



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 12:10 am GMT

PDB ID : 6TDU
EMDB ID : EMD-10467
Title : Cryo-EM structure of Euglena gracilis mitochondrial ATP synthase, full dimer, rotational states 1
Authors : Muhleip, A.; Amunts, A.
Deposited on : 2019-11-10
Resolution : 4.32 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

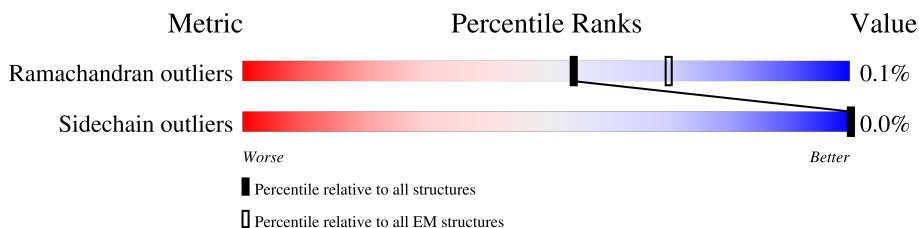
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.32 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.



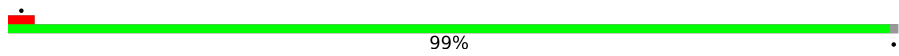
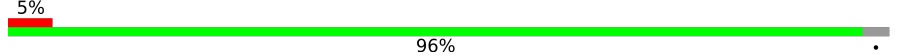
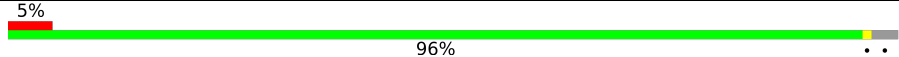
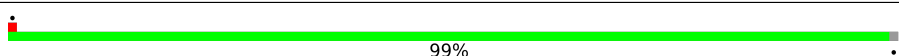
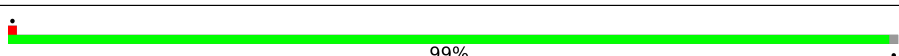
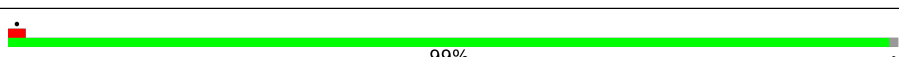
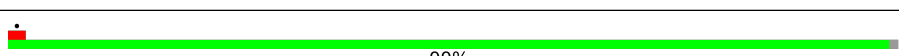
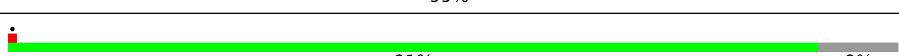
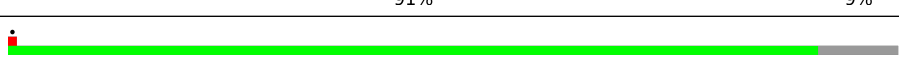
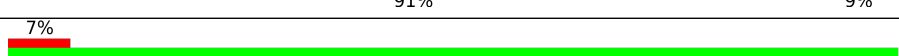
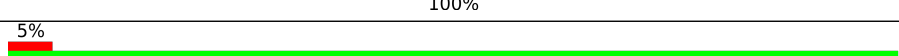
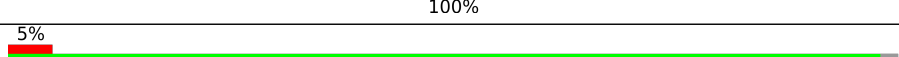
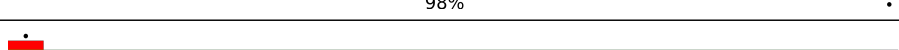
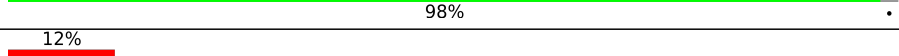
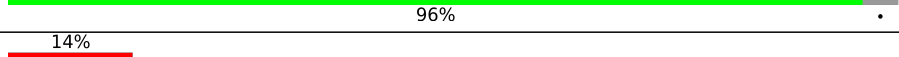
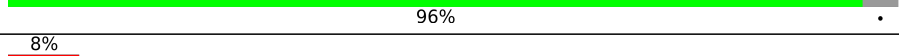


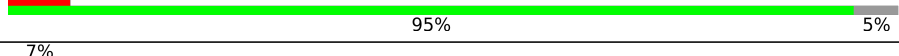
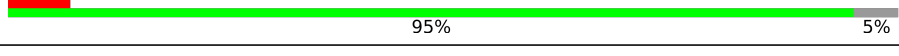
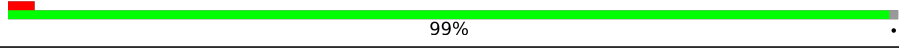
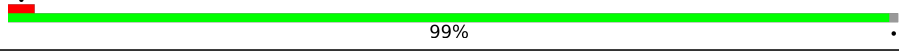



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	D	187	99%
2	d	187	99%
3	E	97	99%
3	e	97	99%
4	F	274	100%
4	f	274	100%
5	G	112	99%

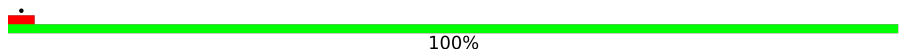
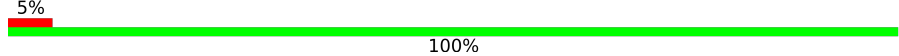
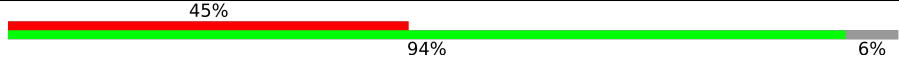
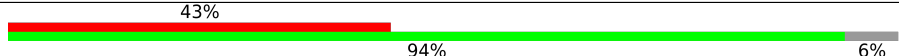
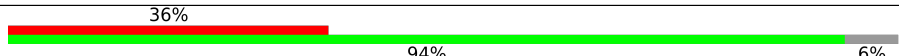
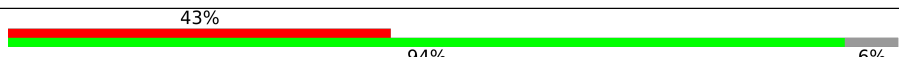
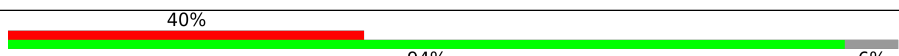
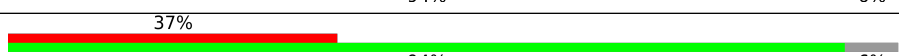
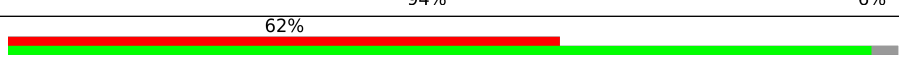
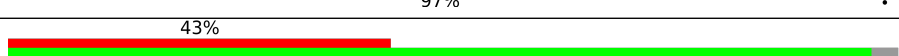
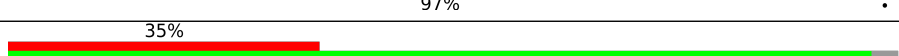
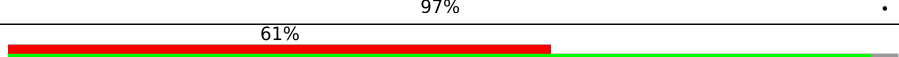
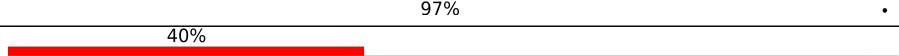
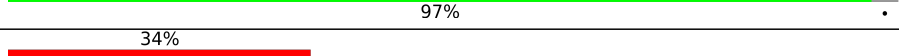
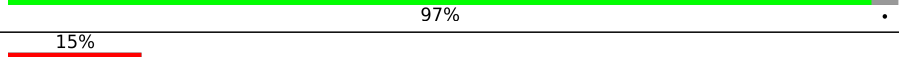
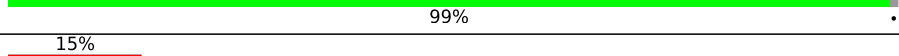
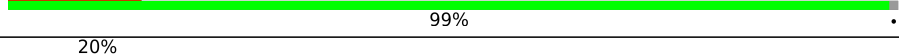
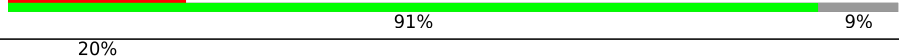
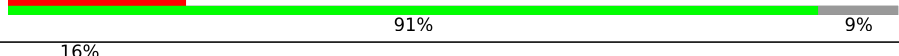
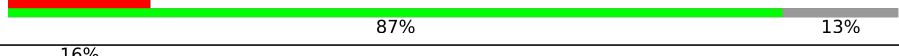

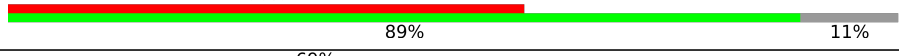

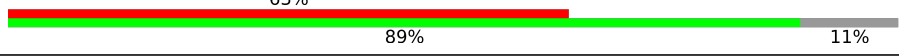
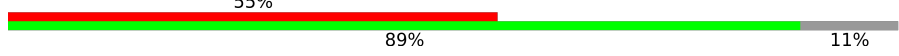
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Mol	Chain	Length	Quality of chain
5	g	112	 99%
6	H	476	 96%
6	h	476	 96%
7	I	98	 99%
7	i	98	 99%
8	J	104	 99%
8	j	104	 99%
9	K	113	 91% 9%
9	k	113	 91% 9%
10	L	57	 100%
10	l	57	 100%
11	M	169	 98%
11	m	169	 98%
12	N	137	 96%
12	n	137	 96%
13	O	116	 86% 14%
13	o	116	 86% 14%
14	P	120	 95% 5%
14	p	120	 95% 5%
15	Q	90	 99%
15	q	90	 99%
16	R	78	 88% 12%
16	r	78	 88% 12%
17	S	74	 88% 12%
17	s	74	 88% 12%

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Mol	Chain	Length	Quality of chain
18	T	66	 100%
18	t	66	 5% 100%
19	AA	561	 45% 94% 6%
19	AB	561	 43% 94% 6%
19	AC	561	 36% 94% 6%
19	BA	561	 43% 94% 6%
19	BB	561	 40% 94% 6%
19	BC	561	 37% 94% 6%
20	AD	501	 62% 97%
20	AE	501	 43% 97%
20	AF	501	 35% 97%
20	BD	501	 61% 97%
20	BE	501	 40% 97%
20	BF	501	 34% 97%
21	AG	306	 15% 99%
21	BG	306	 15% 99%
22	AH	176	 20% 91% 9%
22	BH	176	 20% 91% 9%
23	AI	76	 16% 87% 13%
23	BI	76	 16% 87% 13%
24	AJ	192	 58% 89% 11%
24	AK	192	 69% 89% 11%
24	AL	192	 63% 89% 11%
24	BJ	192	 55% 89% 11%
24	BK	192	 66% 89% 11%

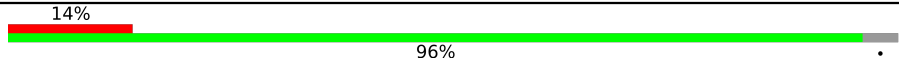
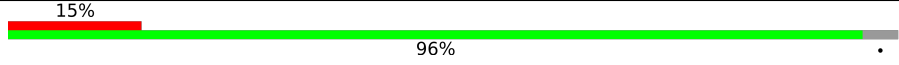
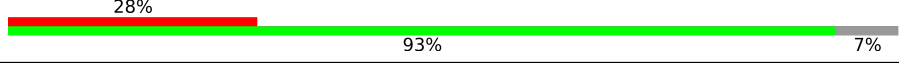
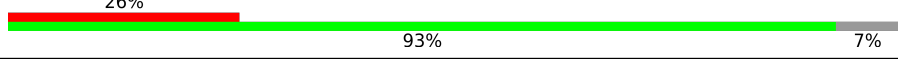
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Mol	Chain	Length	Quality of chain		
24	BL	192	61%	89%	11%
25	AM	267	53%	90%	9%
25	BM	267	52%	90%	9%
26	AN	103	31%	48%	52%
26	BN	103	31%	48%	52%
27	AO	104	21%	78%	22%
27	AP	104	12%	78%	22%
27	AQ	104	16%	78%	22%
27	AR	104	22%	78%	22%
27	AS	104	26%	78%	22%
27	AT	104	27%	78%	22%
27	AU	104	23%	78%	22%
27	AV	104	20%	78%	22%
27	AW	104	23%	78%	22%
27	AX	104	23%	78%	22%
27	BO	104	21%	78%	22%
27	BP	104	14%	78%	22%
27	BQ	104	18%	78%	22%
27	BR	104	20%	78%	22%
27	BS	104	25%	78%	22%
27	BT	104	28%	78%	22%
27	BU	104	23%	78%	22%
27	BV	104	19%	78%	22%
27	BW	104	26%	78%	22%
27	BX	104	23%	78%	22%

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Mol	Chain	Length	Quality of chain
28	B	338	 14% 96% 7%
28	b	338	 15% 96% 7%
29	C	169	 28% 93% 7%
29	c	169	 26% 93% 7%

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 271331 atoms, of which 136237 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	
			Total	C	H	N	O			S
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 ATPTB6.

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

- Molecule 3 is a protein called ATPTB12.

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

- Molecule 4 is a protein called ATP synthase subunit a.

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

- Molecule 5 is a protein called ATP synthase subunit b.

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

- Molecule 6 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace	
6	H	460	Total	C	H	N	O	S	0	0
			7302	2343	3637	607	705	10		
6	h	460	Total	C	H	N	O	S	0	0
			7302	2343	3637	607	705	10		

- Molecule 7 is a protein called ATP synthase subunit f.

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

- Molecule 8 is a protein called ATP synthase subunit i/j.

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

- Molecule 9 is a protein called ATP synthase subunit k.

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

- Molecule 10 is a protein called ATP synthase subunit 8.

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

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

- Molecule 11 is a protein called ATPEG1.

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

- Molecule 12 is a protein called ATPEG2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
12	N	131	Total	C	H	N	O	0	0
			2168	714	1071	198	182		
12	n	131	Total	C	H	N	O	0	0
			2168	714	1071	198	182		

- Molecule 13 is a protein called ATPEG3.

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

- Molecule 14 is a protein called ATPEG4.

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

- Molecule 15 is a protein called ATPEG5.

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

- Molecule 16 is a protein called ATPEG6.

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

- Molecule 17 is a protein called ATPEG7.

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

- Molecule 18 is a protein called ATPEG8.

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

- Molecule 19 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace	
19	AA	526	Total	C	H	N	O	S	0	0
			8291	2611	4196	700	766	18		
19	AB	526	Total	C	H	N	O	S	0	0
			8292	2611	4197	700	766	18		
19	AC	529	Total	C	H	N	O	S	0	0
			8336	2625	4219	703	771	18		
19	BA	526	Total	C	H	N	O	S	0	0
			8291	2611	4196	700	766	18		
19	BB	526	Total	C	H	N	O	S	0	0
			8292	2611	4197	700	766	18		
19	BC	529	Total	C	H	N	O	S	0	0
			8336	2625	4219	703	771	18		

- Molecule 20 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
20	AD	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		
20	AE	487	Total	C	H	N	O	S	0	0
			7408	2318	3730	620	713	27		
20	AF	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		
20	BD	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		
20	BE	487	Total	C	H	N	O	S	0	0
			7408	2318	3730	620	713	27		
20	BF	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		

- Molecule 21 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace	
21	AG	303	Total	C	H	N	O	S	0	0
			4898	1543	2462	420	459	14		
21	BG	303	Total	C	H	N	O	S	0	0
			4898	1543	2462	420	459	14		

- Molecule 22 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
22	AH	160	Total	C	H	N	O	S	0	0
			2448	787	1202	207	251	1		
22	BH	160	Total	C	H	N	O	S	0	0
			2448	787	1202	207	251	1		

- Molecule 23 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	AI	66	Total	C	H	N	O	S	0	0
			1077	346	541	91	98	1		
23	BI	66	Total	C	H	N	O	S	0	0
			1077	346	541	91	98	1		

- Molecule 24 is a protein called p18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	AJ	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace	
24	AK	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
24	AL	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
24	BJ	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
24	BK	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
24	BL	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		

- Molecule 25 is a protein called oligomycin sensitivity conferring protein (OSCP).

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	AM	243	Total	C	H	N	O	S	0	0
			3778	1212	1885	310	370	1		
25	BM	243	Total	C	H	N	O	S	0	0
			3778	1212	1885	310	370	1		

- Molecule 26 is a protein called inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	AN	49	Total	C	H	N	O	S	0	0
			802	247	399	72	82	2		
26	BN	49	Total	C	H	N	O	S	0	0
			802	247	399	72	82	2		

- Molecule 27 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	AO	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AP	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AQ	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AR	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AS	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AT	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	AU	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	AV	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	AW	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	AX	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BO	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BP	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BQ	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BR	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BS	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BT	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BU	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BV	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BW	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0
27	BX	81	Total 1185	C 383	H 605	N 89	O 102	S 6	0	0

- Molecule 28 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	B	326	Total 4813	C 1508	H 2421	N 405	O 474	S 5	0	0
28	b	326	Total 4813	C 1508	H 2421	N 405	O 474	S 5	0	0

- Molecule 29 is a protein called ATPTB4.

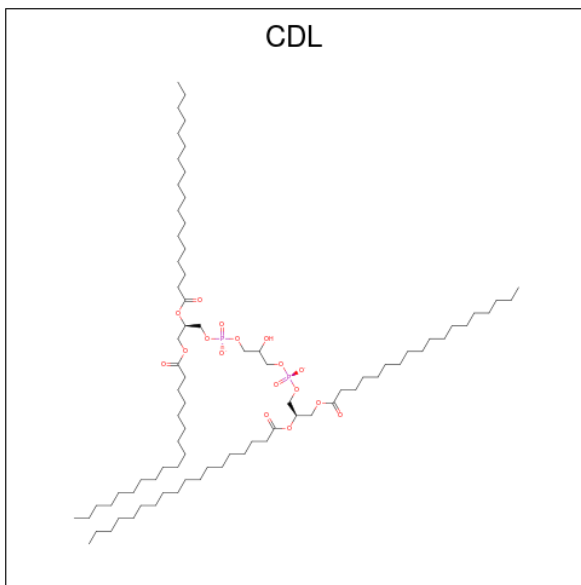
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	C	157	Total 2472	C 781	H 1241	N 211	O 237	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	c	157	2472	781	1241	211	237	2	0	0

- Molecule 30 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



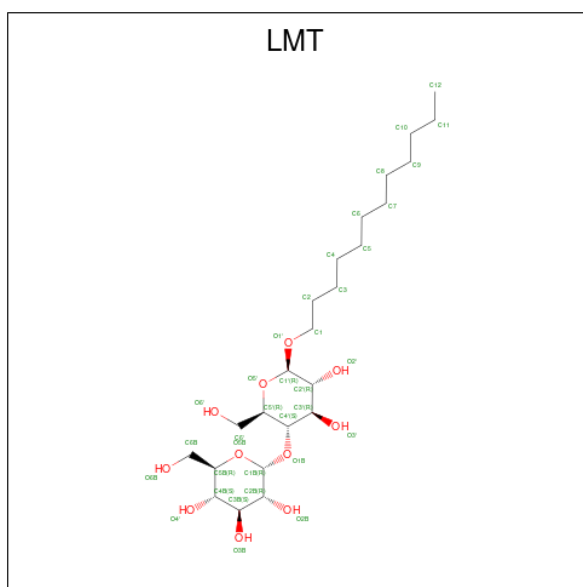
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
30	A	1	820	298	427	85	10	0
30	A	1	820	298	427	85	10	0
30	A	1	820	298	427	85	10	0
30	A	1	820	298	427	85	10	0
30	A	1	820	298	427	85	10	0
30	D	1	228	72	137	17	2	0
30	E	1	95	44	32	17	2	0
30	M	1	312	126	129	51	6	0
30	M	1	312	126	129	51	6	0
30	M	1	312	126	129	51	6	0

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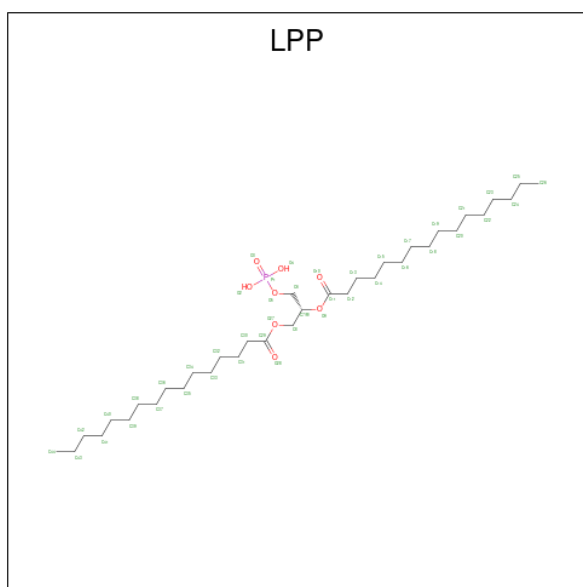
Mol	Chain	Residues	Atoms					AltConf
30	O	1	Total	C	H	O	P	0
			124	46	59	17	2	
30	P	1	Total	C	H	O	P	0
			319	108	173	34	4	
30	P	1	Total	C	H	O	P	0
			319	108	173	34	4	
30	R	1	Total	C	H	O	P	0
			150	57	74	17	2	
30	a	1	Total	C	H	O	P	0
			820	298	427	85	10	
30	a	1	Total	C	H	O	P	0
			820	298	427	85	10	
30	a	1	Total	C	H	O	P	0
			820	298	427	85	10	
30	a	1	Total	C	H	O	P	0
			820	298	427	85	10	
30	a	1	Total	C	H	O	P	0
			820	298	427	85	10	
30	d	1	Total	C	H	O	P	0
			228	72	137	17	2	
30	e	1	Total	C	H	O	P	0
			95	44	32	17	2	
30	m	1	Total	C	H	O	P	0
			152	58	75	17	2	
30	o	1	Total	C	H	O	P	0
			124	46	59	17	2	
30	p	1	Total	C	H	O	P	0
			75	29	27	17	2	
30	r	1	Total	C	H	O	P	0
			150	57	74	17	2	

- Molecule 31 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



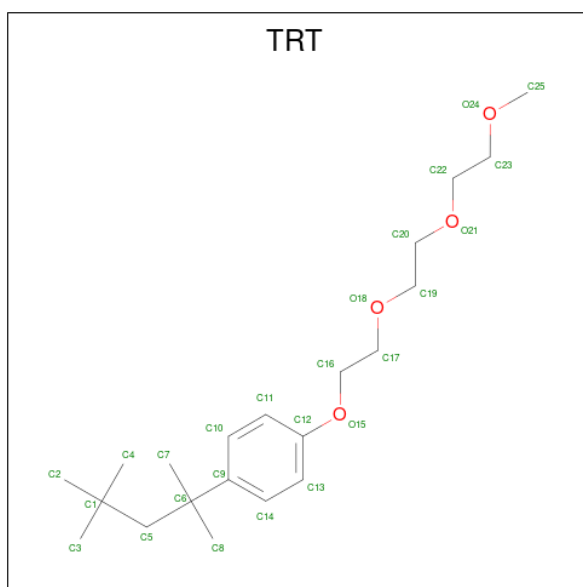
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
31	D	1	81	24	46	11	0
31	F	1	81	24	46	11	0
31	N	1	81	24	46	11	0
31	Q	1	81	24	46	11	0
31	d	1	81	24	46	11	0
31	g	1	81	24	46	11	0
31	n	1	81	24	46	11	0
31	q	1	81	24	46	11	0

- Molecule 32 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
32	F	1	Total 41	C 15	H 17	O 8	P 1	0
32	I	1	Total 111	C 35	H 67	O 8	P 1	0
32	K	1	Total 48	C 22	H 17	O 8	P 1	0
32	N	1	Total 43	C 17	H 17	O 8	P 1	0
32	O	1	Total 114	C 37	H 59	O 16	P 2	0
32	O	1	Total 114	C 37	H 59	O 16	P 2	0
32	f	1	Total 41	C 15	H 17	O 8	P 1	0
32	i	1	Total 111	C 35	H 67	O 8	P 1	0
32	k	1	Total 48	C 22	H 17	O 8	P 1	0
32	n	1	Total 43	C 17	H 17	O 8	P 1	0
32	o	1	Total 114	C 37	H 59	O 16	P 2	0
32	o	1	Total 114	C 37	H 59	O 16	P 2	0

- Molecule 33 is FRAGMENT OF TRITON X-100 (three-letter code: TRT) (formula: C₂₁H₃₆O₄).



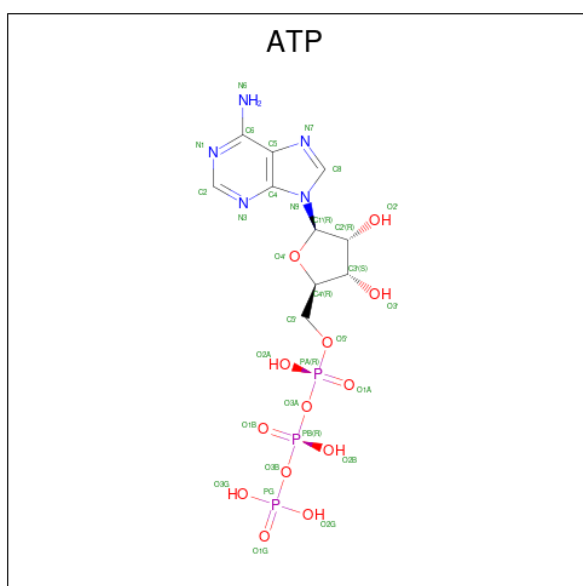
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
33	G	1	122	42	72	8	0
33	G	1	122	42	72	8	0
33	M	1	122	42	72	8	0
33	M	1	122	42	72	8	0
33	N	1	122	42	72	8	0
33	N	1	122	42	72	8	0
33	P	1	61	21	36	4	0
33	g	1	122	42	72	8	0
33	g	1	122	42	72	8	0
33	m	1	122	42	72	8	0
33	m	1	122	42	72	8	0
33	n	1	122	42	72	8	0
33	n	1	122	42	72	8	0
33	p	1	61	21	36	4	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
33	AE	1	Total 61	C 21	H 36	O 4	0
33	AR	1	Total 61	C 21	H 36	O 4	0
33	BE	1	Total 61	C 21	H 36	O 4	0
33	BR	1	Total 61	C 21	H 36	O 4	0

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
34	AA	1	Total 35	C 10	H 4	N 5	O 13	P 3	0
34	AB	1	Total 35	C 10	H 4	N 5	O 13	P 3	0
34	AC	1	Total 35	C 10	H 4	N 5	O 13	P 3	0
34	AF	1	Total 35	C 10	H 4	N 5	O 13	P 3	0
34	BA	1	Total 35	C 10	H 4	N 5	O 13	P 3	0
34	BB	1	Total 35	C 10	H 4	N 5	O 13	P 3	0
34	BC	1	Total 35	C 10	H 4	N 5	O 13	P 3	0

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Mol	Chain	Residues	Atoms						AltConf
34	BF	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	AA	1	Total	Mg	0
			1	1	
35	AB	1	Total	Mg	0
			1	1	
35	AC	1	Total	Mg	0
			1	1	
35	AD	1	Total	Mg	0
			1	1	
35	AF	1	Total	Mg	0
			1	1	
35	BA	1	Total	Mg	0
			1	1	
35	BB	1	Total	Mg	0
			1	1	
35	BC	1	Total	Mg	0
			1	1	
35	BD	1	Total	Mg	0
			1	1	
35	BF	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



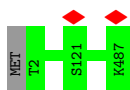
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
36	AD	1	34	10	7	5	10	2	0
36	BD	1	35	10	8	5	10	2	0

3 Residue-property plots [i](#)

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

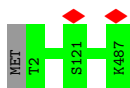
- Molecule 1: ATPTB1

Chain A:  100%



- Molecule 1: ATPTB1

Chain a:  100%



- Molecule 2: ATPTB6

Chain D:  99%



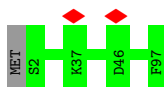
- Molecule 2: ATPTB6

Chain d:  99%

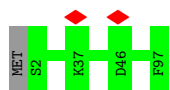


- Molecule 3: ATPTB12

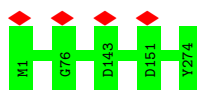
Chain E:  99%



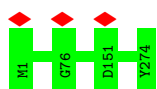
- Molecule 3: ATPTB12



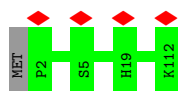
• Molecule 4: ATP synthase subunit a



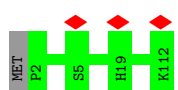
• Molecule 4: ATP synthase subunit a



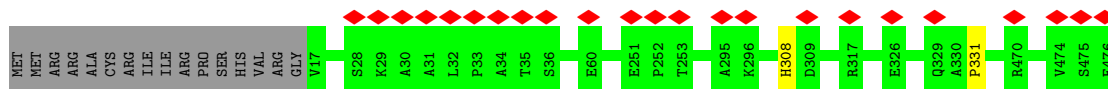
• Molecule 5: ATP synthase subunit b



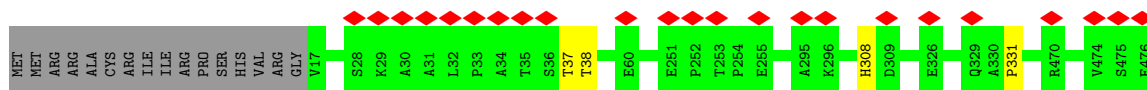
• Molecule 5: ATP synthase subunit b



• Molecule 6: ATP synthase subunit d



• Molecule 6: ATP synthase subunit d



- Molecule 7: ATP synthase subunit f

Chain I:  99%



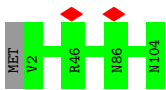
- Molecule 7: ATP synthase subunit f

Chain i:  99%



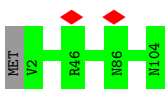
- Molecule 8: ATP synthase subunit i/j

Chain J:  99%

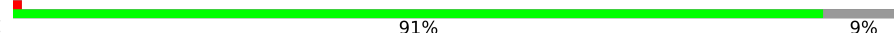


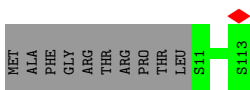
- Molecule 8: ATP synthase subunit i/j

Chain j:  99%




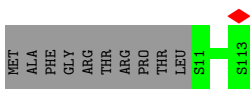
- Molecule 9: ATP synthase subunit k

Chain K:  91%



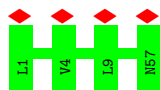
- Molecule 9: ATP synthase subunit k

Chain k:  91%

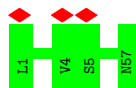


- Molecule 10: ATP synthase subunit 8

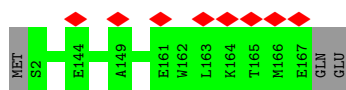
Chain L:  7%



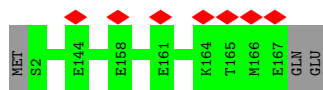
- Molecule 10: ATP synthase subunit 8



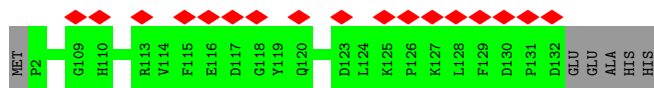
- Molecule 11: ATPEG1



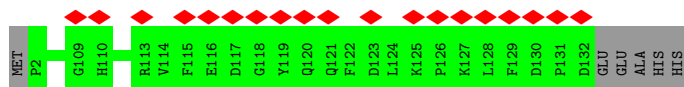
- Molecule 11: ATPEG1



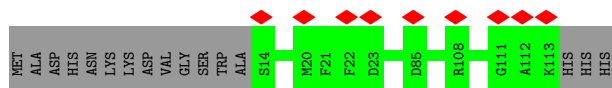
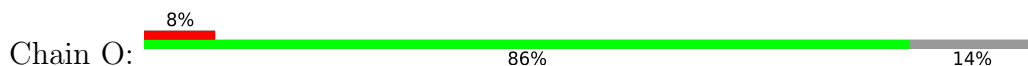
- Molecule 12: ATPEG2



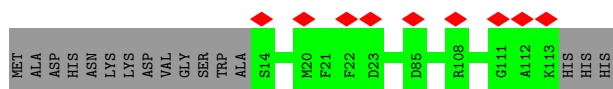
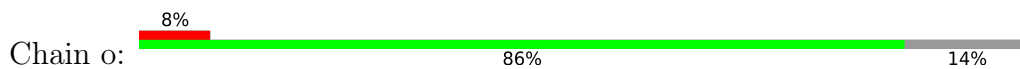
- Molecule 12: ATPEG2



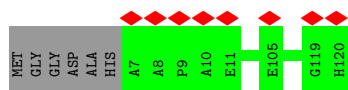
- Molecule 13: ATPEG3



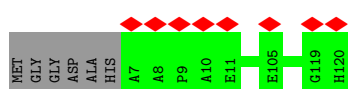
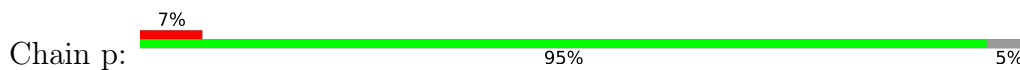
- Molecule 13: ATPEG3



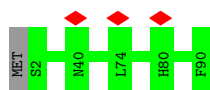
• Molecule 14: ATPEG4



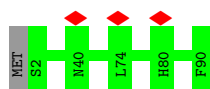
• Molecule 14: ATPEG4



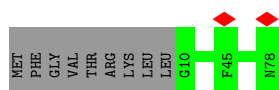
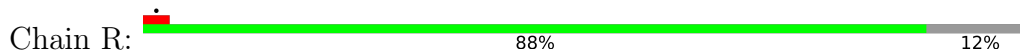
• Molecule 15: ATPEG5



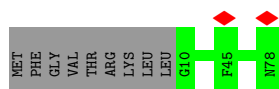
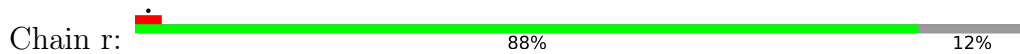
• Molecule 15: ATPEG5



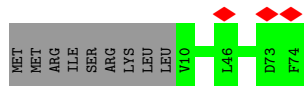
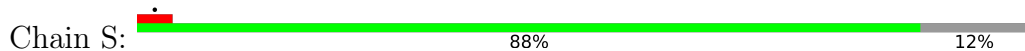
• Molecule 16: ATPEG6



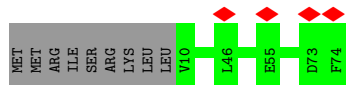
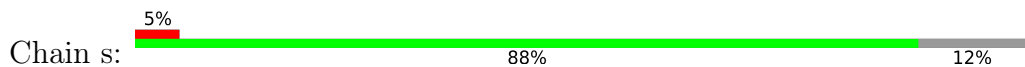
• Molecule 16: ATPEG6



