19	D	0.33	0/2138	0.42	0/2905
19	d	0.33	0/2138	0.42	0/2905
20	M	0.32	0/789	0.41	0/1065
20	m	0.32	0/789	0.41	0/1065
21	N	0.29	0/1280	0.41	0/1734
21	n	0.29	0/1280	0.41	0/1734
22	F	0.30	0/1475	0.42	0/2009
22	f	0.30	0/1475	0.42	0/2009
23	W	0.33	0/778	0.45	0/1057
23	w	0.33	0/778	0.45	0/1057
24	A	0.29	0/3107	0.38	0/4207
24	a	0.29	0/3107	0.38	0/4207
All	All	0.32	0/59218	0.41	0/80184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	131/134 (98%)	128 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	q	131/134 (98%)	128 (98%)	3 (2%)	0	100	100
2	I	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	i	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
3	T	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	t	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
4	G	110/252 (44%)	107 (97%)	3 (3%)	0	100	100
4	g	110/252 (44%)	107 (97%)	3 (3%)	0	100	100
5	O	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
5	o	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
6	K	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
6	k	115/224 (51%)	112 (97%)	3 (3%)	0	100	100
7	J	174/229 (76%)	171 (98%)	3 (2%)	0	100	100
7	j	174/229 (76%)	171 (98%)	3 (2%)	0	100	100
8	S	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	s	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
9	U	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	u	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
10	H	224/239 (94%)	215 (96%)	9 (4%)	0	100	100
10	h	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
11	E	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
11	e	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
12	X	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	x	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
13	B	251/571 (44%)	247 (98%)	4 (2%)	0	100	100
13	b	251/571 (44%)	247 (98%)	4 (2%)	0	100	100
14	R	88/134 (66%)	84 (96%)	4 (4%)	0	100	100
14	r	88/134 (66%)	84 (96%)	4 (4%)	0	100	100
15	P	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	p	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
16	V	108/111 (97%)	108 (100%)	0	0	100	100
16	v	108/111 (97%)	108 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	L	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
17	l	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
18	C	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
18	c	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
19	D	250/310 (81%)	247 (99%)	3 (1%)	0	100	100
19	d	250/310 (81%)	247 (99%)	3 (1%)	0	100	100
20	M	94/205 (46%)	88 (94%)	6 (6%)	0	100	100
20	m	94/205 (46%)	89 (95%)	5 (5%)	0	100	100
21	N	158/166 (95%)	154 (98%)	4 (2%)	0	100	100
21	n	158/166 (95%)	154 (98%)	4 (2%)	0	100	100
22	F	184/267 (69%)	176 (96%)	8 (4%)	0	100	100
22	f	184/267 (69%)	176 (96%)	8 (4%)	0	100	100
23	W	92/106 (87%)	88 (96%)	4 (4%)	0	100	100
23	w	92/106 (87%)	88 (96%)	4 (4%)	0	100	100
24	A	367/536 (68%)	356 (97%)	11 (3%)	0	100	100
24	a	367/536 (68%)	356 (97%)	11 (3%)	0	100	100
All	All	7010/10832 (65%)	6808 (97%)	202 (3%)	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	Q	119/120 (99%)	115 (97%)	4 (3%)	32	66
1	q	119/120 (99%)	115 (97%)	4 (3%)	32	66
2	I	71/197 (36%)	70 (99%)	1 (1%)	62	87
2	i	71/197 (36%)	70 (99%)	1 (1%)	62	87
3	T	77/106 (73%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	t	77/106 (73%)	77 (100%)	0	100	100
4	G	93/214 (44%)	93 (100%)	0	100	100
4	g	93/214 (44%)	93 (100%)	0	100	100
5	O	127/129 (98%)	126 (99%)	1 (1%)	79	93
5	o	127/129 (98%)	126 (99%)	1 (1%)	79	93
6	K	100/175 (57%)	100 (100%)	0	100	100
6	k	100/175 (57%)	100 (100%)	0	100	100
7	J	160/195 (82%)	157 (98%)	3 (2%)	52	82
7	j	160/195 (82%)	157 (98%)	3 (2%)	52	82
8	S	86/113 (76%)	85 (99%)	1 (1%)	67	89
8	s	86/113 (76%)	85 (99%)	1 (1%)	67	89
9	U	76/98 (78%)	76 (100%)	0	100	100
9	u	76/98 (78%)	76 (100%)	0	100	100
10	H	197/204 (97%)	194 (98%)	3 (2%)	60	86
10	h	197/204 (97%)	194 (98%)	3 (2%)	60	86
11	E	118/258 (46%)	116 (98%)	2 (2%)	56	84
11	e	118/258 (46%)	116 (98%)	2 (2%)	56	84
12	X	70/71 (99%)	69 (99%)	1 (1%)	62	87
12	x	70/71 (99%)	69 (99%)	1 (1%)	62	87
13	B	227/491 (46%)	226 (100%)	1 (0%)	89	96
13	b	227/491 (46%)	226 (100%)	1 (0%)	89	96
14	R	80/117 (68%)	80 (100%)	0	100	100
14	r	80/117 (68%)	80 (100%)	0	100	100
15	P	91/113 (80%)	91 (100%)	0	100	100
15	p	91/113 (80%)	91 (100%)	0	100	100
16	V	86/87 (99%)	86 (100%)	0	100	100
16	v	86/87 (99%)	86 (100%)	0	100	100
17	L	177/178 (99%)	176 (99%)	1 (1%)	84	95
17	l	177/178 (99%)	176 (99%)	1 (1%)	84	95
18	C	107/338 (32%)	105 (98%)	2 (2%)	52	82
18	c	107/338 (32%)	105 (98%)	2 (2%)	52	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	D	218/259 (84%)	217 (100%)	1 (0%)	86	95
19	d	218/259 (84%)	217 (100%)	1 (0%)	86	95
20	M	77/156 (49%)	76 (99%)	1 (1%)	65	88
20	m	77/156 (49%)	76 (99%)	1 (1%)	65	88
21	N	138/144 (96%)	137 (99%)	1 (1%)	81	94
21	n	138/144 (96%)	137 (99%)	1 (1%)	81	94
22	F	155/218 (71%)	153 (99%)	2 (1%)	65	88
22	f	155/218 (71%)	153 (99%)	2 (1%)	65	88
23	W	84/89 (94%)	84 (100%)	0	100	100
23	w	84/89 (94%)	84 (100%)	0	100	100
24	A	315/447 (70%)	312 (99%)	3 (1%)	73	91
24	a	315/447 (70%)	312 (99%)	3 (1%)	73	91
All	All	6098/9034 (68%)	6042 (99%)	56 (1%)	74	92

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	17	LEU
24	A	354	ASP
7	J	190	GLN
24	A	208	ASP
20	M	103	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
24	a	310	GLN
2	I	202	GLN
24	A	321	GLN
10	H	209	GLN
22	F	78	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

44 ligands are modelled in this entry.

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$
26	LMT	D	401	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
28	PEE	j	301	-	50,50,50	1.13	6 (12%)	53,55,55	1.13	3 (5%)
26	LMT	X	101	-	36,36,36	1.17	3 (8%)	47,47,47	1.05	2 (4%)
26	LMT	c	403	-	36,36,36	1.11	2 (5%)	47,47,47	1.02	1 (2%)
26	LMT	D	403	-	36,36,36	1.12	2 (5%)	47,47,47	0.90	0
27	CDL	V	202	-	99,99,99	0.89	7 (7%)	105,111,111	1.00	4 (3%)
25	PC1	o	201	-	53,53,53	0.94	3 (5%)	59,61,61	1.03	3 (5%)
27	CDL	u	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)
27	CDL	c	404	-	99,99,99	0.87	7 (7%)	105,111,111	1.04	4 (3%)
27	CDL	C	404	-	99,99,99	0.88	7 (7%)	105,111,111	1.04	4 (3%)
26	LMT	c	401	-	36,36,36	1.09	2 (5%)	47,47,47	1.13	2 (4%)
25	PC1	v	202	-	53,53,53	0.96	4 (7%)	59,61,61	0.95	2 (3%)
26	LMT	C	403	-	36,36,36	1.11	2 (5%)	47,47,47	1.02	1 (2%)
28	PEE	J	302	-	50,50,50	1.14	6 (12%)	53,55,55	1.16	3 (5%)
27	CDL	E	401	-	99,99,99	0.87	8 (8%)	105,111,111	1.02	4 (3%)
26	LMT	O	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.93	1 (2%)
27	CDL	d	402	-	99,99,99	0.87	8 (8%)	105,111,111	1.04	4 (3%)
28	PEE	j	302	-	50,50,50	1.14	6 (12%)	53,55,55	1.16	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LMT	H	301	-	36,36,36	1.13	2 (5%)	47,47,47	0.98	1 (2%)
26	LMT	C	401	-	36,36,36	1.09	2 (5%)	47,47,47	1.13	2 (4%)
27	CDL	b	601	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
28	PEE	c	402	-	50,50,50	1.14	6 (12%)	53,55,55	1.05	2 (3%)
28	PEE	C	402	-	50,50,50	1.14	6 (12%)	53,55,55	1.05	2 (3%)
26	LMT	x	101	-	36,36,36	1.16	3 (8%)	47,47,47	1.05	2 (4%)
28	PEE	J	301	-	50,50,50	1.13	6 (12%)	53,55,55	1.13	3 (5%)
26	LMT	h	301	-	36,36,36	1.13	2 (5%)	47,47,47	0.98	2 (4%)
27	CDL	e	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
27	CDL	O	203	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	5 (4%)
27	CDL	H	302	-	99,99,99	0.87	7 (7%)	105,111,111	1.03	4 (3%)
25	PC1	O	204	5	53,53,53	0.94	4 (7%)	59,61,61	1.00	2 (3%)
27	CDL	B	602	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
25	PC1	o	204	5	53,53,53	0.94	4 (7%)	59,61,61	1.00	2 (3%)
27	CDL	U	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)
25	PC1	V	203	-	53,53,53	0.96	4 (7%)	59,61,61	0.95	2 (3%)
27	CDL	h	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
27	CDL	D	402	-	99,99,99	0.87	8 (8%)	105,111,111	1.04	4 (3%)
26	LMT	d	403	-	36,36,36	1.12	2 (5%)	47,47,47	0.91	0
25	PC1	O	201	-	53,53,53	0.94	3 (5%)	59,61,61	1.04	3 (5%)
26	LMT	o	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.93	1 (2%)
27	CDL	v	201	-	99,99,99	0.89	7 (7%)	105,111,111	1.00	4 (3%)
26	LMT	d	401	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
27	CDL	o	203	-	99,99,99	0.87	7 (7%)	105,111,111	1.05	5 (4%)
27	CDL	V	201	-	99,99,99	0.87	7 (7%)	105,111,111	1.05	4 (3%)
27	CDL	B	601	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)

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
26	LMT	D	401	-	-	12/21/61/61	0/2/2/2
28	PEE	j	301	-	-	20/54/54/54	-
26	LMT	X	101	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMT	c	403	-	-	4/21/61/61	0/2/2/2
26	LMT	D	403	-	-	5/21/61/61	0/2/2/2
27	CDL	V	202	-	-	38/110/110/110	-
25	PC1	o	201	-	-	18/57/57/57	-
27	CDL	u	201	-	-	35/110/110/110	-
27	CDL	c	404	-	-	42/110/110/110	-
27	CDL	C	404	-	-	42/110/110/110	-
26	LMT	c	401	-	-	6/21/61/61	0/2/2/2
25	PC1	v	202	-	-	26/57/57/57	-
26	LMT	C	403	-	-	4/21/61/61	0/2/2/2
28	PEE	J	302	-	-	23/54/54/54	-
27	CDL	E	401	-	-	35/110/110/110	-
26	LMT	O	202	-	-	3/21/61/61	0/2/2/2
27	CDL	d	402	-	-	36/110/110/110	-
28	PEE	j	302	-	-	23/54/54/54	-
26	LMT	H	301	-	-	8/21/61/61	0/2/2/2
26	LMT	C	401	-	-	6/21/61/61	0/2/2/2
27	CDL	b	601	-	-	42/110/110/110	-
28	PEE	c	402	-	-	19/54/54/54	-
28	PEE	C	402	-	-	19/54/54/54	-
26	LMT	x	101	-	-	11/21/61/61	0/2/2/2
28	PEE	J	301	-	-	20/54/54/54	-
26	LMT	h	301	-	-	7/21/61/61	0/2/2/2
27	CDL	e	401	-	-	35/110/110/110	-
27	CDL	O	203	-	-	49/110/110/110	-
27	CDL	H	302	-	-	46/110/110/110	-
25	PC1	O	204	5	-	27/57/57/57	-
27	CDL	B	602	-	-	42/110/110/110	-
25	PC1	o	204	5	-	27/57/57/57	-
27	CDL	U	201	-	-	35/110/110/110	-
25	PC1	V	203	-	-	26/57/57/57	-
27	CDL	h	302	-	-	46/110/110/110	-
27	CDL	D	402	-	-	36/110/110/110	-
26	LMT	d	403	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PC1	O	201	-	-	18/57/57/57	-
26	LMT	o	202	-	-	3/21/61/61	0/2/2/2
27	CDL	v	201	-	-	38/110/110/110	-
26	LMT	d	401	-	-	12/21/61/61	0/2/2/2
27	CDL	o	203	-	-	49/110/110/110	-
27	CDL	V	201	-	-	44/110/110/110	-
27	CDL	B	601	-	-	44/110/110/110	-

The worst 5 of 221 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	402	PEE	C18-C19	3.73	1.53	1.31
28	J	302	PEE	C39-C38	3.73	1.53	1.31
28	j	302	PEE	C39-C38	3.73	1.53	1.31
28	C	402	PEE	C18-C19	3.73	1.53	1.31
28	c	402	PEE	C39-C38	3.72	1.53	1.31

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	402	CDL	OB6-CB5-C51	4.17	120.50	111.50
27	d	402	CDL	OB6-CB5-C51	4.16	120.47	111.50
27	B	602	CDL	OB6-CB5-C51	4.11	120.37	111.50
25	o	204	PC1	O21-C21-C22	4.10	120.34	111.50
27	b	601	CDL	OB6-CB5-C51	4.10	120.33	111.50

There are no chirality outliers.

5 of 1097 torsion outliers are listed below:

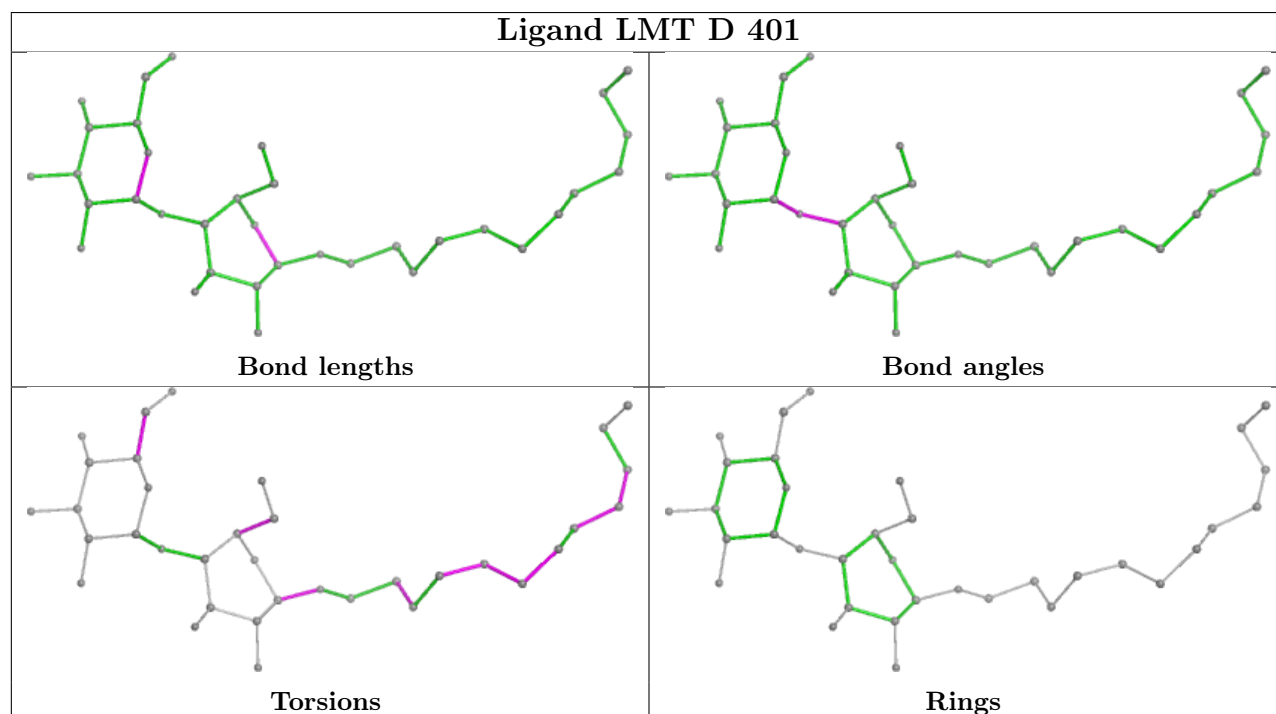
Mol	Chain	Res	Type	Atoms
25	o	201	PC1	O13-C11-C12-N
25	o	201	PC1	C22-C21-O21-C2
25	o	204	PC1	C22-C21-O21-C2
25	v	202	PC1	C1-O11-P-O13
25	v	202	PC1	C12-C11-O13-P

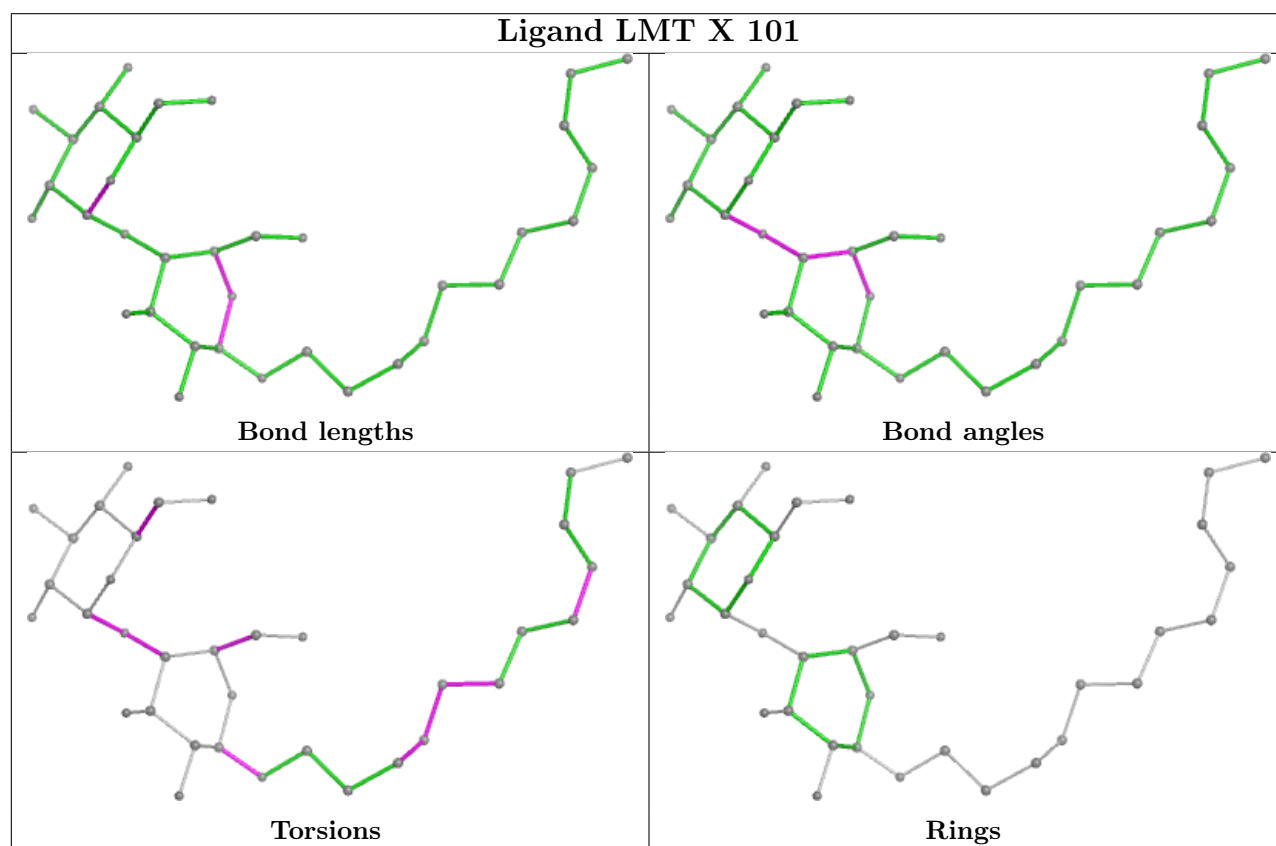
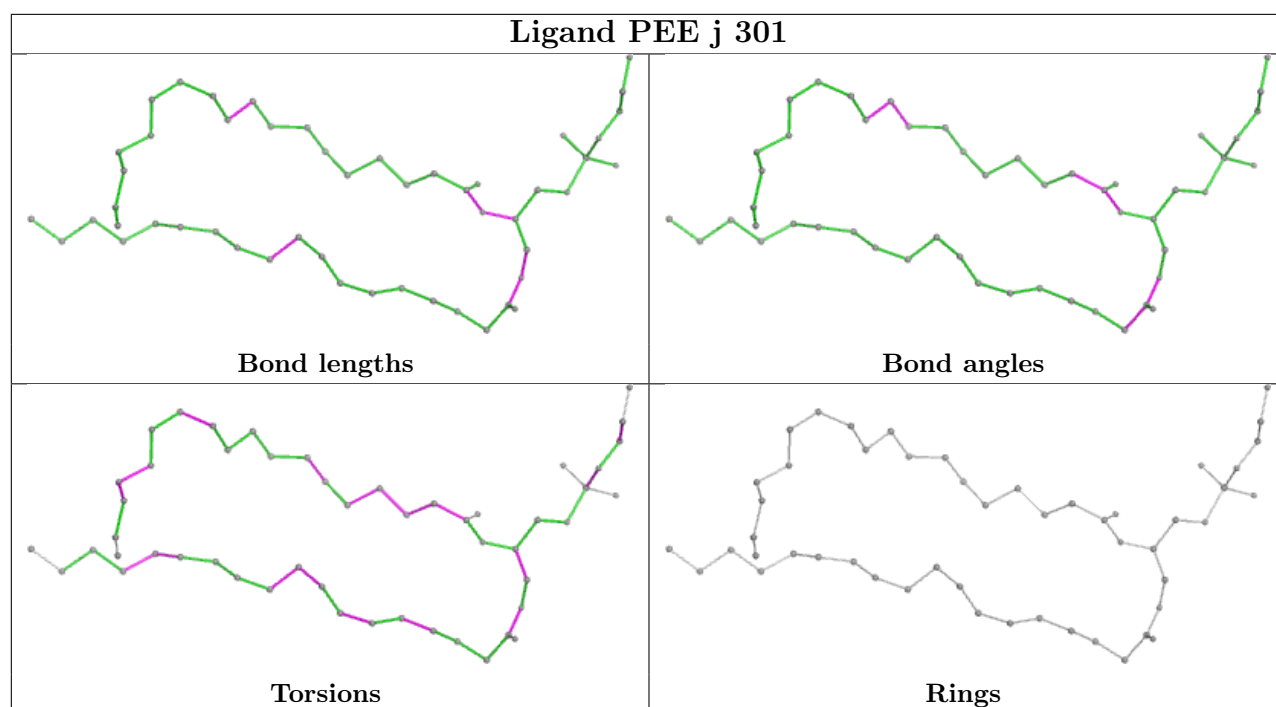
There are no ring outliers.

