



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 11:09 pm GMT

PDB ID : 6TDV
EMDB ID : EMD-10468
Title : Cryo-EM structure of Euglena gracilis mitochondrial ATP synthase, membrane region
Authors : Muhleip, A.; Amunts, A.
Deposited on : 2019-11-10
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation 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 : 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) : 2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

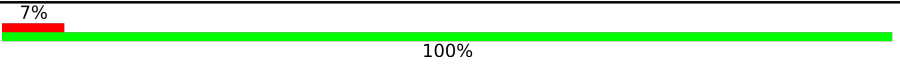
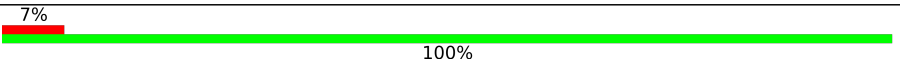
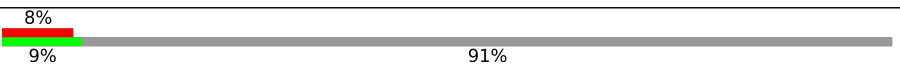
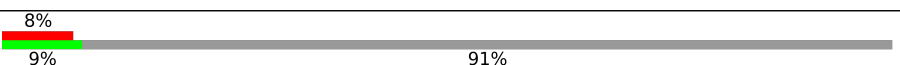
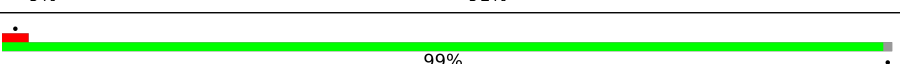
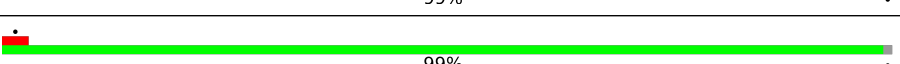
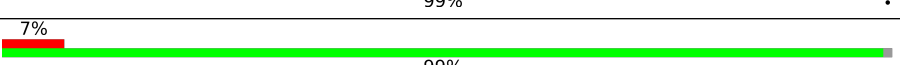
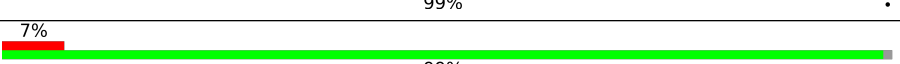
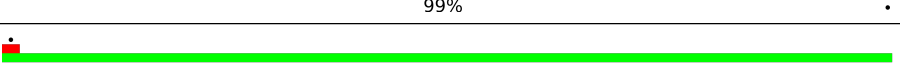
The reported resolution of this entry is 2.80 Å.

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.



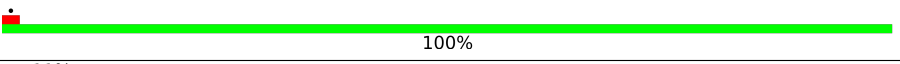
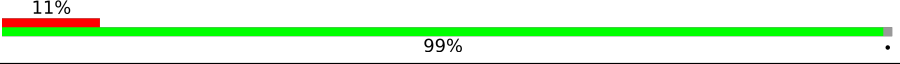
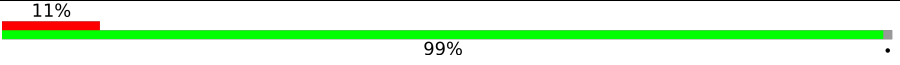
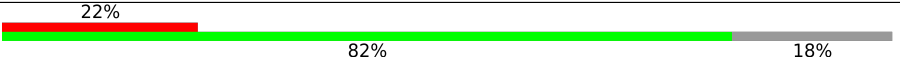
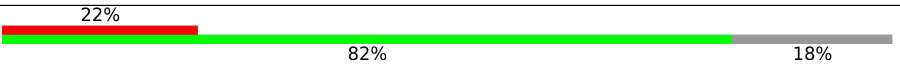
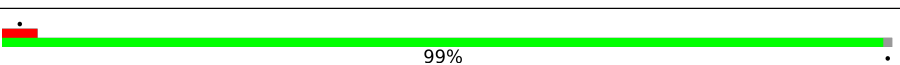
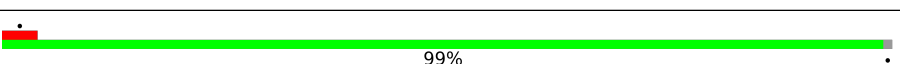
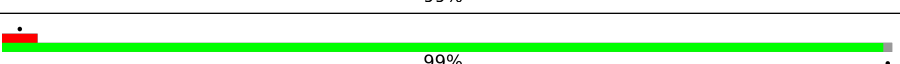
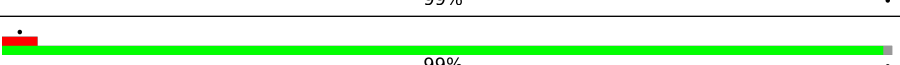
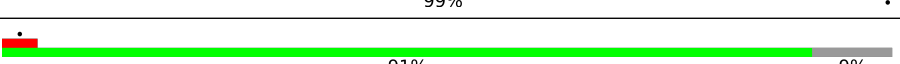
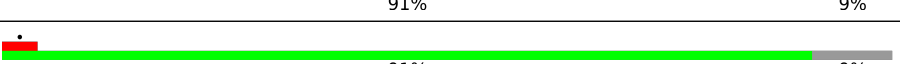
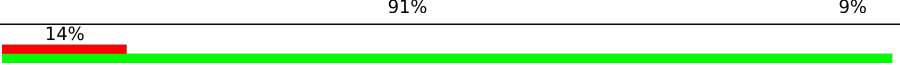
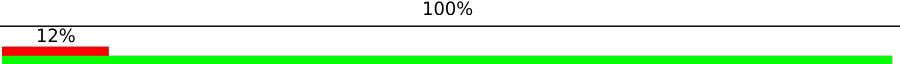
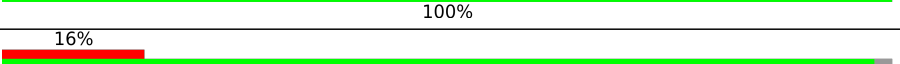
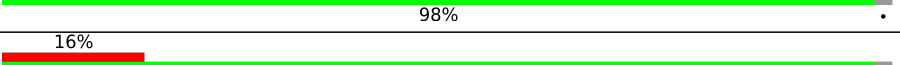
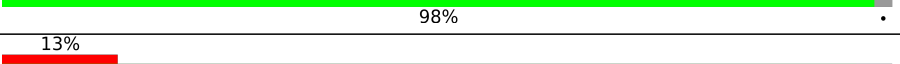
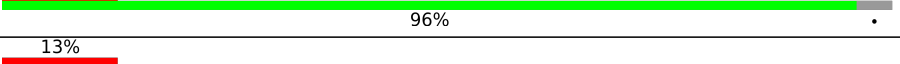
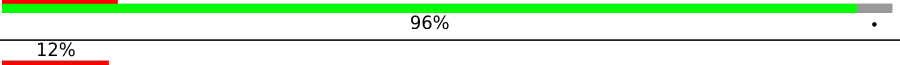

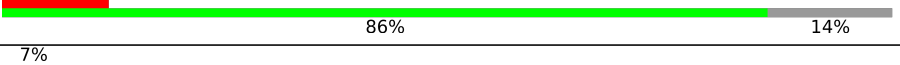
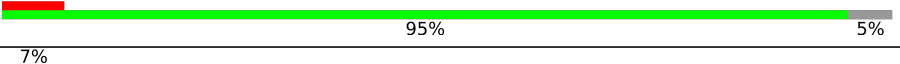
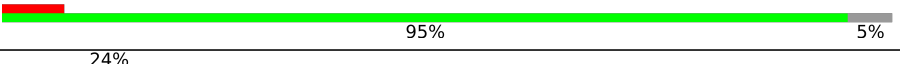
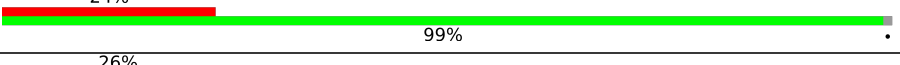
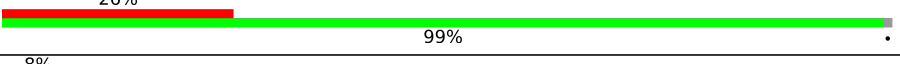

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	487	 100%
1	a	487	 100%
2	B	338	 91%
2	b	338	 91%
3	D	187	 99%
3	d	187	 99%
4	E	97	 99%
4	e	97	 99%
5	F	274	 100%

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Mol	Chain	Length	Quality of chain
5	f	274	
6	G	112	
6	g	112	
7	H	476	
7	h	476	
8	I	98	
8	i	98	
9	J	104	
9	j	104	
10	K	113	
10	k	113	
11	L	57	
11	l	57	
12	M	169	
12	m	169	
13	N	137	
13	n	137	
14	O	116	
14	o	116	
15	P	120	
15	p	120	
16	Q	90	
16	q	90	
17	R	78	
17	r	78	

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Mol	Chain	Length	Quality of chain
18	S	74	<div><div></div><div>7%</div><div>88%</div><div>12%</div></div>
18	s	74	<div><div></div><div>7%</div><div>88%</div><div>12%</div></div>
19	T	66	<div><div></div><div>14%</div><div>100%</div><div></div></div>
19	t	66	<div><div></div><div>14%</div><div>100%</div><div></div></div>

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 95420 atoms, of which 47674 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 ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	486	Total	C	H	N	O	S	0	0
			7864	2525	3919	677	733	10		
1	a	486	Total	C	H	N	O	S	0	0
			7864	2525	3919	677	733	10		

- Molecule 2 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	31	Total	C	H	N	O	0	0
			494	153	243	44	54		
2	b	31	Total	C	H	N	O	0	0
			494	153	243	44	54		

- Molecule 3 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	186	Total	C	H	N	O	S	0	0
			3040	977	1519	269	267	8		
3	d	186	Total	C	H	N	O	S	0	0
			3040	977	1519	269	267	8		

- Molecule 4 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	96	Total	C	H	N	O	S	0	0
			1574	509	777	144	141	3		
4	e	96	Total	C	H	N	O	S	0	0
			1577	510	779	144	141	3		

- Molecule 5 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	274	Total	C	H	N	O	S	0	0
			4639	1566	2327	341	391	14		
5	f	274	Total	C	H	N	O	S	0	0
			4642	1566	2329	342	391	14		

- Molecule 6 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	111	Total	C	H	N	O	S	0	0
			1803	566	924	160	146	7		
6	g	111	Total	C	H	N	O	S	0	0
			1803	566	924	160	146	7		

- Molecule 7 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	388	Total	C	H	N	O	S	0	0
			6165	1987	3059	512	598	9		
7	h	388	Total	C	H	N	O	S	0	0
			6165	1987	3059	512	598	9		

- Molecule 8 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	97	Total	C	H	N	O	S	0	0
			1553	504	771	140	135	3		
8	i	97	Total	C	H	N	O	S	0	0
			1553	504	771	140	135	3		

- Molecule 9 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	103	Total	C	H	N	O	S	0	0
			1734	581	853	151	146	3		
9	j	103	Total	C	H	N	O	S	0	0
			1734	581	853	151	146	3		

- Molecule 10 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	103	Total	C	H	N	O	S	0	0
			1637	530	821	136	144	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	k	103	Total	C	H	N	O	S	0	0
			1637	530	821	136	144	6		

- Molecule 11 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	57	Total	C	H	N	O		0	0
			1008	350	507	69	82			
11	l	57	Total	C	H	N	O		0	0
			1008	350	507	69	82			

- Molecule 12 is a protein called ATPEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	166	Total	C	H	N	O	S	0	0
			2717	887	1354	228	240	8		
12	m	166	Total	C	H	N	O	S	0	0
			2717	887	1354	228	240	8		

- Molecule 13 is a protein called ATPEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	131	Total	C	H	N	O	S	0	0
			2167	714	1070	198	182	3		
13	n	131	Total	C	H	N	O	S	0	0
			2167	714	1070	198	182	3		

- Molecule 14 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	100	Total	C	H	N	O	S	0	0
			1652	556	803	146	145	2		
14	o	100	Total	C	H	N	O	S	0	0
			1652	556	803	146	145	2		

- Molecule 15 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	114	Total	C	H	N	O	S	0	0
			1838	601	912	159	160	6		
15	p	114	Total	C	H	N	O	S	0	0
			1838	601	912	159	160	6		

- Molecule 16 is a protein called ATPEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	89	Total	C	H	N	O	S	0	0
			1476	475	723	137	137	4		
16	q	89	Total	C	H	N	O	S	0	0
			1476	475	723	137	137	4		

- Molecule 17 is a protein called ATPEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	69	Total	C	H	N	O	S	0	0
			1160	374	581	106	97	2		
17	r	69	Total	C	H	N	O	S	0	0
			1160	374	581	106	97	2		

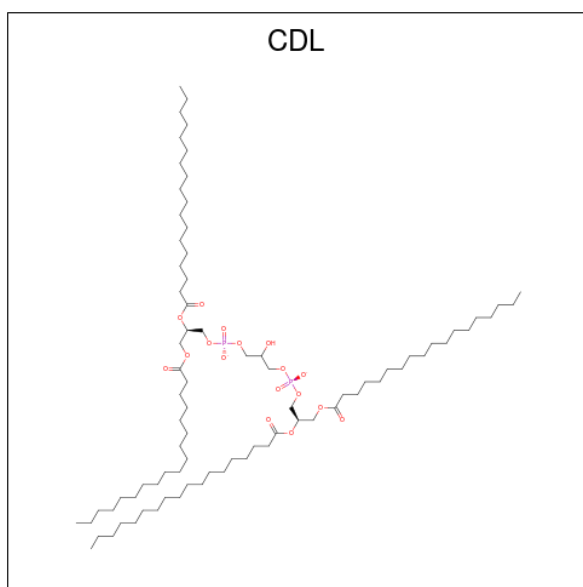
- Molecule 18 is a protein called ATPEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	65	Total	C	H	N	O	S	0	0
			1092	371	541	90	89	1		
18	s	65	Total	C	H	N	O	S	0	0
			1092	371	541	90	89	1		

- Molecule 19 is a protein called ATPEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	66	Total	C	H	N	O	S	0	0
			1080	349	552	95	83	1		
19	t	66	Total	C	H	N	O	S	0	0
			1080	349	552	95	83	1		

- Molecule 20 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



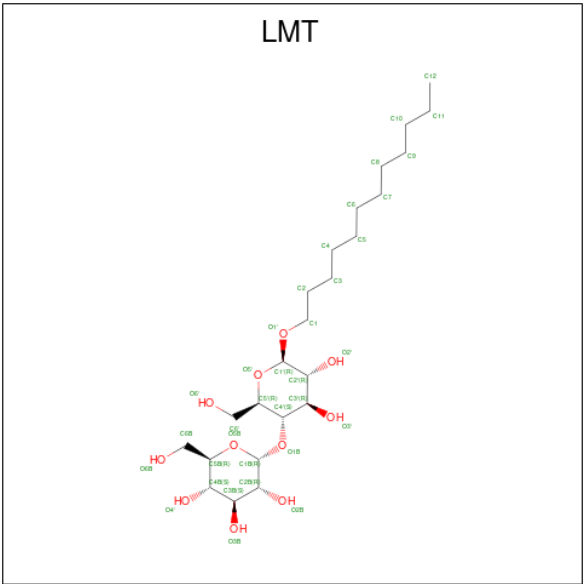
Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	H	O	P	0
			183	62	102	17	2	
20	A	1	Total	C	H	O	P	0
			170	62	89	17	2	
20	A	1	Total	C	H	O	P	0
			184	63	102	17	2	
20	A	1	Total	C	H	O	P	0
			99	44	36	17	2	
20	D	1	Total	C	H	O	P	0
			228	72	137	17	2	
20	D	1	Total	C	H	O	P	0
			184	67	98	17	2	
20	E	1	Total	C	H	O	P	0
			95	44	32	17	2	
20	M	1	Total	C	H	O	P	0
			152	58	75	17	2	
20	M	1	Total	C	H	O	P	0
			80	34	27	17	2	
20	O	1	Total	C	H	O	P	0
			124	46	59	17	2	
20	P	1	Total	C	H	O	P	0
			75	29	27	17	2	
20	R	1	Total	C	H	O	P	0
			150	57	74	17	2	
20	a	1	Total	C	H	O	P	0
			183	62	102	17	2	
20	a	1	Total	C	H	O	P	0
			170	62	89	17	2	

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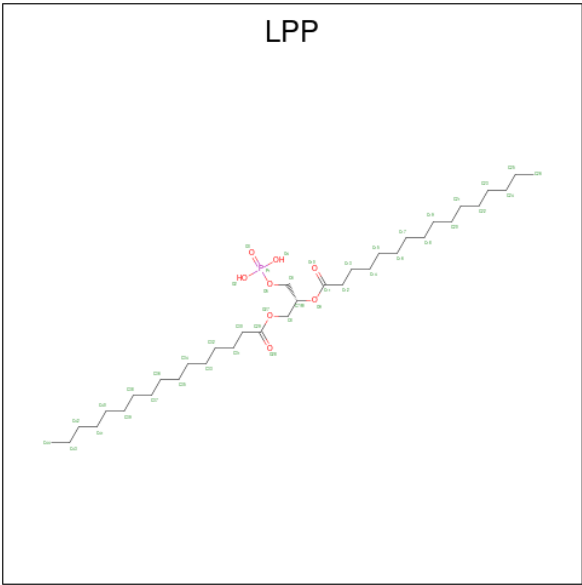
Mol	Chain	Residues	Atoms					AltConf
20	a	1	Total	C	H	O	P	0
			184	63	102	17	2	
20	a	1	Total	C	H	O	P	0
			99	44	36	17	2	
20	d	1	Total	C	H	O	P	0
			228	72	137	17	2	
20	d	1	Total	C	H	O	P	0
			184	67	98	17	2	
20	e	1	Total	C	H	O	P	0
			95	44	32	17	2	
20	m	1	Total	C	H	O	P	0
			152	58	75	17	2	
20	m	1	Total	C	H	O	P	0
			80	34	27	17	2	
20	o	1	Total	C	H	O	P	0
			124	46	59	17	2	
20	p	1	Total	C	H	O	P	0
			244	79	146	17	2	
20	p	1	Total	C	H	O	P	0
			75	29	27	17	2	
20	r	1	Total	C	H	O	P	0
			150	57	74	17	2	

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
21	D	1	Total	C	H	O	0
			81	24	46	11	
21	F	1	Total	C	H	O	0
			81	24	46	11	
21	N	1	Total	C	H	O	0
			81	24	46	11	
21	Q	1	Total	C	H	O	0
			81	24	46	11	
21	d	1	Total	C	H	O	0
			81	24	46	11	
21	f	1	Total	C	H	O	0
			81	24	46	11	
21	n	1	Total	C	H	O	0
			81	24	46	11	
21	q	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 22 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).



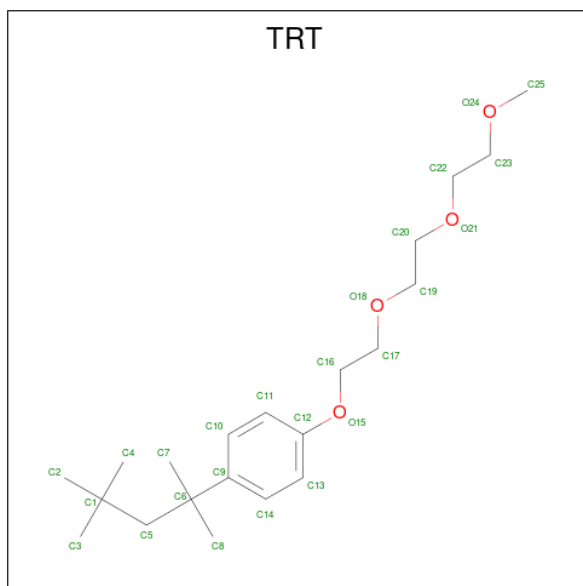
Mol	Chain	Residues	Atoms					AltConf
22	F	1	Total	C	H	O	P	0
			41	15	17	8	1	
22	I	1	Total	C	H	O	P	0
			111	35	67	8	1	
22	N	1	Total	C	H	O	P	0
			43	17	17	8	1	

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Mol	Chain	Residues	Atoms					AltConf
22	O	1	Total	C	H	O	P	0
			40	14	17	8	1	
22	O	1	Total	C	H	O	P	0
			73	23	41	8	1	
22	P	1	Total	C	H	O	P	0
			43	17	17	8	1	
22	R	1	Total	C	H	O	P	0
			48	22	17	8	1	
22	f	1	Total	C	H	O	P	0
			41	15	17	8	1	
22	i	1	Total	C	H	O	P	0
			111	35	67	8	1	
22	o	1	Total	C	H	O	P	0
			40	14	17	8	1	
22	o	1	Total	C	H	O	P	0
			73	23	41	8	1	
22	r	1	Total	C	H	O	P	0
			48	22	17	8	1	

- Molecule 23 is FRAGMENT OF TRITON X-100 (three-letter code: TRT) (formula: C₂₁H₃₆O₄).

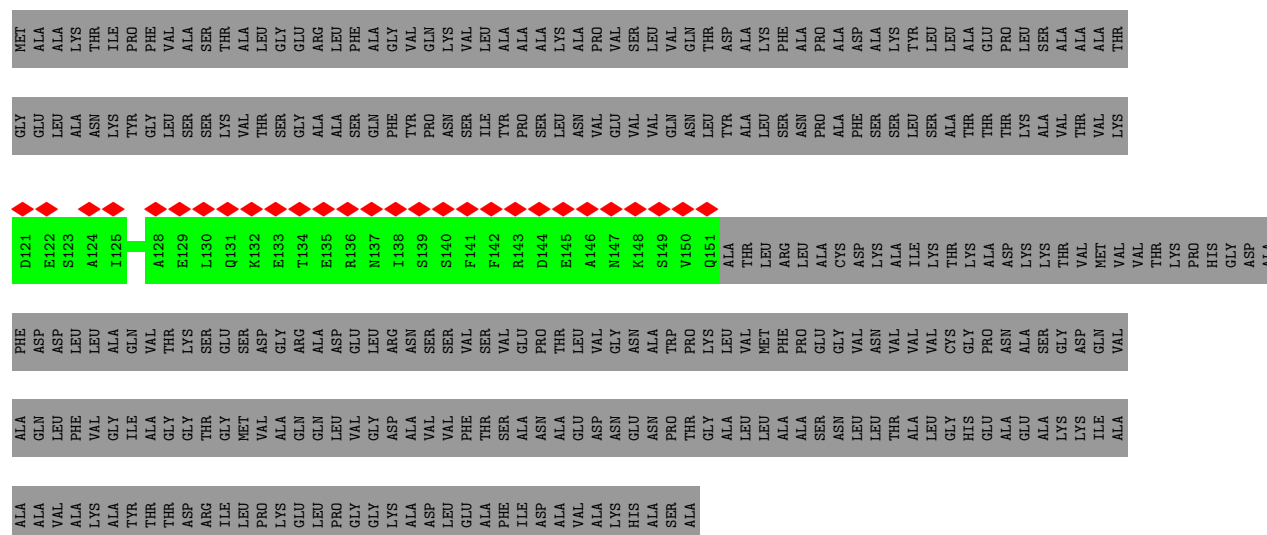


Mol	Chain	Residues	Atoms					AltConf
23	G	1	Total	C	H	O		0
			61	21	36	4		
23	G	1	Total	C	H	O		0
			61	21	36	4		

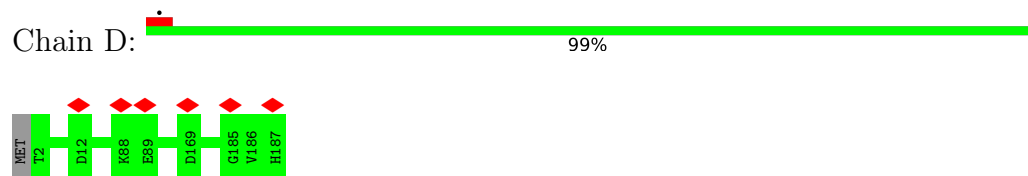
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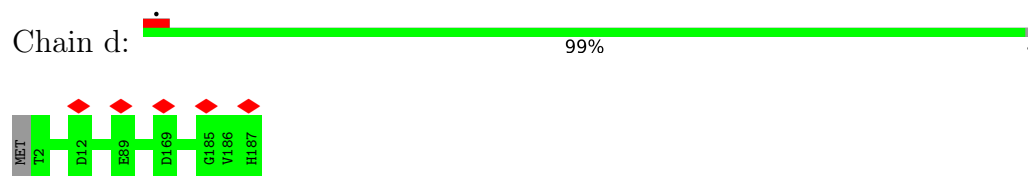
Mol	Chain	Residues	Atoms				AltConf
23	M	1	Total 61	C 21	H 36	O 4	0
23	M	1	Total 61	C 21	H 36	O 4	0
23	N	1	Total 61	C 21	H 36	O 4	0
23	N	1	Total 61	C 21	H 36	O 4	0
23	P	1	Total 61	C 21	H 36	O 4	0
23	R	1	Total 61	C 21	H 36	O 4	0
23	g	1	Total 61	C 21	H 36	O 4	0
23	g	1	Total 61	C 21	H 36	O 4	0
23	m	1	Total 61	C 21	H 36	O 4	0
23	m	1	Total 61	C 21	H 36	O 4	0
23	n	1	Total 61	C 21	H 36	O 4	0
23	n	1	Total 61	C 21	H 36	O 4	0
23	p	1	Total 61	C 21	H 36	O 4	0
23	r	1	Total 61	C 21	H 36	O 4	0



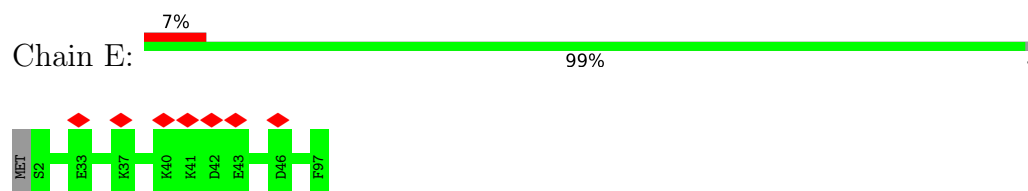
- Molecule 3: ATPTB6



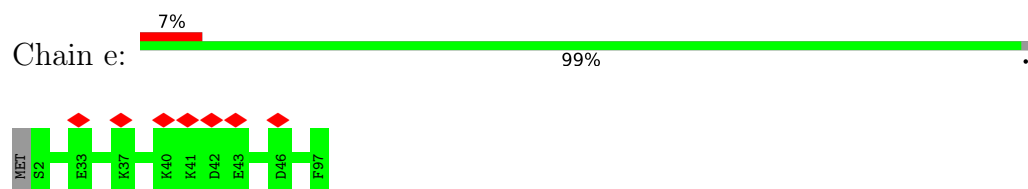
- Molecule 3: ATPTB6



- Molecule 4: ATPTB12

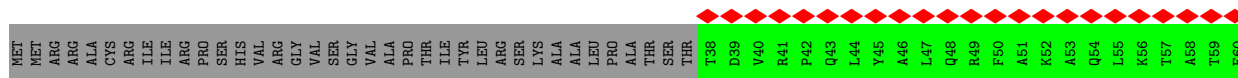


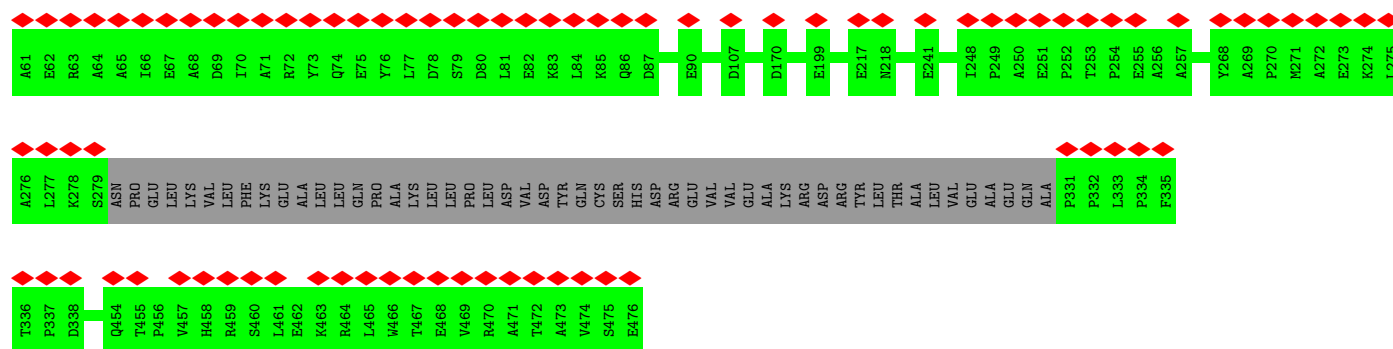
- Molecule 4: ATPTB12



- Molecule 5: subunit a

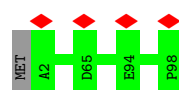






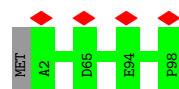
• Molecule 8: subunit f

Chain I: 99%



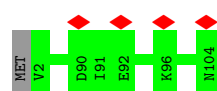
• Molecule 8: subunit f

Chain i: 99%



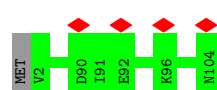
• Molecule 9: subunit i/j

Chain J: 99%



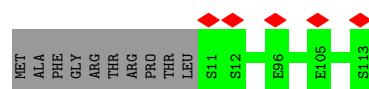
• Molecule 9: subunit i/j

Chain j: 99%




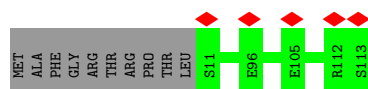
• Molecule 10: subunit k

Chain K: 91%



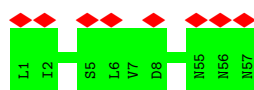
• Molecule 10: subunit k

Chain k:  91% 9%



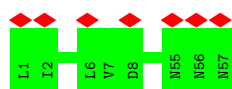
- Molecule 11: subunit 8

Chain L:  14% 100%



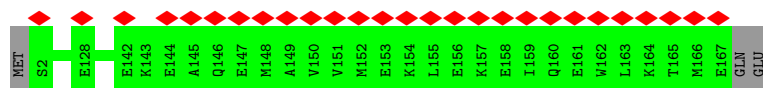
- Molecule 11: subunit 8

Chain l:  12% 100%



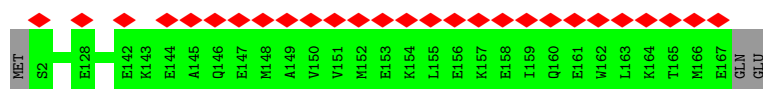
- Molecule 12: ATPEG1

Chain M:  16% 98%



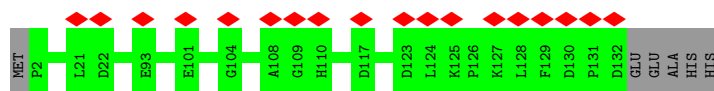
- Molecule 12: ATPEG1

Chain m:  16% 98%



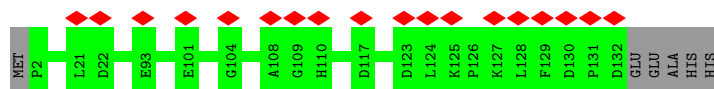
- Molecule 13: ATPEG2

Chain N:  13% 96%

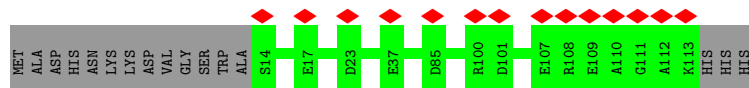
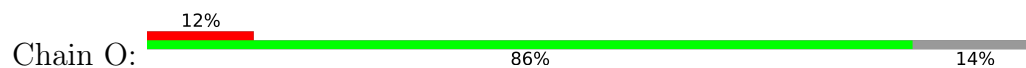


- Molecule 13: ATPEG2

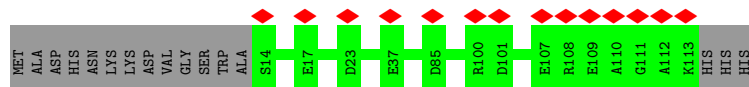
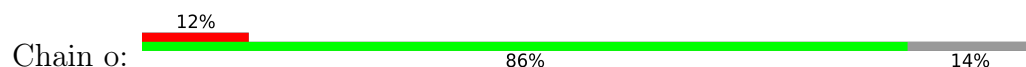
Chain n:  13% 96%



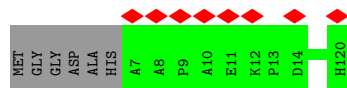
● Molecule 14: ATPEG3



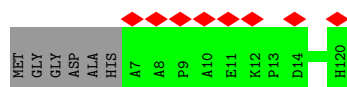
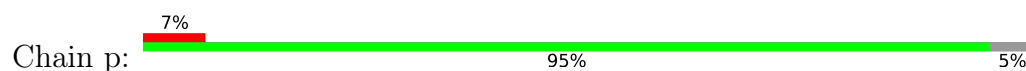
● Molecule 14: ATPEG3



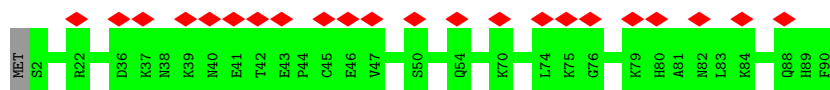
● Molecule 15: ATPEG4



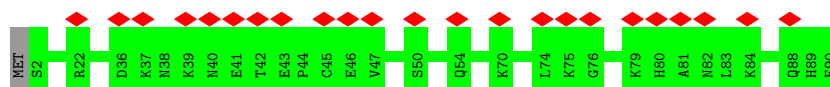
● Molecule 15: ATPEG4



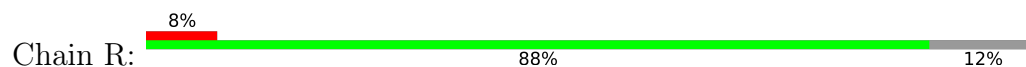
● Molecule 16: ATPEG5

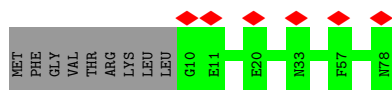


● Molecule 16: ATPEG5

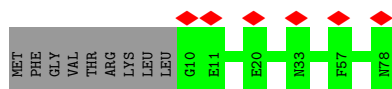
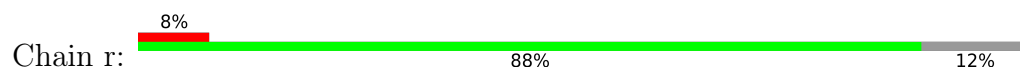


● Molecule 17: ATPEG6

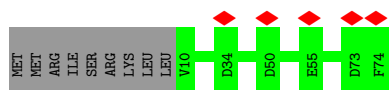
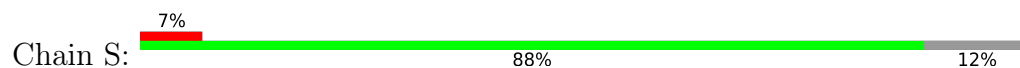




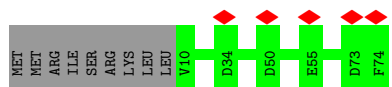
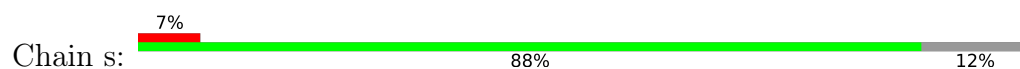
● Molecule 17: ATPEG6



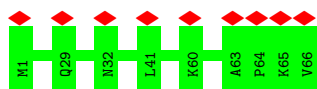
● Molecule 18: ATPEG7



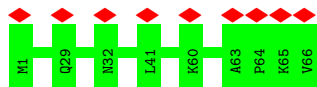
● Molecule 18: ATPEG7



● Molecule 19: ATPEG8



● Molecule 19: ATPEG8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	150242	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 ($e^-/\text{\AA}^2$)	36.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/4047	0.49	0/5500
1	a	0.35	0/4047	0.50	0/5500
2	B	0.24	0/252	0.37	0/335
2	b	0.25	0/252	0.37	0/335
3	D	0.34	0/1559	0.52	0/2106
3	d	0.34	0/1559	0.52	0/2106
4	E	0.32	0/819	0.47	0/1096
4	e	0.31	0/821	0.46	0/1100
5	F	0.37	0/2377	0.46	0/3228
5	f	0.37	0/2379	0.46	0/3233
6	G	0.34	0/901	0.57	0/1218
6	g	0.34	0/901	0.57	0/1218
7	H	0.33	0/3185	0.47	0/4352
7	h	0.33	0/3185	0.47	0/4352
8	I	0.35	0/804	0.47	0/1084
8	i	0.35	0/804	0.47	0/1084
9	J	0.34	0/918	0.46	0/1255
9	j	0.34	0/918	0.46	0/1255
10	K	0.32	0/839	0.45	0/1135
10	k	0.32	0/839	0.45	0/1135
11	L	0.40	0/518	0.46	0/711
11	l	0.40	0/518	0.46	0/711
12	M	0.33	0/1399	0.45	0/1895
12	m	0.34	0/1399	0.45	0/1895
13	N	0.34	0/1137	0.47	0/1540
13	n	0.34	0/1137	0.48	0/1540
14	O	0.32	0/881	0.44	0/1193
14	o	0.32	0/881	0.44	0/1193
15	P	0.36	0/955	0.49	0/1292
15	p	0.36	0/955	0.49	0/1292
16	Q	0.29	0/774	0.51	0/1040
16	q	0.29	0/774	0.51	0/1040

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.30	0/594	0.51	0/798
17	r	0.30	0/594	0.51	0/798
18	S	0.34	0/575	0.48	0/785
18	s	0.34	0/575	0.48	0/785
19	T	0.33	0/543	0.52	0/730
19	t	0.33	0/543	0.52	0/730
All	All	0.34	0/46158	0.48	0/62595

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	A	484/487 (99%)	467 (96%)	17 (4%)	0	100	100
1	a	484/487 (99%)	467 (96%)	17 (4%)	0	100	100
2	B	29/338 (9%)	29 (100%)	0	0	100	100
2	b	29/338 (9%)	29 (100%)	0	0	100	100
3	D	184/187 (98%)	180 (98%)	4 (2%)	0	100	100
3	d	184/187 (98%)	180 (98%)	4 (2%)	0	100	100
4	E	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
4	e	94/97 (97%)	91 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	270/274 (98%)	262 (97%)	8 (3%)	0	100	100
5	f	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
6	G	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
6	g	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
7	H	384/476 (81%)	380 (99%)	4 (1%)	0	100	100
7	h	384/476 (81%)	380 (99%)	4 (1%)	0	100	100
8	I	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
8	i	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
9	J	101/104 (97%)	99 (98%)	2 (2%)	0	100	100
9	j	101/104 (97%)	99 (98%)	2 (2%)	0	100	100
10	K	101/113 (89%)	99 (98%)	2 (2%)	0	100	100
10	k	101/113 (89%)	99 (98%)	2 (2%)	0	100	100
11	L	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
11	l	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
12	M	164/169 (97%)	164 (100%)	0	0	100	100
12	m	164/169 (97%)	164 (100%)	0	0	100	100
13	N	129/137 (94%)	124 (96%)	5 (4%)	0	100	100
13	n	129/137 (94%)	124 (96%)	5 (4%)	0	100	100
14	O	98/116 (84%)	95 (97%)	3 (3%)	0	100	100
14	o	98/116 (84%)	95 (97%)	3 (3%)	0	100	100
15	P	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
15	p	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
16	Q	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
16	q	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
17	R	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
17	r	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
18	S	63/74 (85%)	61 (97%)	2 (3%)	0	100	100
18	s	63/74 (85%)	61 (97%)	2 (3%)	0	100	100
19	T	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
19	t	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
All	All	5382/6386 (84%)	5241 (97%)	141 (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	A	426/427 (100%)	426 (100%)	0	100	100
1	a	426/427 (100%)	426 (100%)	0	100	100
2	B	28/259 (11%)	28 (100%)	0	100	100
2	b	28/259 (11%)	28 (100%)	0	100	100
3	D	159/160 (99%)	159 (100%)	0	100	100
3	d	159/160 (99%)	159 (100%)	0	100	100
4	E	80/82 (98%)	80 (100%)	0	100	100
4	e	81/82 (99%)	81 (100%)	0	100	100
5	F	258/259 (100%)	258 (100%)	0	100	100
5	f	259/259 (100%)	259 (100%)	0	100	100
6	G	98/99 (99%)	98 (100%)	0	100	100
6	g	98/99 (99%)	98 (100%)	0	100	100
7	H	339/414 (82%)	339 (100%)	0	100	100
7	h	339/414 (82%)	339 (100%)	0	100	100
8	I	82/83 (99%)	82 (100%)	0	100	100
8	i	82/83 (99%)	82 (100%)	0	100	100
9	J	94/95 (99%)	94 (100%)	0	100	100
9	j	94/95 (99%)	94 (100%)	0	100	100
10	K	89/97 (92%)	89 (100%)	0	100	100
10	k	89/97 (92%)	89 (100%)	0	100	100
11	L	56/56 (100%)	56 (100%)	0	100	100
11	l	56/56 (100%)	56 (100%)	0	100	100
12	M	137/140 (98%)	137 (100%)	0	100	100
12	m	137/140 (98%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	N	114/119 (96%)	114 (100%)	0	100	100
13	n	114/119 (96%)	114 (100%)	0	100	100
14	O	90/103 (87%)	90 (100%)	0	100	100
14	o	90/103 (87%)	90 (100%)	0	100	100
15	P	96/99 (97%)	96 (100%)	0	100	100
15	p	96/99 (97%)	96 (100%)	0	100	100
16	Q	82/83 (99%)	82 (100%)	0	100	100
16	q	82/83 (99%)	82 (100%)	0	100	100
17	R	59/67 (88%)	59 (100%)	0	100	100
17	r	59/67 (88%)	59 (100%)	0	100	100
18	S	59/68 (87%)	59 (100%)	0	100	100
18	s	59/68 (87%)	59 (100%)	0	100	100
19	T	54/54 (100%)	54 (100%)	0	100	100
19	t	54/54 (100%)	54 (100%)	0	100	100
All	All	4802/5528 (87%)	4802 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	32	ASN
5	f	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

61 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$
21	LMT	N	204	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	5 (10%)
20	CDL	a	503	-	80,80,99	0.97	8 (10%)	85,91,111	1.04	4 (4%)
21	LMT	n	201	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	3 (6%)
23	TRT	P	203	-	25,25,25	1.25	3 (12%)	33,33,33	4.75	8 (24%)
20	CDL	E	101	-	62,62,99	1.08	8 (12%)	68,74,111	1.11	4 (5%)
23	TRT	N	202	-	25,25,25	0.61	0	33,33,33	0.64	0
20	CDL	a	504	-	62,62,99	1.10	8 (12%)	68,74,111	1.17	4 (5%)
22	LPP	O	203	-	31,31,43	1.25	3 (9%)	35,36,48	1.11	2 (5%)
23	TRT	r	103	-	25,25,25	0.53	0	33,33,33	0.83	1 (3%)
20	CDL	d	201	-	90,90,99	0.91	8 (8%)	96,102,111	1.04	4 (4%)
20	CDL	e	101	-	62,62,99	1.08	8 (12%)	68,74,111	1.11	4 (5%)
20	CDL	m	202	-	52,52,99	1.19	8 (15%)	58,64,111	1.24	4 (6%)
23	TRT	g	201	-	25,25,25	0.53	0	33,33,33	0.80	1 (3%)
20	CDL	a	501	-	80,80,99	0.96	7 (8%)	86,92,111	1.11	5 (5%)
22	LPP	I	101	-	43,43,43	1.11	2 (4%)	47,48,48	0.98	2 (4%)
20	CDL	A	504	-	62,62,99	1.09	8 (12%)	68,74,111	1.17	4 (5%)
20	CDL	D	202	-	84,84,99	0.95	8 (9%)	90,96,111	1.03	4 (4%)
20	CDL	M	204	-	52,52,99	1.19	8 (15%)	58,64,111	1.25	4 (6%)
22	LPP	F	301	-	23,23,43	1.37	3 (13%)	27,28,48	1.19	2 (7%)
20	CDL	A	503	-	80,80,99	0.97	8 (10%)	85,91,111	1.05	4 (4%)
22	LPP	f	301	-	23,23,43	1.37	3 (13%)	27,28,48	1.20	2 (7%)
21	LMT	Q	101	-	36,36,36	1.17	6 (16%)	47,47,47	1.01	2 (4%)
23	TRT	m	204	-	25,25,25	0.54	0	33,33,33	0.79	1 (3%)
23	TRT	G	201	-	25,25,25	0.53	0	33,33,33	0.79	1 (3%)
21	LMT	q	101	-	36,36,36	1.17	6 (16%)	47,47,47	1.00	2 (4%)
21	LMT	f	302	-	36,36,36	1.18	5 (13%)	47,47,47	0.95	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LPP	i	101	-	43,43,43	1.11	3 (6%)	47,48,48	0.98	2 (4%)
23	TRT	M	202	-	25,25,25	0.54	0	33,33,33	0.79	1 (3%)
23	TRT	g	202	-	25,25,25	0.60	0	33,33,33	0.69	0
20	CDL	D	201	-	90,90,99	0.91	8 (8%)	96,102,111	1.03	4 (4%)
23	TRT	p	203	-	25,25,25	1.25	3 (12%)	33,33,33	4.75	8 (24%)
20	CDL	A	501	-	80,80,99	0.97	7 (8%)	86,92,111	1.11	5 (5%)
20	CDL	R	101	-	75,75,99	1.00	8 (10%)	81,87,111	1.05	4 (4%)
20	CDL	P	201	-	47,47,99	1.24	8 (17%)	53,59,111	1.29	5 (9%)
20	CDL	r	101	-	75,75,99	1.00	8 (10%)	81,87,111	1.03	4 (4%)
22	LPP	O	202	-	22,22,43	1.39	3 (13%)	26,27,48	1.17	2 (7%)
22	LPP	R	102	-	30,30,43	1.25	4 (13%)	34,35,48	1.22	2 (5%)
22	LPP	r	102	-	30,30,43	1.24	4 (13%)	34,35,48	1.22	2 (5%)
22	LPP	o	203	-	31,31,43	1.26	4 (12%)	35,36,48	1.11	2 (5%)
21	LMT	D	203	-	36,36,36	1.19	5 (13%)	47,47,47	0.91	1 (2%)
23	TRT	R	103	-	25,25,25	0.53	0	33,33,33	0.83	1 (3%)
23	TRT	n	203	-	25,25,25	0.60	0	33,33,33	0.63	0
20	CDL	p	201	-	97,97,99	0.89	8 (8%)	103,109,111	1.00	4 (3%)
23	TRT	m	203	-	25,25,25	0.55	0	33,33,33	0.70	1 (3%)
22	LPP	o	202	-	22,22,43	1.39	2 (9%)	26,27,48	1.17	2 (7%)
20	CDL	a	502	-	80,80,99	0.97	8 (10%)	86,92,111	1.08	4 (4%)
20	CDL	p	202	-	47,47,99	1.23	8 (17%)	53,59,111	1.28	5 (9%)
22	LPP	N	203	-	25,25,43	1.34	3 (12%)	29,30,48	1.24	2 (6%)
23	TRT	G	202	-	25,25,25	0.59	0	33,33,33	0.69	0
20	CDL	d	202	-	84,84,99	0.95	7 (8%)	90,96,111	1.01	4 (4%)
21	LMT	d	203	-	36,36,36	1.19	5 (13%)	47,47,47	0.91	1 (2%)
23	TRT	M	201	-	25,25,25	0.55	0	33,33,33	0.70	1 (3%)
21	LMT	F	302	-	36,36,36	1.18	5 (13%)	47,47,47	0.95	2 (4%)
22	LPP	P	202	-	25,25,43	1.33	3 (12%)	29,30,48	1.24	2 (6%)
23	TRT	n	202	-	25,25,25	0.51	0	33,33,33	0.87	1 (3%)
20	CDL	m	201	-	76,76,99	0.99	8 (10%)	82,88,111	1.09	4 (4%)
20	CDL	M	203	-	76,76,99	0.99	8 (10%)	82,88,111	1.09	4 (4%)
20	CDL	o	201	-	64,64,99	1.07	8 (12%)	70,76,111	1.08	4 (5%)
23	TRT	N	201	-	25,25,25	0.50	0	33,33,33	0.87	1 (3%)
20	CDL	A	502	-	80,80,99	0.98	8 (10%)	86,92,111	1.08	4 (4%)
20	CDL	O	201	-	64,64,99	1.07	8 (12%)	70,76,111	1.07	4 (5%)