• Molecule 17: ATPEG7



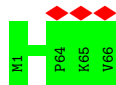
• Molecule 17: ATPEG7



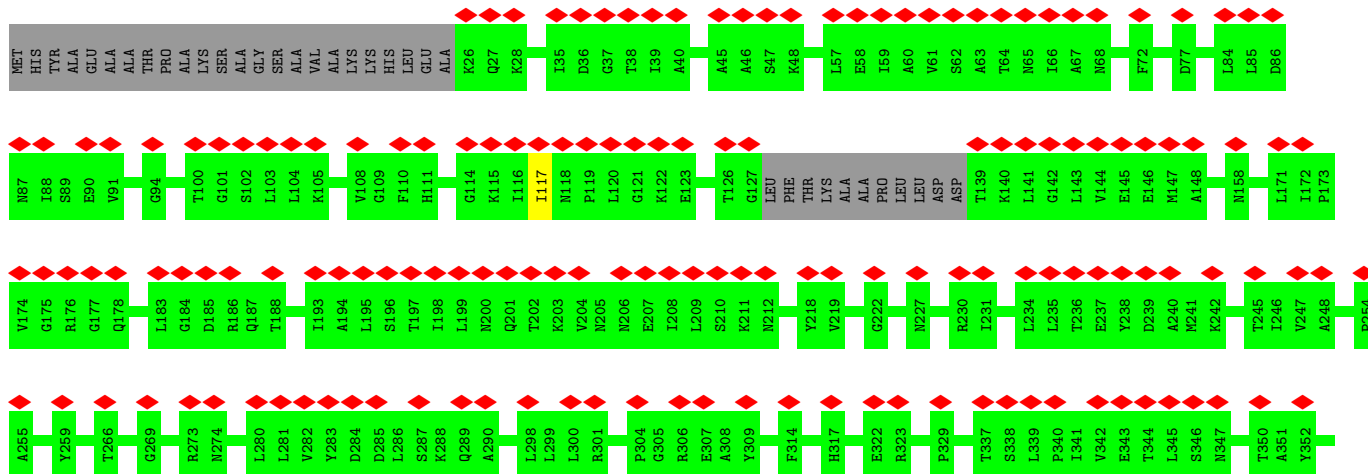
• Molecule 18: ATPEG8

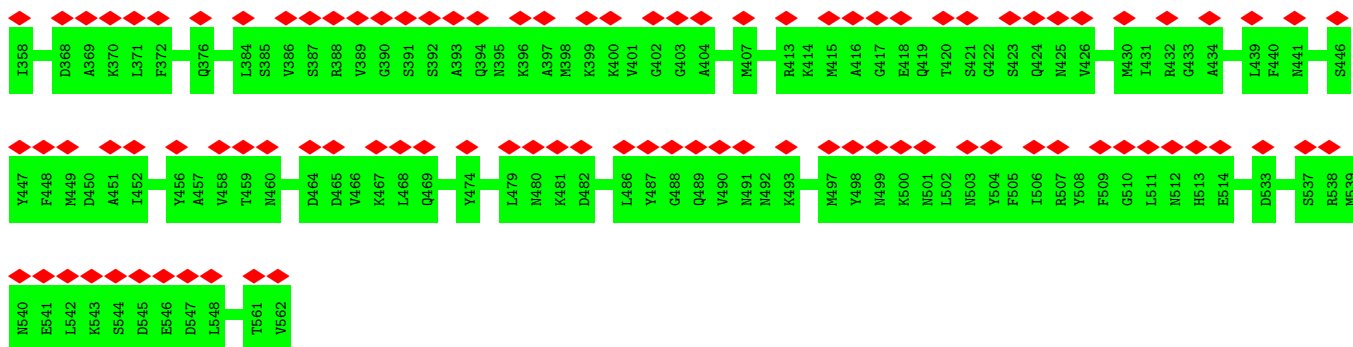


• Molecule 18: ATPEG8

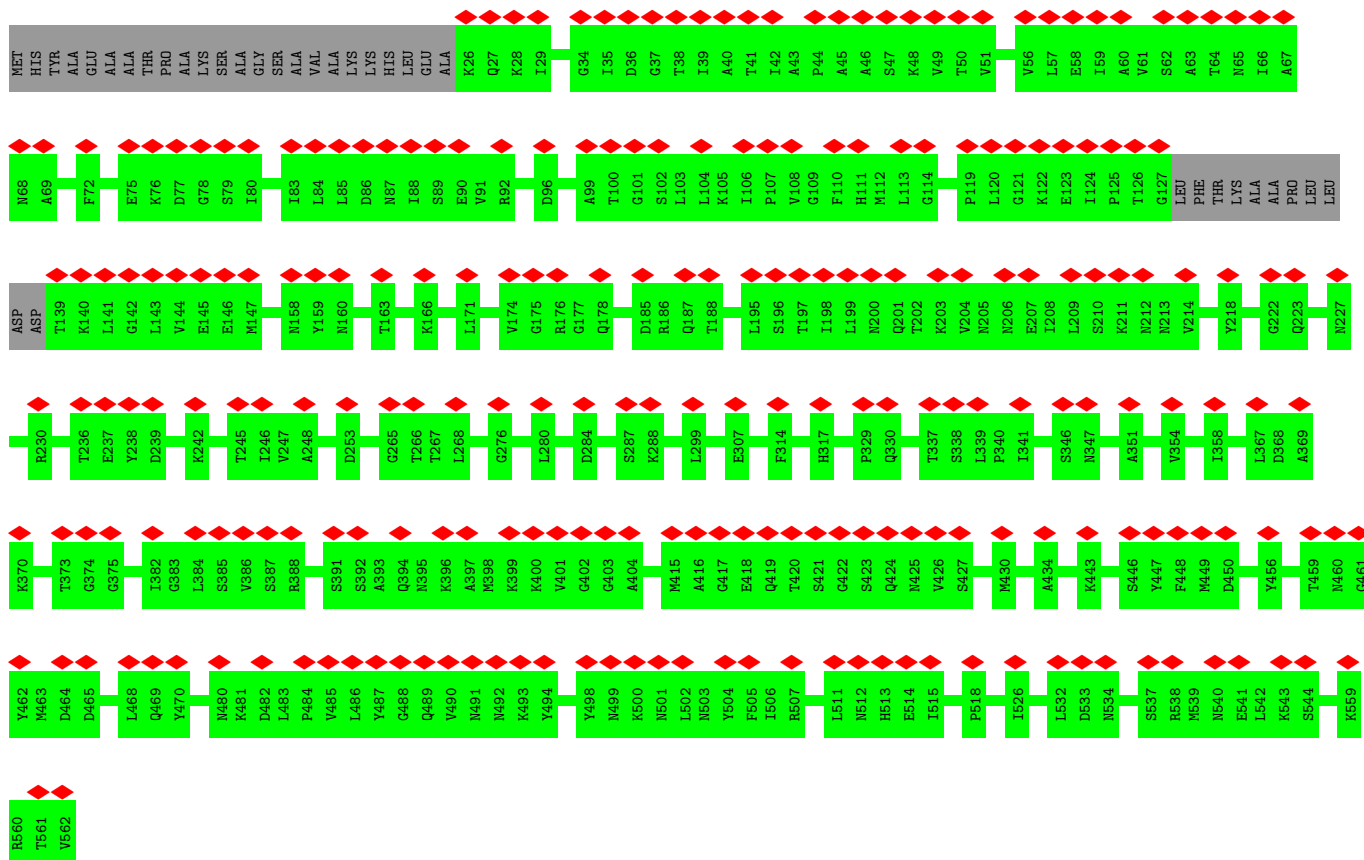


• Molecule 19: ATP synthase subunit alpha

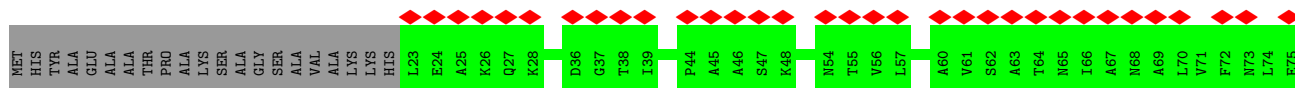


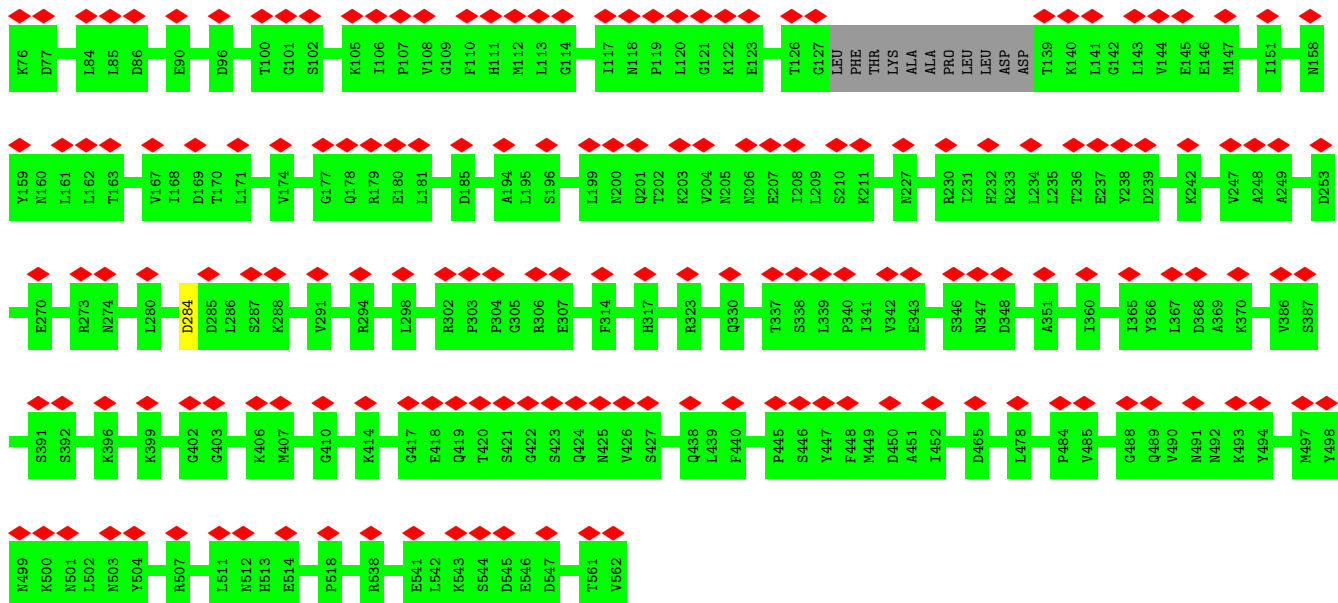


• Molecule 19: ATP synthase subunit alpha

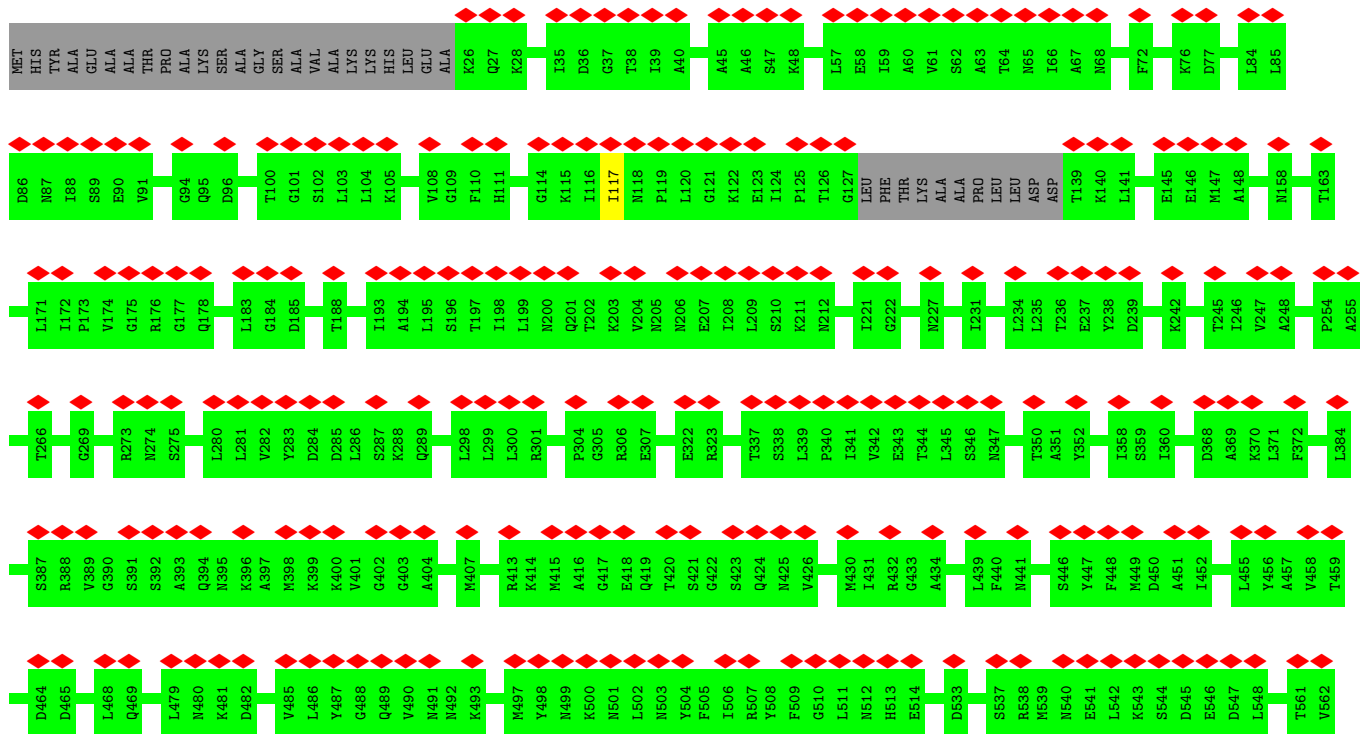
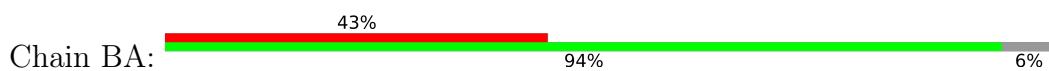


• Molecule 19: ATP synthase subunit alpha

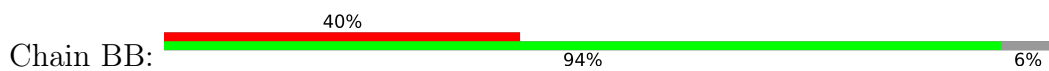


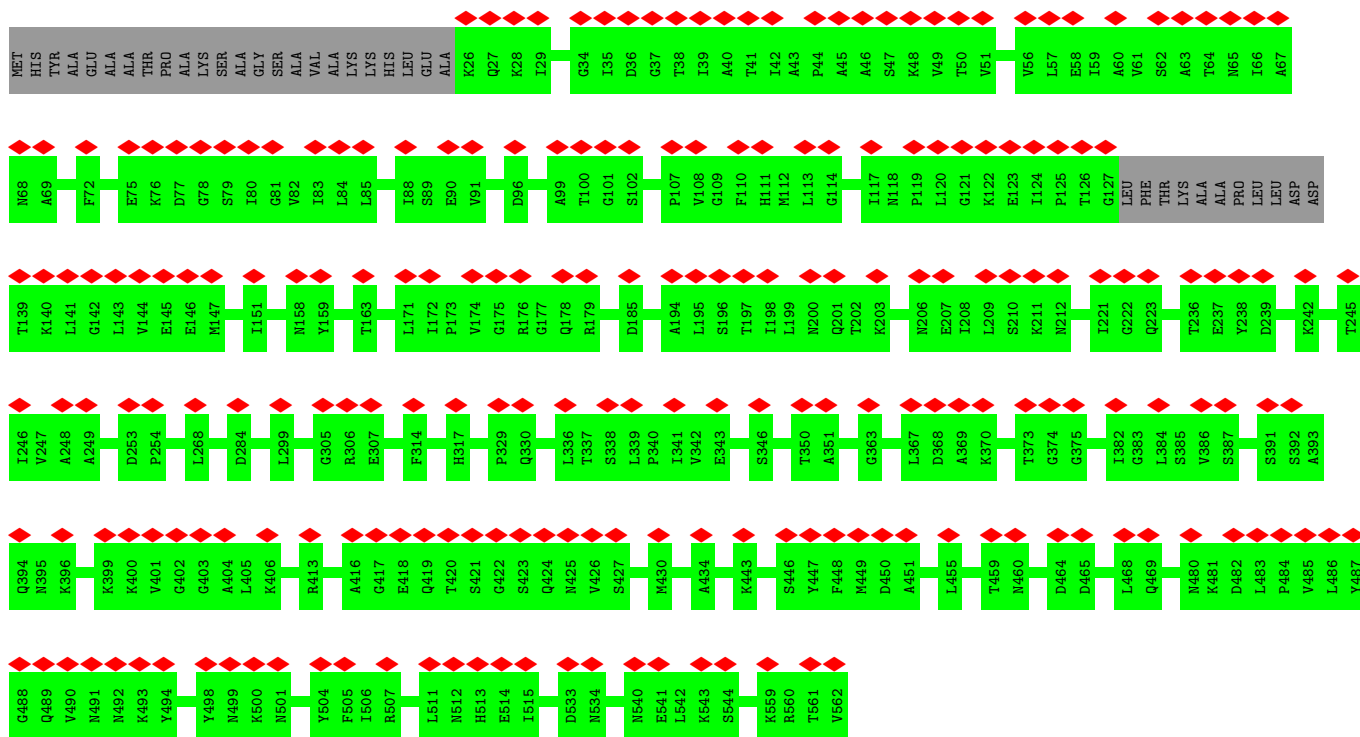


• Molecule 19: ATP synthase subunit alpha

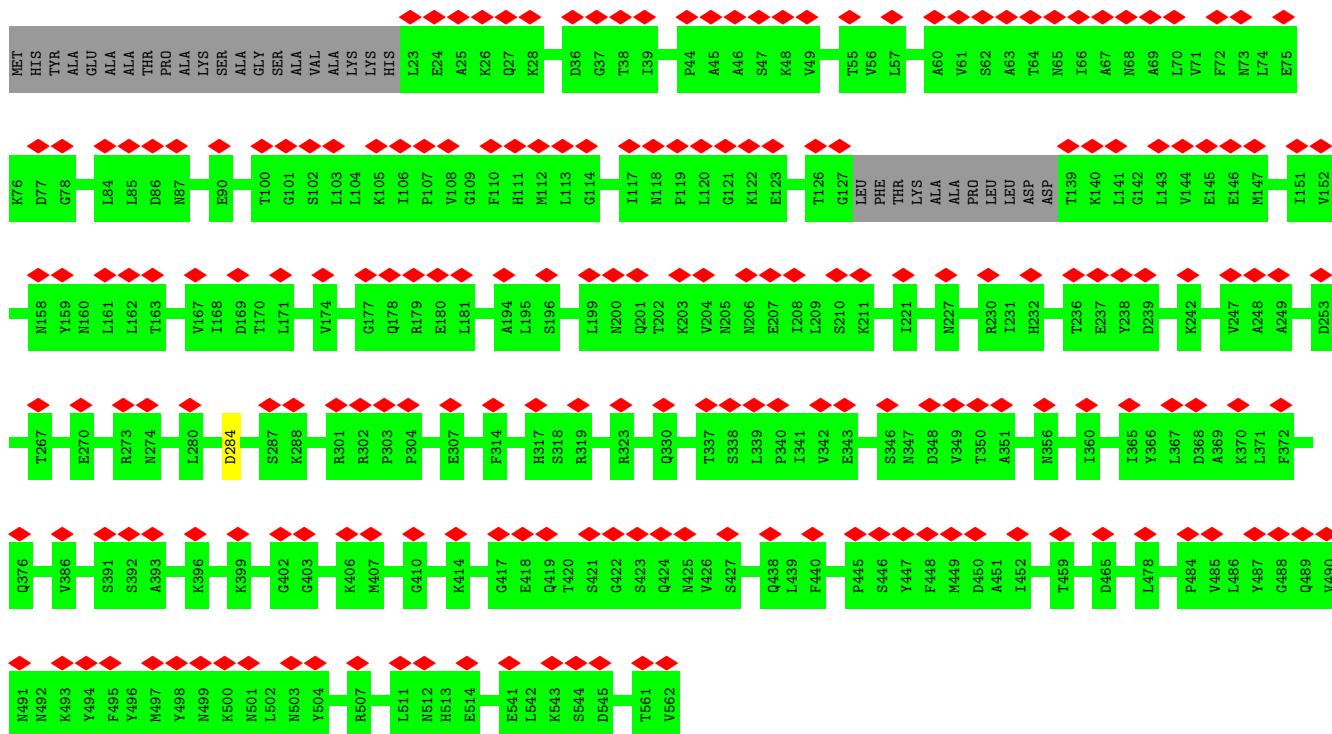
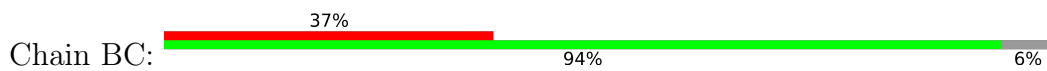


• Molecule 19: ATP synthase subunit alpha

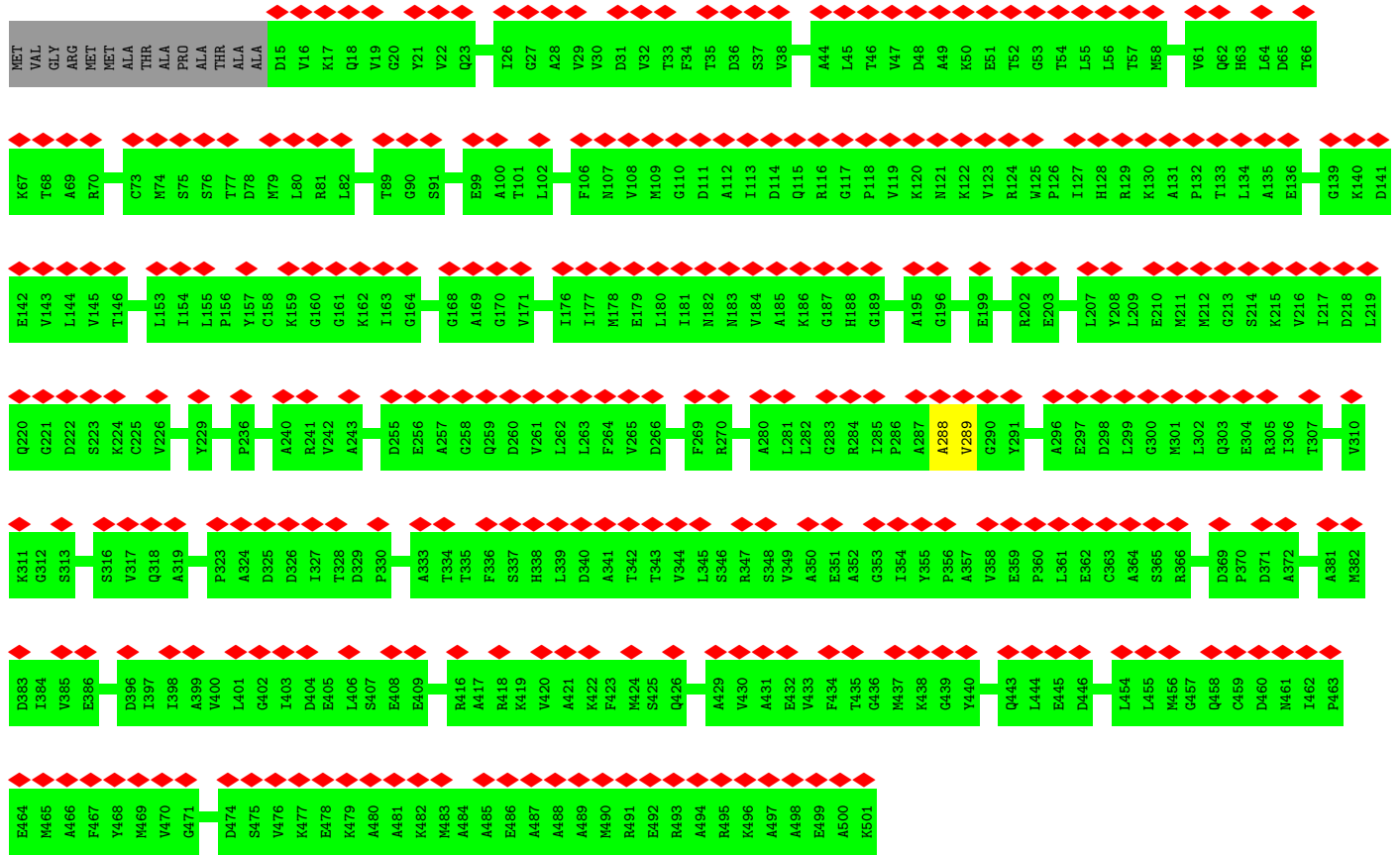




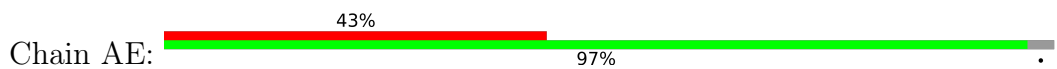
• Molecule 19: ATP synthase subunit alpha



• Molecule 20: ATP synthase subunit beta

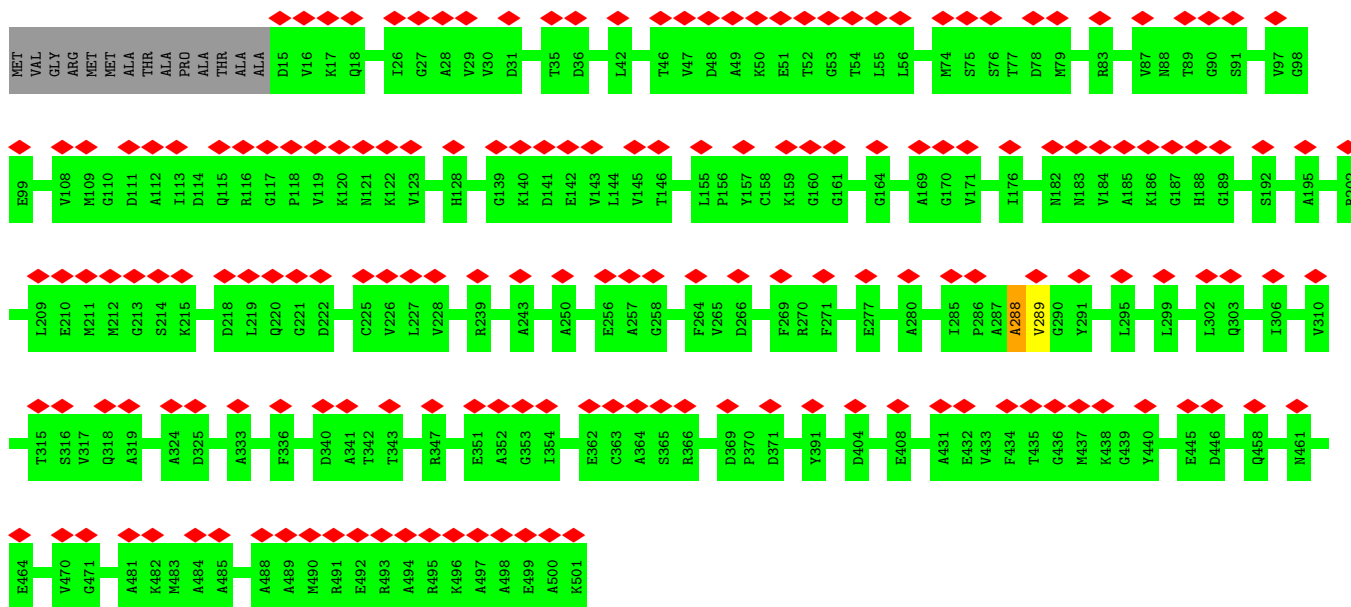


- Molecule 20: ATP synthase subunit beta

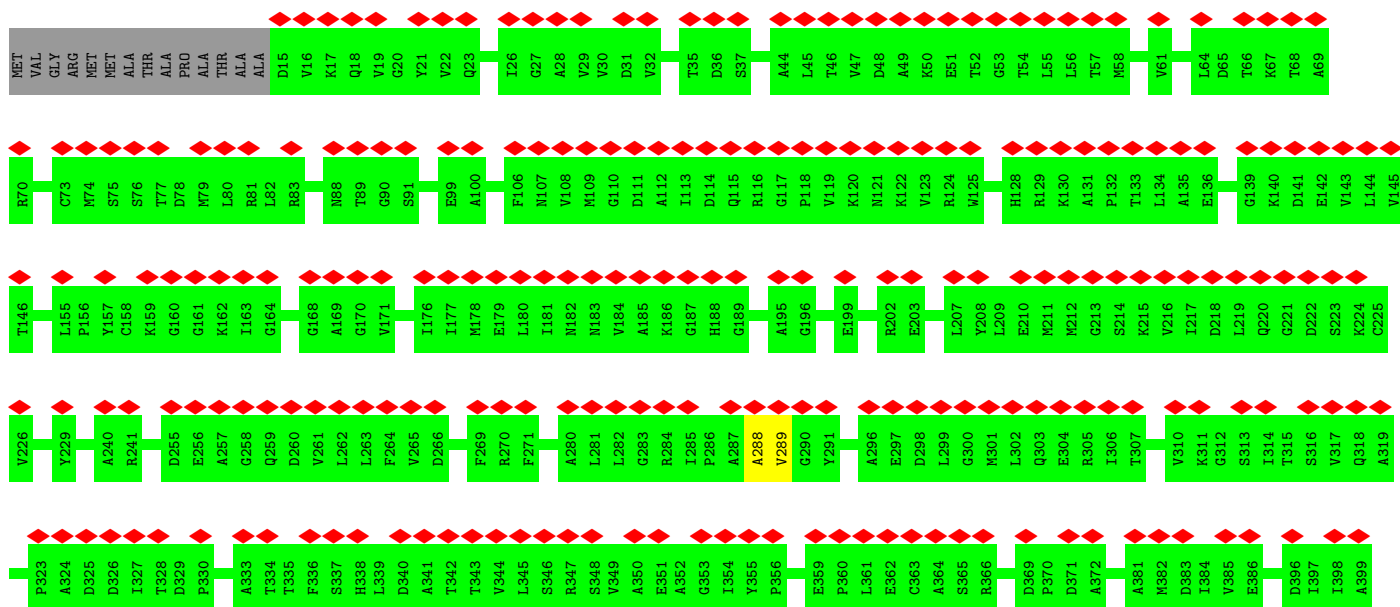


R495
K496
A497
A498
E499
A500
K501

• Molecule 20: ATP synthase subunit beta

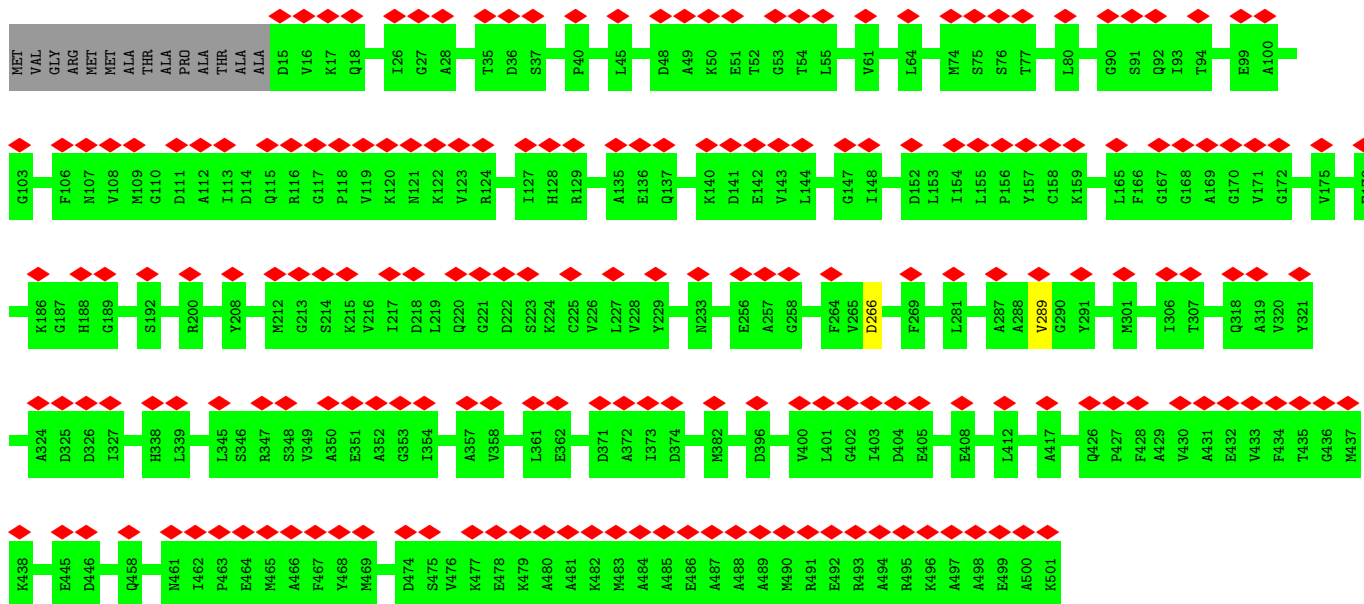
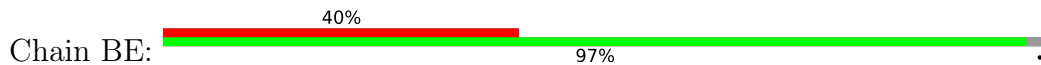


• Molecule 20: ATP synthase subunit beta

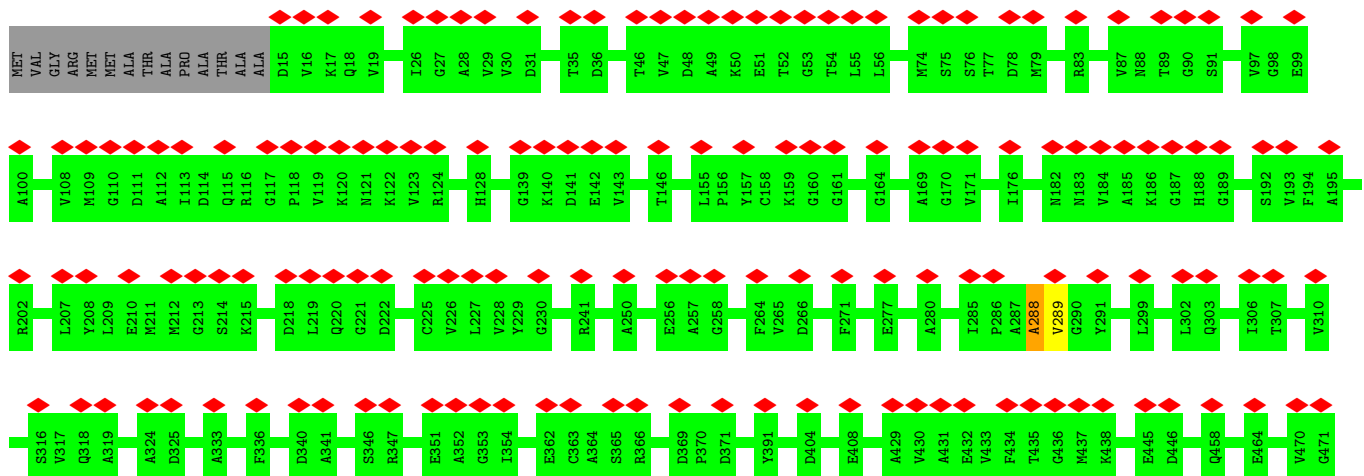




• Molecule 20: ATP synthase subunit beta

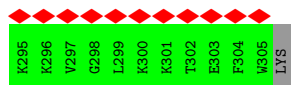
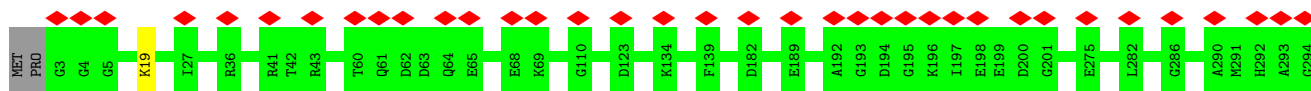


• Molecule 20: ATP synthase subunit beta

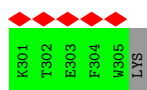
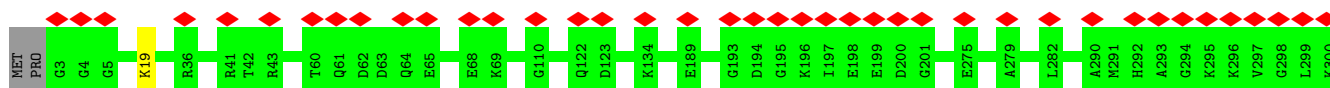




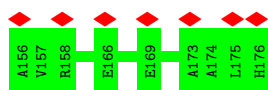
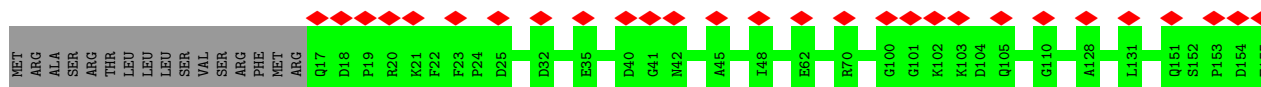
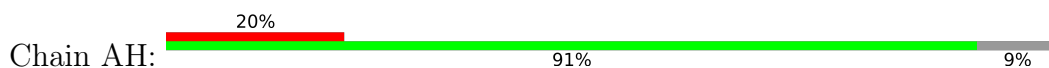
- Molecule 21: ATP synthase subunit gamma



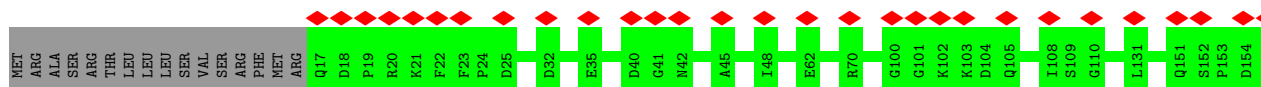
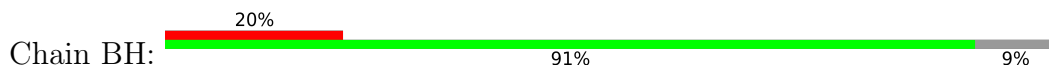
- Molecule 21: ATP synthase subunit gamma



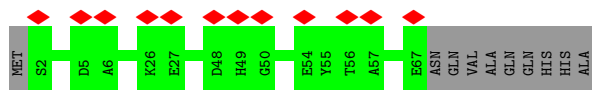
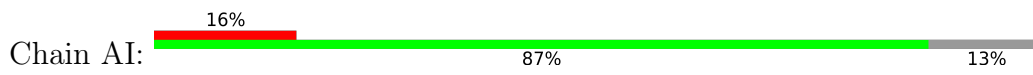
- Molecule 22: ATP synthase subunit delta



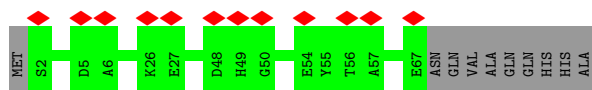
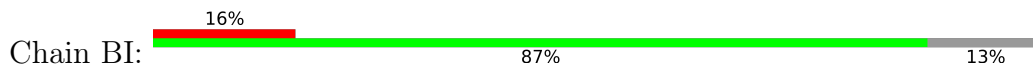
- Molecule 22: ATP synthase subunit delta



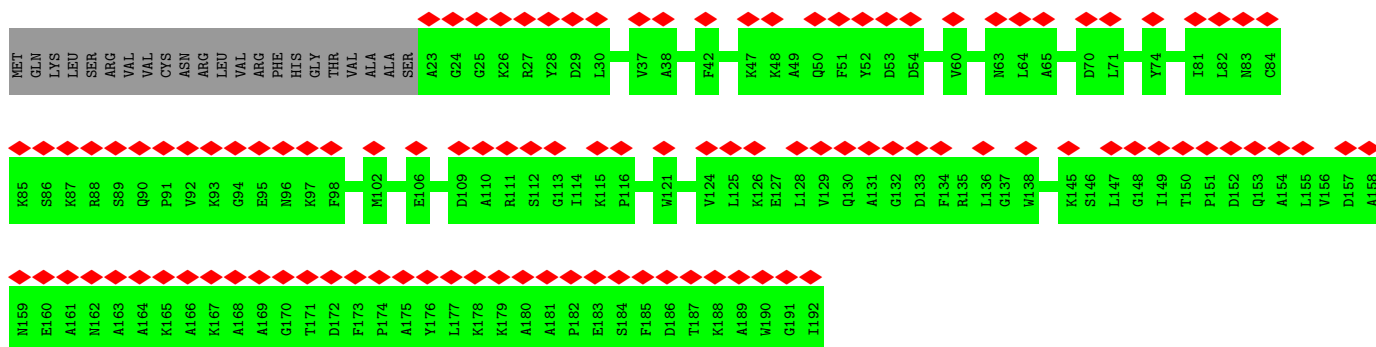
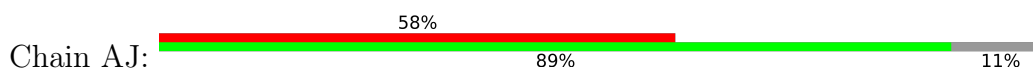
- Molecule 23: ATP synthase subunit epsilon



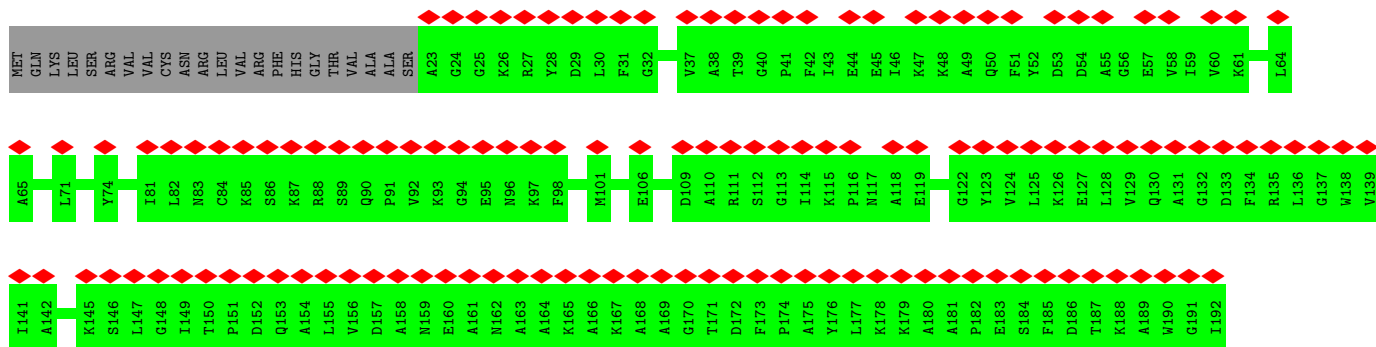
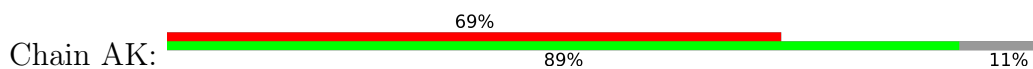
• Molecule 23: ATP synthase subunit epsilon



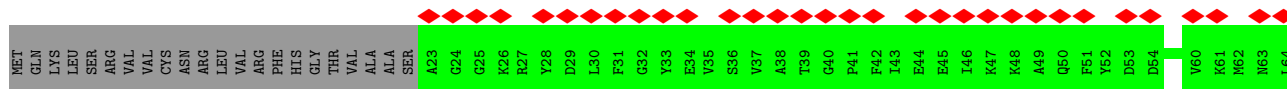
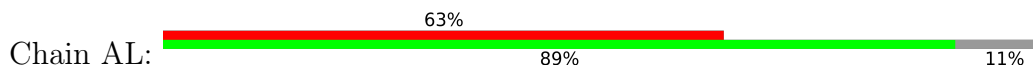
• Molecule 24: p18