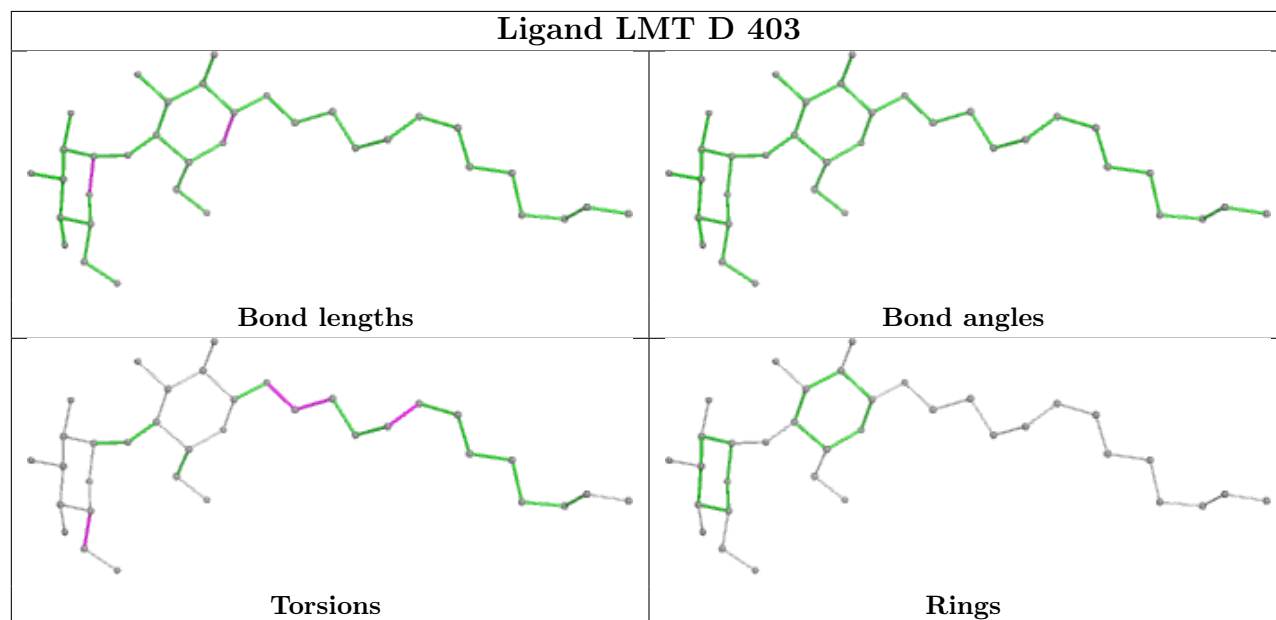
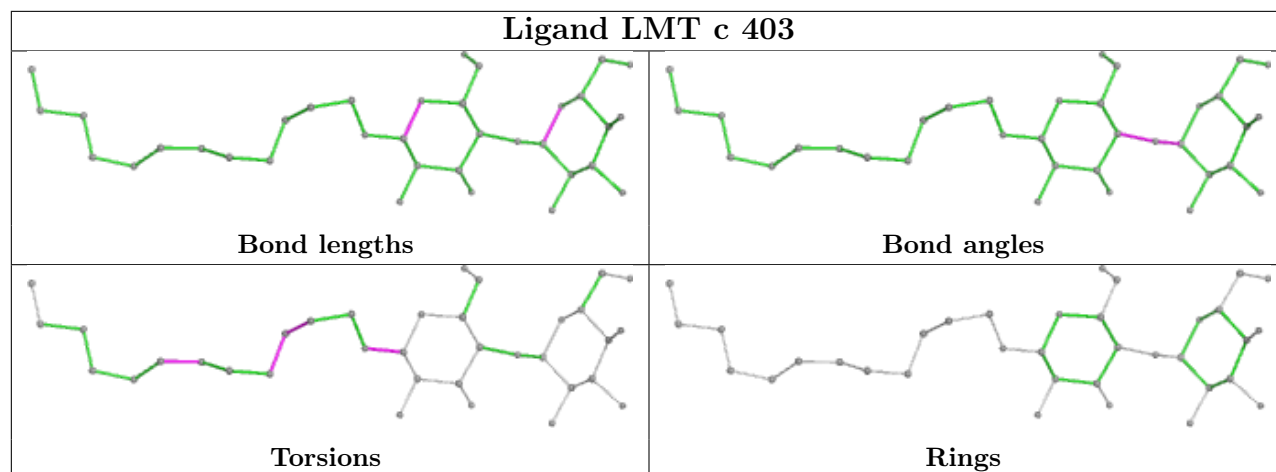
No monomer is involved in short contacts.

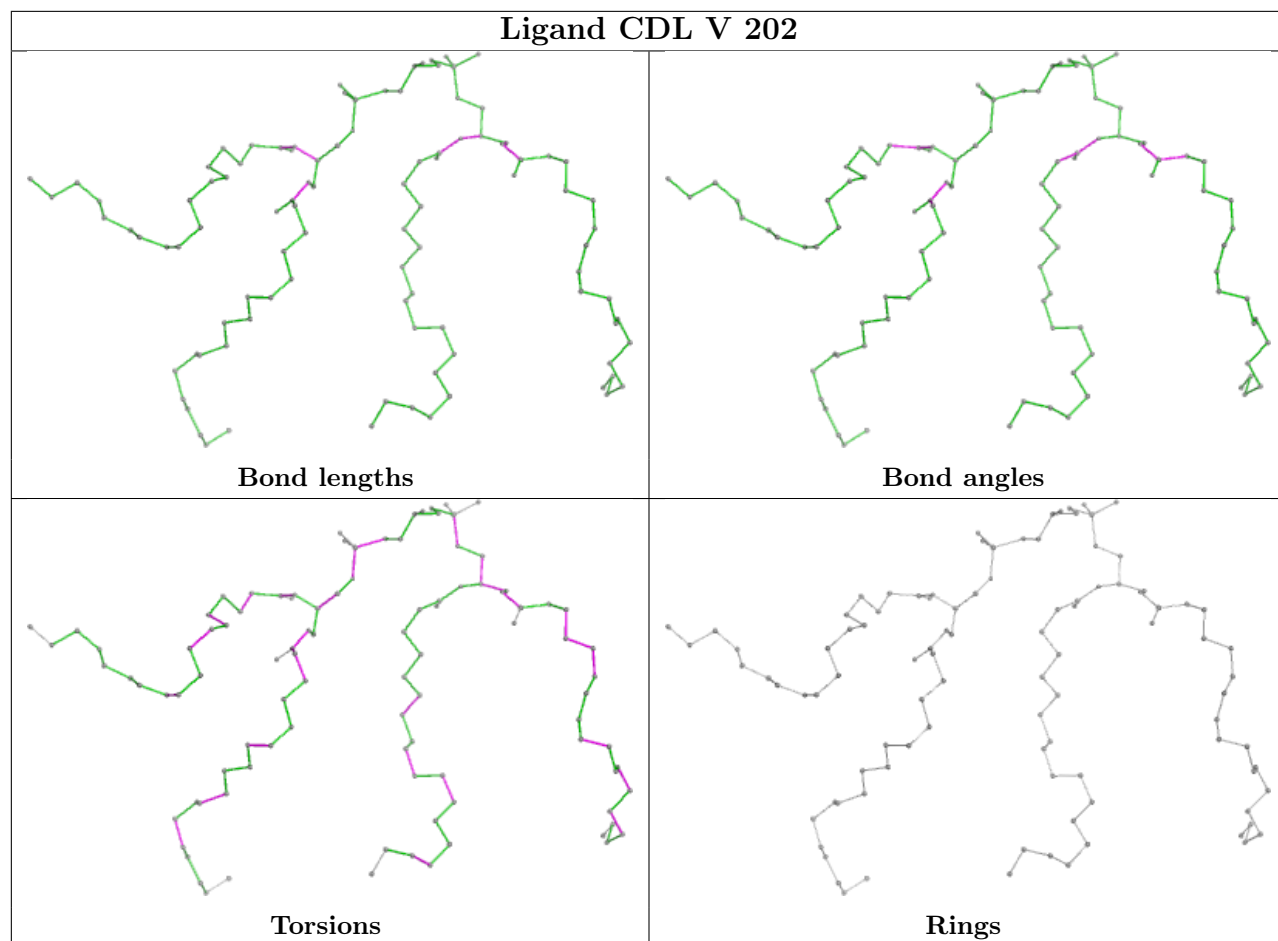
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

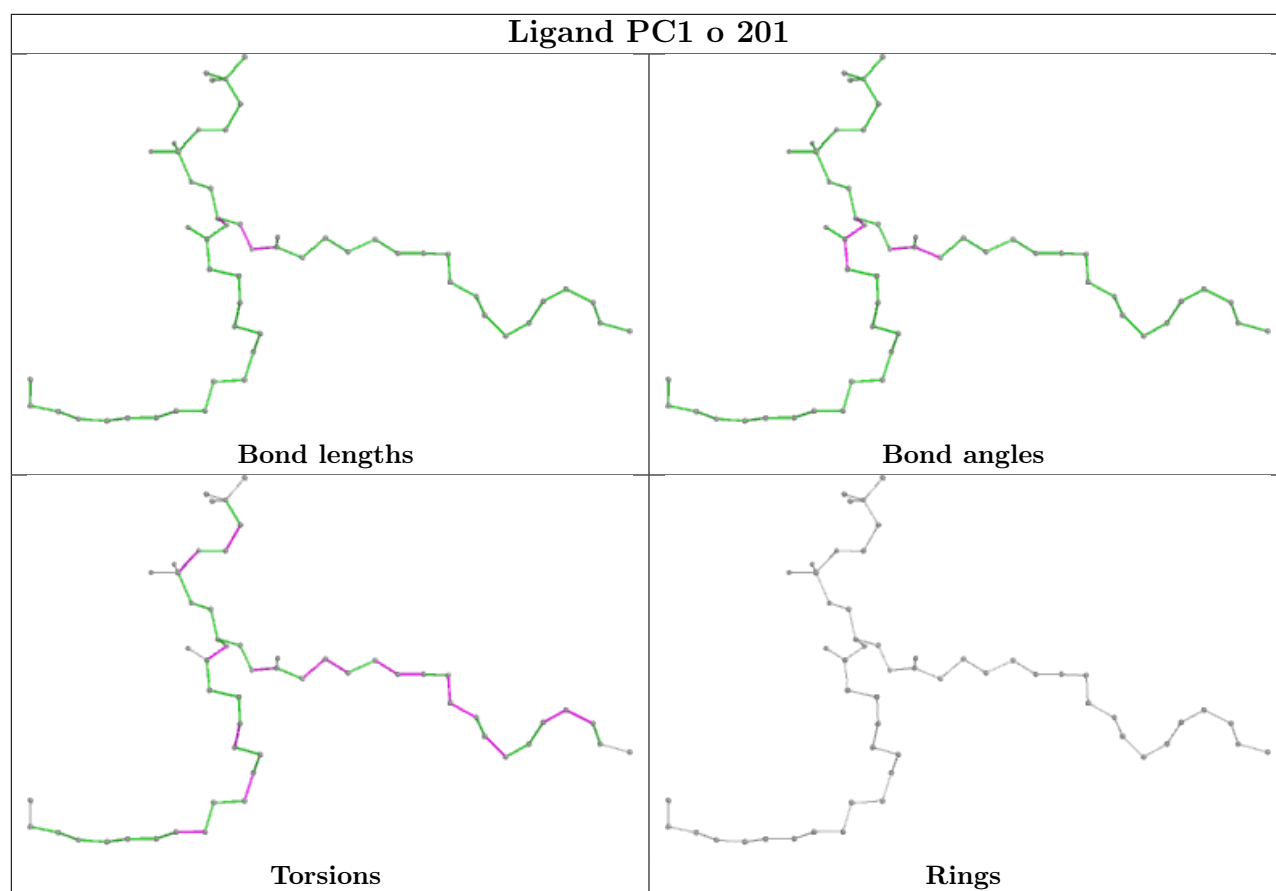


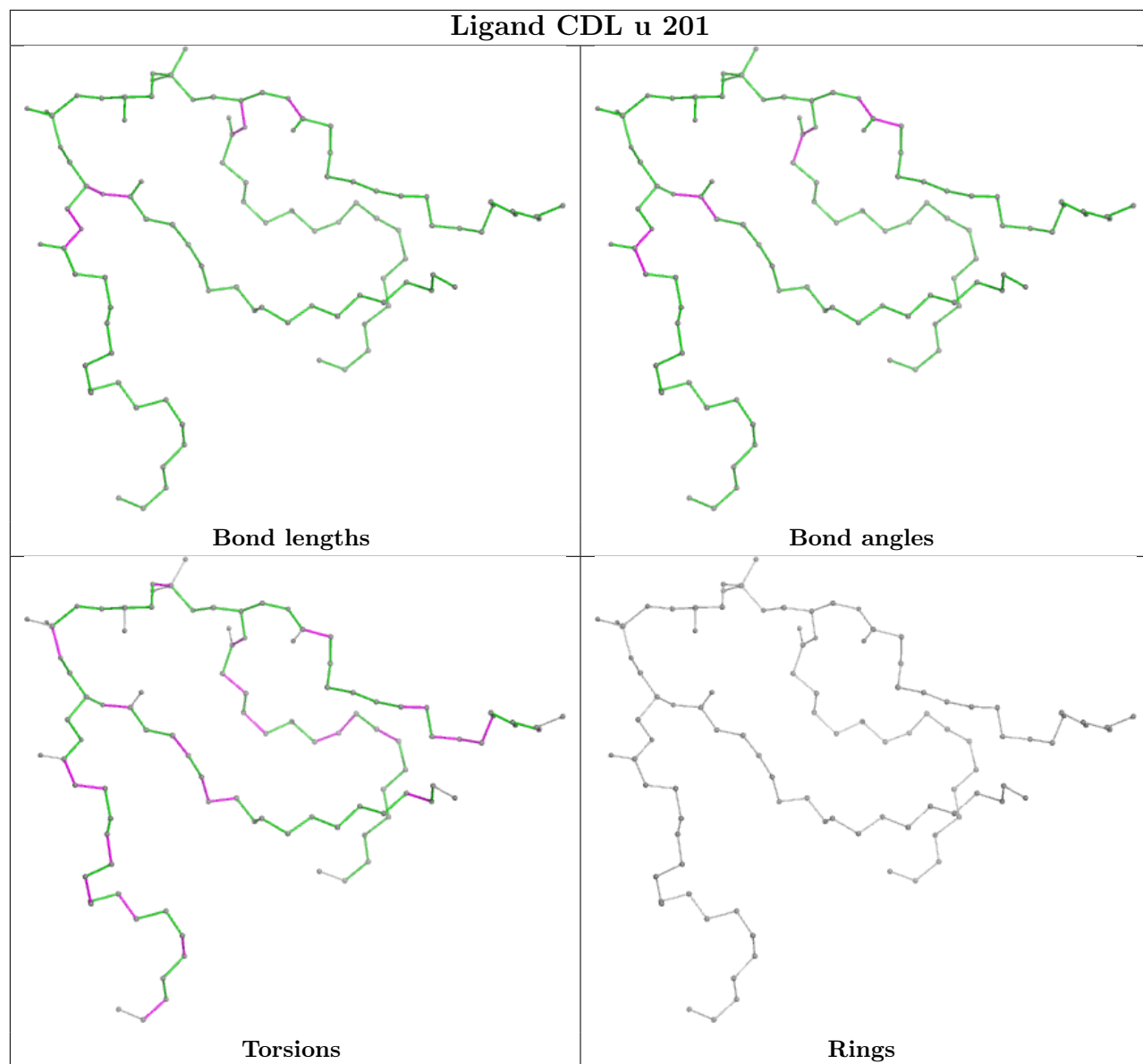


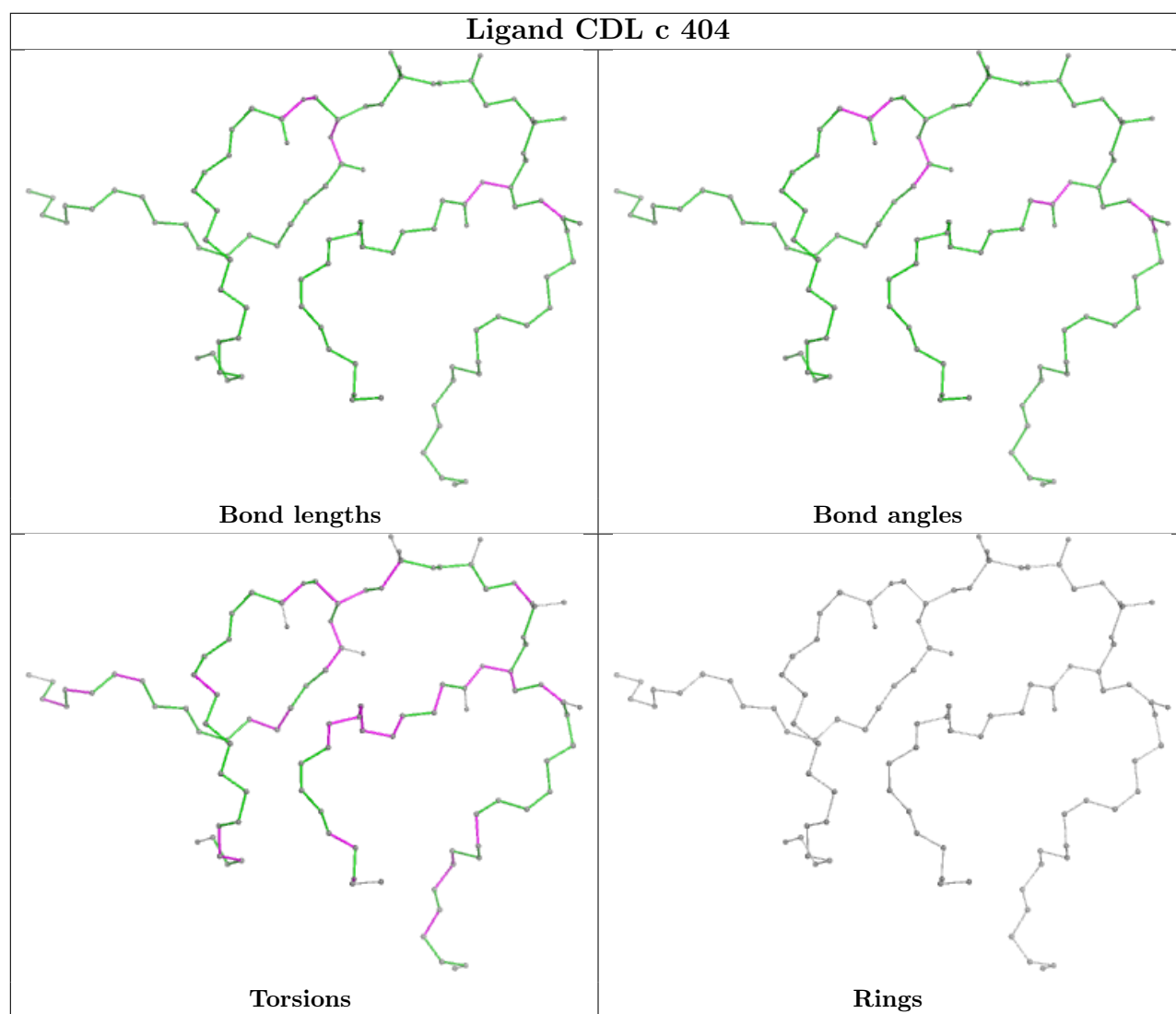


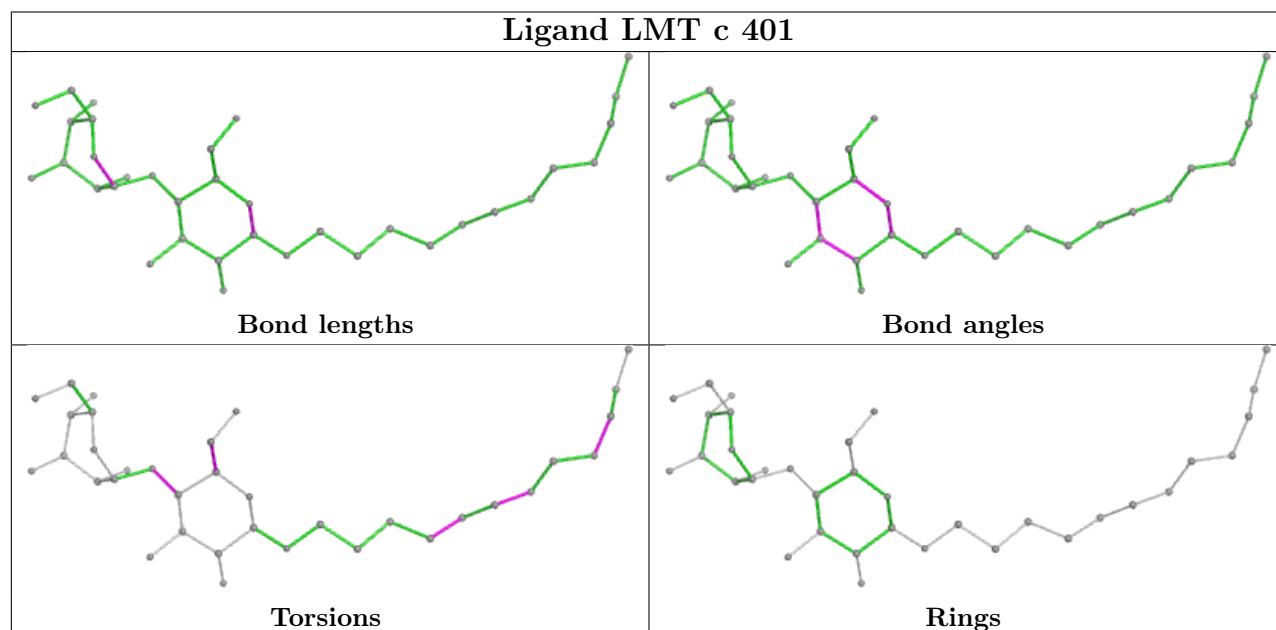
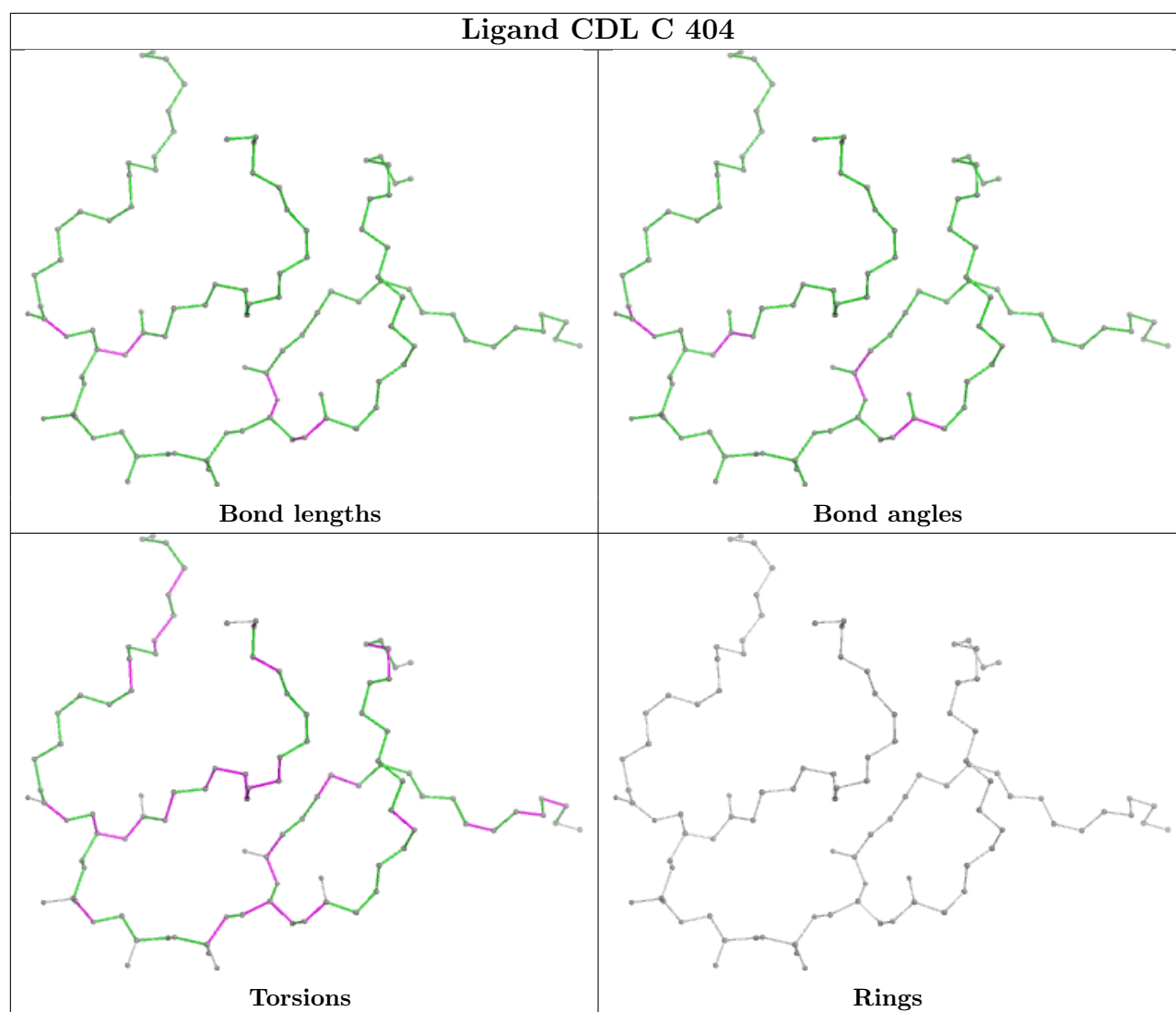