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
21	LMT	N	204	-	-	9/21/61/61	0/2/2/2
20	CDL	a	503	-	-	34/89/89/110	-
21	LMT	n	201	-	-	9/21/61/61	0/2/2/2
23	TRT	P	203	-	-	15/23/23/23	0/1/1/1
20	CDL	E	101	-	-	42/73/73/110	-
23	TRT	N	202	-	-	14/23/23/23	0/1/1/1
20	CDL	a	504	-	-	34/73/73/110	-
22	LPP	O	203	-	-	14/33/33/45	-
23	TRT	r	103	-	-	9/23/23/23	0/1/1/1
20	CDL	d	201	-	-	36/101/101/110	-
20	CDL	e	101	-	-	43/73/73/110	-
20	CDL	m	202	-	-	31/63/63/110	-
23	TRT	g	201	-	-	8/23/23/23	0/1/1/1
20	CDL	a	501	-	-	30/91/91/110	-
22	LPP	I	101	-	-	14/45/45/45	-
20	CDL	A	504	-	-	34/73/73/110	-
20	CDL	D	202	-	-	43/95/95/110	-
20	CDL	M	204	-	-	31/63/63/110	-
22	LPP	F	301	-	-	5/25/25/45	-
20	CDL	A	503	-	-	34/89/89/110	-
22	LPP	f	301	-	-	5/25/25/45	-
21	LMT	Q	101	-	-	6/21/61/61	0/2/2/2
23	TRT	m	204	-	-	8/23/23/23	0/1/1/1
23	TRT	G	201	-	-	8/23/23/23	0/1/1/1
21	LMT	q	101	-	-	6/21/61/61	0/2/2/2
21	LMT	f	302	-	-	8/21/61/61	0/2/2/2
22	LPP	i	101	-	-	14/45/45/45	-
23	TRT	M	202	-	-	8/23/23/23	0/1/1/1
23	TRT	g	202	-	-	16/23/23/23	0/1/1/1
20	CDL	D	201	-	-	39/101/101/110	-
23	TRT	p	203	-	-	15/23/23/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CDL	A	501	-	-	29/91/91/110	-
20	CDL	R	101	-	-	36/86/86/110	-
20	CDL	P	201	-	-	27/57/57/110	-
20	CDL	r	101	-	-	37/86/86/110	-
22	LPP	O	202	-	-	10/24/24/45	-
22	LPP	R	102	-	-	13/32/32/45	-
22	LPP	r	102	-	-	13/32/32/45	-
22	LPP	o	203	-	-	14/33/33/45	-
21	LMT	D	203	-	-	8/21/61/61	0/2/2/2
23	TRT	R	103	-	-	9/23/23/23	0/1/1/1
23	TRT	n	203	-	-	14/23/23/23	0/1/1/1
20	CDL	p	201	-	-	46/108/108/110	-
23	TRT	m	203	-	-	10/23/23/23	0/1/1/1
22	LPP	o	202	-	-	10/24/24/45	-
20	CDL	a	502	-	-	33/91/91/110	-
20	CDL	p	202	-	-	25/57/57/110	-
22	LPP	N	203	-	-	12/27/27/45	-
23	TRT	G	202	-	-	16/23/23/23	0/1/1/1
20	CDL	d	202	-	-	44/95/95/110	-
21	LMT	d	203	-	-	8/21/61/61	0/2/2/2
23	TRT	M	201	-	-	10/23/23/23	0/1/1/1
21	LMT	F	302	-	-	8/21/61/61	0/2/2/2
22	LPP	P	202	-	-	12/27/27/45	-
23	TRT	n	202	-	-	7/23/23/23	0/1/1/1
20	CDL	m	201	-	-	41/87/87/110	-
20	CDL	M	203	-	-	41/87/87/110	-
20	CDL	o	201	-	-	37/75/75/110	-
23	TRT	N	201	-	-	7/23/23/23	0/1/1/1
20	CDL	A	502	-	-	31/91/91/110	-
20	CDL	O	201	-	-	34/75/75/110	-

All (284) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	203	TRT	C6-C9	4.14	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	p	203	TRT	C6-C9	4.14	1.60	1.53
22	P	202	LPP	O9-C11	3.36	1.43	1.34
22	N	203	LPP	O9-C11	3.34	1.43	1.34
22	I	101	LPP	O9-C11	3.25	1.43	1.34
22	i	101	LPP	O9-C11	3.25	1.43	1.34
22	r	102	LPP	O9-C11	3.20	1.43	1.34
22	R	102	LPP	O9-C11	3.20	1.43	1.34
22	o	202	LPP	O9-C11	3.18	1.43	1.34
22	O	202	LPP	O9-C11	3.18	1.43	1.34
22	O	203	LPP	O9-C11	3.18	1.43	1.34
22	o	203	LPP	O9-C11	3.17	1.43	1.34
22	F	301	LPP	O9-C11	3.14	1.43	1.34
22	f	301	LPP	O9-C11	3.14	1.43	1.34
21	n	201	LMT	O3'-C3'	-2.99	1.35	1.43
22	i	101	LPP	O27-C29	2.97	1.42	1.33
21	N	204	LMT	O3'-C3'	-2.97	1.36	1.43
22	I	101	LPP	O27-C29	2.96	1.42	1.33
22	o	203	LPP	O27-C29	2.93	1.41	1.33
22	o	202	LPP	O27-C29	2.92	1.41	1.33
22	O	203	LPP	O27-C29	2.91	1.41	1.33
22	O	202	LPP	O27-C29	2.89	1.41	1.33
21	D	203	LMT	O3'-C3'	-2.87	1.36	1.43
21	d	203	LMT	O3'-C3'	-2.84	1.36	1.43
22	F	301	LPP	O27-C29	2.79	1.41	1.33
20	D	202	CDL	OB6-CB4	-2.79	1.39	1.46
22	f	301	LPP	O27-C29	2.78	1.41	1.33
20	d	202	CDL	OB6-CB4	-2.78	1.39	1.46
20	A	501	CDL	OB6-CB4	-2.77	1.39	1.46
20	a	501	CDL	OB6-CB4	-2.77	1.39	1.46
22	R	102	LPP	O27-C29	2.76	1.41	1.33
21	F	302	LMT	O3'-C3'	-2.76	1.36	1.43
22	N	203	LPP	O27-C29	2.75	1.41	1.33
22	P	202	LPP	O27-C29	2.75	1.41	1.33
22	r	102	LPP	O27-C29	2.75	1.41	1.33
20	d	201	CDL	OB6-CB4	-2.74	1.39	1.46
21	f	302	LMT	O3'-C3'	-2.73	1.36	1.43
21	q	101	LMT	O3'-C3'	-2.71	1.36	1.43
20	D	201	CDL	OB6-CB4	-2.71	1.39	1.46
21	Q	101	LMT	O3'-C3'	-2.70	1.36	1.43
20	m	201	CDL	OA6-CA4	-2.64	1.40	1.46
20	M	203	CDL	OA6-CA4	-2.63	1.40	1.46
20	m	202	CDL	OA6-CA4	-2.63	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	204	CDL	OA6-CA4	-2.62	1.40	1.46
21	D	203	LMT	O2'-C2'	-2.61	1.36	1.43
21	d	203	LMT	O2'-C2'	-2.61	1.36	1.43
20	m	201	CDL	OB6-CB4	-2.60	1.40	1.46
21	f	302	LMT	O2B-C2B	-2.59	1.36	1.43
21	F	302	LMT	O2B-C2B	-2.59	1.36	1.43
20	P	201	CDL	OB6-CB4	-2.59	1.40	1.46
21	d	203	LMT	O2B-C2B	-2.59	1.36	1.43
21	D	203	LMT	O2B-C2B	-2.57	1.36	1.43
20	p	201	CDL	OB6-CB4	-2.56	1.40	1.46
20	a	501	CDL	OA6-CA4	-2.56	1.40	1.46
20	p	202	CDL	OB6-CB4	-2.56	1.40	1.46
20	A	501	CDL	OA6-CA4	-2.56	1.40	1.46
20	M	204	CDL	OB6-CB4	-2.55	1.40	1.46
20	m	202	CDL	OB6-CB4	-2.55	1.40	1.46
20	M	203	CDL	OB6-CB4	-2.55	1.40	1.46
20	a	504	CDL	OB6-CB4	-2.53	1.40	1.46
20	o	201	CDL	OB6-CB4	-2.52	1.40	1.46
20	A	504	CDL	OB6-CB4	-2.51	1.40	1.46
20	D	201	CDL	OA6-CA4	-2.50	1.40	1.46
20	r	101	CDL	OB6-CB4	-2.49	1.40	1.46
20	R	101	CDL	OB6-CB4	-2.49	1.40	1.46
20	A	503	CDL	OB6-CB4	-2.49	1.40	1.46
20	a	504	CDL	OA6-CA4	-2.49	1.40	1.46
20	A	504	CDL	OA8-CA7	2.49	1.40	1.33
20	d	201	CDL	OA6-CA4	-2.49	1.40	1.46
20	O	201	CDL	OB6-CB4	-2.49	1.40	1.46
20	a	504	CDL	OA8-CA7	2.49	1.40	1.33
20	A	502	CDL	OB8-CB7	2.47	1.40	1.33
20	a	502	CDL	OB8-CB7	2.47	1.40	1.33
20	a	503	CDL	OB6-CB4	-2.45	1.40	1.46
21	F	302	LMT	O3B-C3B	-2.45	1.37	1.43
21	N	204	LMT	O2B-C2B	-2.45	1.37	1.43
20	A	504	CDL	OA6-CA4	-2.45	1.40	1.46
21	n	201	LMT	O2B-C2B	-2.44	1.37	1.43
20	p	201	CDL	OA6-CA4	-2.44	1.40	1.46
20	a	502	CDL	OB6-CB4	-2.44	1.40	1.46
20	r	101	CDL	OB8-CB7	2.43	1.40	1.33
20	E	101	CDL	OB6-CB4	-2.43	1.40	1.46
20	m	201	CDL	OA8-CA7	2.43	1.40	1.33
20	A	502	CDL	OB6-CB4	-2.42	1.40	1.46
21	N	204	LMT	O2'-C2'	-2.41	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	f	302	LMT	O3B-C3B	-2.41	1.37	1.43
20	a	504	CDL	OB8-CB7	2.41	1.40	1.33
20	r	101	CDL	OA6-CA4	-2.41	1.40	1.46
20	O	201	CDL	OA8-CA7	2.41	1.40	1.33
20	R	101	CDL	OB8-CB7	2.41	1.40	1.33
20	M	204	CDL	OB8-CB7	2.40	1.40	1.33
20	O	201	CDL	OB8-CB7	2.40	1.40	1.33
21	n	201	LMT	O2'-C2'	-2.40	1.37	1.43
20	D	201	CDL	OA8-CA7	2.40	1.40	1.33
21	q	101	LMT	O3B-C3B	-2.40	1.37	1.43
21	Q	101	LMT	O3B-C3B	-2.40	1.37	1.43
20	d	202	CDL	OA8-CA7	2.39	1.40	1.33
20	A	504	CDL	OB8-CB7	2.39	1.40	1.33
20	M	203	CDL	OA8-CA7	2.39	1.40	1.33
20	e	101	CDL	OB6-CB4	-2.39	1.40	1.46
20	R	101	CDL	OA6-CA4	-2.39	1.40	1.46
20	P	201	CDL	OA6-CA5	2.39	1.41	1.34
20	D	201	CDL	OB8-CB7	2.39	1.40	1.33
20	D	202	CDL	OB8-CB7	2.39	1.40	1.33
20	E	101	CDL	OB8-CB7	2.39	1.40	1.33
20	d	201	CDL	OA8-CA7	2.39	1.40	1.33
20	m	202	CDL	OB8-CB7	2.38	1.40	1.33
20	o	201	CDL	OB8-CB7	2.38	1.40	1.33
20	P	201	CDL	OA8-CA7	2.38	1.40	1.33
20	d	202	CDL	OB8-CB7	2.38	1.40	1.33
20	e	101	CDL	OB8-CB7	2.38	1.40	1.33
20	P	201	CDL	OB8-CB7	2.37	1.40	1.33
20	d	201	CDL	OB8-CB7	2.37	1.40	1.33
20	p	202	CDL	OA8-CA7	2.37	1.40	1.33
20	o	201	CDL	OA6-CA4	-2.37	1.40	1.46
20	r	101	CDL	OA8-CA6	-2.37	1.39	1.45
21	N	204	LMT	O3B-C3B	-2.36	1.37	1.43
20	o	201	CDL	OA8-CA7	2.36	1.40	1.33
20	p	202	CDL	OB8-CB7	2.36	1.40	1.33
20	O	201	CDL	OA6-CA4	-2.36	1.40	1.46
20	D	202	CDL	OA8-CA7	2.35	1.40	1.33
20	e	101	CDL	OA8-CA7	2.35	1.40	1.33
21	n	201	LMT	O3B-C3B	-2.35	1.37	1.43
21	F	302	LMT	O2'-C2'	-2.35	1.37	1.43
20	A	502	CDL	OA8-CA6	-2.35	1.39	1.45
20	M	203	CDL	OB8-CB7	2.35	1.40	1.33
20	a	502	CDL	OB6-CB5	2.35	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	502	CDL	OA6-CA4	-2.35	1.40	1.46
20	A	502	CDL	OB6-CB5	2.35	1.40	1.34
20	E	101	CDL	OA8-CA7	2.34	1.40	1.33
20	a	503	CDL	OA8-CA7	2.34	1.40	1.33
20	m	201	CDL	OB8-CB7	2.34	1.40	1.33
20	M	204	CDL	OA8-CA7	2.33	1.40	1.33
20	a	501	CDL	OB8-CB7	2.33	1.40	1.33
21	D	203	LMT	O3B-C3B	-2.33	1.37	1.43
21	d	203	LMT	O3B-C3B	-2.33	1.37	1.43
21	f	302	LMT	O2'-C2'	-2.33	1.37	1.43
20	A	501	CDL	OA8-CA7	2.33	1.40	1.33
20	a	502	CDL	OA8-CA6	-2.33	1.39	1.45
20	p	201	CDL	OA8-CA7	2.33	1.40	1.33
21	Q	101	LMT	O4'-C4B	-2.33	1.37	1.43
20	A	501	CDL	OA8-CA6	-2.33	1.39	1.45
20	A	503	CDL	OA8-CA7	2.33	1.40	1.33
20	p	201	CDL	OB8-CB7	2.32	1.40	1.33
20	R	101	CDL	OA8-CA6	-2.32	1.39	1.45
20	p	202	CDL	OA6-CA5	2.32	1.40	1.34
20	a	503	CDL	OA8-CA6	-2.32	1.39	1.45
20	D	202	CDL	OA8-CA6	-2.31	1.39	1.45
20	a	501	CDL	OA8-CA7	2.31	1.40	1.33
20	A	501	CDL	OB8-CB7	2.31	1.40	1.33
20	a	503	CDL	OB8-CB7	2.31	1.40	1.33
20	A	503	CDL	OA8-CA6	-2.31	1.39	1.45
20	P	201	CDL	OB6-CB5	2.31	1.40	1.35
20	A	503	CDL	OB8-CB7	2.30	1.40	1.33
20	A	502	CDL	OA8-CA7	2.30	1.40	1.33
21	f	302	LMT	O4'-C4B	-2.30	1.37	1.43
20	m	202	CDL	OA8-CA7	2.30	1.40	1.33
20	a	501	CDL	OA8-CA6	-2.30	1.39	1.45
21	q	101	LMT	O4'-C4B	-2.29	1.37	1.43
20	D	202	CDL	OA6-CA4	-2.29	1.40	1.46
21	F	302	LMT	O4'-C4B	-2.29	1.37	1.43
20	e	101	CDL	OA6-CA4	-2.29	1.40	1.46
21	Q	101	LMT	O2B-C2B	-2.28	1.37	1.43
20	r	101	CDL	OA8-CA7	2.28	1.40	1.33
20	e	101	CDL	OB6-CB5	2.28	1.40	1.34
21	q	101	LMT	O2B-C2B	-2.28	1.37	1.43
20	p	201	CDL	OA8-CA6	-2.28	1.40	1.45
20	R	101	CDL	OA6-CA5	2.28	1.40	1.34
21	D	203	LMT	O4'-C4B	-2.28	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	204	CDL	OA8-CA6	-2.27	1.40	1.45
20	p	202	CDL	OB6-CB5	2.27	1.40	1.35
21	d	203	LMT	O4'-C4B	-2.27	1.37	1.43
21	q	101	LMT	O2'-C2'	-2.27	1.37	1.43
20	R	101	CDL	OA8-CA7	2.27	1.40	1.33
20	a	504	CDL	OB6-CB5	2.27	1.40	1.34
20	E	101	CDL	OB6-CB5	2.27	1.40	1.34
20	r	101	CDL	OA6-CA5	2.27	1.40	1.34
20	E	101	CDL	OA6-CA4	-2.26	1.40	1.46
20	A	504	CDL	OB6-CB5	2.25	1.40	1.34
20	A	503	CDL	OA6-CA4	-2.25	1.41	1.46
20	d	202	CDL	OA6-CA4	-2.25	1.41	1.46
20	A	502	CDL	OA6-CA4	-2.25	1.41	1.46
20	a	502	CDL	OA8-CA7	2.25	1.39	1.33
20	m	202	CDL	OA8-CA6	-2.25	1.40	1.45
20	d	202	CDL	OA8-CA6	-2.25	1.40	1.45
21	Q	101	LMT	O2'-C2'	-2.24	1.37	1.43
20	E	101	CDL	OA6-CA5	2.23	1.40	1.34
20	a	503	CDL	OB8-CB6	-2.23	1.40	1.45
20	a	503	CDL	OA6-CA4	-2.23	1.41	1.46
20	o	201	CDL	OB6-CB5	2.23	1.40	1.34
20	p	201	CDL	OA6-CA5	2.23	1.40	1.34
20	A	502	CDL	OA6-CA5	2.22	1.40	1.34
20	O	201	CDL	OB6-CB5	2.22	1.40	1.34
20	D	202	CDL	OA6-CA5	2.22	1.40	1.34
20	e	101	CDL	OA6-CA5	2.21	1.40	1.34
20	a	501	CDL	OA6-CA5	2.21	1.40	1.34
23	p	203	TRT	C8-C6	2.21	1.60	1.53
20	A	501	CDL	OB8-CB6	-2.21	1.40	1.45
20	o	201	CDL	OA6-CA5	2.21	1.40	1.34
20	p	202	CDL	OA6-CA4	-2.20	1.41	1.46
23	P	203	TRT	C8-C6	2.20	1.59	1.53
20	m	201	CDL	OB6-CB5	2.20	1.40	1.34
20	A	503	CDL	OB8-CB6	-2.20	1.40	1.45
20	a	501	CDL	OB8-CB6	-2.20	1.40	1.45
20	d	202	CDL	OA6-CA5	2.20	1.40	1.34
20	P	201	CDL	OB8-CB6	-2.20	1.40	1.45
20	a	502	CDL	OA6-CA5	2.20	1.40	1.34
20	p	202	CDL	OB8-CB6	-2.20	1.40	1.45
20	a	504	CDL	OA6-CA5	2.19	1.40	1.34
21	N	204	LMT	O4'-C4B	-2.19	1.37	1.43
20	e	101	CDL	OA8-CA6	-2.19	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	204	CDL	OA6-CA5	2.19	1.40	1.34
20	A	503	CDL	OA6-CA5	2.19	1.40	1.34
20	d	202	CDL	OB8-CB6	-2.19	1.40	1.45
23	p	203	TRT	C7-C6	2.19	1.59	1.53
20	D	202	CDL	OB8-CB6	-2.19	1.40	1.45
20	m	202	CDL	OA6-CA5	2.19	1.40	1.34
20	A	501	CDL	OA6-CA5	2.18	1.40	1.34
20	p	201	CDL	OB8-CB6	-2.18	1.40	1.45
20	a	504	CDL	OA8-CA6	-2.18	1.40	1.45
20	D	201	CDL	OA6-CA5	2.18	1.40	1.34
20	a	503	CDL	OA6-CA5	2.17	1.40	1.34
23	P	203	TRT	C7-C6	2.17	1.59	1.53
20	M	204	CDL	OB6-CB5	2.17	1.40	1.34
20	A	504	CDL	OA8-CA6	-2.17	1.40	1.45
20	r	101	CDL	OB6-CB5	2.17	1.40	1.34
20	d	201	CDL	OA6-CA5	2.17	1.40	1.34
20	A	504	CDL	OA6-CA5	2.17	1.40	1.34
20	M	203	CDL	OB6-CB5	2.17	1.40	1.34
20	m	202	CDL	OB6-CB5	2.17	1.40	1.34
20	A	502	CDL	OB8-CB6	-2.16	1.40	1.45
20	R	101	CDL	OB6-CB5	2.16	1.40	1.34
20	P	201	CDL	OA6-CA4	-2.16	1.41	1.46
20	a	504	CDL	OB8-CB6	-2.16	1.40	1.45
20	o	201	CDL	OA8-CA6	-2.16	1.40	1.45
20	O	201	CDL	OA6-CA5	2.15	1.40	1.34
21	n	201	LMT	O4'-C4B	-2.15	1.37	1.43
20	a	503	CDL	OB6-CB5	2.15	1.40	1.34
20	m	202	CDL	OB8-CB6	-2.14	1.40	1.45
20	E	101	CDL	OA8-CA6	-2.14	1.40	1.45
20	a	502	CDL	OB8-CB6	-2.14	1.40	1.45
20	A	504	CDL	OB8-CB6	-2.13	1.40	1.45
20	p	201	CDL	OB6-CB5	2.13	1.40	1.34
20	A	503	CDL	OB6-CB5	2.12	1.40	1.34
20	M	204	CDL	OB8-CB6	-2.12	1.40	1.45
20	D	201	CDL	OA8-CA6	-2.12	1.40	1.45
20	O	201	CDL	OA8-CA6	-2.11	1.40	1.45
20	d	201	CDL	OA8-CA6	-2.11	1.40	1.45
20	P	201	CDL	OA8-CA6	-2.11	1.40	1.45
20	E	101	CDL	OB8-CB6	-2.10	1.40	1.45
21	q	101	LMT	O1'-C1'	-2.10	1.36	1.40
20	M	203	CDL	OA8-CA6	-2.10	1.40	1.45
20	m	201	CDL	OB8-CB6	-2.10	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	m	201	CDL	OA6-CA5	2.10	1.40	1.34
21	Q	101	LMT	O1'-C1'	-2.10	1.36	1.40
20	m	201	CDL	OA8-CA6	-2.09	1.40	1.45
20	M	203	CDL	OB8-CB6	-2.09	1.40	1.45
20	M	203	CDL	OA6-CA5	2.09	1.40	1.34
20	o	201	CDL	OB8-CB6	-2.08	1.40	1.45
20	e	101	CDL	OB8-CB6	-2.08	1.40	1.45
22	o	203	LPP	O9-C7	-2.07	1.41	1.46
22	O	203	LPP	O9-C7	-2.07	1.41	1.46
20	r	101	CDL	OB8-CB6	-2.07	1.40	1.45
20	R	101	CDL	OB8-CB6	-2.07	1.40	1.45
20	O	201	CDL	OB8-CB6	-2.07	1.40	1.45
22	R	102	LPP	O9-C7	-2.06	1.41	1.46
20	p	202	CDL	OA8-CA6	-2.05	1.40	1.45
20	D	201	CDL	OB8-CB6	-2.04	1.40	1.45
22	F	301	LPP	O9-C7	-2.04	1.41	1.46
22	f	301	LPP	O9-C7	-2.03	1.41	1.46
20	d	201	CDL	OB6-CB5	2.03	1.40	1.34
22	N	203	LPP	P1-O5	2.02	1.66	1.60
22	R	102	LPP	C12-C11	2.02	1.56	1.50
21	N	204	LMT	O1'-C1'	-2.02	1.36	1.40
21	n	201	LMT	O1'-C1'	-2.02	1.36	1.40
22	i	101	LPP	O9-C7	-2.01	1.41	1.46
22	r	102	LPP	C12-C11	2.01	1.56	1.50
20	d	201	CDL	OB8-CB6	-2.01	1.40	1.45
22	o	203	LPP	P1-O5	2.01	1.66	1.60
22	r	102	LPP	O9-C7	-2.01	1.41	1.46
20	D	201	CDL	OB6-CB5	2.01	1.40	1.34
20	D	202	CDL	OB6-CB5	2.01	1.40	1.34
22	O	202	LPP	O9-C7	-2.01	1.41	1.46
22	P	202	LPP	P1-O5	2.00	1.66	1.60

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	203	TRT	C7-C6-C8	16.40	152.16	107.28
23	p	203	TRT	C7-C6-C8	16.39	152.14	107.28
23	P	203	TRT	C5-C6-C9	12.47	139.47	111.93
23	p	203	TRT	C5-C6-C9	12.47	139.46	111.93
23	p	203	TRT	C8-C6-C9	-11.32	81.81	110.20
23	P	203	TRT	C8-C6-C9	-11.31	81.85	110.20
23	P	203	TRT	C7-C6-C9	-11.00	82.62	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	p	203	TRT	C7-C6-C9	-10.99	82.65	110.20
20	P	201	CDL	OB6-CB5-C51	4.84	119.99	111.09
20	p	202	CDL	OB6-CB5-C51	4.84	119.98	111.09
20	M	204	CDL	OA6-CA5-C11	4.66	121.55	111.50
20	m	202	CDL	OA6-CA5-C11	4.55	121.31	111.50
23	p	203	TRT	C8-C6-C5	-4.50	88.00	109.08
23	P	203	TRT	C8-C6-C5	-4.50	88.01	109.08
23	P	203	TRT	C7-C6-C5	-4.30	88.94	109.08
23	p	203	TRT	C7-C6-C5	-4.30	88.94	109.08
20	a	504	CDL	OA6-CA5-C11	4.23	120.63	111.50
20	A	504	CDL	OA6-CA5-C11	4.22	120.59	111.50
22	P	202	LPP	O9-C11-C12	4.20	120.54	111.50
22	N	203	LPP	O9-C11-C12	4.19	120.53	111.50
22	r	102	LPP	O9-C11-C12	4.14	120.42	111.50
22	R	102	LPP	O9-C11-C12	4.13	120.41	111.50
20	O	201	CDL	OB6-CB5-C51	4.05	120.24	111.50
20	o	201	CDL	OB6-CB5-C51	4.05	120.22	111.50
20	R	101	CDL	OA6-CA5-C11	4.04	120.20	111.50
20	e	101	CDL	OA6-CA5-C11	4.04	120.20	111.50
20	a	502	CDL	OB6-CB5-C51	4.02	120.16	111.50
20	A	502	CDL	OB6-CB5-C51	3.98	120.09	111.50
20	E	101	CDL	OA6-CA5-C11	3.98	120.08	111.50
20	A	501	CDL	OA6-CA5-C11	3.97	120.05	111.50
20	a	501	CDL	OA6-CA5-C11	3.94	119.99	111.50
20	m	202	CDL	OB6-CB5-C51	3.89	119.89	111.50
20	p	201	CDL	OB6-CB5-C51	3.89	119.89	111.50
22	O	203	LPP	O9-C11-C12	3.89	119.87	111.50
20	M	204	CDL	OB6-CB5-C51	3.87	119.85	111.50
22	o	203	LPP	O9-C11-C12	3.87	119.84	111.50
20	r	101	CDL	OA6-CA5-C11	3.86	119.82	111.50
20	a	504	CDL	OB6-CB5-C51	3.81	119.71	111.50
20	A	504	CDL	OB6-CB5-C51	3.80	119.69	111.50
20	m	201	CDL	OB6-CB5-C51	3.78	119.64	111.50
20	M	203	CDL	OB6-CB5-C51	3.77	119.62	111.50
20	a	503	CDL	OA6-CA5-C11	3.75	119.58	111.50
20	A	503	CDL	OA6-CA5-C11	3.75	119.58	111.50
20	d	201	CDL	OB6-CB5-C51	3.75	119.58	111.50
20	D	201	CDL	OB6-CB5-C51	3.73	119.53	111.50
20	d	201	CDL	OA6-CA5-C11	3.70	119.47	111.50
20	D	201	CDL	OA6-CA5-C11	3.70	119.47	111.50
20	P	201	CDL	OA6-CA5-C11	3.69	119.46	111.50
22	f	301	LPP	O9-C11-C12	3.69	119.46	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	202	LPP	O9-C11-C12	3.68	119.44	111.50
22	o	202	LPP	O9-C11-C12	3.68	119.43	111.50
20	m	201	CDL	OA6-CA5-C11	3.67	119.42	111.50
20	M	203	CDL	OA6-CA5-C11	3.66	119.40	111.50
22	F	301	LPP	O9-C11-C12	3.66	119.40	111.50
20	R	101	CDL	OB6-CB5-C51	3.65	119.37	111.50
20	r	101	CDL	OB6-CB5-C51	3.65	119.36	111.50
20	a	501	CDL	OB6-CB5-C51	3.64	119.35	111.50
20	A	503	CDL	OB6-CB5-C51	3.64	119.34	111.50
20	a	503	CDL	OB6-CB5-C51	3.64	119.33	111.50
20	A	501	CDL	OB6-CB5-C51	3.63	119.33	111.50
20	a	502	CDL	OA6-CA5-C11	3.61	119.27	111.50
20	e	101	CDL	OB6-CB5-C51	3.60	119.26	111.50
20	p	202	CDL	OA6-CA5-C11	3.60	119.25	111.50
20	E	101	CDL	OB6-CB5-C51	3.56	119.18	111.50
20	A	502	CDL	OA6-CA5-C11	3.49	119.03	111.50
20	p	201	CDL	OA6-CA5-C11	3.45	118.94	111.50
23	p	203	TRT	C1-C5-C6	-3.42	111.62	123.91
23	P	203	TRT	C1-C5-C6	-3.41	111.65	123.91
22	i	101	LPP	O9-C11-C12	3.37	118.77	111.50
22	I	101	LPP	O9-C11-C12	3.37	118.75	111.50
20	o	201	CDL	OA8-CA7-C31	3.26	119.94	111.38
20	D	202	CDL	OB6-CB5-C51	3.26	118.53	111.50
20	d	202	CDL	OB6-CB5-C51	3.26	118.53	111.50
20	O	201	CDL	OA6-CA5-C11	3.22	118.44	111.50
20	o	201	CDL	OA6-CA5-C11	3.22	118.44	111.50
20	a	504	CDL	OA8-CA7-C31	3.20	121.95	111.91
20	A	504	CDL	OA8-CA7-C31	3.16	121.83	111.91
20	D	202	CDL	OA6-CA5-C11	3.11	118.21	111.50
20	O	201	CDL	OA8-CA7-C31	3.08	119.47	111.38
20	d	202	CDL	OA6-CA5-C11	2.98	117.92	111.50
20	d	201	CDL	OA8-CA7-C31	2.87	120.93	111.91
20	D	201	CDL	OA8-CA7-C31	2.87	120.90	111.91
20	M	203	CDL	OA8-CA7-C31	2.87	120.90	111.91
20	m	201	CDL	OA8-CA7-C31	2.86	120.87	111.91
20	A	503	CDL	OB8-CB7-C71	2.85	120.86	111.91
20	a	503	CDL	OB8-CB7-C71	2.84	120.81	111.91
20	M	204	CDL	OA8-CA7-C31	2.82	120.76	111.91
20	m	202	CDL	OA8-CA7-C31	2.77	120.60	111.91
20	D	202	CDL	OB8-CB7-C71	2.75	120.53	111.91
20	p	201	CDL	OB8-CB7-C71	2.73	120.48	111.91
20	a	501	CDL	OA8-CA7-C31	2.73	120.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	501	CDL	OA8-CA7-C31	2.71	120.41	111.91
22	f	301	LPP	O27-C29-C30	2.69	120.35	111.91
20	A	502	CDL	OB8-CB7-C71	2.68	120.31	111.91
20	a	502	CDL	OB8-CB7-C71	2.68	120.31	111.91
22	F	301	LPP	O27-C29-C30	2.67	120.29	111.91
20	M	203	CDL	OB8-CB7-C71	2.65	120.23	111.91
20	m	201	CDL	OB8-CB7-C71	2.64	120.20	111.91
20	d	202	CDL	OB8-CB7-C71	2.61	120.11	111.91
20	P	201	CDL	OA8-CA7-C31	2.61	120.09	111.91
20	e	101	CDL	OB8-CB7-C71	2.60	120.07	111.91
20	p	202	CDL	OA8-CA7-C31	2.60	120.07	111.91
21	n	201	LMT	C3B-C4B-C5B	-2.59	105.61	110.24
21	N	204	LMT	C3B-C4B-C5B	-2.59	105.62	110.24
20	p	202	CDL	OB8-CB7-C71	2.59	120.02	111.91
23	P	203	TRT	C14-C9-C6	2.59	126.28	121.53
20	E	101	CDL	OB8-CB7-C71	2.58	120.02	111.91
23	p	203	TRT	C14-C9-C6	2.57	126.25	121.53
20	M	204	CDL	OB8-CB7-C71	2.57	119.97	111.91
20	m	202	CDL	OB8-CB7-C71	2.57	119.96	111.91
20	A	501	CDL	OB8-CB7-C71	2.56	119.94	111.91
20	P	201	CDL	OB8-CB7-C71	2.56	119.93	111.91
20	a	504	CDL	OB8-CB7-C71	2.55	119.92	111.91
20	A	502	CDL	OA8-CA7-C31	2.55	119.92	111.91
20	p	201	CDL	OA8-CA7-C31	2.55	119.90	111.91
20	a	501	CDL	OB8-CB7-C71	2.54	119.89	111.91
22	N	203	LPP	O27-C29-C30	2.54	119.86	111.91
20	A	504	CDL	OB8-CB7-C71	2.54	119.86	111.91
22	P	202	LPP	O27-C29-C30	2.53	119.85	111.91
23	n	202	TRT	C5-C6-C9	-2.52	106.37	111.93
20	o	201	CDL	OB8-CB7-C71	2.51	119.79	111.91
20	O	201	CDL	OB8-CB7-C71	2.50	119.76	111.91
20	P	201	CDL	CB4-OB6-CB5	-2.49	113.25	117.90
23	N	201	TRT	C5-C6-C9	-2.49	106.42	111.93
22	o	203	LPP	O27-C29-C30	2.49	119.72	111.91
22	r	102	LPP	O27-C29-C30	2.48	119.70	111.91
22	O	203	LPP	O27-C29-C30	2.48	119.69	111.91
20	p	202	CDL	CB4-OB6-CB5	-2.48	113.28	117.90
20	a	502	CDL	OA8-CA7-C31	2.47	119.67	111.91
22	R	102	LPP	O27-C29-C30	2.47	119.66	111.91
20	d	202	CDL	OA8-CA7-C31	2.45	119.60	111.91
20	D	202	CDL	OA8-CA7-C31	2.44	119.58	111.91
20	R	101	CDL	OB8-CB7-C71	2.43	119.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	r	101	CDL	OB8-CB7-C71	2.43	119.52	111.91
20	a	503	CDL	OA8-CA7-C31	2.42	119.51	111.91
20	A	503	CDL	OA8-CA7-C31	2.42	119.49	111.91
20	A	501	CDL	CB4-OB6-CB5	-2.41	111.85	117.79
21	Q	101	LMT	C3B-C4B-C5B	-2.39	105.97	110.24
21	q	101	LMT	C3B-C4B-C5B	-2.38	106.00	110.24
22	o	202	LPP	O27-C29-C30	2.38	119.36	111.91
20	e	101	CDL	OA8-CA7-C31	2.37	119.36	111.91
20	E	101	CDL	OA8-CA7-C31	2.37	119.34	111.91
20	a	501	CDL	CB4-OB6-CB5	-2.37	111.97	117.79
23	m	203	TRT	C5-C6-C9	2.37	117.15	111.93
22	O	202	LPP	O27-C29-C30	2.35	119.29	111.91
23	M	201	TRT	C5-C6-C9	2.35	117.11	111.93
20	R	101	CDL	OA8-CA7-C31	2.33	119.23	111.91
21	N	204	LMT	C3'-C4'-C5'	-2.33	105.59	110.93
20	r	101	CDL	OA8-CA7-C31	2.32	119.20	111.91
22	i	101	LPP	O27-C29-C30	2.32	119.19	111.91
22	I	101	LPP	O27-C29-C30	2.32	119.18	111.91
21	n	201	LMT	C3'-C4'-C5'	-2.32	105.61	110.93
23	R	103	TRT	C5-C6-C9	-2.29	106.87	111.93
23	r	103	TRT	C5-C6-C9	-2.29	106.88	111.93
20	d	201	CDL	OB8-CB7-C71	2.28	119.07	111.91
20	D	201	CDL	OB8-CB7-C71	2.22	118.87	111.91
21	q	101	LMT	C3'-C4'-C5'	-2.17	105.95	110.93
21	Q	101	LMT	C3'-C4'-C5'	-2.17	105.96	110.93
21	f	302	LMT	C3B-C4B-C5B	-2.14	106.43	110.24
21	F	302	LMT	C3B-C4B-C5B	-2.13	106.44	110.24
23	m	204	TRT	C5-C6-C9	-2.12	107.25	111.93
23	M	202	TRT	C5-C6-C9	-2.11	107.27	111.93
21	f	302	LMT	C3'-C4'-C5'	-2.09	106.12	110.93
21	F	302	LMT	C3'-C4'-C5'	-2.09	106.14	110.93
21	n	201	LMT	O5B-C5B-C6B	2.06	111.55	106.44
23	G	201	TRT	C5-C6-C9	-2.05	107.39	111.93
21	d	203	LMT	C3'-C4'-C5'	-2.05	106.23	110.93
21	D	203	LMT	C3'-C4'-C5'	-2.05	106.23	110.93
21	N	204	LMT	O5B-C5B-C6B	2.05	111.52	106.44
23	g	201	TRT	C5-C6-C9	-2.03	107.44	111.93
21	N	204	LMT	O5B-C1B-C2B	2.01	114.60	110.35
21	N	204	LMT	C1B-C2B-C3B	2.01	114.17	110.00

There are no chirality outliers.