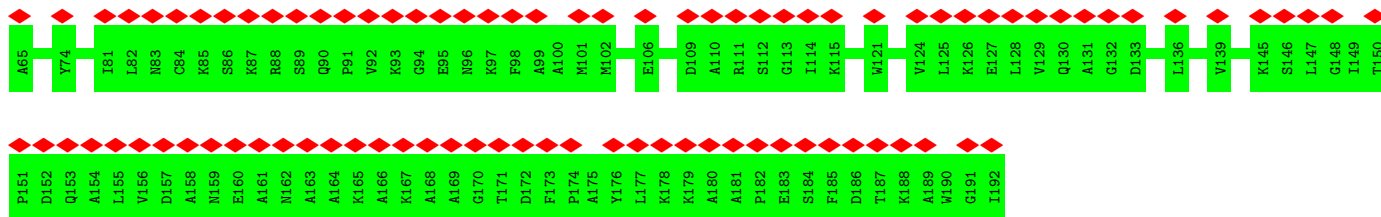


• Molecule 24: p18

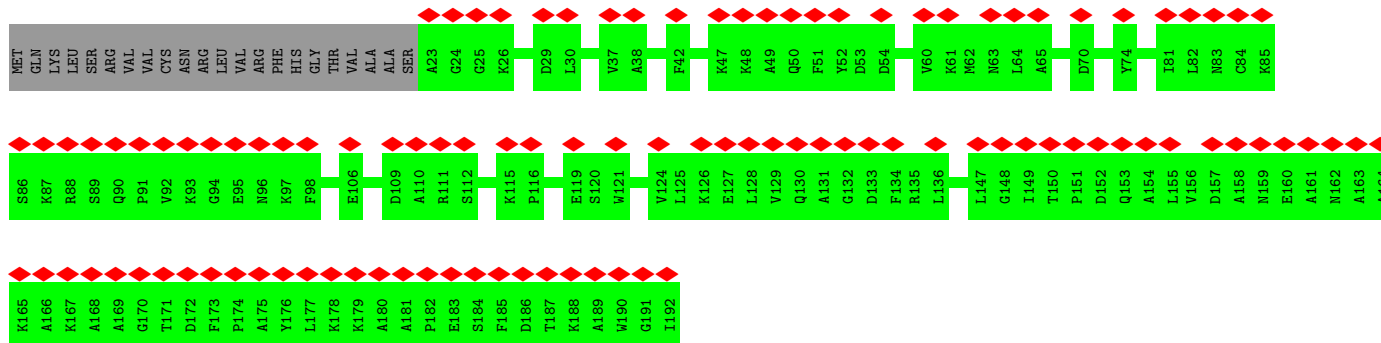
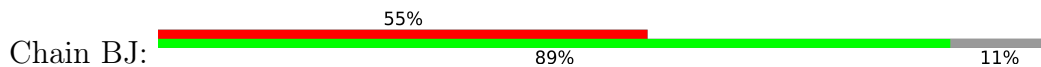


• Molecule 24: p18

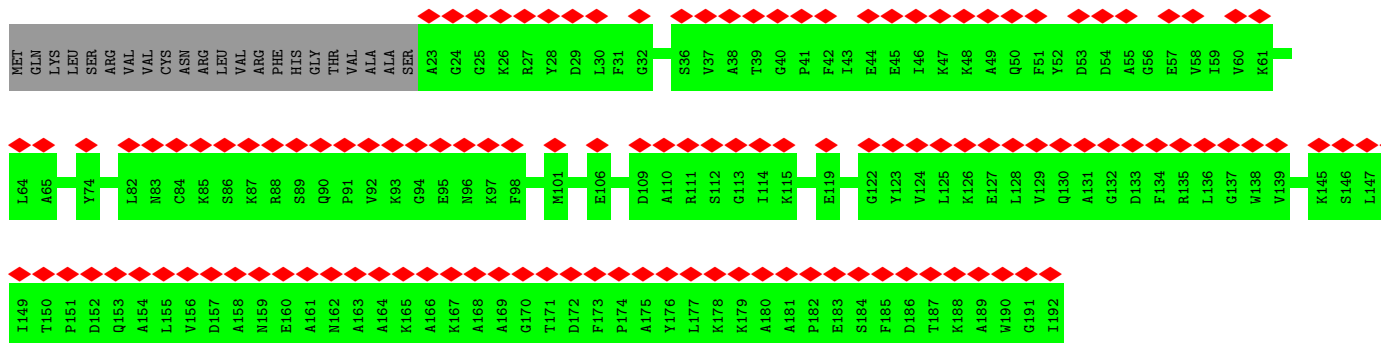
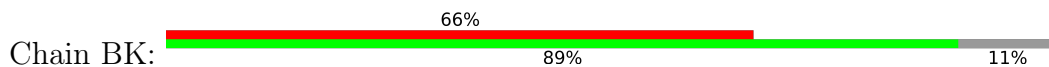




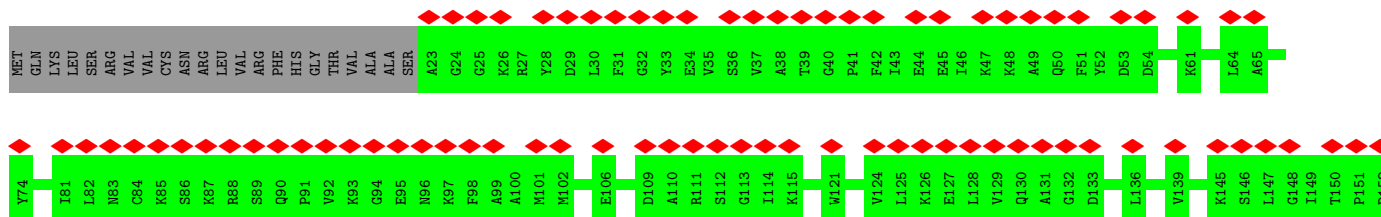
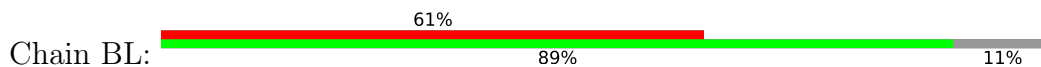
• Molecule 24: p18



• Molecule 24: p18

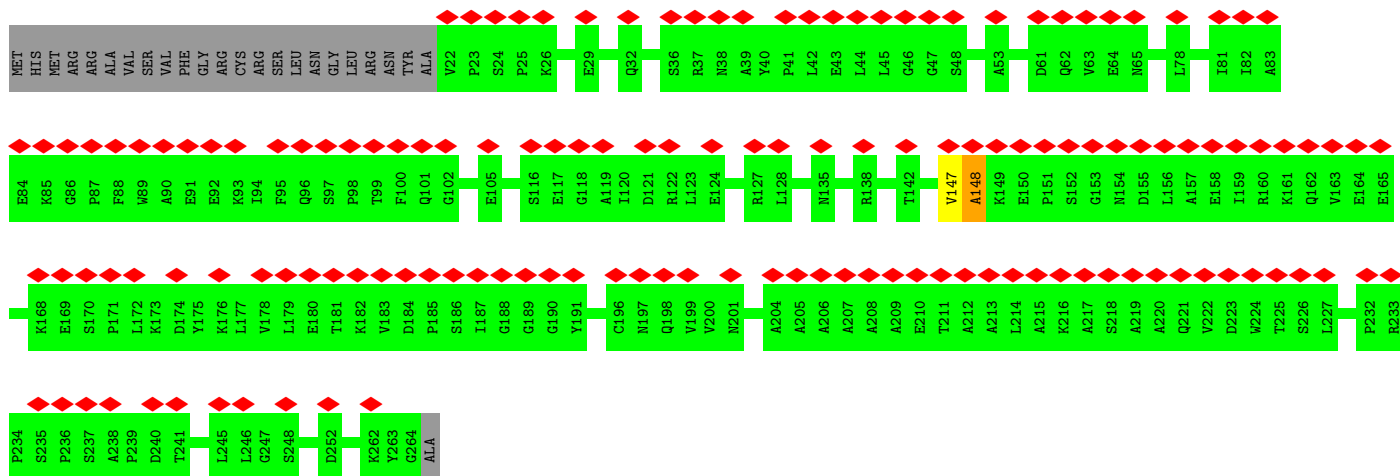
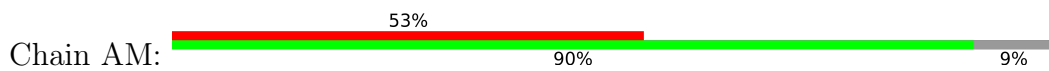


• Molecule 24: p18

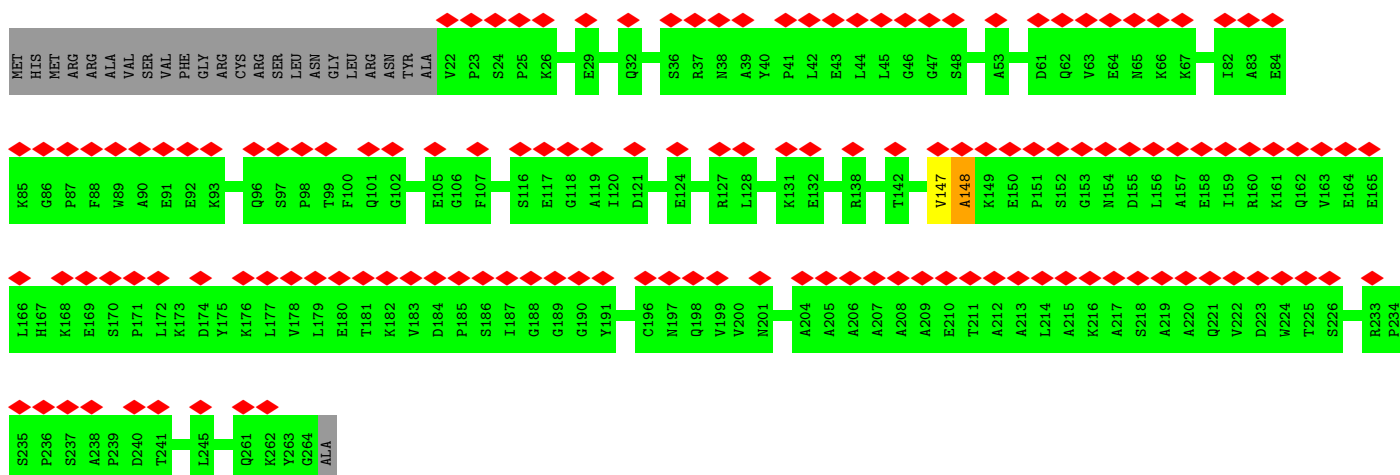
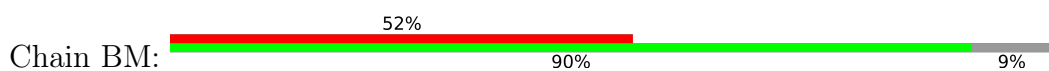




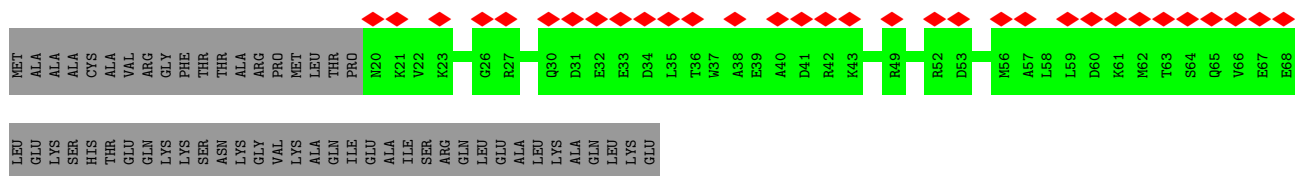
• Molecule 25: oligomycin sensitivity conferring protein (OSCP)



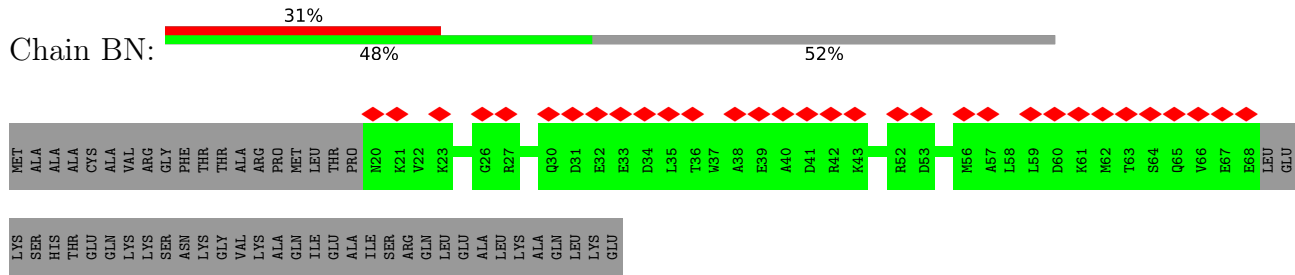
• Molecule 25: oligomycin sensitivity conferring protein (OSCP)



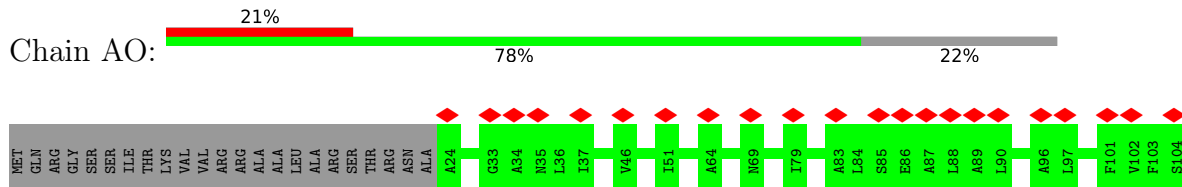
• Molecule 26: inhibitor of F1 (IF1)



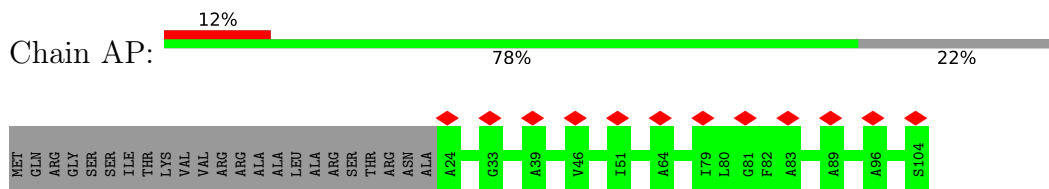
• Molecule 26: inhibitor of F1 (IF1)



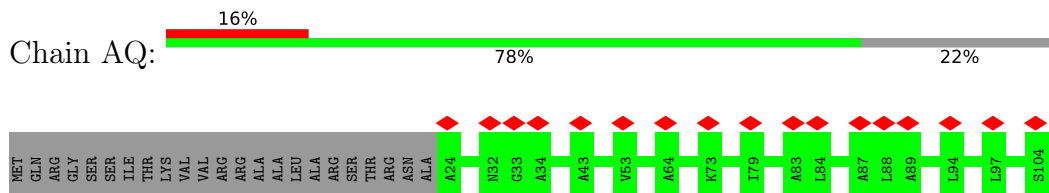
• Molecule 27: ATP synthase subunit c



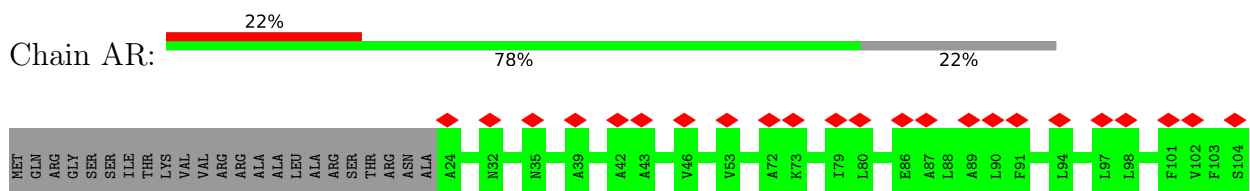
• Molecule 27: ATP synthase subunit c



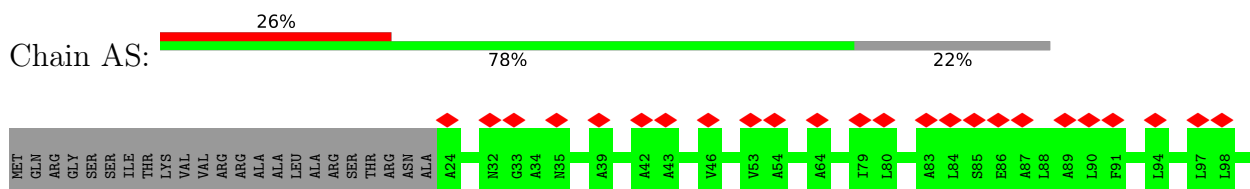
• Molecule 27: ATP synthase subunit c

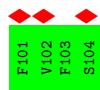


• Molecule 27: ATP synthase subunit c

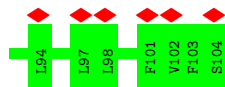
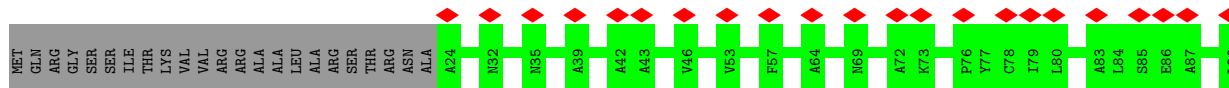
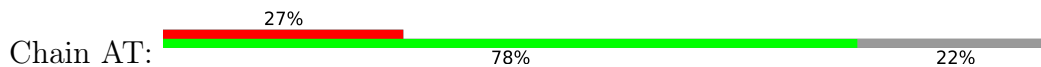


• Molecule 27: ATP synthase subunit c

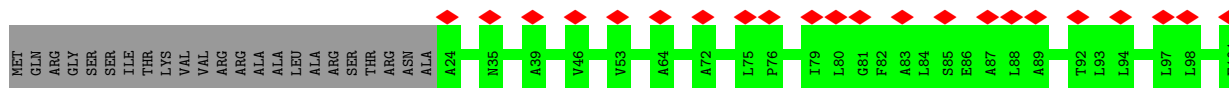
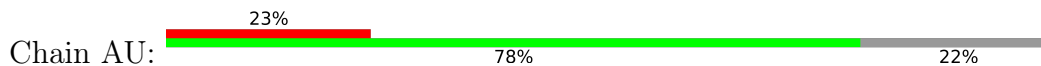




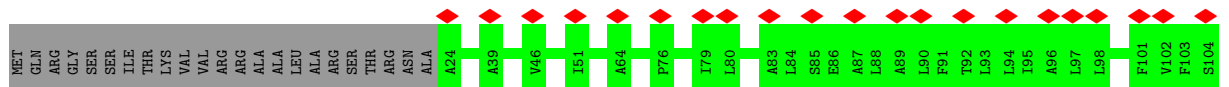
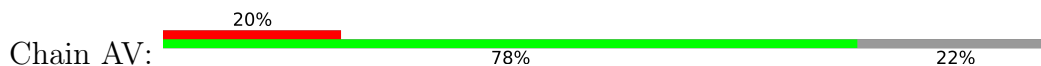
• Molecule 27: ATP synthase subunit c



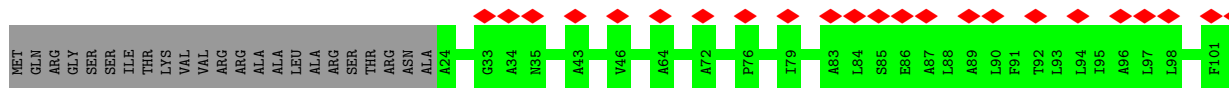
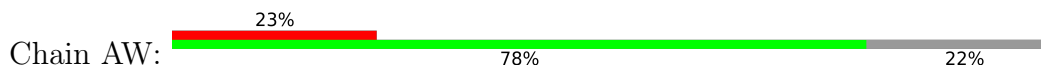
• Molecule 27: ATP synthase subunit c



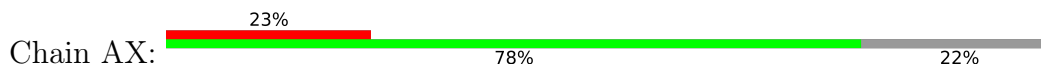
• Molecule 27: ATP synthase subunit c

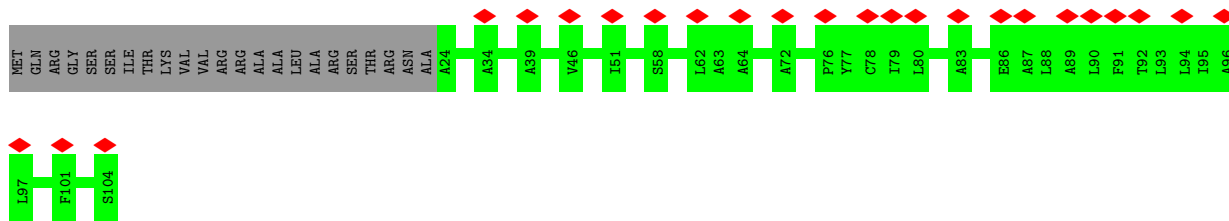


• Molecule 27: ATP synthase subunit c

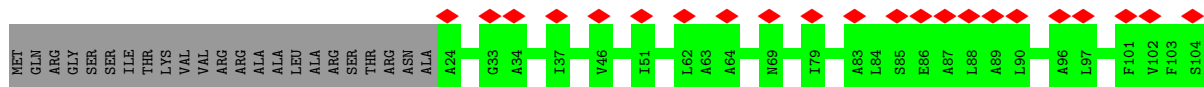
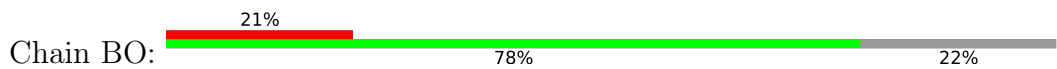


• Molecule 27: ATP synthase subunit c

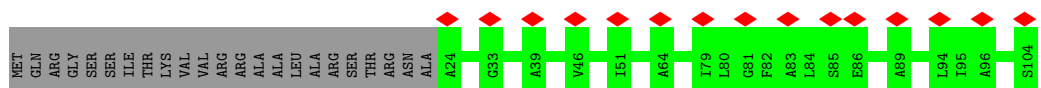
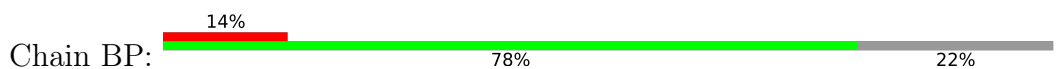




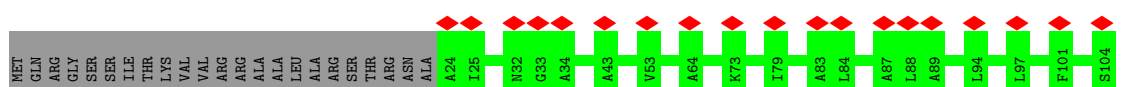
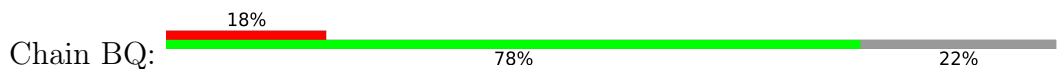
• Molecule 27: ATP synthase subunit c



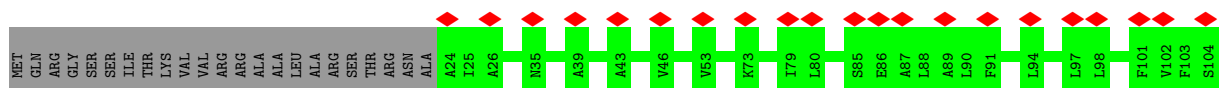
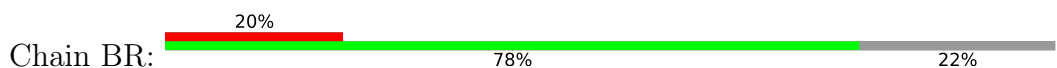
• Molecule 27: ATP synthase subunit c



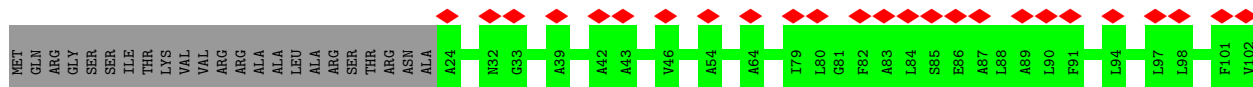
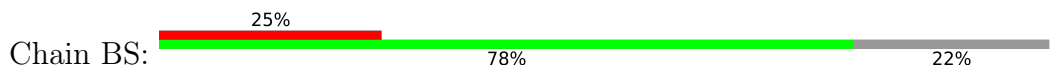
• Molecule 27: ATP synthase subunit c



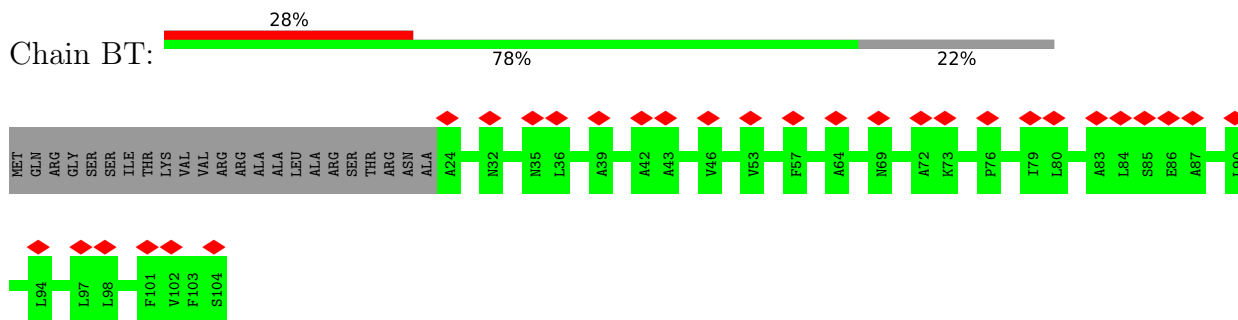
• Molecule 27: ATP synthase subunit c



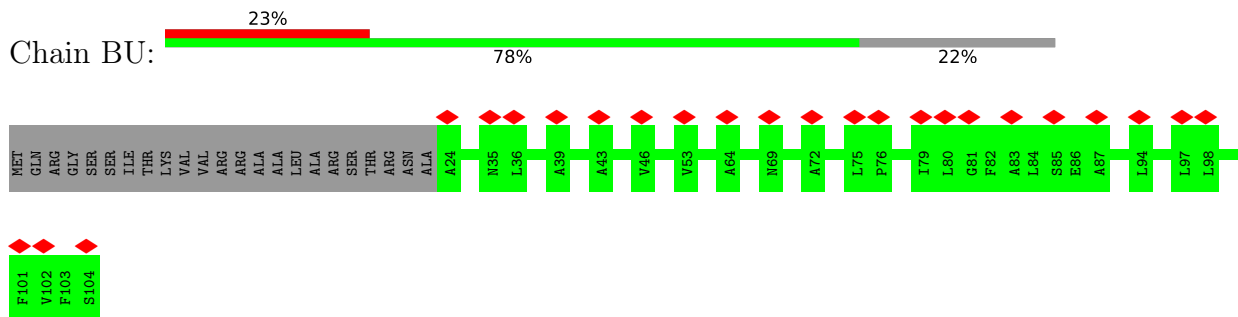
• Molecule 27: ATP synthase subunit c



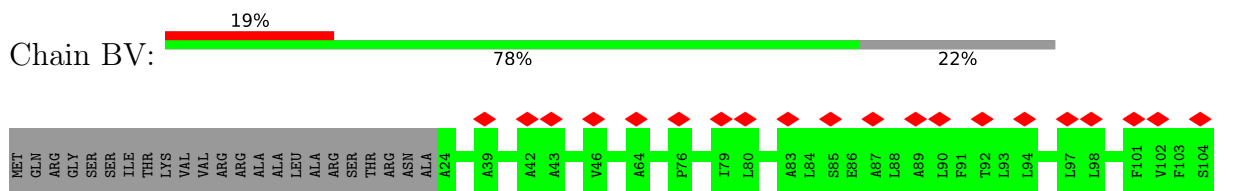
• Molecule 27: ATP synthase subunit c



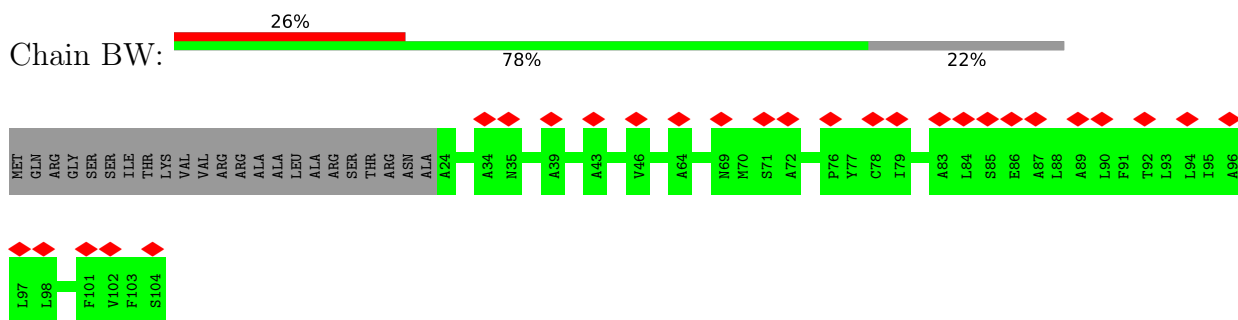
• Molecule 27: ATP synthase subunit c



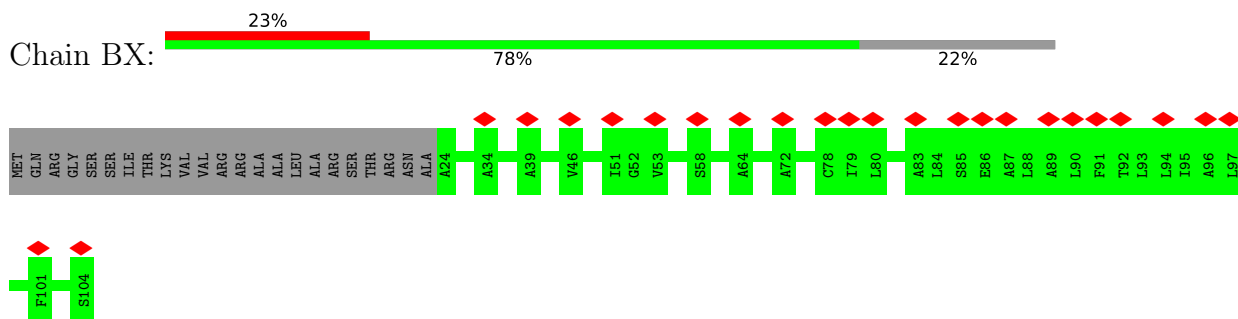
• Molecule 27: ATP synthase subunit c



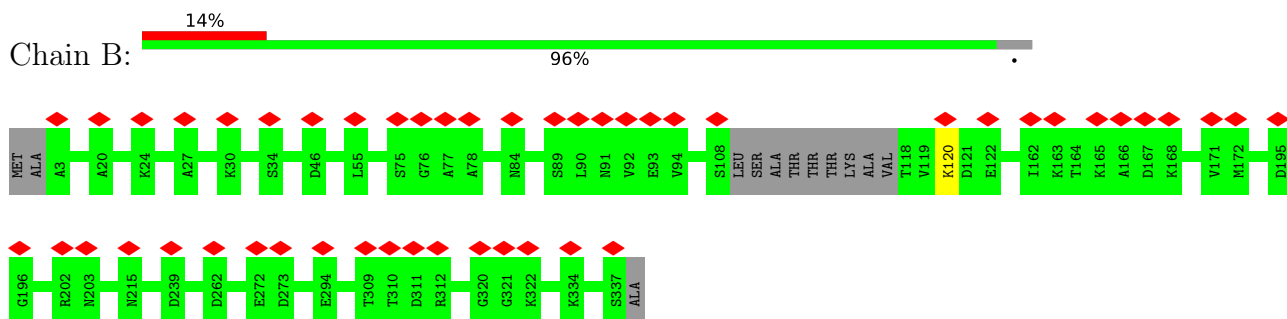
• Molecule 27: ATP synthase subunit c



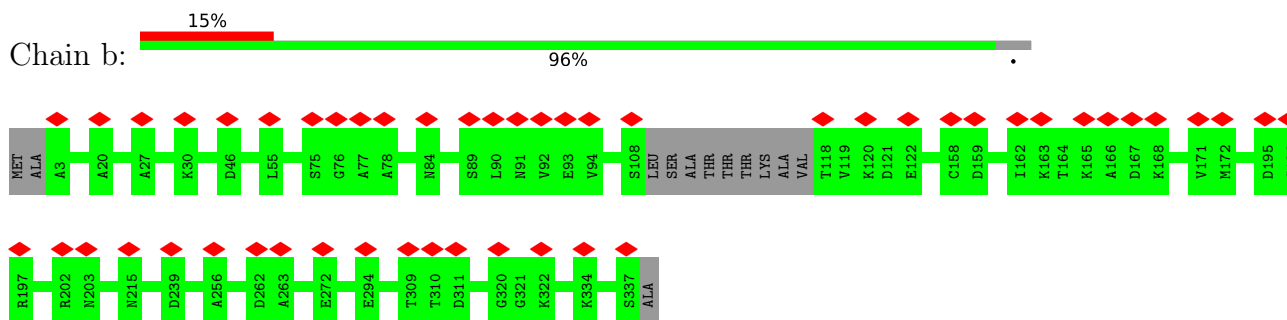
• Molecule 27: ATP synthase subunit c



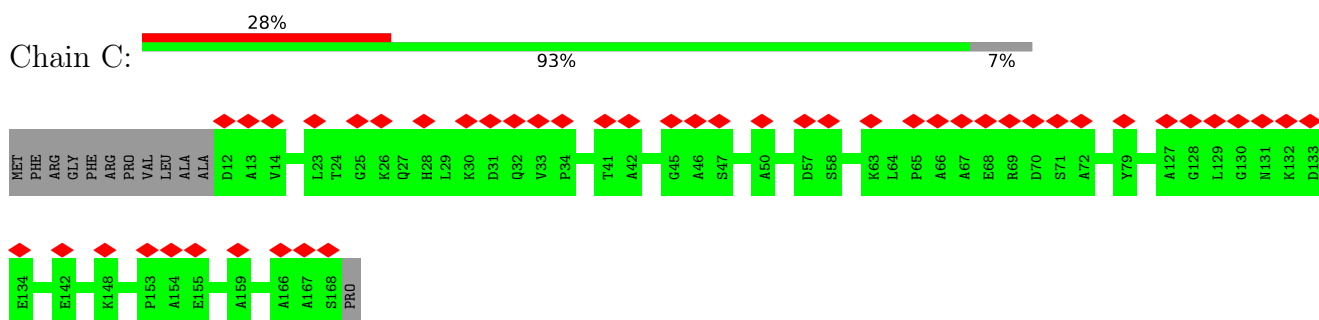
• Molecule 28: ATPTB3



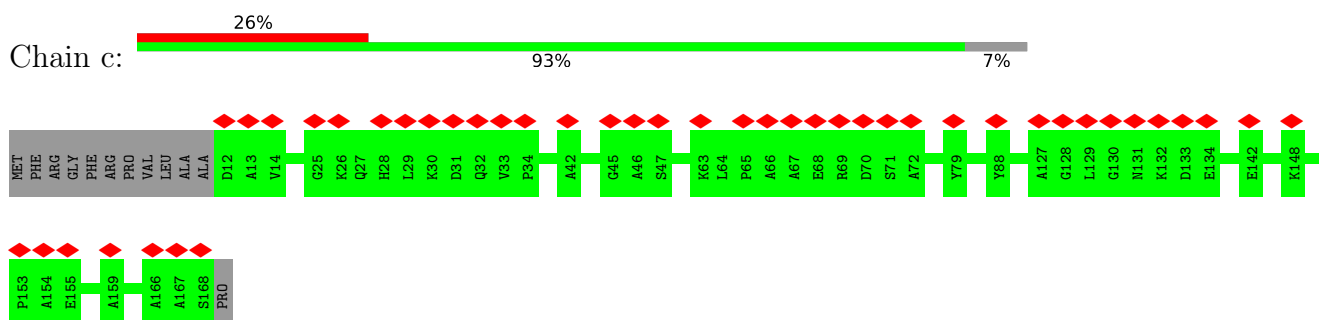
• Molecule 28: ATPTB3



• Molecule 29: ATPTB4



• Molecule 29: ATPTB4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	27232	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	0.129	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	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: CDL, ATP, MG, ADP, TRT, LMT, LPP

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	0.33	0/4047	0.50	0/5500
1	a	0.33	0/4047	0.50	0/5500
2	D	0.30	0/1559	0.53	0/2106
2	d	0.30	0/1559	0.52	0/2106
3	E	0.28	0/821	0.46	0/1100
3	e	0.27	0/821	0.46	0/1100
4	F	0.37	0/2379	0.49	0/3233
4	f	0.37	0/2379	0.48	0/3233
5	G	0.34	0/901	0.55	0/1218
5	g	0.34	0/901	0.56	0/1218
6	H	0.31	0/3755	0.49	0/5132
6	h	0.31	0/3755	0.49	0/5132
7	I	0.32	0/804	0.50	0/1084
7	i	0.32	0/804	0.50	0/1084
8	J	0.33	0/918	0.48	0/1255
8	j	0.32	0/918	0.47	0/1255
9	K	0.28	0/839	0.44	0/1135
9	k	0.28	0/839	0.44	0/1135
10	L	0.39	0/518	0.48	0/711
10	l	0.39	0/518	0.48	0/711
11	M	0.34	0/1399	0.45	0/1895
11	m	0.34	0/1399	0.45	0/1895
12	N	0.33	0/1137	0.48	0/1540
12	n	0.33	0/1137	0.48	0/1540
13	O	0.30	0/881	0.46	0/1193
13	o	0.30	0/881	0.46	0/1193
14	P	0.36	0/955	0.50	0/1292
14	p	0.36	0/955	0.50	0/1292
15	Q	0.27	0/774	0.52	0/1040
15	q	0.27	0/774	0.52	0/1040
16	R	0.28	0/594	0.51	0/798
16	r	0.28	0/594	0.50	0/798