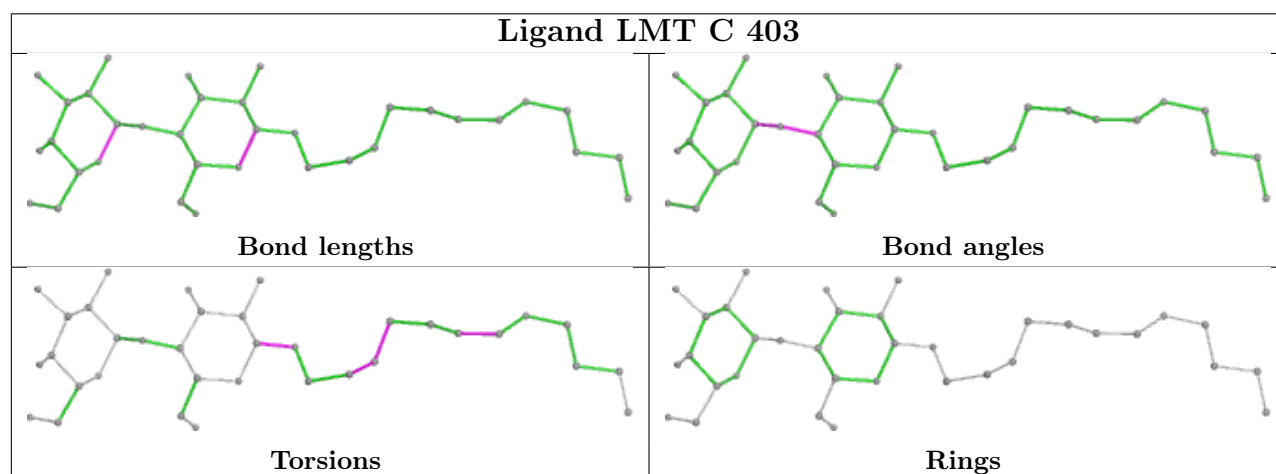
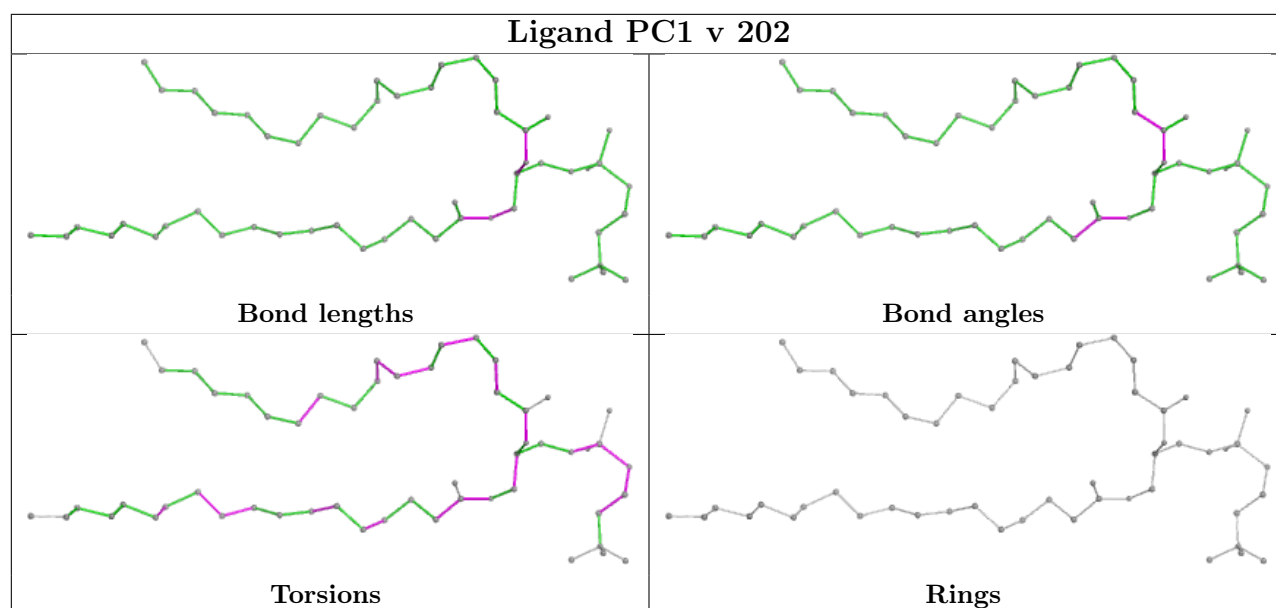


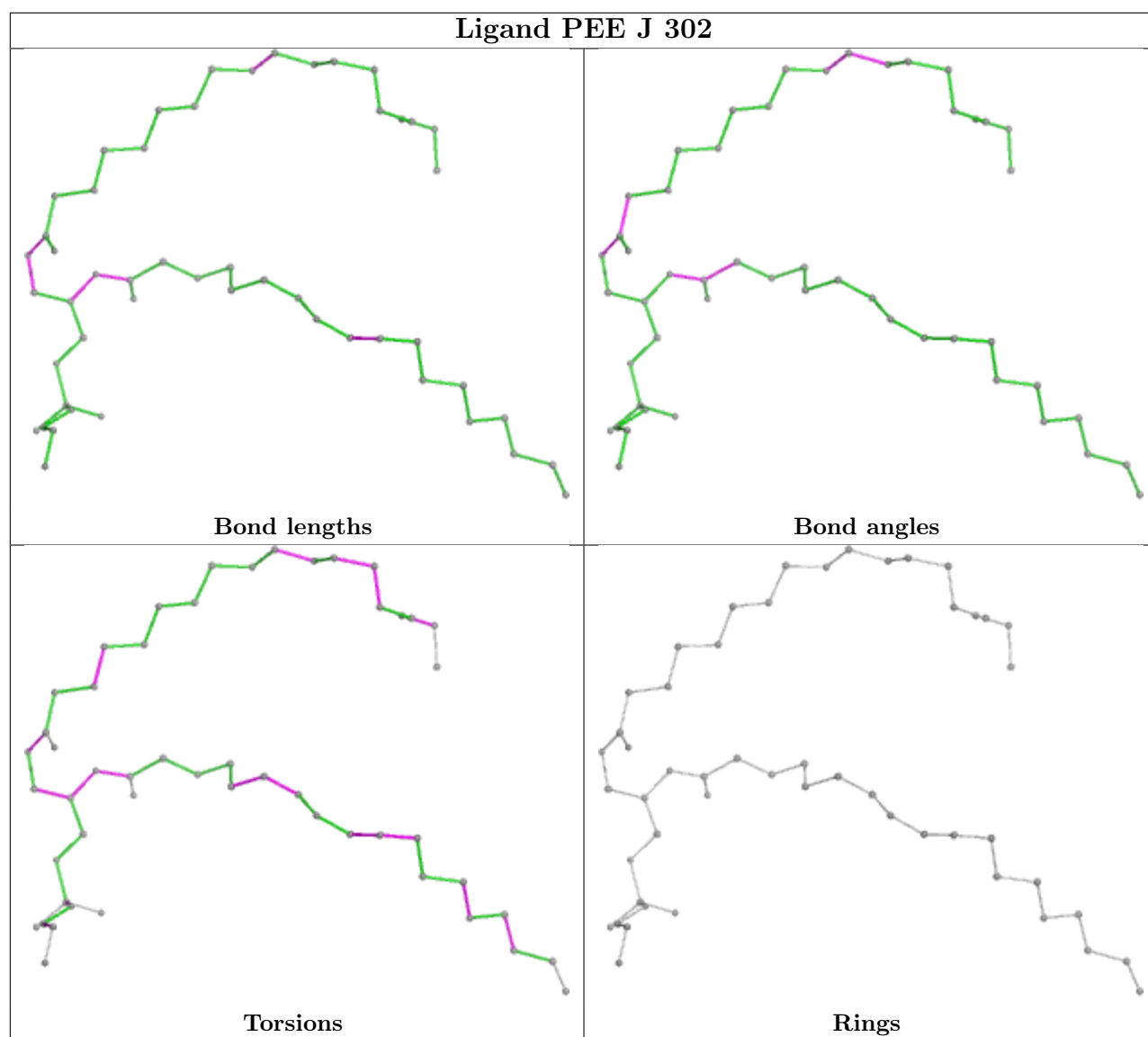


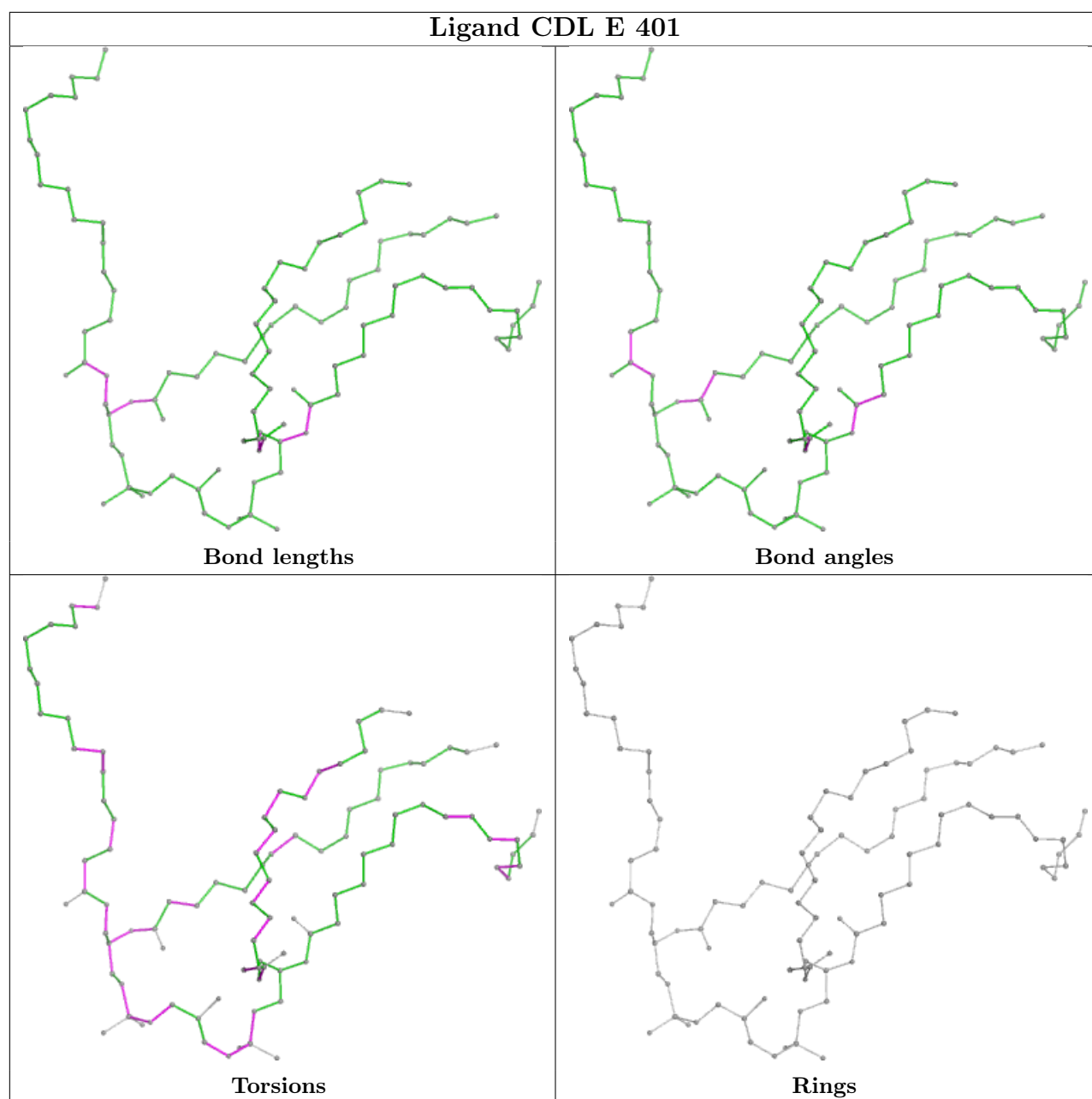


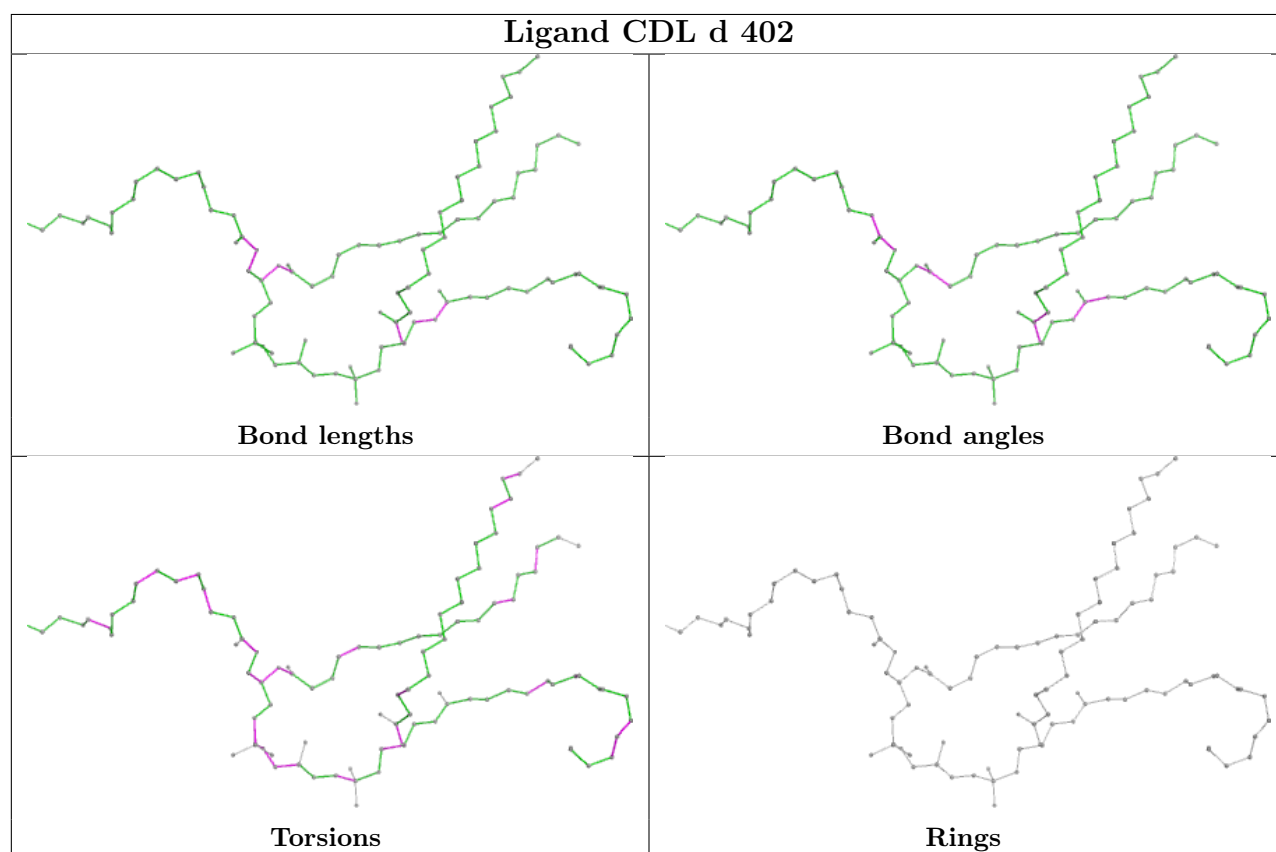
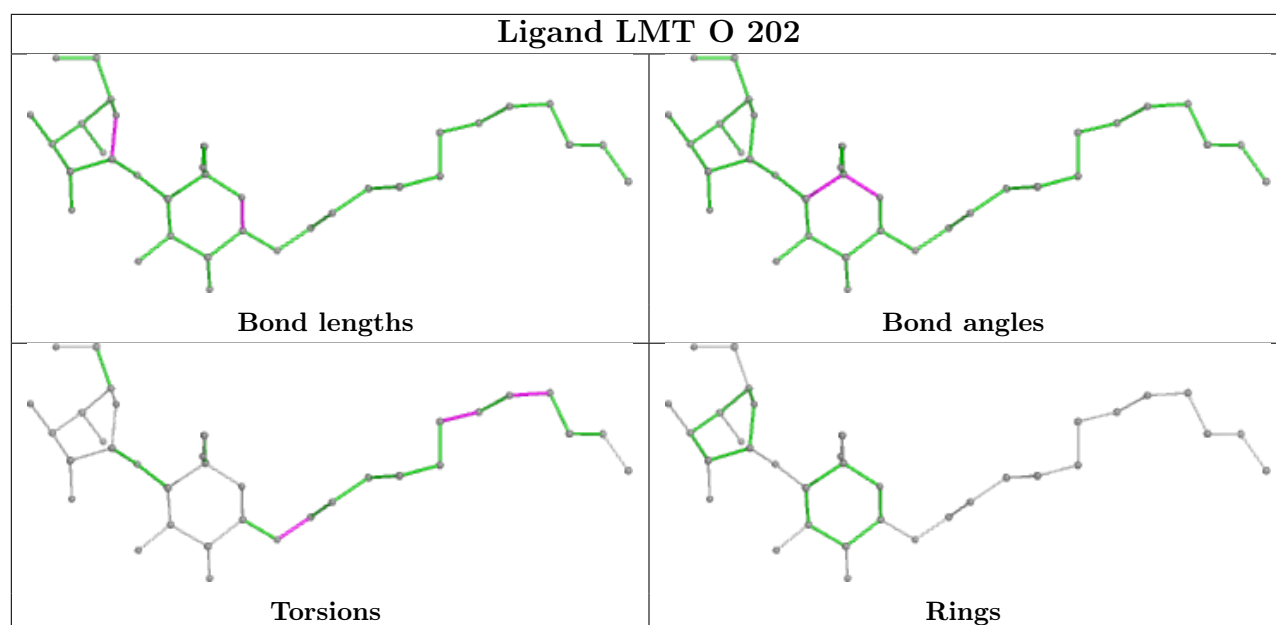




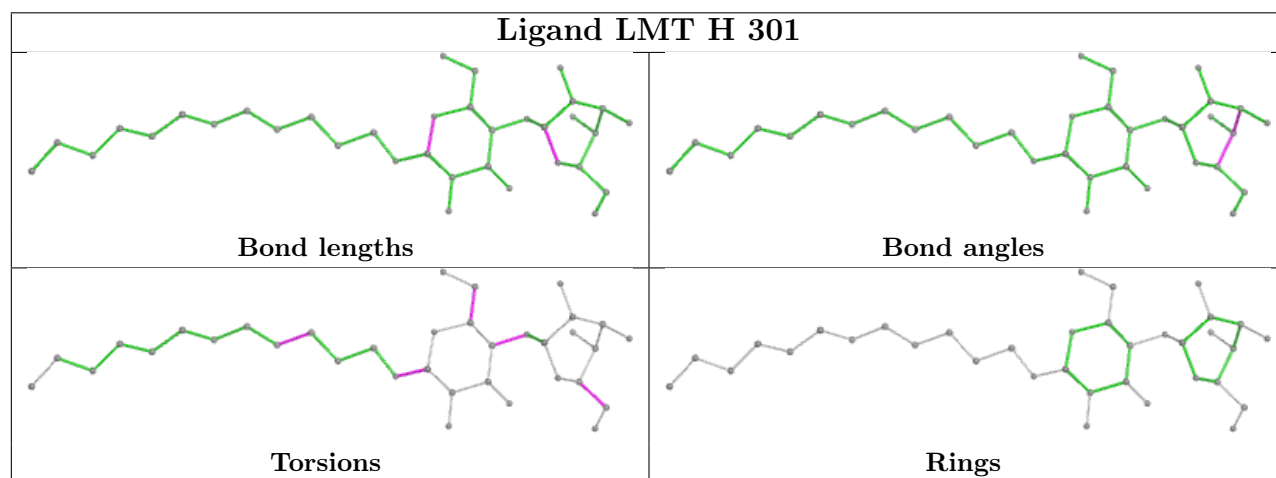
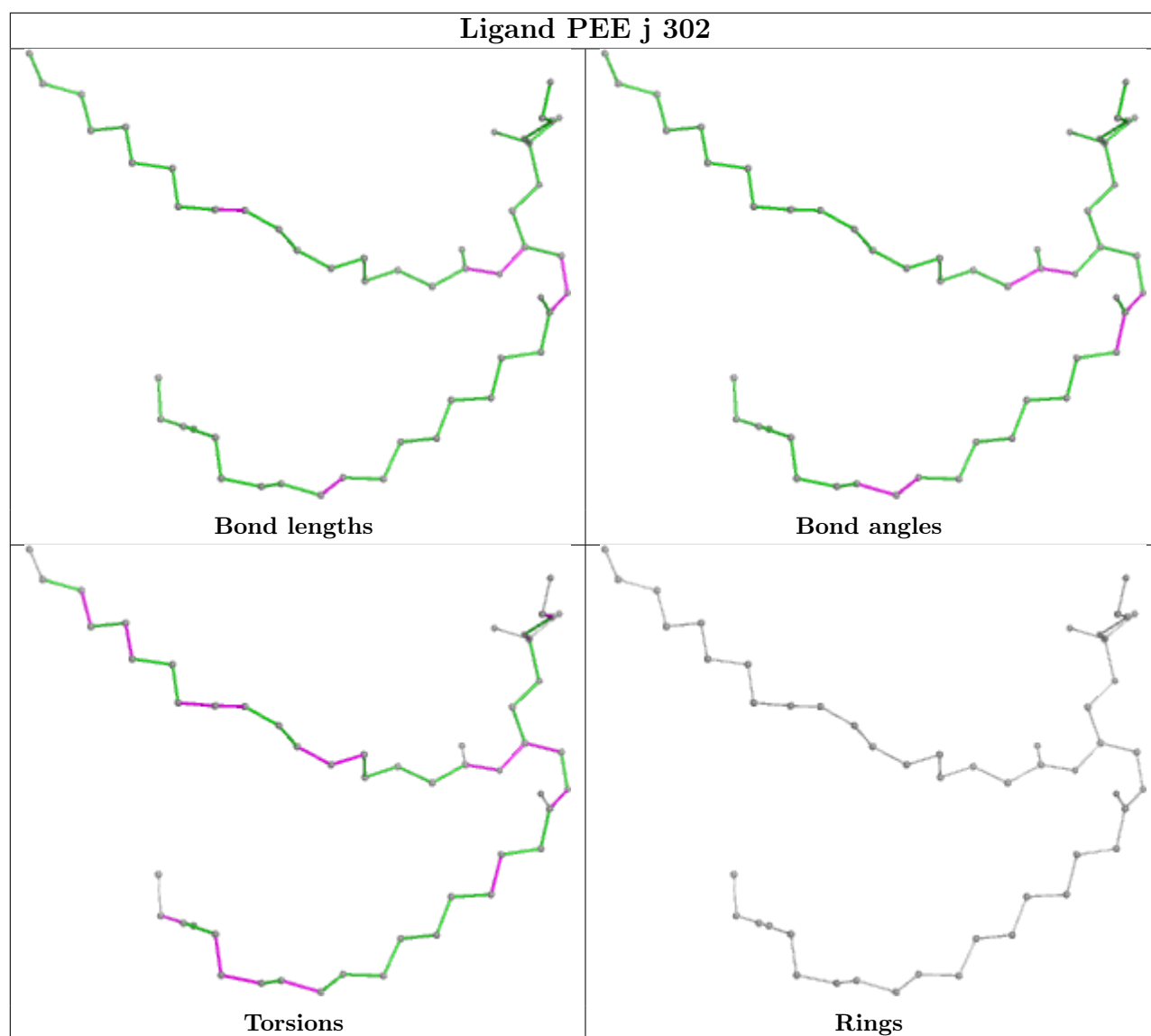