All (1264) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	501	CDL	CB2-OB2-PB2-OB3
20	A	501	CDL	CB3-OB5-PB2-OB3
20	A	501	CDL	C51-CB5-OB6-CB4
20	A	502	CDL	O1-C1-CB2-OB2
20	A	502	CDL	CA3-OA5-PA1-OA3
20	A	502	CDL	OA7-CA5-OA6-CA4
20	A	502	CDL	C11-CA5-OA6-CA4
20	A	502	CDL	CB2-OB2-PB2-OB3
20	A	502	CDL	OB7-CB5-OB6-CB4
20	A	503	CDL	CA2-OA2-PA1-OA3
20	A	503	CDL	CB3-OB5-PB2-OB3
20	A	504	CDL	O1-C1-CB2-OB2
20	A	504	CDL	CA2-C1-CB2-OB2
20	A	504	CDL	OA7-CA5-OA6-CA4
20	A	504	CDL	CB3-OB5-PB2-OB4
20	D	201	CDL	CA2-OA2-PA1-OA3
20	D	201	CDL	CA2-OA2-PA1-OA4
20	D	201	CDL	CB2-OB2-PB2-OB3
20	D	202	CDL	O1-C1-CA2-OA2
20	D	202	CDL	CA2-OA2-PA1-OA3
20	D	202	CDL	CA3-OA5-PA1-OA2
20	D	202	CDL	CA3-OA5-PA1-OA4
20	D	202	CDL	C51-CB5-OB6-CB4
20	E	101	CDL	O1-C1-CB2-OB2
20	E	101	CDL	CA3-OA5-PA1-OA3
20	E	101	CDL	CB2-OB2-PB2-OB3
20	E	101	CDL	CB3-OB5-PB2-OB4
20	E	101	CDL	OB5-CB3-CB4-OB6
20	M	203	CDL	CA2-OA2-PA1-OA4
20	M	203	CDL	CB3-OB5-PB2-OB4
20	M	203	CDL	OB5-CB3-CB4-OB6
20	M	204	CDL	CA3-OA5-PA1-OA3
20	M	204	CDL	CB2-OB2-PB2-OB3
20	M	204	CDL	CB3-OB5-PB2-OB2
20	M	204	CDL	CB3-OB5-PB2-OB3
20	M	204	CDL	CB3-OB5-PB2-OB4
20	O	201	CDL	CA3-OA5-PA1-OA3
20	O	201	CDL	CA3-OA5-PA1-OA4
20	O	201	CDL	CB2-OB2-PB2-OB3
20	O	201	CDL	CB2-OB2-PB2-OB4
20	O	201	CDL	CB3-OB5-PB2-OB3
20	O	201	CDL	CB3-OB5-PB2-OB4
20	P	201	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
20	P	201	CDL	CA3-OA5-PA1-OA3
20	P	201	CDL	OA9-CA7-OA8-CA6
20	P	201	CDL	CB2-OB2-PB2-OB3
20	P	201	CDL	CB2-OB2-PB2-OB4
20	P	201	CDL	OB7-CB5-OB6-CB4
20	P	201	CDL	C51-CB5-OB6-CB4
20	R	101	CDL	CB2-OB2-PB2-OB5
20	a	501	CDL	CB2-OB2-PB2-OB3
20	a	501	CDL	CB3-OB5-PB2-OB3
20	a	501	CDL	C51-CB5-OB6-CB4
20	a	502	CDL	C11-CA5-OA6-CA4
20	a	502	CDL	CB2-OB2-PB2-OB3
20	a	502	CDL	CB2-OB2-PB2-OB5
20	a	502	CDL	OB7-CB5-OB6-CB4
20	a	503	CDL	CA2-OA2-PA1-OA3
20	a	503	CDL	CB3-OB5-PB2-OB2
20	a	503	CDL	CB3-OB5-PB2-OB3
20	a	504	CDL	O1-C1-CB2-OB2
20	a	504	CDL	CA2-C1-CB2-OB2
20	a	504	CDL	OA7-CA5-OA6-CA4
20	a	504	CDL	CB3-OB5-PB2-OB4
20	d	201	CDL	CA2-OA2-PA1-OA3
20	d	201	CDL	CA2-OA2-PA1-OA4
20	d	201	CDL	CB2-OB2-PB2-OB3
20	d	202	CDL	CA2-OA2-PA1-OA3
20	d	202	CDL	CA3-OA5-PA1-OA2
20	d	202	CDL	CA3-OA5-PA1-OA4
20	d	202	CDL	C51-CB5-OB6-CB4
20	e	101	CDL	O1-C1-CB2-OB2
20	e	101	CDL	CA3-OA5-PA1-OA3
20	e	101	CDL	CB2-OB2-PB2-OB3
20	e	101	CDL	CB3-OB5-PB2-OB4
20	e	101	CDL	OB5-CB3-CB4-OB6
20	m	201	CDL	CA2-OA2-PA1-OA4
20	m	201	CDL	CB3-OB5-PB2-OB4
20	m	201	CDL	OB5-CB3-CB4-OB6
20	m	202	CDL	CA3-OA5-PA1-OA3
20	m	202	CDL	CB2-OB2-PB2-OB3
20	m	202	CDL	CB3-OB5-PB2-OB2
20	m	202	CDL	CB3-OB5-PB2-OB3
20	m	202	CDL	CB3-OB5-PB2-OB4
20	o	201	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
20	o	201	CDL	CA2-OA2-PA1-OA4
20	o	201	CDL	CA3-OA5-PA1-OA2
20	o	201	CDL	CA3-OA5-PA1-OA3
20	o	201	CDL	CA3-OA5-PA1-OA4
20	o	201	CDL	CB2-OB2-PB2-OB3
20	o	201	CDL	CB2-OB2-PB2-OB4
20	o	201	CDL	CB3-OB5-PB2-OB3
20	o	201	CDL	CB3-OB5-PB2-OB4
20	p	201	CDL	CA3-OA5-PA1-OA4
20	p	201	CDL	OA5-CA3-CA4-OA6
20	p	201	CDL	CB3-OB5-PB2-OB3
20	p	201	CDL	CB3-OB5-PB2-OB4
20	p	202	CDL	CA2-OA2-PA1-OA3
20	p	202	CDL	CA3-OA5-PA1-OA3
20	p	202	CDL	CB2-OB2-PB2-OB3
20	p	202	CDL	CB2-OB2-PB2-OB4
20	p	202	CDL	C51-CB5-OB6-CB4
20	r	101	CDL	CB2-OB2-PB2-OB5
21	N	204	LMT	C2'-C1'-O1'-C1
21	N	204	LMT	O5'-C1'-O1'-C1
21	n	201	LMT	C2'-C1'-O1'-C1
21	n	201	LMT	O5'-C1'-O1'-C1
22	I	101	LPP	C6-O5-P1-O2
22	O	203	LPP	C6-O5-P1-O2
22	O	203	LPP	C6-O5-P1-O4
22	O	203	LPP	O5-C6-C7-O9
22	R	102	LPP	O10-C11-O9-C7
22	i	101	LPP	C6-O5-P1-O2
22	o	203	LPP	C6-O5-P1-O2
22	o	203	LPP	C6-O5-P1-O4
22	o	203	LPP	O5-C6-C7-O9
22	r	102	LPP	O10-C11-O9-C7
20	p	202	CDL	OB7-CB5-OB6-CB4
20	M	204	CDL	OA9-CA7-OA8-CA6
20	m	202	CDL	OA9-CA7-OA8-CA6
22	R	102	LPP	O28-C29-O27-C8
22	r	102	LPP	O28-C29-O27-C8
20	p	202	CDL	C31-CA7-OA8-CA6
21	Q	101	LMT	C4B-C5B-C6B-O6B
21	q	101	LMT	C4B-C5B-C6B-O6B
20	A	501	CDL	OA9-CA7-OA8-CA6
20	D	201	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
20	M	203	CDL	OA9-CA7-OA8-CA6
20	a	501	CDL	OA9-CA7-OA8-CA6
20	d	201	CDL	OA9-CA7-OA8-CA6
20	m	201	CDL	OA9-CA7-OA8-CA6
20	p	201	CDL	OA9-CA7-OA8-CA6
20	p	201	CDL	OB9-CB7-OB8-CB6
20	p	202	CDL	OA9-CA7-OA8-CA6
20	A	501	CDL	OB7-CB5-OB6-CB4
20	D	202	CDL	OB7-CB5-OB6-CB4
20	a	501	CDL	OB7-CB5-OB6-CB4
20	a	502	CDL	OA7-CA5-OA6-CA4
20	d	202	CDL	OB7-CB5-OB6-CB4
20	A	501	CDL	C31-CA7-OA8-CA6
20	D	201	CDL	C31-CA7-OA8-CA6
20	M	203	CDL	C31-CA7-OA8-CA6
20	M	204	CDL	C31-CA7-OA8-CA6
20	P	201	CDL	C31-CA7-OA8-CA6
20	a	501	CDL	C31-CA7-OA8-CA6
20	d	201	CDL	C31-CA7-OA8-CA6
20	m	201	CDL	C31-CA7-OA8-CA6
20	m	202	CDL	C31-CA7-OA8-CA6
20	p	201	CDL	C71-CB7-OB8-CB6
22	R	102	LPP	C30-C29-O27-C8
22	r	102	LPP	C30-C29-O27-C8
20	A	502	CDL	C51-CB5-OB6-CB4
20	A	504	CDL	C11-CA5-OA6-CA4
20	a	502	CDL	C51-CB5-OB6-CB4
20	a	504	CDL	C11-CA5-OA6-CA4
22	R	102	LPP	C12-C11-O9-C7
22	r	102	LPP	C12-C11-O9-C7
23	P	203	TRT	C4-C1-C5-C6
23	p	203	TRT	C4-C1-C5-C6
21	Q	101	LMT	O5B-C5B-C6B-O6B
21	q	101	LMT	O5B-C5B-C6B-O6B
21	N	204	LMT	O5'-C5'-C6'-O6'
21	n	201	LMT	O5'-C5'-C6'-O6'
20	P	201	CDL	C71-CB7-OB8-CB6
20	p	201	CDL	C31-CA7-OA8-CA6
20	p	202	CDL	C71-CB7-OB8-CB6
22	N	203	LPP	O28-C29-O27-C8
22	P	202	LPP	O28-C29-O27-C8
20	A	503	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
20	O	201	CDL	O1-C1-CA2-OA2
20	a	502	CDL	O1-C1-CB2-OB2
20	a	503	CDL	O1-C1-CA2-OA2
20	d	202	CDL	O1-C1-CA2-OA2
20	D	202	CDL	C71-CB7-OB8-CB6
20	R	101	CDL	C31-CA7-OA8-CA6
20	d	202	CDL	C71-CB7-OB8-CB6
20	r	101	CDL	C31-CA7-OA8-CA6
22	N	203	LPP	C30-C29-O27-C8
22	P	202	LPP	C30-C29-O27-C8
21	D	203	LMT	O5B-C5B-C6B-O6B
21	d	203	LMT	O5B-C5B-C6B-O6B
20	A	502	CDL	C74-C75-C76-C77
20	a	502	CDL	C74-C75-C76-C77
23	P	203	TRT	C2-C1-C5-C6
23	p	203	TRT	C2-C1-C5-C6
20	d	202	CDL	OB9-CB7-OB8-CB6
20	p	202	CDL	OB9-CB7-OB8-CB6
22	R	102	LPP	C37-C38-C39-C40
22	r	102	LPP	C37-C38-C39-C40
21	F	302	LMT	O5B-C5B-C6B-O6B
21	f	302	LMT	O5B-C5B-C6B-O6B
23	P	203	TRT	O15-C16-C17-O18
23	p	203	TRT	O15-C16-C17-O18
20	D	202	CDL	OB9-CB7-OB8-CB6
20	P	201	CDL	OB9-CB7-OB8-CB6
20	M	204	CDL	C71-C72-C73-C74
20	m	202	CDL	C71-C72-C73-C74
20	R	101	CDL	OA9-CA7-OA8-CA6
20	r	101	CDL	OA9-CA7-OA8-CA6
23	G	202	TRT	O21-C22-C23-O24
23	g	202	TRT	O21-C22-C23-O24
23	r	103	TRT	C13-C12-O15-C16
23	P	203	TRT	O21-C22-C23-O24
23	R	103	TRT	C13-C12-O15-C16
23	p	203	TRT	O21-C22-C23-O24
21	D	203	LMT	C4B-C5B-C6B-O6B
20	d	202	CDL	C75-C76-C77-C78
23	G	201	TRT	O18-C19-C20-O21
23	R	103	TRT	C11-C12-O15-C16
23	g	201	TRT	O18-C19-C20-O21
20	M	203	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
20	m	201	CDL	C11-CA5-OA6-CA4
21	d	203	LMT	C4B-C5B-C6B-O6B
20	D	202	CDL	C75-C76-C77-C78
23	r	103	TRT	C11-C12-O15-C16
20	A	502	CDL	CA2-C1-CB2-OB2
20	A	503	CDL	CB2-C1-CA2-OA2
20	a	503	CDL	CB2-C1-CA2-OA2
21	N	204	LMT	C4'-C5'-C6'-O6'
21	n	201	LMT	C4'-C5'-C6'-O6'
23	P	203	TRT	C3-C1-C5-C6
23	p	203	TRT	C3-C1-C5-C6
23	R	103	TRT	O21-C22-C23-O24
23	r	103	TRT	O21-C22-C23-O24
20	A	502	CDL	C31-CA7-OA8-CA6
20	A	503	CDL	C31-CA7-OA8-CA6
20	A	503	CDL	C71-CB7-OB8-CB6
20	E	101	CDL	C71-CB7-OB8-CB6
20	a	502	CDL	C31-CA7-OA8-CA6
20	a	503	CDL	C31-CA7-OA8-CA6
20	a	503	CDL	C71-CB7-OB8-CB6
20	e	101	CDL	C71-CB7-OB8-CB6
20	a	501	CDL	C72-C73-C74-C75
20	p	201	CDL	C57-C58-C59-C60
23	N	201	TRT	C13-C12-O15-C16
23	n	202	TRT	C13-C12-O15-C16
20	M	203	CDL	OA5-CA3-CA4-OA6
20	m	201	CDL	OA5-CA3-CA4-OA6
20	A	501	CDL	C72-C73-C74-C75
23	G	201	TRT	C11-C12-O15-C16
23	N	201	TRT	C11-C12-O15-C16
23	P	203	TRT	C13-C12-O15-C16
23	g	201	TRT	C11-C12-O15-C16
23	n	202	TRT	C11-C12-O15-C16
23	p	203	TRT	C13-C12-O15-C16
20	M	203	CDL	O1-C1-CB2-OB2
20	m	201	CDL	O1-C1-CB2-OB2
23	P	203	TRT	C11-C12-O15-C16
23	p	203	TRT	C11-C12-O15-C16
20	a	503	CDL	OB9-CB7-OB8-CB6
23	G	201	TRT	C13-C12-O15-C16
23	M	201	TRT	O15-C16-C17-O18
20	a	504	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
20	A	503	CDL	OB9-CB7-OB8-CB6
23	g	201	TRT	C13-C12-O15-C16
23	m	203	TRT	O15-C16-C17-O18
23	N	202	TRT	O18-C19-C20-O21
23	n	203	TRT	O18-C19-C20-O21
20	A	504	CDL	CB5-C51-C52-C53
20	d	201	CDL	CB5-C51-C52-C53
23	R	103	TRT	O18-C19-C20-O21
23	r	103	TRT	O18-C19-C20-O21
23	G	202	TRT	C11-C12-O15-C16
23	g	202	TRT	C11-C12-O15-C16
20	a	504	CDL	CA5-C11-C12-C13
20	A	503	CDL	CB5-C51-C52-C53
20	A	504	CDL	CA7-C31-C32-C33
20	D	201	CDL	CB5-C51-C52-C53
20	a	503	CDL	CB5-C51-C52-C53
20	a	504	CDL	CA7-C31-C32-C33
20	p	201	CDL	CB5-C51-C52-C53
22	N	203	LPP	C29-C30-C31-C32
22	P	202	LPP	C29-C30-C31-C32
23	G	202	TRT	C13-C12-O15-C16
23	P	203	TRT	C5-C6-C9-C14
23	P	203	TRT	C5-C6-C9-C10
23	p	203	TRT	C5-C6-C9-C14
23	p	203	TRT	C5-C6-C9-C10
20	M	203	CDL	OA7-CA5-OA6-CA4
20	m	201	CDL	OA7-CA5-OA6-CA4
23	g	202	TRT	C13-C12-O15-C16
23	P	203	TRT	C1-C5-C6-C8
23	P	203	TRT	C1-C5-C6-C7
23	p	203	TRT	C1-C5-C6-C8
23	p	203	TRT	C1-C5-C6-C7
20	A	503	CDL	OA9-CA7-OA8-CA6
20	a	503	CDL	OA9-CA7-OA8-CA6
20	e	101	CDL	OB9-CB7-OB8-CB6
20	A	502	CDL	OA9-CA7-OA8-CA6
20	E	101	CDL	OB9-CB7-OB8-CB6
20	a	502	CDL	OA9-CA7-OA8-CA6
20	d	202	CDL	C78-C79-C80-C81
20	A	502	CDL	CB2-OB2-PB2-OB5
20	A	503	CDL	CB3-OB5-PB2-OB2
20	A	504	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
20	D	201	CDL	CA2-OA2-PA1-OA5
20	D	201	CDL	CB2-OB2-PB2-OB5
20	D	202	CDL	CA2-OA2-PA1-OA5
20	D	202	CDL	CB2-OB2-PB2-OB5
20	D	202	CDL	CB3-OB5-PB2-OB2
20	E	101	CDL	CB2-OB2-PB2-OB5
20	E	101	CDL	CB3-OB5-PB2-OB2
20	M	203	CDL	CB3-OB5-PB2-OB2
20	M	204	CDL	CA2-OA2-PA1-OA5
20	M	204	CDL	CA3-OA5-PA1-OA2
20	O	201	CDL	CA2-OA2-PA1-OA5
20	O	201	CDL	CA3-OA5-PA1-OA2
20	O	201	CDL	CB2-OB2-PB2-OB5
20	O	201	CDL	CB3-OB5-PB2-OB2
20	P	201	CDL	CA3-OA5-PA1-OA2
20	P	201	CDL	CB2-OB2-PB2-OB5
20	a	502	CDL	CA3-OA5-PA1-OA2
20	a	504	CDL	CB3-OB5-PB2-OB2
20	d	201	CDL	CA2-OA2-PA1-OA5
20	d	201	CDL	CB2-OB2-PB2-OB5
20	d	202	CDL	CA2-OA2-PA1-OA5
20	d	202	CDL	CB2-OB2-PB2-OB5
20	d	202	CDL	CB3-OB5-PB2-OB2
20	e	101	CDL	CB2-OB2-PB2-OB5
20	e	101	CDL	CB3-OB5-PB2-OB2
20	m	201	CDL	CB3-OB5-PB2-OB2
20	m	202	CDL	CA2-OA2-PA1-OA5
20	m	202	CDL	CA3-OA5-PA1-OA2
20	o	201	CDL	CA2-OA2-PA1-OA5
20	o	201	CDL	CB2-OB2-PB2-OB5
20	o	201	CDL	CB3-OB5-PB2-OB2
20	p	201	CDL	CB2-OB2-PB2-OB5
20	p	201	CDL	CB3-OB5-PB2-OB2
20	p	202	CDL	CA3-OA5-PA1-OA2
20	p	202	CDL	CB2-OB2-PB2-OB5
20	D	202	CDL	C78-C79-C80-C81
20	R	101	CDL	CA5-C11-C12-C13
20	D	202	CDL	CB2-C1-CA2-OA2
20	E	101	CDL	CA2-C1-CB2-OB2
20	d	202	CDL	CB2-C1-CA2-OA2
20	e	101	CDL	CA2-C1-CB2-OB2
20	o	201	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
21	F	302	LMT	C4B-C5B-C6B-O6B
21	f	302	LMT	C4B-C5B-C6B-O6B
23	M	202	TRT	C13-C12-O15-C16
23	m	204	TRT	C13-C12-O15-C16
20	A	503	CDL	C74-C75-C76-C77
20	R	101	CDL	C51-CB5-OB6-CB4
20	r	101	CDL	C51-CB5-OB6-CB4
20	A	503	CDL	C72-C73-C74-C75
20	E	101	CDL	C56-C57-C58-C59
20	E	101	CDL	C72-C73-C74-C75
20	M	203	CDL	C13-C14-C15-C16
20	a	503	CDL	C72-C73-C74-C75
20	a	503	CDL	C74-C75-C76-C77
20	d	202	CDL	C81-C82-C83-C84
20	m	201	CDL	C13-C14-C15-C16
20	m	201	CDL	C32-C33-C34-C35
20	m	201	CDL	C79-C80-C81-C82
20	M	203	CDL	C32-C33-C34-C35
20	M	203	CDL	C79-C80-C81-C82
20	M	204	CDL	C53-C54-C55-C56
20	e	101	CDL	C72-C73-C74-C75
22	I	101	LPP	C21-C22-C23-C24
22	O	203	LPP	C17-C18-C19-C20
22	O	203	LPP	C18-C19-C20-C21
22	o	203	LPP	C17-C18-C19-C20
22	o	203	LPP	C18-C19-C20-C21
20	R	101	CDL	OB7-CB5-OB6-CB4
20	r	101	CDL	OB7-CB5-OB6-CB4
20	D	201	CDL	C17-C18-C19-C20
20	D	202	CDL	C81-C82-C83-C84
20	d	201	CDL	C17-C18-C19-C20
20	m	201	CDL	C71-C72-C73-C74
22	i	101	LPP	C21-C22-C23-C24
20	A	502	CDL	C72-C73-C74-C75
20	M	203	CDL	C71-C72-C73-C74
20	M	203	CDL	C73-C74-C75-C76
20	m	201	CDL	C73-C74-C75-C76
22	I	101	LPP	C35-C36-C37-C38
22	i	101	LPP	C35-C36-C37-C38
20	D	201	CDL	O1-C1-CB2-OB2
20	d	201	CDL	O1-C1-CB2-OB2
20	A	502	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
20	a	502	CDL	C72-C73-C74-C75
20	p	201	CDL	C15-C16-C17-C18
21	F	302	LMT	O1'-C1-C2-C3
21	f	302	LMT	O1'-C1-C2-C3
23	N	202	TRT	C13-C12-O15-C16
23	n	203	TRT	C13-C12-O15-C16
20	D	202	CDL	CA5-C11-C12-C13
20	D	202	CDL	C34-C35-C36-C37
20	D	202	CDL	C37-C38-C39-C40
20	a	502	CDL	C13-C14-C15-C16
20	d	202	CDL	C37-C38-C39-C40
20	r	101	CDL	C55-C56-C57-C58
21	N	204	LMT	C11-C10-C9-C8
21	n	201	LMT	C11-C10-C9-C8
20	A	501	CDL	C17-C18-C19-C20
20	A	502	CDL	C60-C61-C62-C63
20	D	202	CDL	C72-C73-C74-C75
20	R	101	CDL	C55-C56-C57-C58
20	R	101	CDL	C57-C58-C59-C60
20	a	502	CDL	C60-C61-C62-C63
20	d	202	CDL	C72-C73-C74-C75
22	R	102	LPP	C30-C31-C32-C33
22	r	102	LPP	C30-C31-C32-C33
20	A	503	CDL	C33-C34-C35-C36
20	D	201	CDL	C42-C43-C44-C45
20	D	202	CDL	C77-C78-C79-C80
20	O	201	CDL	C71-C72-C73-C74
20	a	501	CDL	C17-C18-C19-C20
20	a	502	CDL	C11-C12-C13-C14
20	a	503	CDL	C33-C34-C35-C36
20	d	202	CDL	C34-C35-C36-C37
20	d	202	CDL	C77-C78-C79-C80
20	e	101	CDL	C71-C72-C73-C74
20	o	201	CDL	C71-C72-C73-C74
20	r	101	CDL	C57-C58-C59-C60
20	A	502	CDL	C11-C12-C13-C14
20	a	503	CDL	C21-C22-C23-C24
20	d	201	CDL	C42-C43-C44-C45
20	p	201	CDL	C18-C19-C20-C21
20	P	201	CDL	OA7-CA5-OA6-CA4
20	E	101	CDL	C11-CA5-OA6-CA4
20	P	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
20	e	101	CDL	C11-CA5-OA6-CA4
20	e	101	CDL	C56-C57-C58-C59
22	r	102	LPP	C32-C33-C34-C35
20	d	202	CDL	CA5-C11-C12-C13
20	p	201	CDL	CA5-C11-C12-C13
20	r	101	CDL	CA5-C11-C12-C13
20	A	503	CDL	C21-C22-C23-C24
20	D	202	CDL	C74-C75-C76-C77
20	E	101	CDL	C71-C72-C73-C74
20	p	201	CDL	C55-C56-C57-C58
22	R	102	LPP	C32-C33-C34-C35
20	A	503	CDL	C52-C53-C54-C55
20	a	503	CDL	C52-C53-C54-C55
20	d	202	CDL	C74-C75-C76-C77
22	R	102	LPP	C11-C12-C13-C14
22	r	102	LPP	C11-C12-C13-C14
20	A	503	CDL	C31-C32-C33-C34
20	M	203	CDL	C74-C75-C76-C77
20	m	201	CDL	C74-C75-C76-C77
23	M	202	TRT	C11-C12-O15-C16
23	m	204	TRT	C11-C12-O15-C16
20	p	201	CDL	C31-C32-C33-C34
20	r	101	CDL	C36-C37-C38-C39
23	G	202	TRT	C5-C6-C9-C10
23	M	201	TRT	C5-C6-C9-C14
23	M	201	TRT	C5-C6-C9-C10
23	g	202	TRT	C5-C6-C9-C10
23	m	203	TRT	C5-C6-C9-C14
23	m	203	TRT	C5-C6-C9-C10
20	a	503	CDL	C31-C32-C33-C34
20	M	204	CDL	CA5-C11-C12-C13
20	m	202	CDL	CA5-C11-C12-C13
20	E	101	CDL	OA7-CA5-OA6-CA4
20	e	101	CDL	OA7-CA5-OA6-CA4
20	R	101	CDL	C36-C37-C38-C39
23	N	202	TRT	C11-C12-O15-C16
23	n	203	TRT	C11-C12-O15-C16
20	D	202	CDL	C11-CA5-OA6-CA4
20	M	204	CDL	C51-CB5-OB6-CB4
20	O	201	CDL	C51-CB5-OB6-CB4
20	p	202	CDL	C11-CA5-OA6-CA4
21	N	204	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
21	q	101	LMT	O5'-C5'-C6'-O6'
20	P	201	CDL	C72-C73-C74-C75
20	R	101	CDL	C74-C75-C76-C77
20	r	101	CDL	C74-C75-C76-C77
21	n	201	LMT	C3-C4-C5-C6
21	Q	101	LMT	O5'-C5'-C6'-O6'
20	M	203	CDL	C77-C78-C79-C80
22	O	203	LPP	C19-C20-C21-C22
20	p	202	CDL	C72-C73-C74-C75
22	o	203	LPP	C19-C20-C21-C22
22	r	102	LPP	C34-C35-C36-C37
23	G	201	TRT	O21-C22-C23-O24
23	N	202	TRT	C5-C6-C9-C10
23	n	203	TRT	C5-C6-C9-C10
20	O	201	CDL	C55-C56-C57-C58
20	m	201	CDL	C77-C78-C79-C80
20	o	201	CDL	C55-C56-C57-C58
22	R	102	LPP	C34-C35-C36-C37
23	g	201	TRT	O21-C22-C23-O24
20	O	201	CDL	OB7-CB5-OB6-CB4
20	p	202	CDL	OA7-CA5-OA6-CA4
20	M	204	CDL	C1-CA2-OA2-PA1
20	m	202	CDL	C1-CA2-OA2-PA1
21	Q	101	LMT	C1-C2-C3-C4
21	q	101	LMT	C1-C2-C3-C4
20	R	101	CDL	C62-C63-C64-C65
20	r	101	CDL	C62-C63-C64-C65
20	a	501	CDL	C34-C35-C36-C37
20	o	201	CDL	C51-CB5-OB6-CB4
21	D	203	LMT	C3-C4-C5-C6
21	d	203	LMT	C3-C4-C5-C6
20	a	501	CDL	CB7-C71-C72-C73
20	A	502	CDL	C73-C74-C75-C76
20	a	502	CDL	C73-C74-C75-C76
20	A	501	CDL	C34-C35-C36-C37
20	A	504	CDL	C74-C75-C76-C77
20	a	504	CDL	C74-C75-C76-C77
20	A	503	CDL	OA7-CA5-OA6-CA4
20	A	503	CDL	OB7-CB5-OB6-CB4
20	D	202	CDL	OA7-CA5-OA6-CA4
20	M	204	CDL	OA7-CA5-OA6-CA4
20	a	503	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
20	a	503	CDL	OB7-CB5-OB6-CB4
20	d	201	CDL	OA7-CA5-OA6-CA4
20	d	201	CDL	OB7-CB5-OB6-CB4
20	d	202	CDL	OA7-CA5-OA6-CA4
20	m	202	CDL	OA7-CA5-OA6-CA4
20	m	202	CDL	OB7-CB5-OB6-CB4
20	o	201	CDL	OB7-CB5-OB6-CB4
20	A	501	CDL	CB7-C71-C72-C73
20	D	201	CDL	C71-CB7-OB8-CB6
20	d	201	CDL	C71-CB7-OB8-CB6
22	O	202	LPP	C30-C29-O27-C8
22	o	202	LPP	C30-C29-O27-C8
22	R	102	LPP	C36-C37-C38-C39
22	r	102	LPP	C36-C37-C38-C39
23	G	202	TRT	C5-C6-C9-C14
23	N	202	TRT	C5-C6-C9-C14
23	g	202	TRT	C5-C6-C9-C14
23	n	203	TRT	C5-C6-C9-C14
20	A	502	CDL	C23-C24-C25-C26
20	O	201	CDL	C20-C21-C22-C23
20	o	201	CDL	C20-C21-C22-C23
20	p	201	CDL	C37-C38-C39-C40
20	a	502	CDL	C23-C24-C25-C26
20	M	203	CDL	C82-C83-C84-C85
20	m	201	CDL	C82-C83-C84-C85
20	A	503	CDL	C71-C72-C73-C74
20	p	201	CDL	C79-C80-C81-C82
20	A	501	CDL	CA7-C31-C32-C33
20	a	501	CDL	CA7-C31-C32-C33
20	A	503	CDL	C11-CA5-OA6-CA4
20	A	503	CDL	C51-CB5-OB6-CB4
20	D	201	CDL	C11-CA5-OA6-CA4
20	D	201	CDL	C51-CB5-OB6-CB4
20	M	203	CDL	C51-CB5-OB6-CB4
20	M	204	CDL	C11-CA5-OA6-CA4
20	O	201	CDL	C11-CA5-OA6-CA4
20	a	503	CDL	C11-CA5-OA6-CA4
20	a	503	CDL	C51-CB5-OB6-CB4
20	d	201	CDL	C11-CA5-OA6-CA4
20	d	201	CDL	C51-CB5-OB6-CB4
20	d	202	CDL	C11-CA5-OA6-CA4
20	m	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	m	202	CDL	C11-CA5-OA6-CA4
20	m	202	CDL	C51-CB5-OB6-CB4
20	o	201	CDL	C11-CA5-OA6-CA4
20	p	201	CDL	C51-CB5-OB6-CB4
22	N	203	LPP	C12-C11-O9-C7
22	P	202	LPP	C12-C11-O9-C7
20	A	502	CDL	OB5-CB3-CB4-OB6
20	a	502	CDL	OB5-CB3-CB4-OB6
22	N	203	LPP	C13-C14-C15-C16
20	A	502	CDL	C20-C21-C22-C23
20	a	502	CDL	C20-C21-C22-C23
22	P	202	LPP	C13-C14-C15-C16
20	D	201	CDL	OA7-CA5-OA6-CA4
20	D	201	CDL	OB7-CB5-OB6-CB4
20	M	203	CDL	OB7-CB5-OB6-CB4
20	M	204	CDL	OB7-CB5-OB6-CB4
20	O	201	CDL	OA7-CA5-OA6-CA4
20	m	201	CDL	OB7-CB5-OB6-CB4
22	N	203	LPP	O10-C11-O9-C7
22	P	202	LPP	O10-C11-O9-C7
20	A	504	CDL	OA6-CA4-CA6-OA8
20	E	101	CDL	OB6-CB4-CB6-OB8
20	a	504	CDL	OA6-CA4-CA6-OA8
20	e	101	CDL	OB6-CB4-CB6-OB8
20	M	204	CDL	C51-C52-C53-C54
20	D	202	CDL	C31-C32-C33-C34
20	D	201	CDL	OB9-CB7-OB8-CB6
22	O	202	LPP	O28-C29-O27-C8
22	o	202	LPP	O28-C29-O27-C8
20	o	201	CDL	OA7-CA5-OA6-CA4
20	p	201	CDL	OB7-CB5-OB6-CB4
20	A	501	CDL	CB3-OB5-PB2-OB2
20	M	203	CDL	CA2-OA2-PA1-OA5
20	M	204	CDL	CB2-OB2-PB2-OB5
20	P	201	CDL	CA2-OA2-PA1-OA5
20	a	501	CDL	CB3-OB5-PB2-OB2
20	m	202	CDL	CB2-OB2-PB2-OB5
20	p	202	CDL	CA2-OA2-PA1-OA5
20	r	101	CDL	CA2-OA2-PA1-OA5
21	n	201	LMT	O5B-C5B-C6B-O6B
20	O	201	CDL	C1-CB2-OB2-PB2
21	N	204	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
20	A	503	CDL	OB5-CB3-CB4-CB6
20	D	201	CDL	OB5-CB3-CB4-CB6
20	M	203	CDL	OA5-CA3-CA4-CA6
20	M	203	CDL	OB5-CB3-CB4-CB6
20	a	503	CDL	OB5-CB3-CB4-CB6
20	d	201	CDL	OB5-CB3-CB4-CB6
20	e	101	CDL	OA5-CA3-CA4-CA6
20	m	201	CDL	OA5-CA3-CA4-CA6
20	m	201	CDL	OB5-CB3-CB4-CB6
22	O	203	LPP	O5-C6-C7-C8
22	o	203	LPP	O5-C6-C7-C8
20	p	201	CDL	C41-C42-C43-C44
20	p	201	CDL	C81-C82-C83-C84
21	d	203	LMT	O1'-C1-C2-C3
20	O	201	CDL	CB2-C1-CA2-OA2
20	a	502	CDL	CA2-C1-CB2-OB2
20	D	202	CDL	C43-C44-C45-C46
20	E	101	CDL	C53-C54-C55-C56
21	D	203	LMT	O1'-C1-C2-C3
20	M	203	CDL	C81-C82-C83-C84
20	d	202	CDL	C43-C44-C45-C46
23	G	201	TRT	O15-C16-C17-O18
20	d	201	CDL	OB9-CB7-OB8-CB6
21	F	302	LMT	C5-C6-C7-C8
21	f	302	LMT	C5-C6-C7-C8
23	g	201	TRT	O15-C16-C17-O18
20	D	202	CDL	CB3-CB4-CB6-OB8
20	M	204	CDL	CB3-CB4-CB6-OB8
20	a	502	CDL	C75-C76-C77-C78
20	m	202	CDL	CB3-CB4-CB6-OB8
20	r	101	CDL	CB3-CB4-CB6-OB8
20	A	502	CDL	C75-C76-C77-C78
20	e	101	CDL	C53-C54-C55-C56
20	p	201	CDL	CA7-C31-C32-C33
20	A	503	CDL	C18-C19-C20-C21
22	N	203	LPP	C32-C33-C34-C35
20	M	204	CDL	C73-C74-C75-C76
20	m	202	CDL	C73-C74-C75-C76
22	P	202	LPP	C32-C33-C34-C35
20	A	504	CDL	CA5-C11-C12-C13
20	m	201	CDL	C81-C82-C83-C84
20	a	504	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
22	I	101	LPP	C31-C32-C33-C34
22	i	101	LPP	C31-C32-C33-C34
20	A	504	CDL	C71-C72-C73-C74
20	M	203	CDL	C72-C73-C74-C75
20	a	504	CDL	C57-C58-C59-C60
20	m	201	CDL	C72-C73-C74-C75
20	o	201	CDL	C1-CB2-OB2-PB2
22	O	203	LPP	C6-O5-P1-O3
22	o	203	LPP	C6-O5-P1-O3
20	D	202	CDL	C53-C54-C55-C56
20	a	503	CDL	C18-C19-C20-C21
20	r	101	CDL	C59-C60-C61-C62
20	M	203	CDL	C71-CB7-OB8-CB6
20	A	504	CDL	C57-C58-C59-C60
20	E	101	CDL	C62-C63-C64-C65
20	d	202	CDL	C53-C54-C55-C56
20	r	101	CDL	C75-C76-C77-C78
20	R	101	CDL	C75-C76-C77-C78
20	R	101	CDL	OA6-CA4-CA6-OA8
20	R	101	CDL	OB6-CB4-CB6-OB8
20	o	201	CDL	OA6-CA4-CA6-OA8
20	r	101	CDL	OA6-CA4-CA6-OA8
20	A	501	CDL	C55-C56-C57-C58
20	R	101	CDL	C59-C60-C61-C62
20	d	202	CDL	C31-C32-C33-C34
20	e	101	CDL	C62-C63-C64-C65
20	A	502	CDL	C31-C32-C33-C34
22	f	301	LPP	C12-C13-C14-C15
22	F	301	LPP	C12-C13-C14-C15
20	E	101	CDL	C12-C11-CA5-OA6
20	O	201	CDL	C15-C16-C17-C18
20	a	501	CDL	C55-C56-C57-C58
20	m	201	CDL	C71-CB7-OB8-CB6
23	M	201	TRT	O18-C19-C20-O21
23	m	203	TRT	O18-C19-C20-O21
20	D	201	CDL	C12-C13-C14-C15
20	m	202	CDL	C51-C52-C53-C54
20	o	201	CDL	C15-C16-C17-C18
22	I	101	LPP	C30-C29-O27-C8
22	i	101	LPP	C30-C29-O27-C8
20	d	201	CDL	C12-C13-C14-C15
22	R	102	LPP	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
22	r	102	LPP	C38-C39-C40-C41
20	A	502	CDL	OB5-CB3-CB4-CB6
20	E	101	CDL	OA5-CA3-CA4-CA6
20	E	101	CDL	OB5-CB3-CB4-CB6
20	a	502	CDL	OB5-CB3-CB4-CB6
20	e	101	CDL	OB5-CB3-CB4-CB6
23	P	203	TRT	C17-C16-O15-C12
23	p	203	TRT	C17-C16-O15-C12
23	P	203	TRT	C22-C23-O24-C25
23	p	203	TRT	C22-C23-O24-C25
20	D	201	CDL	C11-C12-C13-C14
20	p	201	CDL	C20-C21-C22-C23
20	e	101	CDL	C12-C11-CA5-OA6
23	R	103	TRT	C17-C16-O15-C12
23	r	103	TRT	C17-C16-O15-C12
21	F	302	LMT	C2-C1-O1'-C1'
21	f	302	LMT	C2-C1-O1'-C1'
20	a	502	CDL	C31-C32-C33-C34
20	d	201	CDL	C34-C35-C36-C37
20	A	504	CDL	CA3-CA4-CA6-OA8
20	E	101	CDL	CB3-CB4-CB6-OB8
20	R	101	CDL	CB3-CB4-CB6-OB8
20	a	504	CDL	CA3-CA4-CA6-OA8
20	d	202	CDL	CB3-CB4-CB6-OB8
20	e	101	CDL	CB3-CB4-CB6-OB8
20	R	101	CDL	C31-C32-C33-C34
20	A	502	CDL	C77-C78-C79-C80
20	d	201	CDL	C11-C12-C13-C14
20	D	201	CDL	C34-C35-C36-C37
20	r	101	CDL	C31-C32-C33-C34
20	a	502	CDL	C32-C33-C34-C35
20	p	201	CDL	C59-C60-C61-C62
20	A	502	CDL	CA3-OA5-PA1-OA2
20	D	201	CDL	CA3-OA5-PA1-OA2
20	R	101	CDL	CA2-OA2-PA1-OA5
20	a	503	CDL	CA2-OA2-PA1-OA5
20	d	201	CDL	CB3-OB5-PB2-OB2
20	m	201	CDL	CA2-OA2-PA1-OA5
20	p	201	CDL	CA3-OA5-PA1-OA2
20	m	202	CDL	C53-C54-C55-C56
20	D	201	CDL	OB5-CB3-CB4-OB6
20	d	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
22	N	203	LPP	O9-C11-C12-C13
22	P	202	LPP	O9-C11-C12-C13
20	A	501	CDL	C15-C16-C17-C18
22	I	101	LPP	O28-C29-O27-C8
22	i	101	LPP	O28-C29-O27-C8
20	A	504	CDL	C52-C53-C54-C55
20	m	202	CDL	OB6-CB4-CB6-OB8
20	p	201	CDL	OB6-CB4-CB6-OB8
20	r	101	CDL	OB6-CB4-CB6-OB8
23	R	103	TRT	C22-C23-O24-C25
23	r	103	TRT	C22-C23-O24-C25
20	D	202	CDL	C13-C14-C15-C16
20	M	203	CDL	OB9-CB7-OB8-CB6
20	a	501	CDL	C15-C16-C17-C18
20	e	101	CDL	C63-C64-C65-C66
20	E	101	CDL	C1-CB2-OB2-PB2
20	O	201	CDL	C1-CA2-OA2-PA1
20	o	201	CDL	C1-CA2-OA2-PA1
20	p	201	CDL	C1-CA2-OA2-PA1
20	R	101	CDL	CA7-C31-C32-C33
20	e	101	CDL	C51-C52-C53-C54
20	A	501	CDL	OA7-CA5-OA6-CA4
20	A	501	CDL	C11-CA5-OA6-CA4
20	a	501	CDL	C11-CA5-OA6-CA4
20	p	201	CDL	C11-CA5-OA6-CA4
20	E	101	CDL	C63-C64-C65-C66
20	r	101	CDL	CA7-C31-C32-C33
23	R	103	TRT	C1-C5-C6-C8
23	r	103	TRT	C1-C5-C6-C8
20	m	201	CDL	OB9-CB7-OB8-CB6
20	M	204	CDL	OA5-CA3-CA4-CA6
20	p	201	CDL	OA5-CA3-CA4-CA6
23	N	201	TRT	O21-C22-C23-O24
20	p	201	CDL	C74-C75-C76-C77
23	n	202	TRT	O21-C22-C23-O24
23	G	202	TRT	C17-C16-O15-C12
23	g	202	TRT	C17-C16-O15-C12
20	a	501	CDL	OA7-CA5-OA6-CA4
20	p	201	CDL	OA7-CA5-OA6-CA4
20	A	502	CDL	C76-C77-C78-C79
22	R	102	LPP	C35-C36-C37-C38
23	M	202	TRT	O18-C19-C20-O21

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Mol	Chain	Res	Type	Atoms
20	d	202	CDL	C13-C14-C15-C16
21	F	302	LMT	C11-C10-C9-C8
22	I	101	LPP	C23-C24-C25-C26
22	i	101	LPP	C23-C24-C25-C26
22	r	102	LPP	C35-C36-C37-C38
23	m	204	TRT	O18-C19-C20-O21
21	f	302	LMT	C11-C10-C9-C8
22	I	101	LPP	C6-O5-P1-O4
22	i	101	LPP	C6-O5-P1-O4
20	a	504	CDL	C52-C53-C54-C55
22	F	301	LPP	C30-C29-O27-C8
22	f	301	LPP	C30-C29-O27-C8
20	p	201	CDL	C38-C39-C40-C41
20	A	501	CDL	C40-C41-C42-C43
20	a	502	CDL	C77-C78-C79-C80
22	i	101	LPP	C12-C13-C14-C15
20	m	201	CDL	C21-C22-C23-C24
22	I	101	LPP	C12-C13-C14-C15
20	A	502	CDL	CA6-CA4-OA6-CA5
20	A	503	CDL	CA6-CA4-OA6-CA5
20	E	101	CDL	CA6-CA4-OA6-CA5
20	P	201	CDL	CA6-CA4-OA6-CA5
20	a	502	CDL	CA6-CA4-OA6-CA5
20	a	503	CDL	CA6-CA4-OA6-CA5
20	e	101	CDL	CA6-CA4-OA6-CA5
20	p	202	CDL	CA6-CA4-OA6-CA5
20	a	501	CDL	C40-C41-C42-C43
23	G	202	TRT	C20-C19-O18-C17
23	g	202	TRT	C20-C19-O18-C17
20	A	501	CDL	CB4-CB3-OB5-PB2
20	a	501	CDL	CB4-CB3-OB5-PB2
20	e	101	CDL	C1-CB2-OB2-PB2
20	o	201	CDL	CA3-CA4-CA6-OA8
20	p	201	CDL	CB3-CB4-CB6-OB8
22	O	202	LPP	C6-C7-C8-O27
22	o	202	LPP	C6-C7-C8-O27
20	a	501	CDL	C20-C21-C22-C23
20	d	202	CDL	C39-C40-C41-C42
23	m	203	TRT	C13-C12-O15-C16
20	A	503	CDL	OA5-CA3-CA4-OA6
20	E	101	CDL	OA5-CA3-CA4-OA6
20	O	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
20	a	503	CDL	OA5-CA3-CA4-OA6
20	e	101	CDL	OA5-CA3-CA4-OA6
20	o	201	CDL	OB5-CB3-CB4-OB6
20	M	203	CDL	C17-C18-C19-C20
20	m	201	CDL	C17-C18-C19-C20
20	o	201	CDL	C31-CA7-OA8-CA6
23	R	103	TRT	O15-C16-C17-O18
23	M	201	TRT	C13-C12-O15-C16
23	r	103	TRT	O15-C16-C17-O18
20	M	203	CDL	CA2-C1-CB2-OB2
20	m	201	CDL	CA2-C1-CB2-OB2
23	N	202	TRT	C16-C17-O18-C19
23	n	203	TRT	C16-C17-O18-C19
23	M	202	TRT	C16-C17-O18-C19
23	m	204	TRT	C16-C17-O18-C19
20	D	202	CDL	OB6-CB4-CB6-OB8
20	d	202	CDL	OB6-CB4-CB6-OB8
20	M	203	CDL	C21-C22-C23-C24
20	a	502	CDL	C76-C77-C78-C79
22	I	101	LPP	C18-C19-C20-C21
22	i	101	LPP	C18-C19-C20-C21
20	D	202	CDL	C39-C40-C41-C42
20	r	101	CDL	C72-C73-C74-C75
22	F	301	LPP	O28-C29-O27-C8
22	f	301	LPP	O28-C29-O27-C8
20	e	101	CDL	CA7-C31-C32-C33
20	R	101	CDL	C72-C73-C74-C75
23	M	201	TRT	C11-C12-O15-C16
23	m	203	TRT	C11-C12-O15-C16
20	M	204	CDL	C12-C11-CA5-OA6
23	R	103	TRT	C1-C5-C6-C9
23	r	103	TRT	C1-C5-C6-C9
21	D	203	LMT	C6-C7-C8-C9
23	N	202	TRT	C22-C23-O24-C25
23	n	203	TRT	C22-C23-O24-C25
21	d	203	LMT	C6-C7-C8-C9
21	q	101	LMT	C3-C4-C5-C6
20	m	201	CDL	CB7-C71-C72-C73
21	Q	101	LMT	C3-C4-C5-C6
22	O	203	LPP	C12-C13-C14-C15
22	o	203	LPP	C12-C13-C14-C15
20	m	201	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
20	E	101	CDL	CA2-OA2-PA1-OA5
20	E	101	CDL	CA3-OA5-PA1-OA2
20	M	203	CDL	CB2-OB2-PB2-OB5
20	d	201	CDL	CA3-OA5-PA1-OA2
20	e	101	CDL	CA2-OA2-PA1-OA5
20	e	101	CDL	CA3-OA5-PA1-OA2
20	m	201	CDL	CB2-OB2-PB2-OB5
20	p	201	CDL	C53-C54-C55-C56
20	a	501	CDL	C51-C52-C53-C54
20	A	504	CDL	CA4-CA3-OA5-PA1
20	M	204	CDL	CB4-CB3-OB5-PB2
20	a	504	CDL	CA4-CA3-OA5-PA1
20	o	201	CDL	OA9-CA7-OA8-CA6
20	A	502	CDL	CA2-OA2-PA1-OA3
20	A	503	CDL	CA3-OA5-PA1-OA4
20	A	503	CDL	CB2-OB2-PB2-OB3
20	D	201	CDL	CB2-OB2-PB2-OB4
20	D	202	CDL	CA3-OA5-PA1-OA3
20	D	202	CDL	CB2-OB2-PB2-OB3
20	D	202	CDL	CB3-OB5-PB2-OB4
20	E	101	CDL	CA2-OA2-PA1-OA3
20	E	101	CDL	CB2-OB2-PB2-OB4
20	E	101	CDL	CB3-OB5-PB2-OB3
20	M	203	CDL	CA2-OA2-PA1-OA3
20	M	203	CDL	CB3-OB5-PB2-OB3
20	M	204	CDL	CA2-OA2-PA1-OA3
20	O	201	CDL	CA2-OA2-PA1-OA4
20	P	201	CDL	CA2-OA2-PA1-OA4
20	a	502	CDL	CA2-OA2-PA1-OA3
20	a	502	CDL	CA3-OA5-PA1-OA3
20	a	502	CDL	CA3-OA5-PA1-OA4
20	a	503	CDL	CA3-OA5-PA1-OA4
20	d	201	CDL	CB2-OB2-PB2-OB4
20	d	202	CDL	CA3-OA5-PA1-OA3
20	d	202	CDL	CB2-OB2-PB2-OB3
20	d	202	CDL	CB3-OB5-PB2-OB4
20	e	101	CDL	CA2-OA2-PA1-OA3
20	e	101	CDL	CB2-OB2-PB2-OB4
20	e	101	CDL	CB3-OB5-PB2-OB3
20	m	201	CDL	CA2-OA2-PA1-OA3
20	m	201	CDL	CB3-OB5-PB2-OB3
20	m	202	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
20	p	201	CDL	CA3-OA5-PA1-OA3
20	p	201	CDL	CB2-OB2-PB2-OB4
20	p	202	CDL	CA2-OA2-PA1-OA4
20	r	101	CDL	CA2-OA2-PA1-OA4
22	I	101	LPP	C39-C40-C41-C42
20	O	201	CDL	OB5-CB3-CB4-CB6
20	m	202	CDL	OA5-CA3-CA4-CA6
20	o	201	CDL	OB5-CB3-CB4-CB6
22	i	101	LPP	C39-C40-C41-C42
20	A	504	CDL	C53-C54-C55-C56
20	m	201	CDL	C16-C17-C18-C19
20	A	501	CDL	C51-C52-C53-C54
20	p	202	CDL	C32-C33-C34-C35
20	A	502	CDL	C32-C33-C34-C35
20	E	101	CDL	CA7-C31-C32-C33
20	A	501	CDL	C12-C11-CA5-OA6
20	D	201	CDL	C55-C56-C57-C58
20	d	201	CDL	C40-C41-C42-C43
20	o	201	CDL	C17-C18-C19-C20
20	M	203	CDL	C16-C17-C18-C19
23	M	202	TRT	O21-C22-C23-O24
23	m	204	TRT	O21-C22-C23-O24
20	A	502	CDL	CB5-C51-C52-C53
20	M	203	CDL	CB7-C71-C72-C73
20	A	501	CDL	C58-C59-C60-C61
20	M	203	CDL	C75-C76-C77-C78
20	d	201	CDL	C55-C56-C57-C58
20	a	501	CDL	C58-C59-C60-C61
20	a	501	CDL	C12-C11-CA5-OA6
20	O	201	CDL	C17-C18-C19-C20
20	d	202	CDL	C73-C74-C75-C76
20	a	504	CDL	C53-C54-C55-C56
22	O	202	LPP	C13-C14-C15-C16
22	o	202	LPP	C13-C14-C15-C16
20	a	502	CDL	CB5-C51-C52-C53
20	m	202	CDL	C12-C11-CA5-OA6
20	R	101	CDL	CA3-CA4-CA6-OA8
20	p	201	CDL	C76-C77-C78-C79
20	r	101	CDL	CA3-CA4-CA6-OA8
20	M	204	CDL	OB6-CB4-CB6-OB8
20	d	202	CDL	OA6-CA4-CA6-OA8
22	R	102	LPP	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
22	r	102	LPP	C39-C40-C41-C42
20	A	504	CDL	C1-CA2-OA2-PA1
20	a	504	CDL	C1-CA2-OA2-PA1
20	m	202	CDL	CB4-CB3-OB5-PB2
22	O	203	LPP	C23-C24-C25-C26
22	o	203	LPP	C23-C24-C25-C26
20	a	503	CDL	C55-C56-C57-C58
20	D	201	CDL	CB7-C71-C72-C73
20	A	503	CDL	C55-C56-C57-C58
21	Q	101	LMT	C7-C8-C9-C10
21	q	101	LMT	C7-C8-C9-C10
21	N	204	LMT	C2-C3-C4-C5
21	n	201	LMT	C2-C3-C4-C5
20	A	504	CDL	C32-C31-CA7-OA8
20	p	201	CDL	C61-C62-C63-C64
23	G	201	TRT	C16-C17-O18-C19
23	g	201	TRT	C23-C22-O21-C20
23	G	201	TRT	C23-C22-O21-C20
23	g	201	TRT	C16-C17-O18-C19
20	A	504	CDL	C75-C76-C77-C78
20	P	201	CDL	C32-C33-C34-C35
20	a	504	CDL	C75-C76-C77-C78
20	a	504	CDL	C32-C31-CA7-OA8
20	o	201	CDL	C72-C71-CB7-OB8
20	D	202	CDL	CA6-CA4-OA6-CA5
20	O	201	CDL	CA3-CA4-OA6-CA5
20	d	202	CDL	CA6-CA4-OA6-CA5
20	o	201	CDL	CA3-CA4-OA6-CA5
22	N	203	LPP	C8-C7-O9-C11
22	P	202	LPP	C8-C7-O9-C11
20	A	503	CDL	OA5-CA3-CA4-CA6
20	a	503	CDL	OA5-CA3-CA4-CA6
20	r	101	CDL	C63-C64-C65-C66
20	O	201	CDL	C72-C71-CB7-OB8
20	D	202	CDL	C1-CA2-OA2-PA1
20	d	202	CDL	CB4-CB3-OB5-PB2
20	p	202	CDL	CA4-CA3-OA5-PA1
20	A	503	CDL	OB5-CB3-CB4-OB6
20	M	204	CDL	OA5-CA3-CA4-OA6
20	a	503	CDL	OB5-CB3-CB4-OB6
20	R	101	CDL	C63-C64-C65-C66
20	D	202	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
20	a	504	CDL	C59-C60-C61-C62
20	A	501	CDL	C13-C14-C15-C16
20	A	503	CDL	CA2-OA2-PA1-OA5
20	A	504	CDL	CA2-OA2-PA1-OA5
20	R	101	CDL	CA3-OA5-PA1-OA2
20	a	504	CDL	CA2-OA2-PA1-OA5
20	r	101	CDL	CA3-OA5-PA1-OA2
22	O	202	LPP	C14-C15-C16-C17
22	o	202	LPP	C14-C15-C16-C17
20	D	201	CDL	C33-C34-C35-C36
23	P	203	TRT	C1-C5-C6-C9
23	p	203	TRT	C1-C5-C6-C9
20	d	201	CDL	CB7-C71-C72-C73
20	a	501	CDL	C13-C14-C15-C16
20	d	201	CDL	C33-C34-C35-C36
20	A	504	CDL	C59-C60-C61-C62
20	d	202	CDL	C15-C16-C17-C18
23	N	201	TRT	O15-C16-C17-O18
20	P	201	CDL	C71-C72-C73-C74
22	F	301	LPP	C14-C15-C16-C17
22	f	301	LPP	C14-C15-C16-C17
23	g	202	TRT	O15-C16-C17-O18
23	n	202	TRT	O15-C16-C17-O18
20	d	201	CDL	C53-C54-C55-C56
23	G	202	TRT	O15-C16-C17-O18
20	D	202	CDL	CB4-CB3-OB5-PB2
20	P	201	CDL	CA4-CA3-OA5-PA1
20	d	202	CDL	C1-CA2-OA2-PA1
20	D	201	CDL	C40-C41-C42-C43
20	R	101	CDL	C77-C78-C79-C80
20	A	501	CDL	C71-CB7-OB8-CB6
20	p	201	CDL	C42-C43-C44-C45
20	r	101	CDL	C77-C78-C79-C80
20	E	101	CDL	C51-C52-C53-C54
20	A	504	CDL	C31-CA7-OA8-CA6
20	A	501	CDL	OB5-CB3-CB4-CB6
20	a	501	CDL	OB5-CB3-CB4-CB6
20	p	202	CDL	OA5-CA3-CA4-CA6
20	p	201	CDL	C73-C74-C75-C76
20	r	101	CDL	C13-C14-C15-C16
20	d	202	CDL	C71-C72-C73-C74
20	A	501	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
20	D	202	CDL	C15-C16-C17-C18
20	D	201	CDL	C53-C54-C55-C56
20	R	101	CDL	C13-C14-C15-C16
23	M	202	TRT	C1-C5-C6-C9
23	N	201	TRT	C1-C5-C6-C9
23	m	204	TRT	C1-C5-C6-C9
23	n	202	TRT	C1-C5-C6-C9
20	E	101	CDL	C59-C60-C61-C62
20	d	201	CDL	CB2-C1-CA2-OA2
20	p	201	CDL	C83-C84-C85-C86
20	D	202	CDL	C40-C41-C42-C43
20	a	501	CDL	C71-CB7-OB8-CB6
21	D	203	LMT	O5'-C1'-O1'-C1
21	d	203	LMT	O5'-C1'-O1'-C1
20	d	202	CDL	C40-C41-C42-C43
20	A	503	CDL	CA3-OA5-PA1-OA2
20	D	201	CDL	CB3-OB5-PB2-OB2
20	a	503	CDL	CA3-OA5-PA1-OA2
20	A	504	CDL	OA9-CA7-OA8-CA6
20	o	201	CDL	C72-C73-C74-C75
20	D	202	CDL	C32-C31-CA7-OA8
20	O	201	CDL	C52-C51-CB5-OB6
22	o	202	LPP	O10-C11-O9-C7
20	O	201	CDL	C72-C73-C74-C75
20	P	201	CDL	OA5-CA3-CA4-CA6
22	N	203	LPP	C31-C32-C33-C34
22	P	202	LPP	C31-C32-C33-C34
20	A	504	CDL	C56-C57-C58-C59
23	G	201	TRT	C1-C5-C6-C9
23	g	201	TRT	C1-C5-C6-C9
20	a	504	CDL	C56-C57-C58-C59
20	a	501	CDL	OB9-CB7-OB8-CB6
22	O	202	LPP	O10-C11-O9-C7
20	o	201	CDL	C52-C51-CB5-OB6
20	A	504	CDL	C73-C74-C75-C76
20	D	201	CDL	CB2-C1-CA2-OA2
20	D	201	CDL	C22-C23-C24-C25
20	d	201	CDL	C22-C23-C24-C25
22	I	101	LPP	C37-C38-C39-C40
22	i	101	LPP	C37-C38-C39-C40
20	a	504	CDL	C73-C74-C75-C76
20	e	101	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
20	A	502	CDL	C24-C25-C26-C27
20	a	502	CDL	C24-C25-C26-C27
20	d	202	CDL	C32-C31-CA7-OA8
21	D	203	LMT	C1-C2-C3-C4
20	d	201	CDL	C59-C60-C61-C62
20	a	502	CDL	CA5-C11-C12-C13
20	R	101	CDL	C60-C61-C62-C63
20	E	101	CDL	C12-C11-CA5-OA7
20	M	203	CDL	C80-C81-C82-C83
21	d	203	LMT	C1-C2-C3-C4
20	E	101	CDL	C32-C33-C34-C35
20	D	201	CDL	C59-C60-C61-C62
20	r	101	CDL	C60-C61-C62-C63
20	R	101	CDL	C76-C77-C78-C79
20	e	101	CDL	C32-C33-C34-C35
20	p	201	CDL	C52-C53-C54-C55
20	E	101	CDL	C72-C71-CB7-OB8
23	N	201	TRT	C17-C16-O15-C12
23	n	202	TRT	C17-C16-O15-C12
23	N	202	TRT	C1-C5-C6-C9
23	n	203	TRT	C1-C5-C6-C9
21	F	302	LMT	C1-C2-C3-C4
21	f	302	LMT	C1-C2-C3-C4
20	R	101	CDL	C37-C38-C39-C40
20	p	202	CDL	C71-C72-C73-C74
20	e	101	CDL	C12-C11-CA5-OA7
20	O	201	CDL	OA6-CA4-CA6-OA8
22	F	301	LPP	O9-C7-C8-O27
22	f	301	LPP	O9-C7-C8-O27
20	a	504	CDL	C31-CA7-OA8-CA6
20	r	101	CDL	C32-C31-CA7-OA8
23	G	202	TRT	C7-C6-C9-C10
23	g	202	TRT	C7-C6-C9-C10
20	r	101	CDL	C76-C77-C78-C79
21	F	302	LMT	C7-C8-C9-C10
21	f	302	LMT	C7-C8-C9-C10
20	P	201	CDL	C31-C32-C33-C34
20	O	201	CDL	C18-C19-C20-C21
20	R	101	CDL	C32-C31-CA7-OA8
20	e	101	CDL	C60-C61-C62-C63
23	N	202	TRT	C8-C6-C9-C10
23	n	203	TRT	C8-C6-C9-C10