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	S	0.32	0/575	0.48	0/785
17	s	0.32	0/575	0.48	0/785
18	T	0.31	0/543	0.50	0/730
18	t	0.31	0/543	0.49	0/730
19	AA	0.27	0/4164	0.53	1/5635 (0.0%)
19	AB	0.27	0/4164	0.52	0/5635
19	AC	0.27	0/4186	0.53	0/5665
19	BA	0.27	0/4164	0.53	1/5635 (0.0%)
19	BB	0.27	0/4164	0.51	0/5635
19	BC	0.27	0/4186	0.53	0/5665
20	AD	0.28	0/3732	0.54	0/5056
20	AE	0.28	0/3732	0.53	0/5056
20	AF	0.28	0/3732	0.54	0/5056
20	BD	0.28	0/3732	0.54	0/5056
20	BE	0.28	0/3732	0.53	0/5056
20	BF	0.28	0/3732	0.54	0/5056
21	AG	0.27	0/2476	0.52	0/3337
21	BG	0.27	0/2476	0.52	0/3337
22	AH	0.27	0/1270	0.51	0/1720
22	BH	0.27	0/1270	0.51	0/1720
23	AI	0.27	0/549	0.50	0/744
23	BI	0.27	0/549	0.49	0/744
24	AJ	0.26	0/1328	0.44	0/1792
24	AK	0.27	0/1328	0.47	0/1792
24	AL	0.27	0/1328	0.47	0/1792
24	BJ	0.27	0/1328	0.44	0/1792
24	BK	0.27	0/1328	0.47	0/1792
24	BL	0.27	0/1328	0.47	0/1792
25	AM	0.28	0/1933	0.51	0/2623
25	BM	0.28	0/1933	0.51	0/2623
26	AN	0.27	0/408	0.51	0/547
26	BN	0.26	0/408	0.51	0/547
27	AO	0.29	0/590	0.52	0/802
27	AP	0.30	0/590	0.50	0/802
27	AQ	0.30	0/590	0.52	0/802
27	AR	0.29	0/590	0.53	0/802
27	AS	0.27	0/590	0.47	0/802
27	AT	0.28	0/590	0.49	0/802
27	AU	0.27	0/590	0.46	0/802
27	AV	0.27	0/590	0.47	0/802
27	AW	0.27	0/590	0.52	0/802
27	AX	0.27	0/590	0.50	0/802
27	BO	0.29	0/590	0.52	0/802

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BP	0.30	0/590	0.49	0/802
27	BQ	0.30	0/590	0.51	0/802
27	BR	0.28	0/590	0.53	0/802
27	BS	0.27	0/590	0.47	0/802
27	BT	0.28	0/590	0.49	0/802
27	BU	0.27	0/590	0.46	0/802
27	BV	0.27	0/590	0.46	0/802
27	BW	0.27	0/590	0.52	0/802
27	BX	0.27	0/590	0.50	0/802
28	B	0.26	0/2428	0.50	0/3298
28	b	0.27	0/2428	0.50	0/3298
29	C	0.26	0/1253	0.48	0/1691
29	c	0.26	0/1253	0.49	0/1691
All	All	0.29	0/134620	0.51	2/182412 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	AC	0	1
19	BC	0	1
20	AE	0	1
20	AF	0	1
20	BE	0	1
20	BF	0	1
25	AM	0	2
25	BM	0	2
All	All	0	10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BA	117	ILE	C-N-CA	9.65	145.84	121.70
19	AA	117	ILE	C-N-CA	9.61	145.71	121.70

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	AC	284	ASP	Peptide
20	AE	266	ASP	Peptide
20	AF	288	ALA	Peptide
25	AM	147	VAL	Peptide
25	AM	148	ALA	Peptide

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%)	468 (97%)	16 (3%)	0	100	100
1	a	484/487 (99%)	468 (97%)	16 (3%)	0	100	100
2	D	184/187 (98%)	179 (97%)	5 (3%)	0	100	100
2	d	184/187 (98%)	179 (97%)	5 (3%)	0	100	100
3	E	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
3	e	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
4	F	272/274 (99%)	261 (96%)	11 (4%)	0	100	100
4	f	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
5	G	109/112 (97%)	109 (100%)	0	0	100	100
5	g	109/112 (97%)	109 (100%)	0	0	100	100
6	H	458/476 (96%)	447 (98%)	10 (2%)	1 (0%)	47	81
6	h	458/476 (96%)	445 (97%)	10 (2%)	3 (1%)	22	62
7	I	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
7	i	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
8	J	101/104 (97%)	98 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	j	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
9	K	101/113 (89%)	100 (99%)	1 (1%)	0	100	100
9	k	101/113 (89%)	100 (99%)	1 (1%)	0	100	100
10	L	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
10	l	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
11	M	164/169 (97%)	164 (100%)	0	0	100	100
11	m	164/169 (97%)	164 (100%)	0	0	100	100
12	N	129/137 (94%)	128 (99%)	1 (1%)	0	100	100
12	n	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
13	O	98/116 (84%)	94 (96%)	4 (4%)	0	100	100
13	o	98/116 (84%)	94 (96%)	4 (4%)	0	100	100
14	P	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
14	p	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
15	Q	87/90 (97%)	79 (91%)	8 (9%)	0	100	100
15	q	87/90 (97%)	79 (91%)	8 (9%)	0	100	100
16	R	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
16	r	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
17	S	63/74 (85%)	63 (100%)	0	0	100	100
17	s	63/74 (85%)	63 (100%)	0	0	100	100
18	T	64/66 (97%)	64 (100%)	0	0	100	100
18	t	64/66 (97%)	64 (100%)	0	0	100	100
19	AA	522/561 (93%)	502 (96%)	20 (4%)	0	100	100
19	AB	522/561 (93%)	497 (95%)	25 (5%)	0	100	100
19	AC	525/561 (94%)	505 (96%)	20 (4%)	0	100	100
19	BA	522/561 (93%)	501 (96%)	21 (4%)	0	100	100
19	BB	522/561 (93%)	499 (96%)	23 (4%)	0	100	100
19	BC	525/561 (94%)	506 (96%)	19 (4%)	0	100	100
20	AD	485/501 (97%)	468 (96%)	15 (3%)	2 (0%)	34	72
20	AE	485/501 (97%)	459 (95%)	25 (5%)	1 (0%)	47	81
20	AF	485/501 (97%)	467 (96%)	16 (3%)	2 (0%)	34	72
20	BD	485/501 (97%)	466 (96%)	17 (4%)	2 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	BE	485/501 (97%)	460 (95%)	24 (5%)	1 (0%)	47	81
20	BF	485/501 (97%)	467 (96%)	16 (3%)	2 (0%)	34	72
21	AG	301/306 (98%)	294 (98%)	7 (2%)	0	100	100
21	BG	301/306 (98%)	294 (98%)	7 (2%)	0	100	100
22	AH	158/176 (90%)	148 (94%)	10 (6%)	0	100	100
22	BH	158/176 (90%)	147 (93%)	11 (7%)	0	100	100
23	AI	64/76 (84%)	60 (94%)	4 (6%)	0	100	100
23	BI	64/76 (84%)	60 (94%)	4 (6%)	0	100	100
24	AJ	168/192 (88%)	166 (99%)	2 (1%)	0	100	100
24	AK	168/192 (88%)	167 (99%)	1 (1%)	0	100	100
24	AL	168/192 (88%)	165 (98%)	3 (2%)	0	100	100
24	BJ	168/192 (88%)	165 (98%)	3 (2%)	0	100	100
24	BK	168/192 (88%)	167 (99%)	1 (1%)	0	100	100
24	BL	168/192 (88%)	165 (98%)	3 (2%)	0	100	100
25	AM	241/267 (90%)	230 (95%)	10 (4%)	1 (0%)	34	72
25	BM	241/267 (90%)	230 (95%)	10 (4%)	1 (0%)	34	72
26	AN	47/103 (46%)	46 (98%)	1 (2%)	0	100	100
26	BN	47/103 (46%)	46 (98%)	1 (2%)	0	100	100
27	AO	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AP	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AQ	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AR	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	AS	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	AT	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AU	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AV	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	AW	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AX	79/104 (76%)	76 (96%)	3 (4%)	0	100	100
27	BO	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BP	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BQ	79/104 (76%)	78 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BR	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	BS	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	BT	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BU	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BV	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	BW	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BX	79/104 (76%)	76 (96%)	3 (4%)	0	100	100
28	B	322/338 (95%)	297 (92%)	24 (8%)	1 (0%)	41	76
28	b	322/338 (95%)	299 (93%)	23 (7%)	0	100	100
29	C	155/169 (92%)	147 (95%)	8 (5%)	0	100	100
29	c	155/169 (92%)	147 (95%)	8 (5%)	0	100	100
All	All	16686/18184 (92%)	16110 (96%)	559 (3%)	17 (0%)	54	85

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	h	38	THR
20	AD	289	VAL
20	AF	289	VAL
25	AM	148	ALA
28	B	120	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/427 (100%)	426 (100%)	0	100	100
1	a	426/427 (100%)	426 (100%)	0	100	100
2	D	159/160 (99%)	159 (100%)	0	100	100
2	d	159/160 (99%)	159 (100%)	0	100	100
3	E	81/82 (99%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	e	81/82 (99%)	81 (100%)	0	100	100
4	F	259/259 (100%)	259 (100%)	0	100	100
4	f	259/259 (100%)	259 (100%)	0	100	100
5	G	98/99 (99%)	98 (100%)	0	100	100
5	g	98/99 (99%)	98 (100%)	0	100	100
6	H	400/414 (97%)	399 (100%)	1 (0%)	92	95
6	h	400/414 (97%)	399 (100%)	1 (0%)	92	95
7	I	82/83 (99%)	82 (100%)	0	100	100
7	i	82/83 (99%)	82 (100%)	0	100	100
8	J	94/95 (99%)	94 (100%)	0	100	100
8	j	94/95 (99%)	94 (100%)	0	100	100
9	K	89/97 (92%)	89 (100%)	0	100	100
9	k	89/97 (92%)	89 (100%)	0	100	100
10	L	56/56 (100%)	56 (100%)	0	100	100
10	l	56/56 (100%)	56 (100%)	0	100	100
11	M	137/140 (98%)	137 (100%)	0	100	100
11	m	137/140 (98%)	137 (100%)	0	100	100
12	N	114/119 (96%)	114 (100%)	0	100	100
12	n	114/119 (96%)	114 (100%)	0	100	100
13	O	90/103 (87%)	90 (100%)	0	100	100
13	o	90/103 (87%)	90 (100%)	0	100	100
14	P	96/99 (97%)	96 (100%)	0	100	100
14	p	96/99 (97%)	96 (100%)	0	100	100
15	Q	82/83 (99%)	82 (100%)	0	100	100
15	q	82/83 (99%)	82 (100%)	0	100	100
16	R	59/67 (88%)	59 (100%)	0	100	100
16	r	59/67 (88%)	59 (100%)	0	100	100
17	S	59/68 (87%)	59 (100%)	0	100	100
17	s	59/68 (87%)	59 (100%)	0	100	100
18	T	54/54 (100%)	54 (100%)	0	100	100
18	t	54/54 (100%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AA	450/474 (95%)	450 (100%)	0	100	100
19	AB	450/474 (95%)	450 (100%)	0	100	100
19	AC	452/474 (95%)	452 (100%)	0	100	100
19	BA	450/474 (95%)	450 (100%)	0	100	100
19	BB	450/474 (95%)	450 (100%)	0	100	100
19	BC	452/474 (95%)	452 (100%)	0	100	100
20	AD	397/405 (98%)	397 (100%)	0	100	100
20	AE	397/405 (98%)	397 (100%)	0	100	100
20	AF	397/405 (98%)	397 (100%)	0	100	100
20	BD	397/405 (98%)	397 (100%)	0	100	100
20	BE	397/405 (98%)	397 (100%)	0	100	100
20	BF	397/405 (98%)	397 (100%)	0	100	100
21	AG	261/264 (99%)	260 (100%)	1 (0%)	91	94
21	BG	261/264 (99%)	260 (100%)	1 (0%)	91	94
22	AH	131/146 (90%)	131 (100%)	0	100	100
22	BH	131/146 (90%)	131 (100%)	0	100	100
23	AI	58/66 (88%)	58 (100%)	0	100	100
23	BI	58/66 (88%)	58 (100%)	0	100	100
24	AJ	132/151 (87%)	132 (100%)	0	100	100
24	AK	132/151 (87%)	132 (100%)	0	100	100
24	AL	132/151 (87%)	132 (100%)	0	100	100
24	BJ	132/151 (87%)	132 (100%)	0	100	100
24	BK	132/151 (87%)	132 (100%)	0	100	100
24	BL	132/151 (87%)	132 (100%)	0	100	100
25	AM	202/221 (91%)	202 (100%)	0	100	100
25	BM	202/221 (91%)	202 (100%)	0	100	100
26	AN	44/87 (51%)	44 (100%)	0	100	100
26	BN	44/87 (51%)	44 (100%)	0	100	100
27	AO	58/76 (76%)	58 (100%)	0	100	100
27	AP	58/76 (76%)	58 (100%)	0	100	100
27	AQ	58/76 (76%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	AR	58/76 (76%)	58 (100%)	0	100	100
27	AS	58/76 (76%)	58 (100%)	0	100	100
27	AT	58/76 (76%)	58 (100%)	0	100	100
27	AU	58/76 (76%)	58 (100%)	0	100	100
27	AV	58/76 (76%)	58 (100%)	0	100	100
27	AW	58/76 (76%)	58 (100%)	0	100	100
27	AX	58/76 (76%)	58 (100%)	0	100	100
27	BO	58/76 (76%)	58 (100%)	0	100	100
27	BP	58/76 (76%)	58 (100%)	0	100	100
27	BQ	58/76 (76%)	58 (100%)	0	100	100
27	BR	58/76 (76%)	58 (100%)	0	100	100
27	BS	58/76 (76%)	58 (100%)	0	100	100
27	BT	58/76 (76%)	58 (100%)	0	100	100
27	BU	58/76 (76%)	58 (100%)	0	100	100
27	BV	58/76 (76%)	58 (100%)	0	100	100
27	BW	58/76 (76%)	58 (100%)	0	100	100
27	BX	58/76 (76%)	58 (100%)	0	100	100
28	B	251/259 (97%)	251 (100%)	0	100	100
28	b	251/259 (97%)	251 (100%)	0	100	100
29	C	128/137 (93%)	128 (100%)	0	100	100
29	c	128/137 (93%)	128 (100%)	0	100	100
All	All	14058/15070 (93%)	14054 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	H	308	HIS
6	h	308	HIS
21	AG	19	LYS
21	BG	19	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
20	AE	303	GLN
20	BF	426	GLN
20	AF	426	GLN
21	BG	162	ASN
19	BC	356	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 10 are monoatomic - leaving 73 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CDL	a	505	-	84,84,99	0.95	7 (8%)	90,96,111	0.97	4 (4%)
30	CDL	P	202	-	97,97,99	0.89	8 (8%)	103,109,111	0.98	4 (3%)
34	ATP	BB	601	35	26,33,33	0.95	1 (3%)	31,52,52	1.47	4 (12%)
30	CDL	A	501	-	80,80,99	0.96	7 (8%)	86,92,111	1.08	5 (5%)
30	CDL	d	201	-	90,90,99	0.92	7 (7%)	96,102,111	1.02	4 (4%)
30	CDL	M	204	-	76,76,99	0.99	8 (10%)	82,88,111	1.11	4 (4%)
31	LMT	D	202	-	36,36,36	1.17	6 (16%)	47,47,47	0.92	0
31	LMT	d	202	-	36,36,36	1.16	6 (16%)	47,47,47	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	TRT	N	202	-	25,25,25	0.60	0	33,33,33	1.00	1 (3%)
30	CDL	m	201	-	76,76,99	1.00	8 (10%)	82,88,111	1.09	4 (4%)
31	LMT	F	302	-	36,36,36	1.15	5 (13%)	47,47,47	0.92	2 (4%)
33	TRT	BE	600	-	25,25,25	0.66	1 (4%)	33,33,33	1.04	1 (3%)
30	CDL	P	201	-	47,47,99	1.24	8 (17%)	53,59,111	1.30	5 (9%)
34	ATP	BA	601	35	26,33,33	0.93	1 (3%)	31,52,52	1.54	4 (12%)
31	LMT	g	201	-	36,36,36	1.15	5 (13%)	47,47,47	0.93	2 (4%)
31	LMT	n	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.94	2 (4%)
32	LPP	k	201	-	30,30,43	1.26	3 (10%)	34,35,48	1.18	2 (5%)
30	CDL	D	201	-	90,90,99	0.92	7 (7%)	96,102,111	1.02	4 (4%)
32	LPP	f	301	-	23,23,43	1.38	3 (13%)	27,28,48	1.12	2 (7%)
30	CDL	O	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.07	4 (5%)
33	TRT	N	201	-	25,25,25	0.51	0	33,33,33	1.05	3 (9%)
32	LPP	O	203	-	31,31,43	1.26	4 (12%)	35,36,48	1.01	2 (5%)
33	TRT	m	203	-	25,25,25	0.55	0	33,33,33	0.93	2 (6%)
33	TRT	P	203	-	25,25,25	1.23	3 (12%)	33,33,33	4.76	9 (27%)
30	CDL	A	504	-	62,62,99	1.10	7 (11%)	68,74,111	1.19	4 (5%)
34	ATP	AB	601	35	26,33,33	0.95	1 (3%)	31,52,52	1.47	4 (12%)
30	CDL	A	502	-	80,80,99	0.97	7 (8%)	86,92,111	1.12	4 (4%)
30	CDL	A	505	-	84,84,99	0.96	8 (9%)	90,96,111	0.98	4 (4%)
33	TRT	m	202	-	25,25,25	0.58	0	33,33,33	0.69	0
32	LPP	O	202	-	22,22,43	1.42	4 (18%)	26,27,48	1.21	2 (7%)
33	TRT	n	204	-	25,25,25	0.59	0	33,33,33	1.04	1 (3%)
30	CDL	e	101	-	62,62,99	1.09	8 (12%)	68,74,111	1.13	4 (5%)
33	TRT	M	202	-	25,25,25	0.58	0	33,33,33	0.69	0
36	ADP	AD	601	35	24,29,29	0.91	1 (4%)	29,45,45	1.73	6 (20%)
30	CDL	M	205	-	52,52,99	1.20	8 (15%)	58,64,111	1.24	4 (6%)
30	CDL	r	101	-	75,75,99	1.00	8 (10%)	81,87,111	1.14	4 (4%)
33	TRT	g	202	-	25,25,25	0.51	0	33,33,33	0.82	1 (3%)
34	ATP	AC	601	35	26,33,33	0.92	1 (3%)	31,52,52	1.50	4 (12%)
32	LPP	n	201	-	25,25,43	1.35	3 (12%)	29,30,48	1.24	2 (6%)
30	CDL	R	101	-	75,75,99	1.00	8 (10%)	81,87,111	1.14	4 (4%)
32	LPP	K	201	-	30,30,43	1.26	3 (10%)	34,35,48	1.18	2 (5%)
33	TRT	M	203	-	25,25,25	0.55	0	33,33,33	0.95	2 (6%)
33	TRT	G	202	-	25,25,25	0.60	0	33,33,33	0.82	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ATP	BC	601	35	26,33,33	0.93	1 (3%)	31,52,52	1.50	4 (12%)
30	CDL	a	504	-	62,62,99	1.10	7 (11%)	68,74,111	1.19	4 (5%)
32	LPP	I	101	-	43,43,43	1.13	3 (6%)	47,48,48	1.00	2 (4%)
30	CDL	a	502	-	80,80,99	0.97	8 (10%)	86,92,111	1.12	4 (4%)
33	TRT	AR	201	-	25,25,25	0.54	0	33,33,33	0.93	2 (6%)
31	LMT	Q	101	-	36,36,36	1.18	5 (13%)	47,47,47	1.02	3 (6%)
33	TRT	AE	600	-	25,25,25	0.66	1 (4%)	33,33,33	1.04	1 (3%)
36	ADP	BD	601	35	24,29,29	0.90	1 (4%)	29,45,45	1.75	6 (20%)
32	LPP	o	203	-	31,31,43	1.26	4 (12%)	35,36,48	0.99	2 (5%)
33	TRT	g	203	-	25,25,25	0.60	0	33,33,33	0.82	1 (3%)
32	LPP	N	203	-	25,25,43	1.34	3 (12%)	29,30,48	1.24	2 (6%)
30	CDL	A	503	-	80,80,99	0.96	8 (10%)	85,91,111	1.06	4 (4%)
30	CDL	a	501	-	80,80,99	0.96	7 (8%)	86,92,111	1.09	5 (5%)
30	CDL	a	503	-	80,80,99	0.97	8 (10%)	85,91,111	1.07	4 (4%)
33	TRT	p	202	-	25,25,25	1.21	3 (12%)	33,33,33	4.78	9 (27%)
32	LPP	i	101	-	43,43,43	1.13	3 (6%)	47,48,48	1.00	2 (4%)
34	ATP	AA	601	35	26,33,33	0.93	1 (3%)	31,52,52	1.54	4 (12%)
32	LPP	F	301	-	23,23,43	1.38	3 (13%)	27,28,48	1.13	2 (7%)
30	CDL	E	101	-	62,62,99	1.09	8 (12%)	68,74,111	1.12	4 (5%)
30	CDL	o	201	-	64,64,99	1.08	7 (10%)	70,76,111	1.09	4 (5%)
31	LMT	q	101	-	36,36,36	1.17	5 (13%)	47,47,47	1.00	2 (4%)
33	TRT	n	203	-	25,25,25	0.51	0	33,33,33	1.06	3 (9%)
30	CDL	p	201	-	47,47,99	1.24	8 (17%)	53,59,111	1.30	5 (9%)
33	TRT	G	201	-	25,25,25	0.51	0	33,33,33	0.82	1 (3%)
34	ATP	BF	601	35	26,33,33	0.96	1 (3%)	31,52,52	1.73	5 (16%)
34	ATP	AF	601	35	26,33,33	0.95	1 (3%)	31,52,52	1.71	4 (12%)
31	LMT	N	204	-	36,36,36	1.24	6 (16%)	47,47,47	0.96	2 (4%)
32	LPP	o	202	-	22,22,43	1.42	4 (18%)	26,27,48	1.23	2 (7%)
30	CDL	M	201	-	52,52,99	1.20	8 (15%)	58,64,111	1.26	4 (6%)
33	TRT	BR	201	-	25,25,25	0.54	0	33,33,33	0.94	2 (6%)

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
30	CDL	a	505	-	-	43/95/95/110	-
30	CDL	P	202	-	-	44/108/108/110	-
34	ATP	BB	601	35	-	2/18/38/38	0/3/3/3
30	CDL	A	501	-	-	26/91/91/110	-
30	CDL	d	201	-	-	39/101/101/110	-
30	CDL	M	204	-	-	39/87/87/110	-
31	LMT	D	202	-	-	9/21/61/61	0/2/2/2
31	LMT	d	202	-	-	9/21/61/61	0/2/2/2
33	TRT	N	202	-	-	15/23/23/23	0/1/1/1
30	CDL	m	201	-	-	39/87/87/110	-
31	LMT	F	302	-	-	9/21/61/61	0/2/2/2
33	TRT	BE	600	-	-	9/23/23/23	0/1/1/1
30	CDL	P	201	-	-	27/57/57/110	-
34	ATP	BA	601	35	-	0/18/38/38	0/3/3/3
31	LMT	g	201	-	-	10/21/61/61	0/2/2/2
31	LMT	n	202	-	-	10/21/61/61	0/2/2/2
32	LPP	k	201	-	-	13/32/32/45	-
30	CDL	D	201	-	-	39/101/101/110	-
32	LPP	f	301	-	-	8/25/25/45	-
30	CDL	O	201	-	-	36/75/75/110	-
33	TRT	N	201	-	-	9/23/23/23	0/1/1/1
32	LPP	O	203	-	-	8/33/33/45	-
33	TRT	m	203	-	-	9/23/23/23	0/1/1/1
33	TRT	P	203	-	-	15/23/23/23	0/1/1/1
30	CDL	A	504	-	-	28/73/73/110	-
34	ATP	AB	601	35	-	2/18/38/38	0/3/3/3
30	CDL	A	502	-	-	30/91/91/110	-
30	CDL	A	505	-	-	42/95/95/110	-
33	TRT	m	202	-	-	12/23/23/23	0/1/1/1
32	LPP	O	202	-	-	9/24/24/45	-
33	TRT	n	204	-	-	15/23/23/23	0/1/1/1
30	CDL	e	101	-	-	40/73/73/110	-
33	TRT	M	202	-	-	12/23/23/23	0/1/1/1
36	ADP	AD	601	35	-	0/12/32/32	0/3/3/3
30	CDL	M	205	-	-	30/63/63/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CDL	r	101	-	-	36/86/86/110	-
33	TRT	g	202	-	-	7/23/23/23	0/1/1/1
34	ATP	AC	601	35	-	2/18/38/38	0/3/3/3
32	LPP	n	201	-	-	15/27/27/45	-
30	CDL	R	101	-	-	36/86/86/110	-
32	LPP	K	201	-	-	13/32/32/45	-
33	TRT	M	203	-	-	9/23/23/23	0/1/1/1
33	TRT	G	202	-	-	15/23/23/23	0/1/1/1
34	ATP	BC	601	35	-	2/18/38/38	0/3/3/3
30	CDL	a	504	-	-	28/73/73/110	-
32	LPP	I	101	-	-	14/45/45/45	-
30	CDL	a	502	-	-	28/91/91/110	-
33	TRT	AR	201	-	-	10/23/23/23	0/1/1/1
31	LMT	Q	101	-	-	7/21/61/61	0/2/2/2
33	TRT	AE	600	-	-	9/23/23/23	0/1/1/1
36	ADP	BD	601	35	-	0/12/32/32	0/3/3/3
32	LPP	o	203	-	-	8/33/33/45	-
33	TRT	g	203	-	-	15/23/23/23	0/1/1/1
32	LPP	N	203	-	-	15/27/27/45	-
30	CDL	A	503	-	-	32/89/89/110	-
30	CDL	a	501	-	-	27/91/91/110	-
30	CDL	a	503	-	-	32/89/89/110	-
33	TRT	p	202	-	-	15/23/23/23	0/1/1/1
32	LPP	i	101	-	-	14/45/45/45	-
34	ATP	AA	601	35	-	0/18/38/38	0/3/3/3
32	LPP	F	301	-	-	8/25/25/45	-
30	CDL	E	101	-	-	38/73/73/110	-
30	CDL	o	201	-	-	38/75/75/110	-
31	LMT	q	101	-	-	7/21/61/61	0/2/2/2
33	TRT	n	203	-	-	9/23/23/23	0/1/1/1
30	CDL	p	201	-	-	29/57/57/110	-
33	TRT	G	201	-	-	7/23/23/23	0/1/1/1
34	ATP	BF	601	35	-	3/18/38/38	0/3/3/3
34	ATP	AF	601	35	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	N	204	-	-	10/21/61/61	0/2/2/2
32	LPP	o	202	-	-	7/24/24/45	-
30	CDL	M	201	-	-	30/63/63/110	-
33	TRT	BR	201	-	-	11/23/23/23	0/1/1/1

The worst 5 of 293 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	P	203	TRT	C6-C9	3.97	1.59	1.53
33	p	202	TRT	C6-C9	3.84	1.59	1.53
32	i	101	LPP	O9-C11	3.45	1.44	1.34
32	I	101	LPP	O9-C11	3.41	1.43	1.34
32	O	202	LPP	O9-C11	3.35	1.43	1.34

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
33	P	203	TRT	C7-C6-C8	15.69	150.20	107.28
33	p	202	TRT	C7-C6-C8	15.11	148.64	107.28
33	p	202	TRT	C5-C6-C9	14.29	143.47	111.93
33	P	203	TRT	C5-C6-C9	13.37	141.46	111.93
33	P	203	TRT	C8-C6-C9	-11.41	81.58	110.20

There are no chirality outliers.

5 of 1276 torsion outliers are listed below:

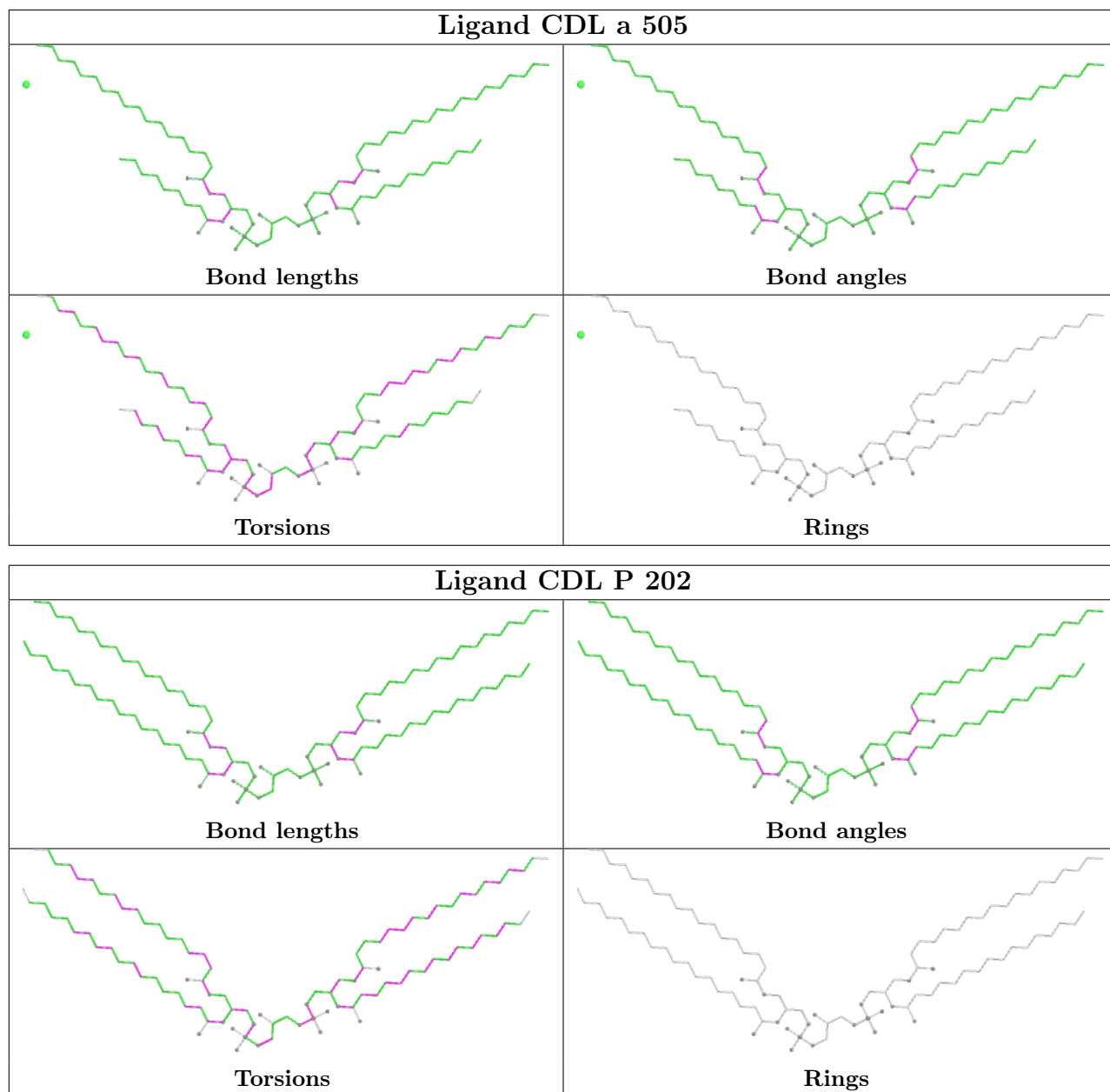
Mol	Chain	Res	Type	Atoms
30	A	501	CDL	CB2-OB2-PB2-OB3
30	A	501	CDL	C51-CB5-OB6-CB4
30	A	502	CDL	CB2-OB2-PB2-OB3
30	A	502	CDL	CB3-OB5-PB2-OB3
30	A	502	CDL	OB7-CB5-OB6-CB4

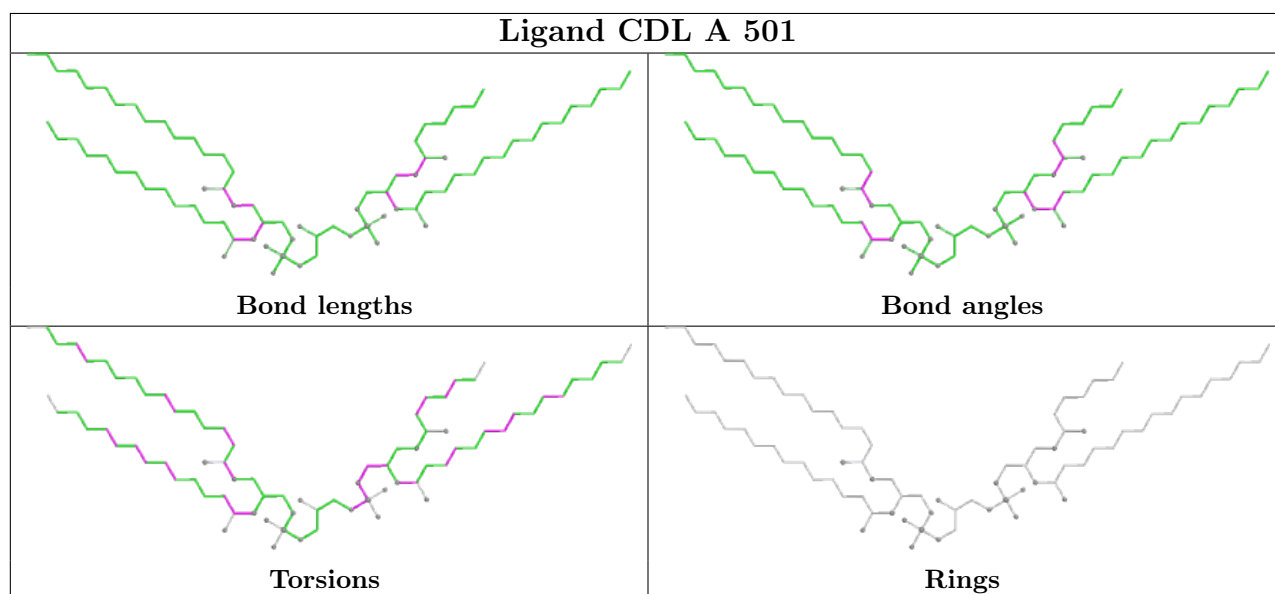
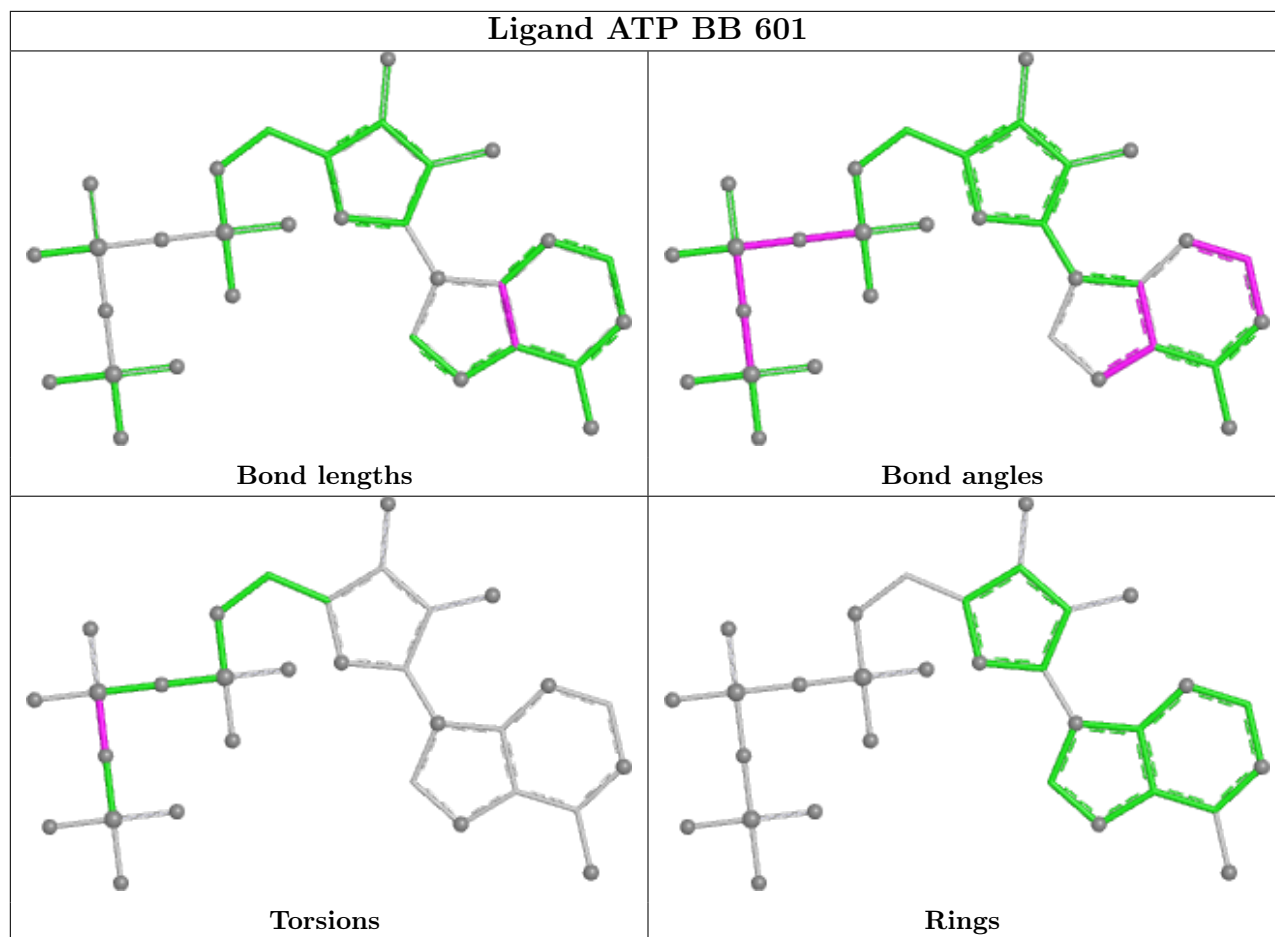
There are no ring outliers.

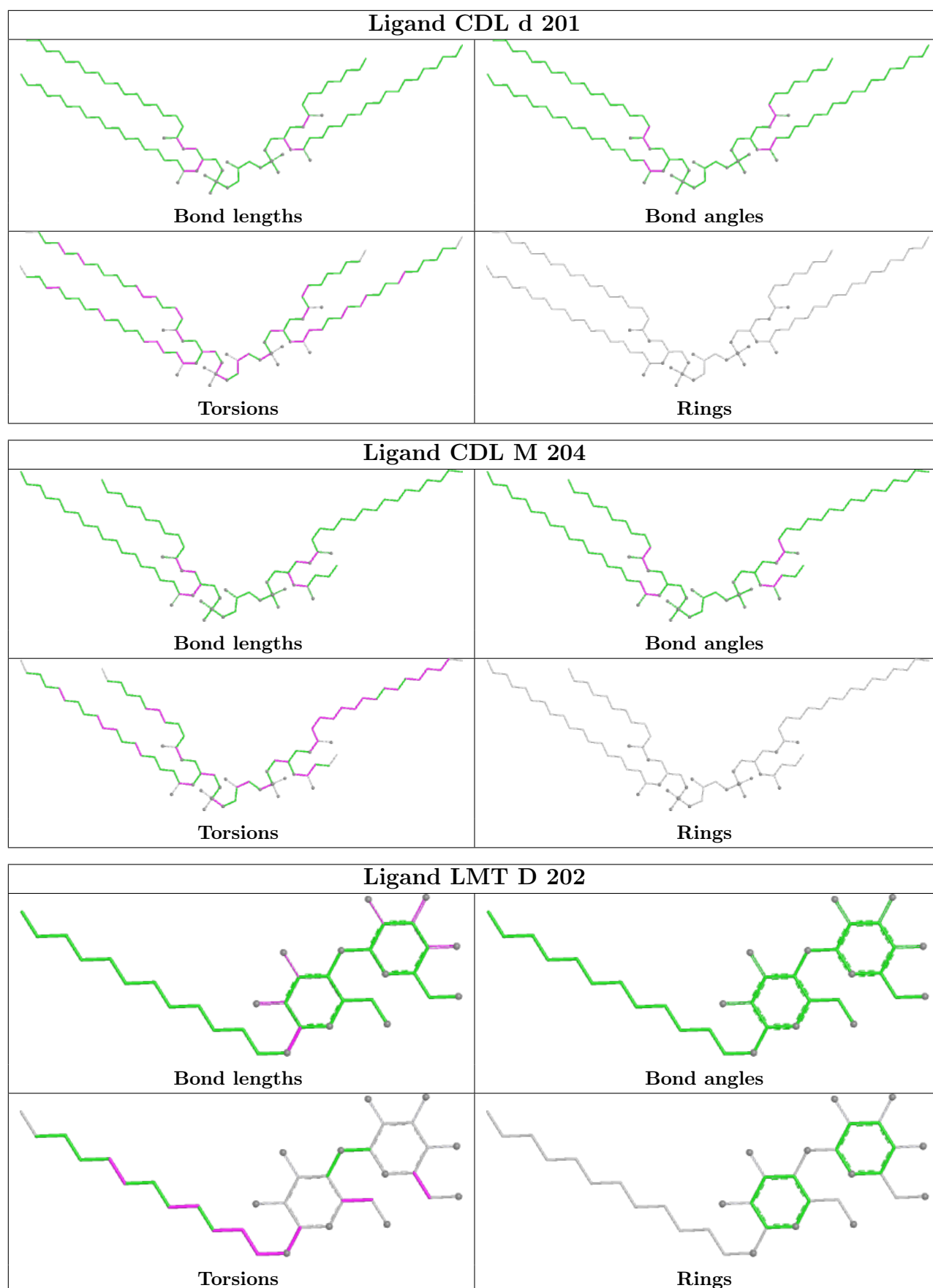
No monomer is involved in short contacts.