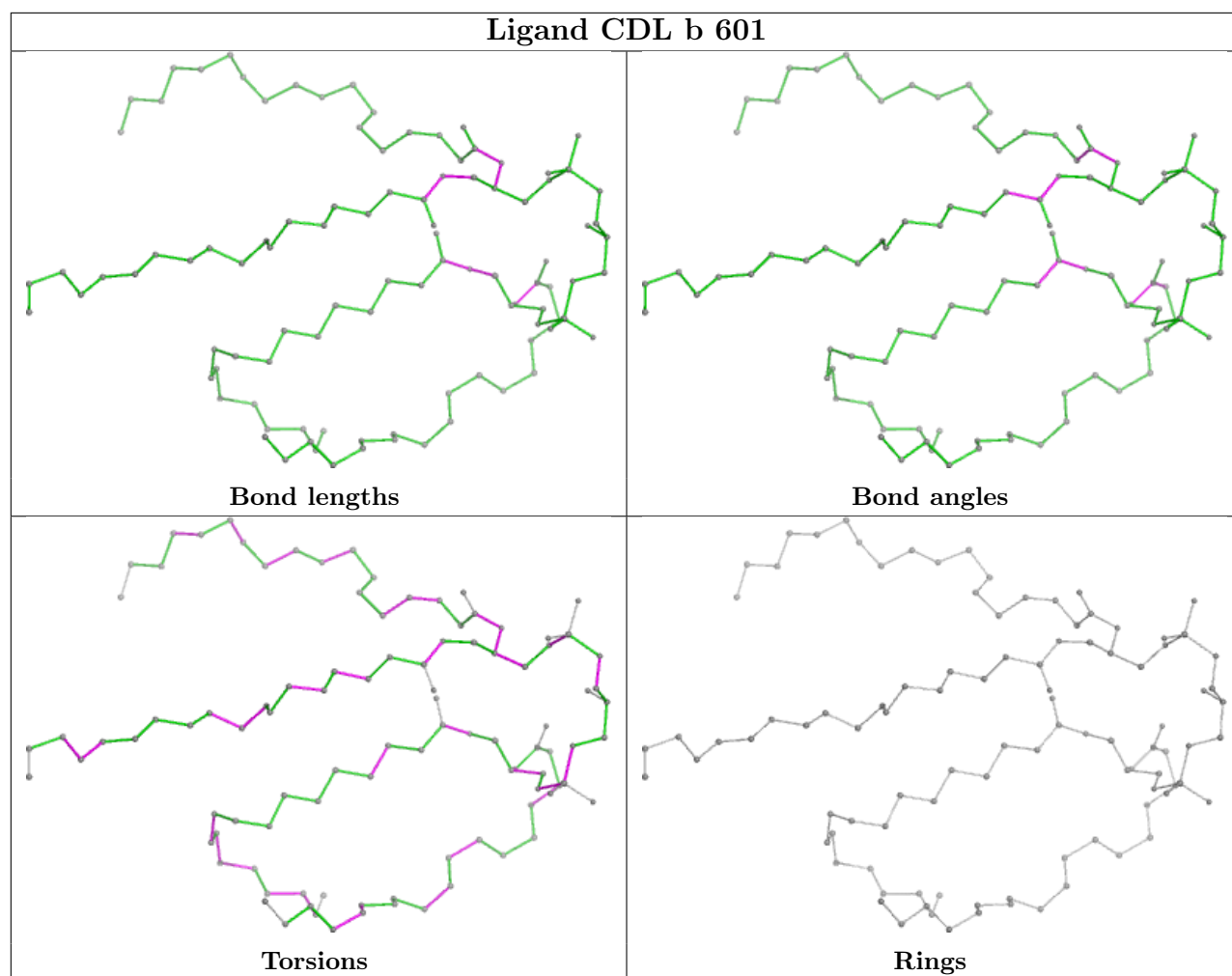
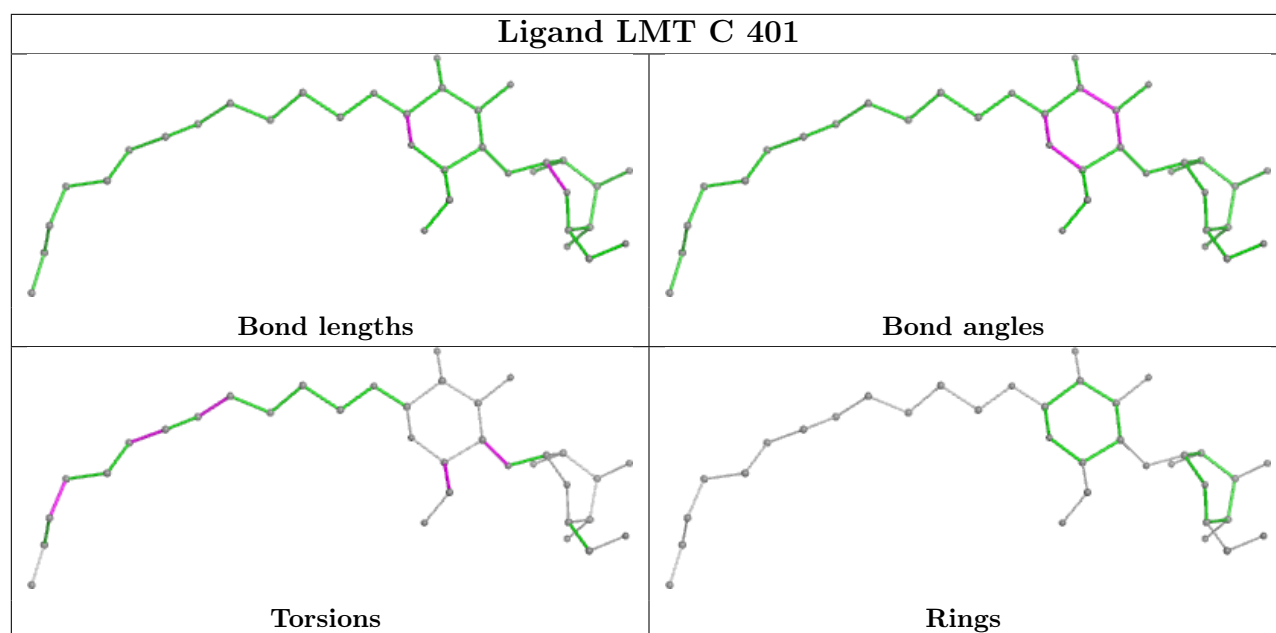


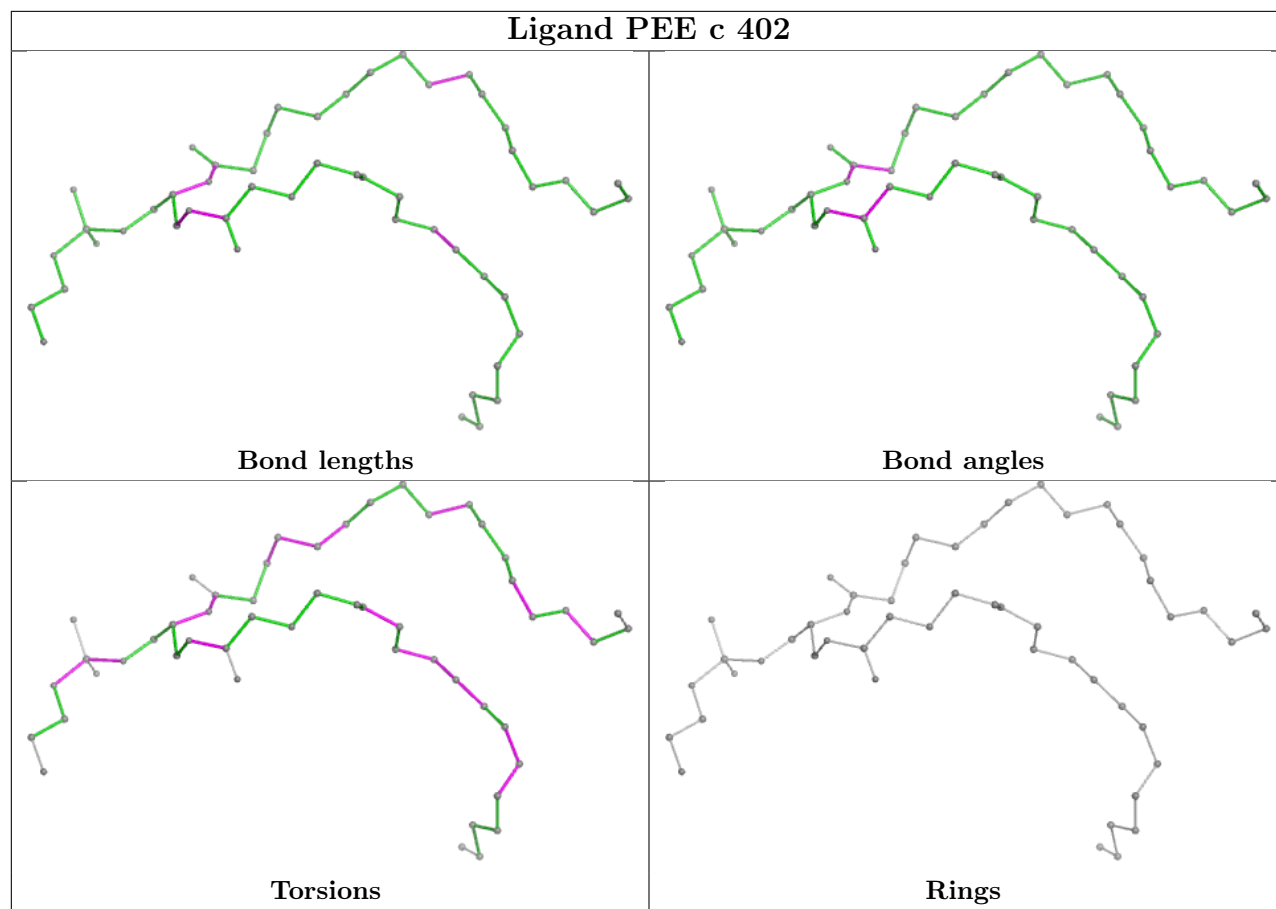


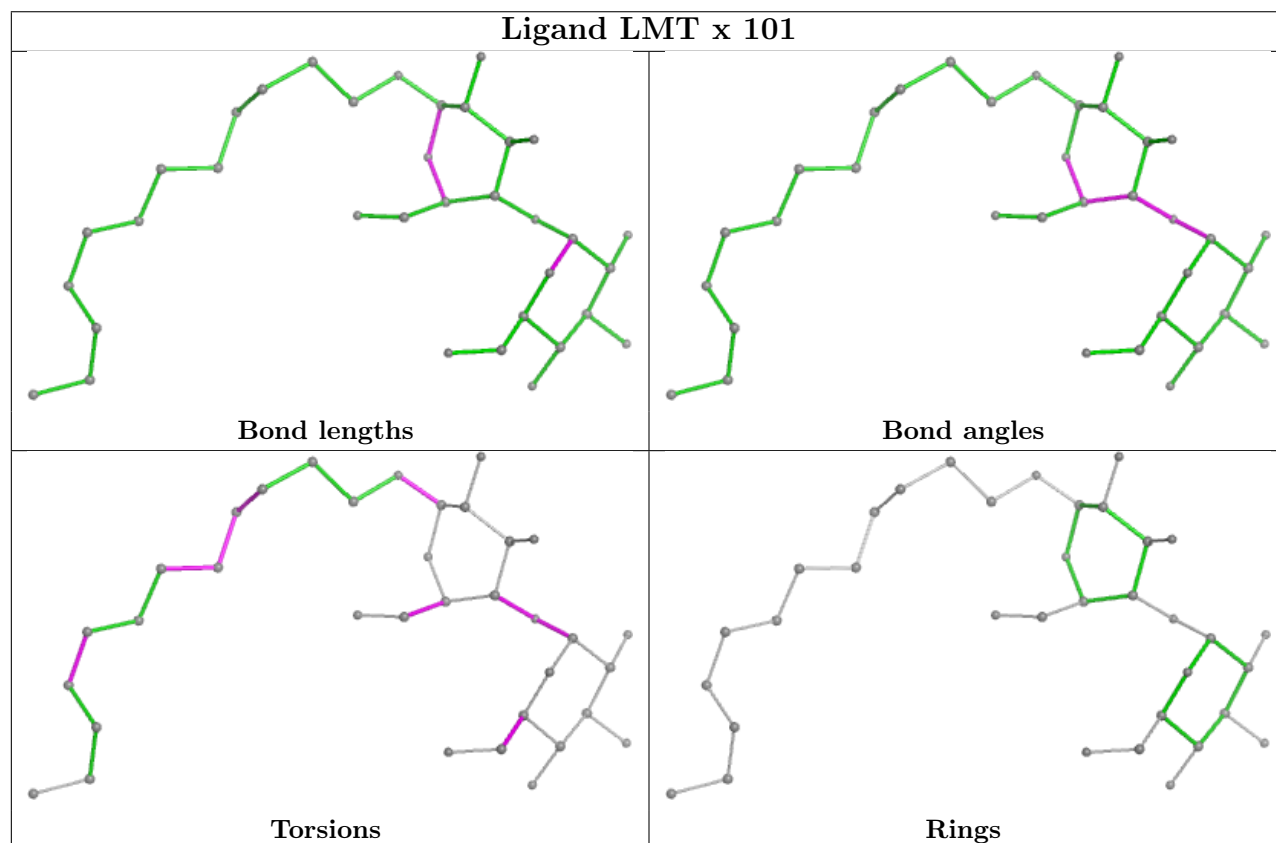
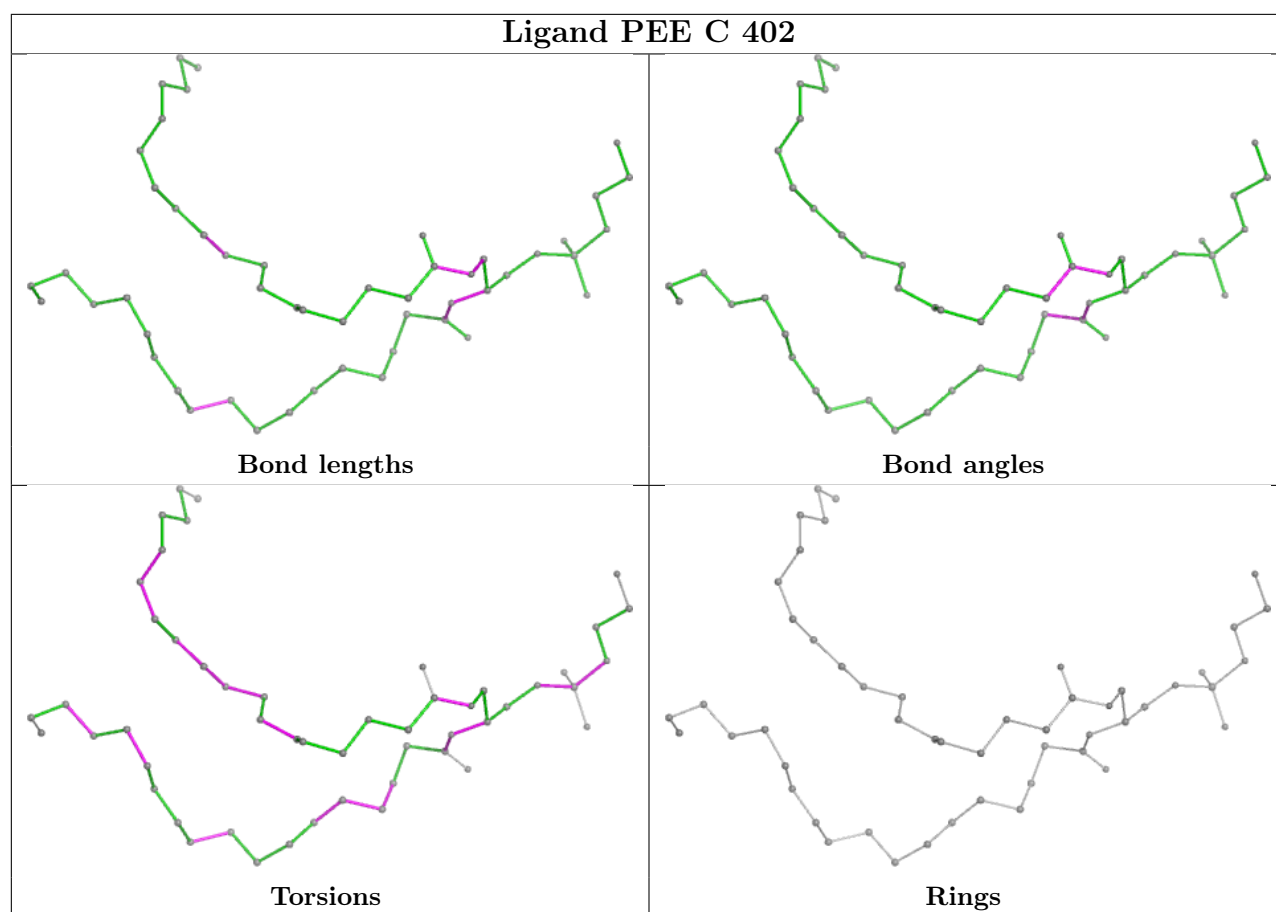