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Mol	Chain	Res	Type	Atoms
20	E	101	CDL	C60-C61-C62-C63
20	D	202	CDL	C71-C72-C73-C74
20	a	504	CDL	CB7-C71-C72-C73
23	N	201	TRT	O18-C19-C20-O21
23	n	202	TRT	O18-C19-C20-O21
22	O	203	LPP	C14-C15-C16-C17
20	a	504	CDL	OA9-CA7-OA8-CA6
20	e	101	CDL	C72-C71-CB7-OB8
20	D	202	CDL	C12-C13-C14-C15
20	a	503	CDL	C71-C72-C73-C74
20	o	201	CDL	C18-C19-C20-C21
20	E	101	CDL	C73-C74-C75-C76
22	o	203	LPP	C14-C15-C16-C17
20	A	504	CDL	OB7-CB5-OB6-CB4
20	a	504	CDL	OB7-CB5-OB6-CB4
22	O	203	LPP	O10-C11-O9-C7
22	o	203	LPP	O10-C11-O9-C7
23	G	202	TRT	C7-C6-C9-C14
23	M	201	TRT	C7-C6-C9-C10
23	g	202	TRT	C7-C6-C9-C14
23	m	203	TRT	C7-C6-C9-C10
20	A	504	CDL	CB7-C71-C72-C73
20	M	203	CDL	C72-C71-CB7-OB8
20	m	201	CDL	C80-C81-C82-C83
20	r	101	CDL	C32-C33-C34-C35
20	D	202	CDL	C32-C33-C34-C35
23	N	202	TRT	C7-C6-C9-C14
23	n	203	TRT	C7-C6-C9-C14
20	d	201	CDL	C13-C14-C15-C16
23	P	203	TRT	O18-C19-C20-O21
23	p	203	TRT	O18-C19-C20-O21
20	A	501	CDL	CB3-CB4-CB6-OB8
20	A	501	CDL	C19-C20-C21-C22
20	m	201	CDL	C72-C71-CB7-OB8
20	m	202	CDL	C52-C51-CB5-OB6
22	O	203	LPP	C21-C22-C23-C24
22	o	203	LPP	C21-C22-C23-C24
23	G	202	TRT	C1-C5-C6-C9
23	g	202	TRT	C1-C5-C6-C9
23	g	202	TRT	C2-C1-C5-C6
20	d	201	CDL	C56-C57-C58-C59
23	N	202	TRT	C7-C6-C9-C10

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Mol	Chain	Res	Type	Atoms
23	n	203	TRT	C7-C6-C9-C10
20	A	504	CDL	C52-C51-CB5-OB6
22	N	203	LPP	O10-C11-C12-C13
22	P	202	LPP	O10-C11-C12-C13
20	D	201	CDL	C13-C14-C15-C16
20	a	504	CDL	C52-C51-CB5-OB6
20	D	201	CDL	C56-C57-C58-C59
20	O	201	CDL	C13-C14-C15-C16
20	e	101	CDL	C73-C74-C75-C76
22	O	202	LPP	O5-C6-C7-C8
22	o	202	LPP	O5-C6-C7-C8
23	N	202	TRT	C8-C6-C9-C14
23	n	203	TRT	C8-C6-C9-C14
20	M	204	CDL	C52-C51-CB5-OB6
22	N	203	LPP	O9-C7-C8-O27
22	O	202	LPP	O9-C7-C8-O27
22	P	202	LPP	O9-C7-C8-O27
23	G	202	TRT	C2-C1-C5-C6
20	O	201	CDL	C12-C13-C14-C15
20	d	202	CDL	C12-C13-C14-C15
20	o	201	CDL	C13-C14-C15-C16
23	M	202	TRT	C1-C5-C6-C8
20	A	503	CDL	C23-C24-C25-C26
22	O	202	LPP	C12-C11-O9-C7
20	a	504	CDL	C72-C73-C74-C75
20	E	101	CDL	OB7-CB5-OB6-CB4
23	M	202	TRT	O15-C16-C17-O18
23	m	204	TRT	O15-C16-C17-O18
20	A	501	CDL	C54-C55-C56-C57
20	A	504	CDL	C72-C73-C74-C75
20	o	201	CDL	C12-C13-C14-C15
20	a	501	CDL	C54-C55-C56-C57
20	m	201	CDL	C72-C71-CB7-OB9
23	M	201	TRT	C8-C6-C9-C14
20	R	101	CDL	C51-C52-C53-C54
22	o	202	LPP	C12-C11-O9-C7
20	M	203	CDL	C72-C71-CB7-OB9
20	d	202	CDL	C32-C33-C34-C35
20	r	101	CDL	C52-C51-CB5-OB6
23	m	203	TRT	C7-C6-C9-C14
20	R	101	CDL	C53-C54-C55-C56
20	a	503	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	r	101	CDL	C53-C54-C55-C56
23	m	204	TRT	C1-C5-C6-C8
23	M	201	TRT	C7-C6-C9-C14
23	m	203	TRT	C8-C6-C9-C14
20	R	101	CDL	C32-C31-CA7-OA9
23	N	202	TRT	O15-C16-C17-O18
23	n	203	TRT	O15-C16-C17-O18
23	M	201	TRT	C8-C6-C9-C10
23	m	203	TRT	C8-C6-C9-C10
20	a	501	CDL	C19-C20-C21-C22
20	A	504	CDL	C55-C56-C57-C58
23	g	202	TRT	C8-C6-C9-C14
20	e	101	CDL	C31-CA7-OA8-CA6
20	A	504	CDL	C52-C51-CB5-OB7
20	a	504	CDL	C52-C51-CB5-OB7
20	m	202	CDL	C52-C51-CB5-OB7
21	N	204	LMT	C5'-C4'-O1B-C1B
20	a	501	CDL	CB3-CB4-CB6-OB8
23	G	202	TRT	C8-C6-C9-C14
20	r	101	CDL	C32-C31-CA7-OA9
21	n	201	LMT	C5'-C4'-O1B-C1B
20	r	101	CDL	C51-C52-C53-C54
20	R	101	CDL	C52-C51-CB5-OB6
23	N	202	TRT	O21-C22-C23-O24
23	n	203	TRT	O21-C22-C23-O24
20	A	501	CDL	CA2-OA2-PA1-OA3
20	A	504	CDL	CA2-OA2-PA1-OA3
20	A	504	CDL	CB2-OB2-PB2-OB3
20	E	101	CDL	CA2-OA2-PA1-OA4
20	M	203	CDL	CB2-OB2-PB2-OB3
20	R	101	CDL	CA2-OA2-PA1-OA4
20	R	101	CDL	CA3-OA5-PA1-OA3
20	a	501	CDL	CA2-OA2-PA1-OA3
20	a	503	CDL	CB2-OB2-PB2-OB3
20	a	504	CDL	CA2-OA2-PA1-OA3
20	a	504	CDL	CB2-OB2-PB2-OB3
20	e	101	CDL	CA2-OA2-PA1-OA4
20	m	201	CDL	CB2-OB2-PB2-OB3
20	p	201	CDL	CB2-OB2-PB2-OB3
20	r	101	CDL	CA3-OA5-PA1-OA3
22	o	202	LPP	O9-C7-C8-O27
20	M	204	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
22	o	203	LPP	C15-C16-C17-C18
22	O	203	LPP	C15-C16-C17-C18
20	D	201	CDL	C72-C71-CB7-OB8
20	m	202	CDL	C71-CB7-OB8-CB6
23	g	202	TRT	C8-C6-C9-C10
23	G	202	TRT	C8-C6-C9-C10
20	D	201	CDL	C52-C51-CB5-OB6
20	p	202	CDL	C12-C11-CA5-OA6
20	E	101	CDL	C54-C55-C56-C57
20	r	101	CDL	C33-C34-C35-C36
22	I	101	LPP	C19-C20-C21-C22
22	i	101	LPP	C19-C20-C21-C22
23	G	202	TRT	C23-C22-O21-C20
20	A	503	CDL	C12-C11-CA5-OA6
20	P	201	CDL	C12-C11-CA5-OA6
20	m	201	CDL	C52-C51-CB5-OB6
20	p	202	CDL	C72-C71-CB7-OB8
22	I	101	LPP	O27-C29-C30-C31
22	i	101	LPP	O27-C29-C30-C31
20	m	202	CDL	OB9-CB7-OB8-CB6
23	g	202	TRT	C23-C22-O21-C20
20	M	204	CDL	C1-CB2-OB2-PB2
22	O	202	LPP	O5-C6-C7-O9
22	o	202	LPP	O5-C6-C7-O9
20	P	201	CDL	C72-C71-CB7-OB9
20	R	101	CDL	C52-C51-CB5-OB7
20	M	203	CDL	C52-C51-CB5-OB6
20	P	201	CDL	C72-C71-CB7-OB8
20	r	101	CDL	C52-C51-CB5-OB7
20	a	504	CDL	C55-C56-C57-C58
21	D	203	LMT	C2-C1-O1'-C1'
21	d	203	LMT	C2-C1-O1'-C1'
20	d	201	CDL	C52-C51-CB5-OB6
20	p	201	CDL	C32-C33-C34-C35
20	D	201	CDL	C72-C71-CB7-OB9
20	p	202	CDL	C12-C11-CA5-OA7
20	e	101	CDL	C54-C55-C56-C57
20	D	201	CDL	C32-C31-CA7-OA8
20	M	204	CDL	C32-C31-CA7-OA8
20	m	202	CDL	C32-C31-CA7-OA8
23	G	202	TRT	O18-C19-C20-O21
23	g	202	TRT	O18-C19-C20-O21

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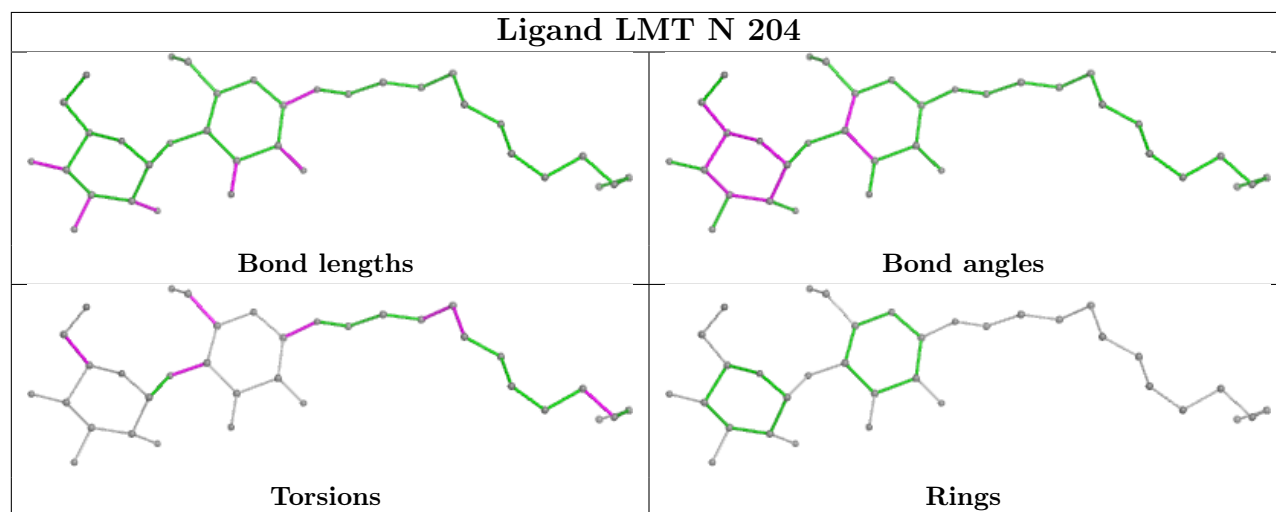
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Mol	Chain	Res	Type	Atoms
20	P	201	CDL	C12-C11-CA5-OA7
20	e	101	CDL	C31-C32-C33-C34
20	a	503	CDL	C12-C11-CA5-OA6

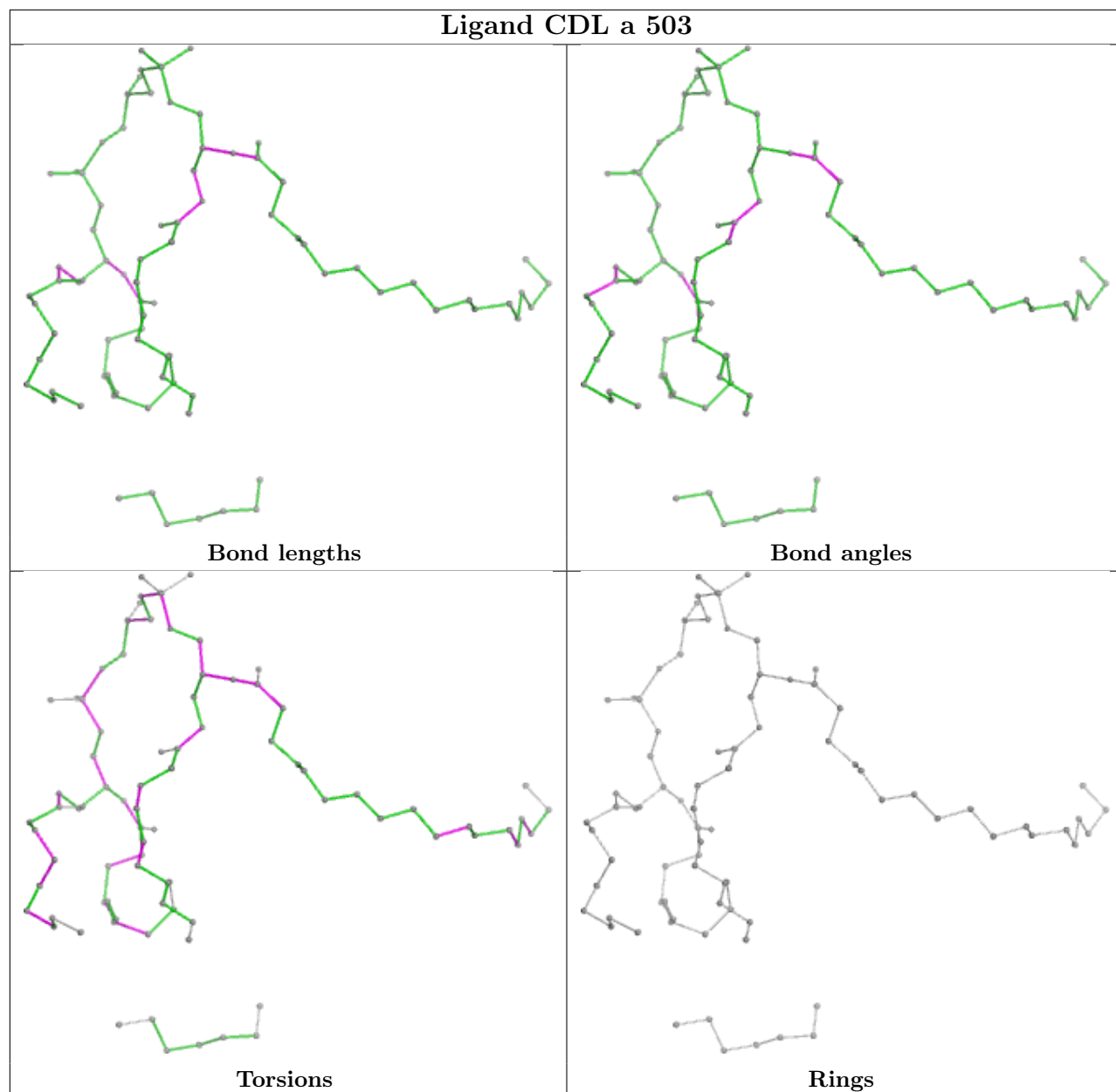
There are no ring outliers.

No monomer is involved in short contacts.

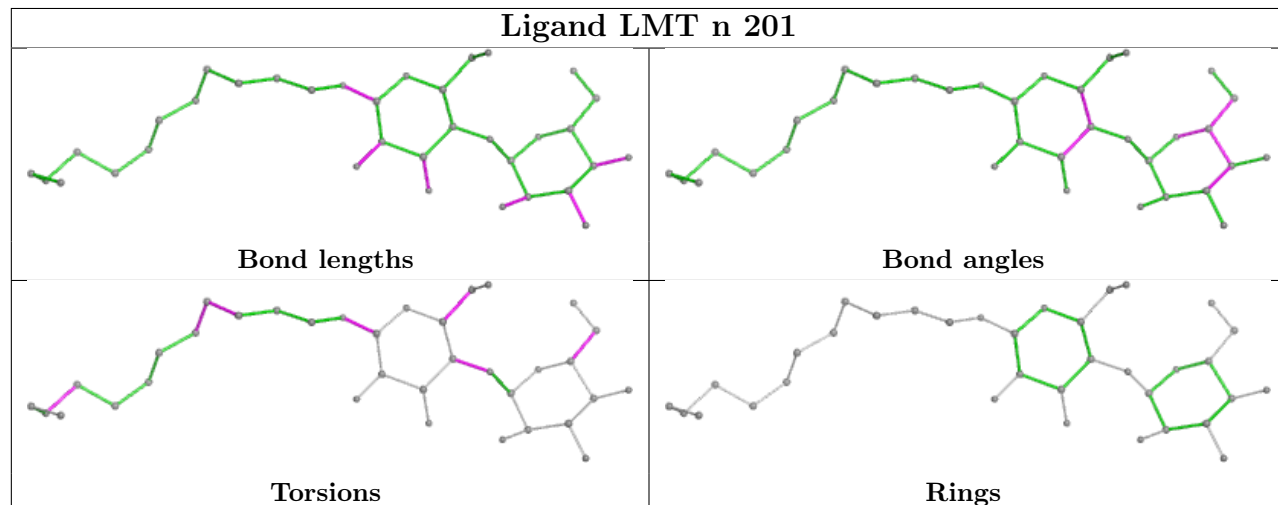
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

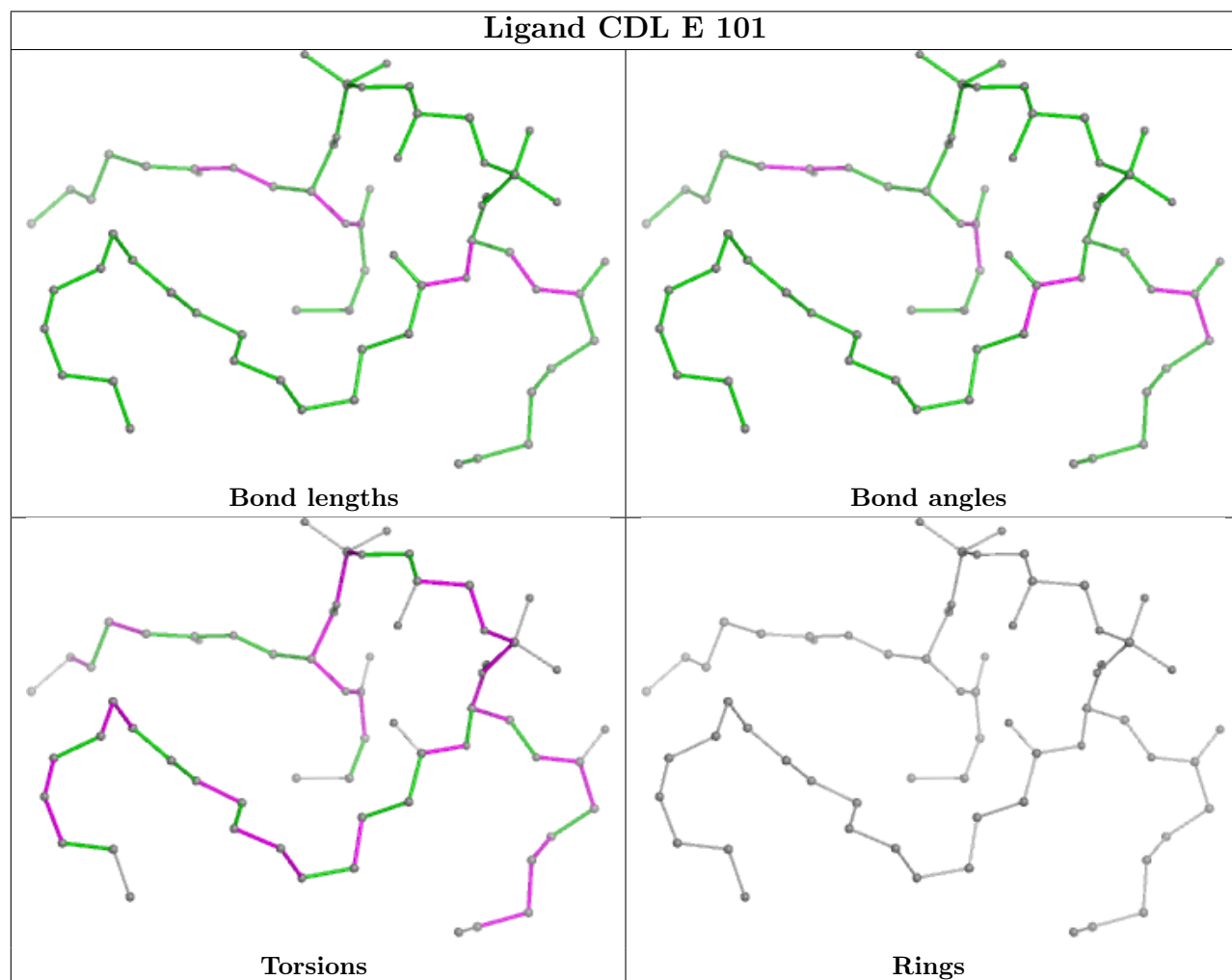
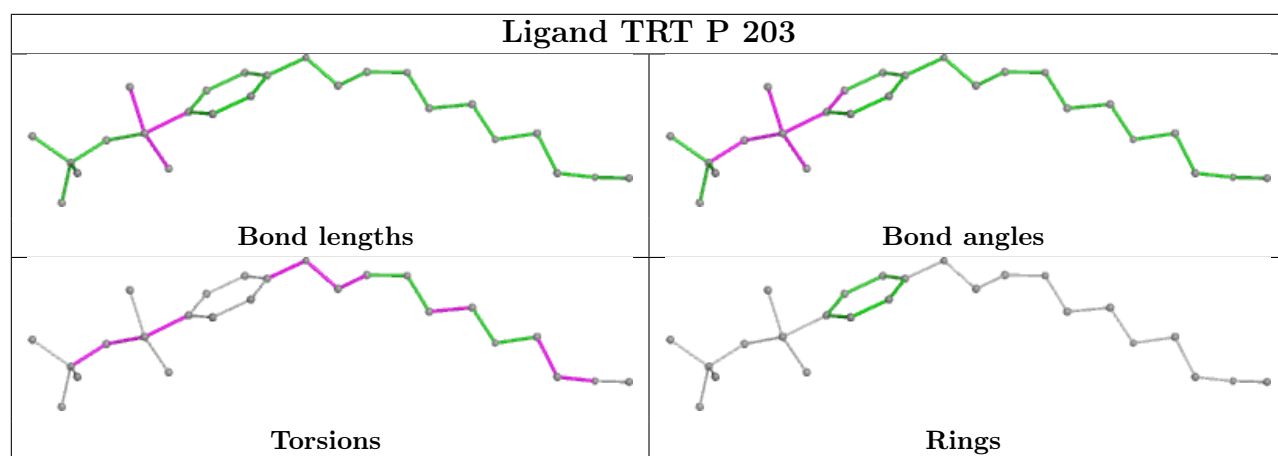


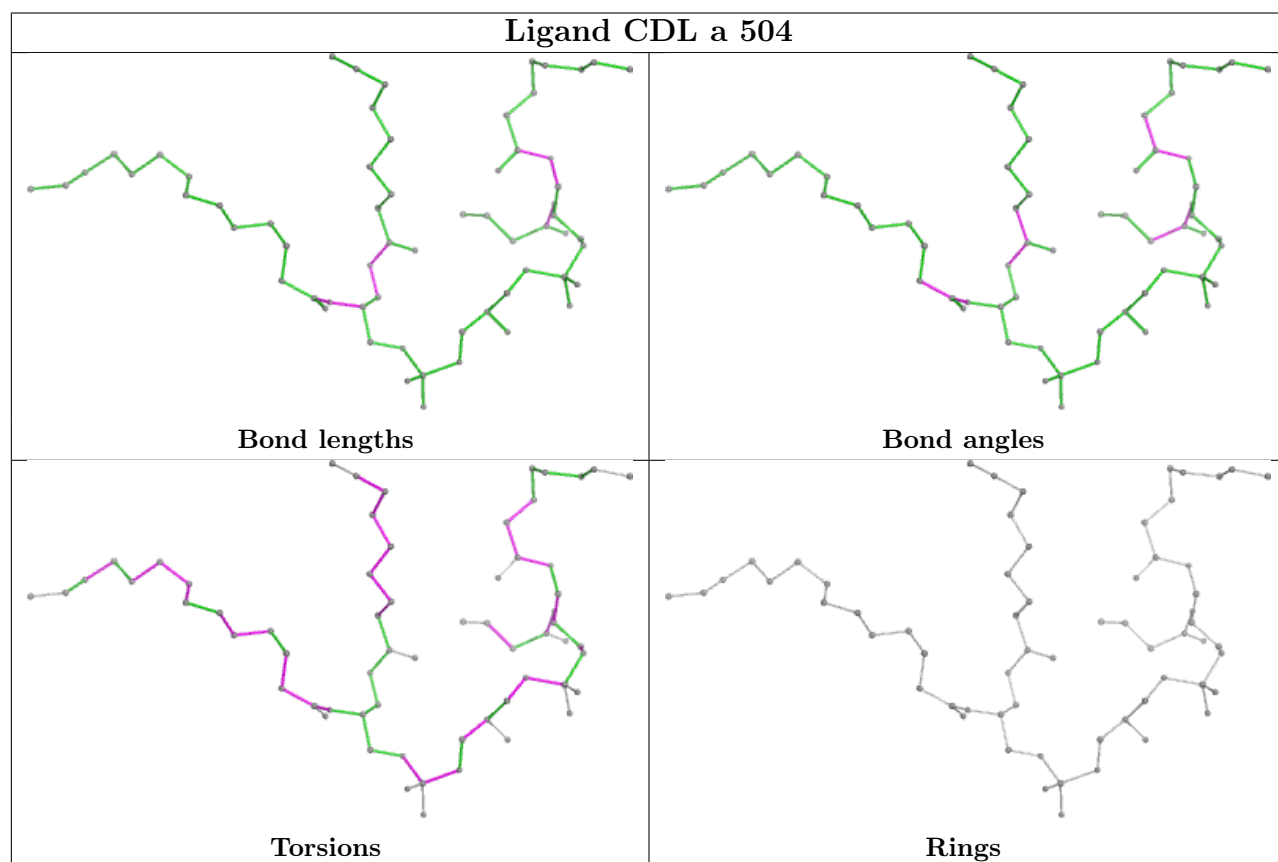
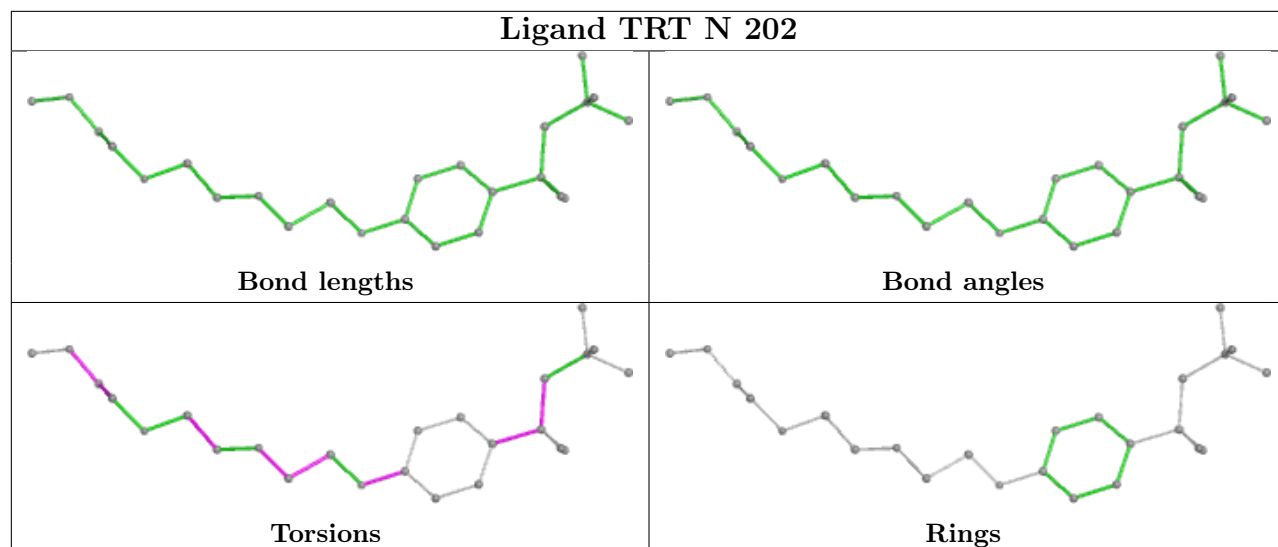
Ligand CDL a 503

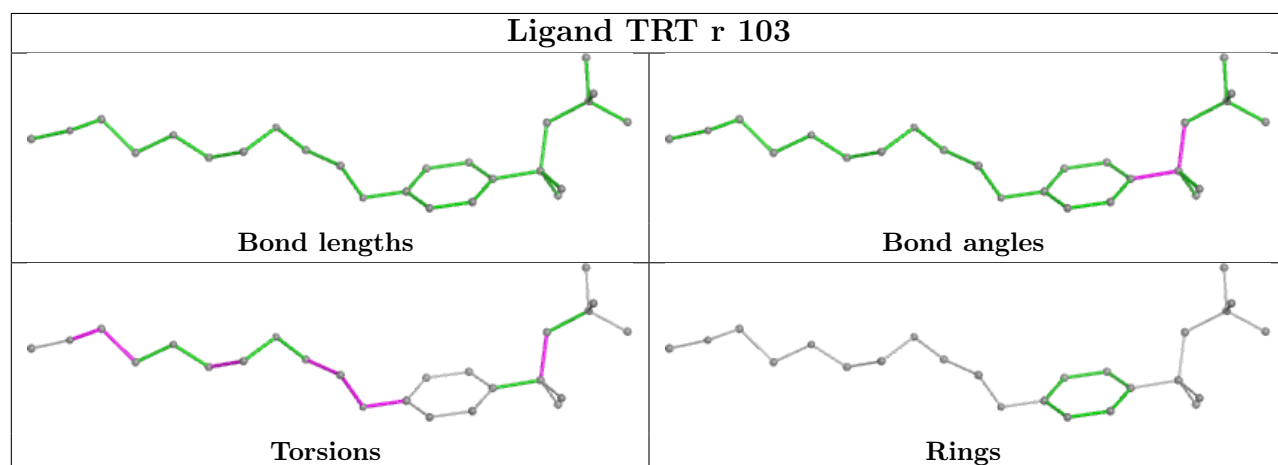
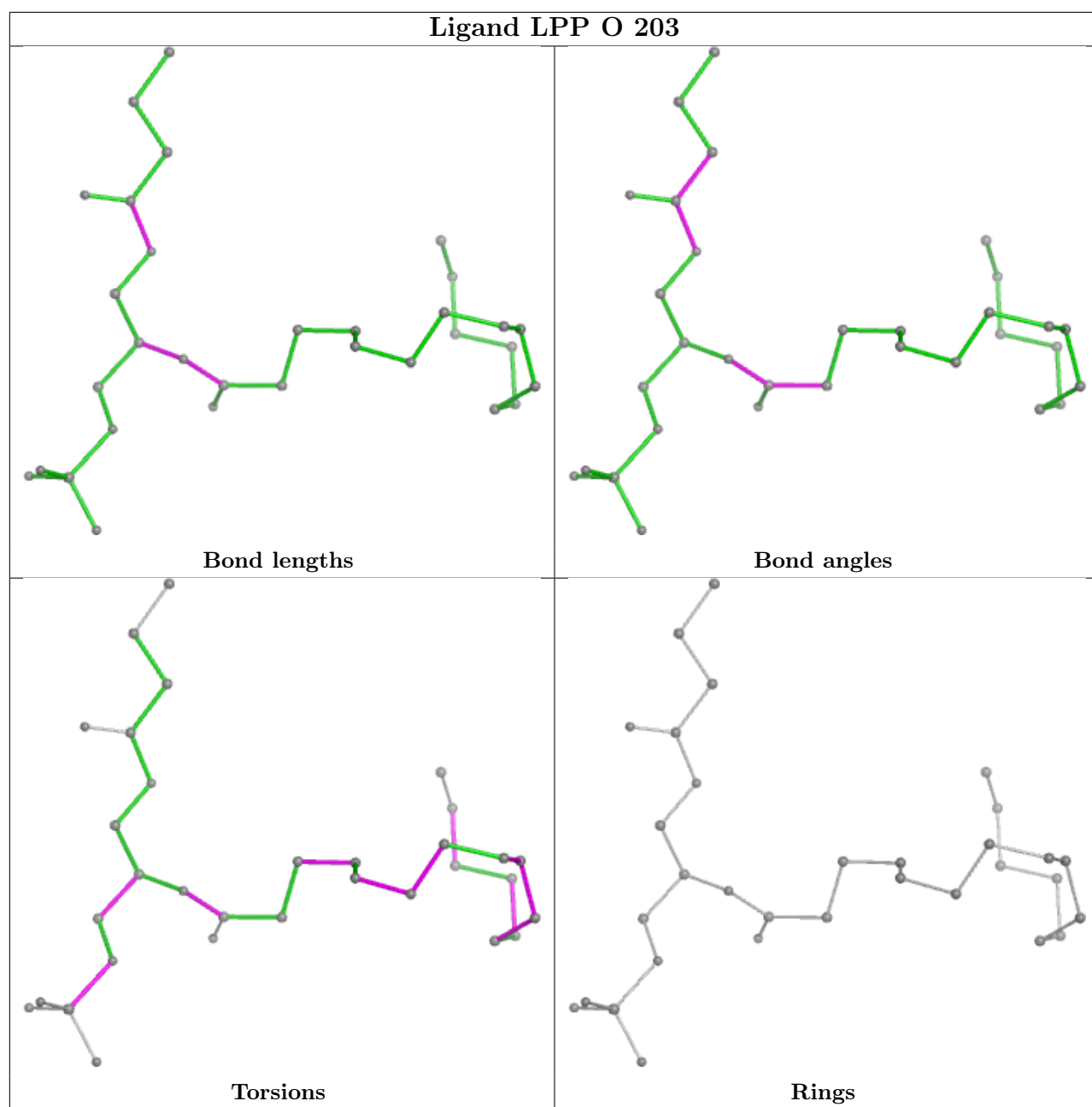


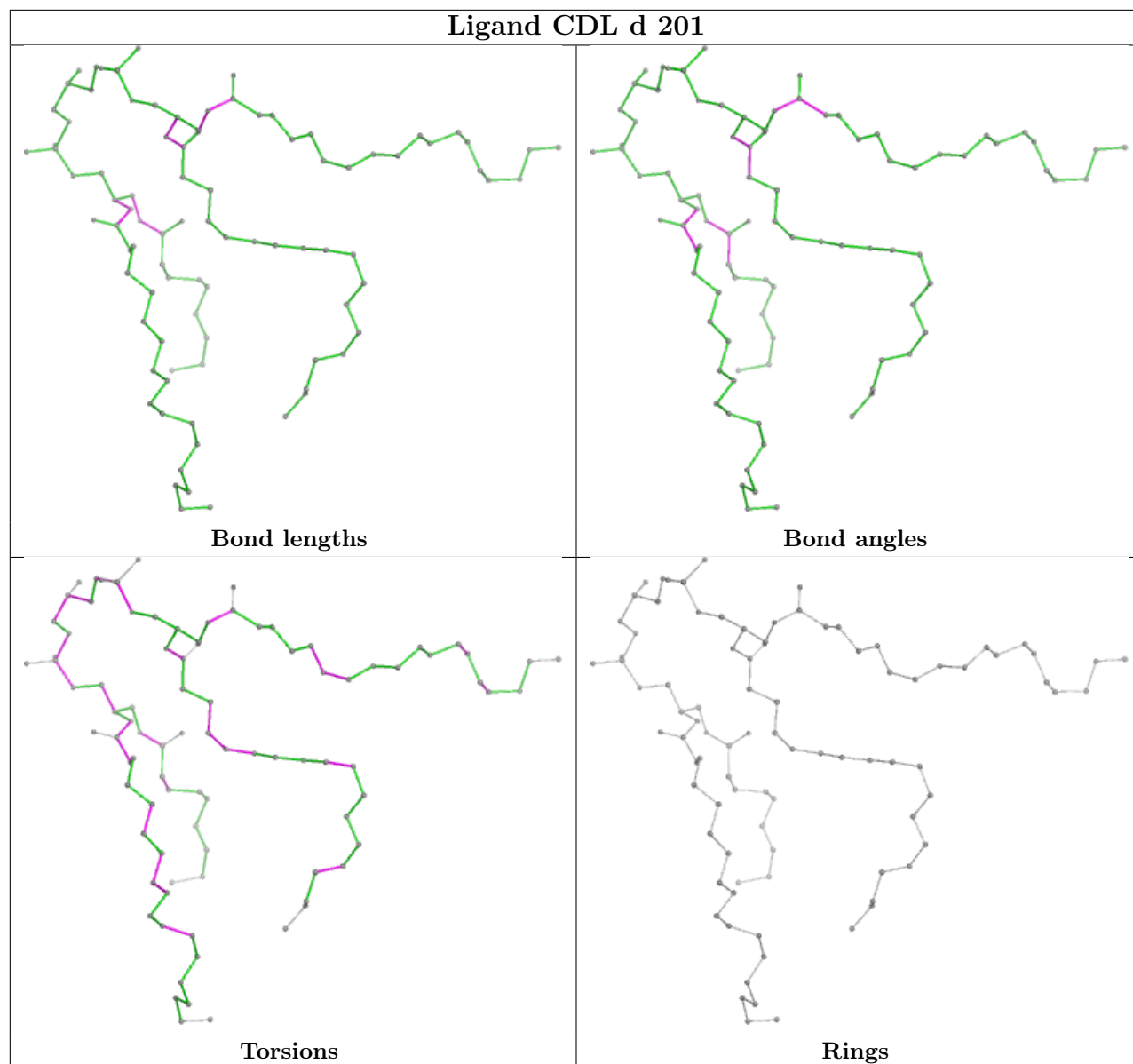
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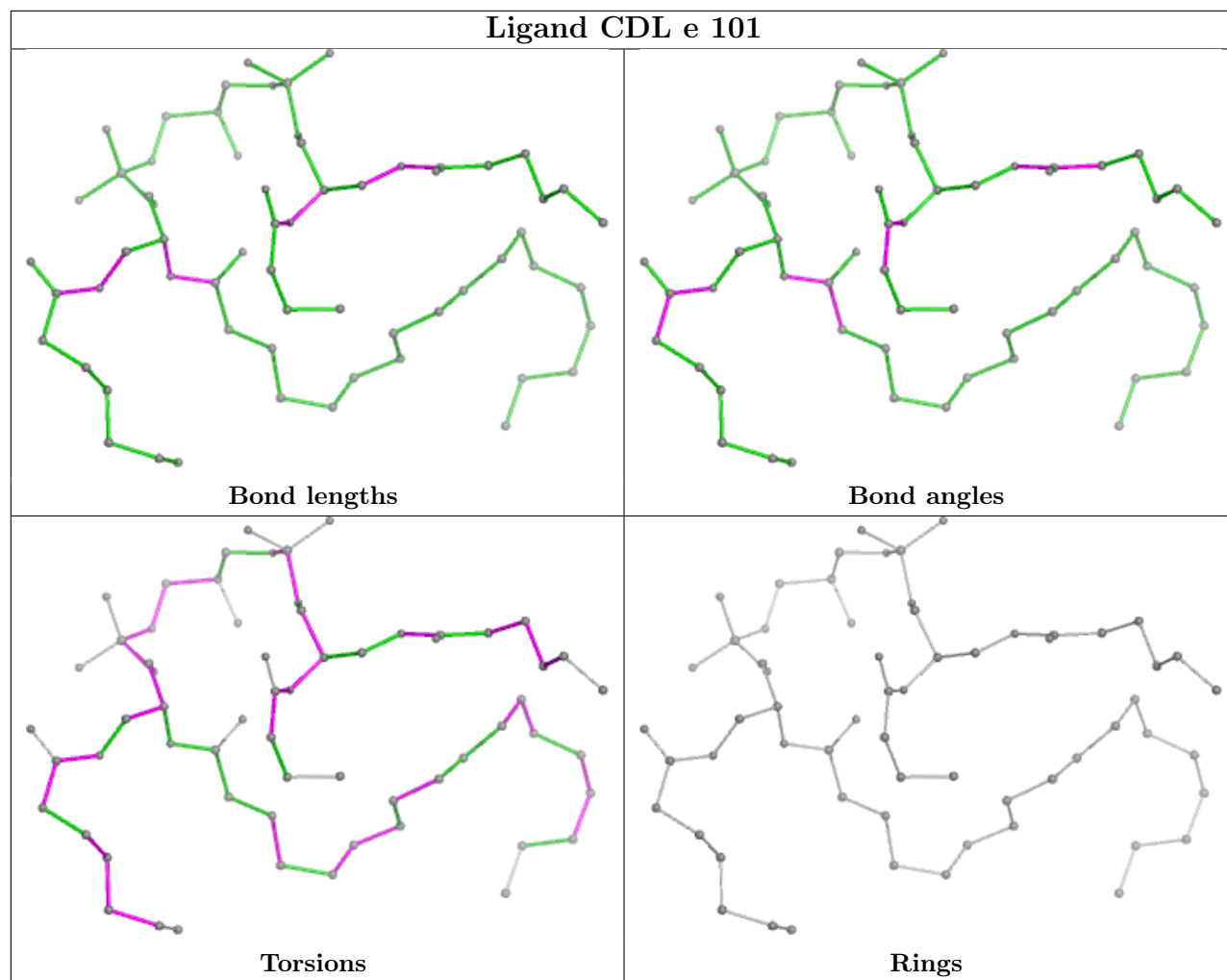