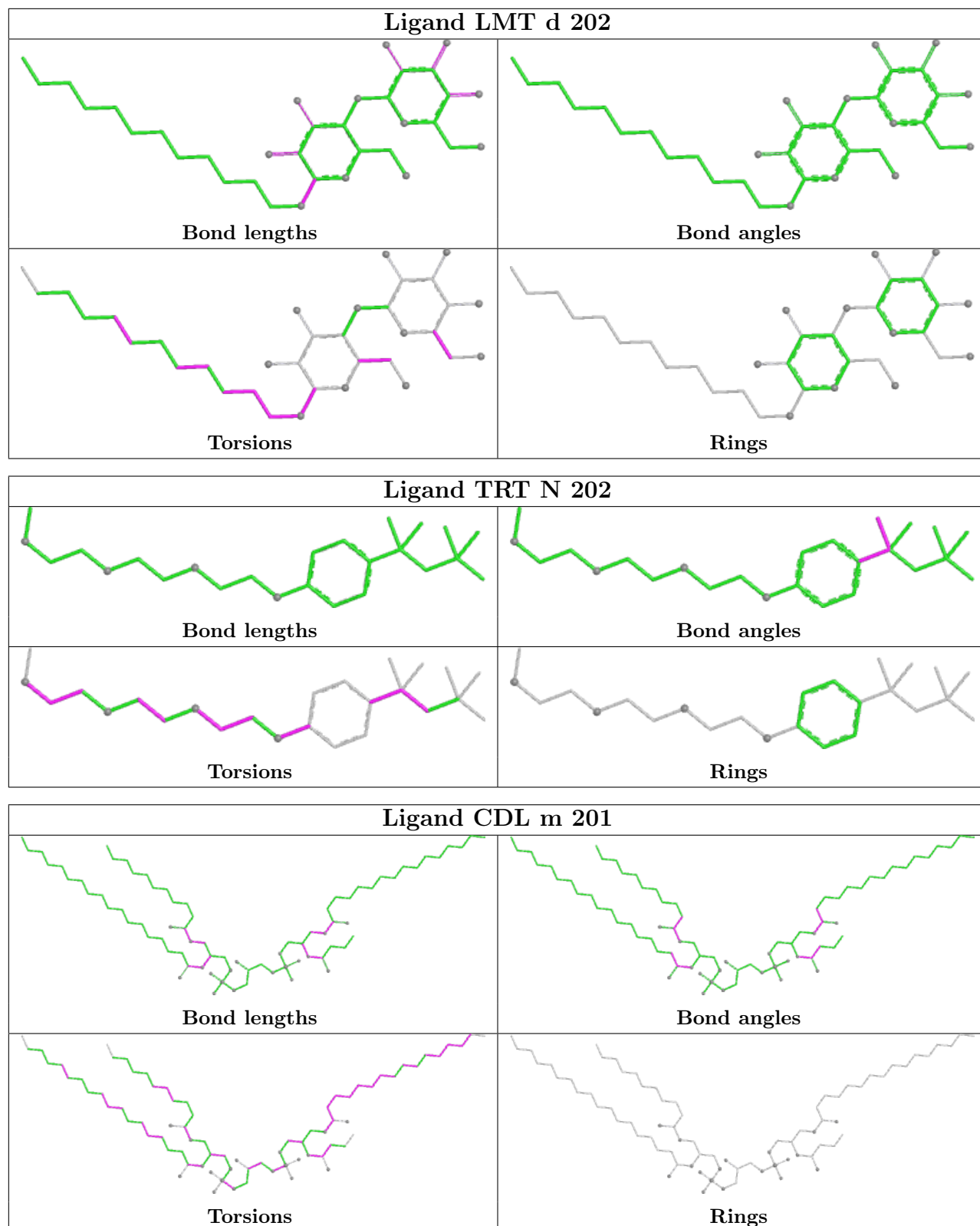
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

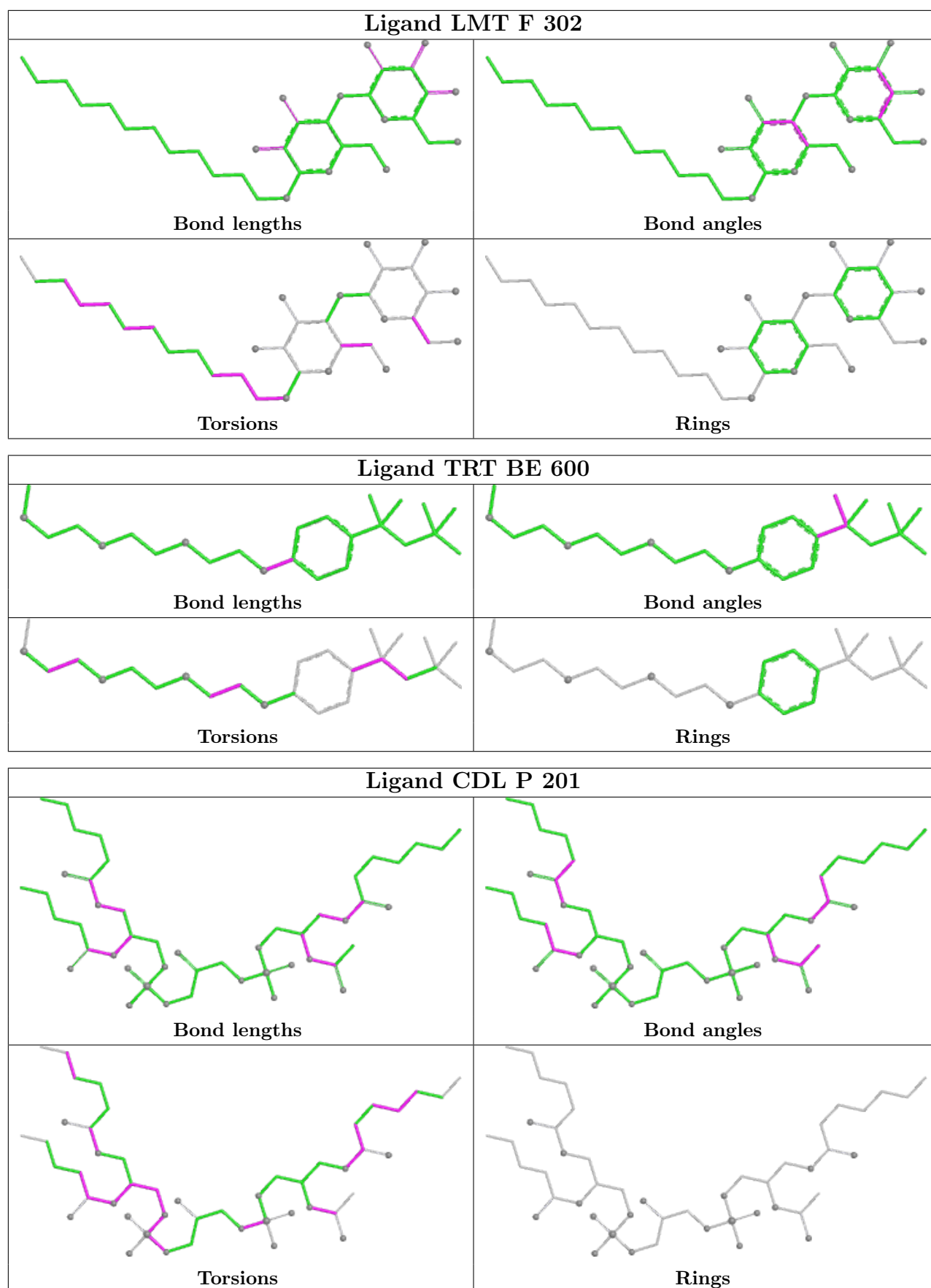
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

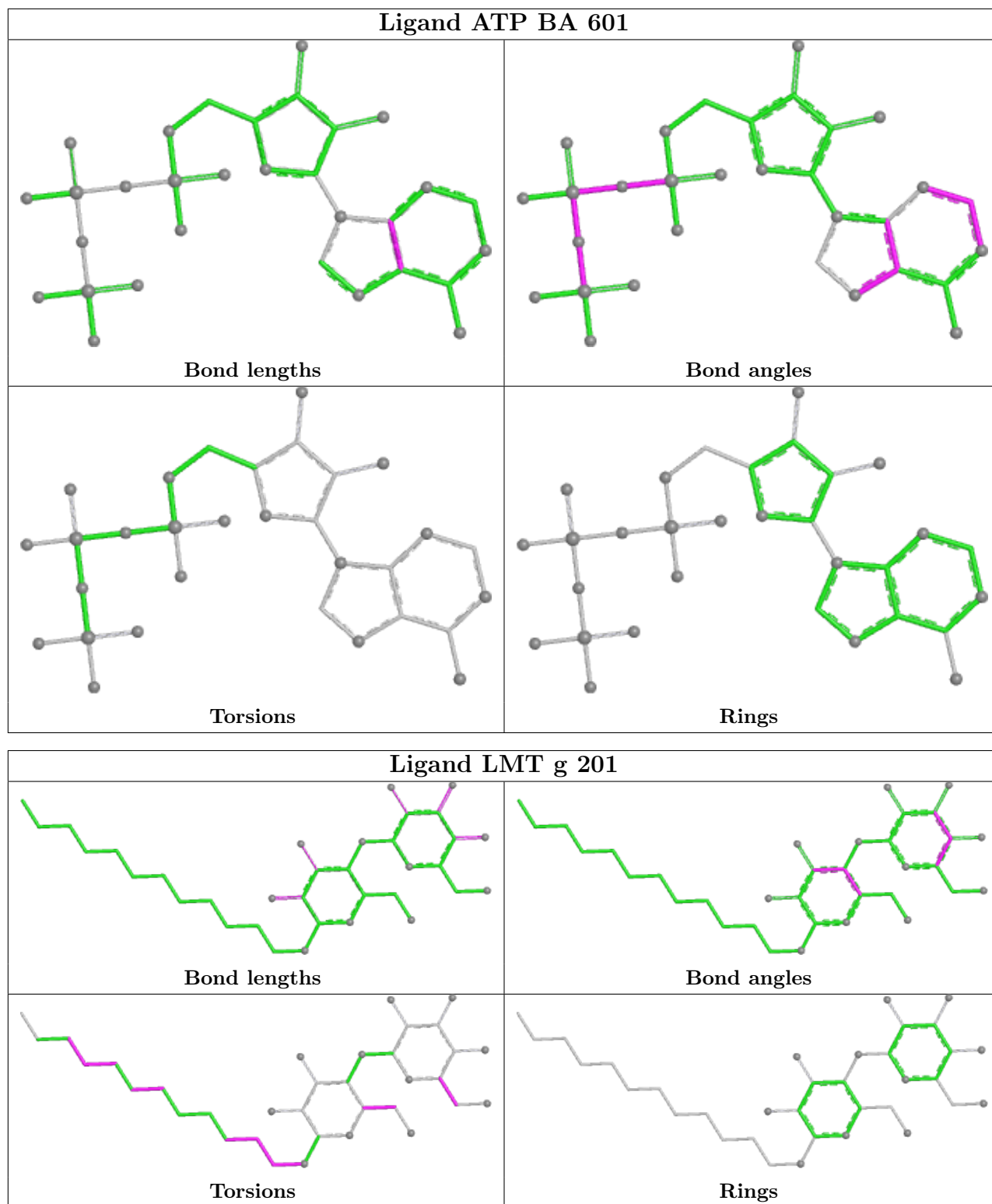


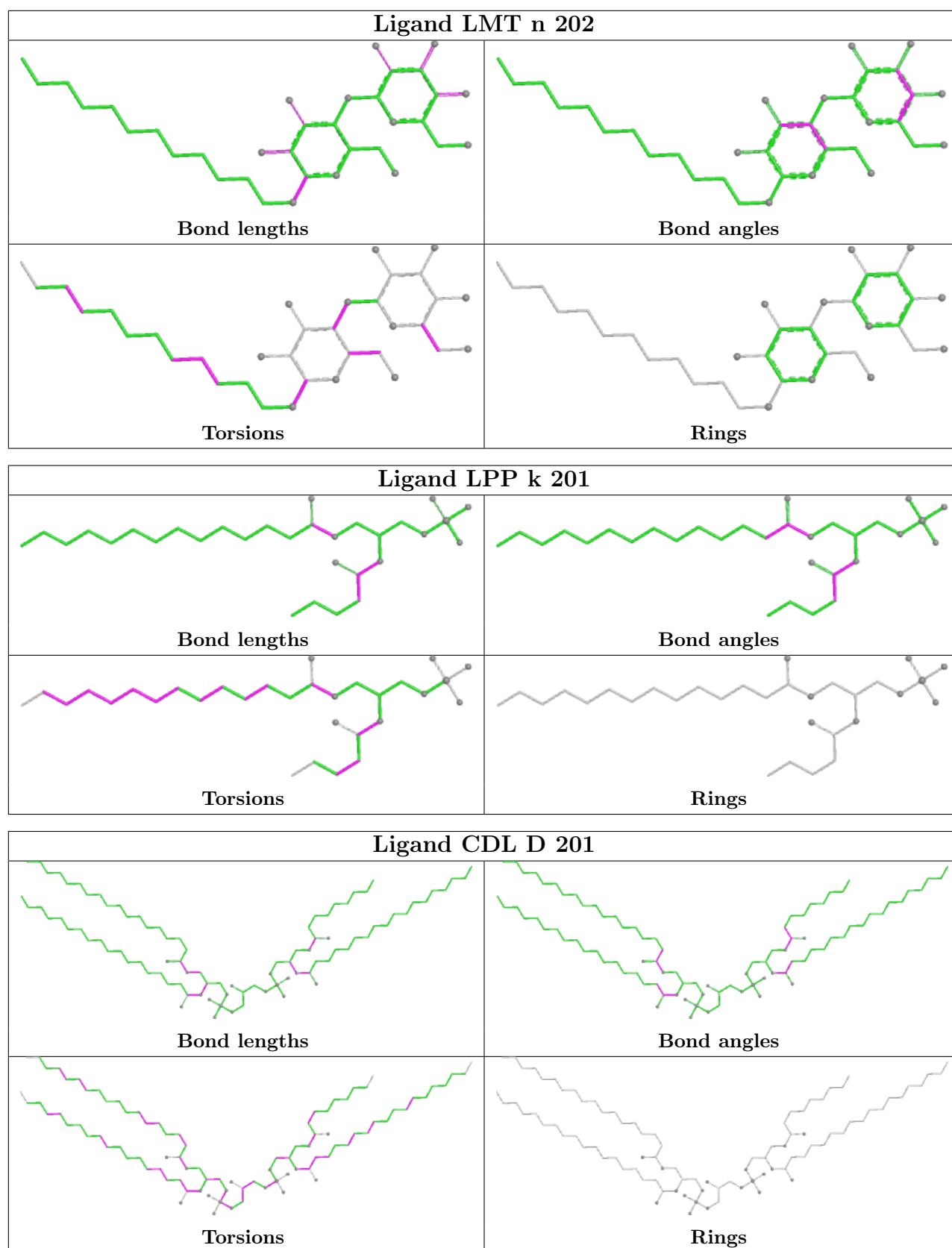


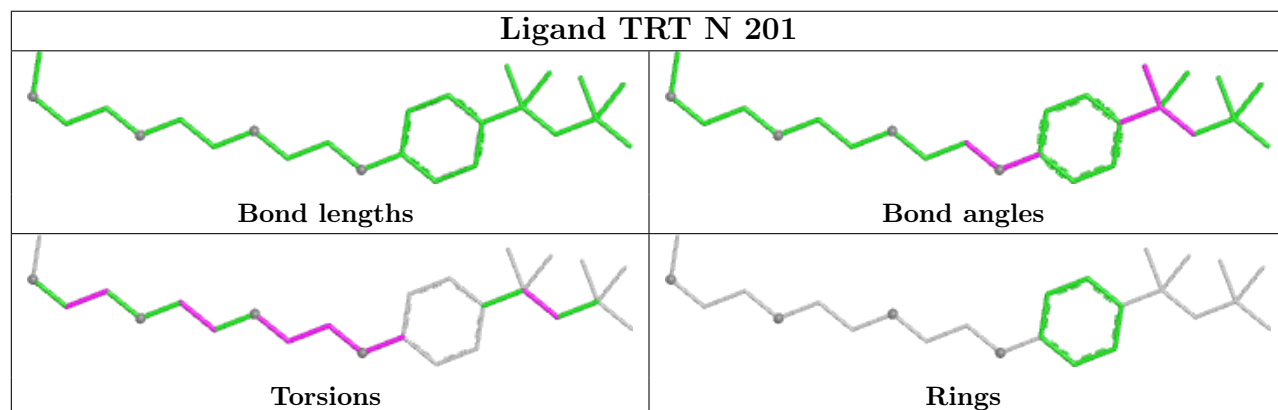
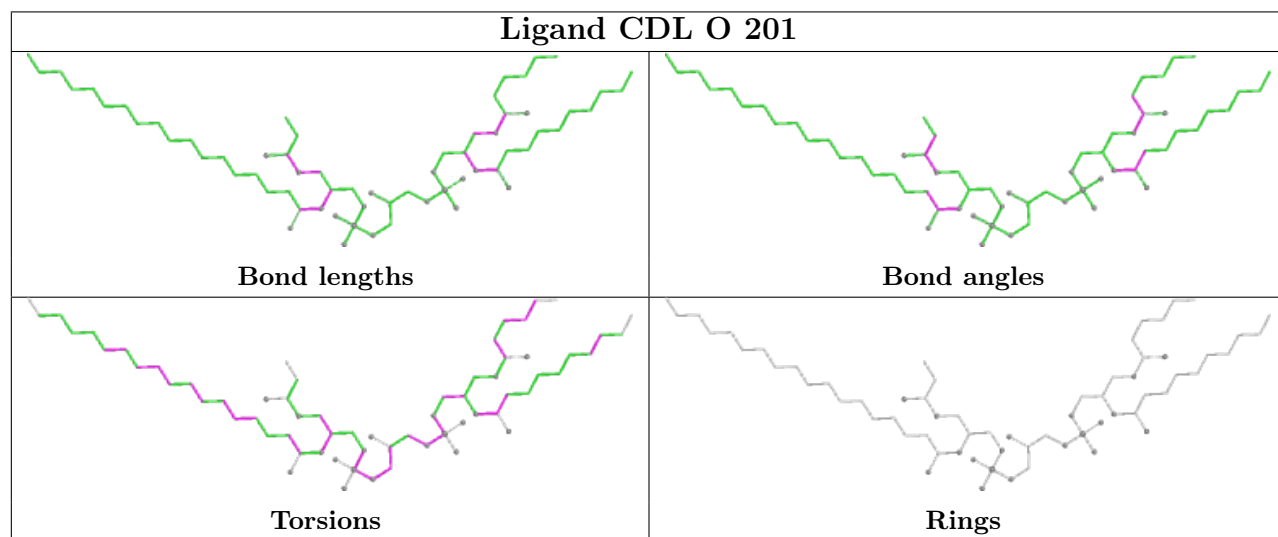
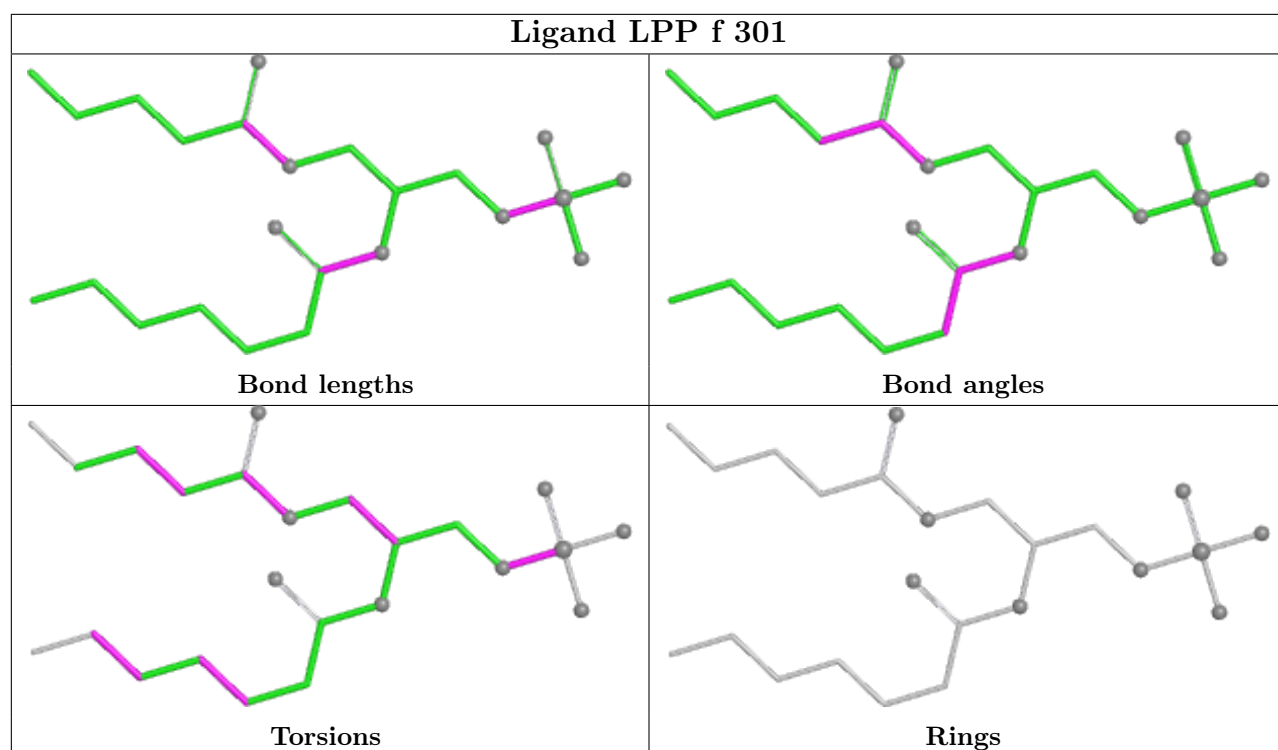


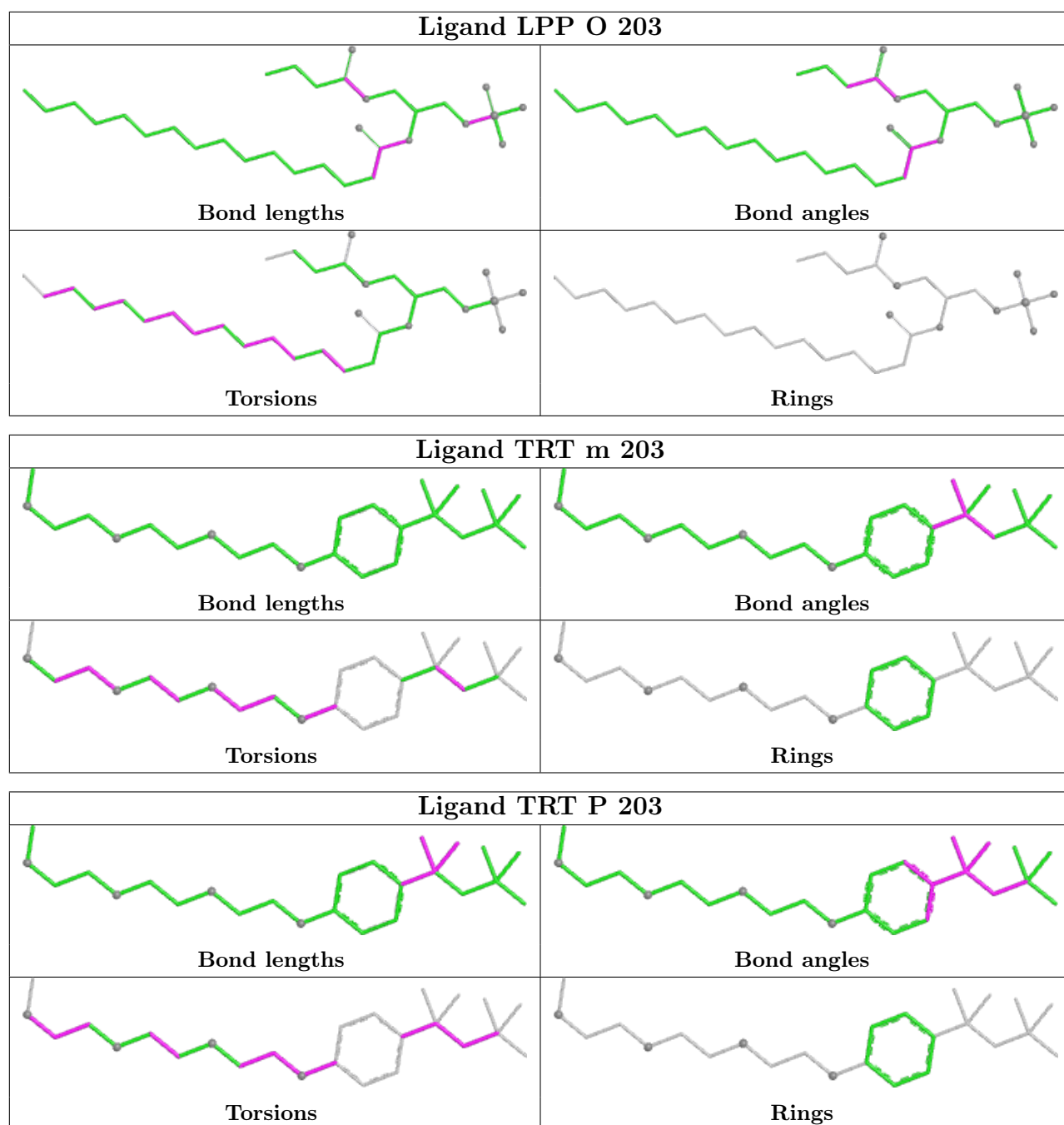


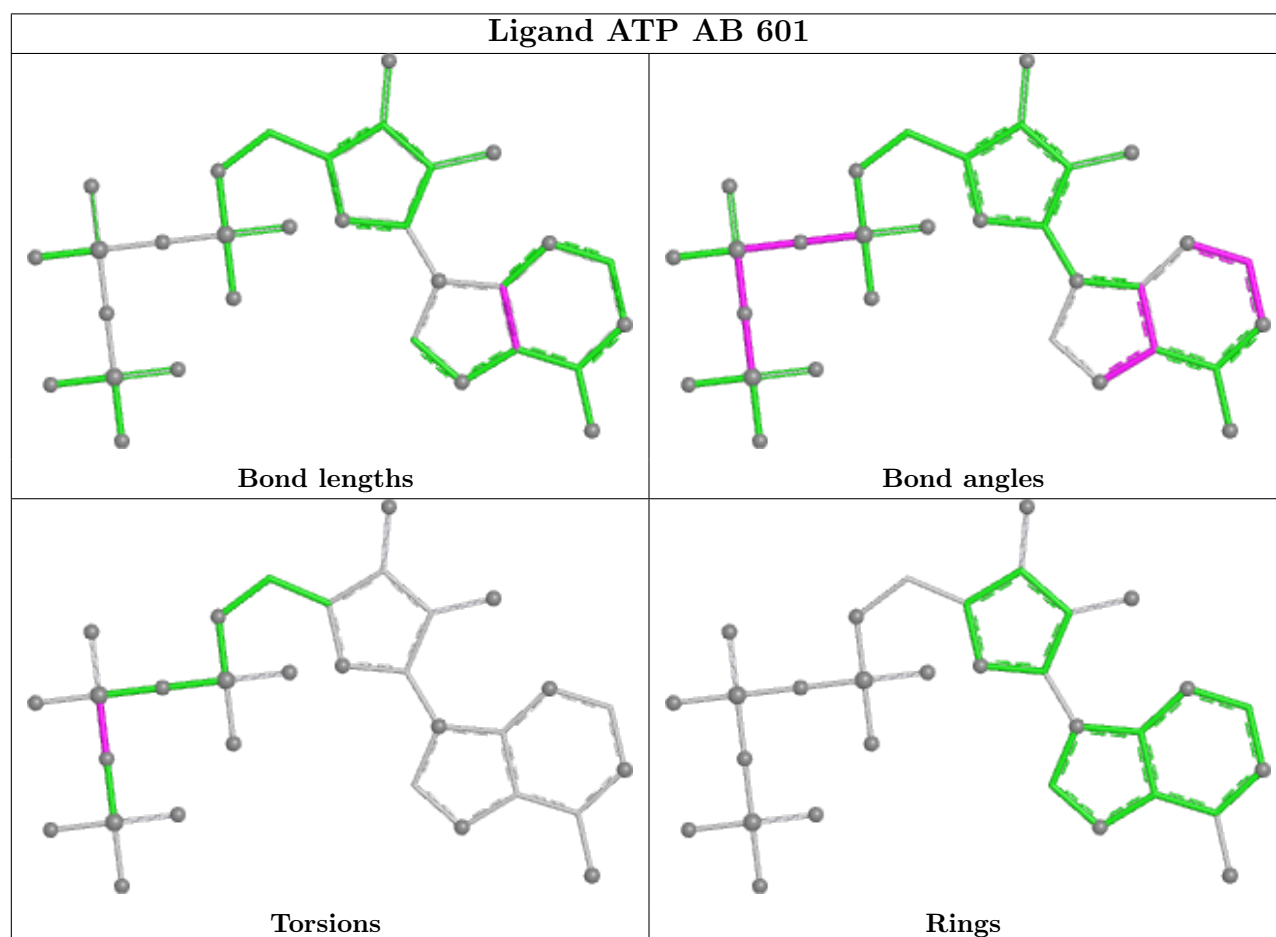
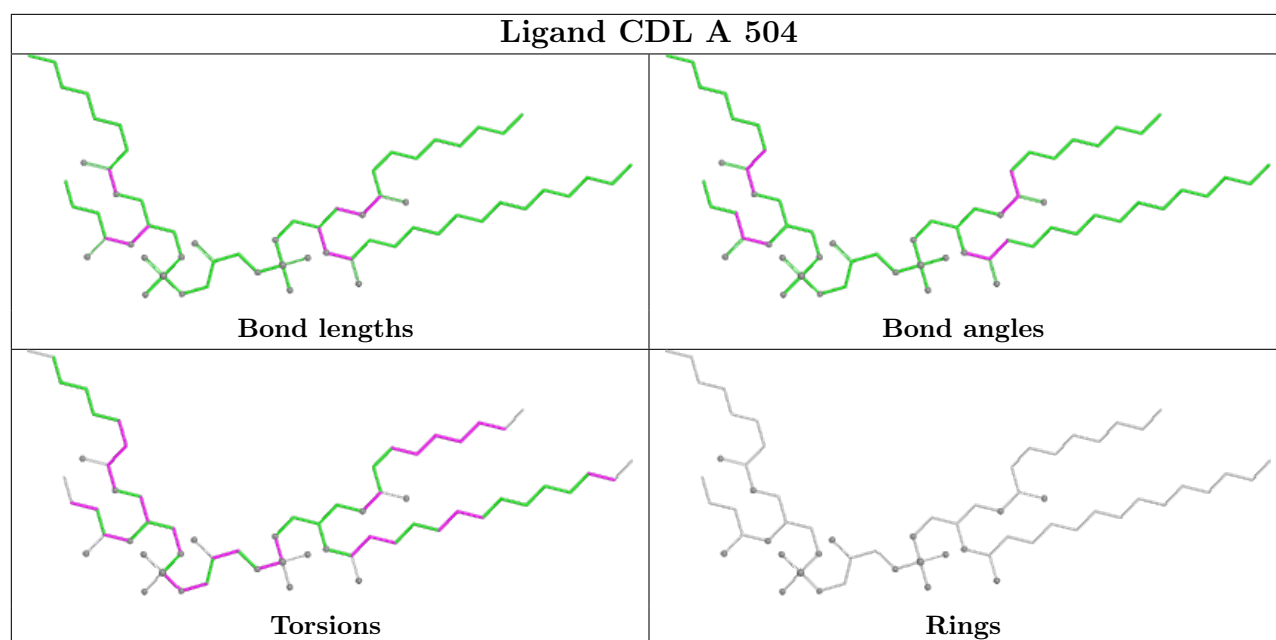