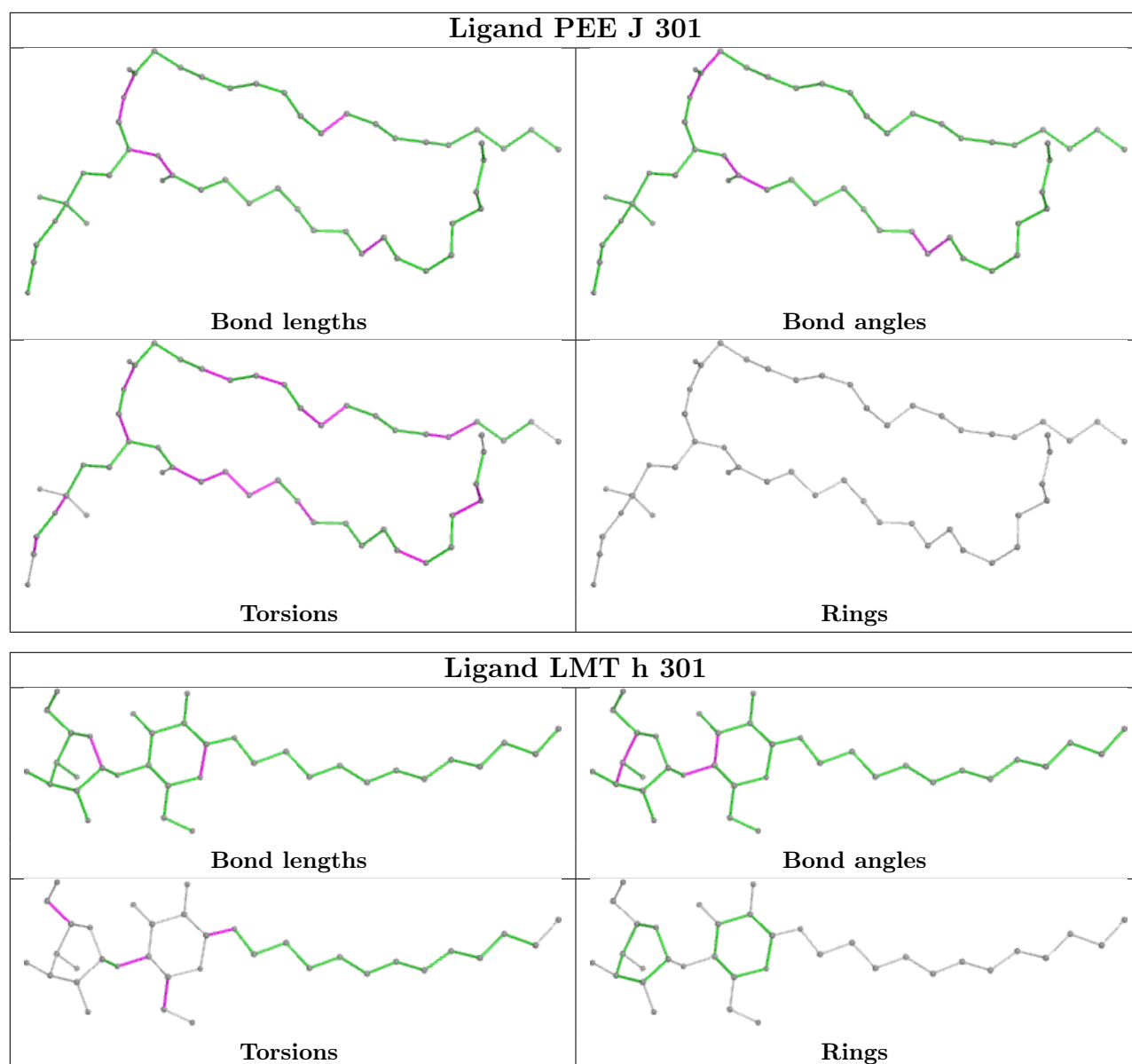


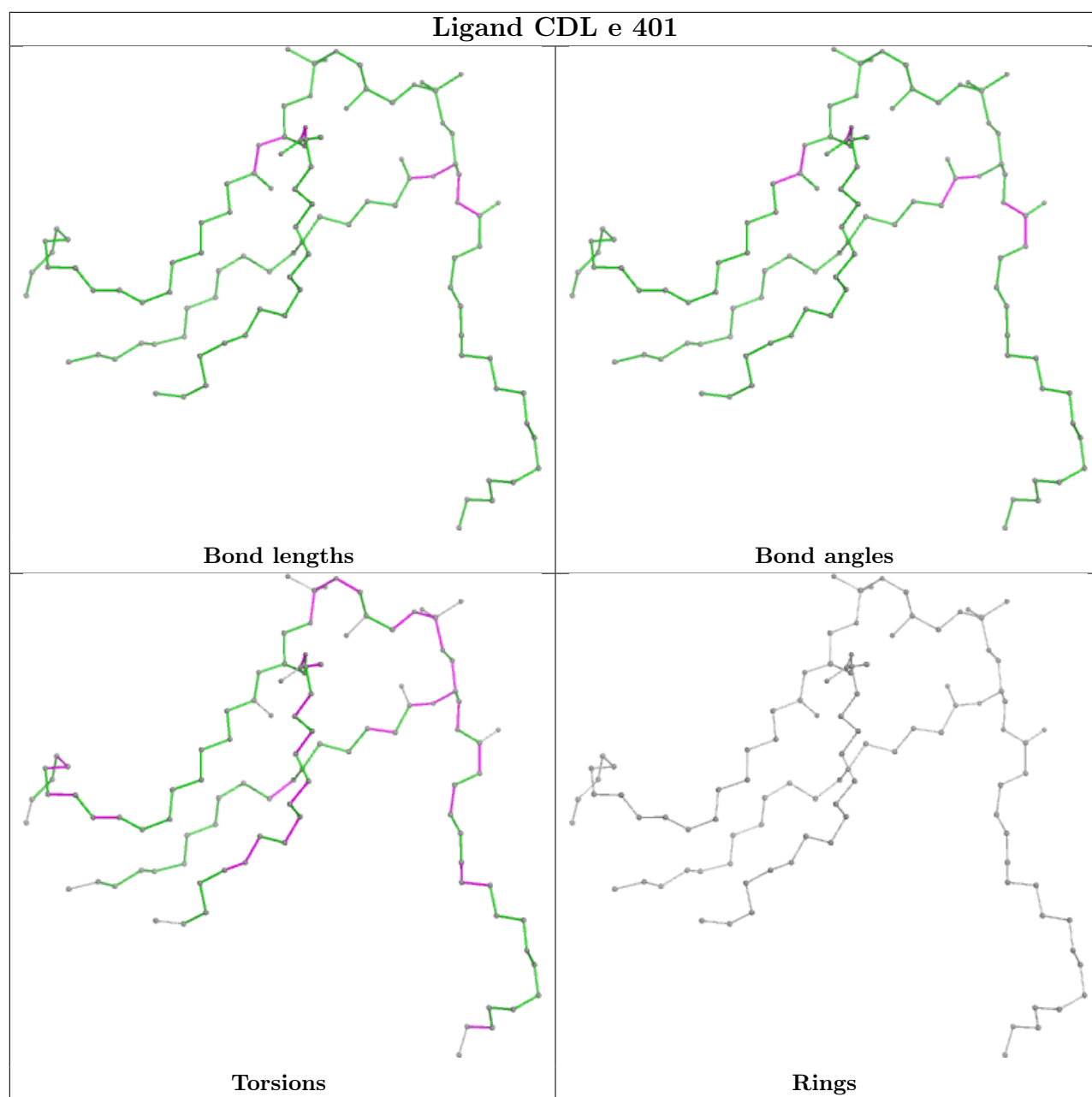


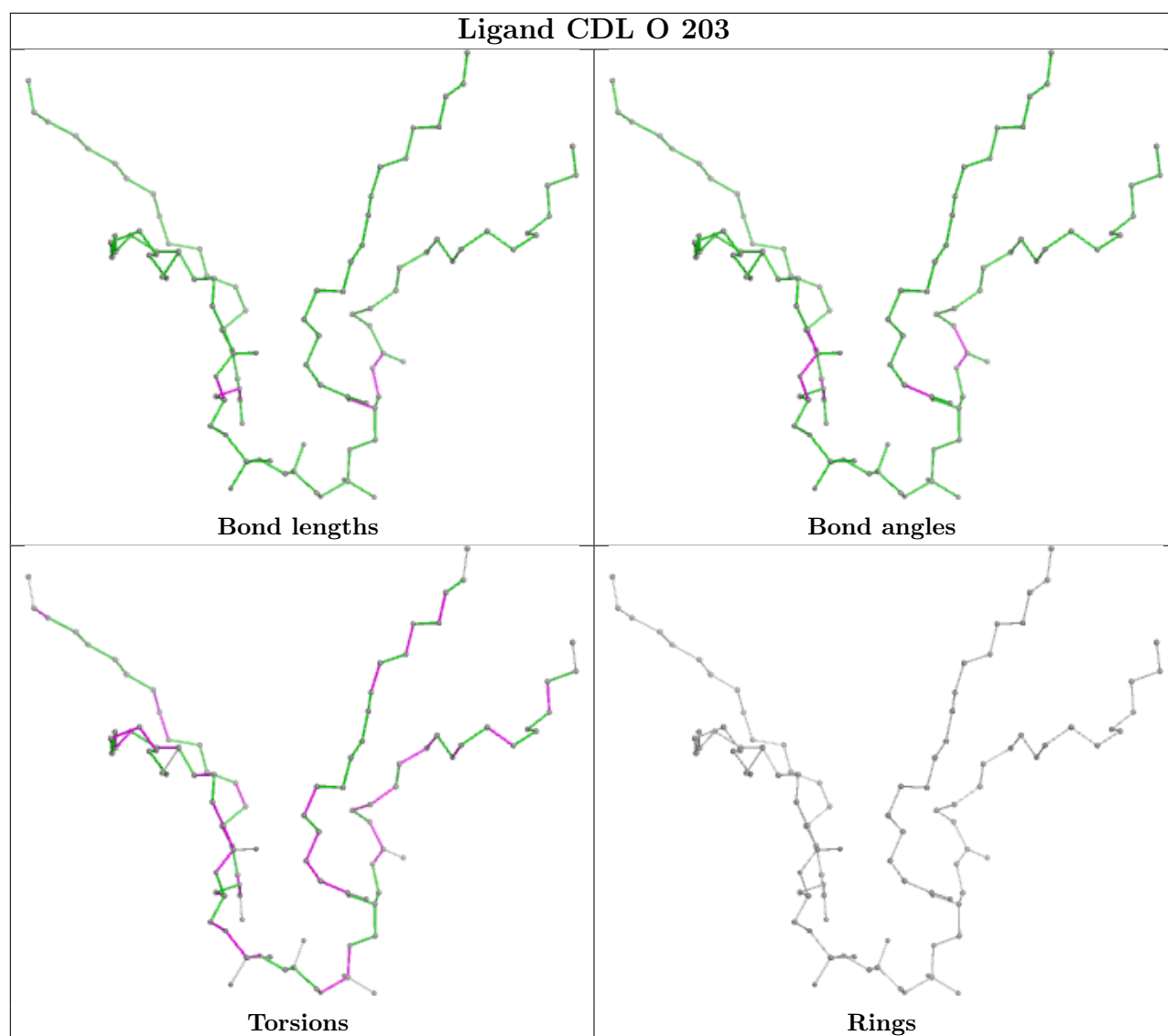


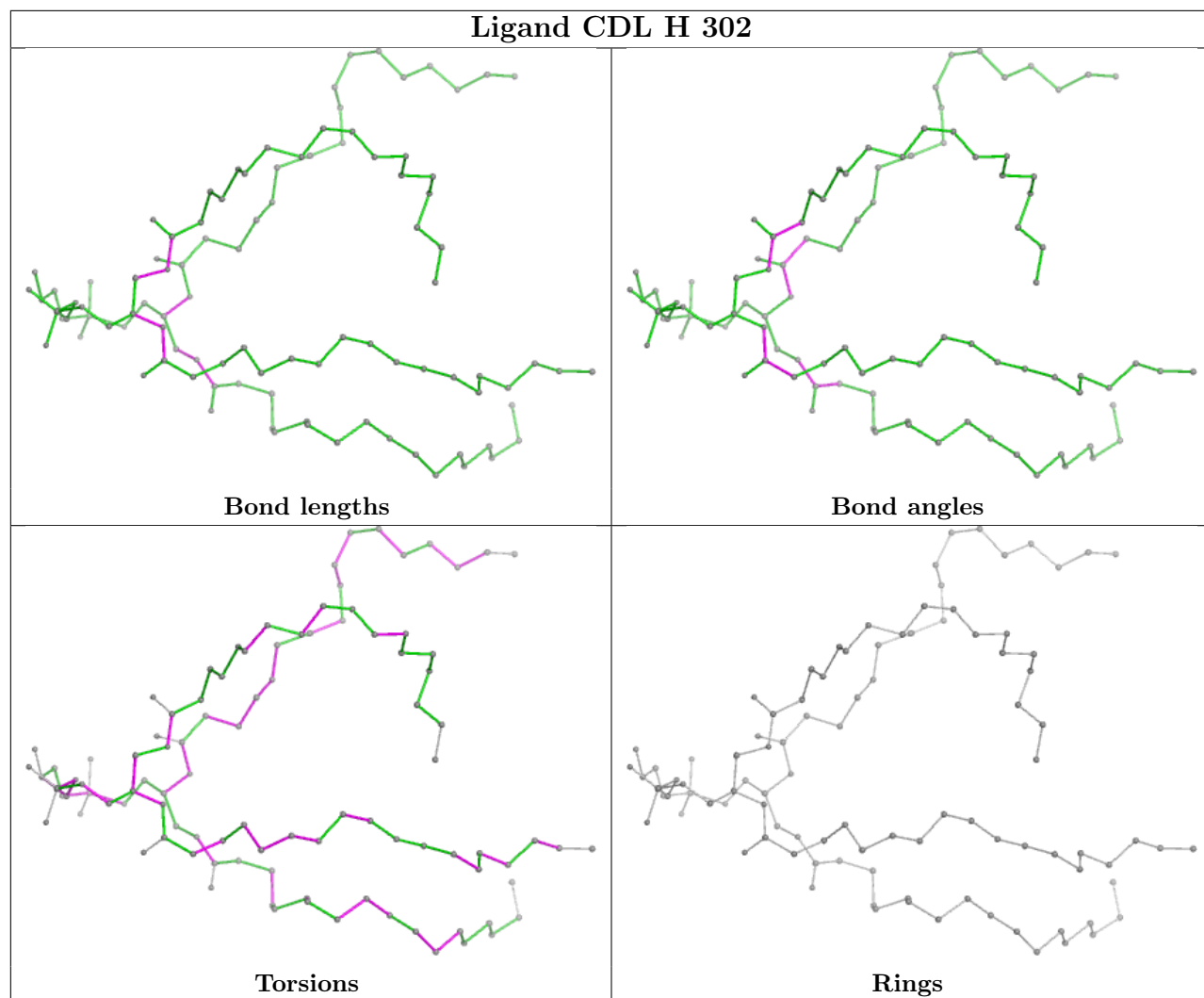




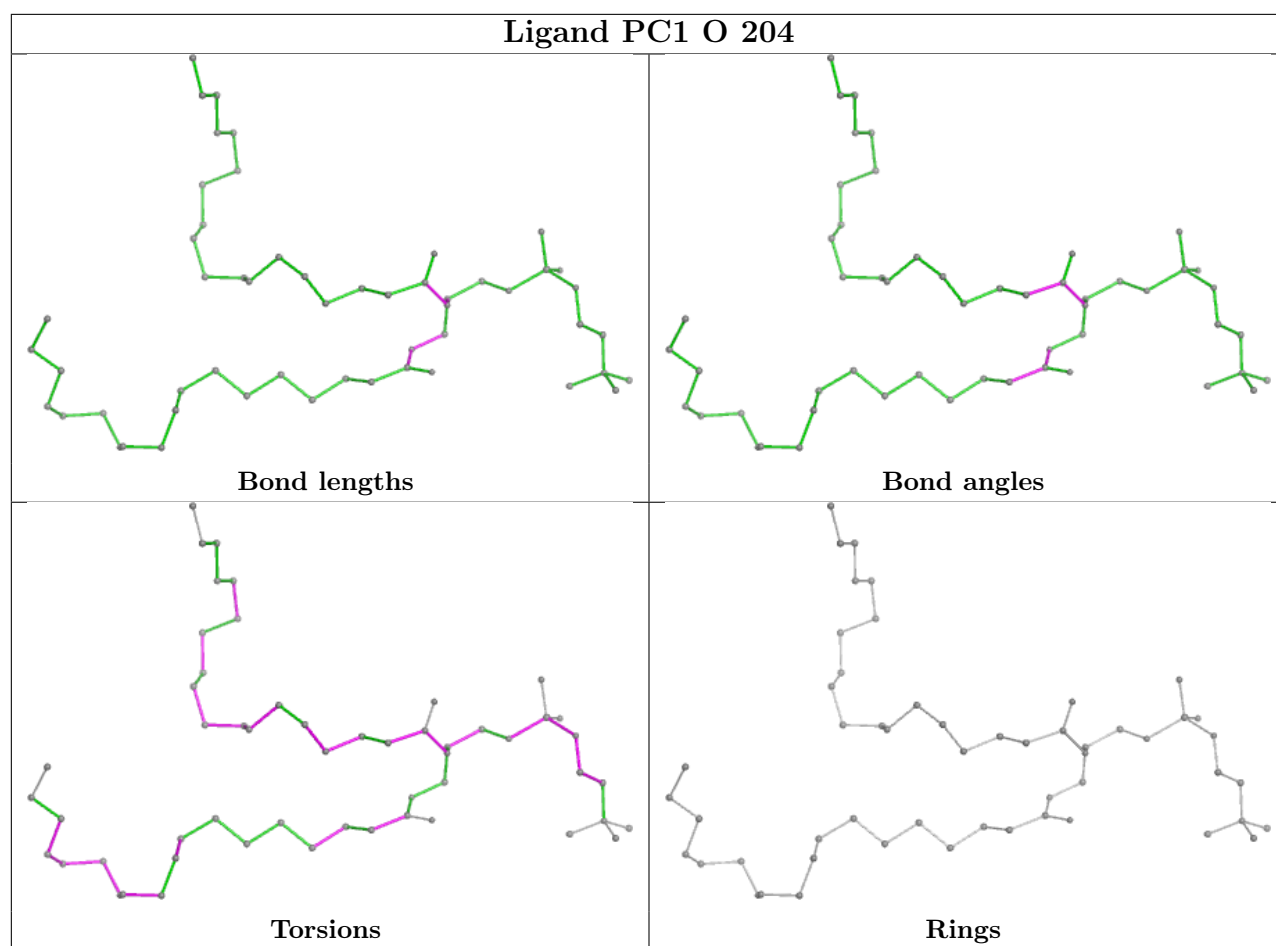


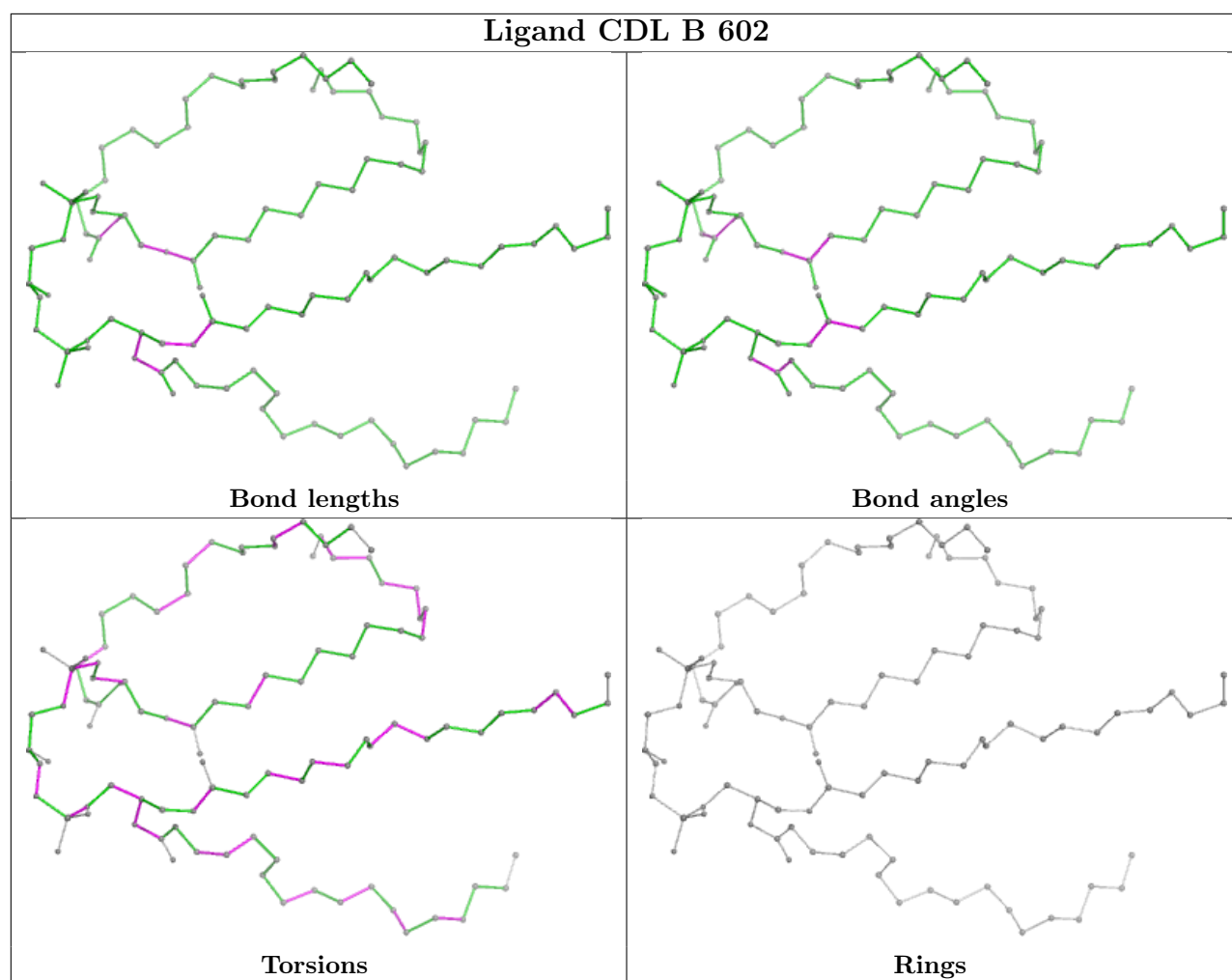


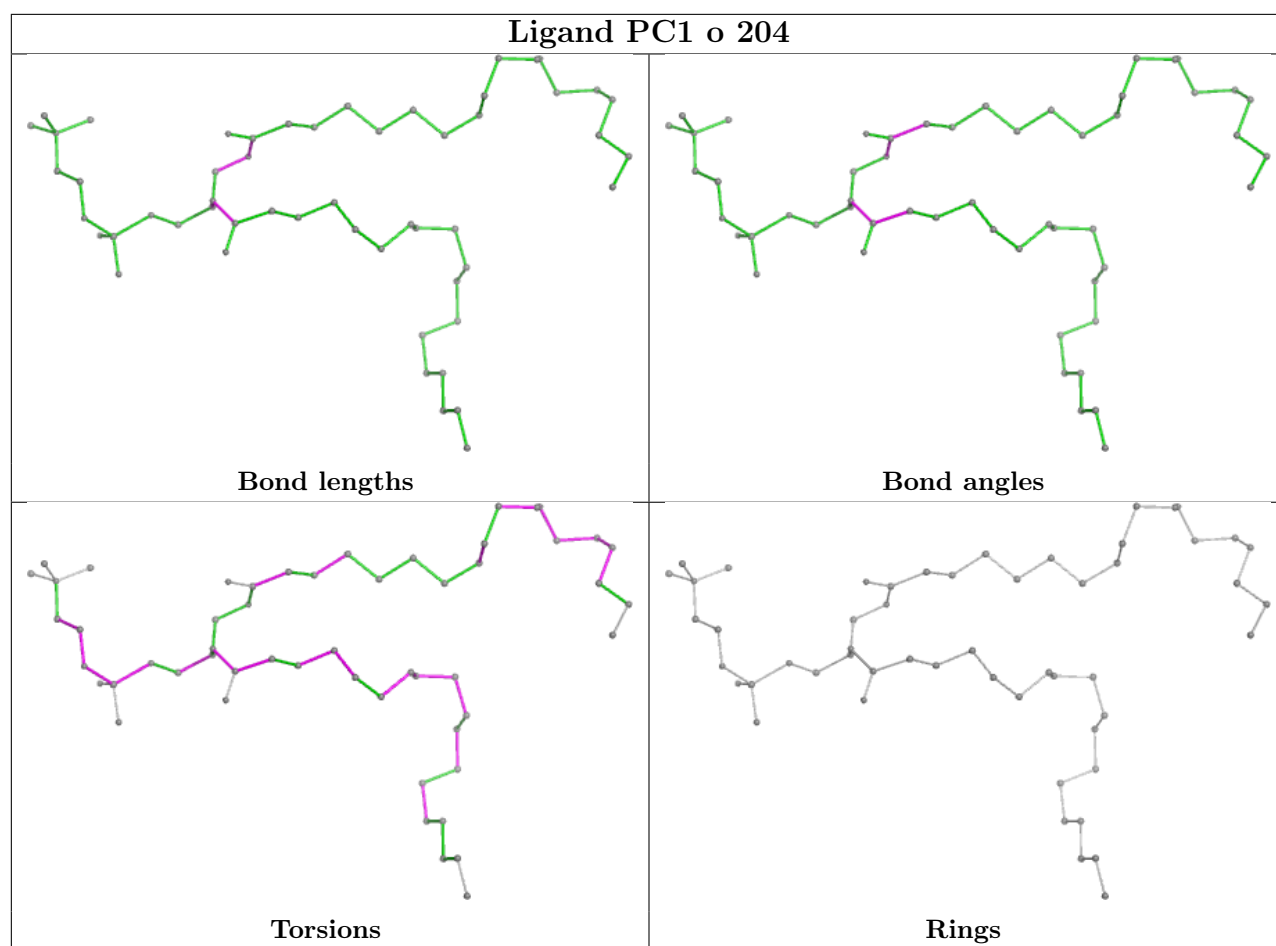


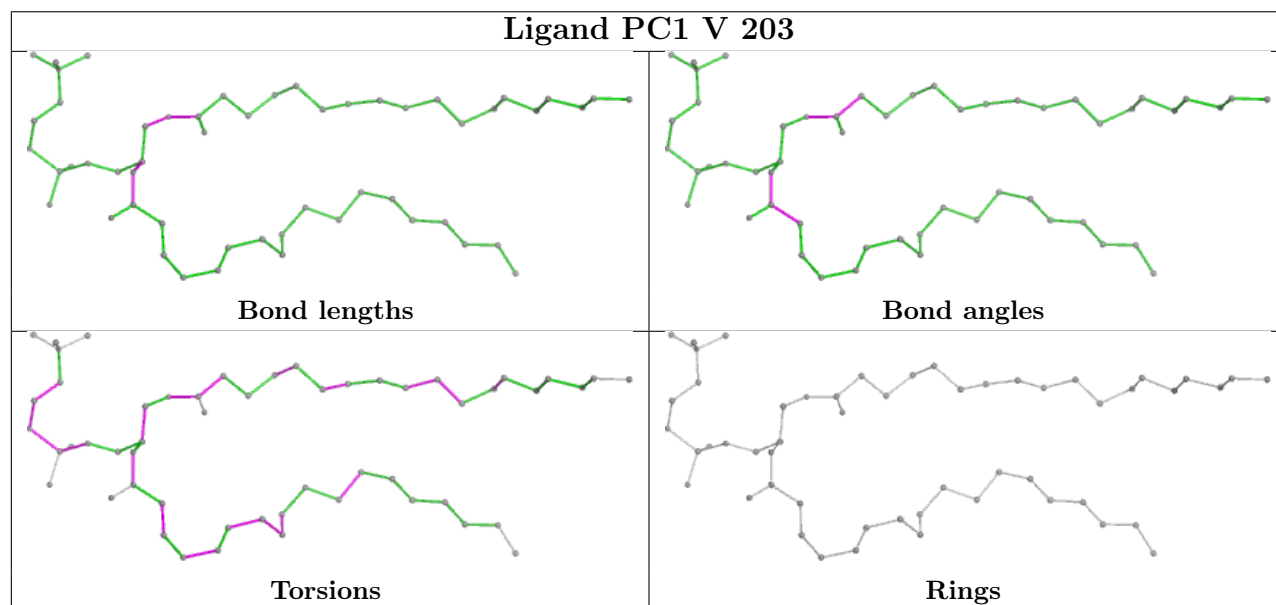
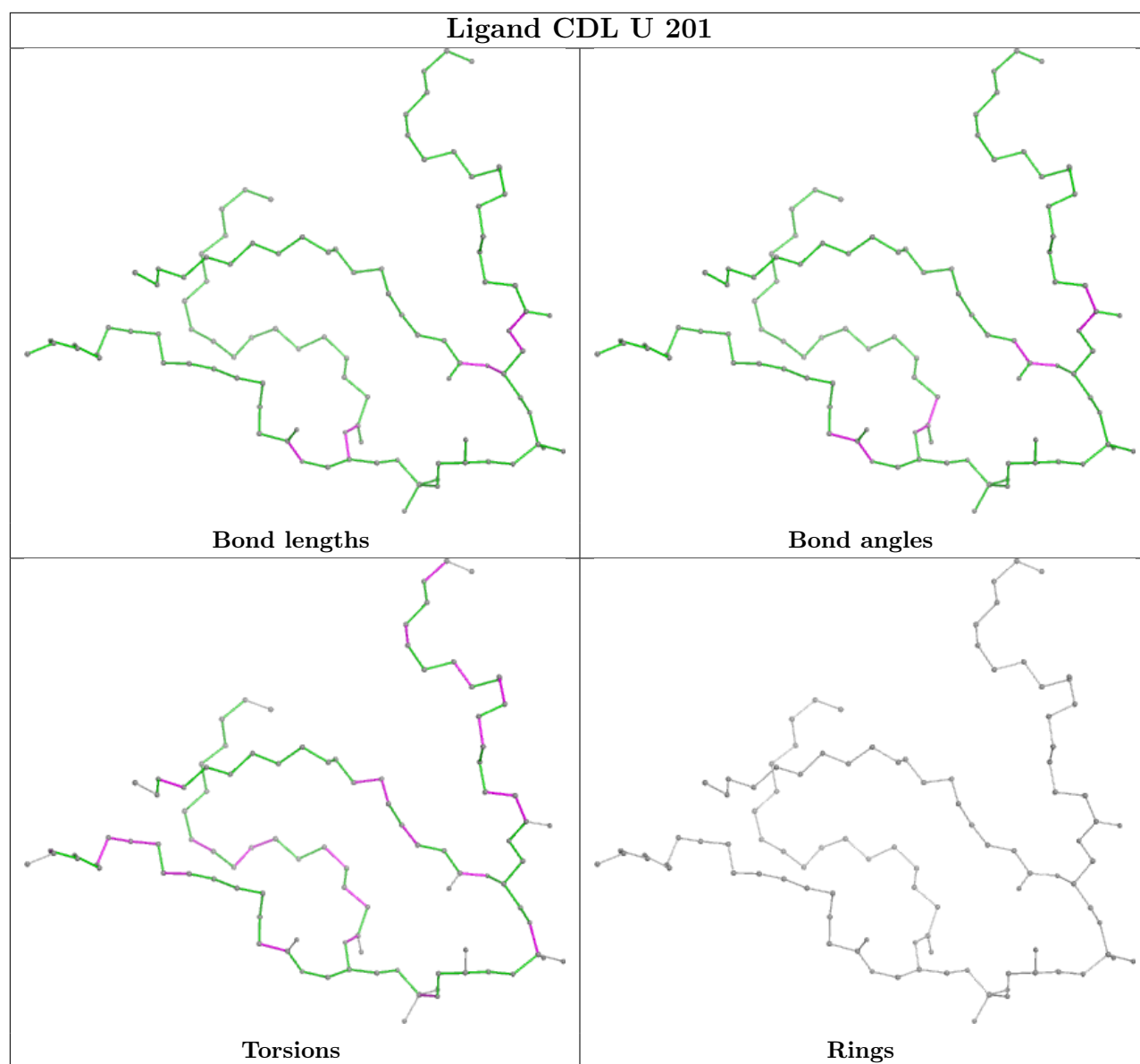