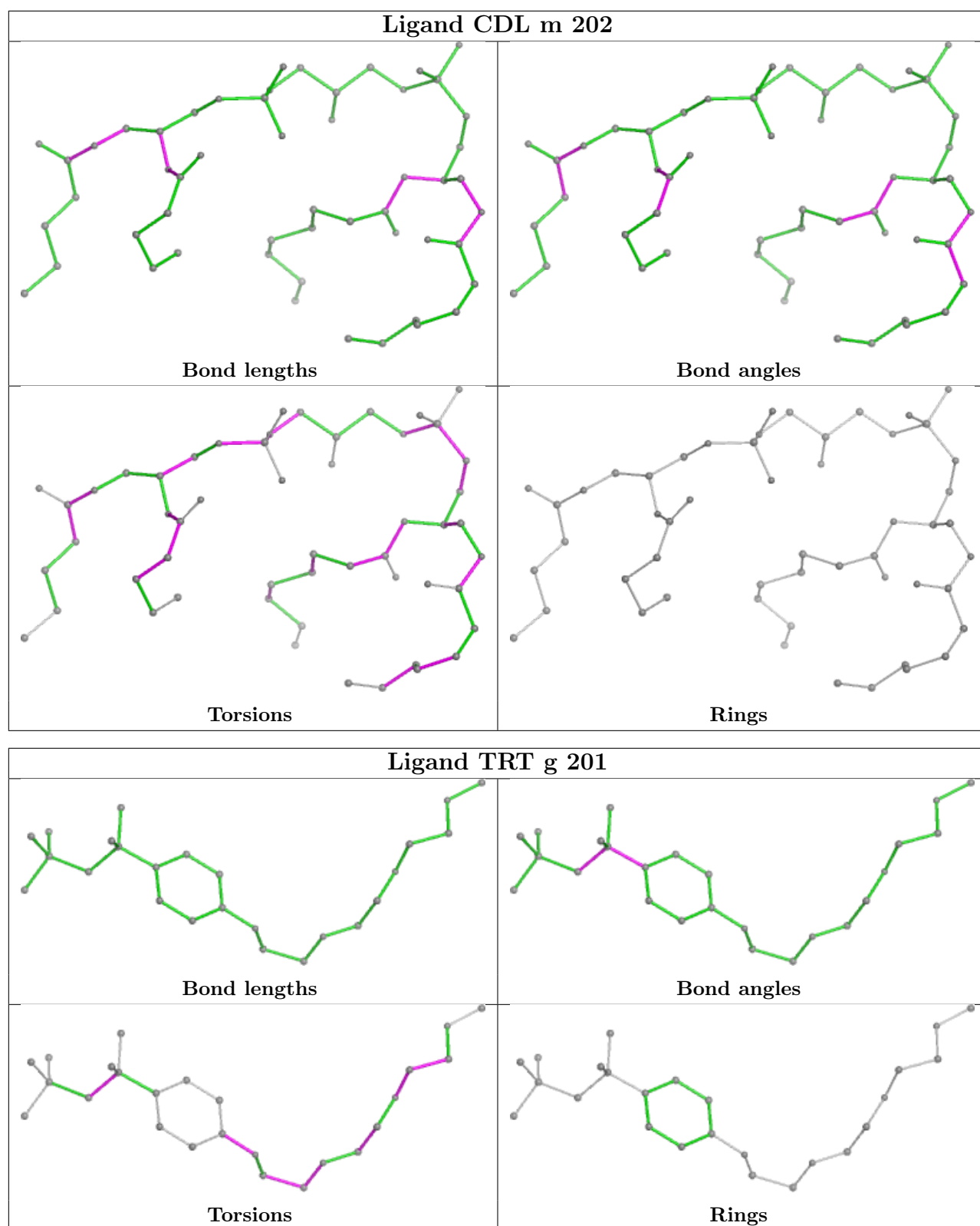


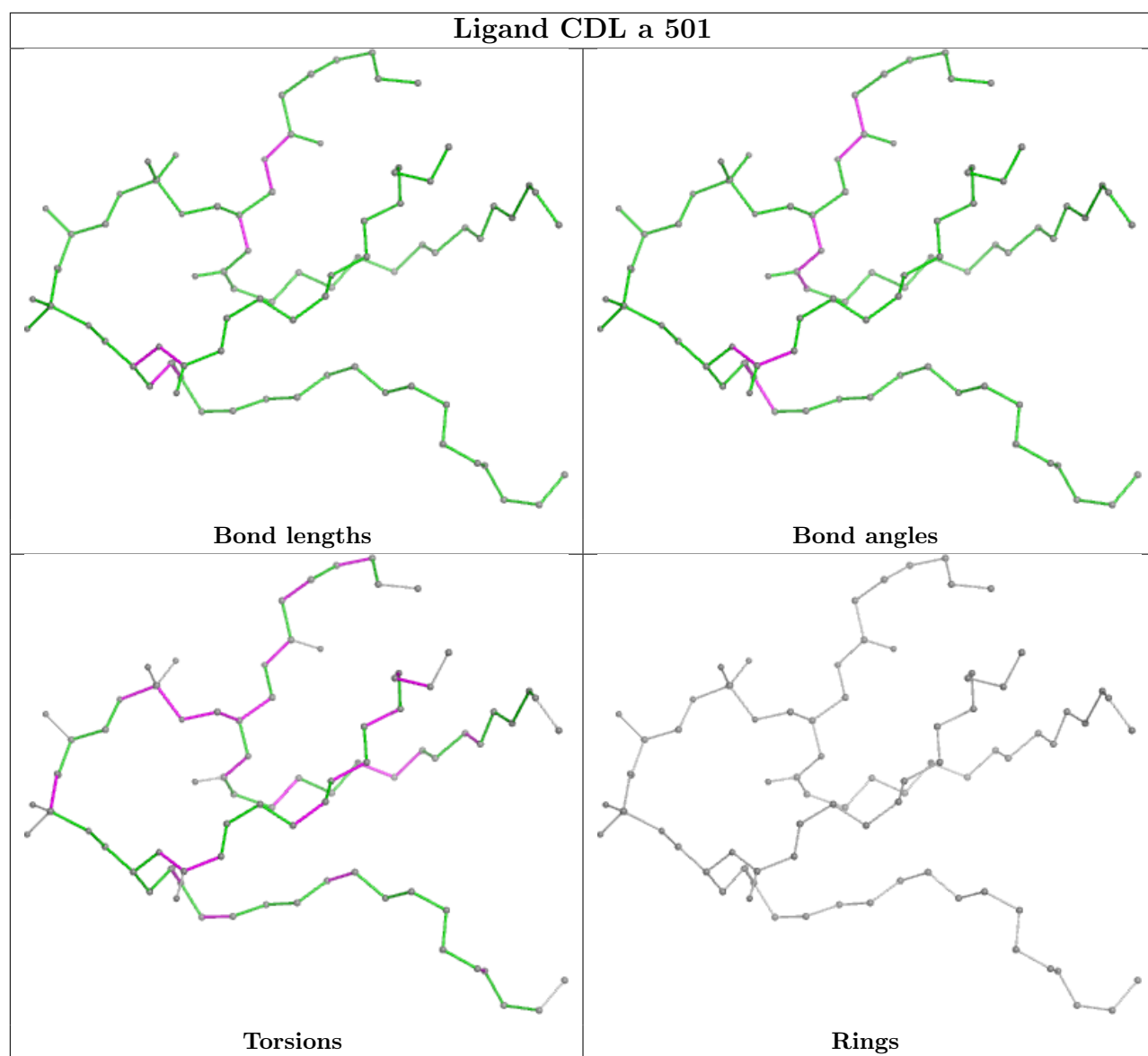


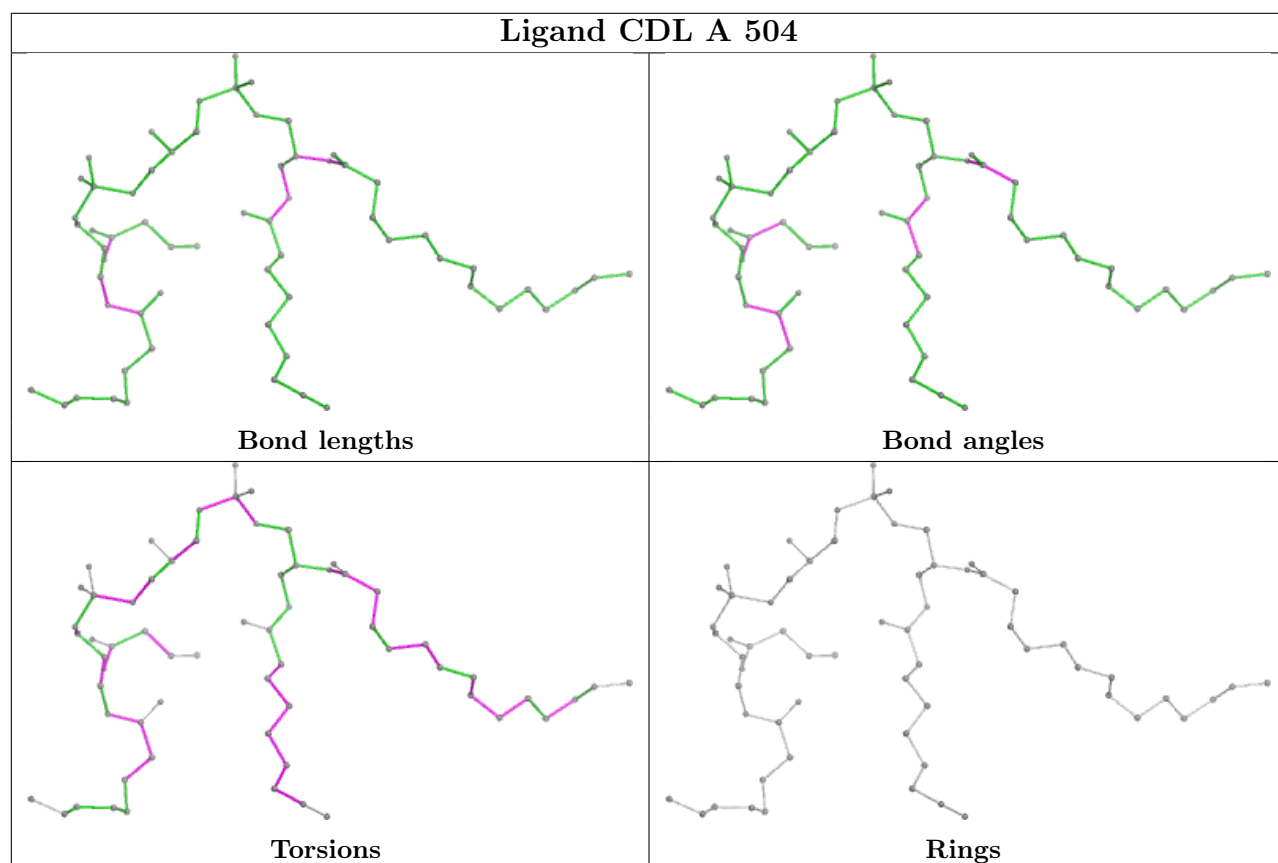
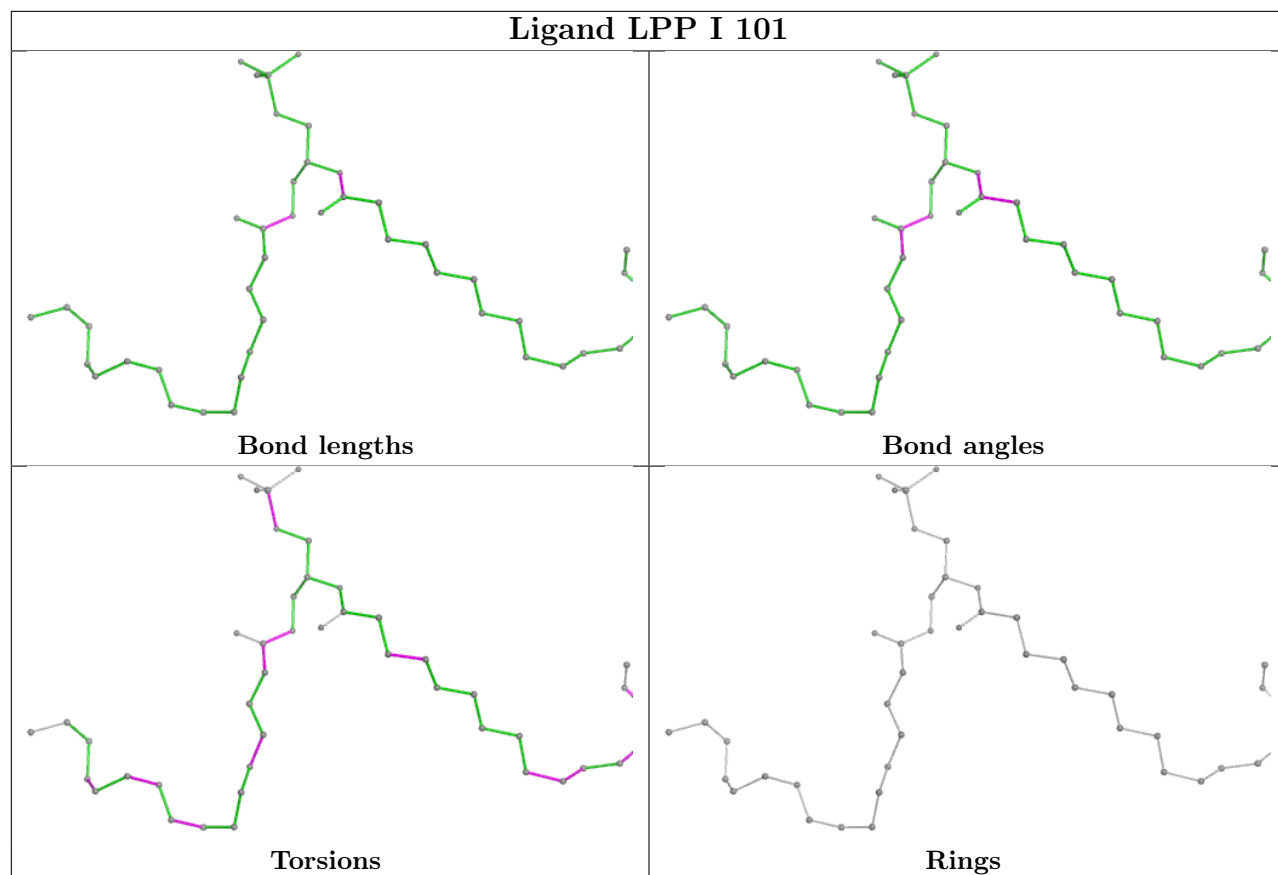


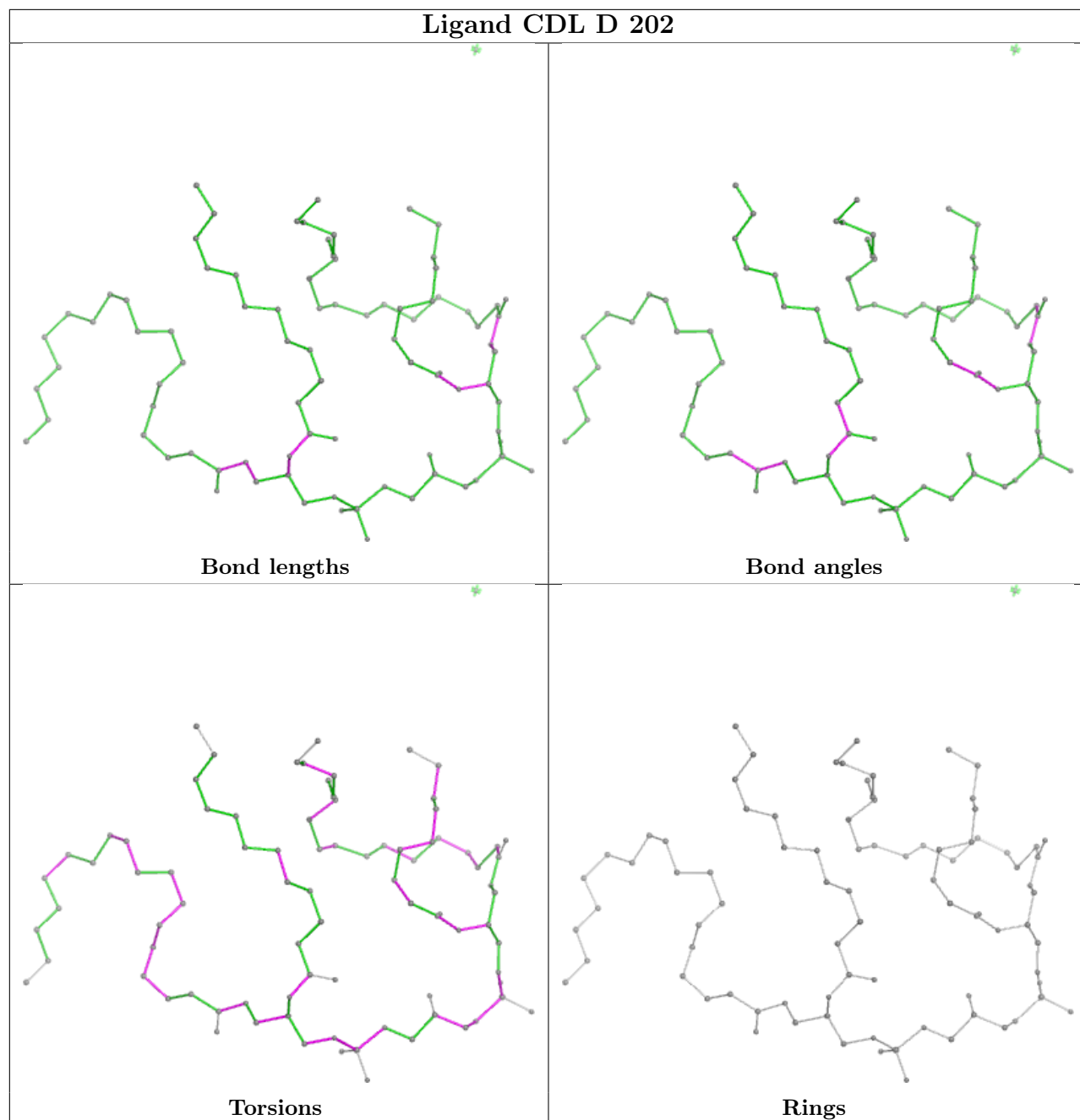


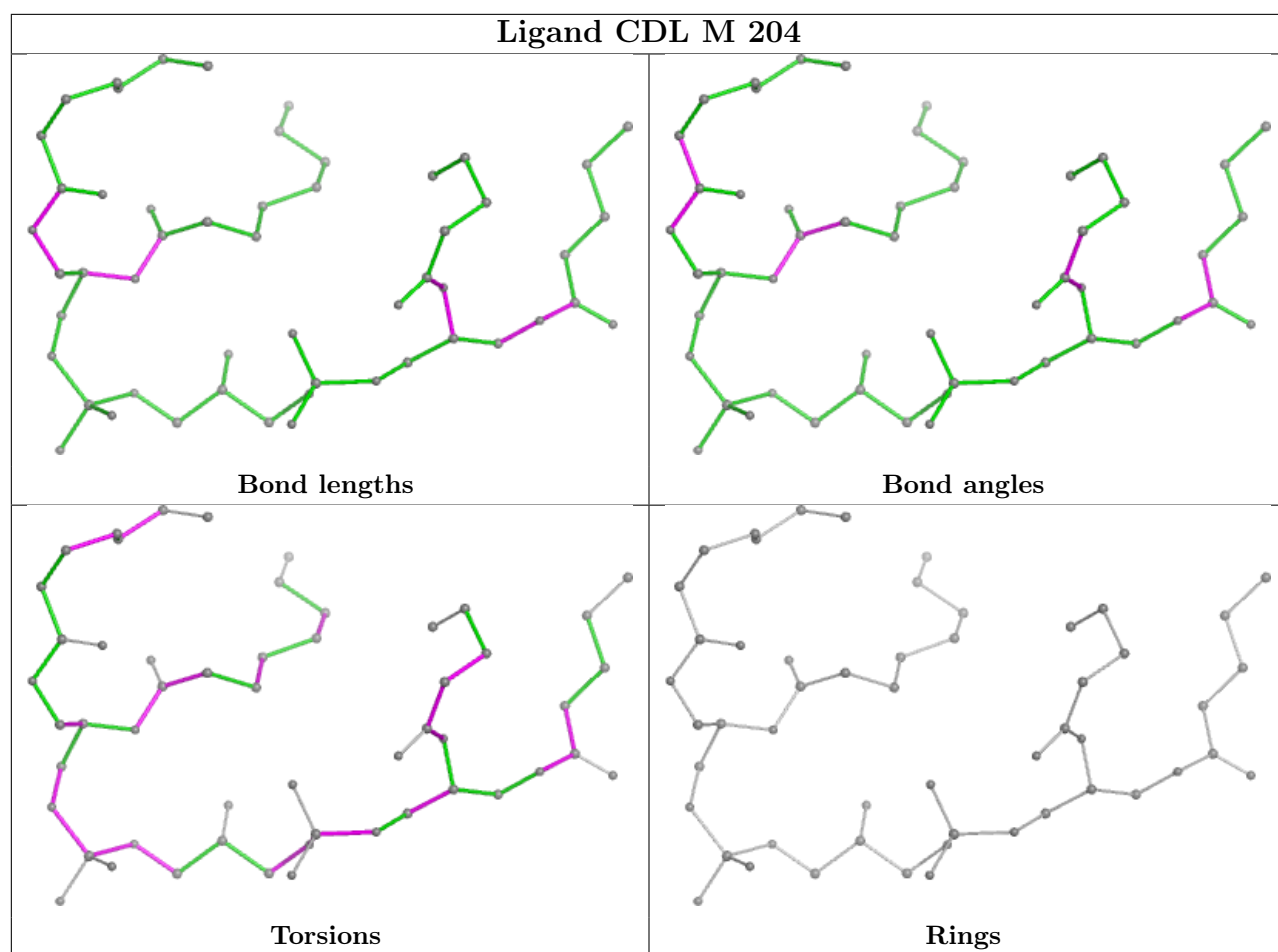


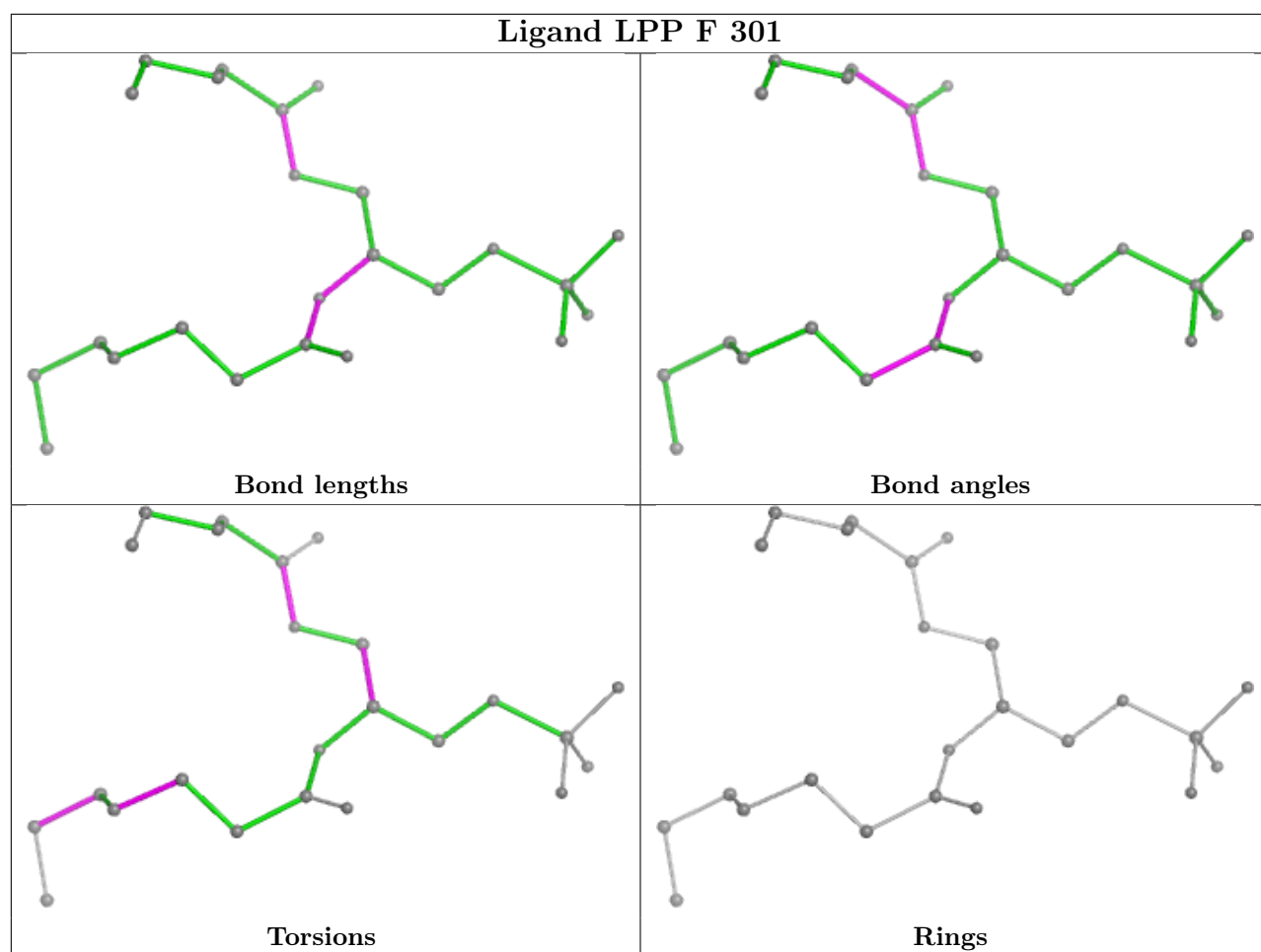


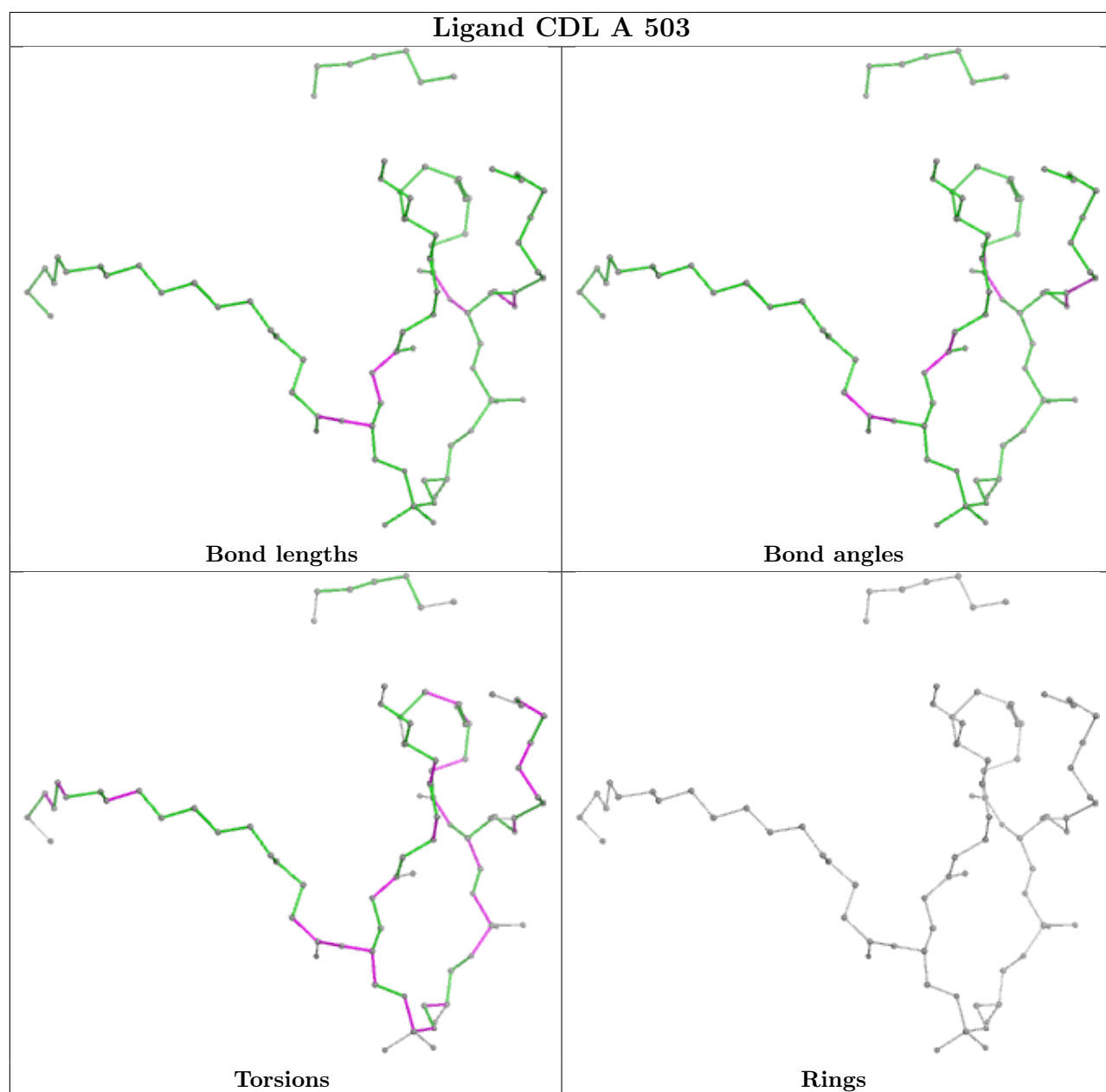


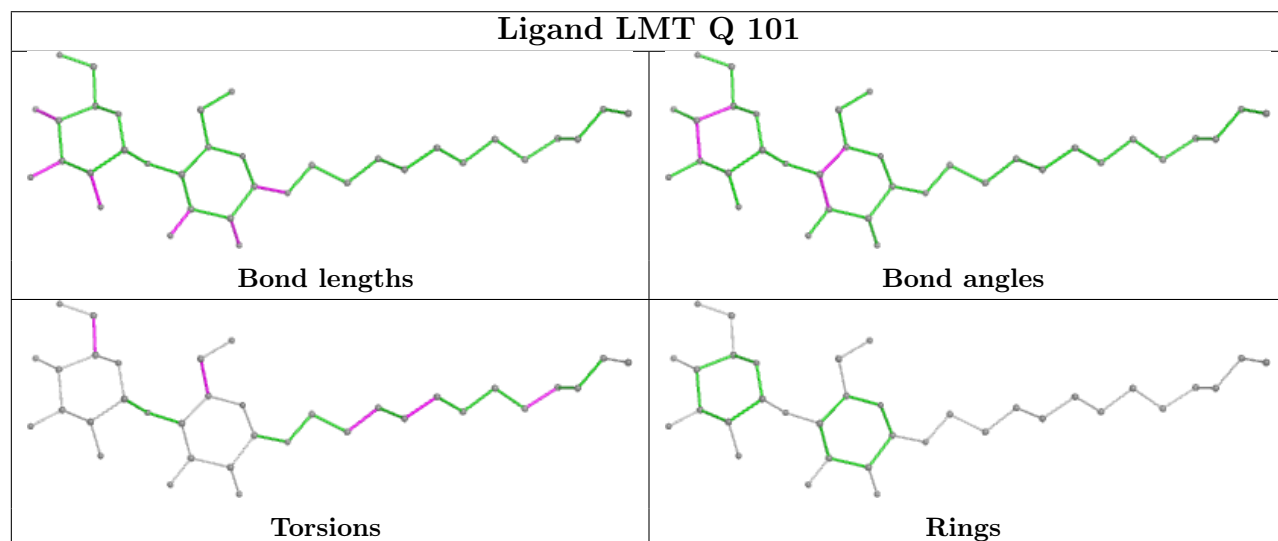
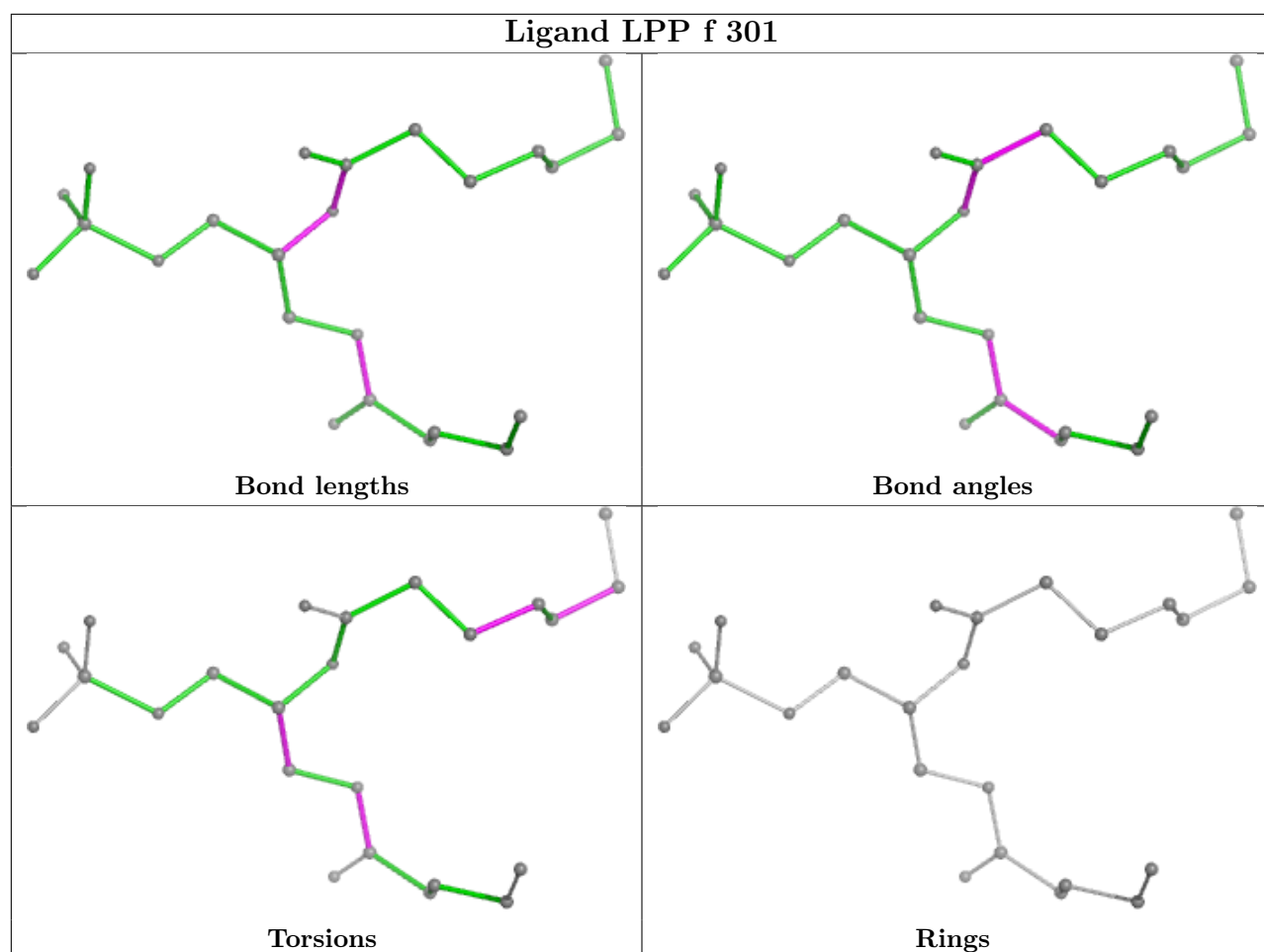


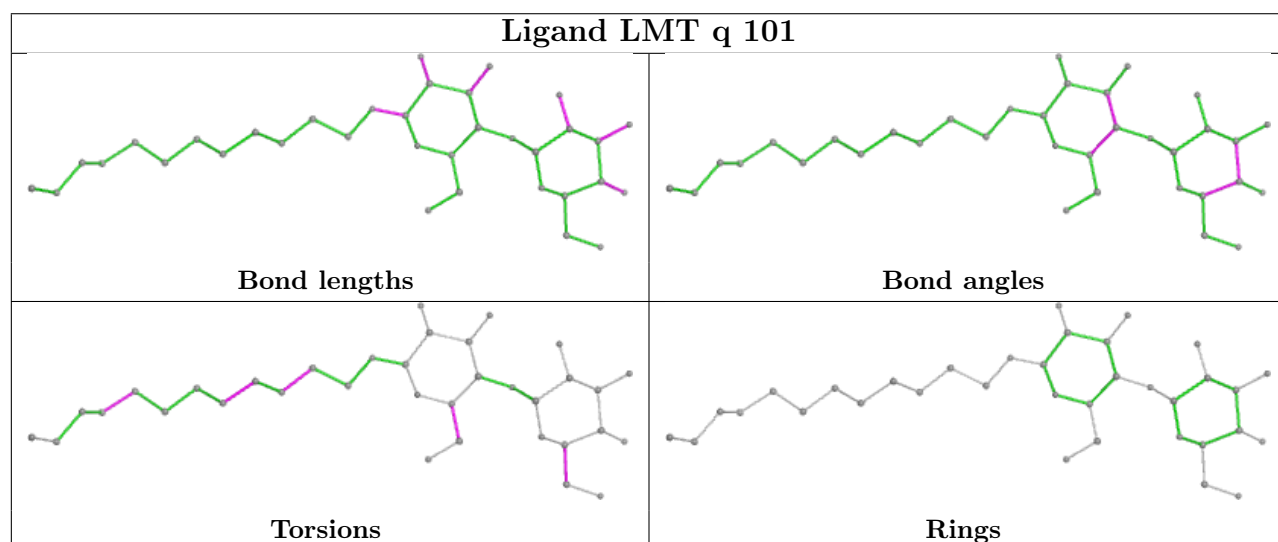
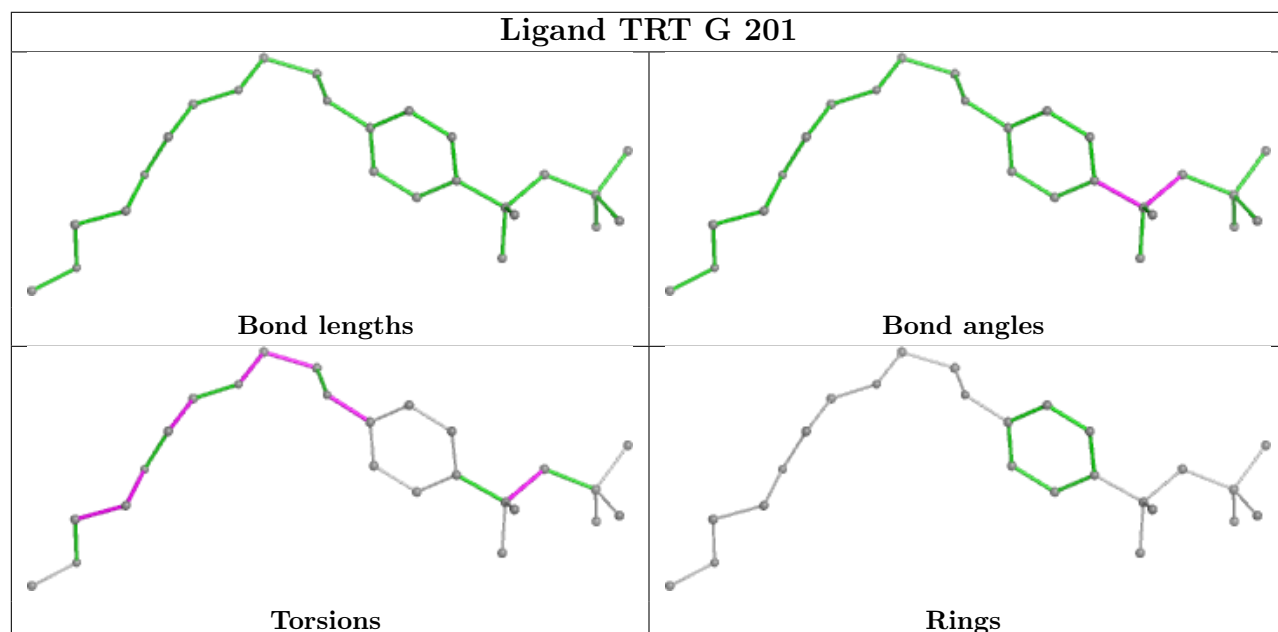
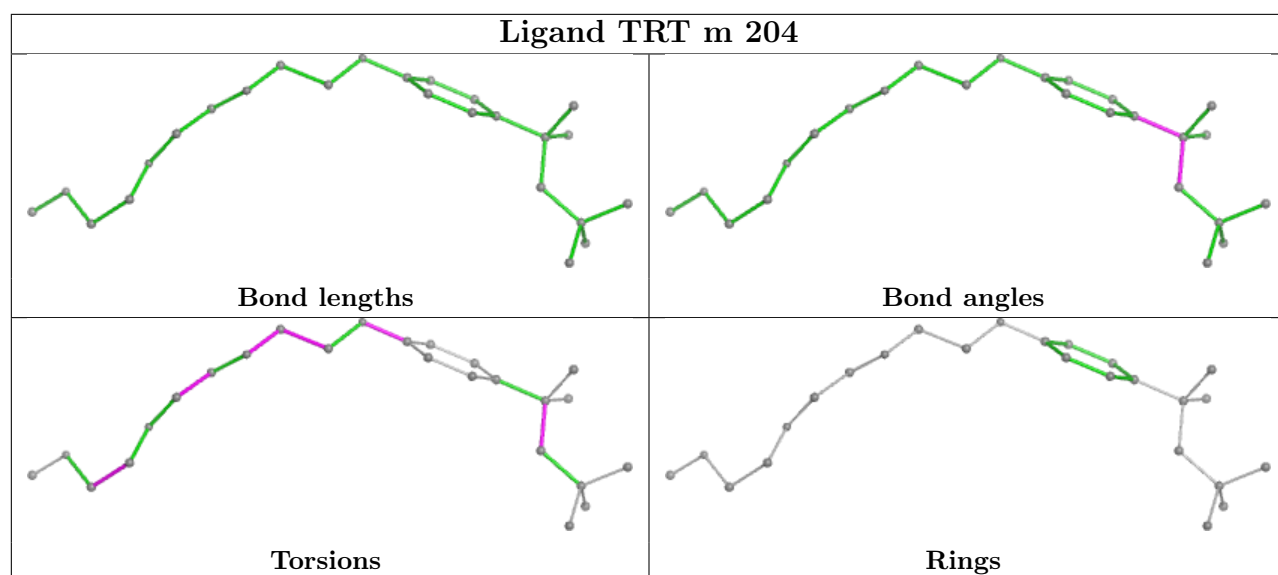