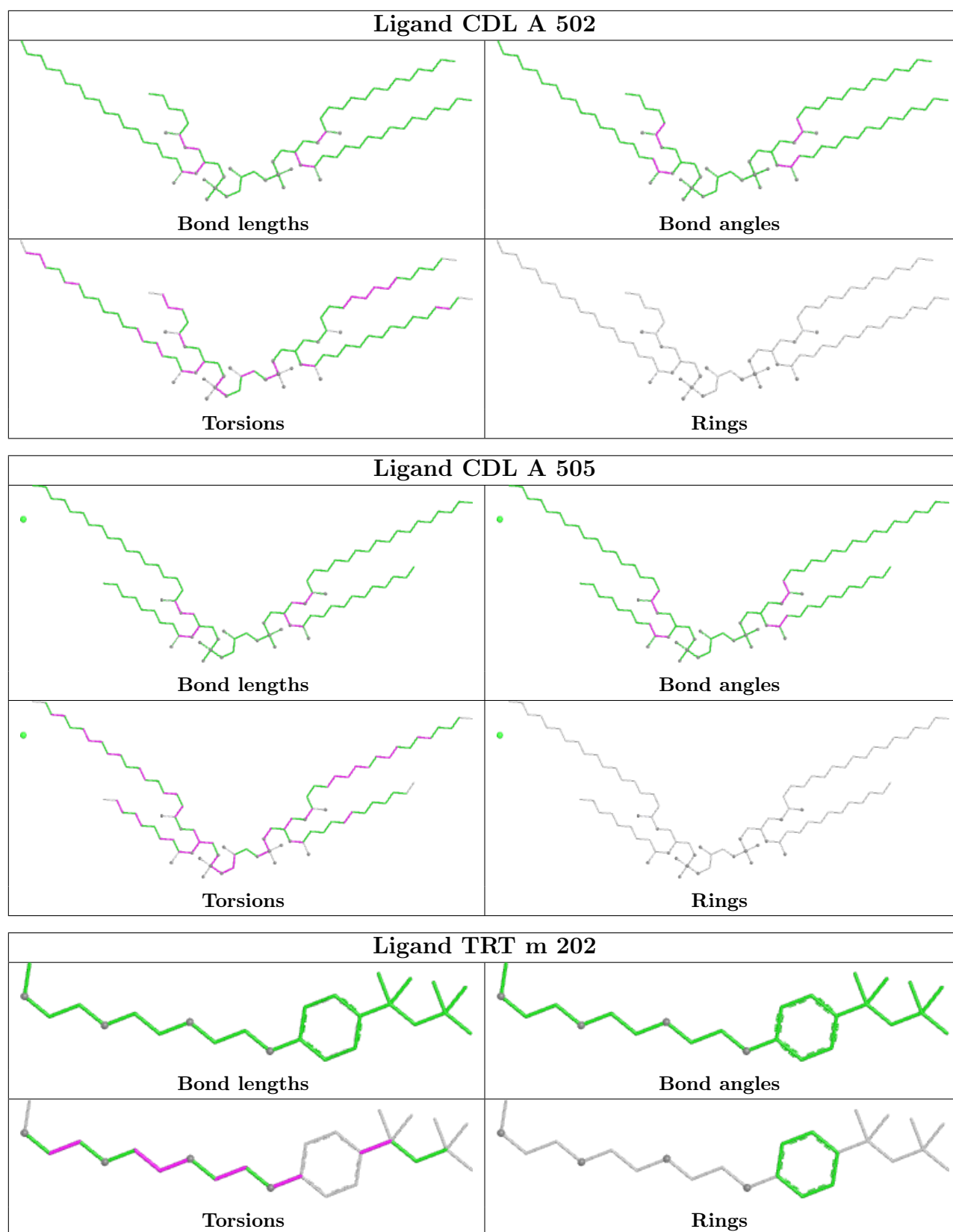


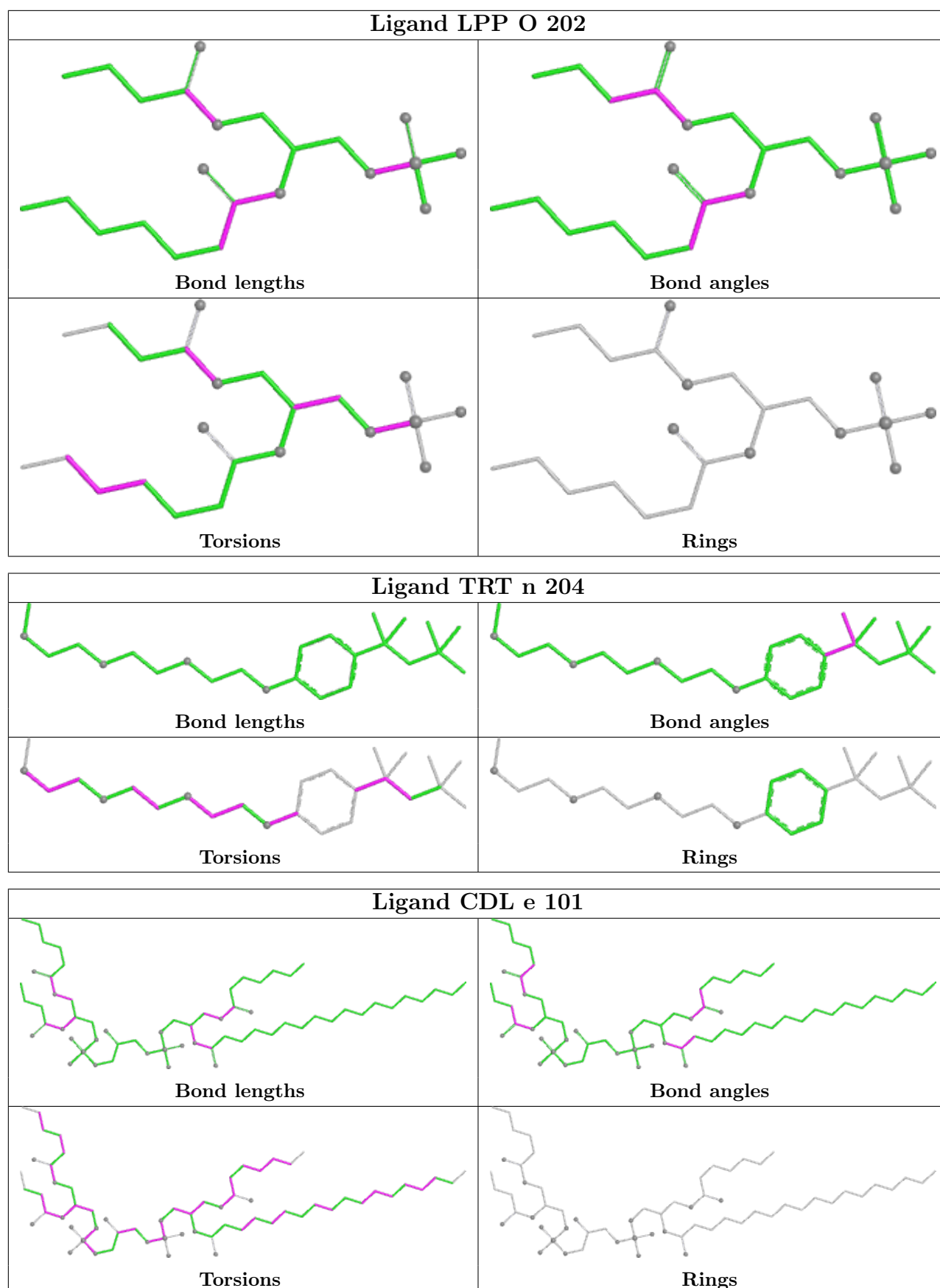


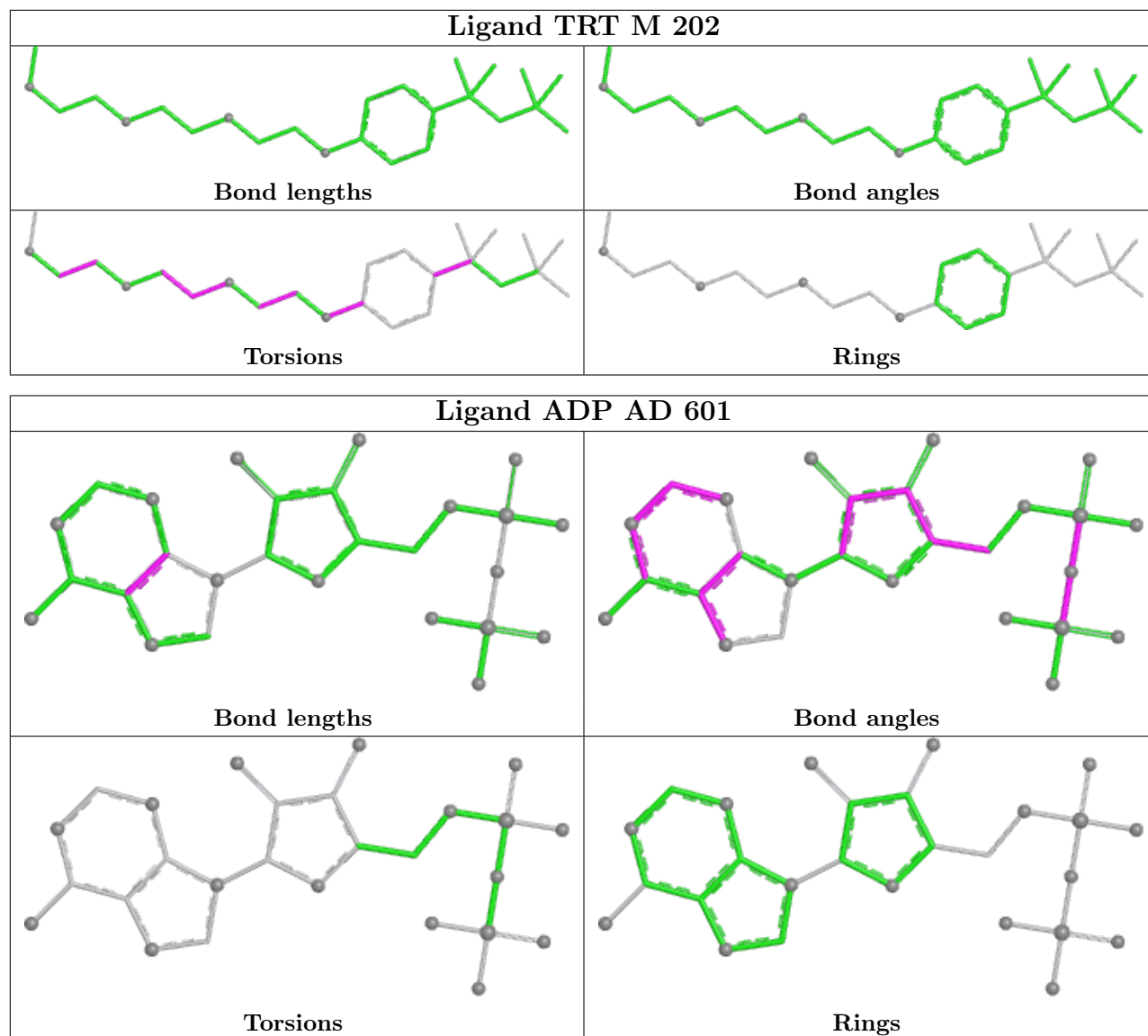


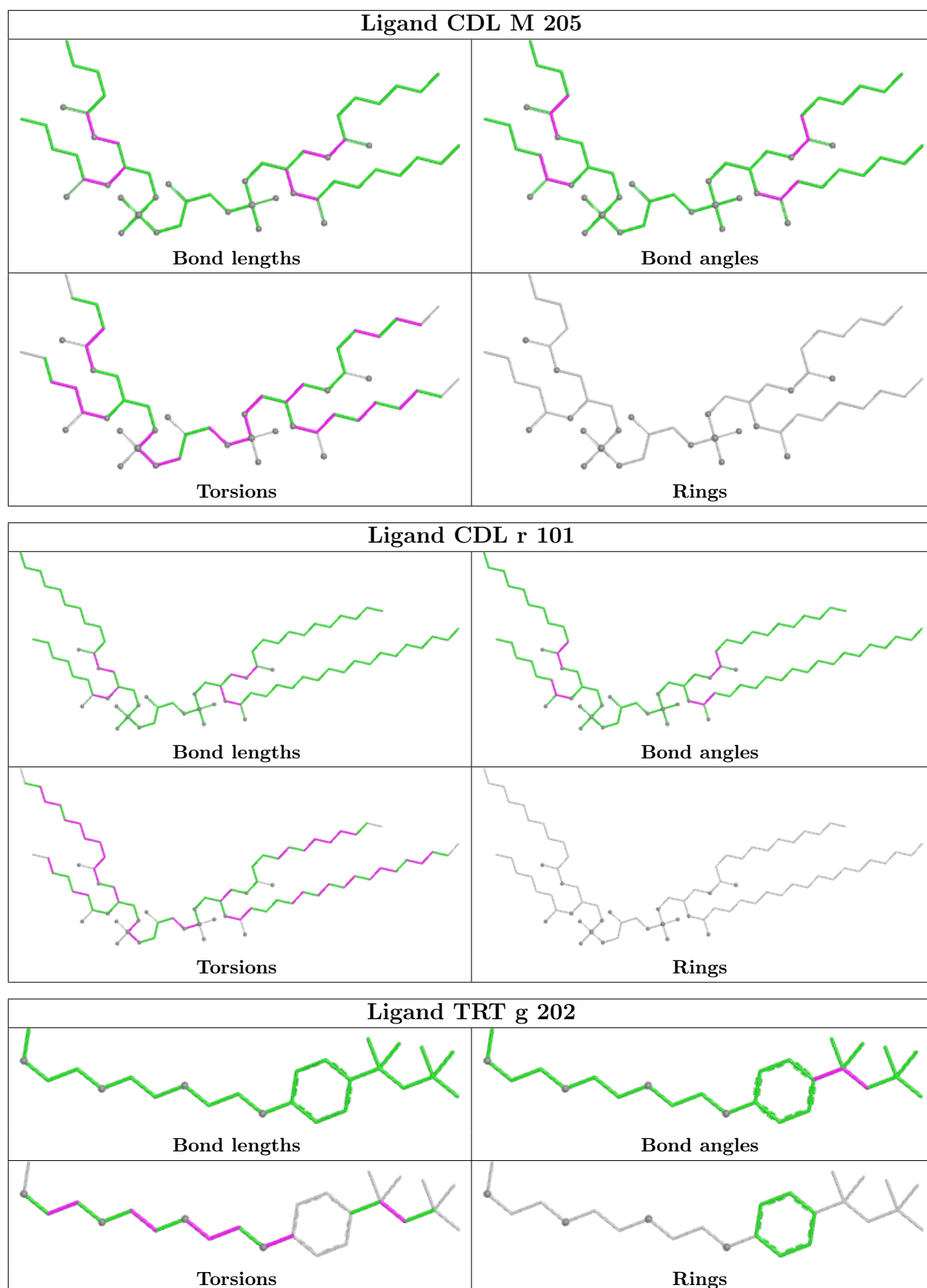


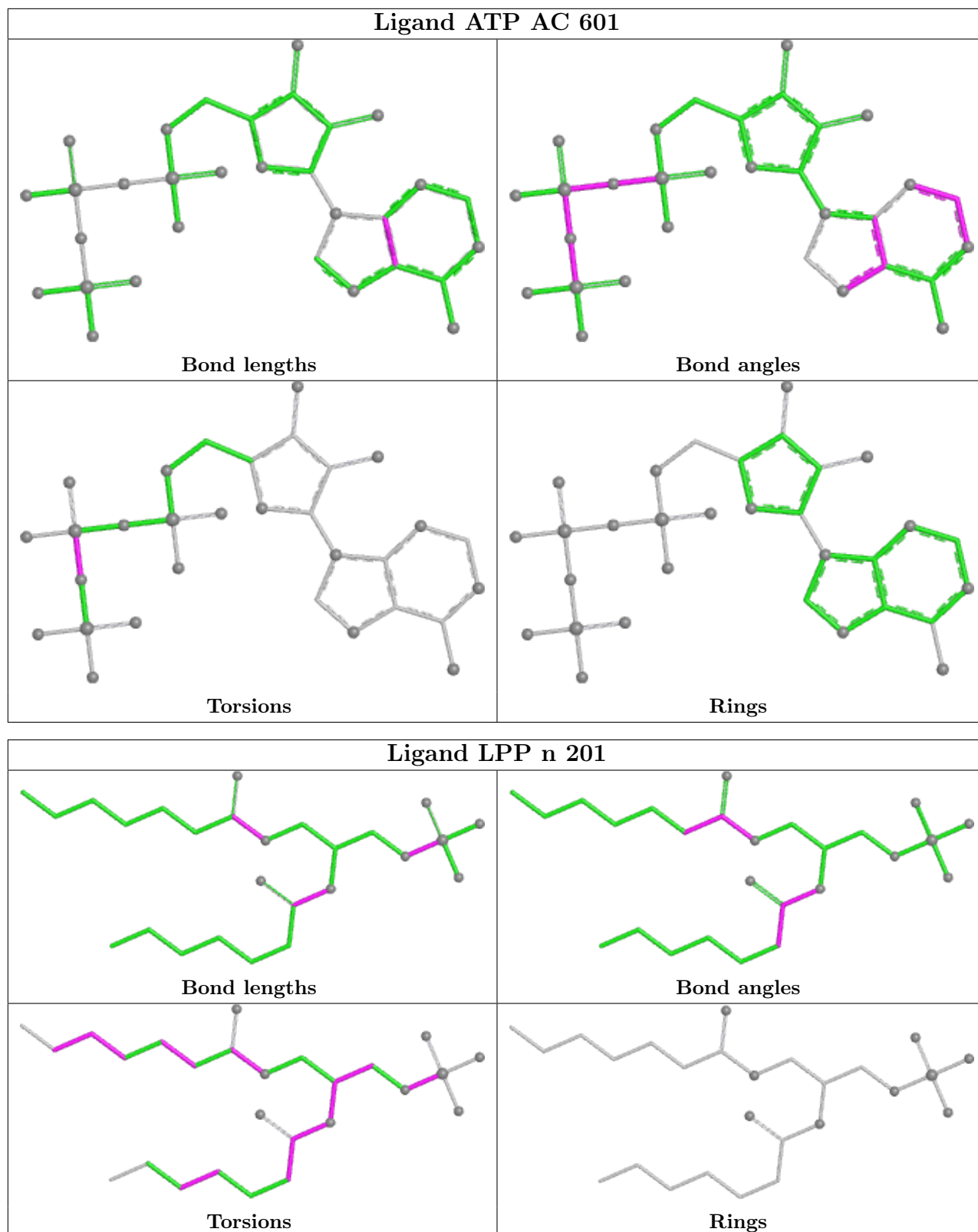


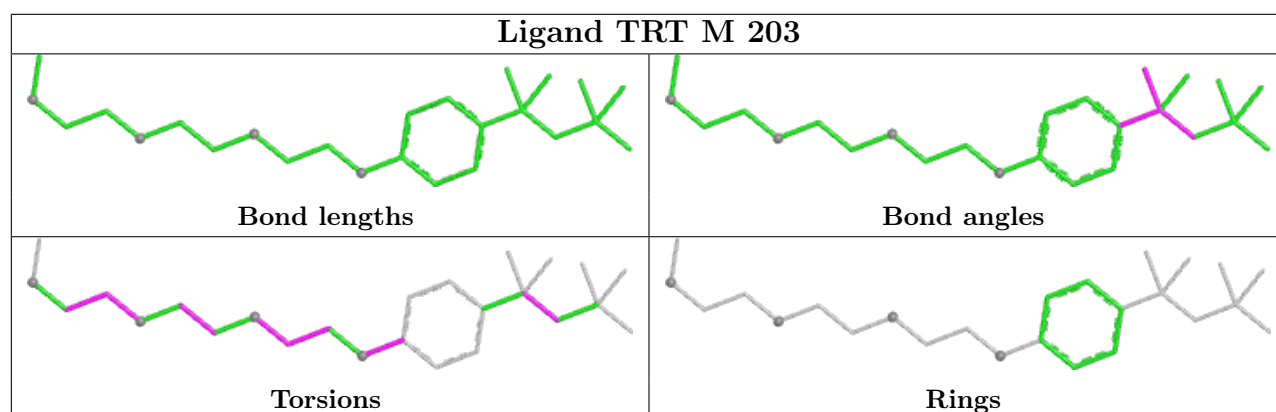
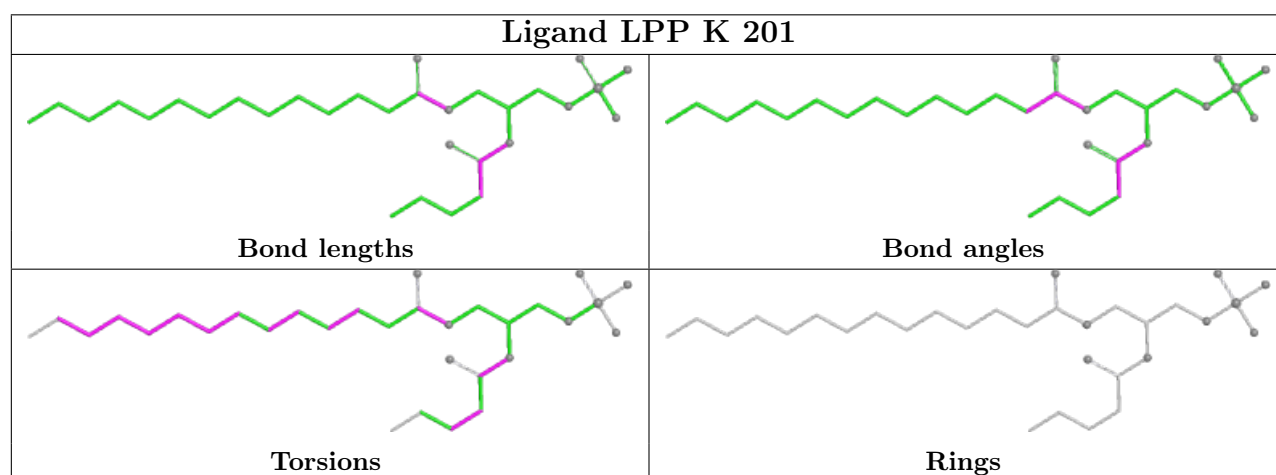
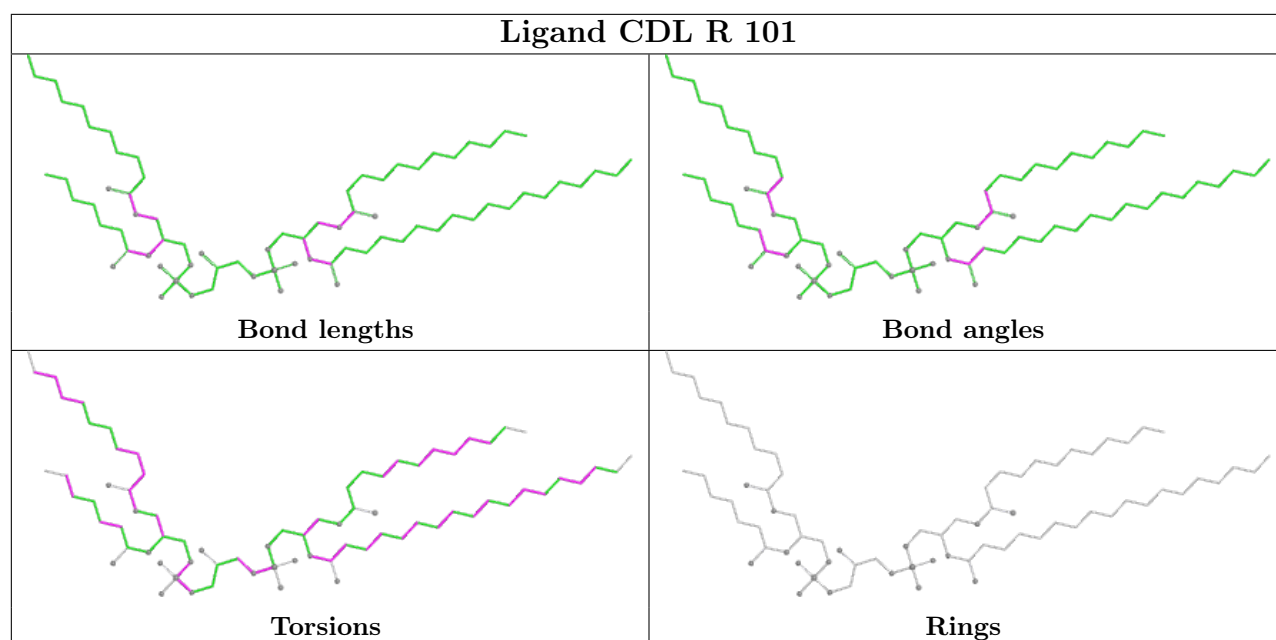


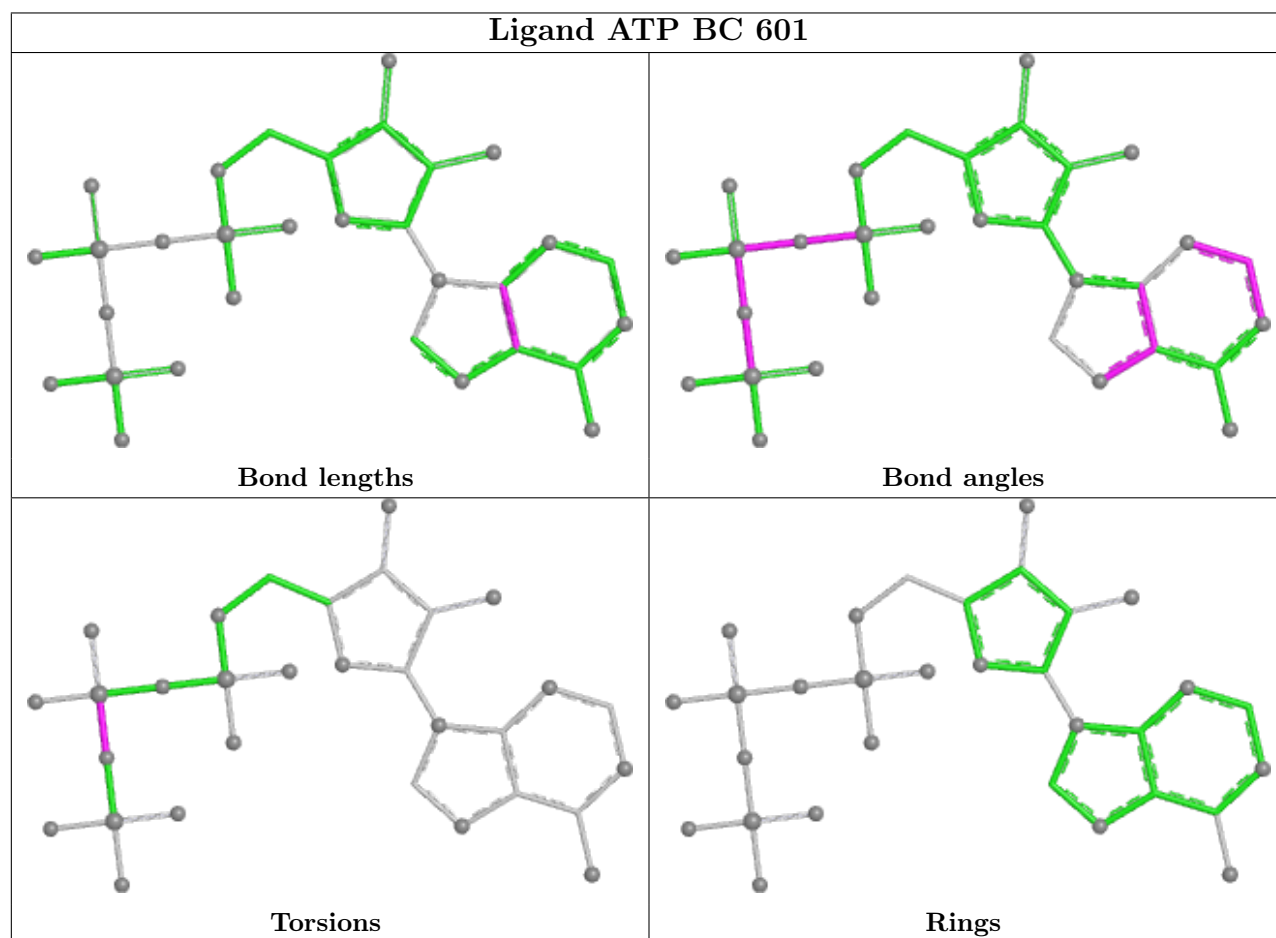
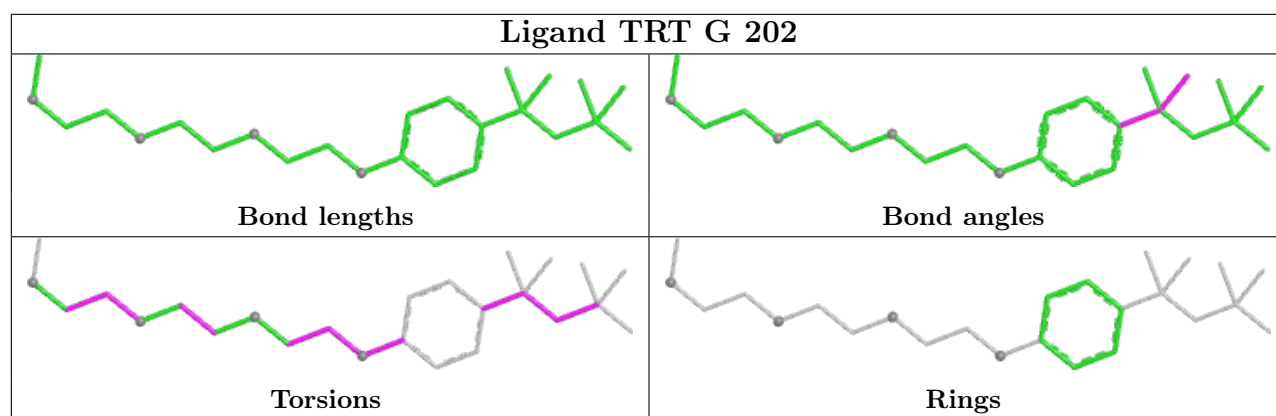


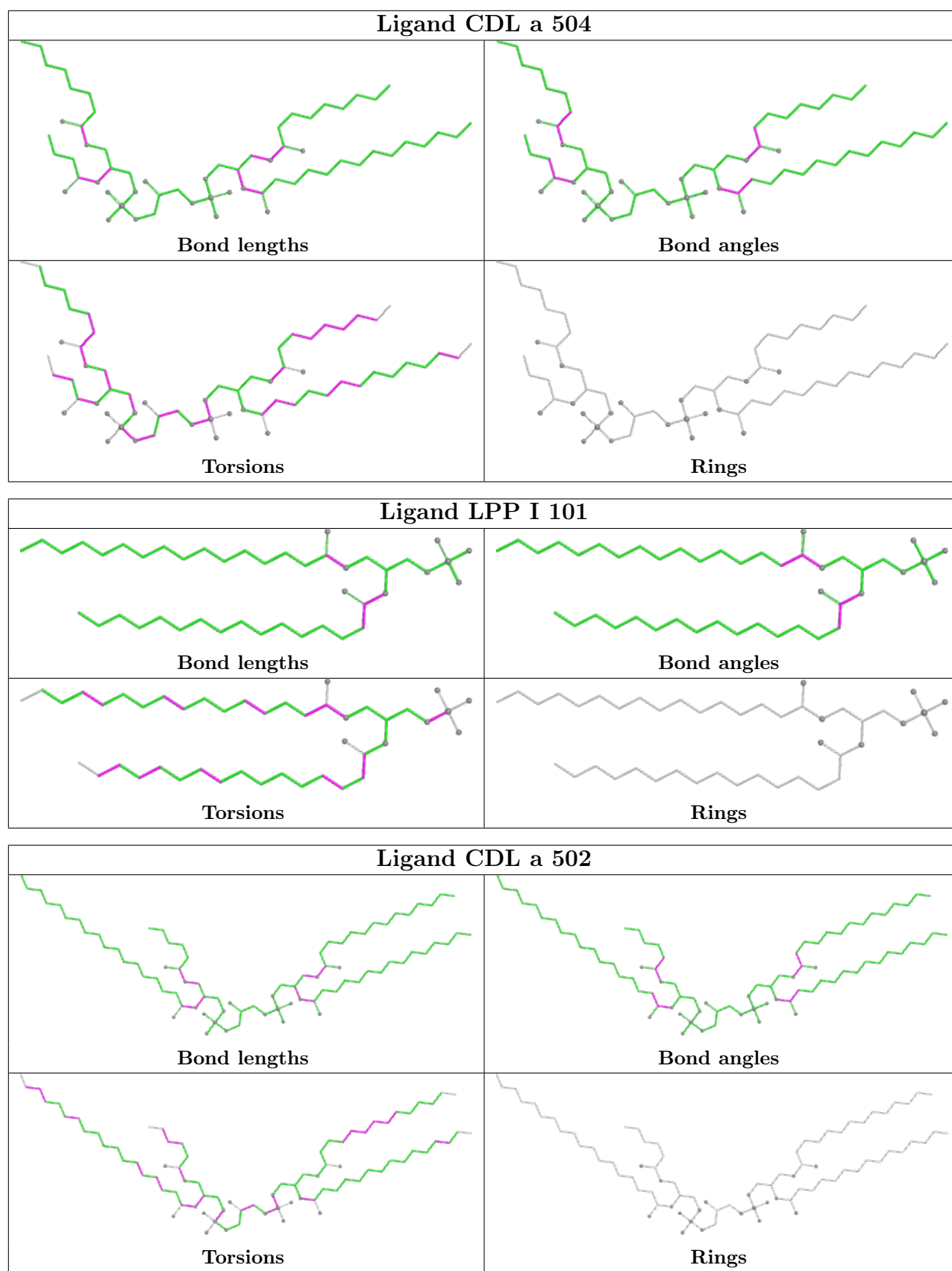


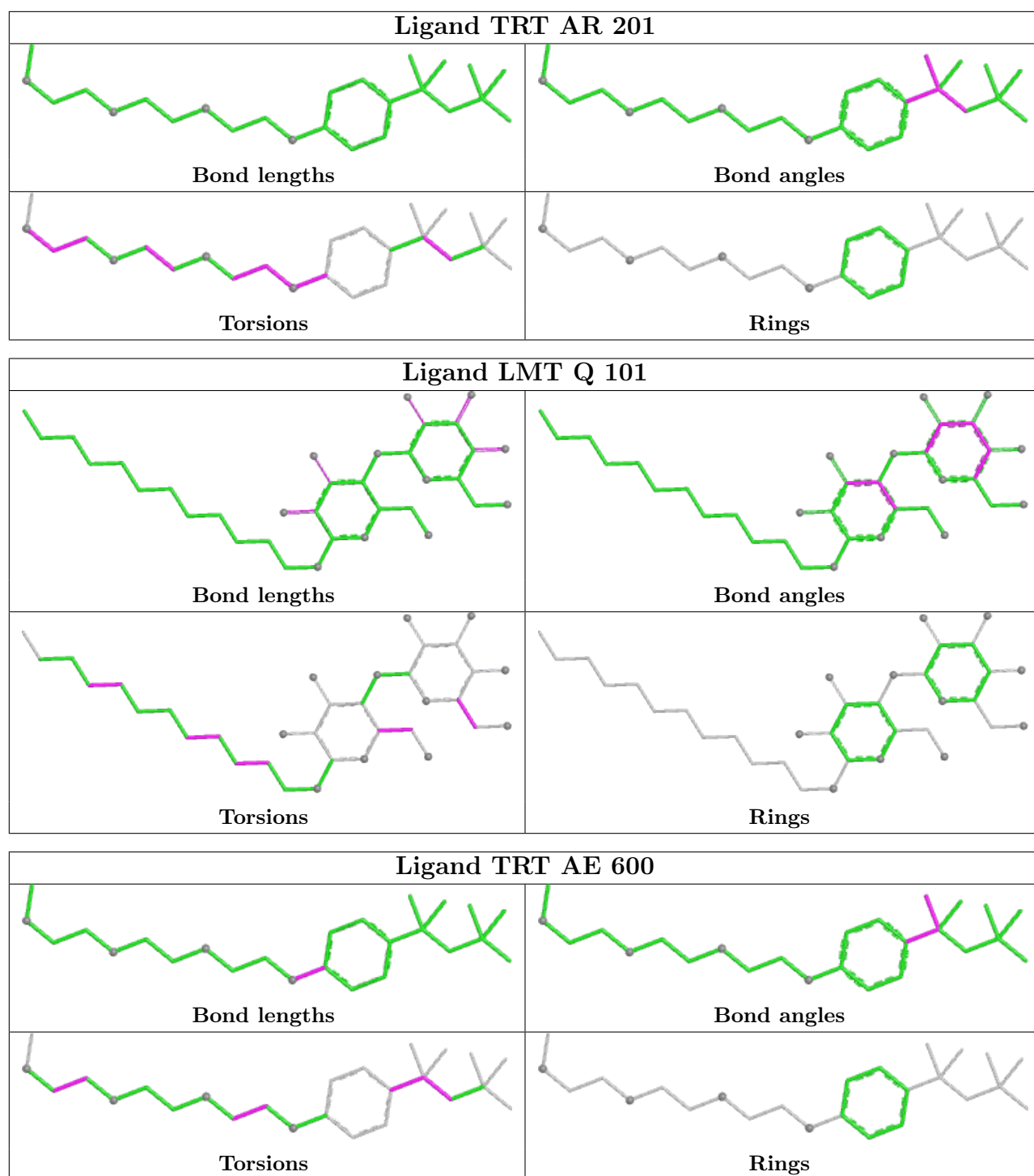


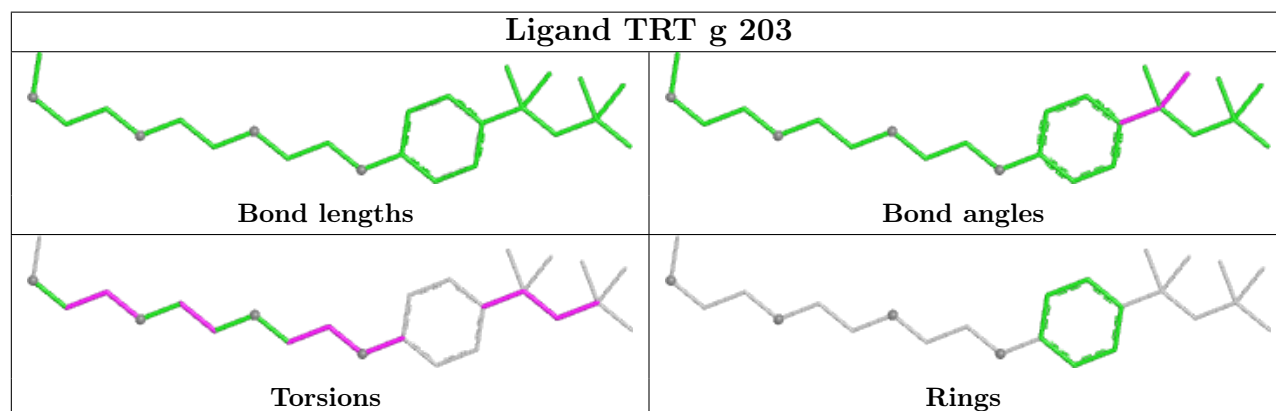
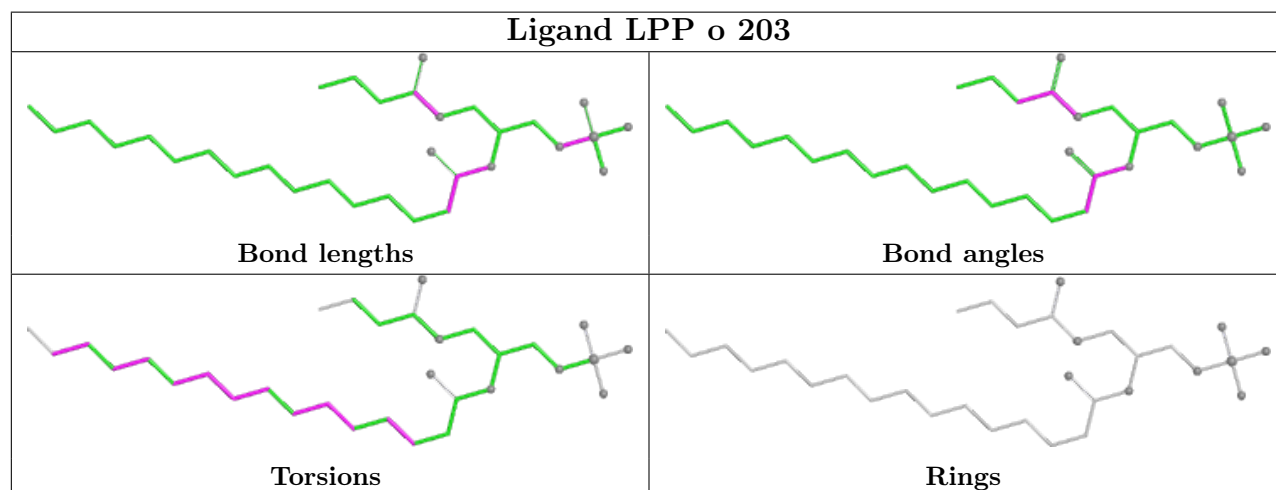
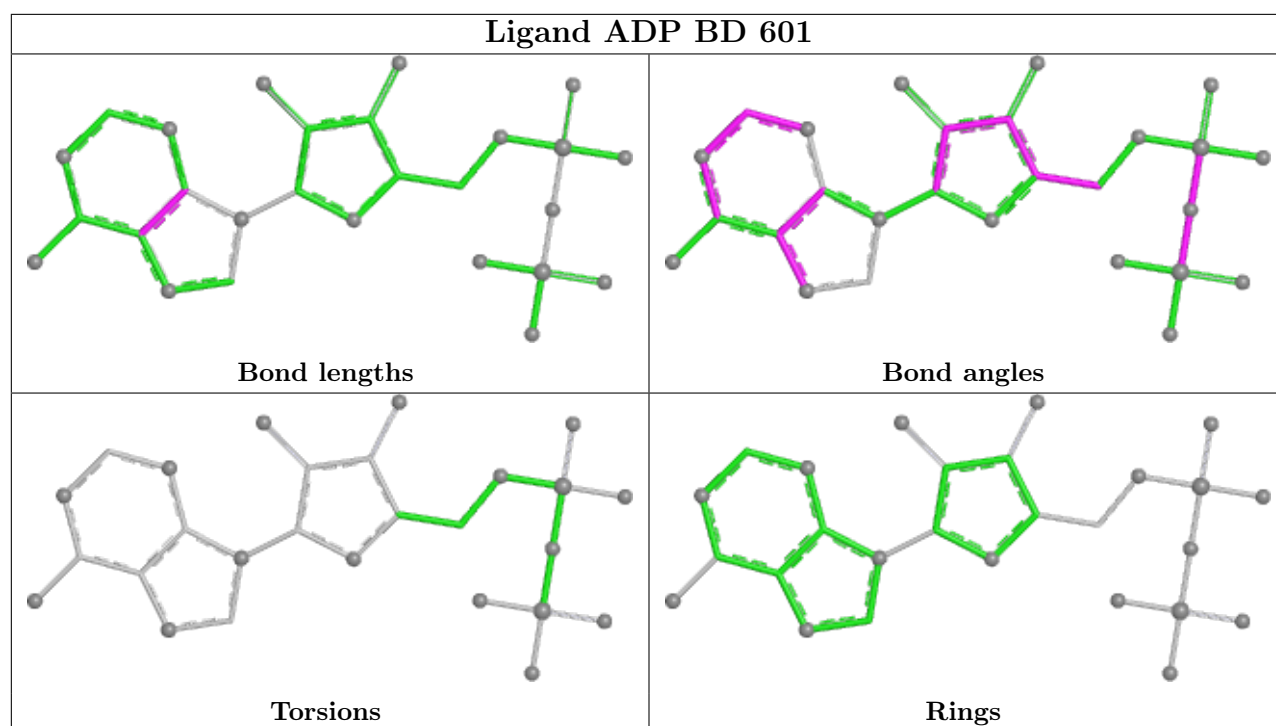