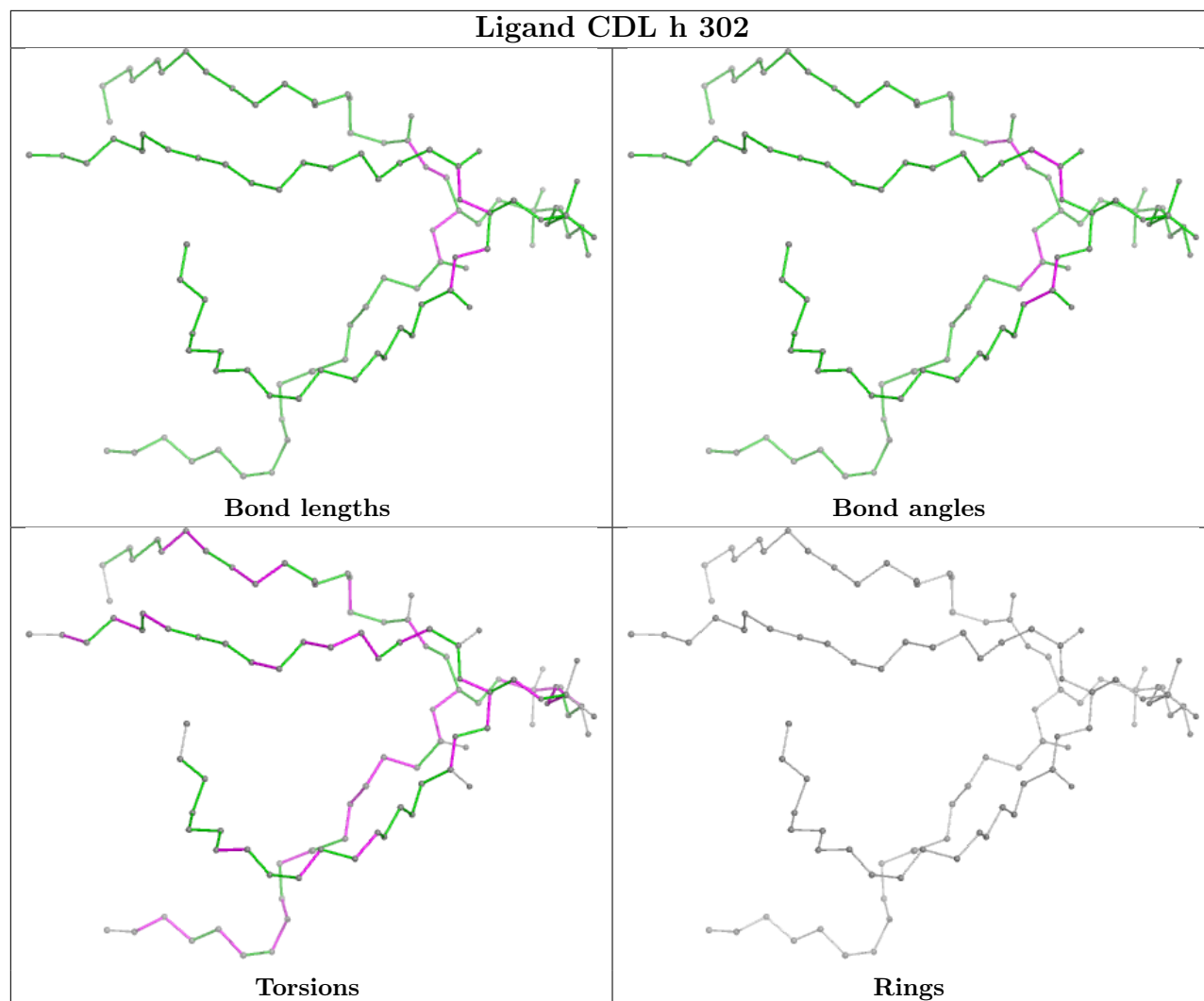


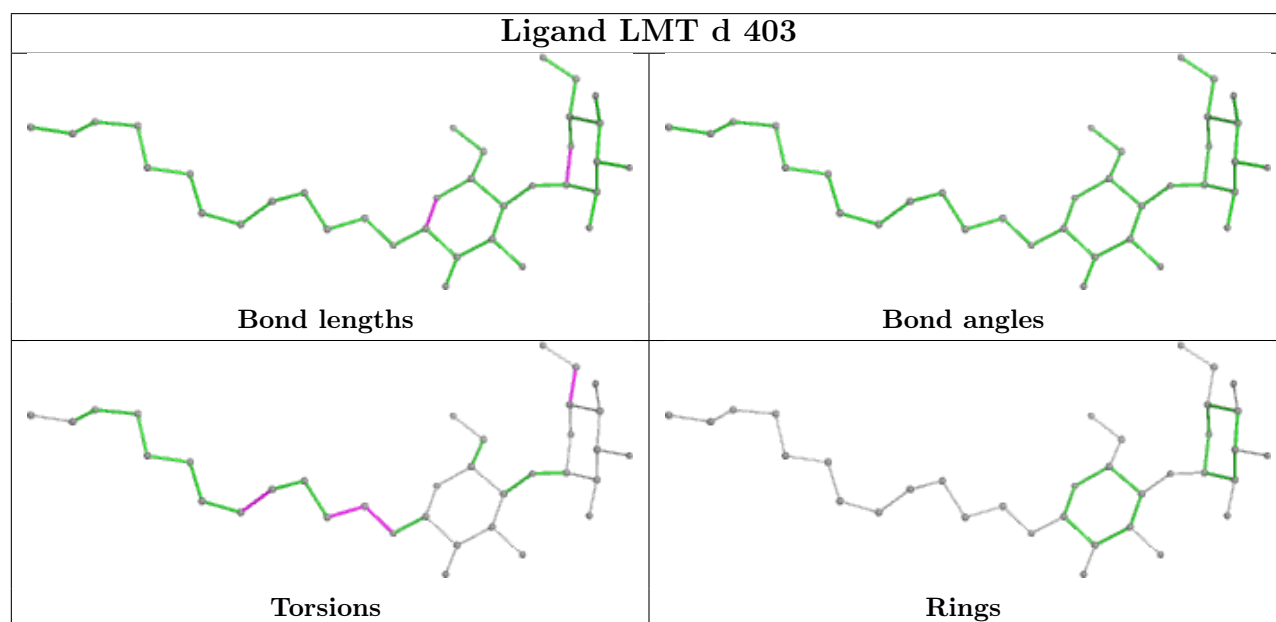
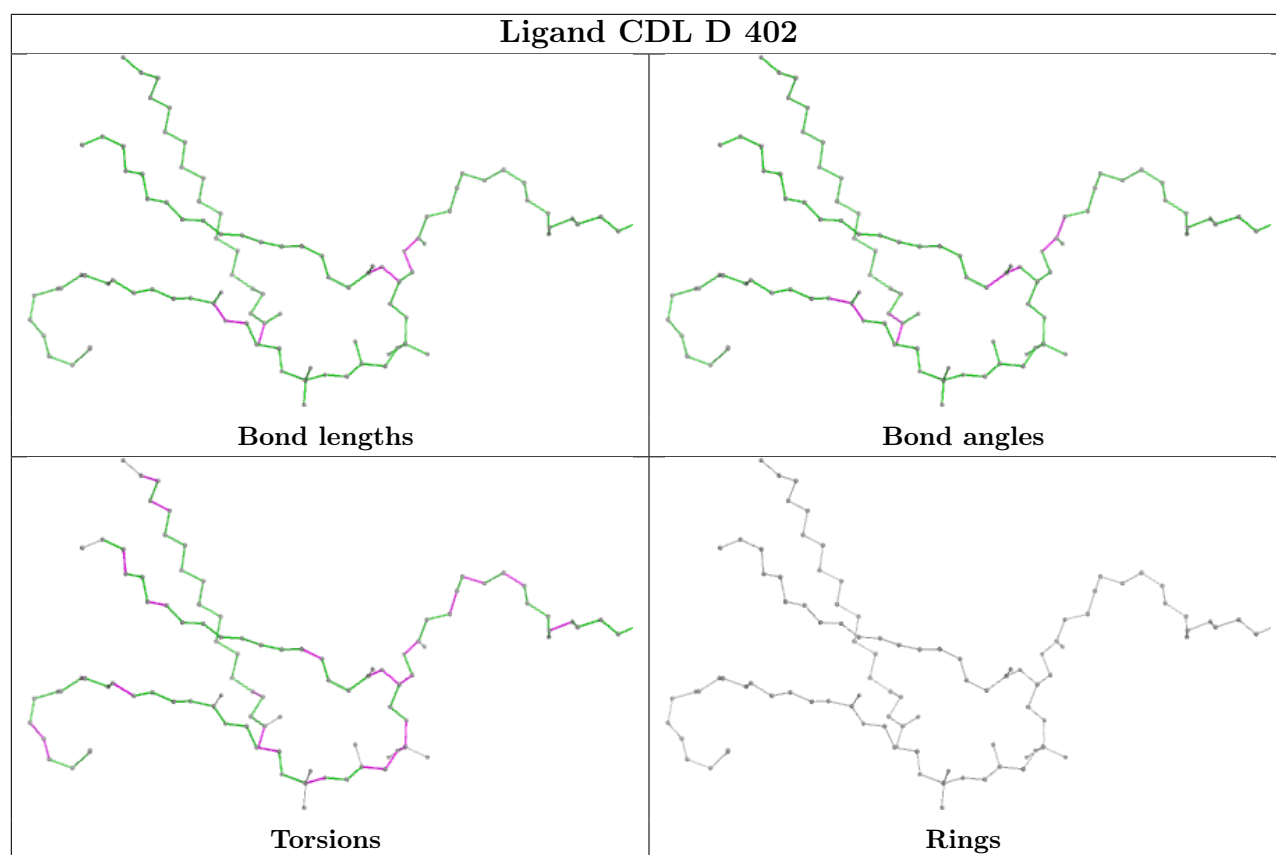


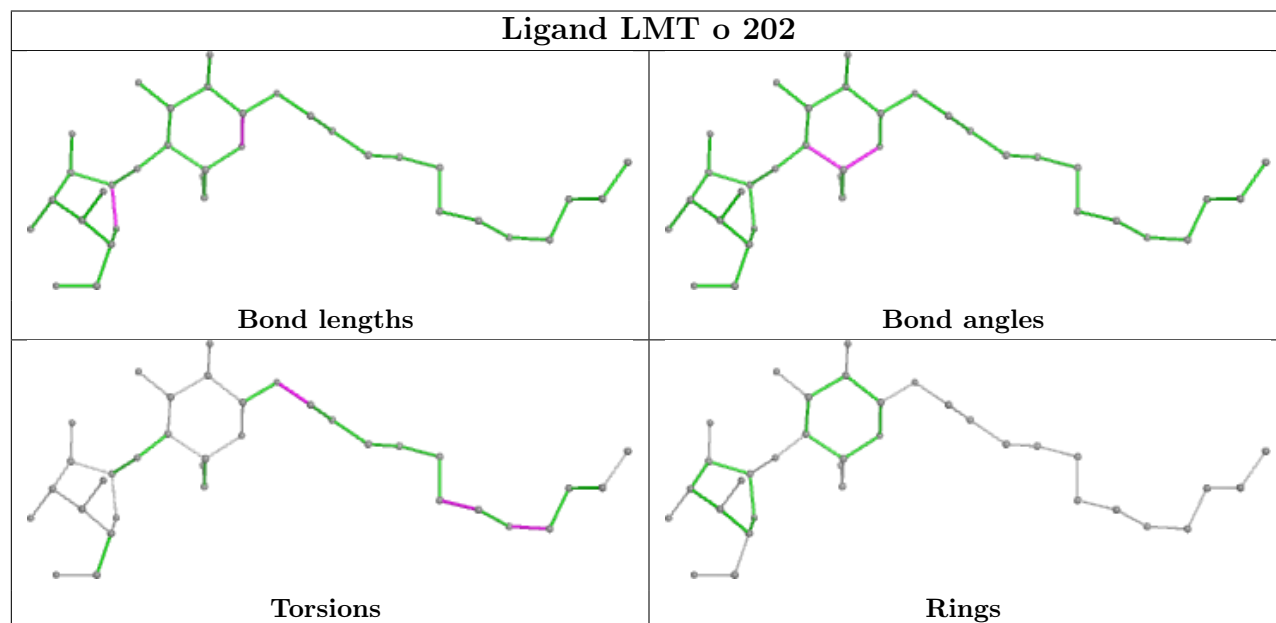
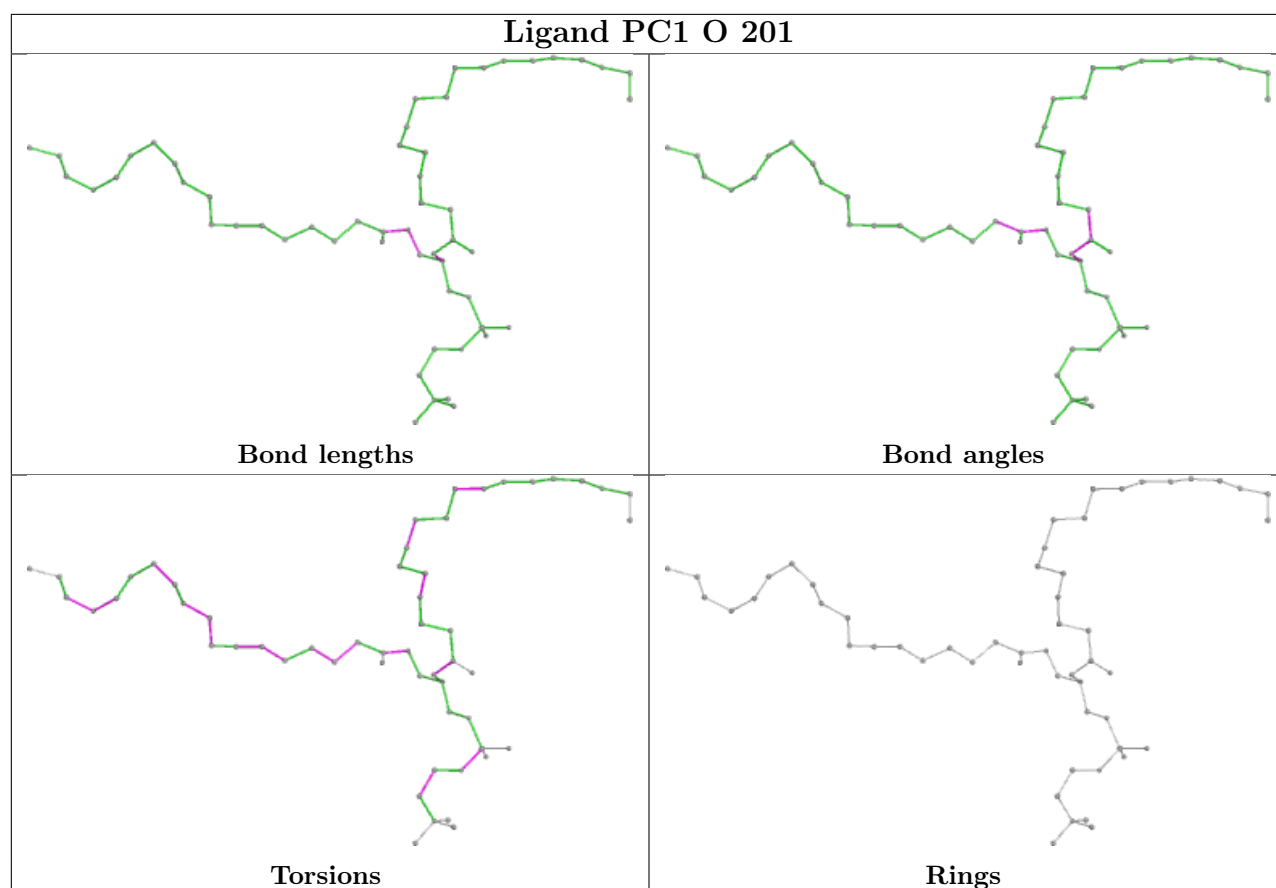


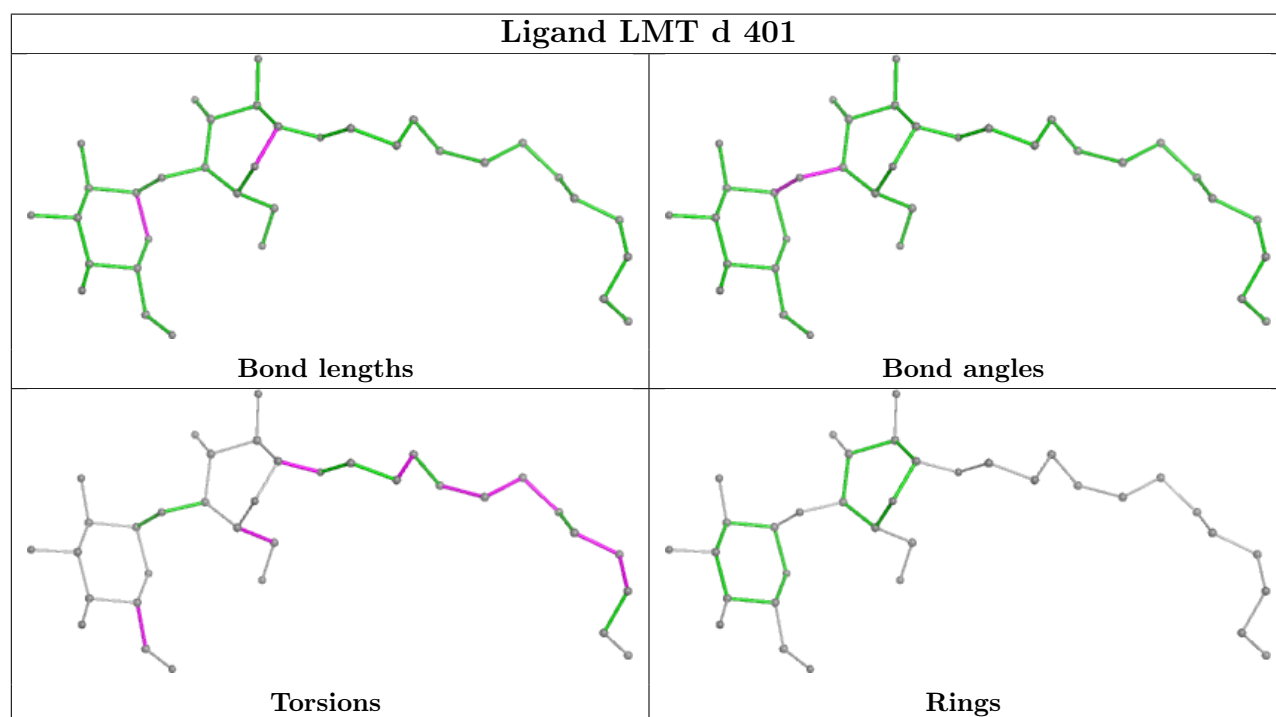
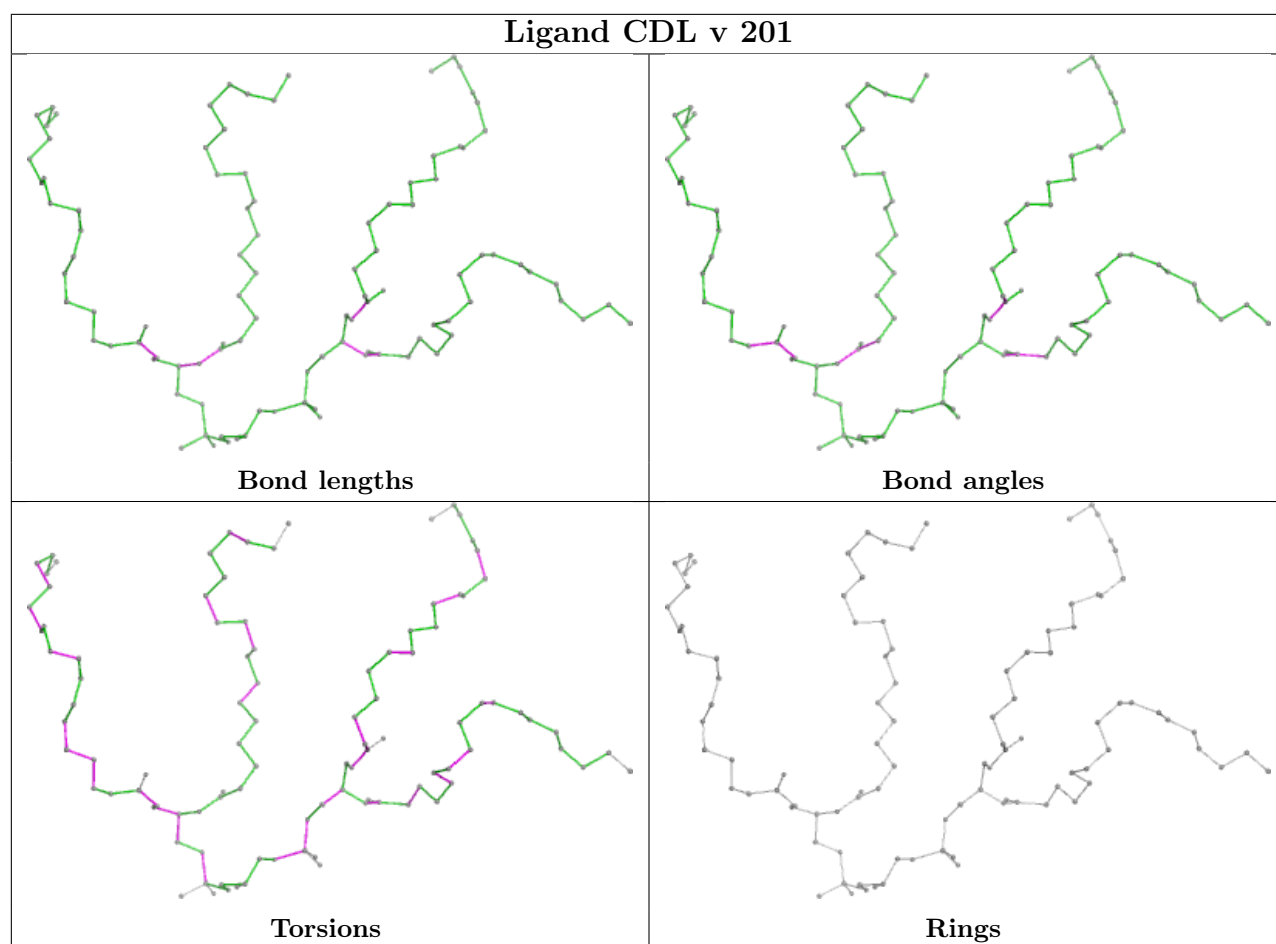