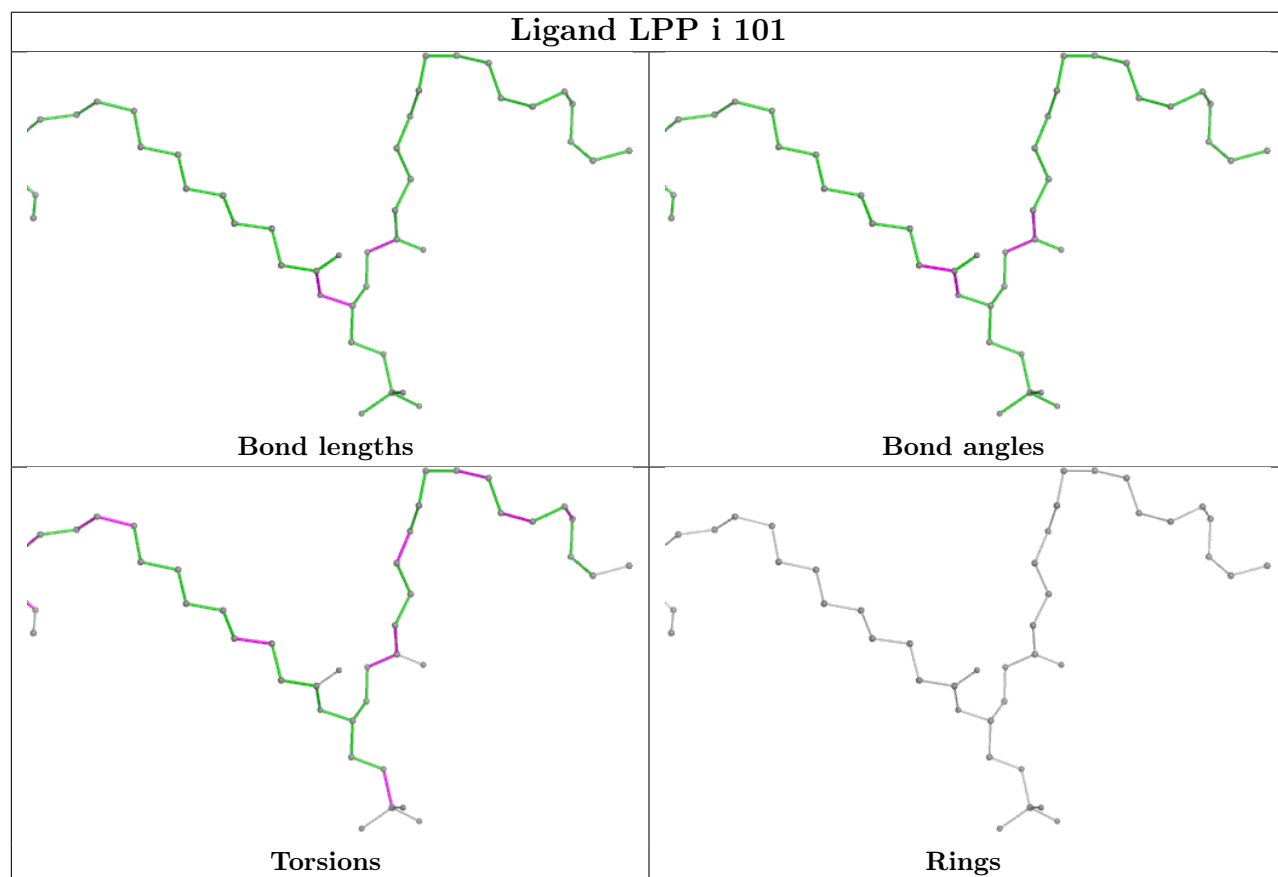
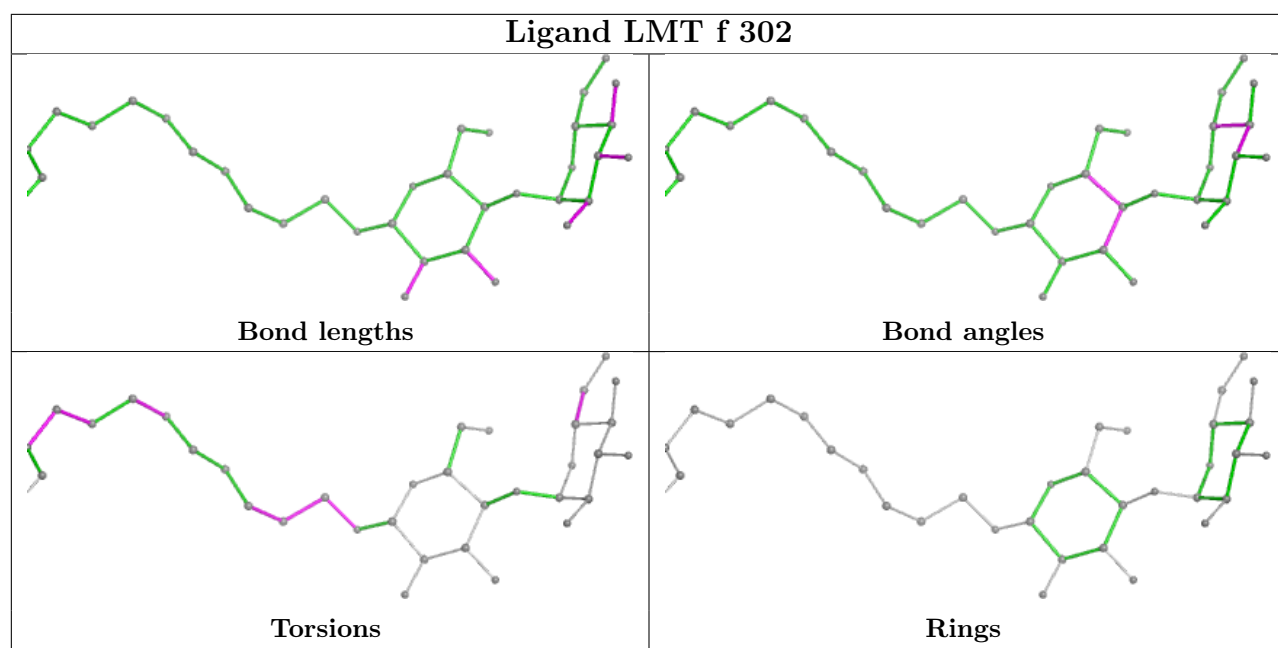


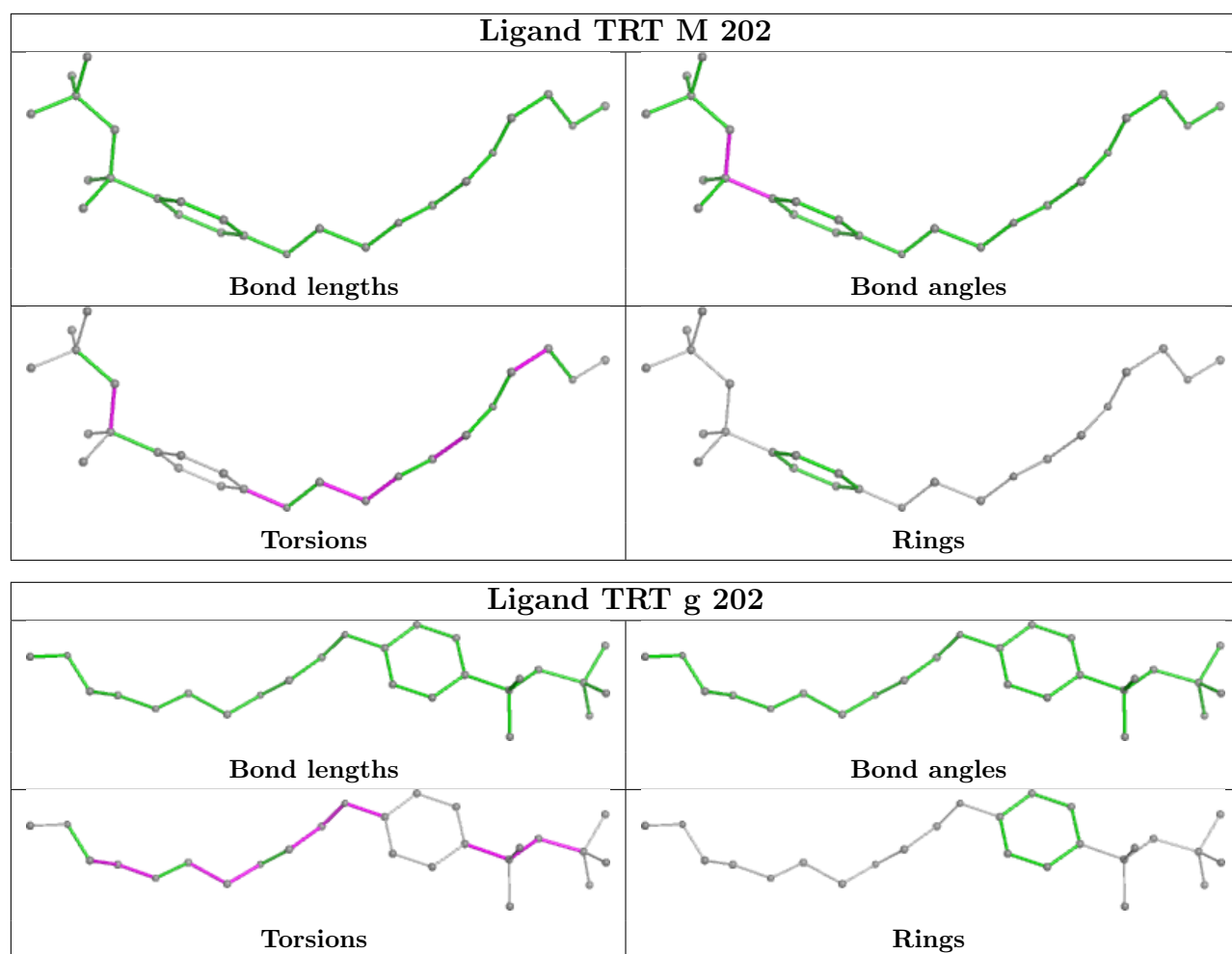


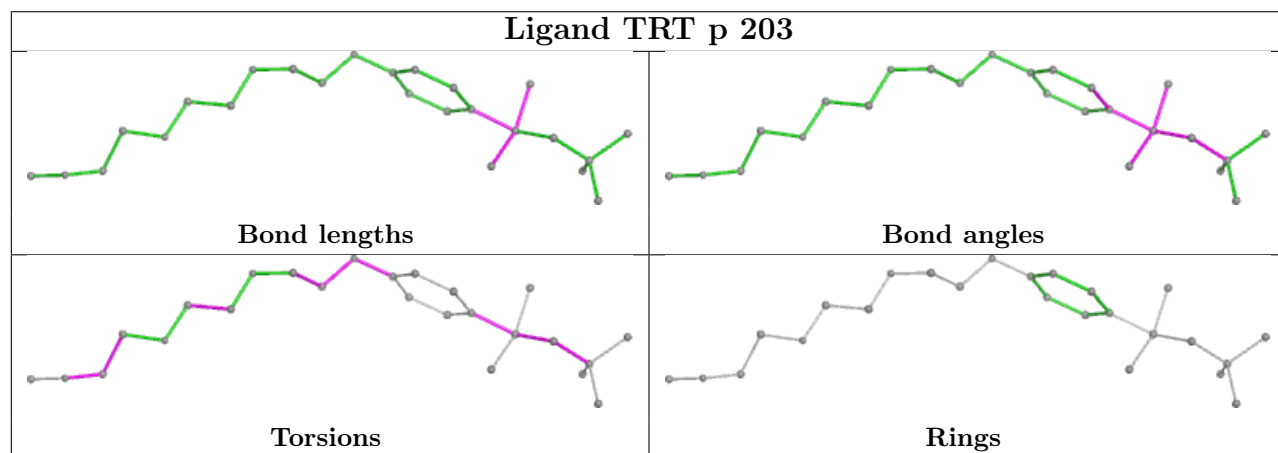
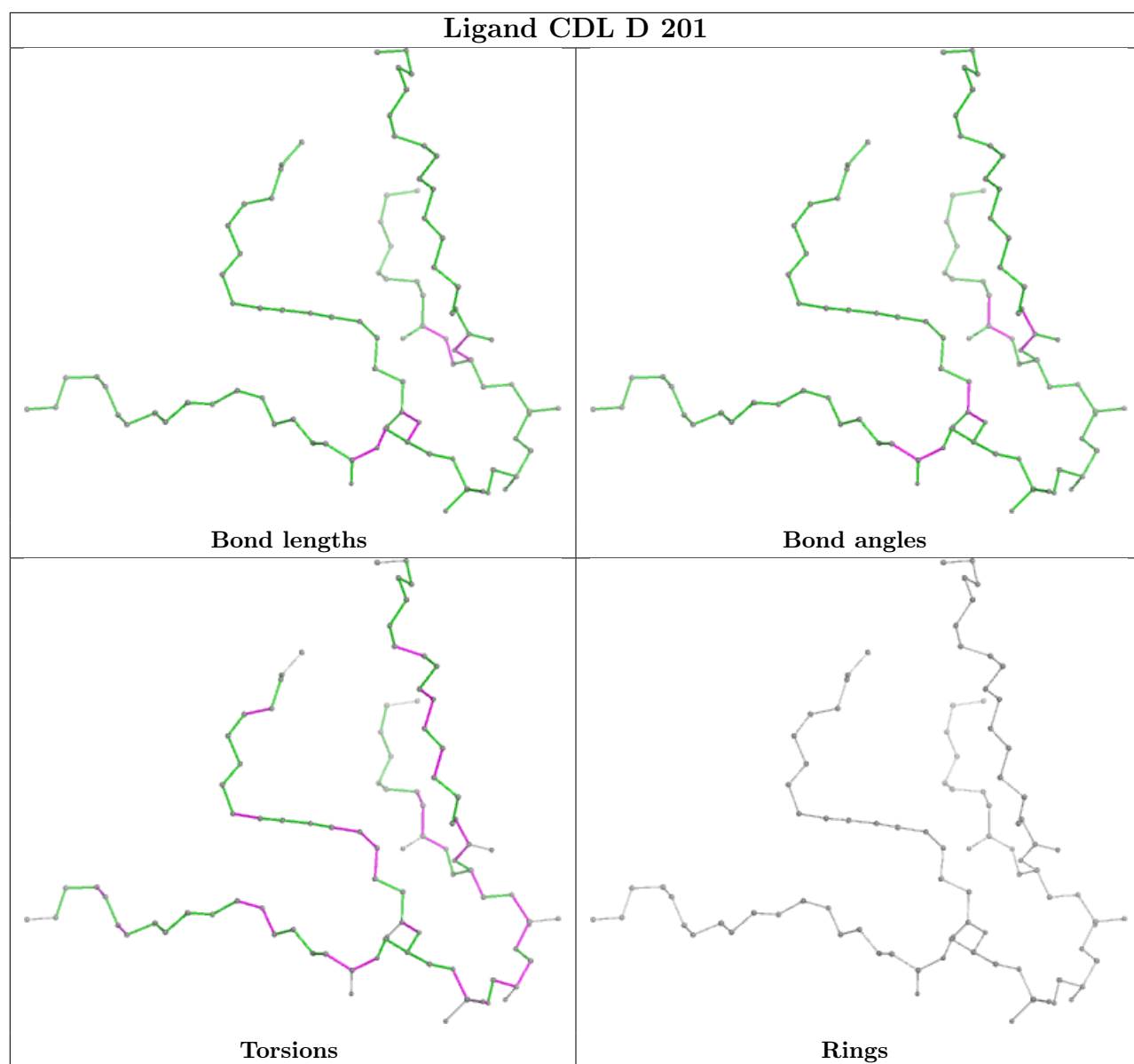


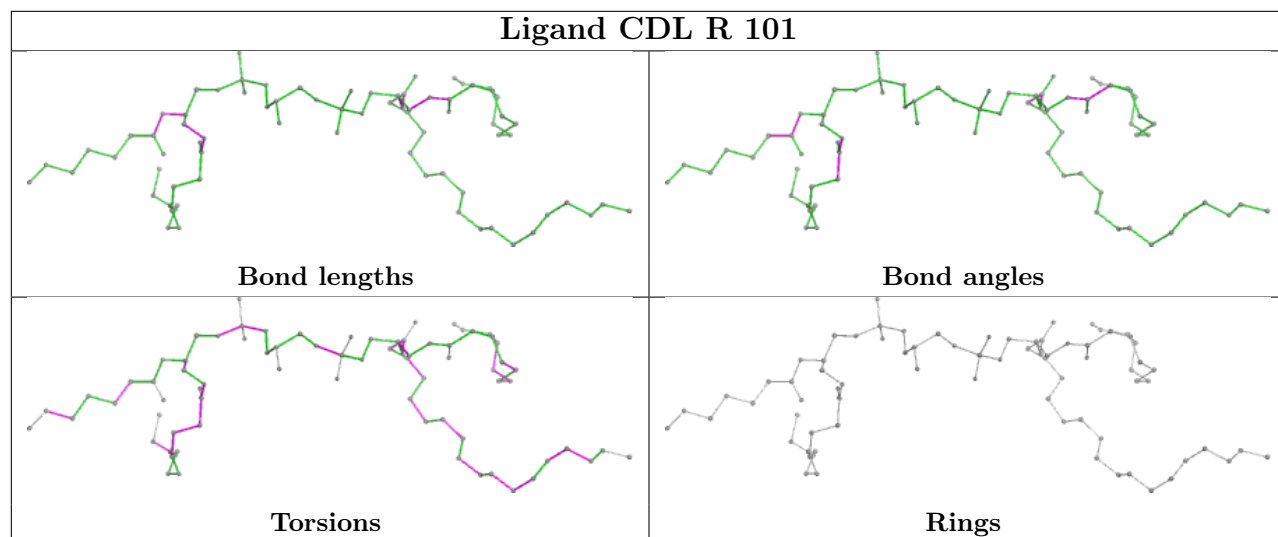
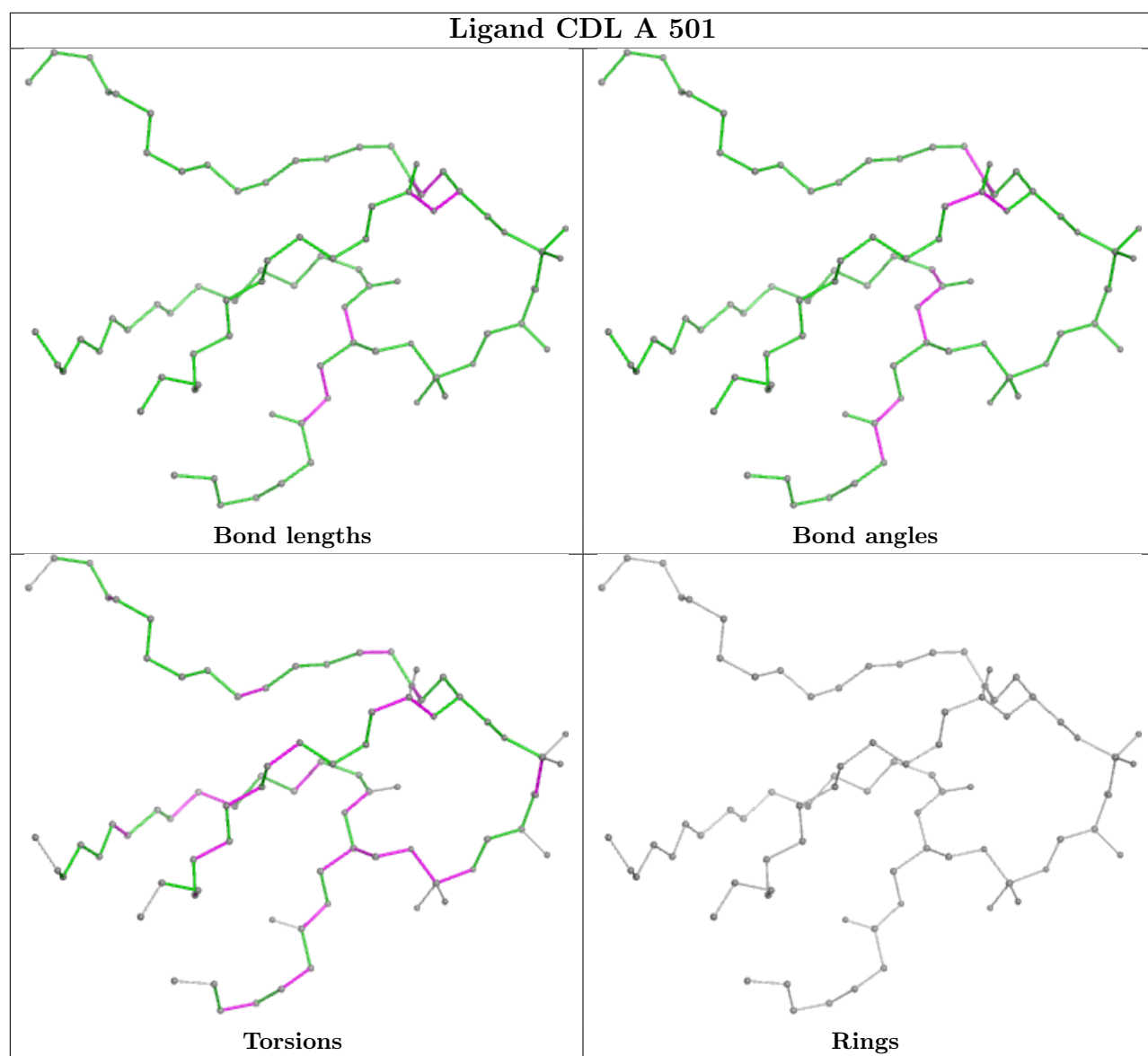


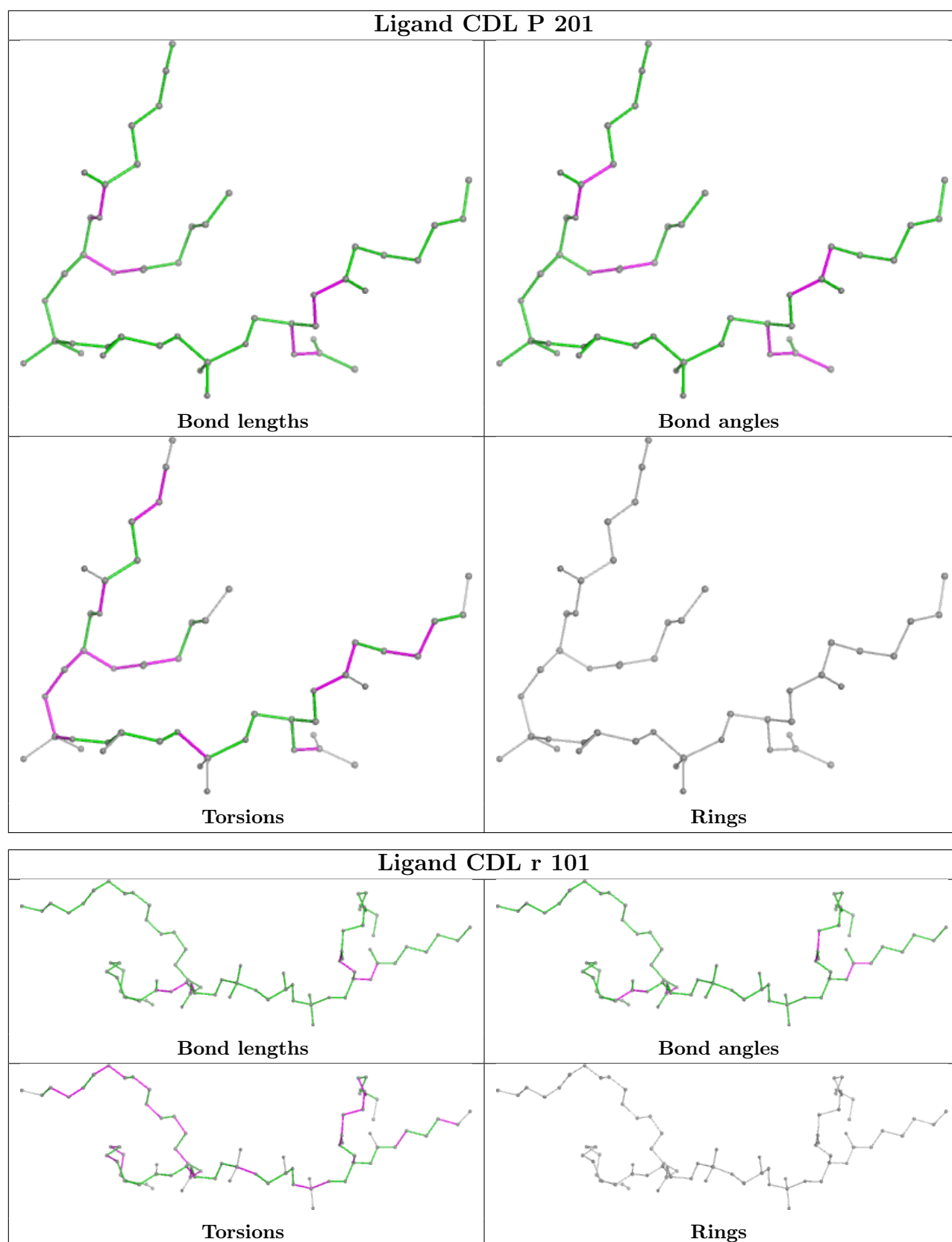


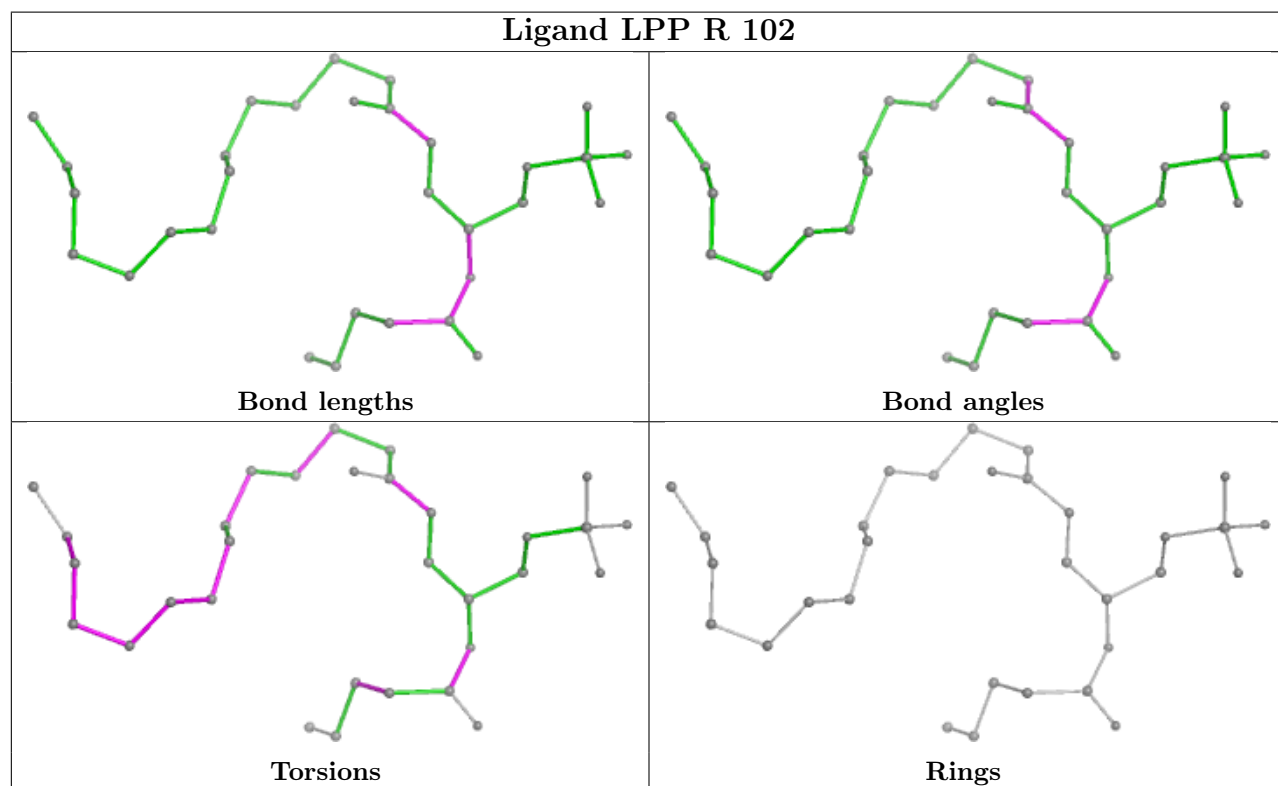
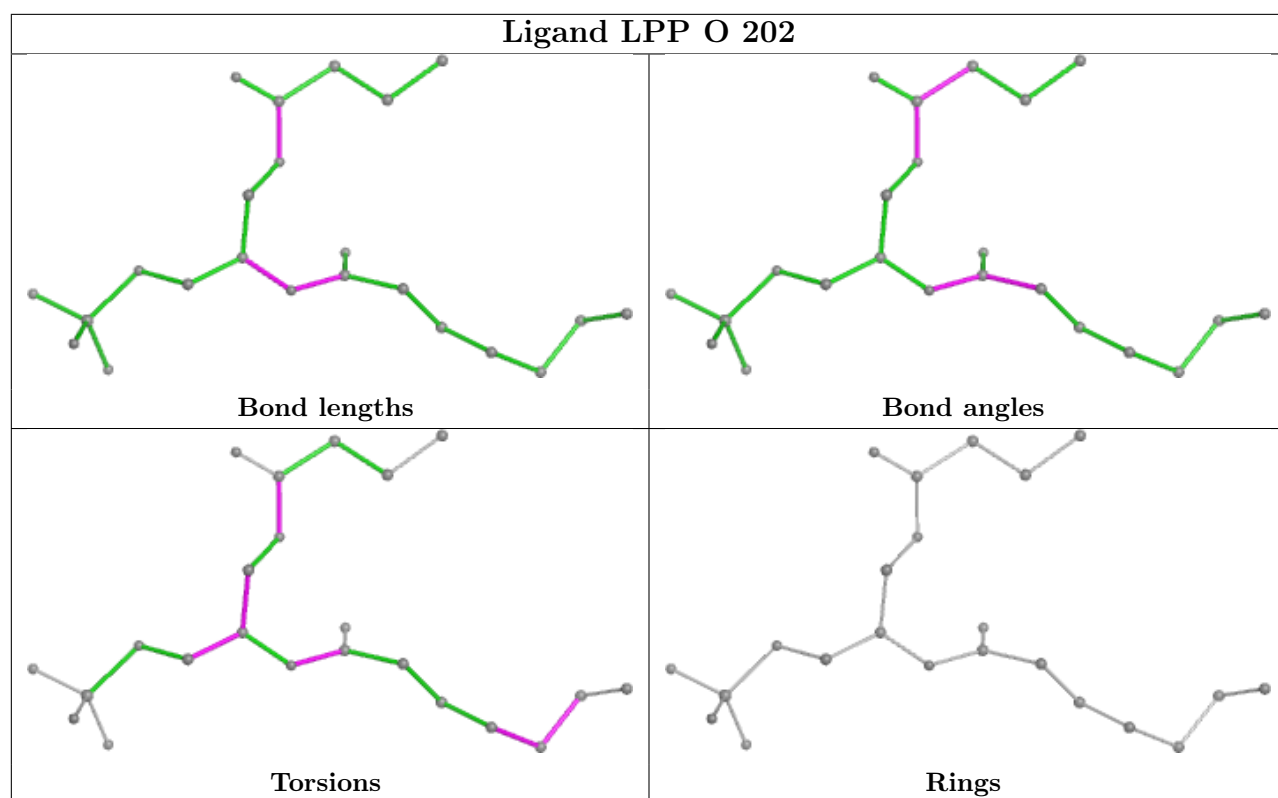


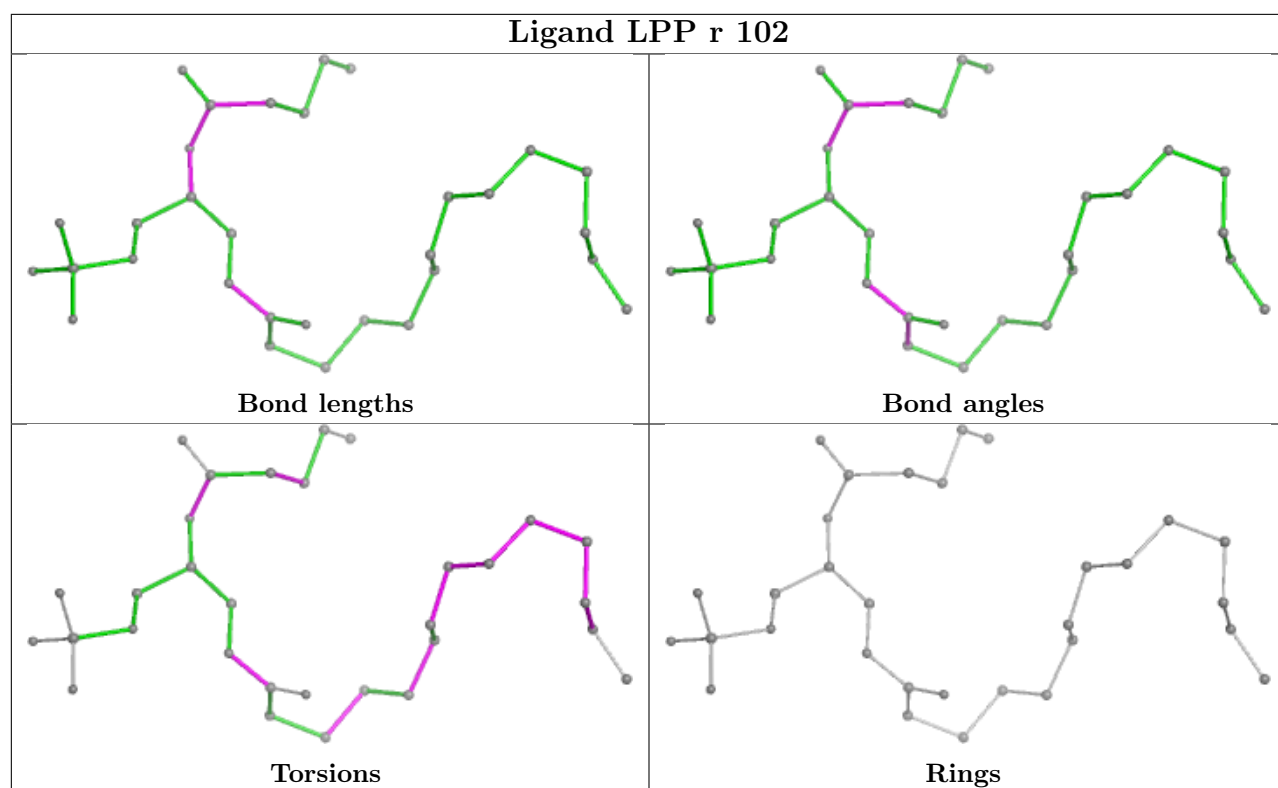


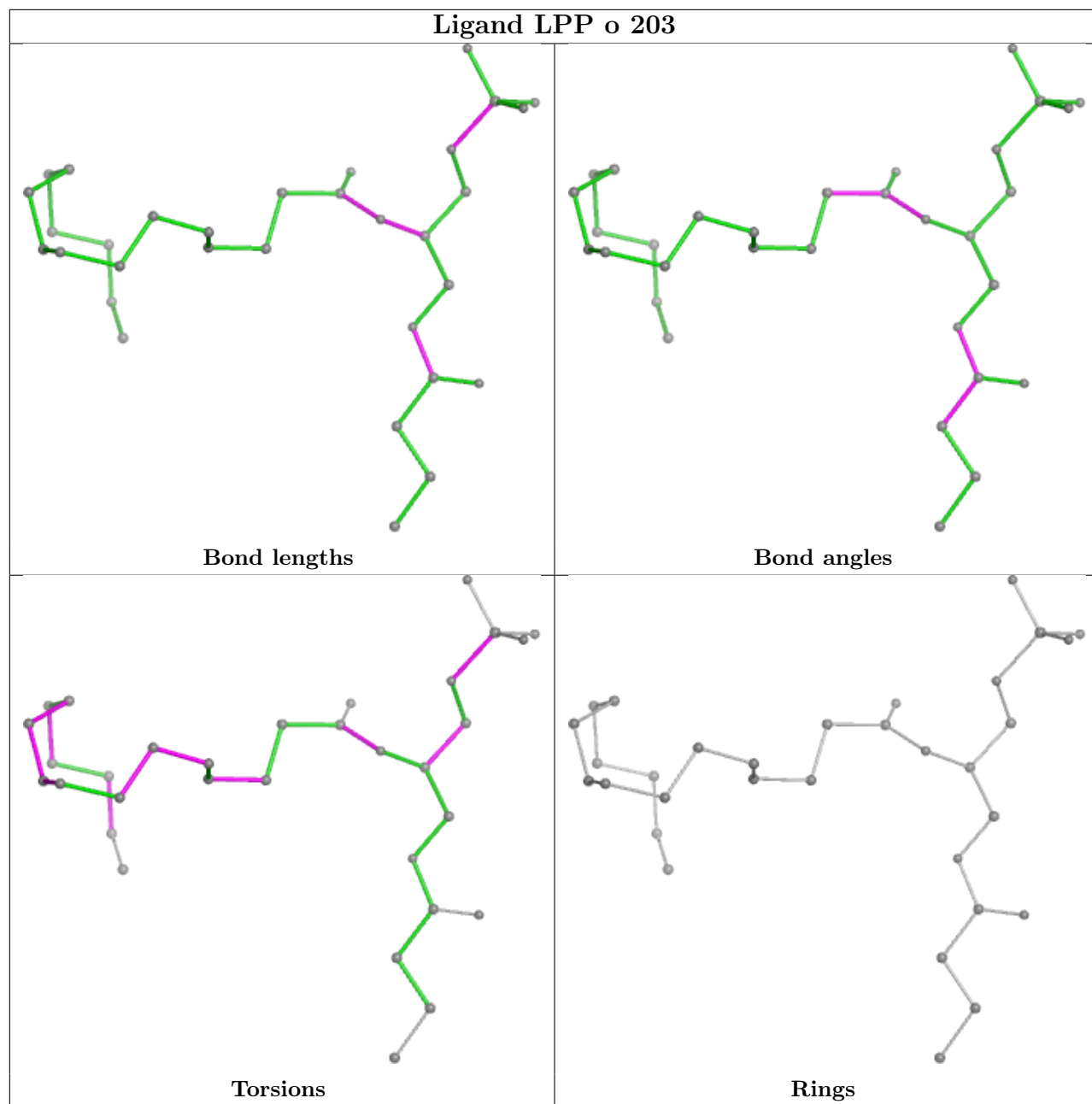


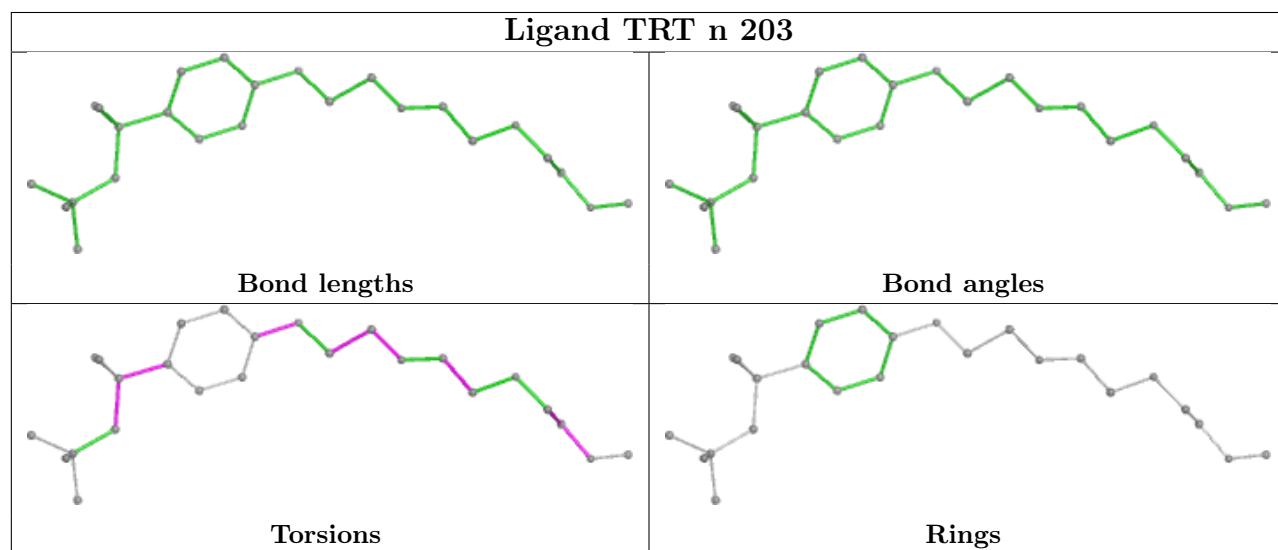
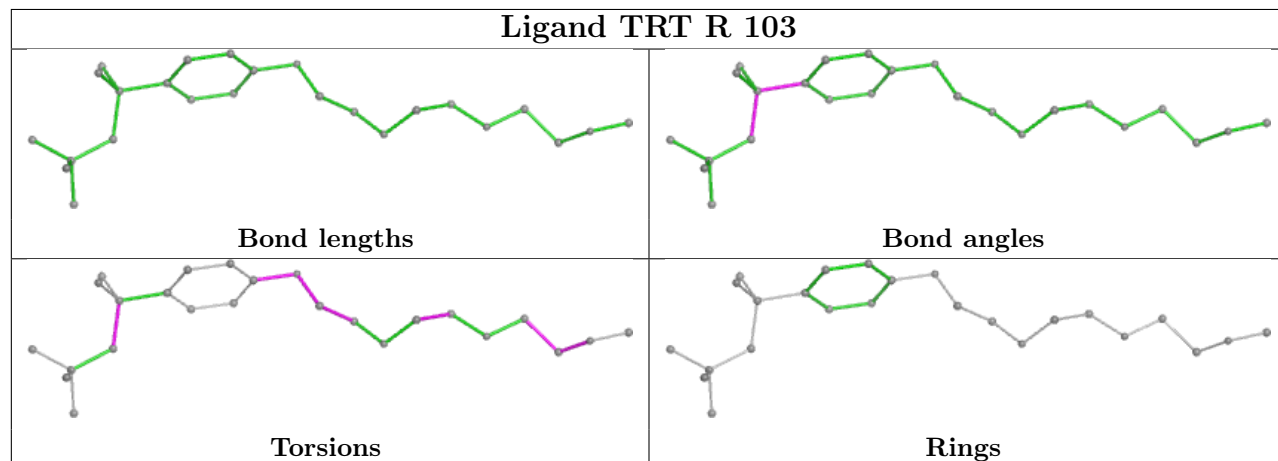
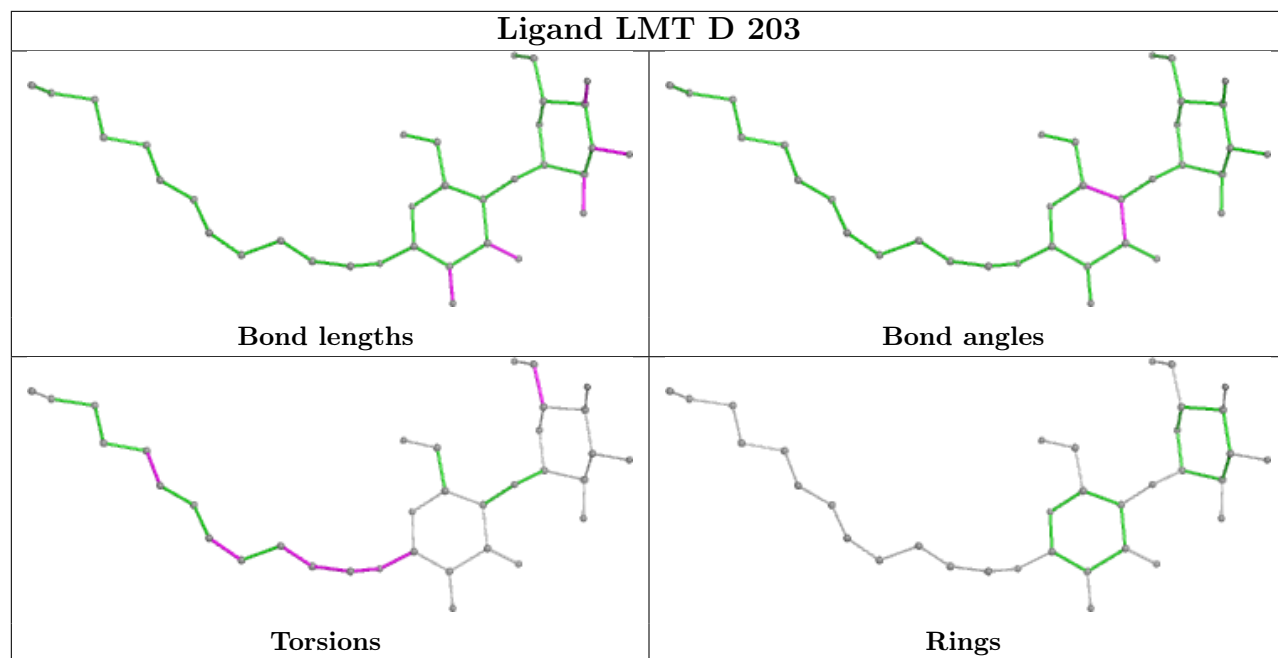