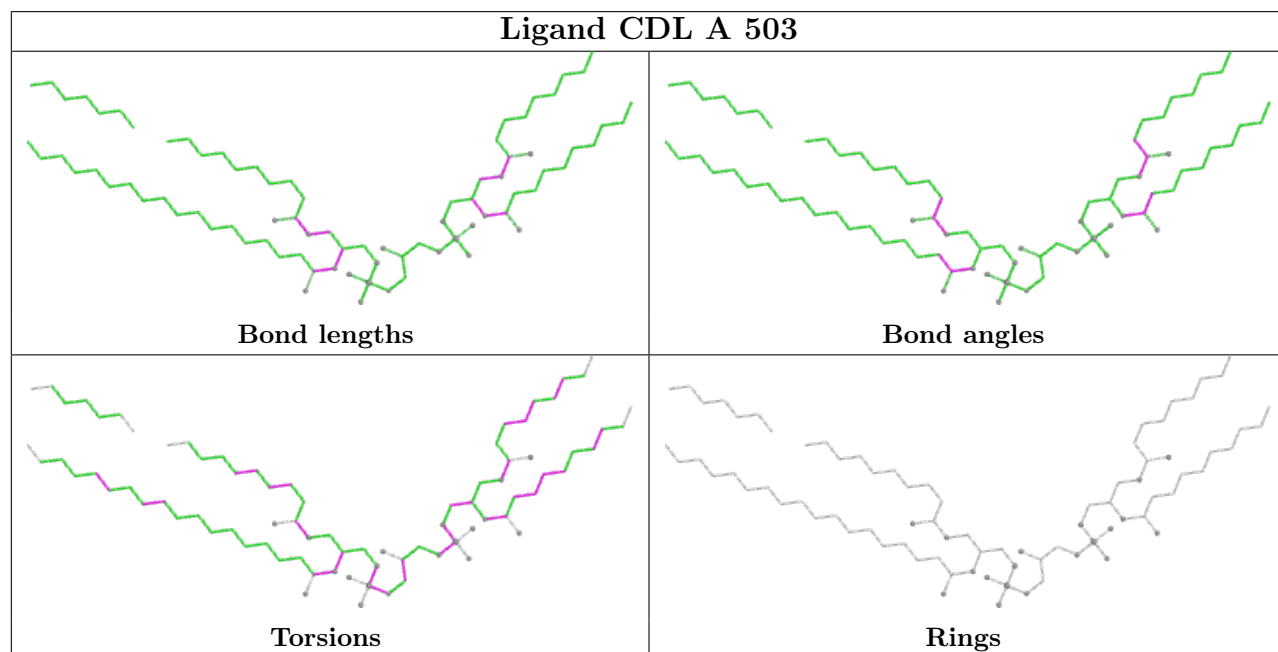
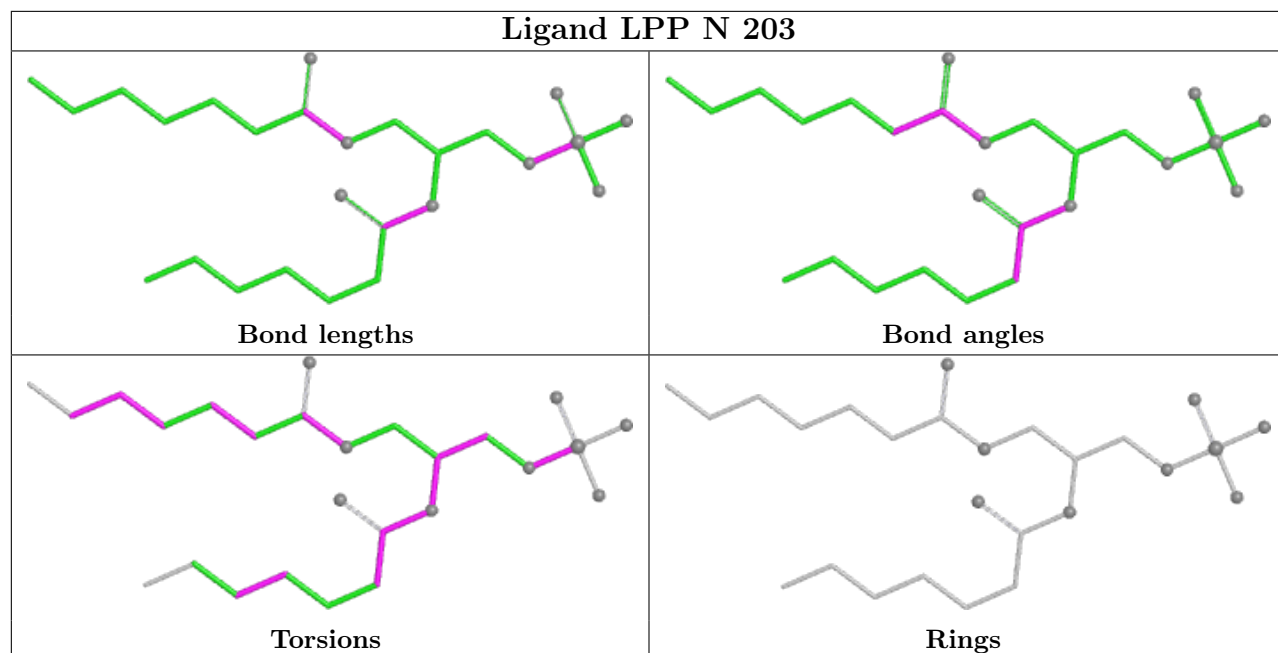


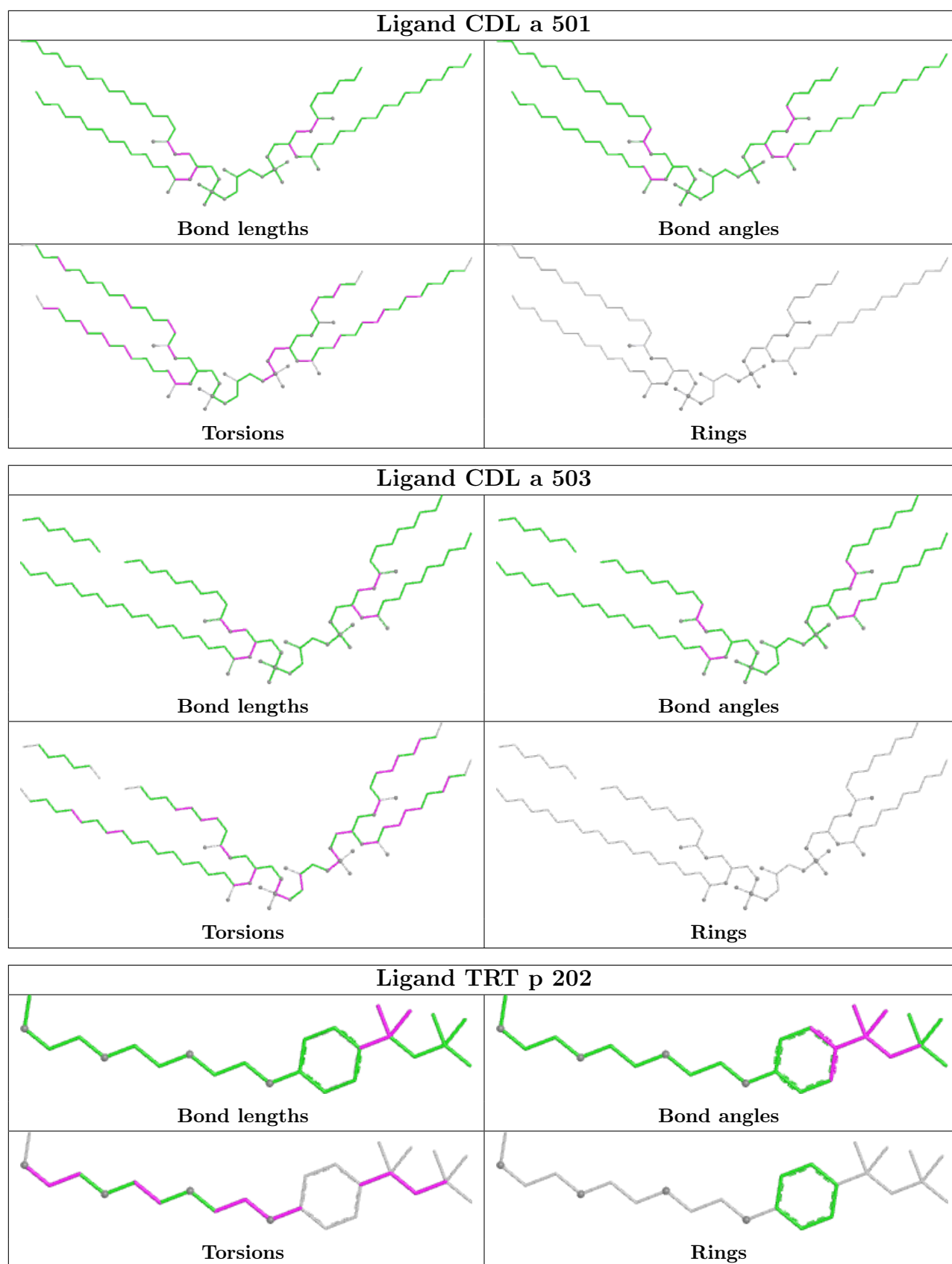


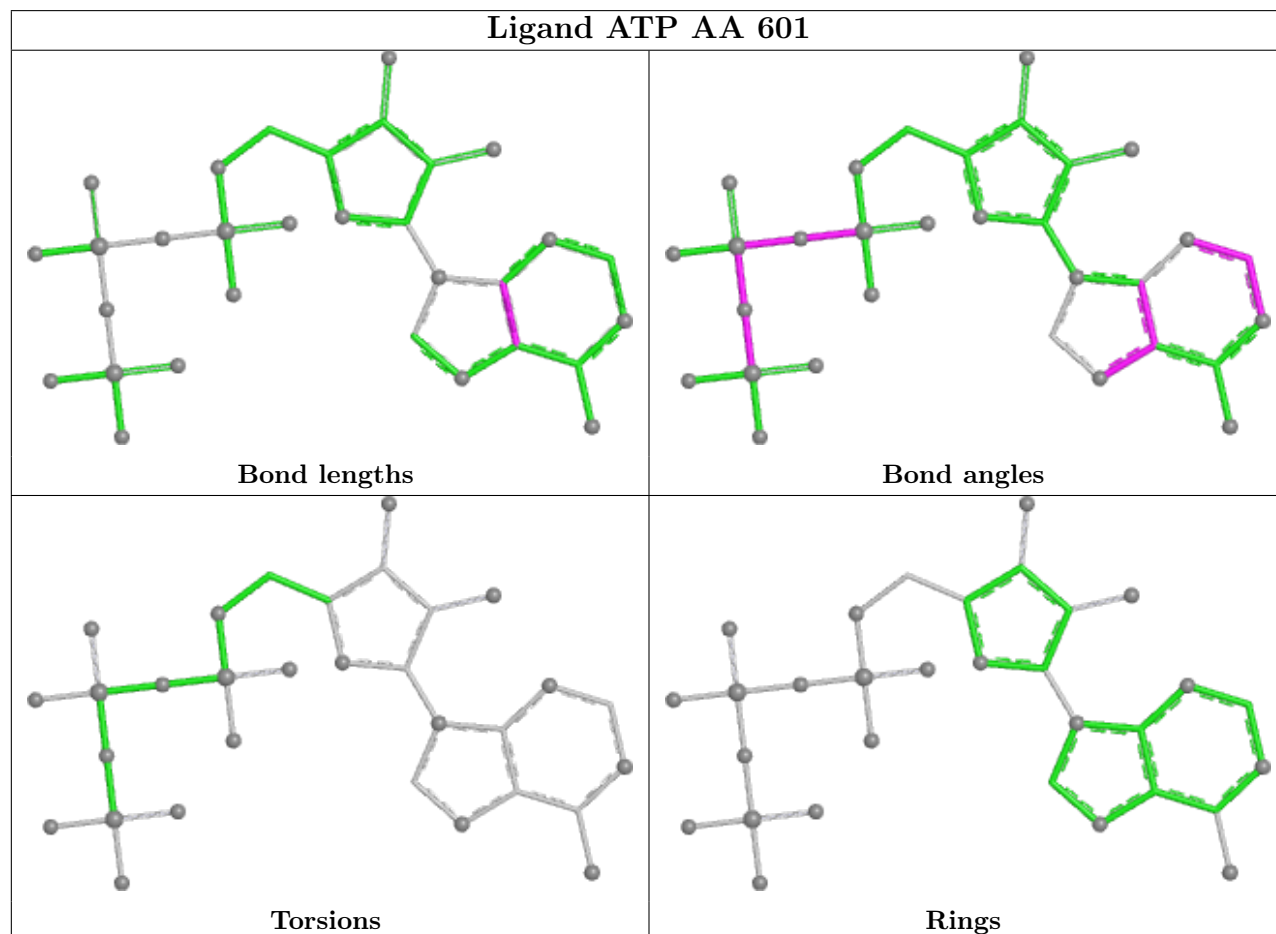
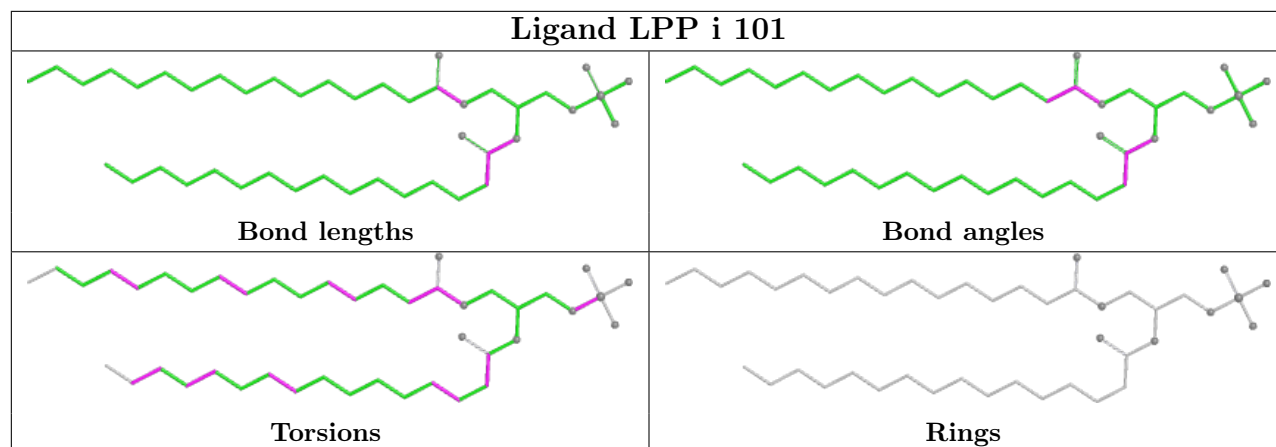


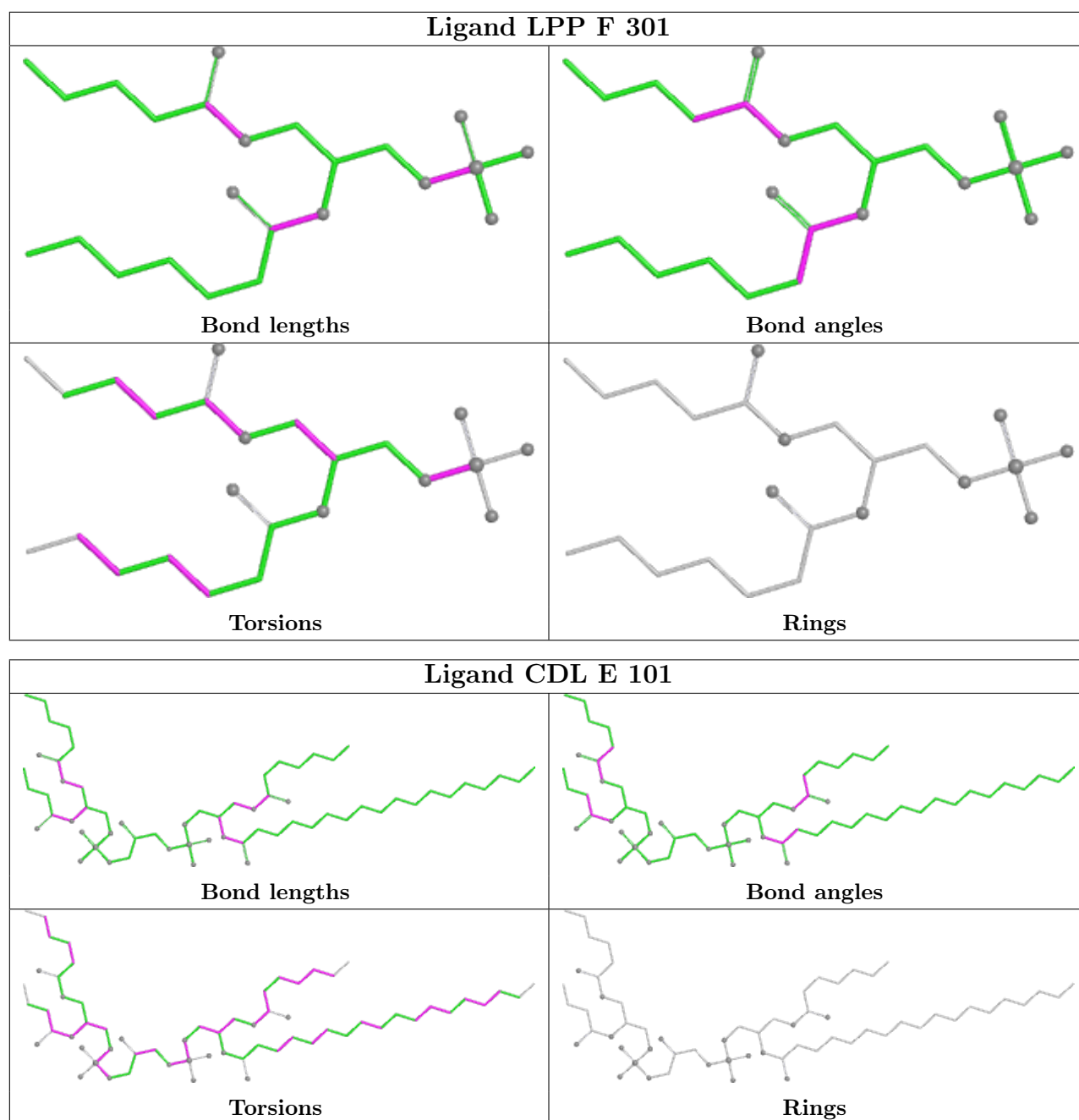


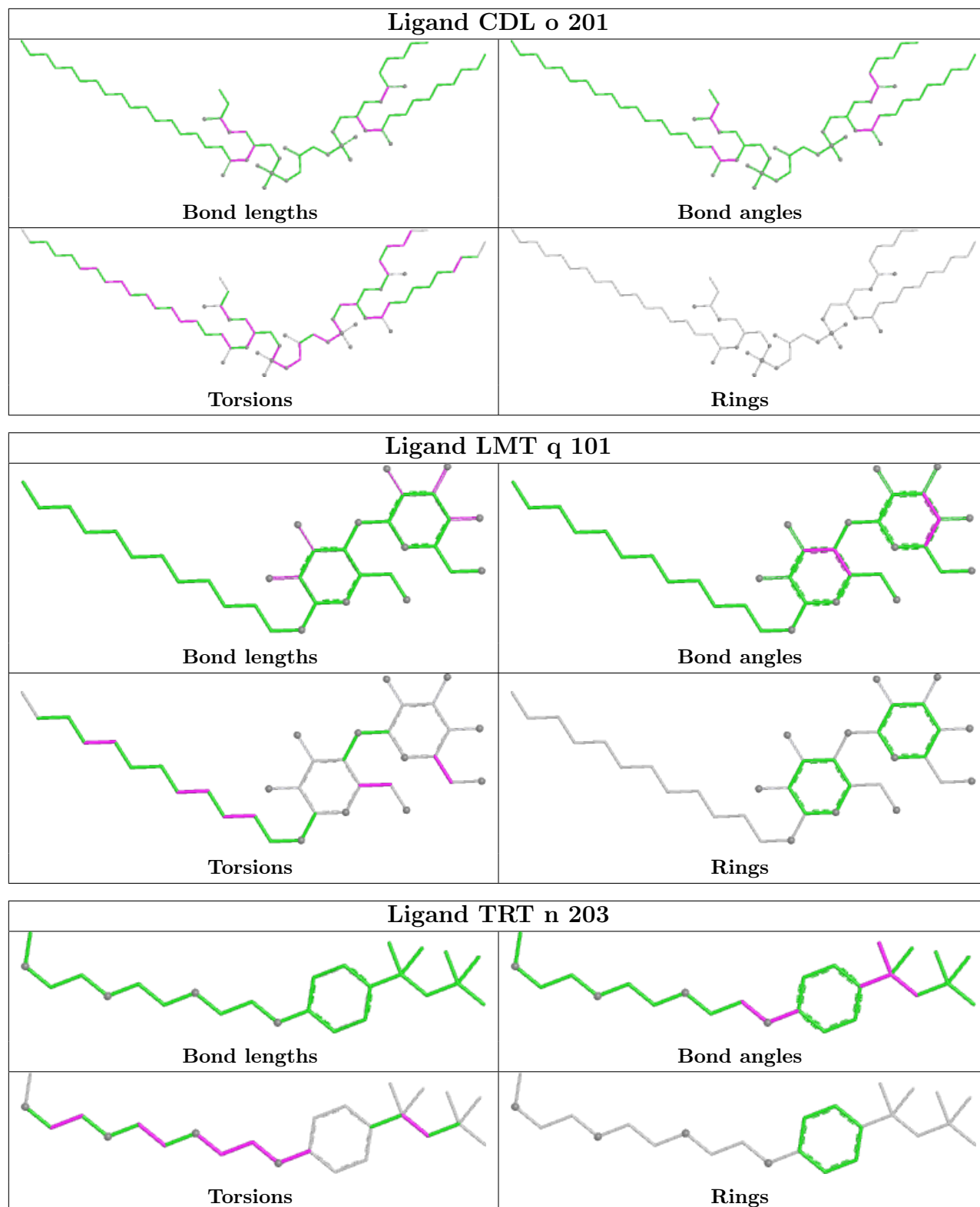


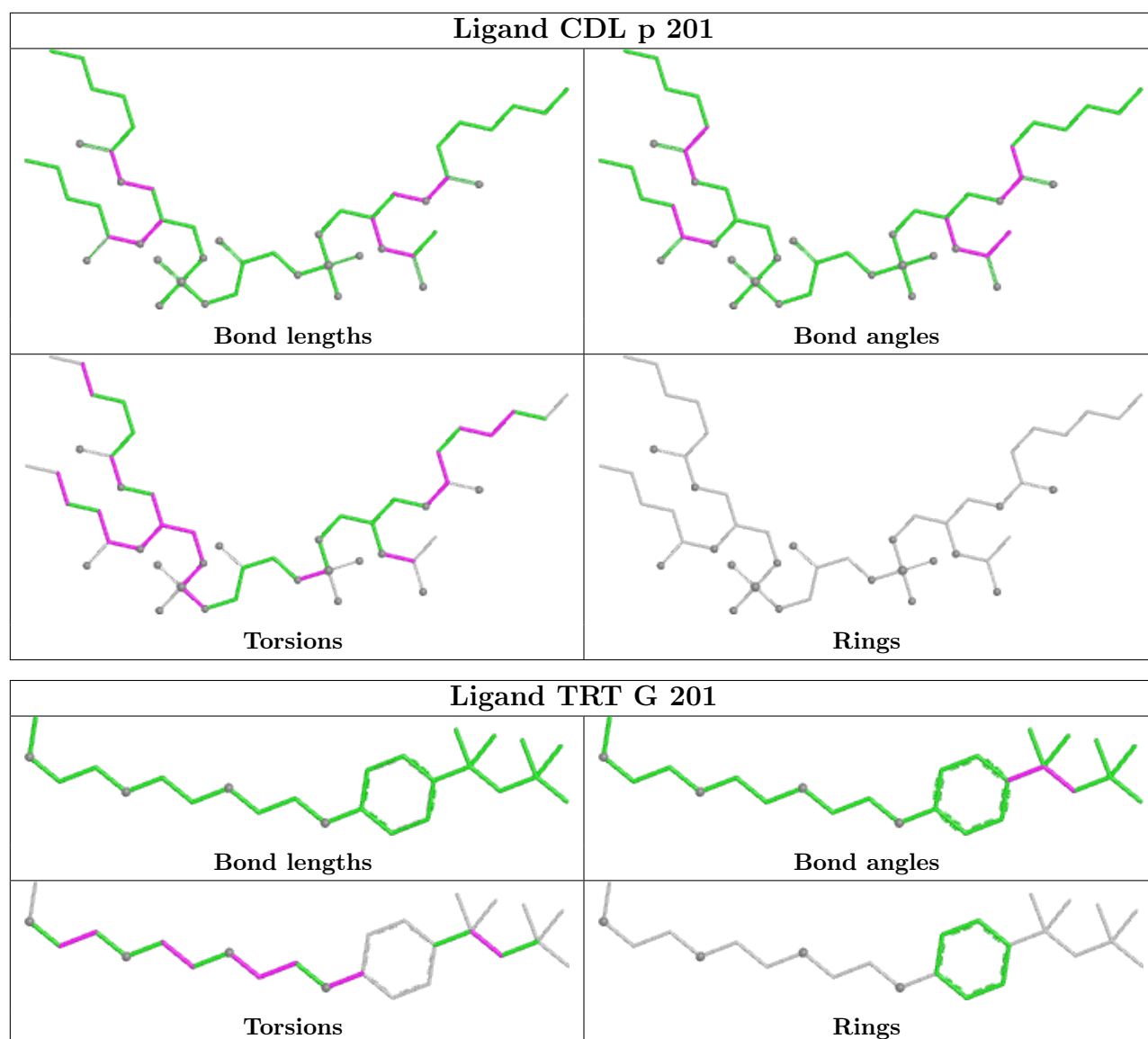


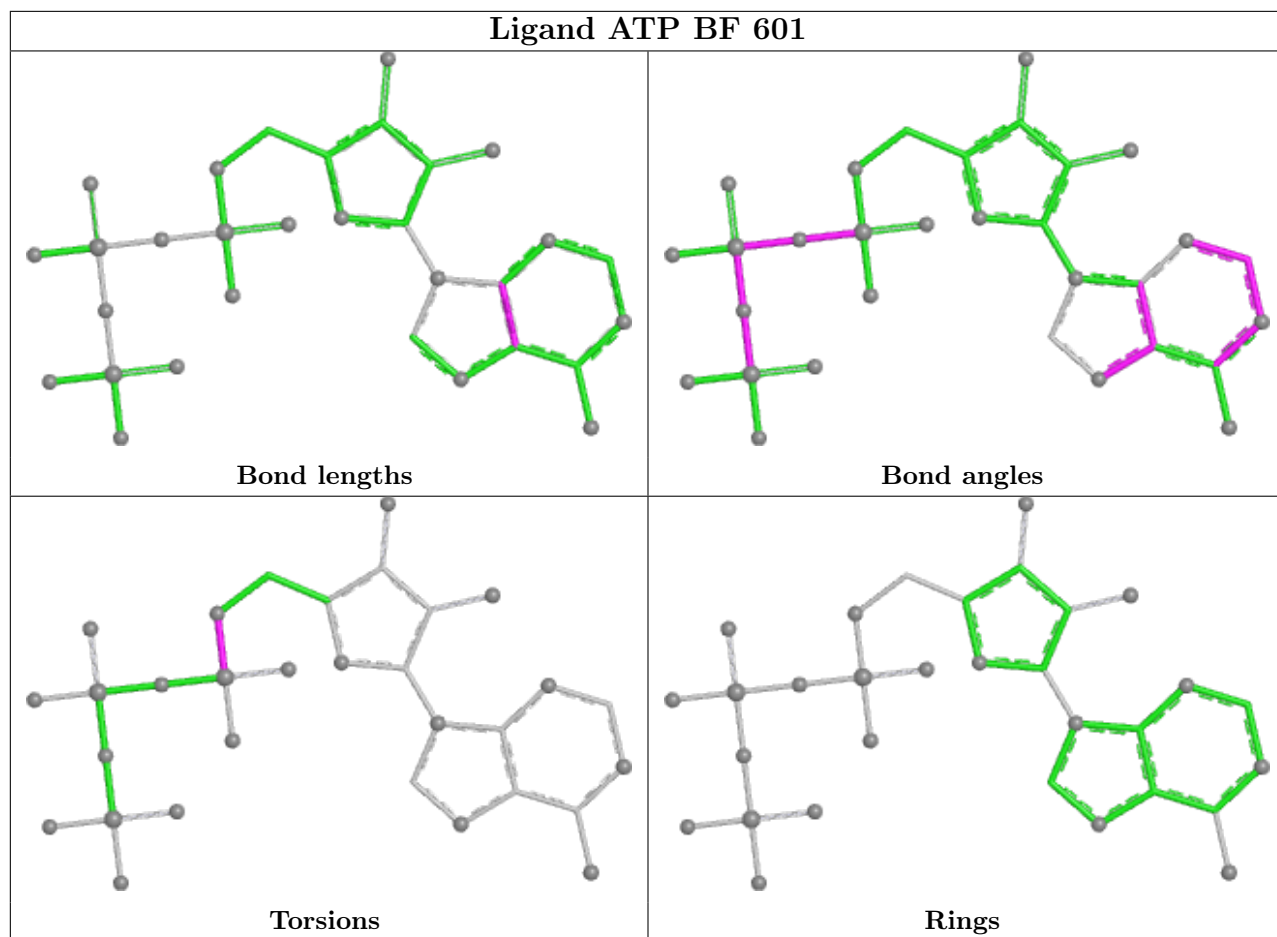


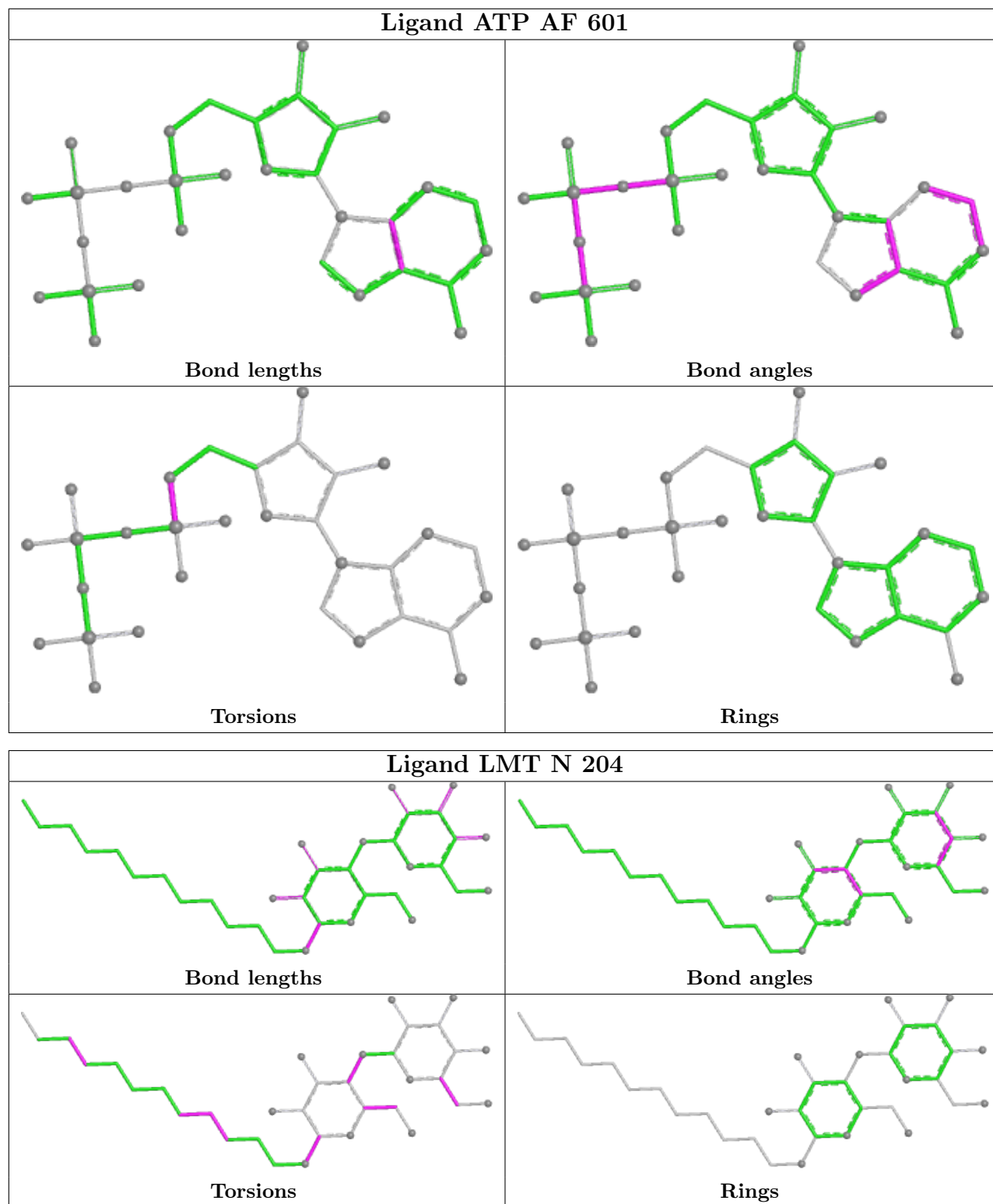


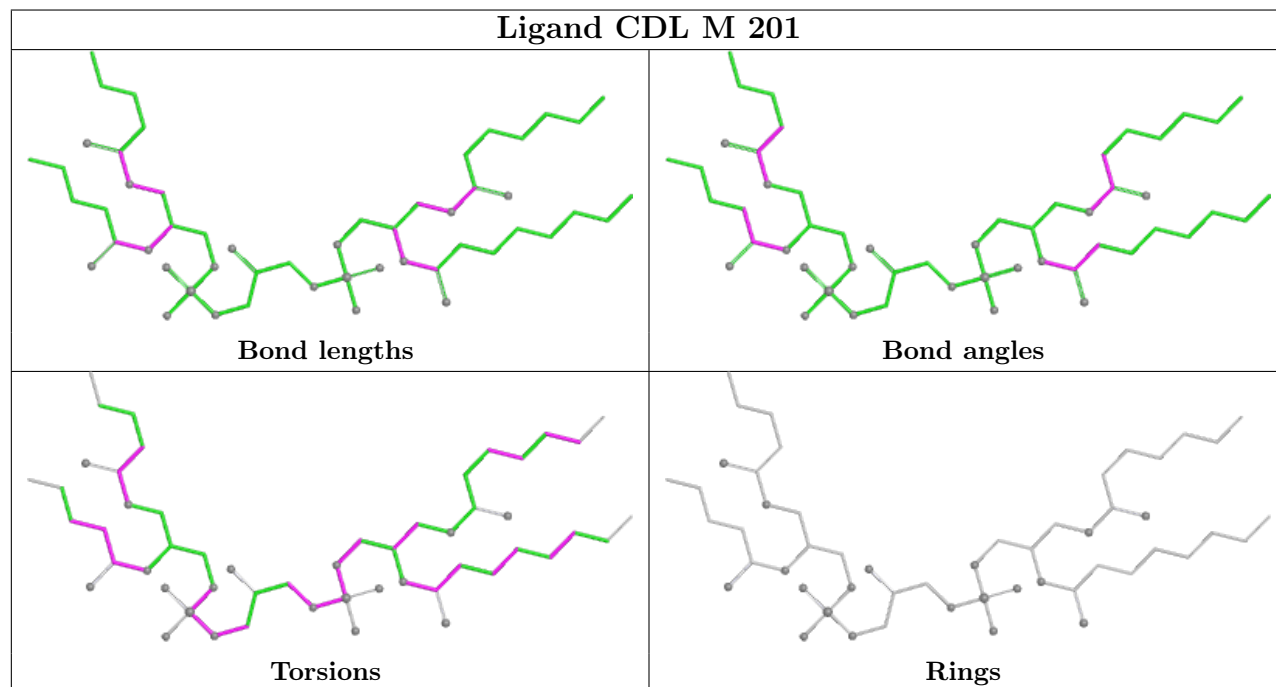
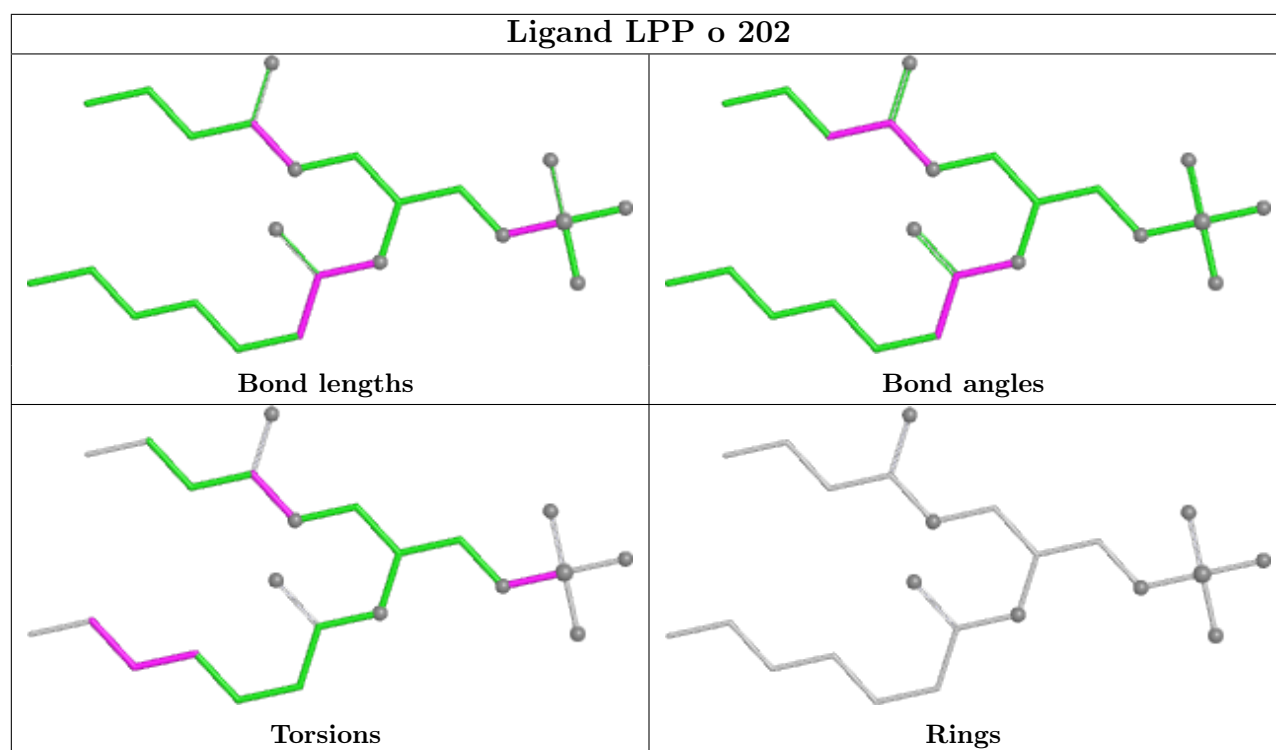


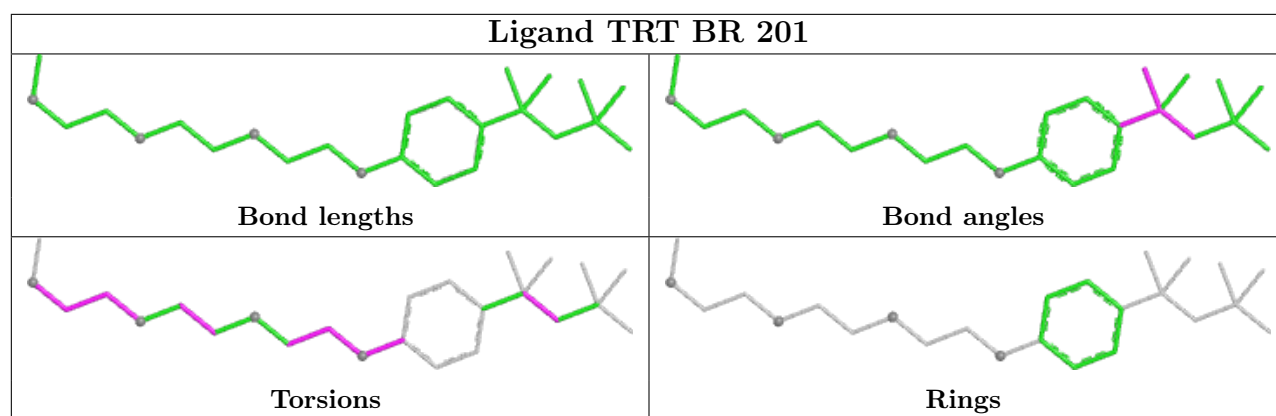












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

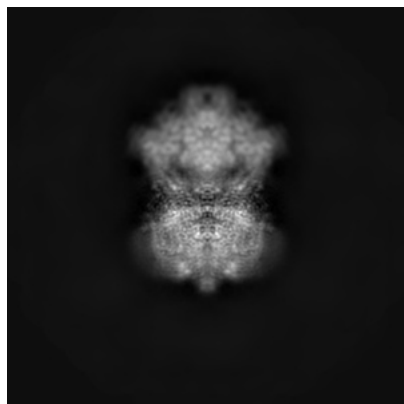
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10467. These allow visual inspection of the internal detail of the map and identification of artifacts.