## Ligand CDL h 302

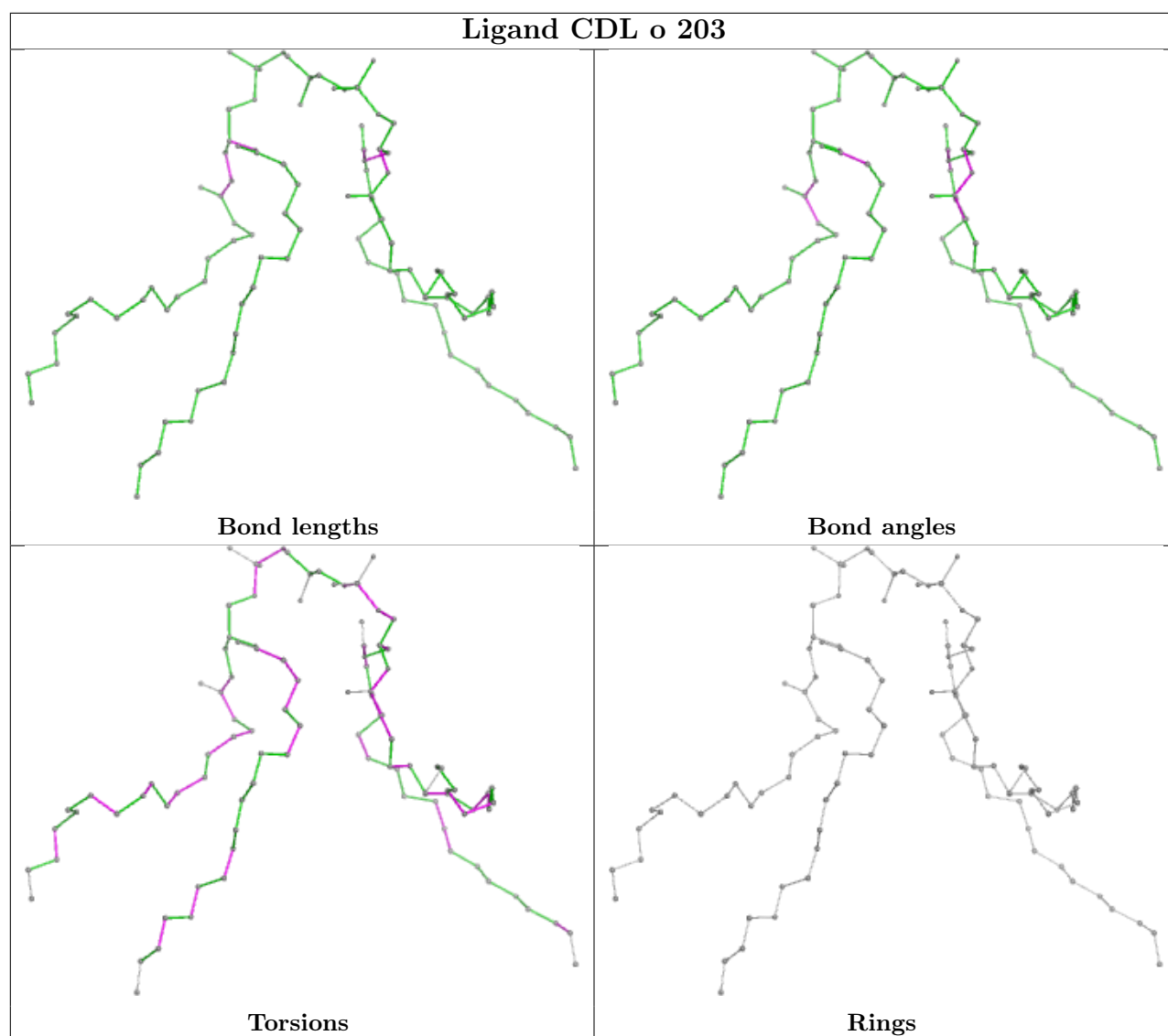


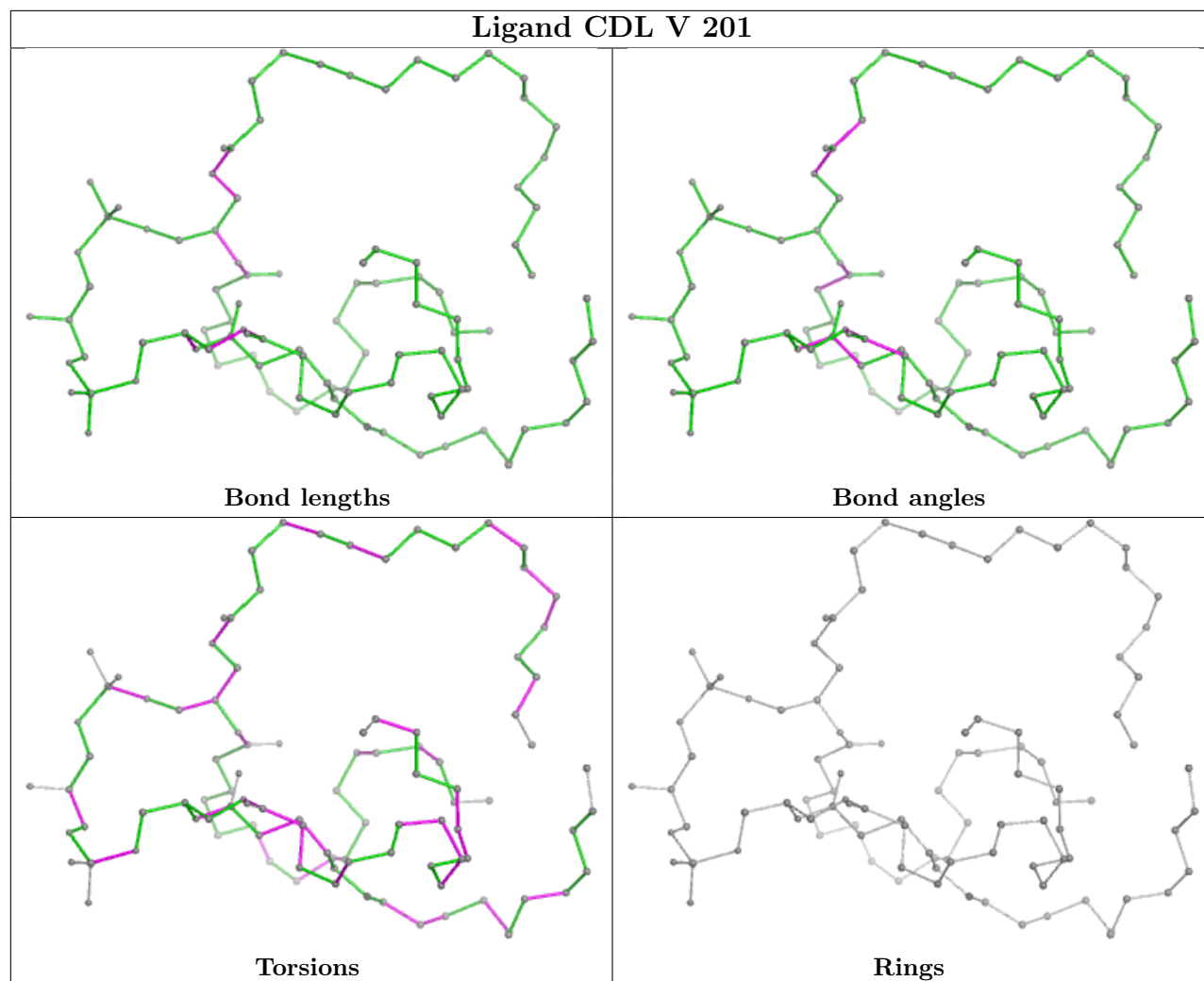


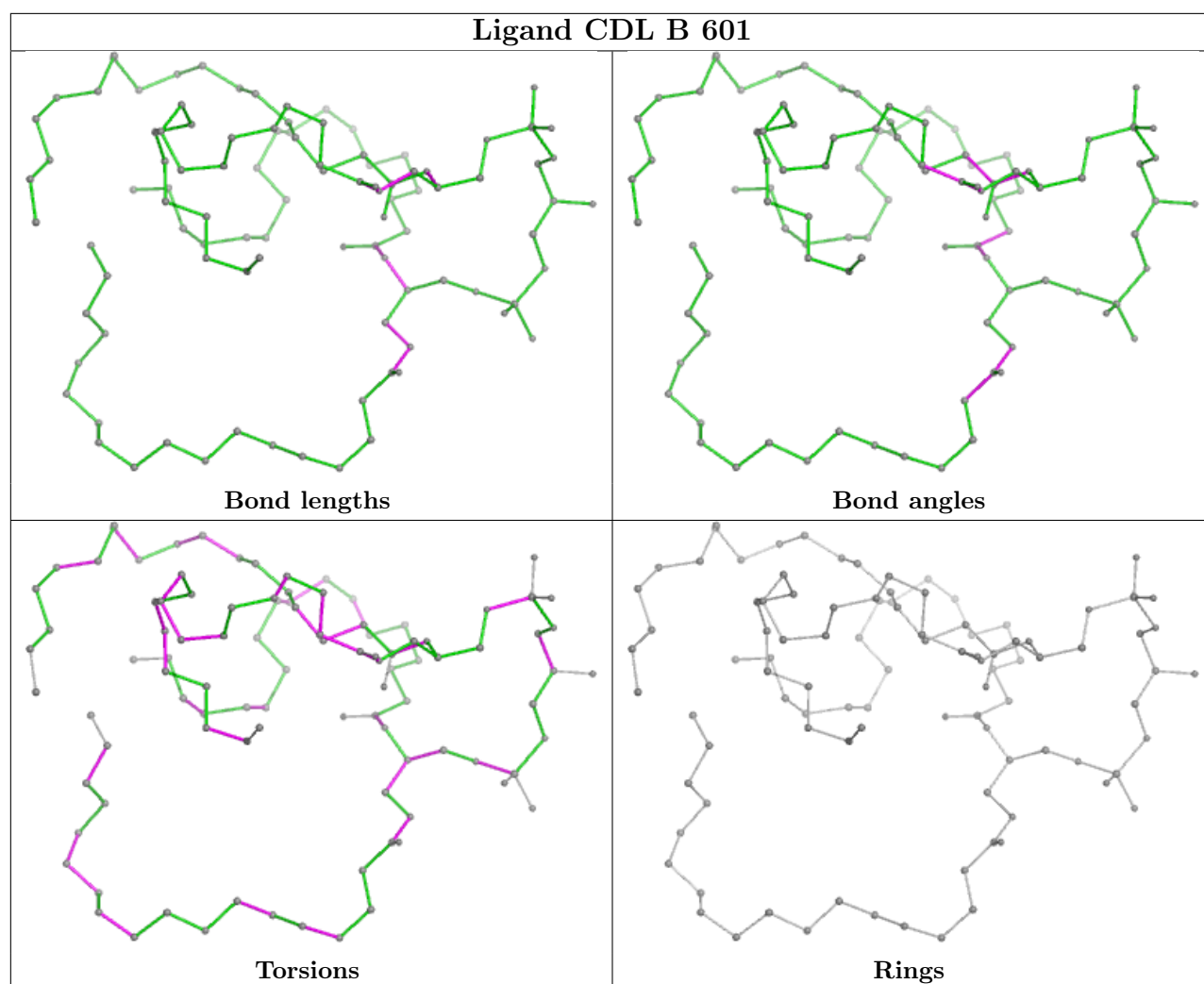












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

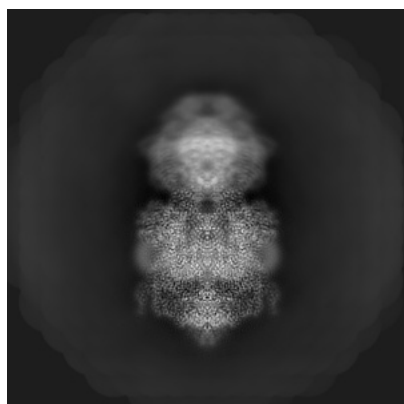
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10520. These allow visual inspection of the internal detail of the map and identification of artifacts.

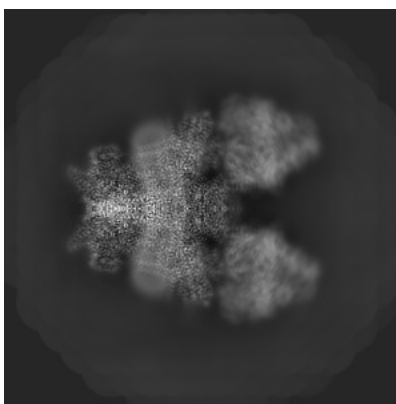
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

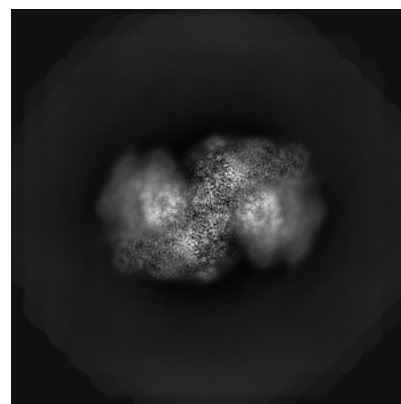
#### 6.1.1 Primary map



X

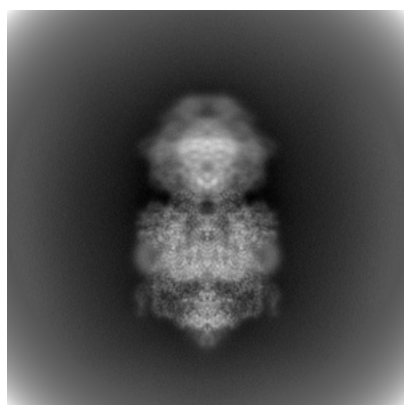


Y

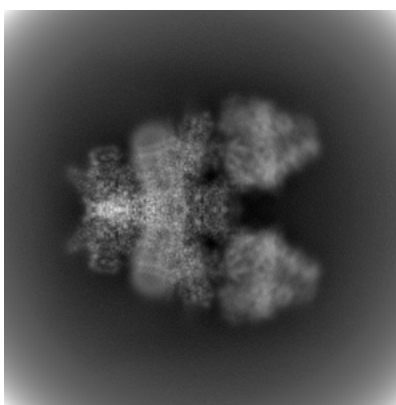


Z

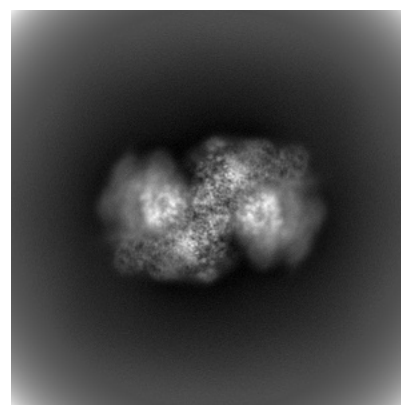
#### 6.1.2 Raw map



X



Y

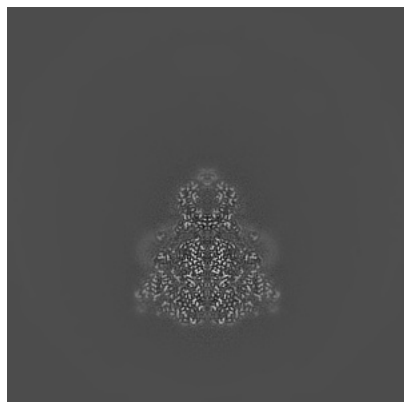


Z

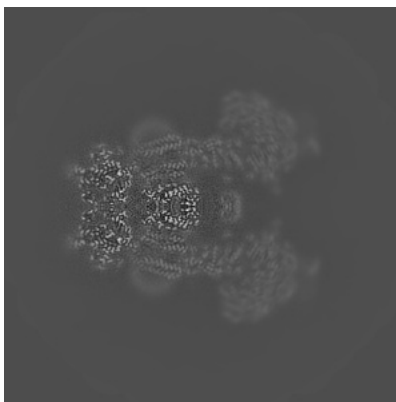
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

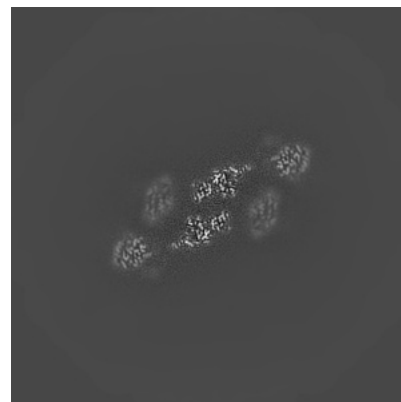
### 6.2.1 Primary map



X Index: 280

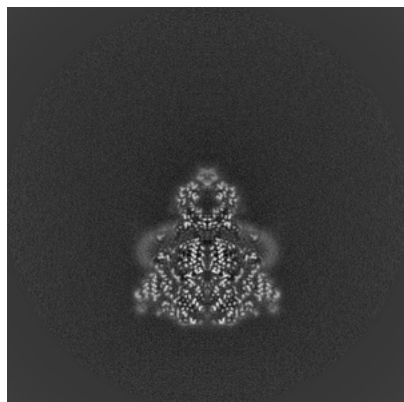


Y Index: 280

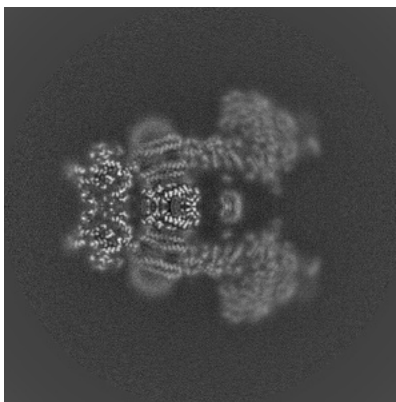


Z Index: 280

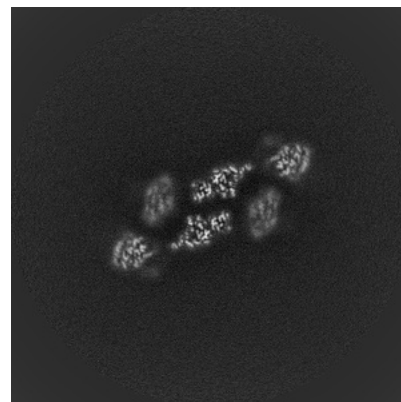
### 6.2.2 Raw map



X Index: 280



Y Index: 280

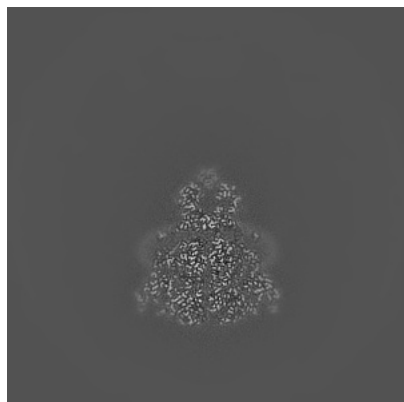


Z Index: 280

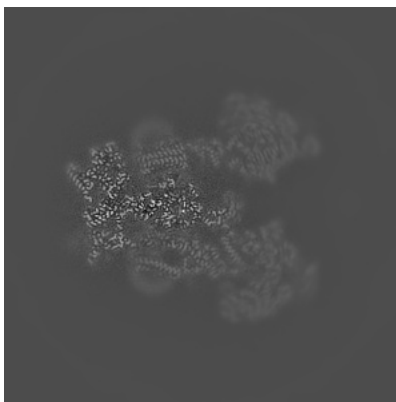
The images above show central slices of the map in three orthogonal directions.

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

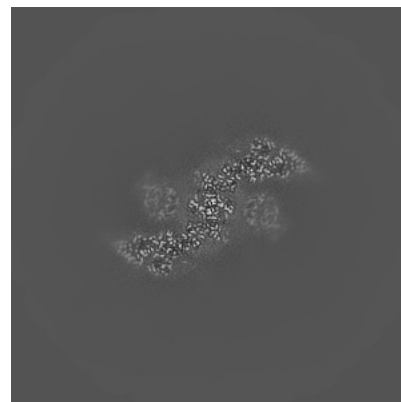
### 6.3.1 Primary map



X Index: 282

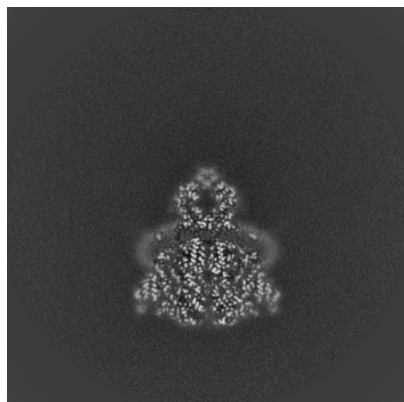


Y Index: 289

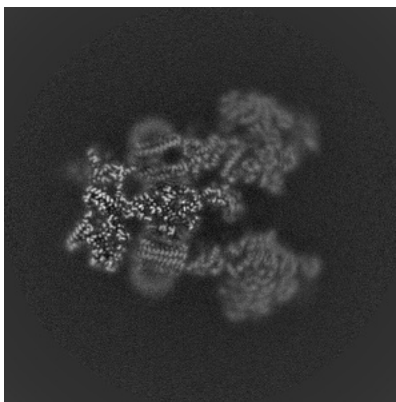


Z Index: 252

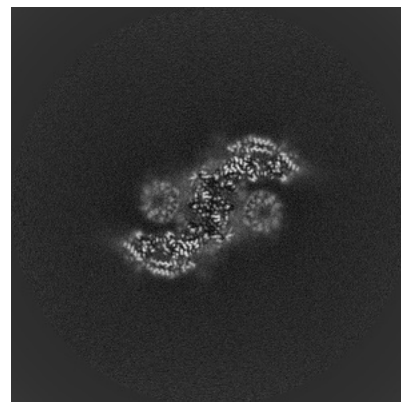
### 6.3.2 Raw map



X Index: 279



Y Index: 271

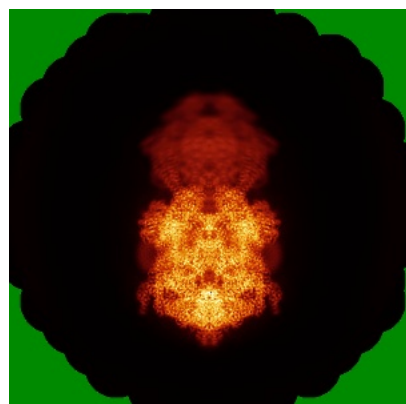


Z Index: 248

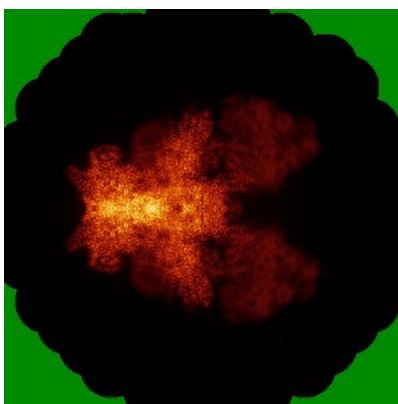
The images above show the largest variance slices of the map in three orthogonal directions.

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

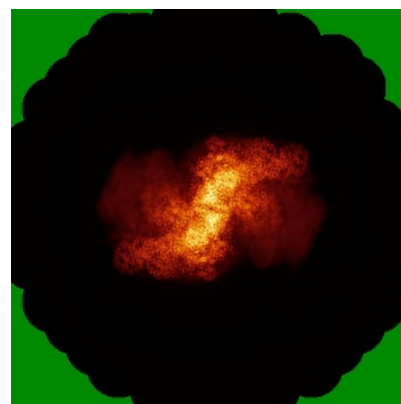
### 6.4.1 Primary map



X

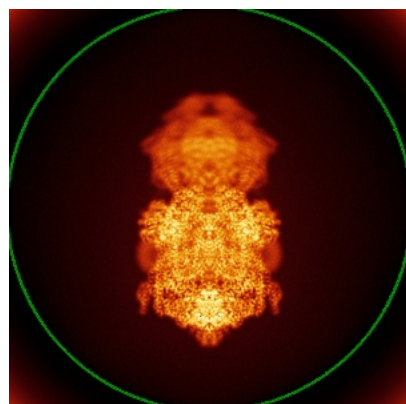


Y

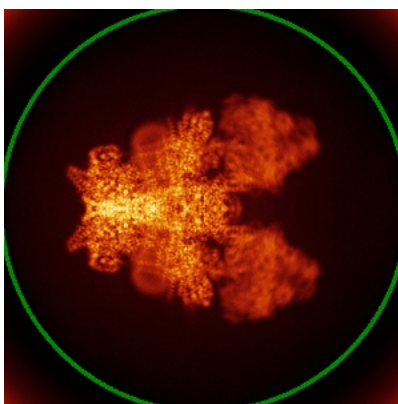


Z

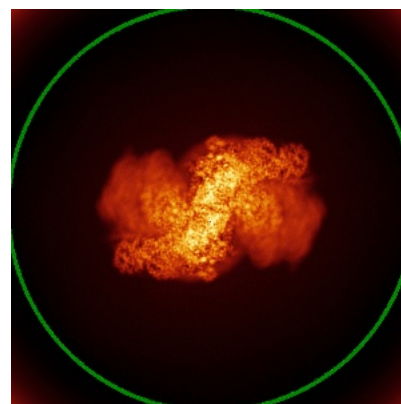
### 6.4.2 Raw map



X



Y



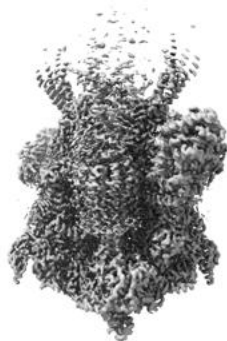
Z

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



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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



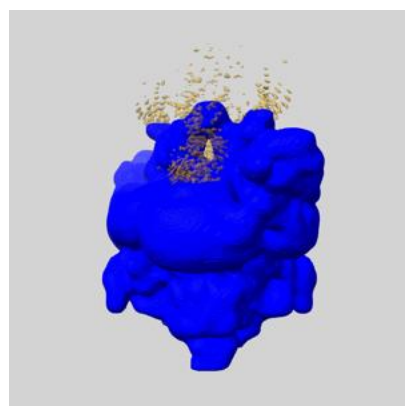
## 6.6 Mask visualisation [i](#)

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

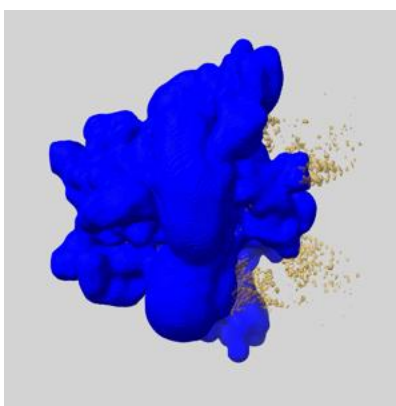
A mask typically either:

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

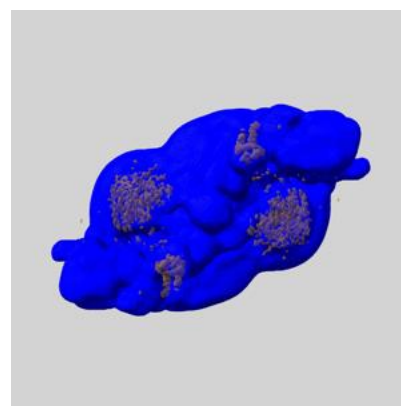
### 6.6.1 emd\_10520\_msk\_1.map [i](#)