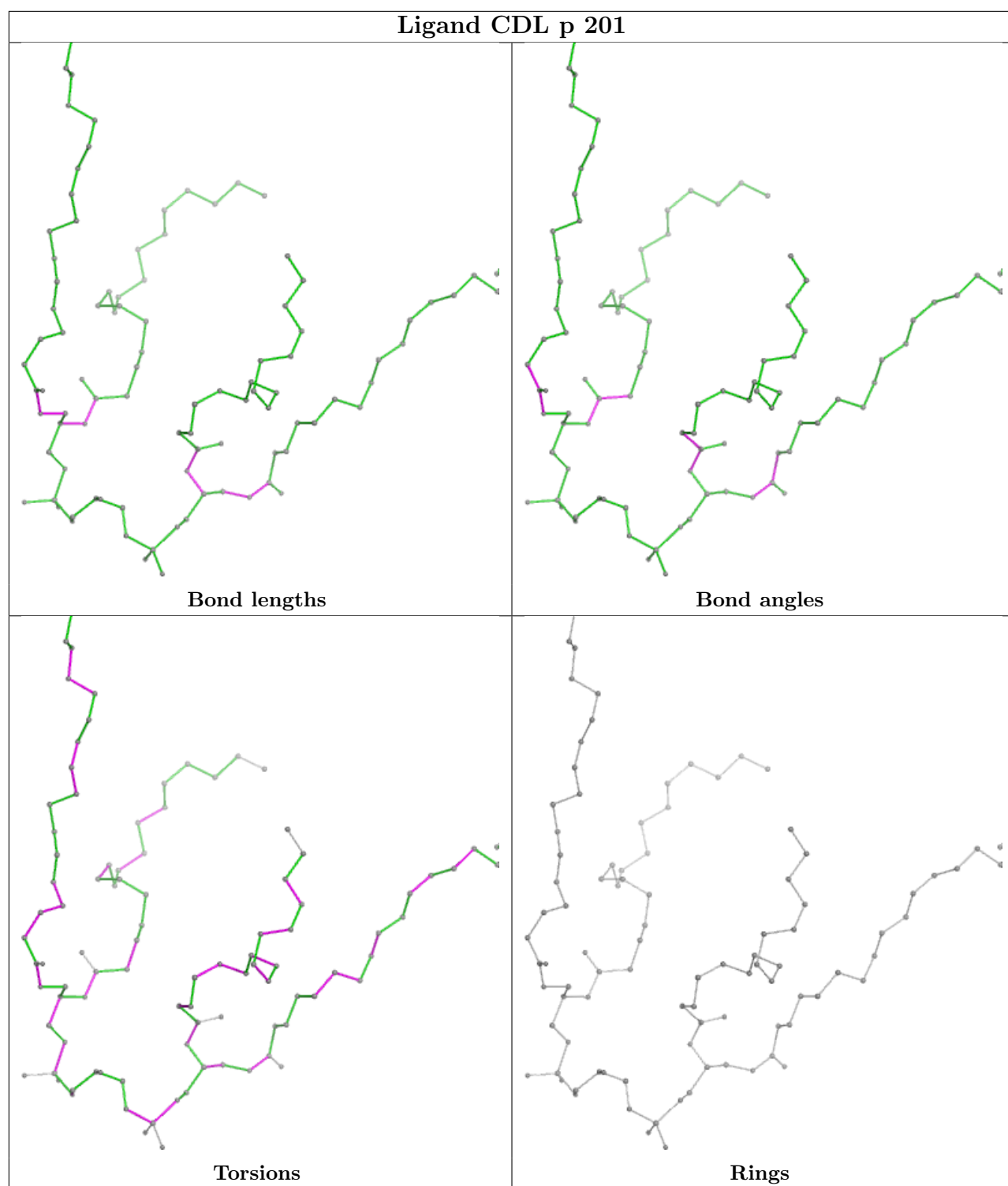


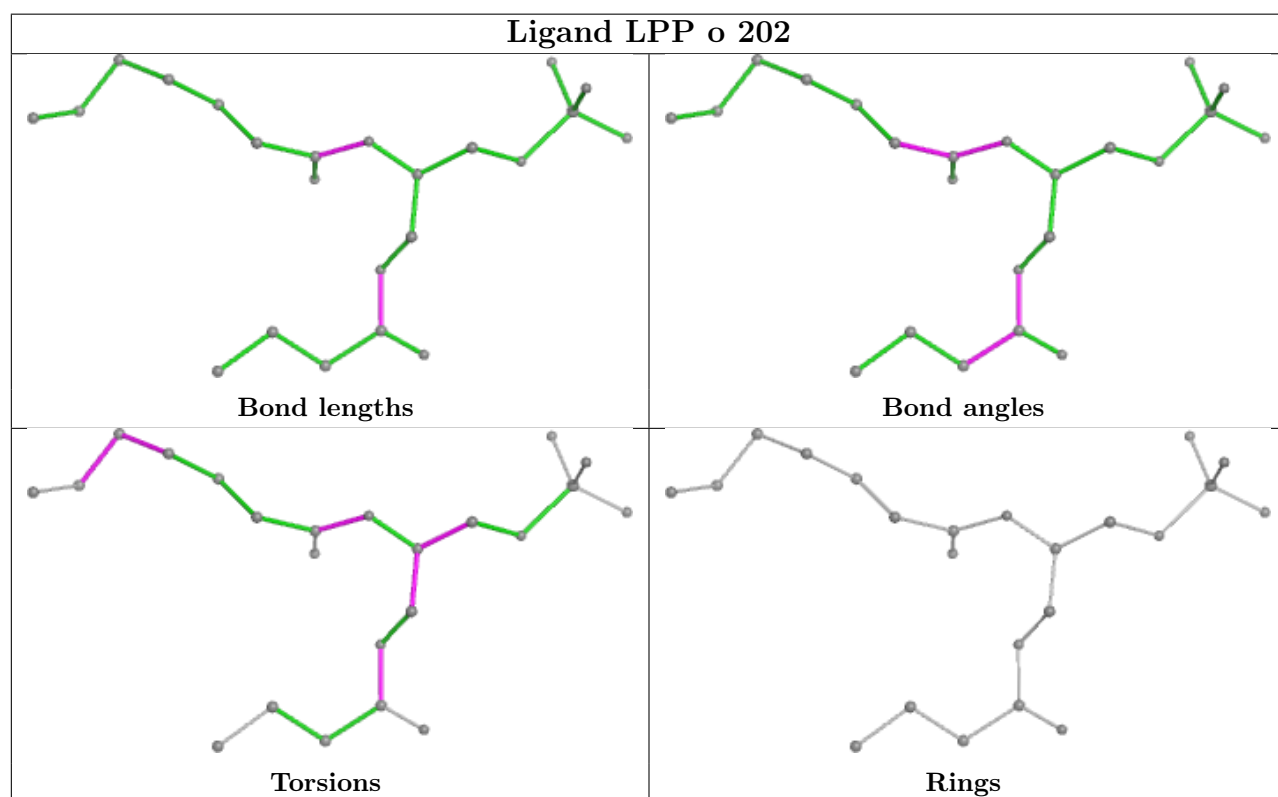
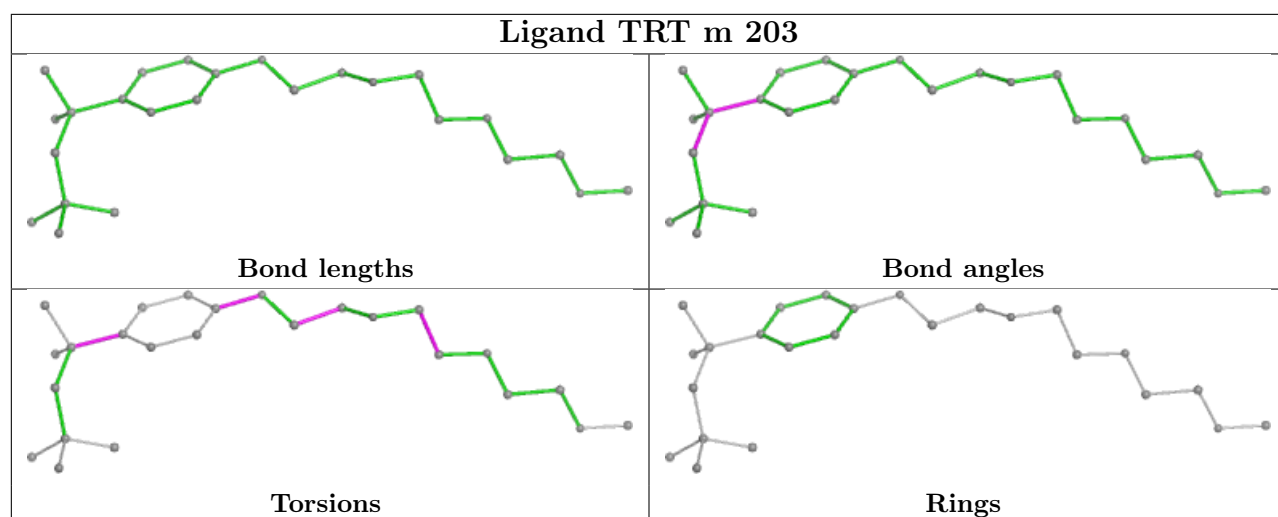


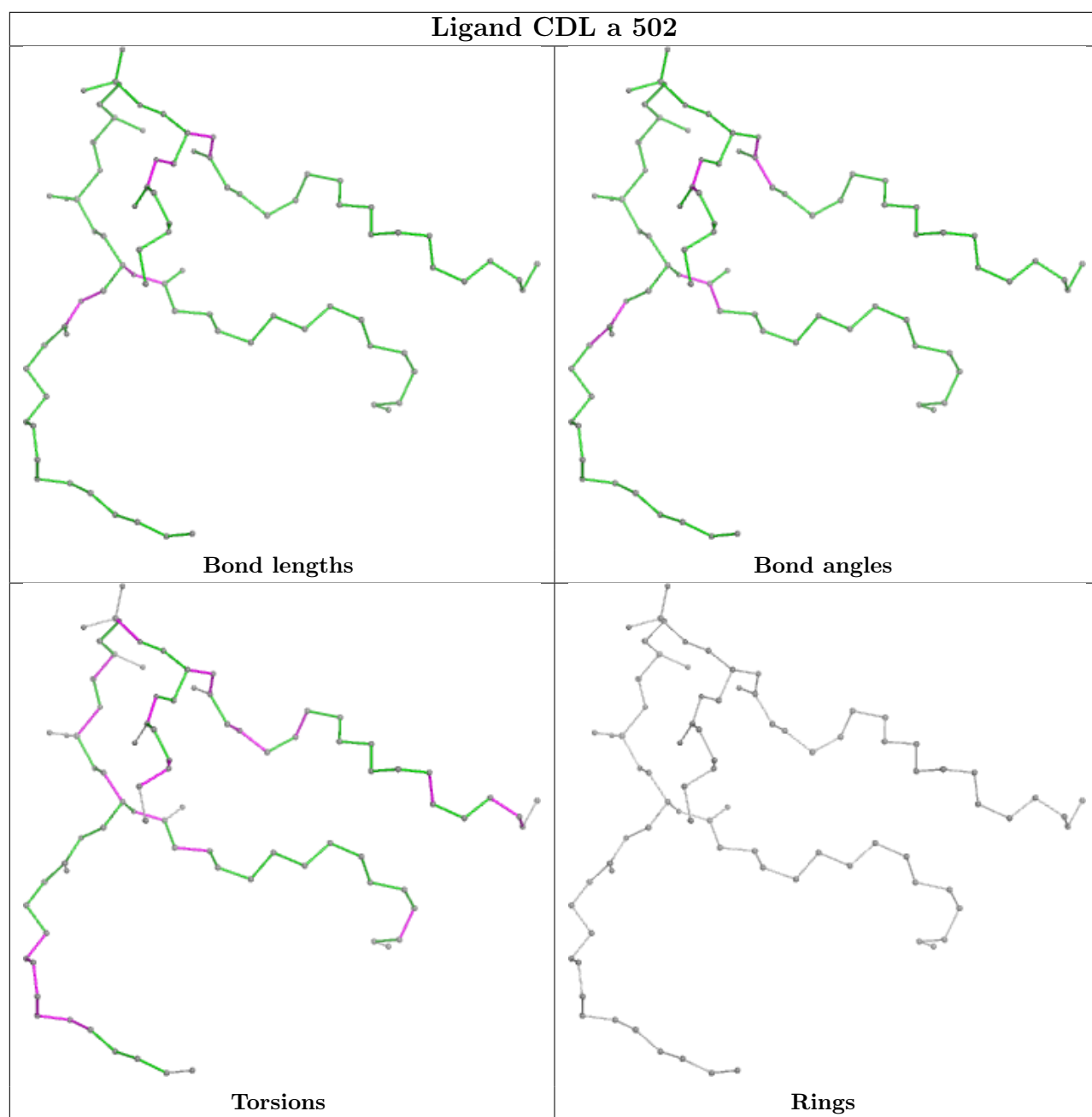


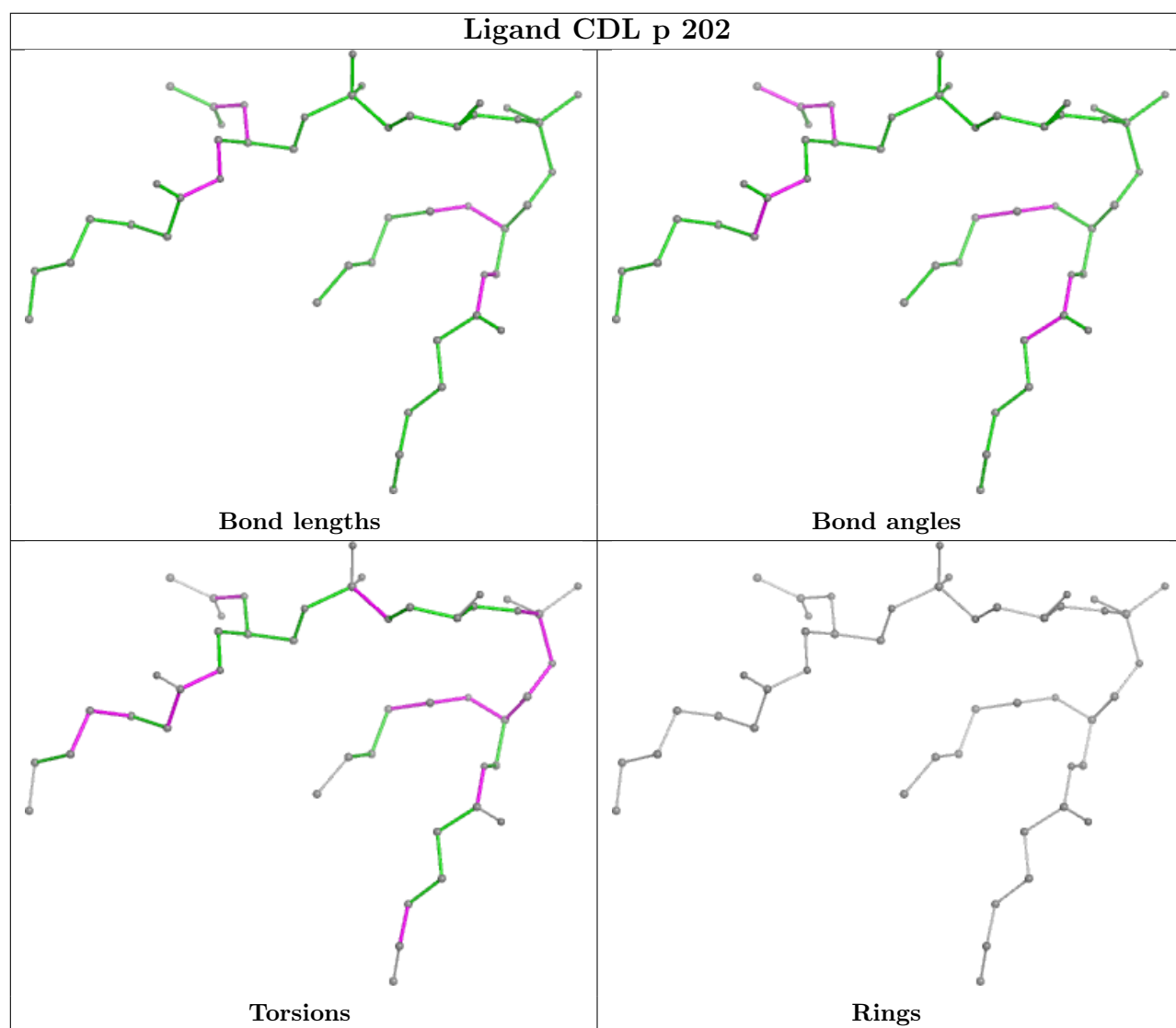


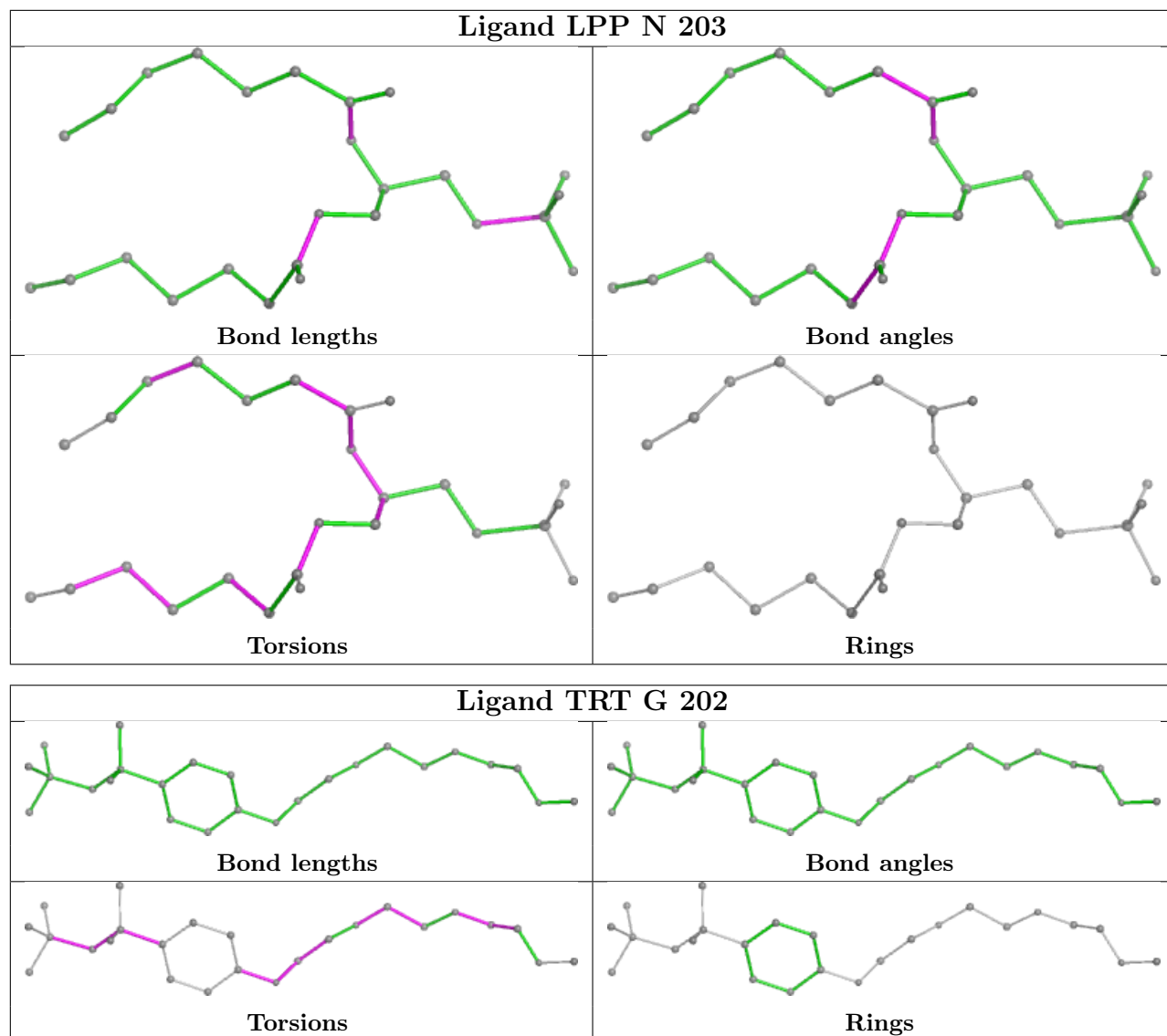


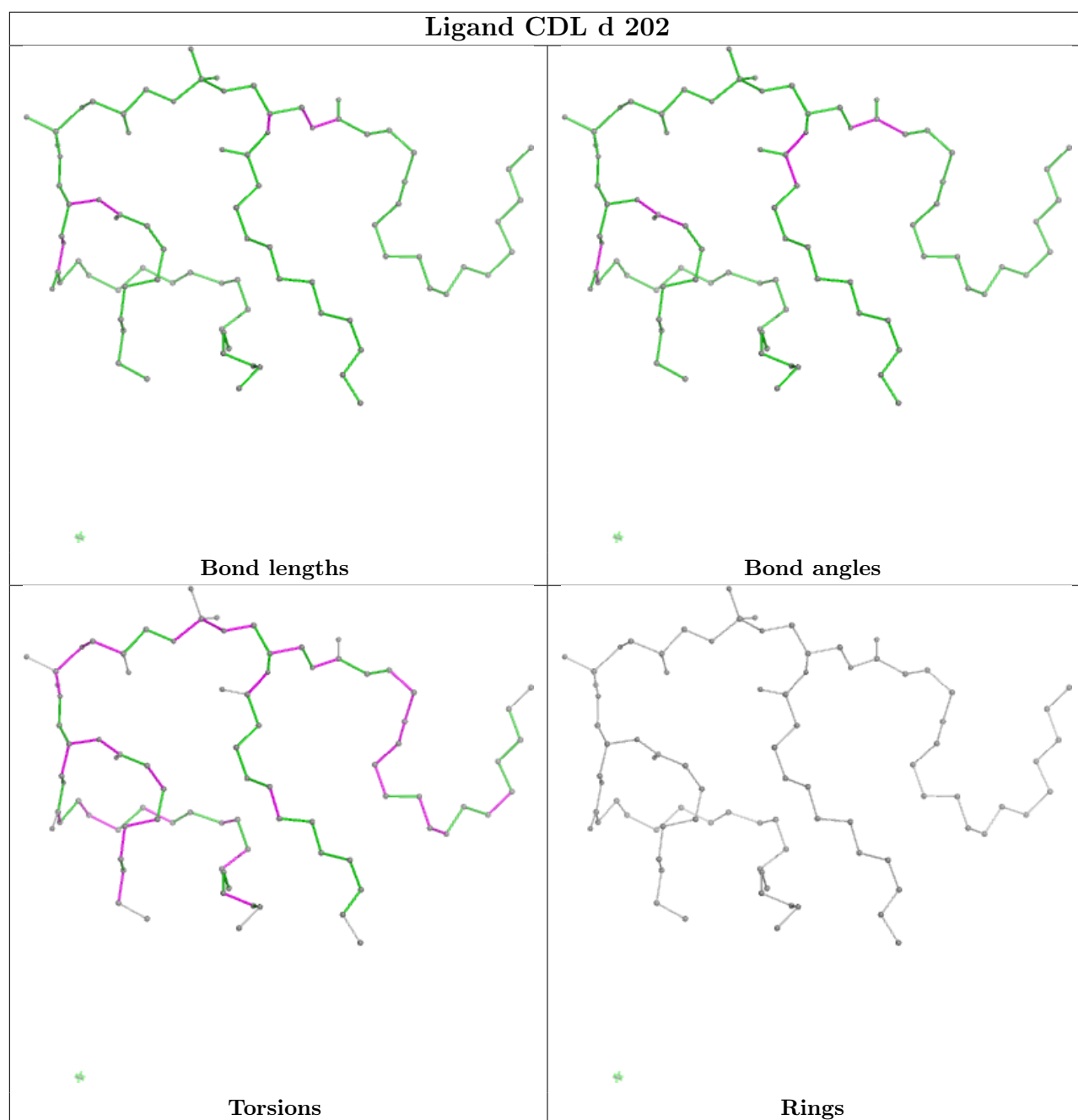


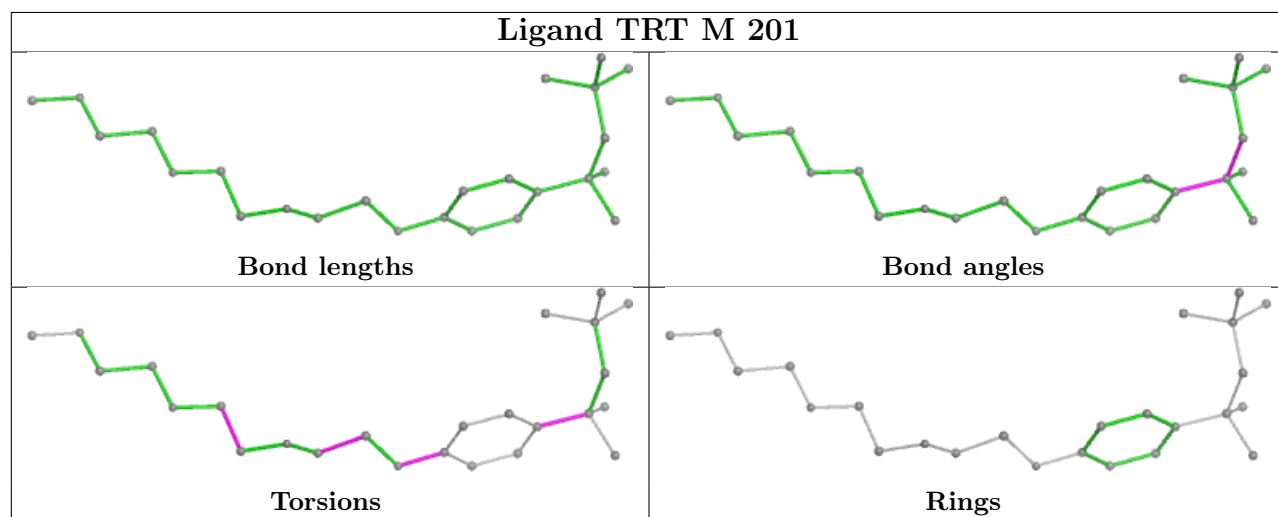
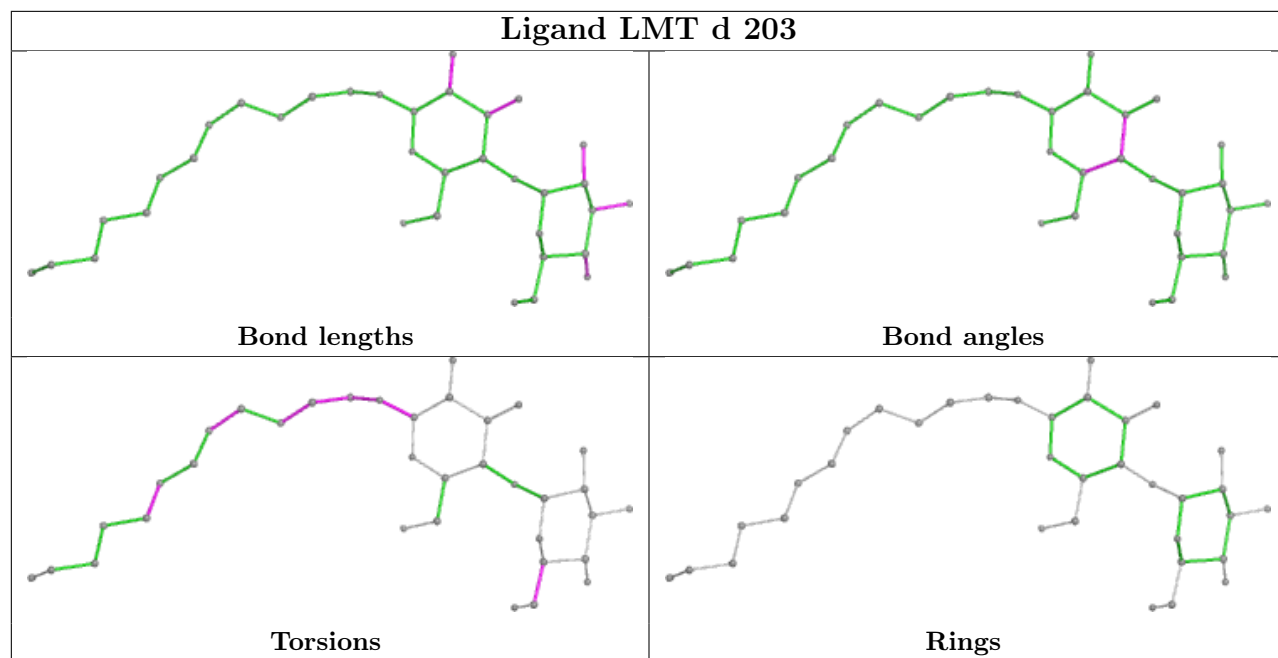


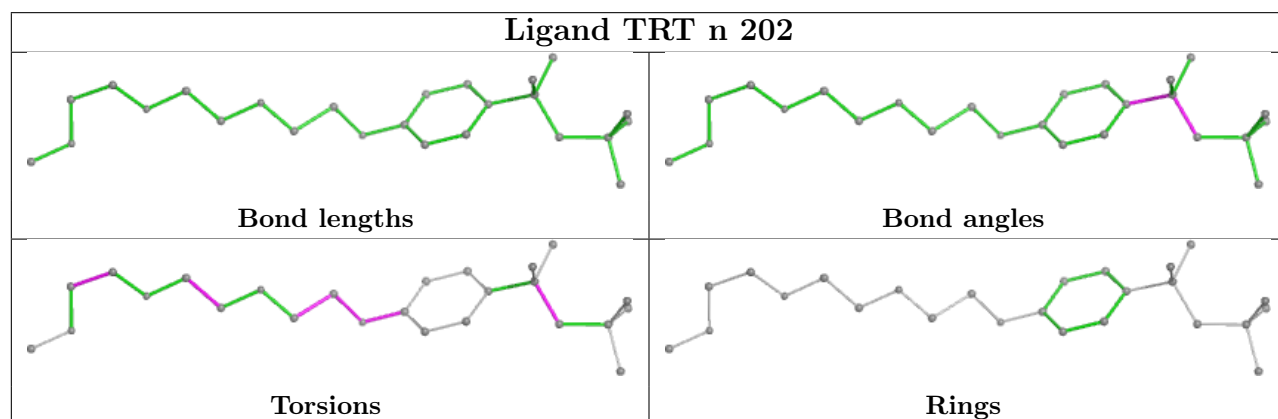
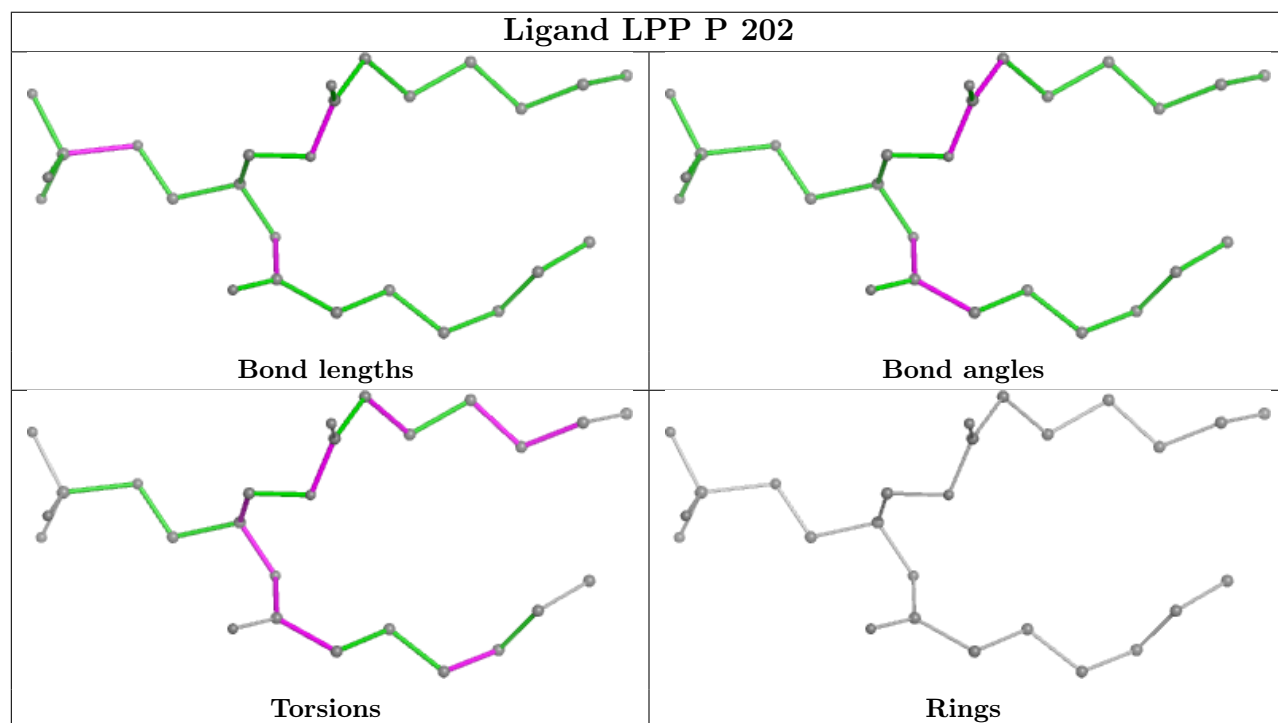
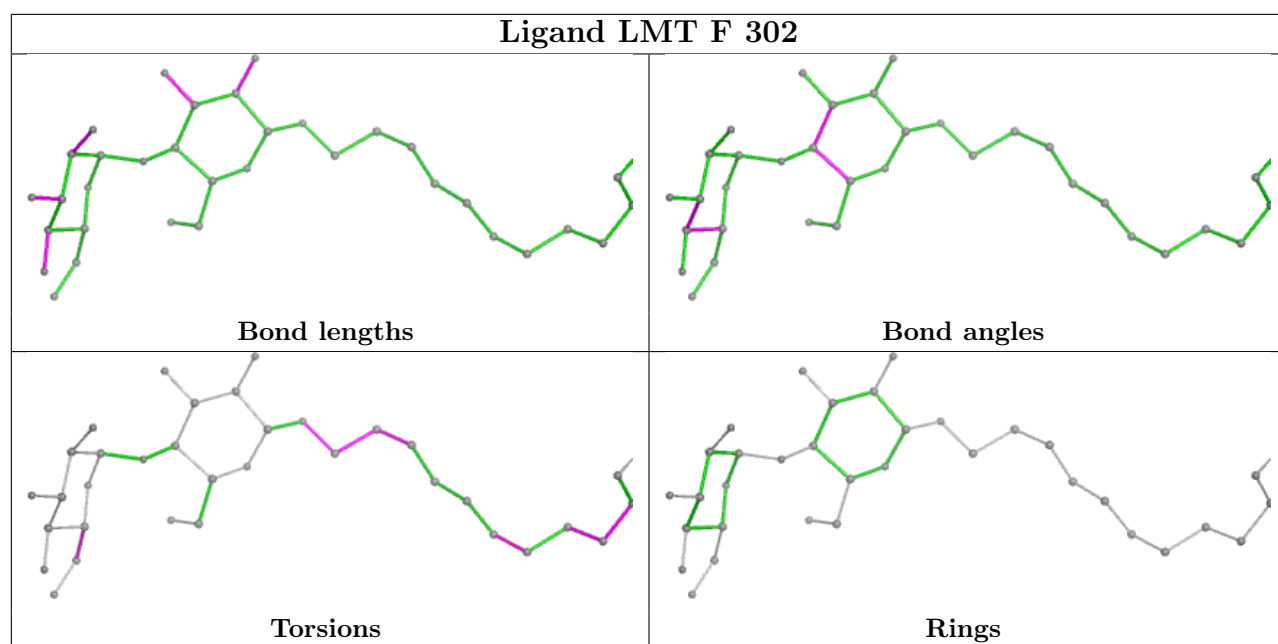


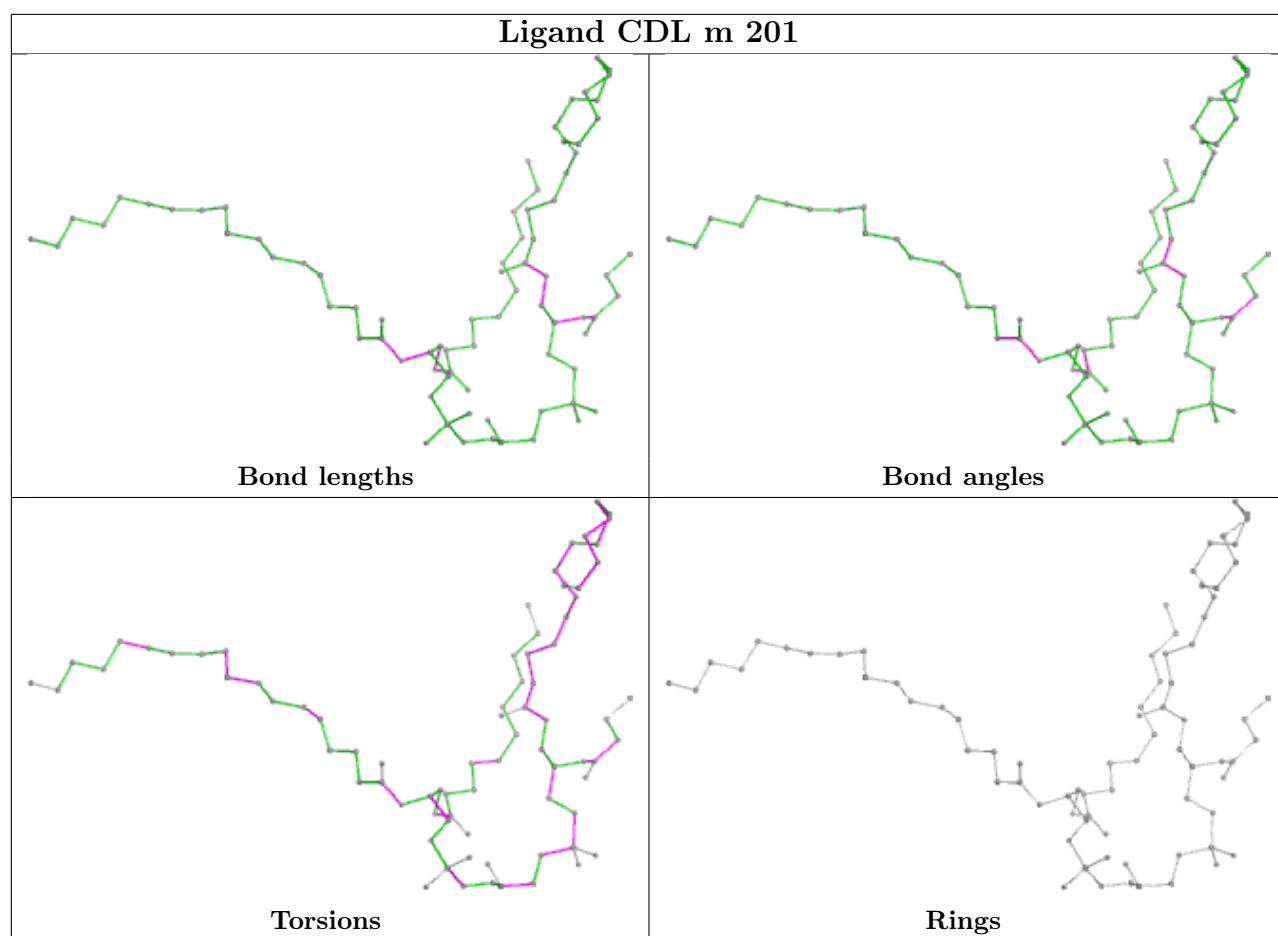


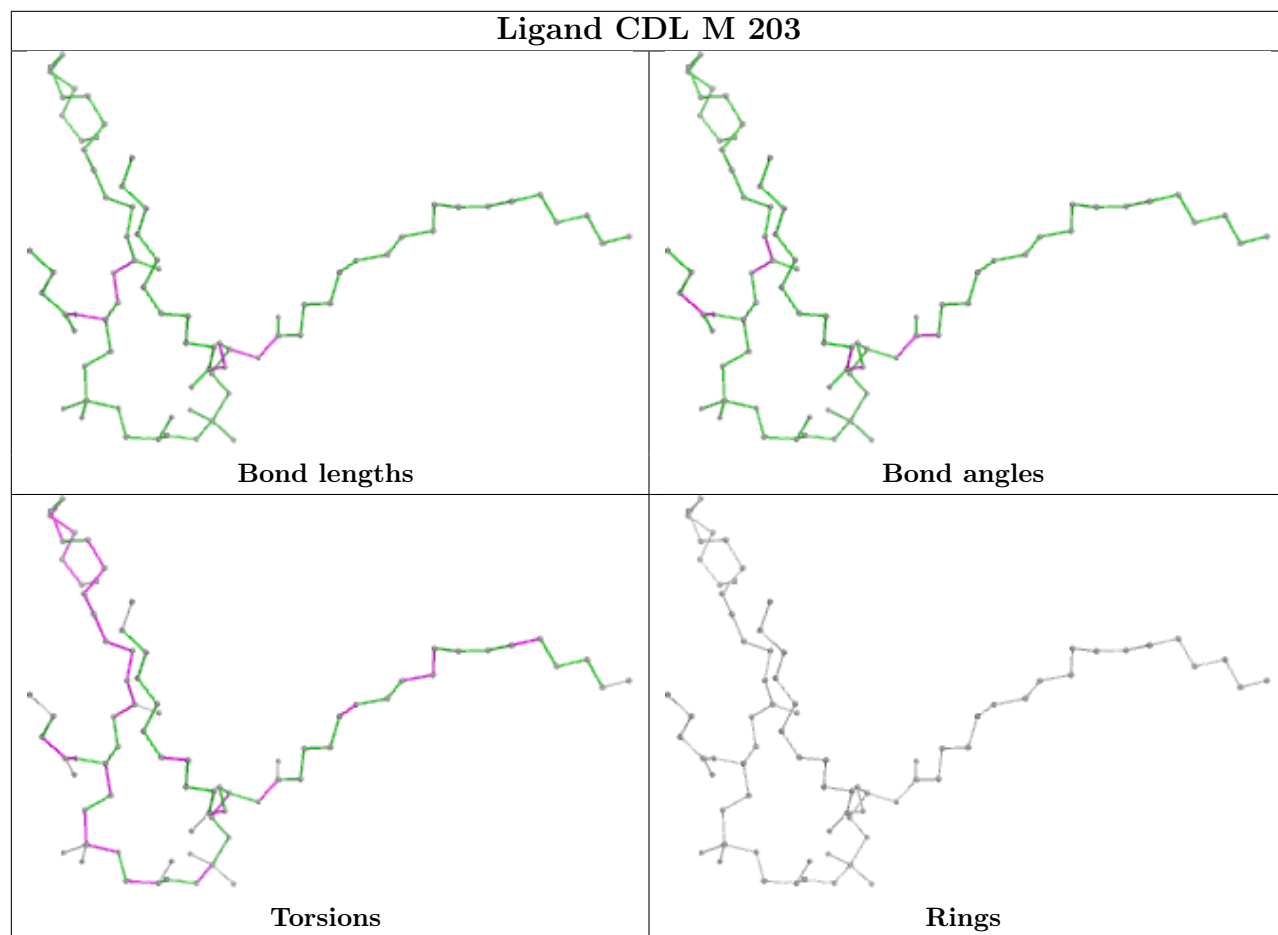


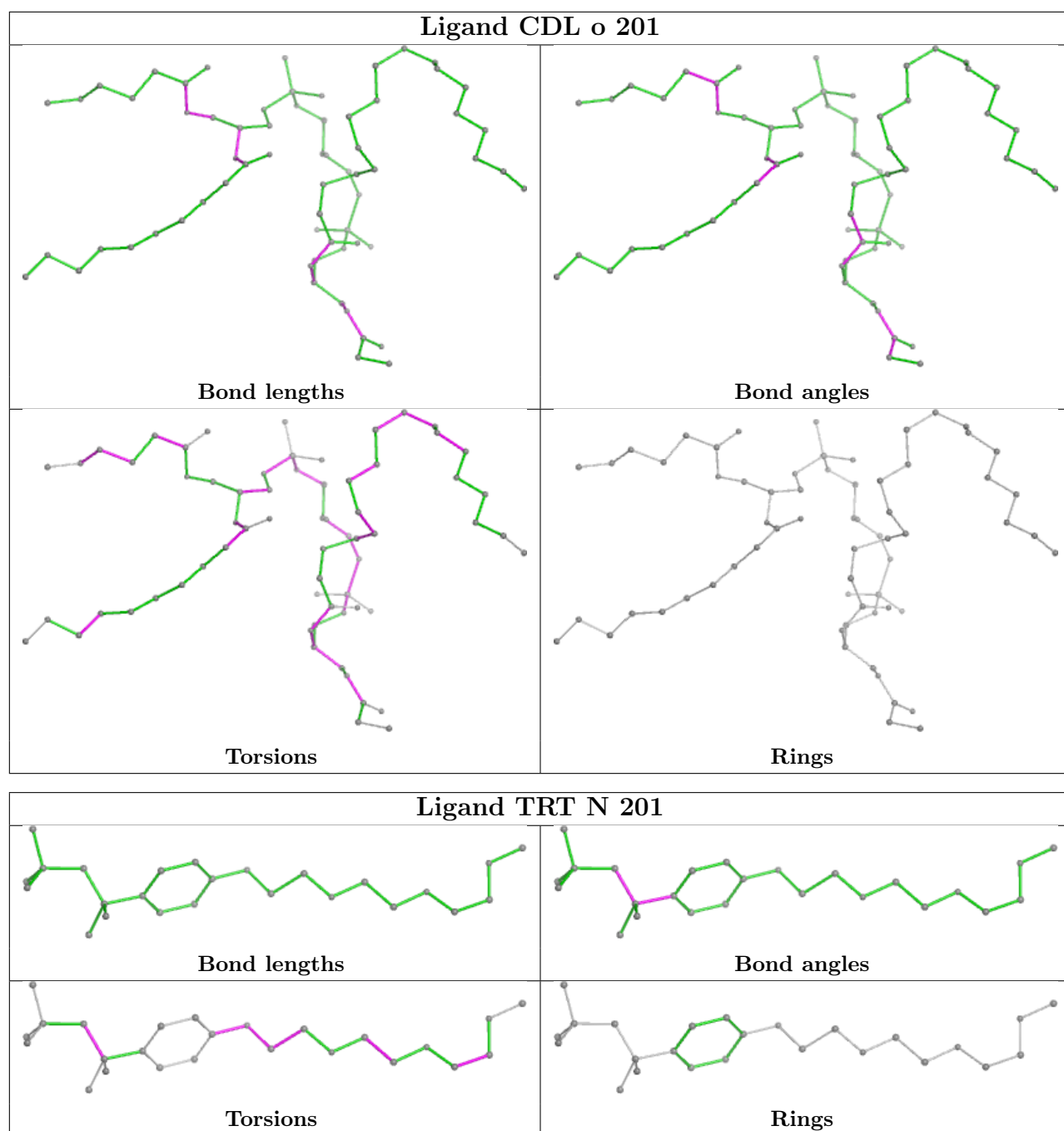


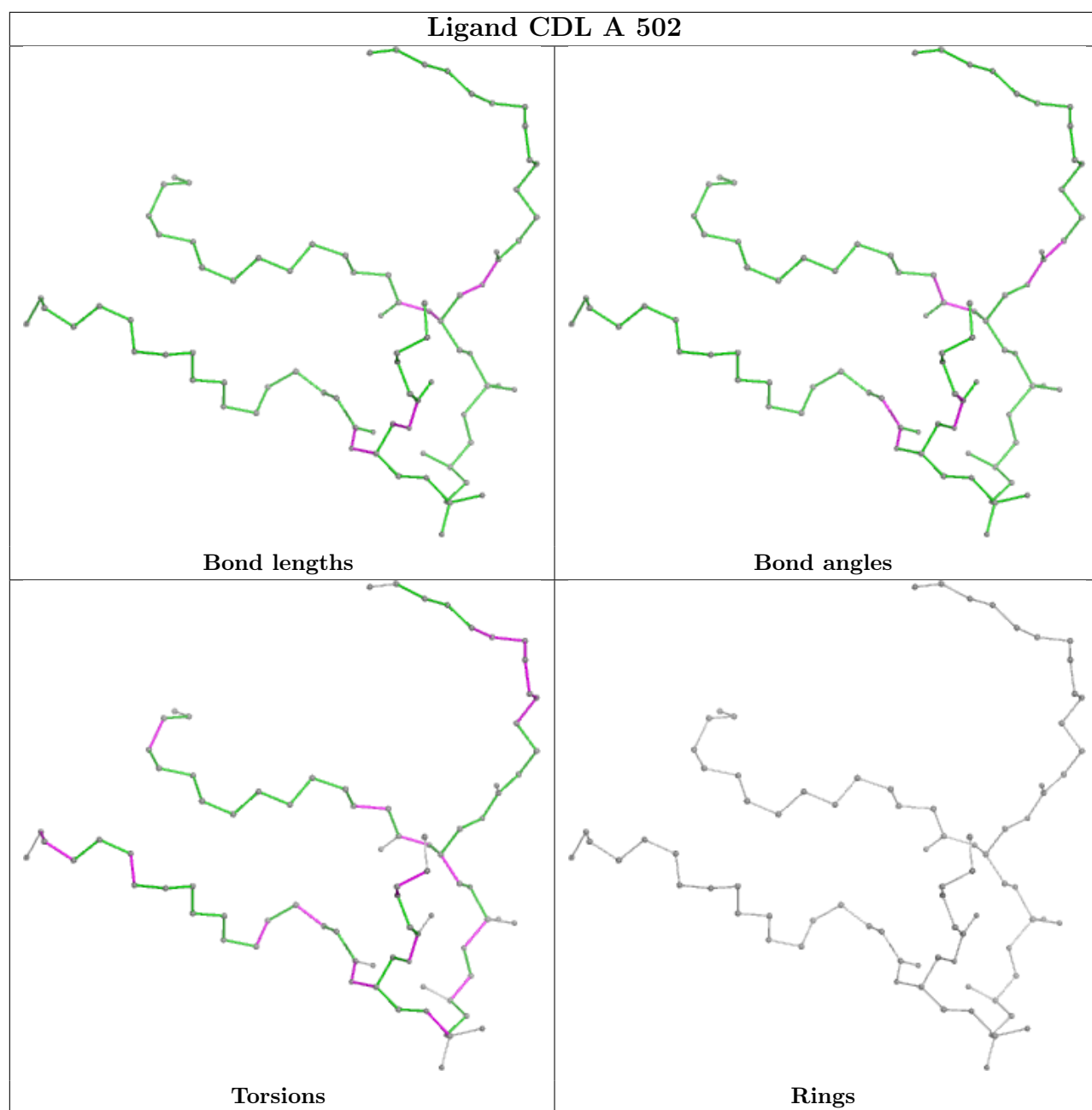


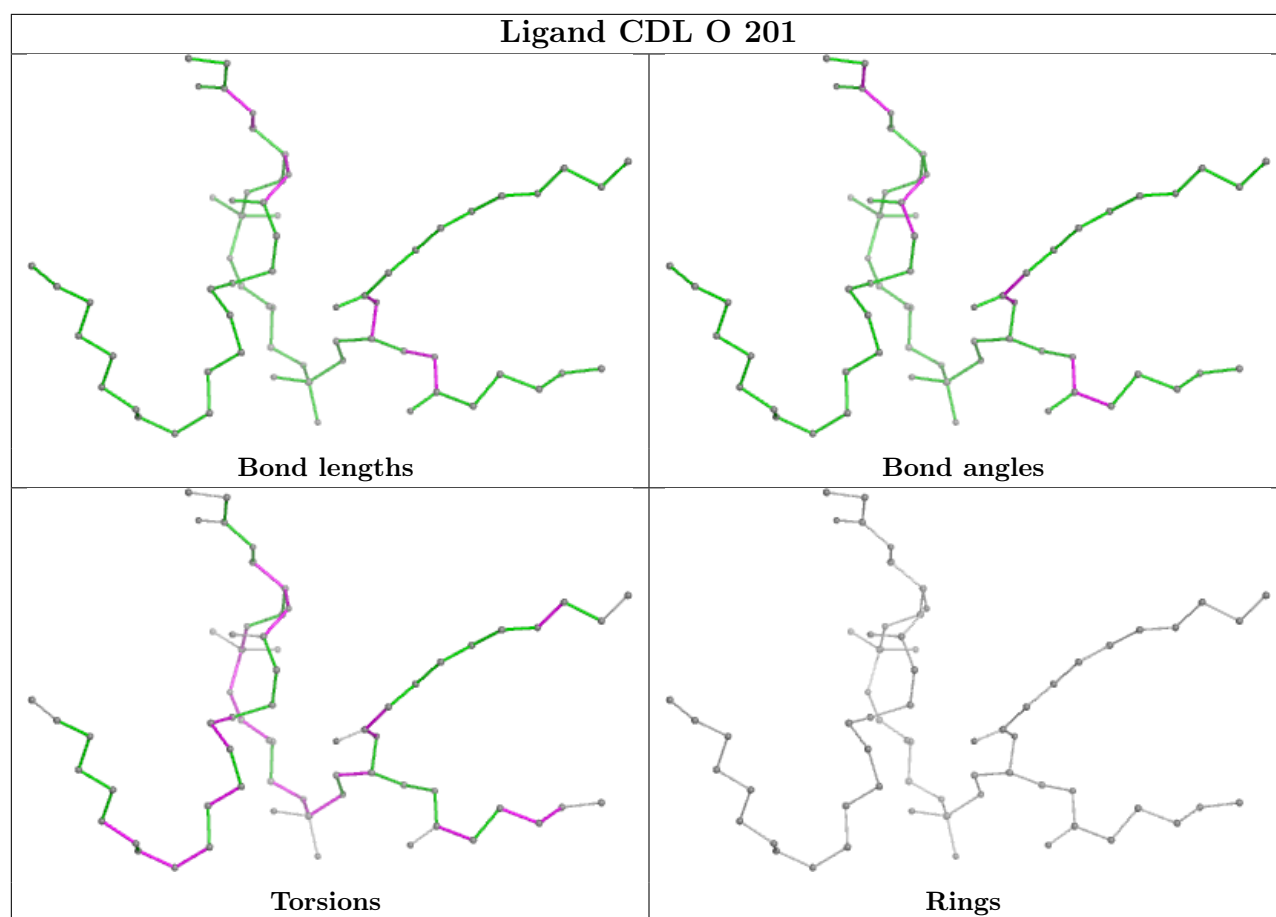












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

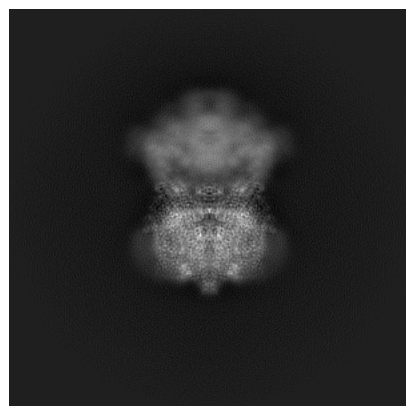
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10468. These allow visual inspection of the internal detail of the map and identification of artifacts.