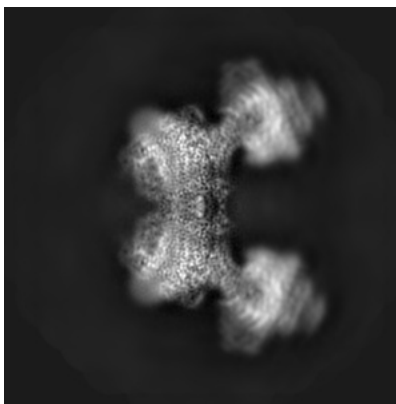
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

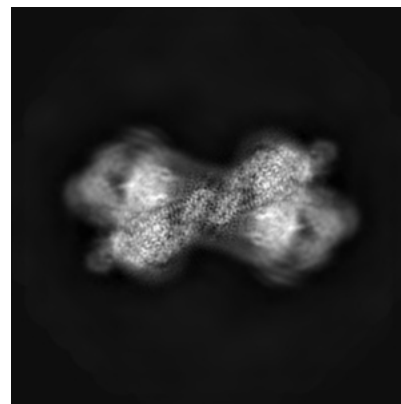
6.1.1 Primary map



X

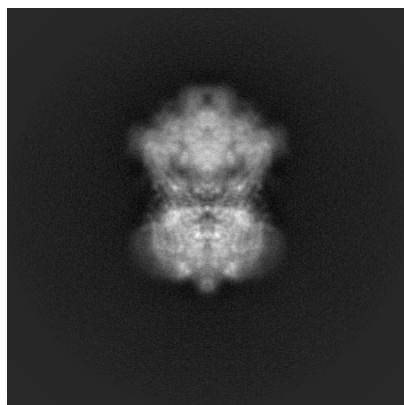


Y

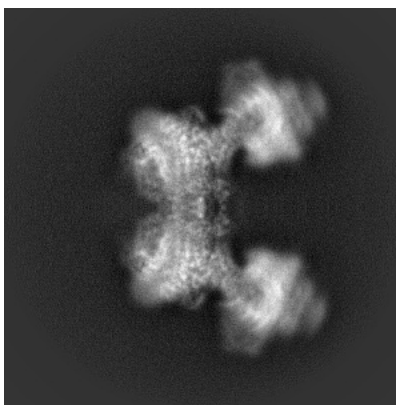


Z

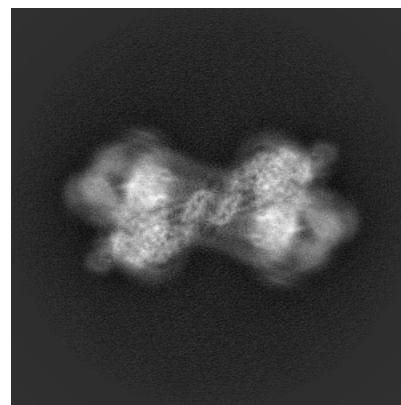
6.1.2 Raw map



X



Y

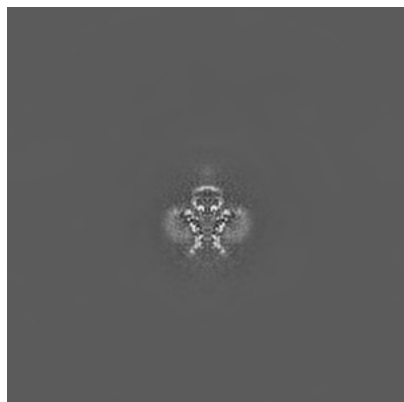


Z

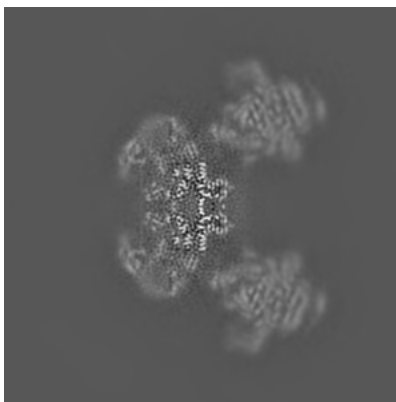
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 220

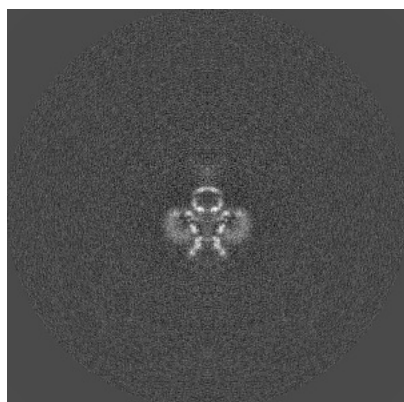


Y Index: 220

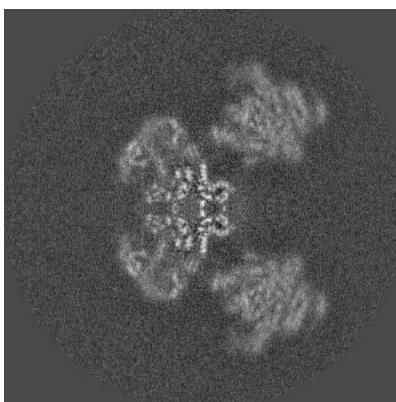


Z Index: 220

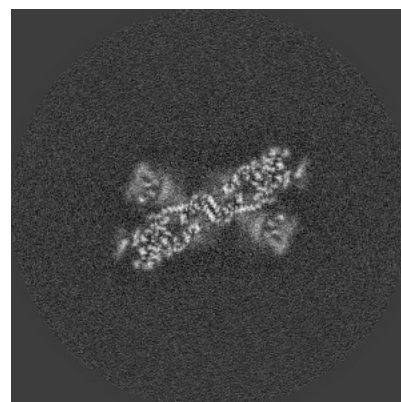
6.2.2 Raw map



X Index: 220



Y Index: 220

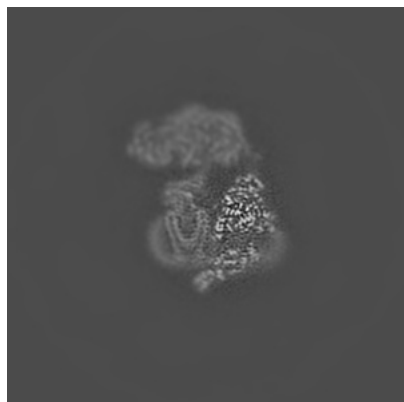


Z Index: 220

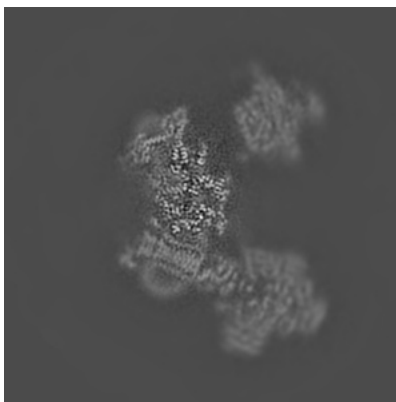
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

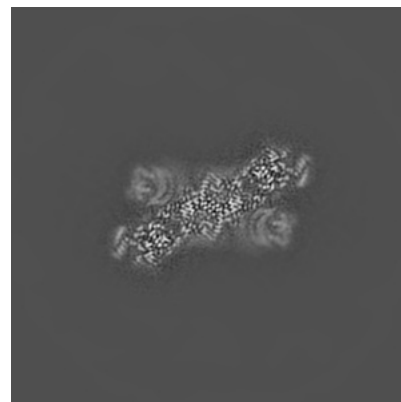
6.3.1 Primary map



X Index: 283

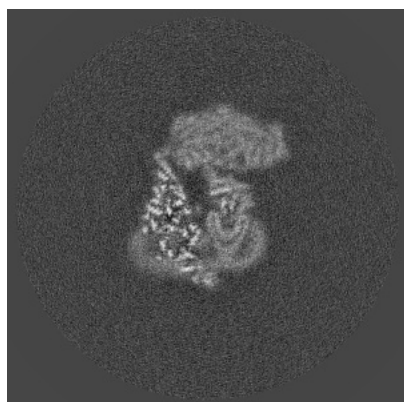


Y Index: 230

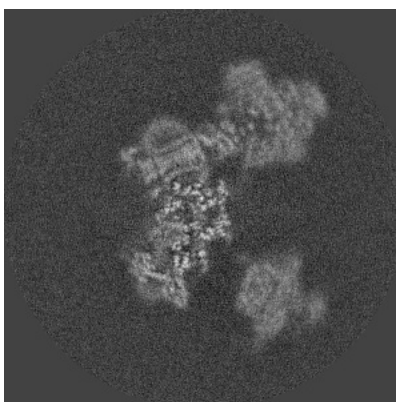


Z Index: 215

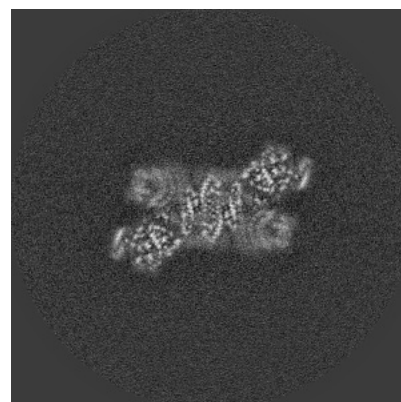
6.3.2 Raw map



X Index: 152



Y Index: 210



Z Index: 215

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



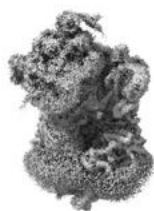
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

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

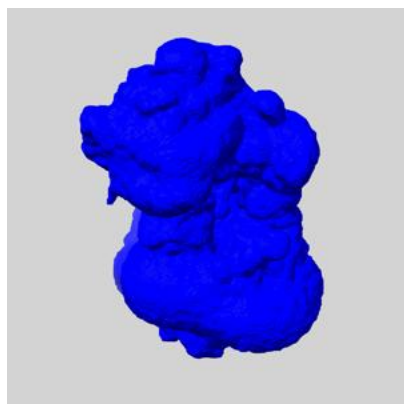
6.5 Mask visualisation [i](#)

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

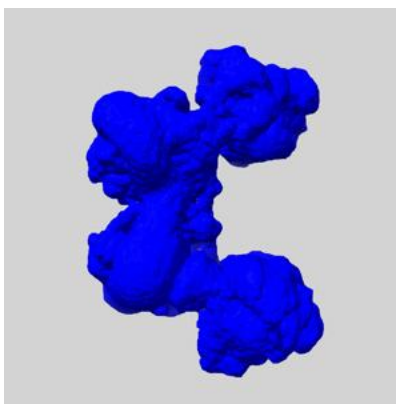
A mask typically either:

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

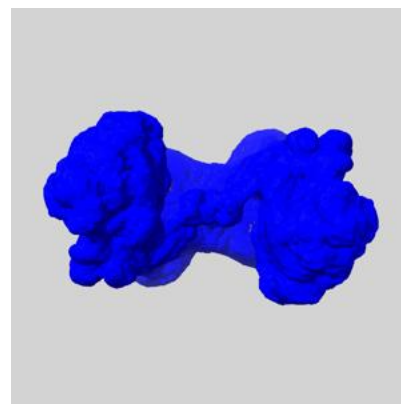
6.5.1 emd_10467_msk_1.map [i](#)



X



Y

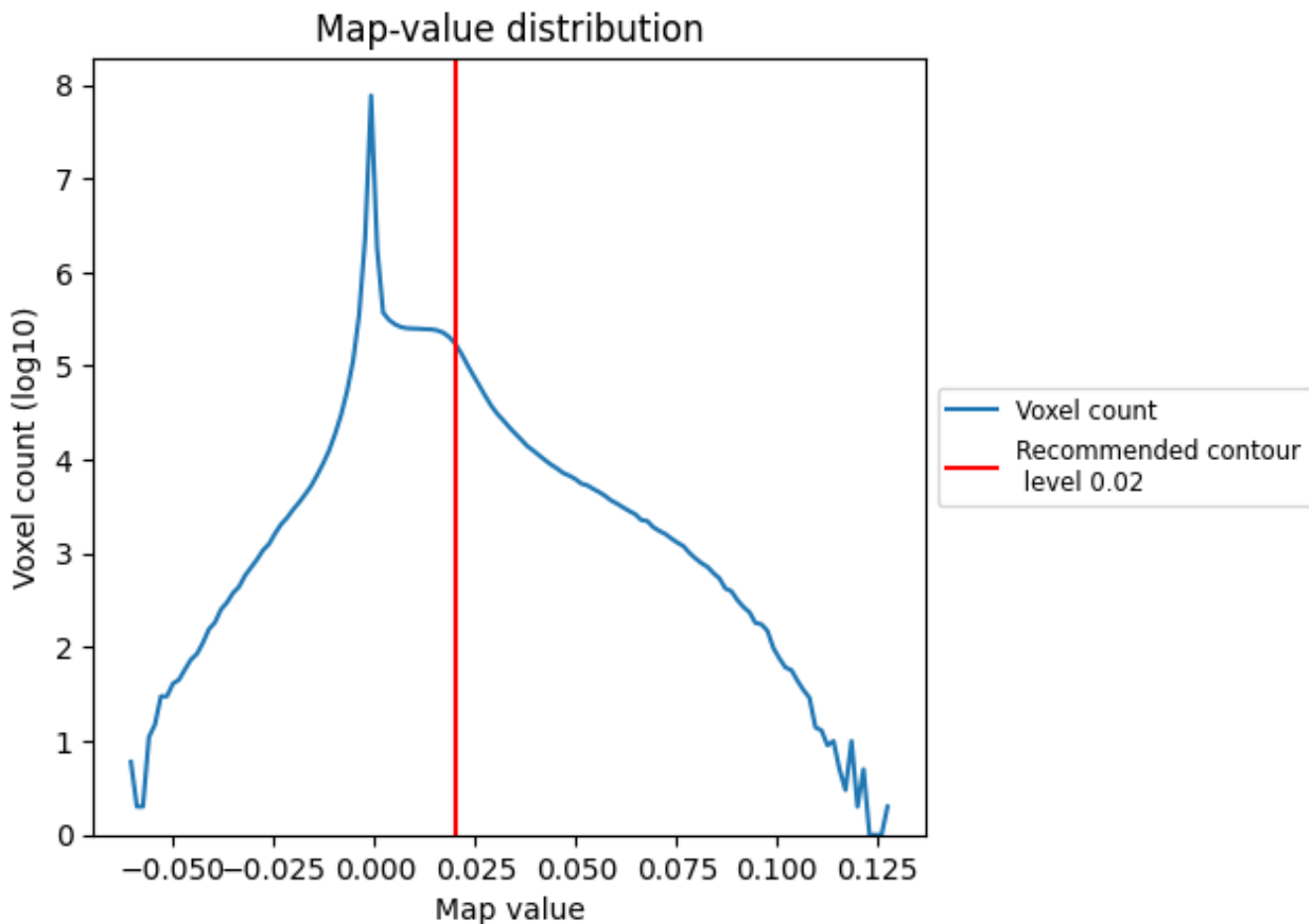


Z

7 Map analysis [i](#)

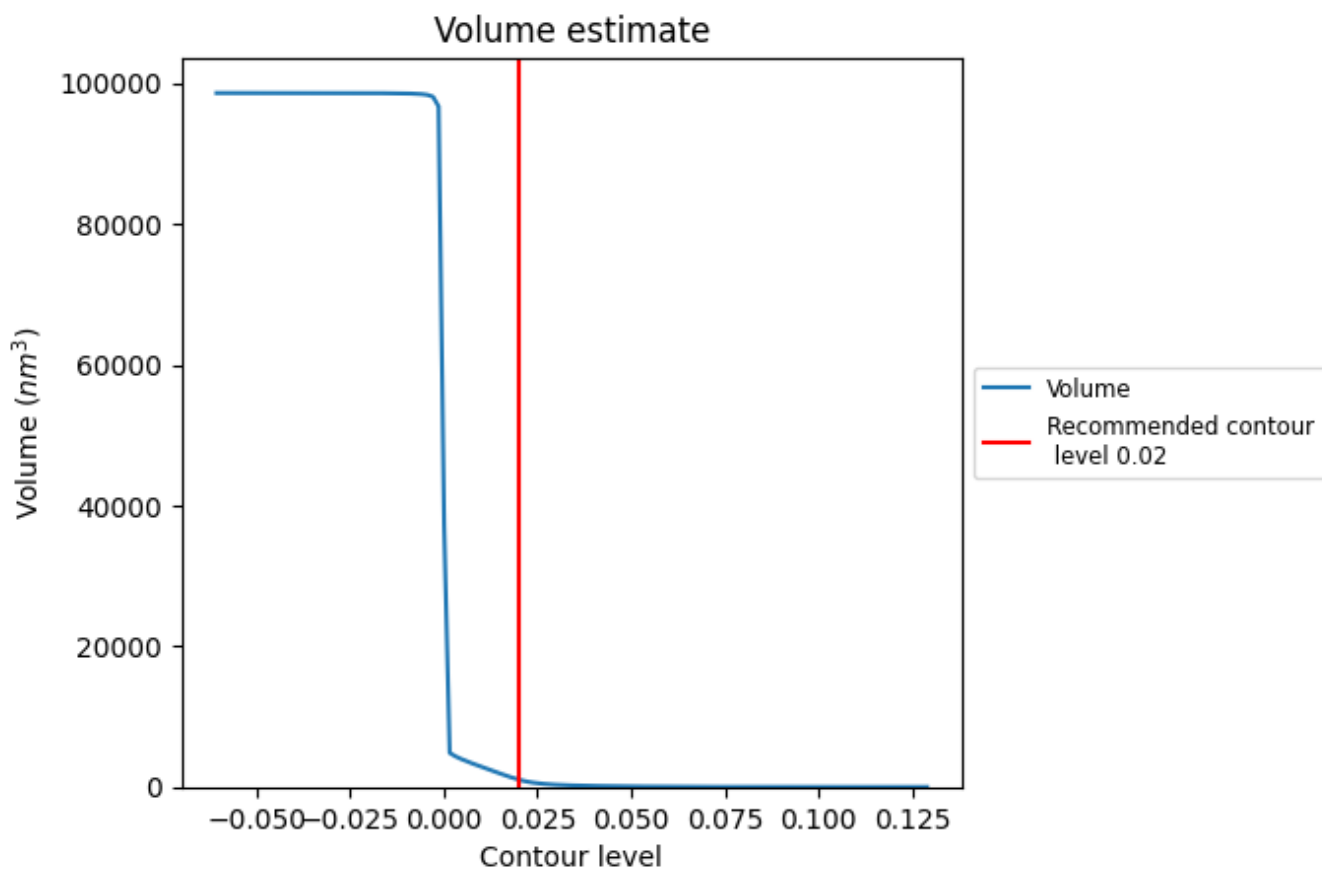
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

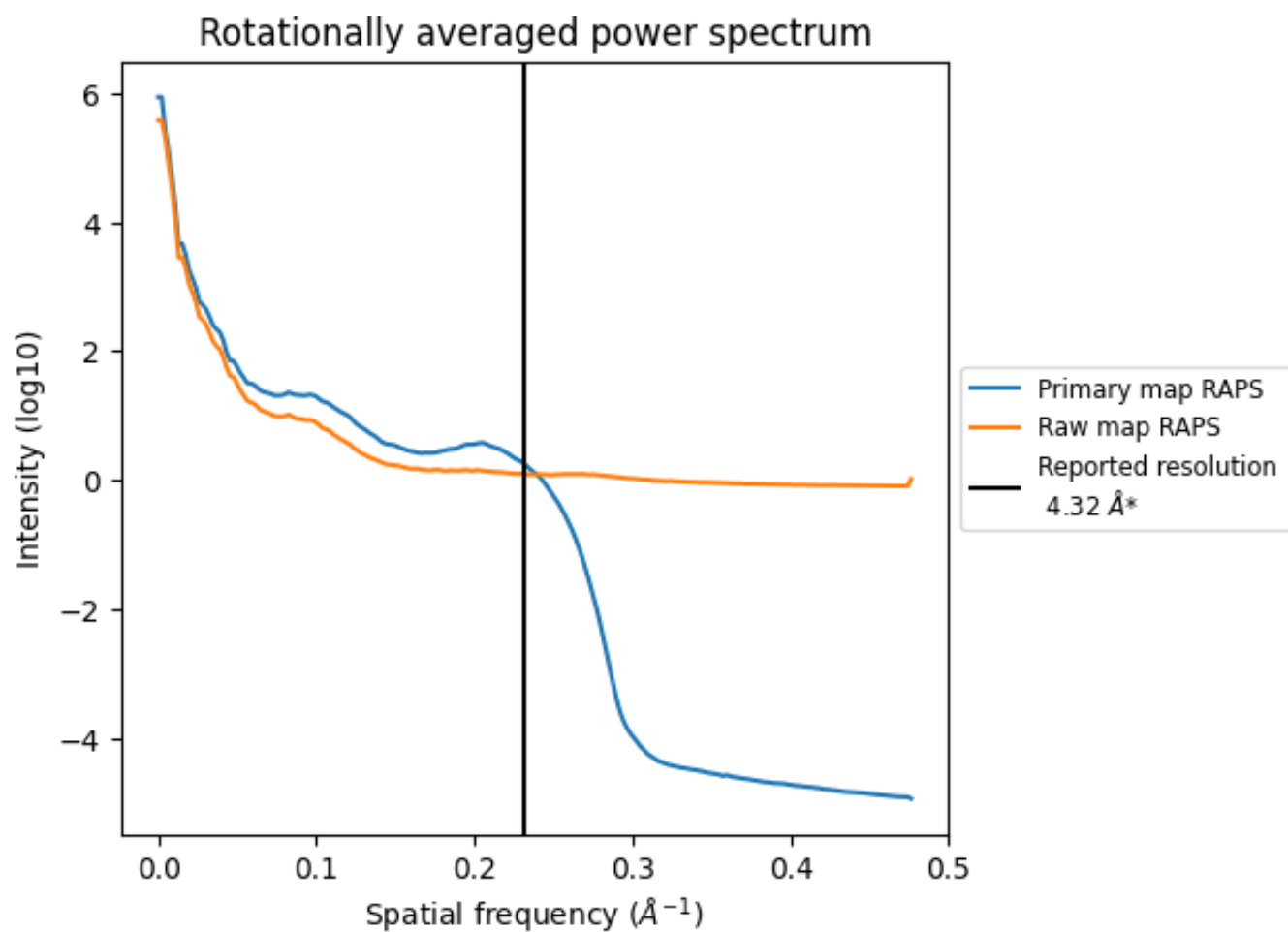
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1048 nm³; this corresponds to an approximate mass of 947 kDa.

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

7.3 Rotationally averaged power spectrum i

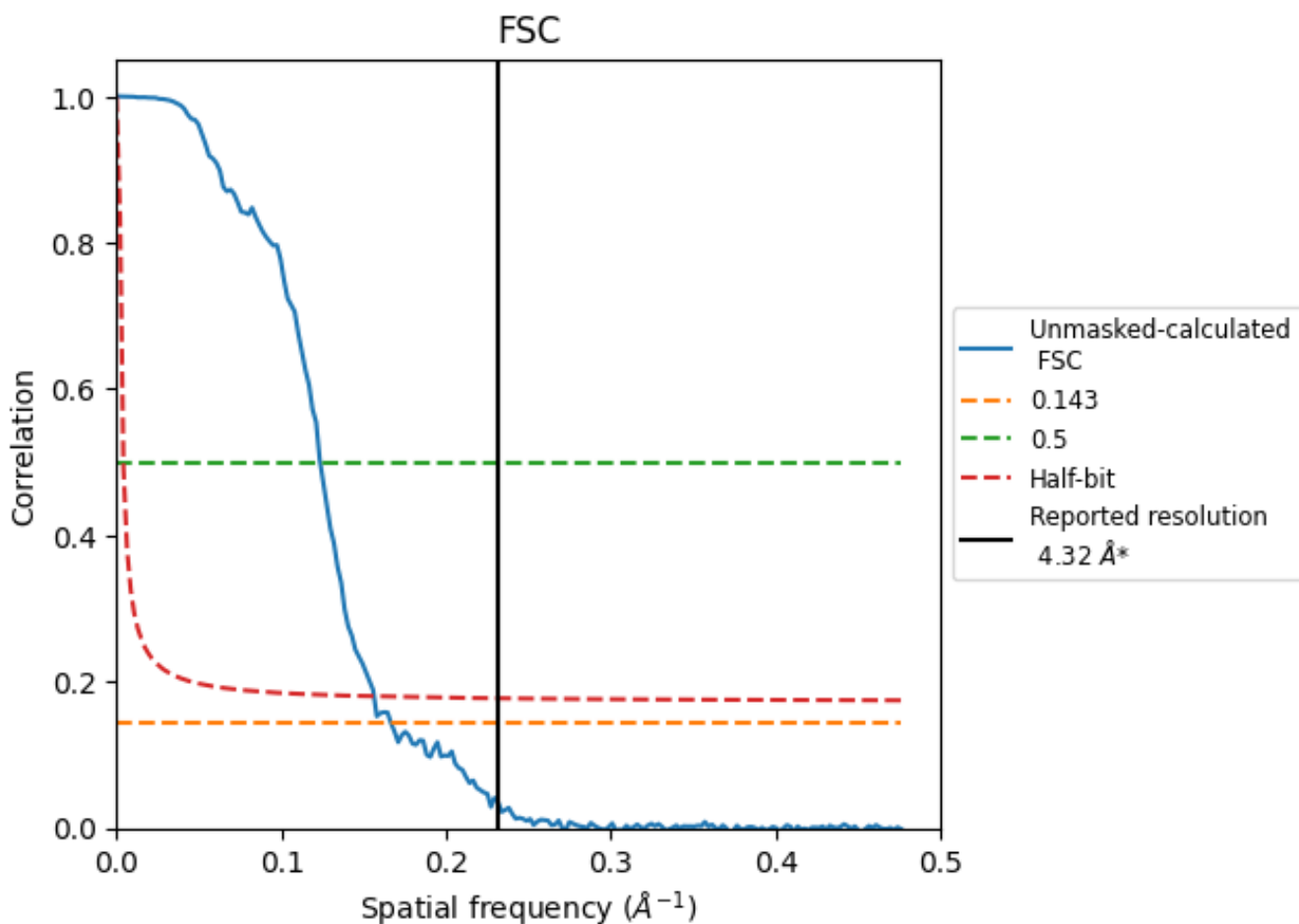


*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

8.2 Resolution estimates [i](#)

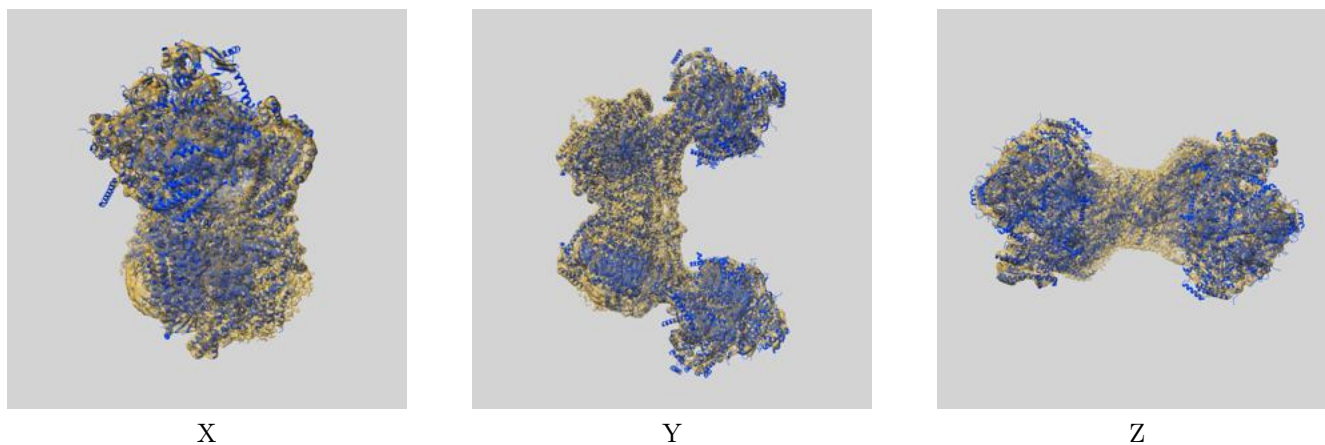
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.00	8.09	6.39

*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 6.00 differs from the reported value 4.32 by more than 10 %

9 Map-model fit [i](#)

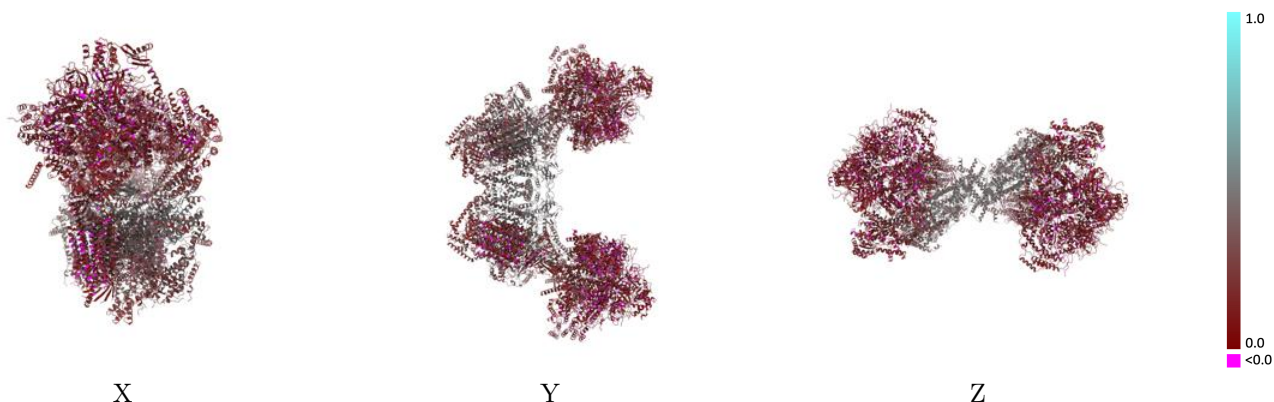
This section contains information regarding the fit between EMDB map EMD-10467 and PDB model 6TDU. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



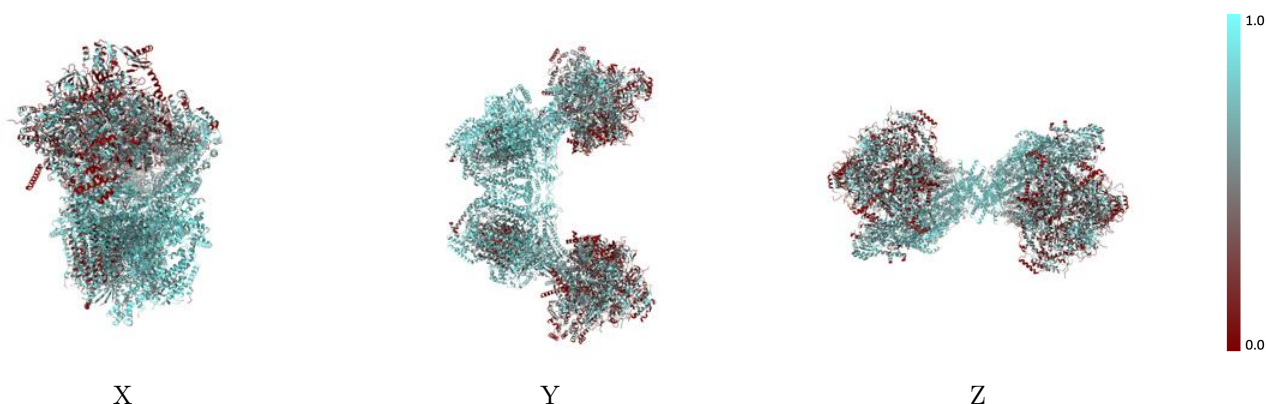
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



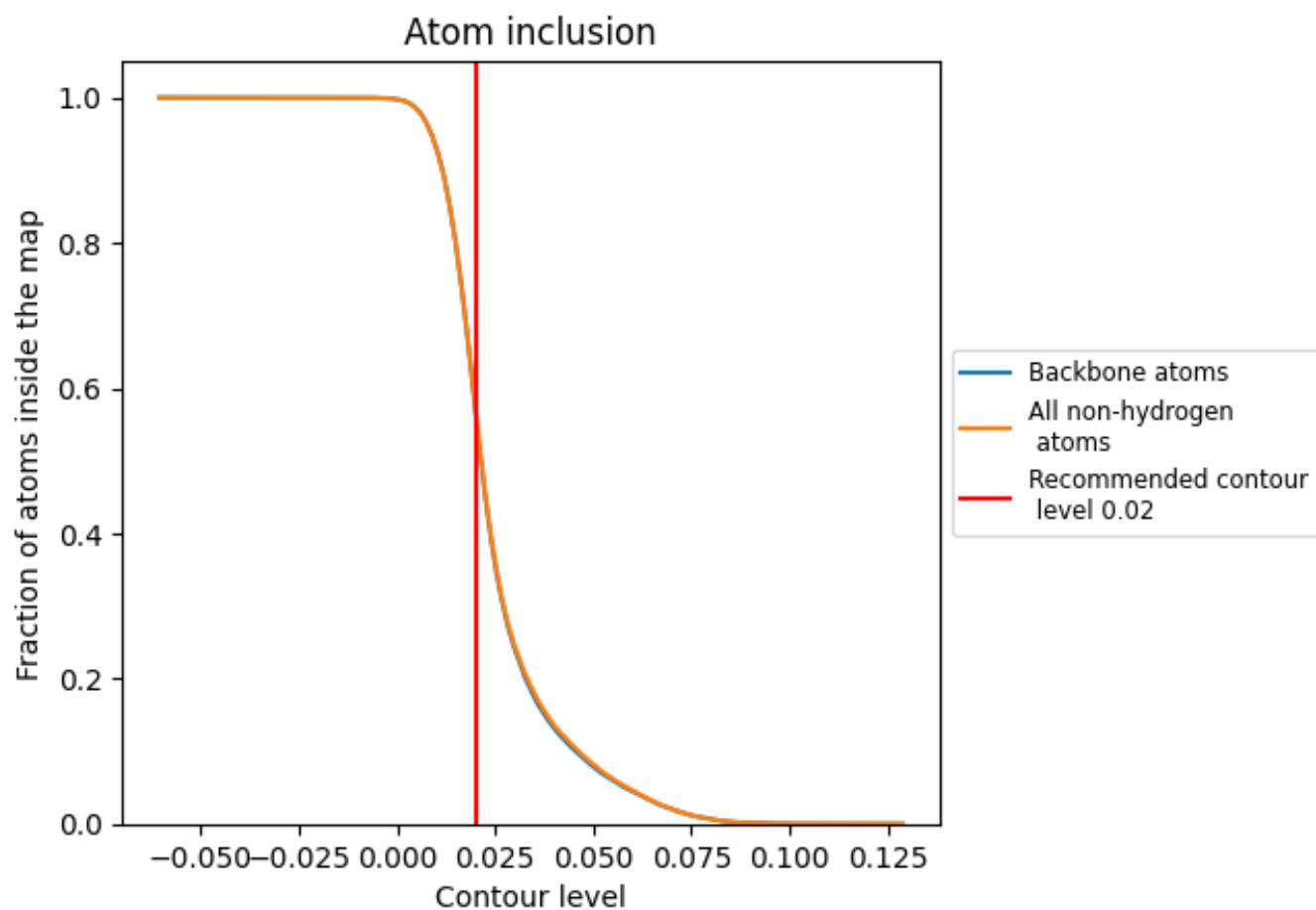
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 57% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5712	 0.2360
A	 0.8072	 0.4010
AA	 0.4295	 0.1310
AB	 0.4391	 0.1380
AC	 0.4913	 0.1490
AD	 0.3203	 0.1280
AE	 0.4388	 0.1470
AF	 0.4903	 0.1650
AG	 0.6324	 0.2230
AH	 0.6003	 0.1930
AI	 0.6111	 0.2330
AJ	 0.3055	 0.1400
AK	 0.2104	 0.1420
AL	 0.2611	 0.1490
AM	 0.3491	 0.1510
AN	 0.2926	 0.1840
AO	 0.6000	 0.2070
AP	 0.6661	 0.2470
AQ	 0.6313	 0.2490
AR	 0.5833	 0.2310
AS	 0.5496	 0.1840
AT	 0.5530	 0.1540
AU	 0.6052	 0.1700
AV	 0.6104	 0.1770
AW	 0.5565	 0.1910
AX	 0.5861	 0.1840
B	 0.6301	 0.1900
BA	 0.4391	 0.1340
BB	 0.4490	 0.1450
BC	 0.4873	 0.1440
BD	 0.3178	 0.1300
BE	 0.4459	 0.1570
BF	 0.5001	 0.1640
BG	 0.6425	 0.2250
BH	 0.6011	 0.2070



























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Chain	Atom inclusion	Q-score
BI	 0.6130	 0.2390
BJ	 0.3040	 0.1460
BK	 0.2206	 0.1400
BL	 0.2720	 0.1510
BM	 0.3458	 0.1560
BN	 0.3053	 0.1850
BO	 0.5948	 0.2010
BP	 0.6643	 0.2400
BQ	 0.6330	 0.2550
BR	 0.6083	 0.2350
BS	 0.5461	 0.1710
BT	 0.5461	 0.1360
BU	 0.5913	 0.1570
BV	 0.6035	 0.1670
BW	 0.5513	 0.1790
BX	 0.5965	 0.1840
C	 0.5397	 0.1490
D	 0.7799	 0.3460
E	 0.7676	 0.3060
F	 0.7923	 0.4060
G	 0.8163	 0.3970
H	 0.7634	 0.3340
I	 0.8027	 0.3950
J	 0.7648	 0.3630
K	 0.7914	 0.3400
L	 0.7923	 0.4220
M	 0.7769	 0.3750
N	 0.7206	 0.3800
O	 0.7074	 0.3290
P	 0.7581	 0.4120
Q	 0.7442	 0.2500
R	 0.7543	 0.3370
S	 0.7751	 0.3860
T	 0.8038	 0.3810
a	 0.8034	 0.4000
b	 0.6331	 0.1890
c	 0.5446	 0.1530
d	 0.7774	 0.3460
e	 0.7700	 0.3040
f	 0.7922	 0.4060
g	 0.8019	 0.3930
h	 0.7629	 0.3350

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Chain	Atom inclusion	Q-score
i	 0.7953	 0.3930
j	 0.7707	 0.3600
k	 0.7890	 0.3360
l	 0.7984	 0.4150
m	 0.7895	 0.3740
n	 0.7062	 0.3810
o	 0.7074	 0.3300
p	 0.7840	 0.4170
q	 0.7416	 0.2500
r	 0.7465	 0.3370
s	 0.7695	 0.3910
t	 0.7942	 0.3770