X



Y

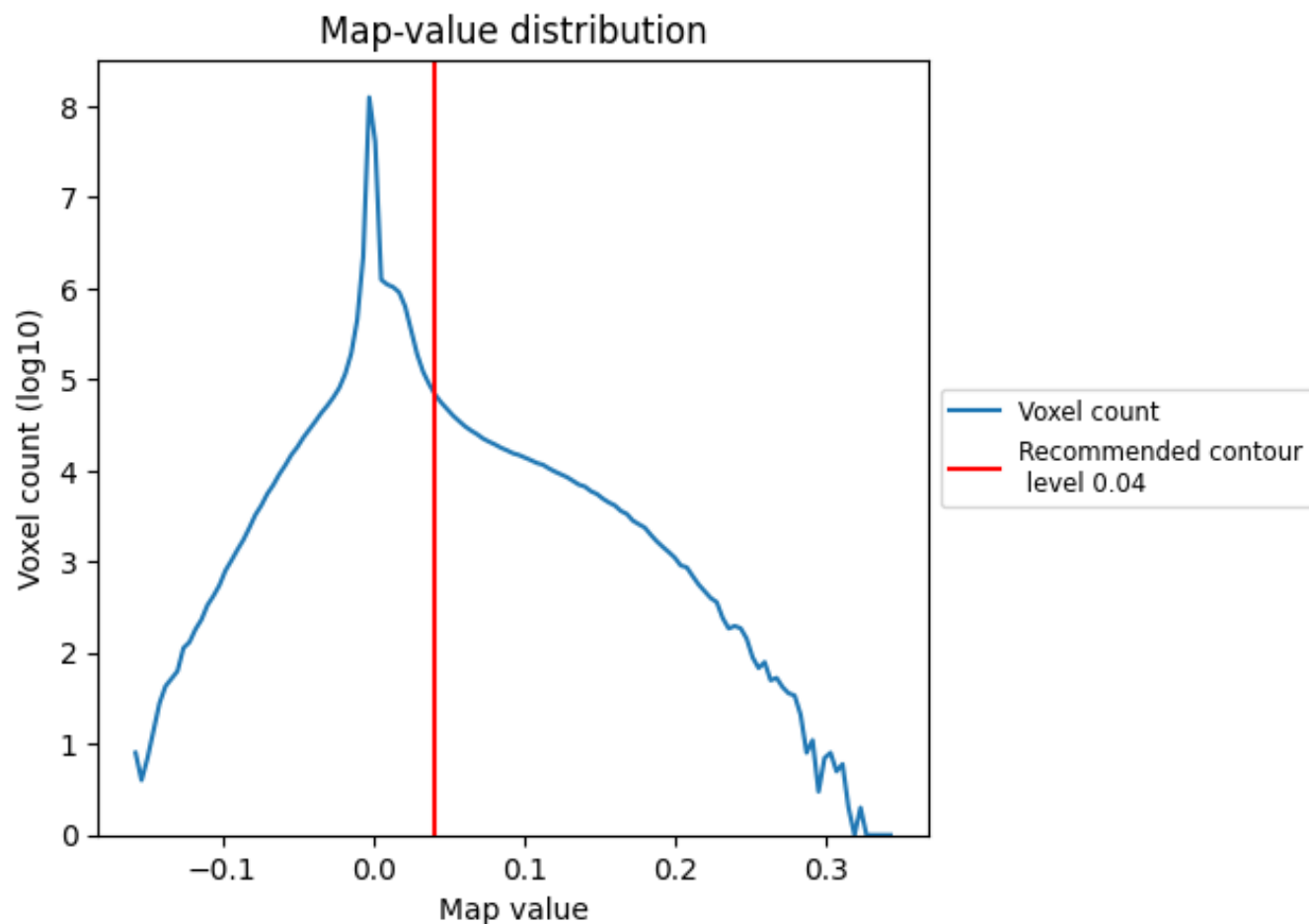


Z

## 7 Map analysis [i](#)

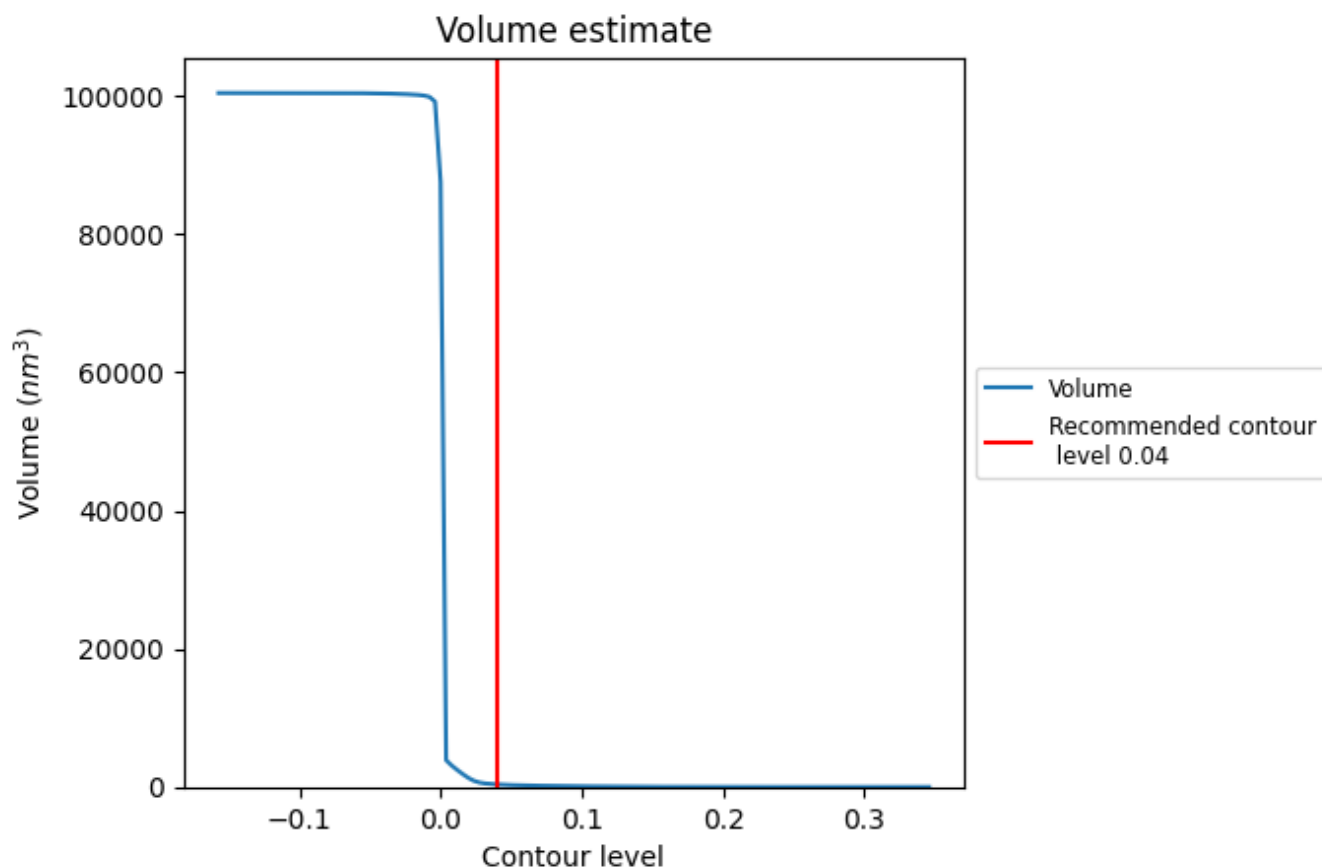
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

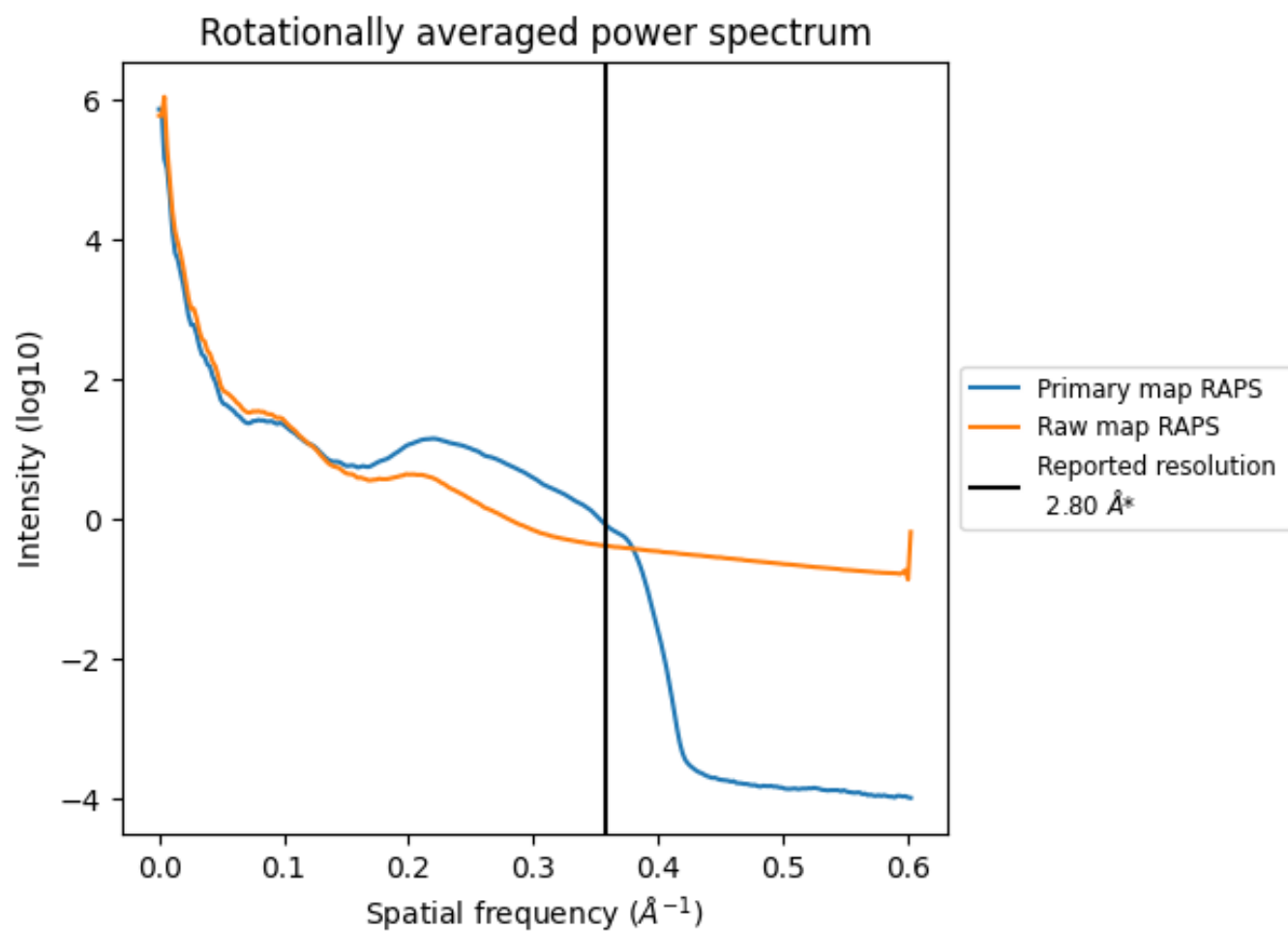
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365  $\text{nm}^3$ ; this corresponds to an approximate mass of 329 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 ⓘ

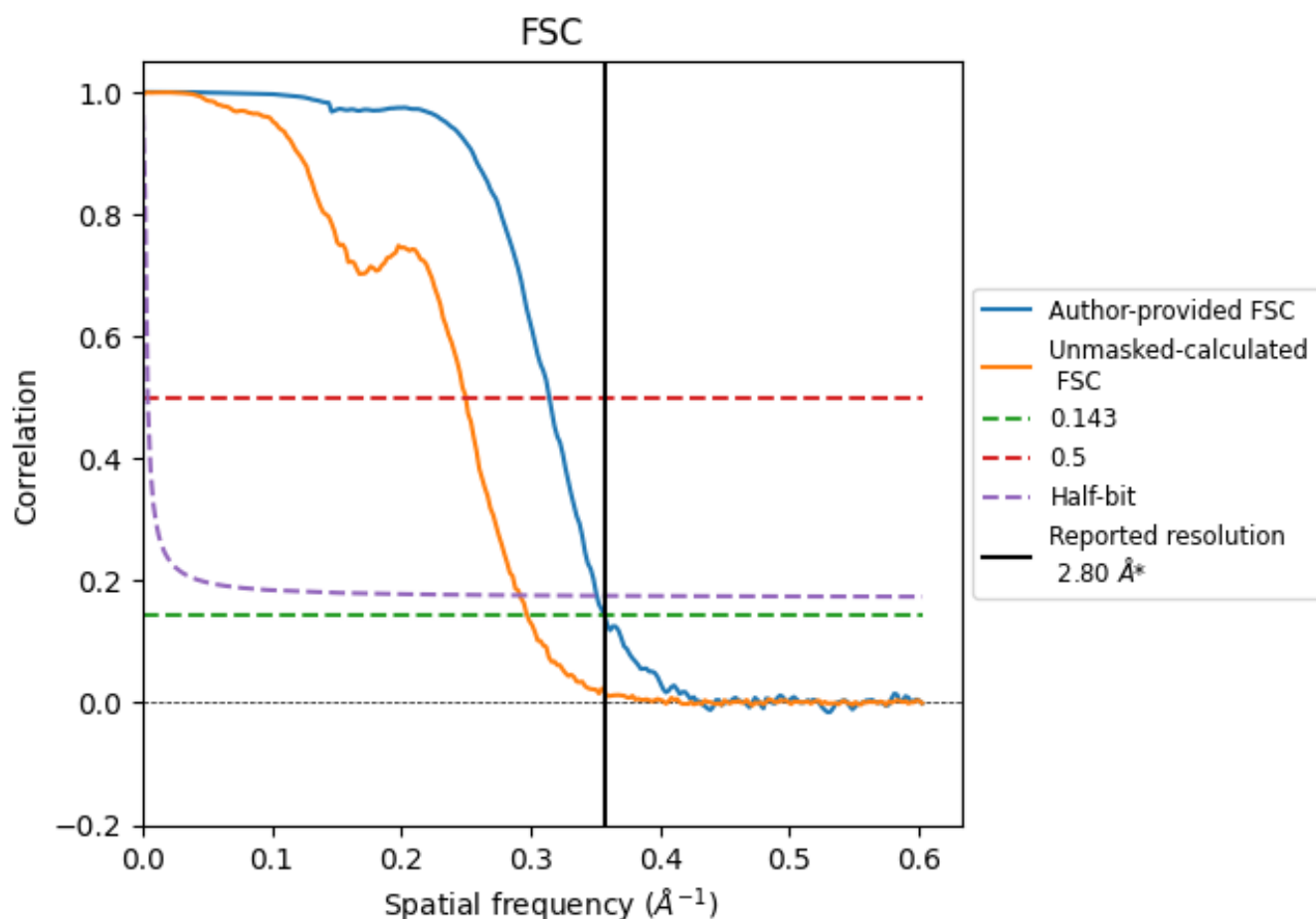


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

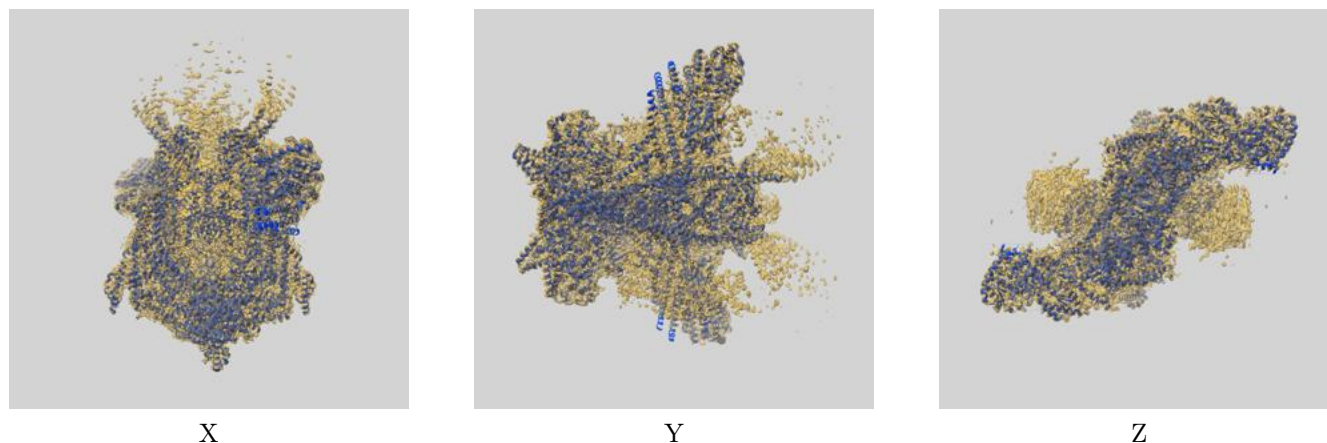
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.18	2.85
Unmasked-calculated*	3.36	4.00	3.43

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.8 by more than 10 %

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

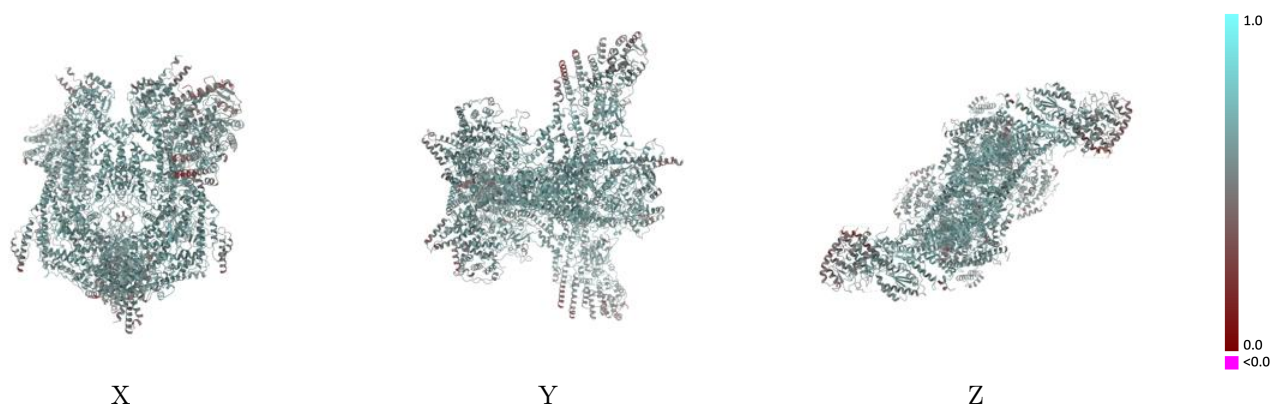
This section contains information regarding the fit between EMDB map EMD-10520 and PDB model 6TMG. Per-residue inclusion information can be found in section [3](#) on page [16](#).

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



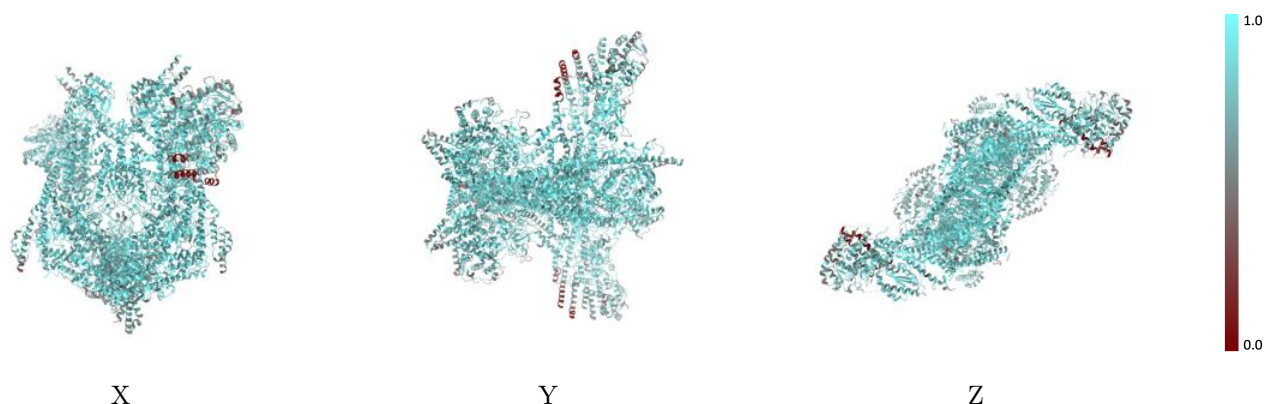
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

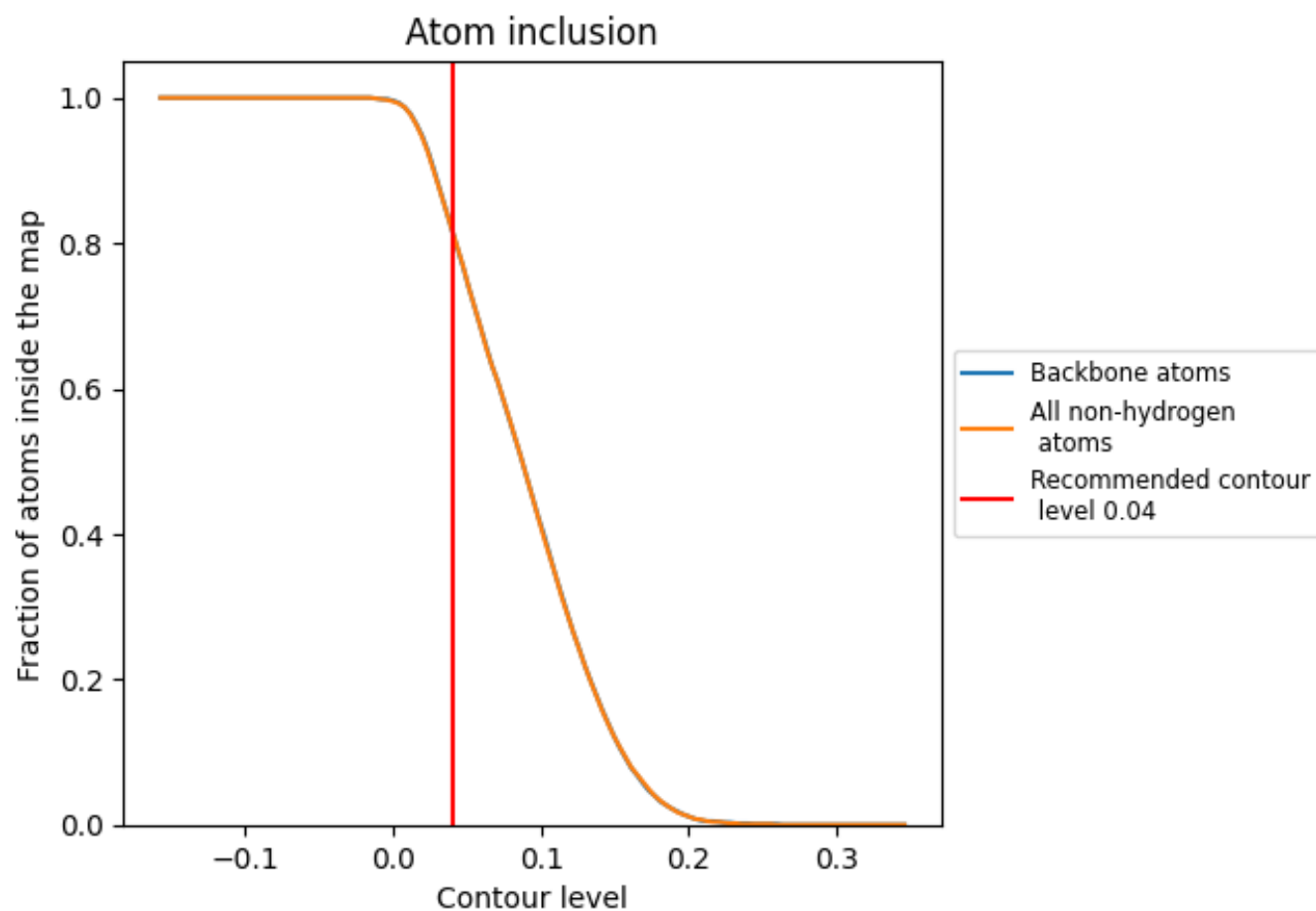
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.5890
A	 0.7430	 0.5380
B	 0.8250	 0.5940
C	 0.7290	 0.5550
D	 0.8560	 0.6130
E	 0.8560	 0.6140
F	 0.8180	 0.5770
G	 0.8440	 0.5920
H	 0.8720	 0.6180
I	 0.7610	 0.5490
J	 0.9210	 0.6520
K	 0.7460	 0.5820
L	 0.8650	 0.6020
M	 0.8940	 0.6290
N	 0.7650	 0.5560
O	 0.7930	 0.5800
P	 0.8690	 0.6010
Q	 0.7190	 0.5150
R	 0.8430	 0.5950
S	 0.8360	 0.5860
T	 0.7700	 0.5560
U	 0.8200	 0.5840
V	 0.8290	 0.6100
W	 0.9230	 0.6320
X	 0.8610	 0.6130
a	 0.7410	 0.5390
b	 0.8330	 0.6010
c	 0.7300	 0.5560
d	 0.8570	 0.6120
e	 0.8550	 0.6160
f	 0.8170	 0.5760
g	 0.8500	 0.5940
h	 0.8710	 0.6190
i	 0.7660	 0.5510
j	 0.9230	 0.6510



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Chain	Atom inclusion	Q-score
k	 0.7410	 0.5810
l	 0.8630	 0.6010
m	 0.8910	 0.6270
n	 0.7640	 0.5560
o	 0.7940	 0.5830
p	 0.8700	 0.6030
q	 0.7110	 0.5160
r	 0.8380	 0.5930
s	 0.8330	 0.5840
t	 0.7540	 0.5540
u	 0.8230	 0.5860
v	 0.8510	 0.6170
w	 0.9190	 0.6320
x	 0.8580	 0.6110