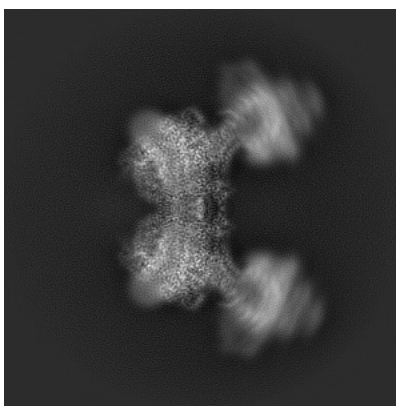
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

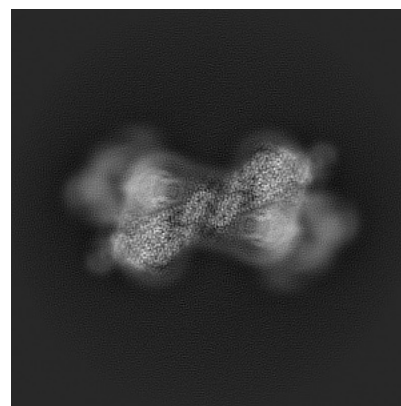
6.1.1 Primary map



X

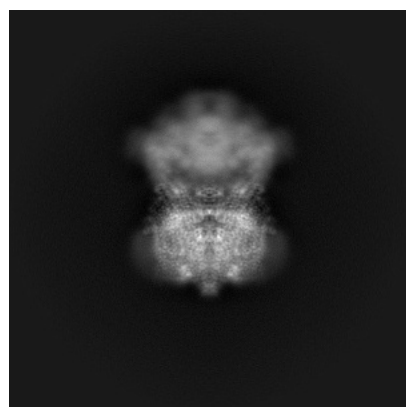


Y

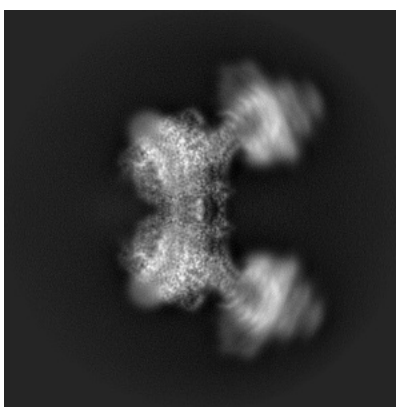


Z

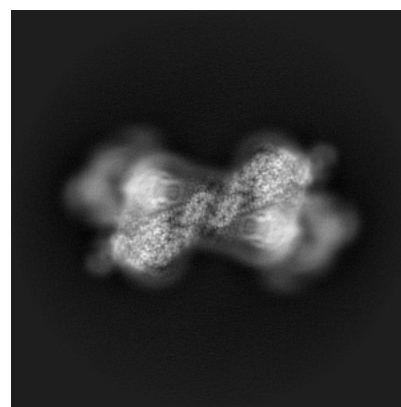
6.1.2 Raw map



X



Y

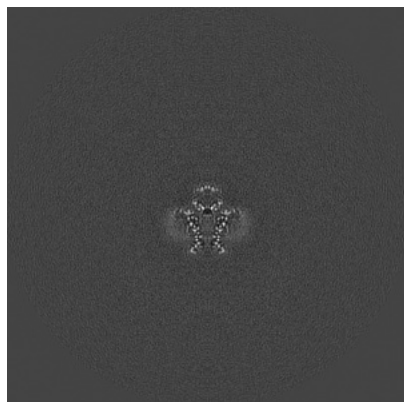


Z

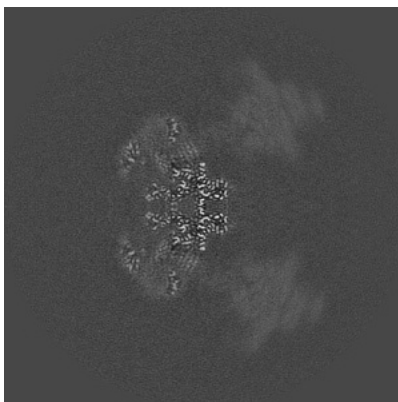
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

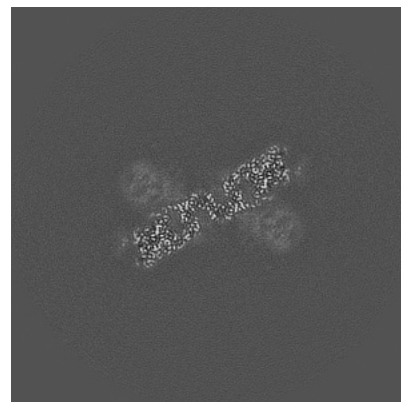
6.2.1 Primary map



X Index: 220

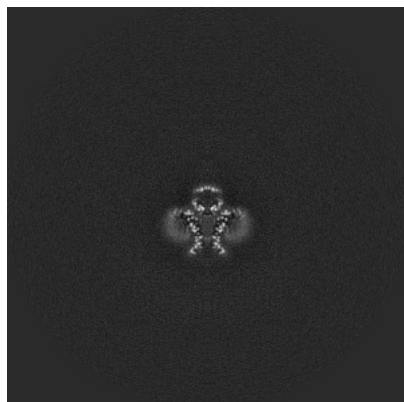


Y Index: 220

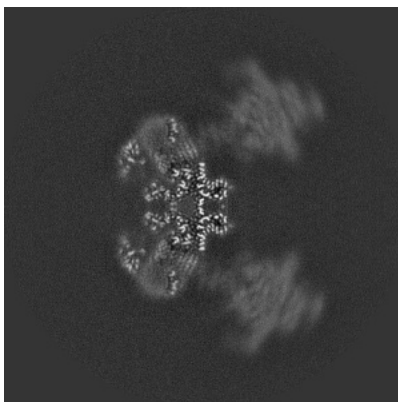


Z Index: 220

6.2.2 Raw map



X Index: 220



Y Index: 220

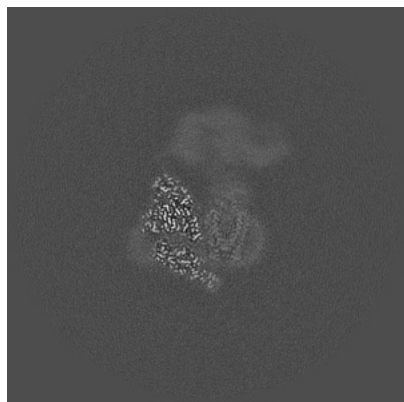


Z Index: 220

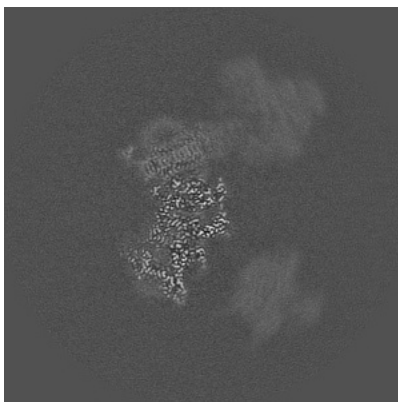
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

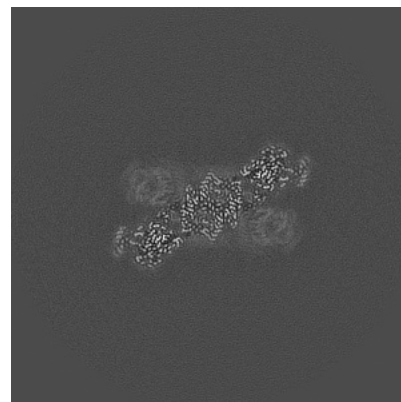
6.3.1 Primary map



X Index: 158

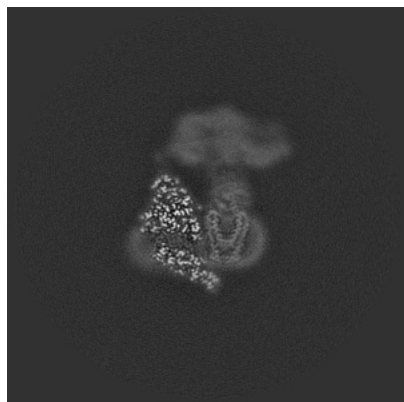


Y Index: 210

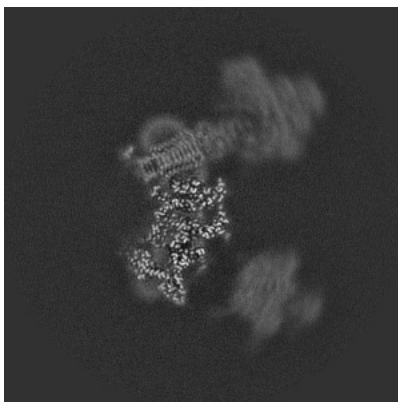


Z Index: 214

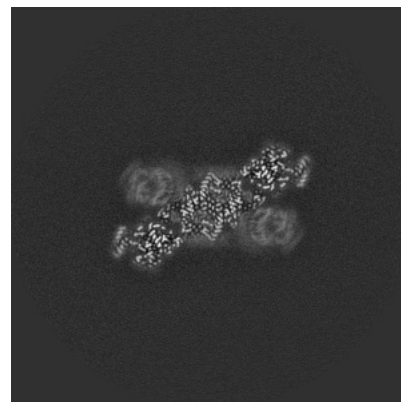
6.3.2 Raw map



X Index: 157



Y Index: 209

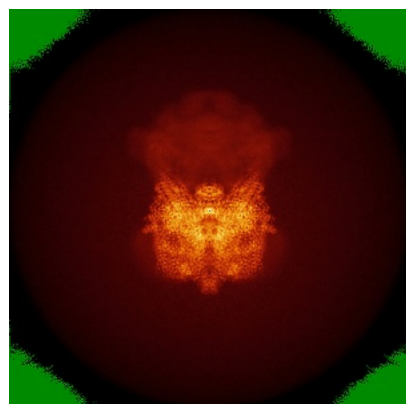


Z Index: 214

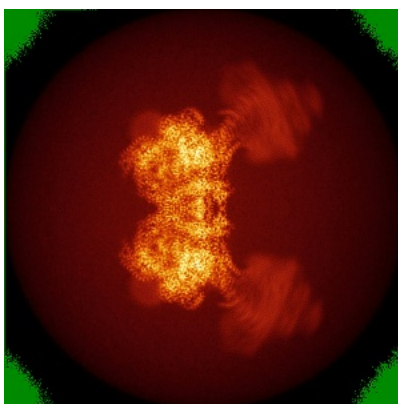
The images above show the largest variance slices of the map in three orthogonal directions.

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

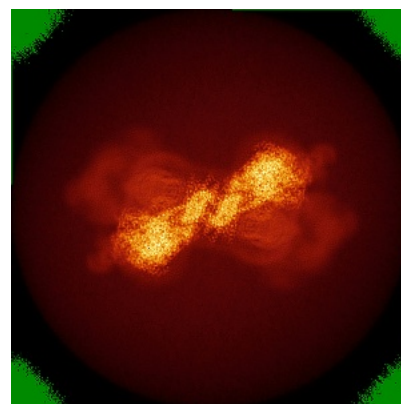
6.4.1 Primary map



X



Y



Z

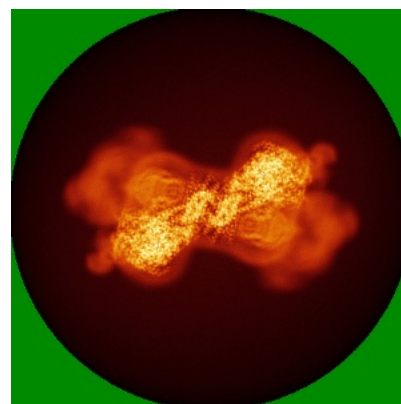
6.4.2 Raw map



X



Y

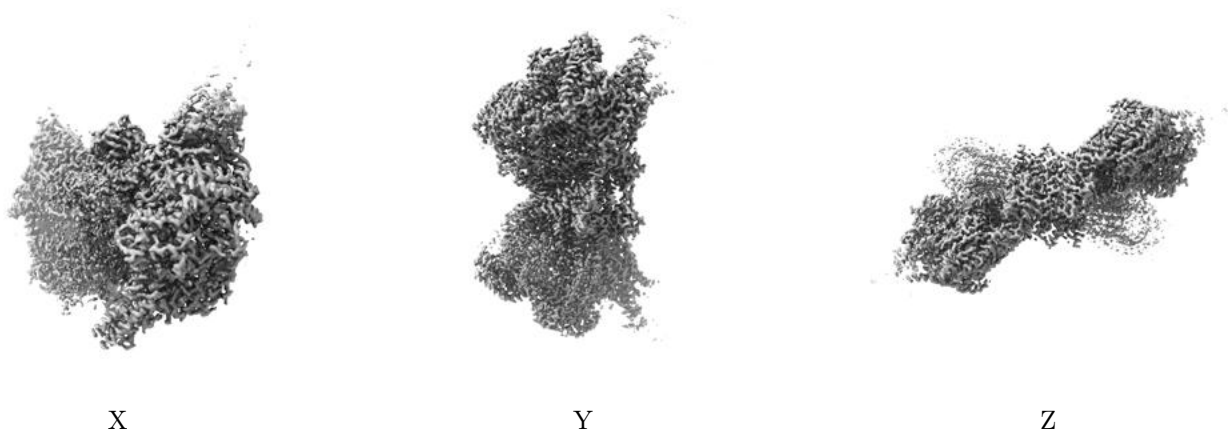


Z

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

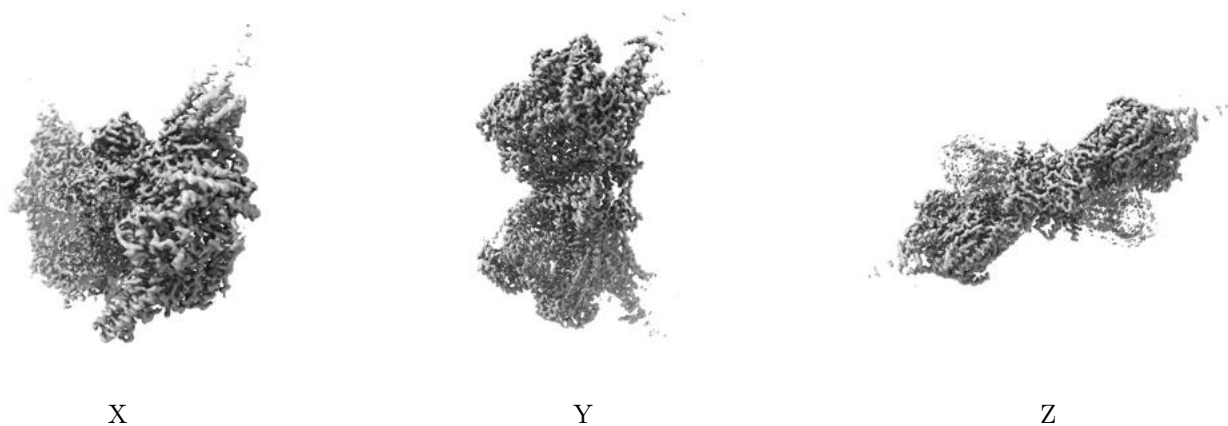
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

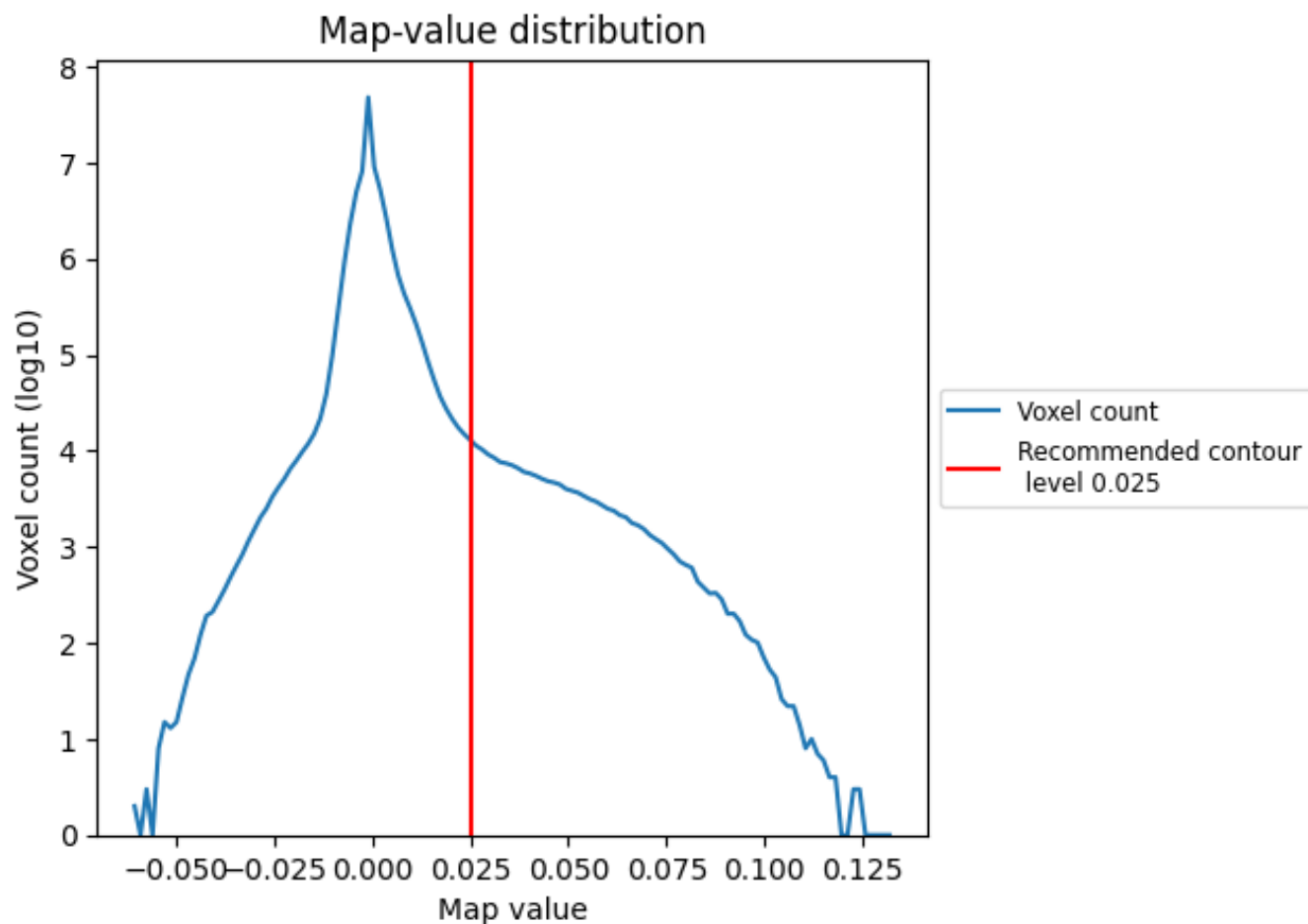
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

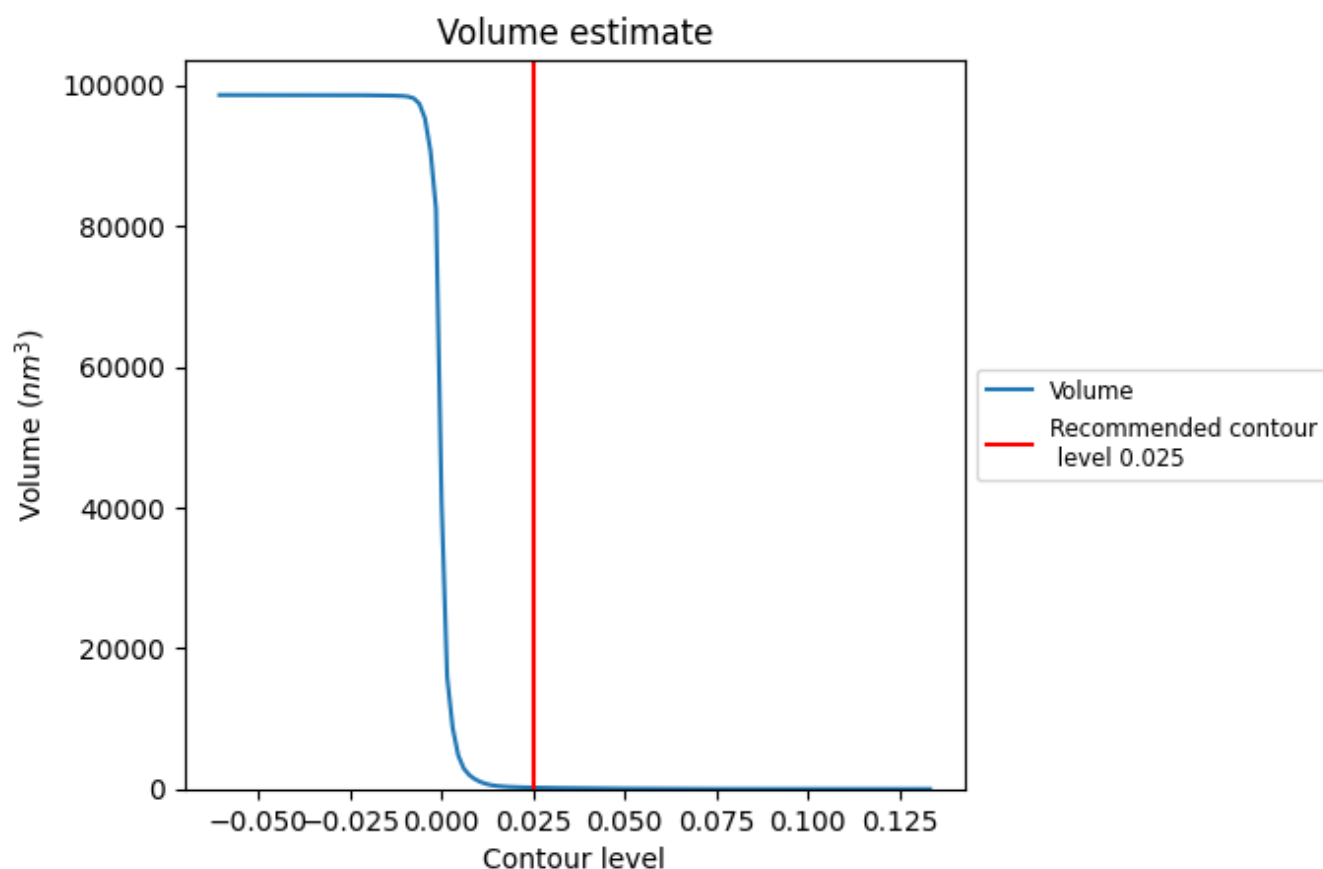
This section contains the results of statistical analysis of the map.

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.

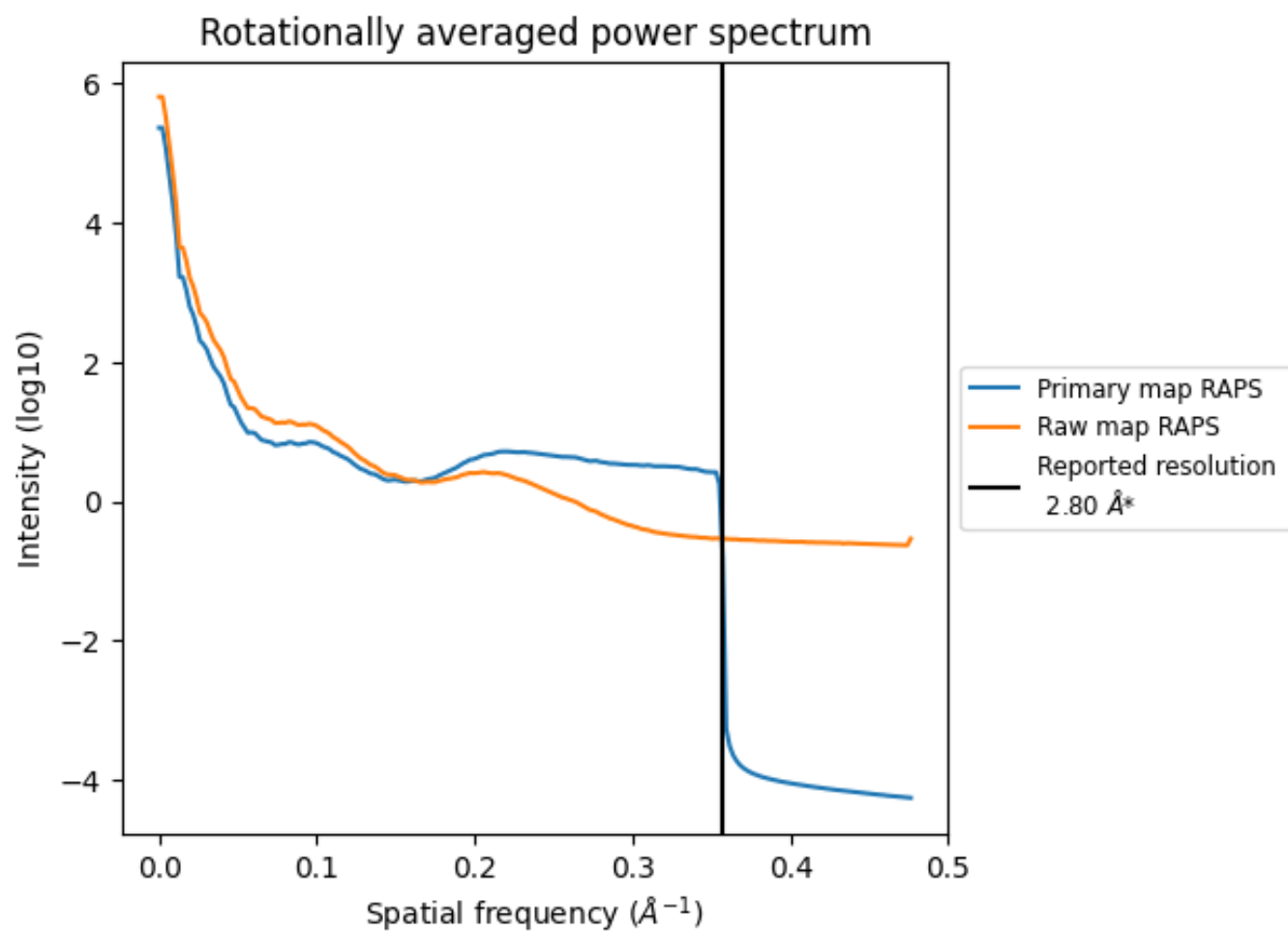
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm^3 ; this corresponds to an approximate mass of 173 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 ⓘ

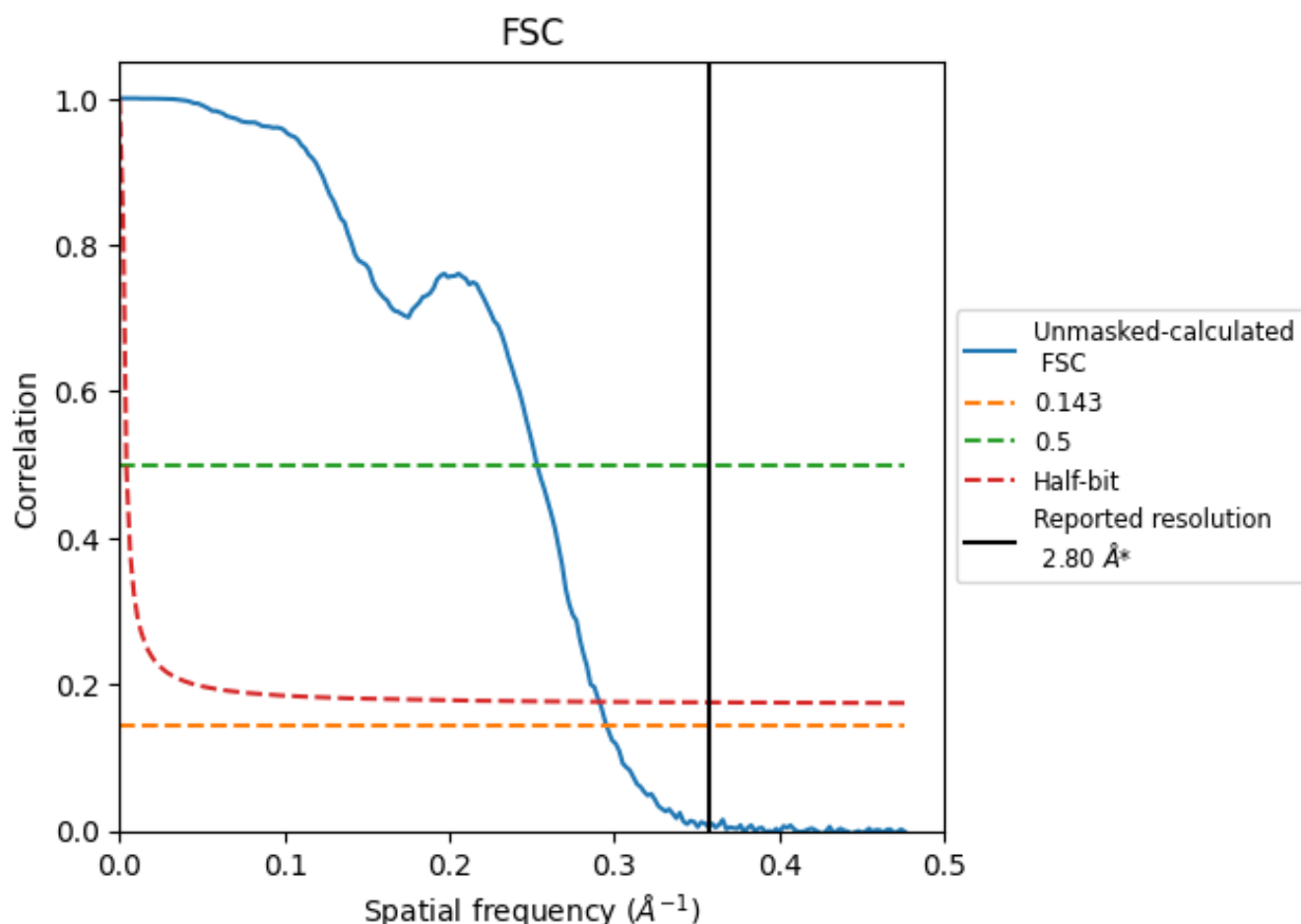


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

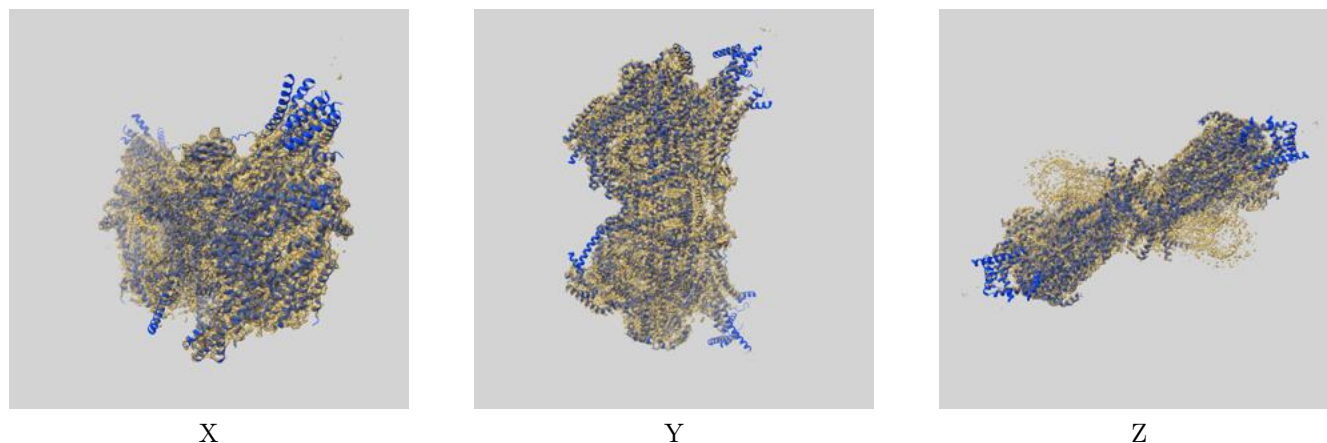
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.95	3.44

*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 3.38 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

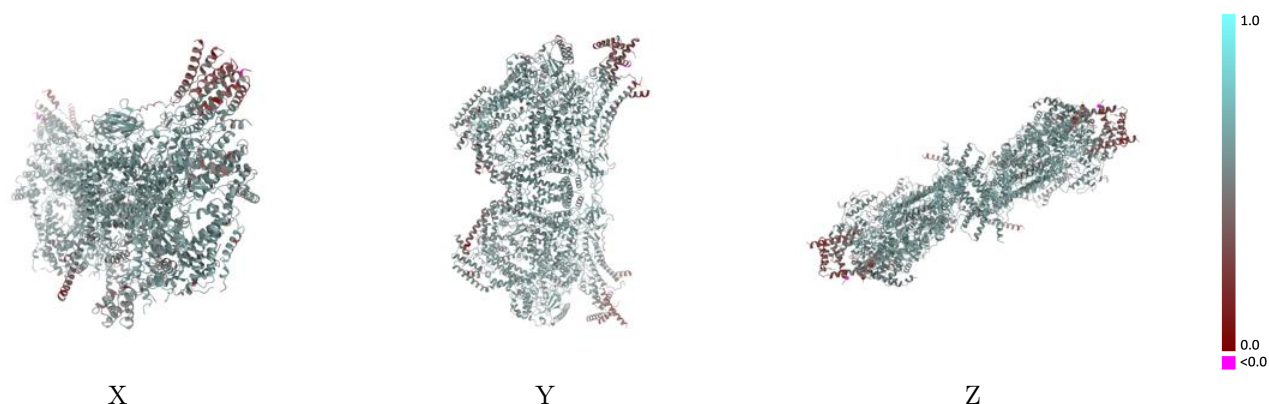
This section contains information regarding the fit between EMDB map EMD-10468 and PDB model 6TDV. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



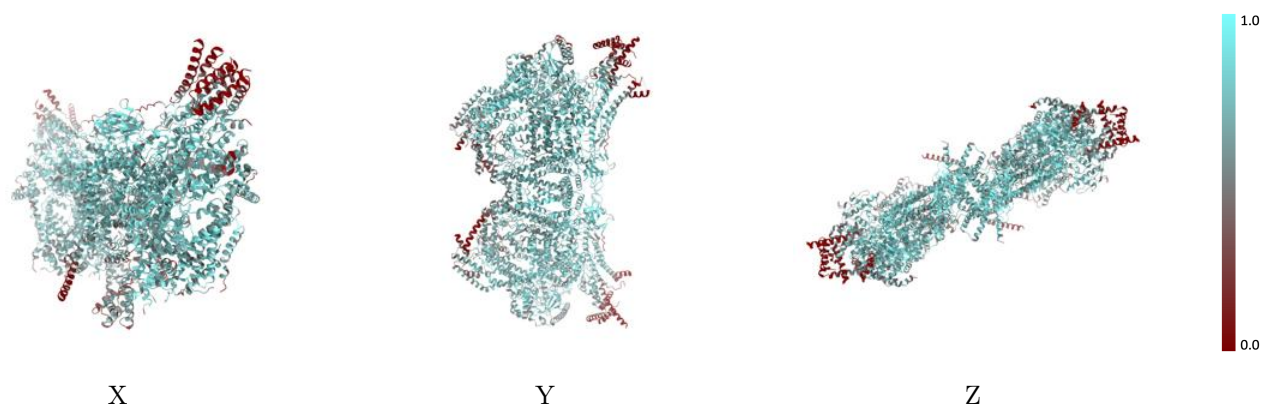
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



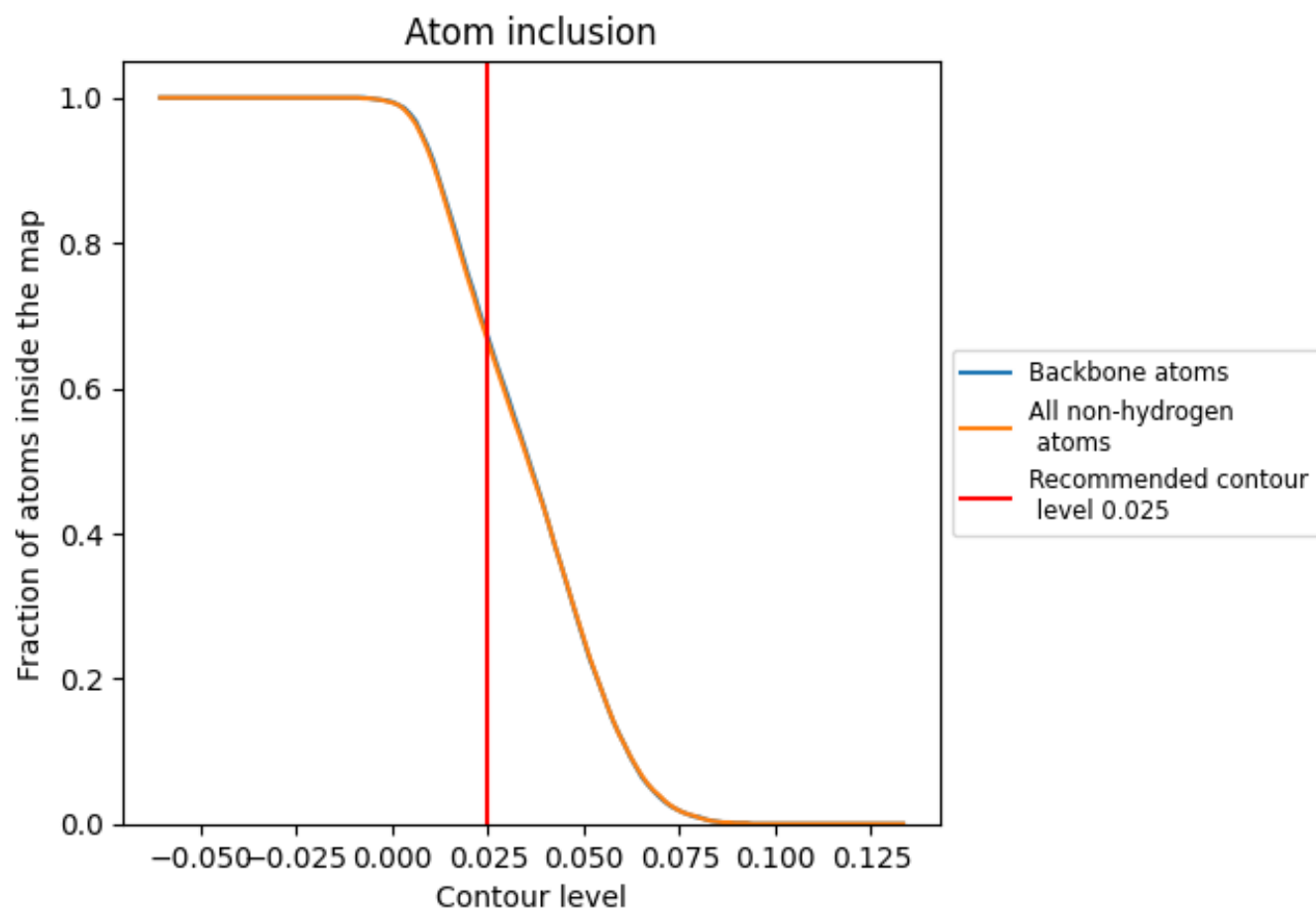
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 66% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.5580
A	 0.6970	 0.5680
B	 0.1210	 0.3190
D	 0.7070	 0.5750
E	 0.6790	 0.5630
F	 0.7500	 0.5880
G	 0.6710	 0.5580
H	 0.5710	 0.5090
I	 0.7140	 0.5740
J	 0.7450	 0.5960
K	 0.7150	 0.5700
L	 0.7070	 0.5760
M	 0.6170	 0.5500
N	 0.6530	 0.5720
O	 0.6210	 0.5540
P	 0.7080	 0.5750
Q	 0.5480	 0.4960
R	 0.6090	 0.5520
S	 0.7360	 0.5960
T	 0.7060	 0.5710
a	 0.6970	 0.5700
b	 0.1210	 0.3130
d	 0.7080	 0.5750
e	 0.6780	 0.5630
f	 0.7500	 0.5880
g	 0.6710	 0.5580
h	 0.5730	 0.5080
i	 0.7140	 0.5770
j	 0.7450	 0.5930
k	 0.7140	 0.5740
l	 0.7070	 0.5750
m	 0.6220	 0.5480
n	 0.6570	 0.5760
o	 0.6210	 0.5540
p	 0.6640	 0.5740



Continued on next page...

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Chain	Atom inclusion	Q-score
q	 0.5480	 0.4990
r	 0.6090	 0.5530
s	 0.7340	 0.5990
t	 0.7120	 0.5730