



Full wwPDB EM Validation 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

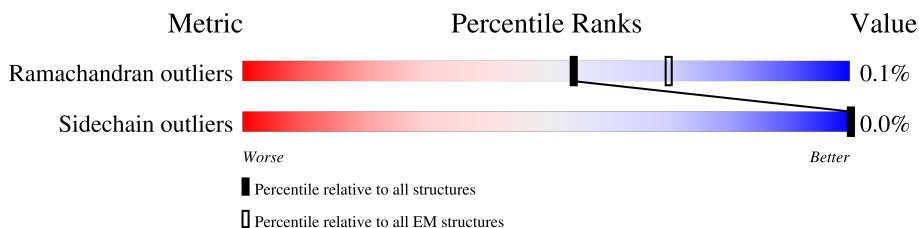
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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



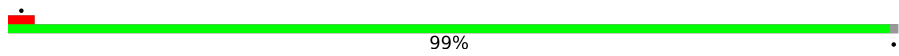
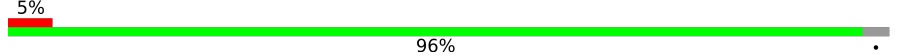
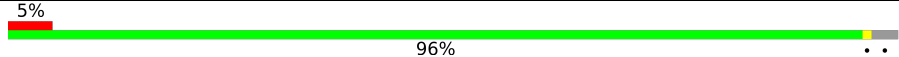
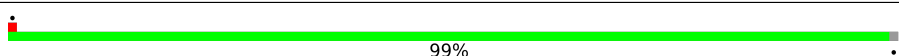
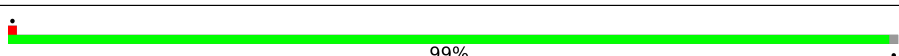
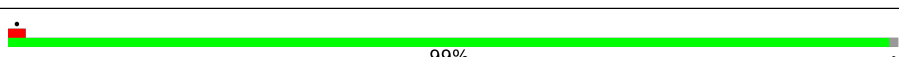
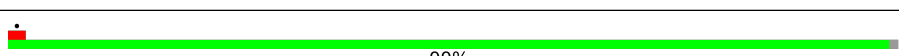
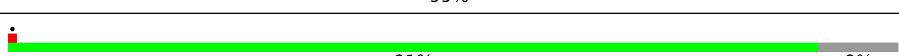
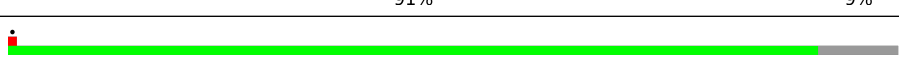
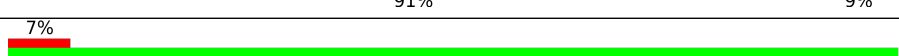
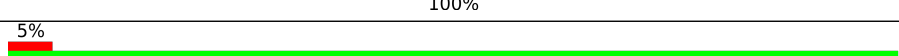
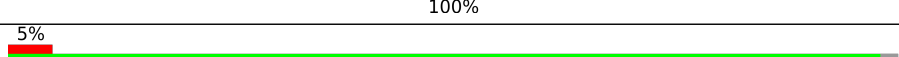
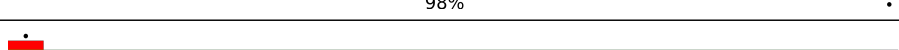
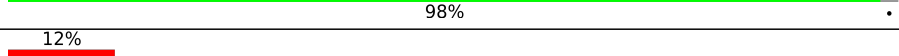
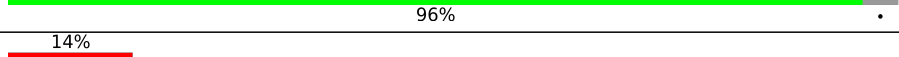
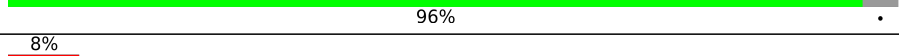


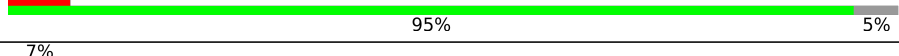
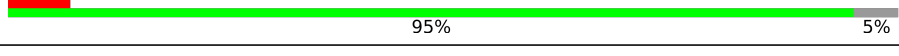
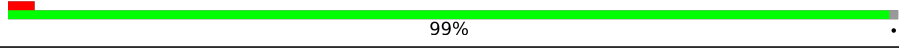
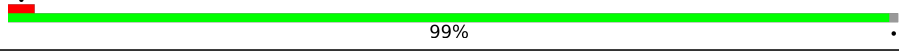



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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%

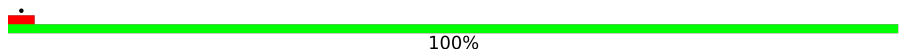
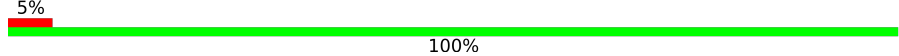
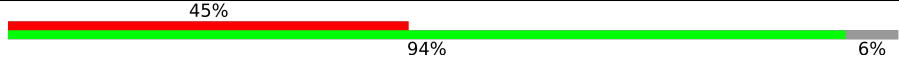
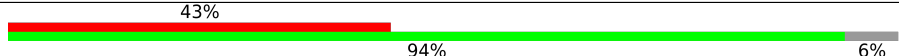
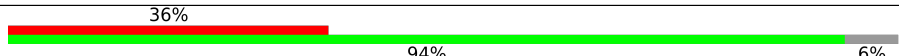
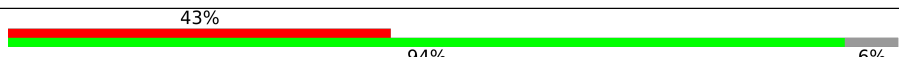
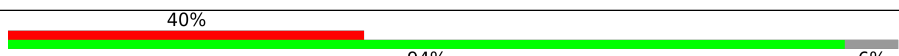
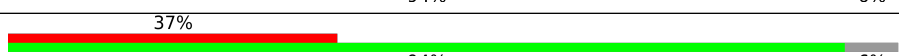
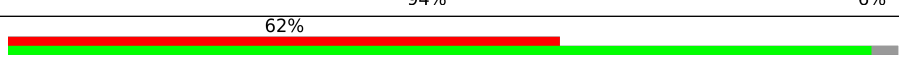
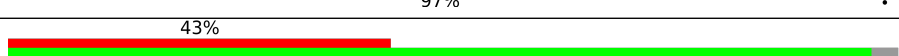
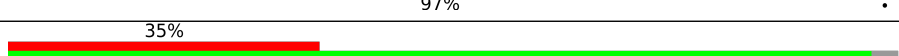
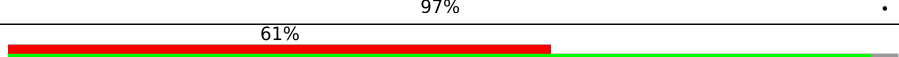
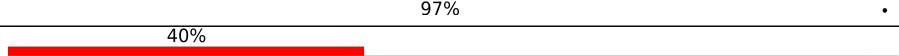
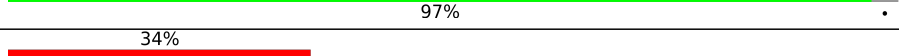
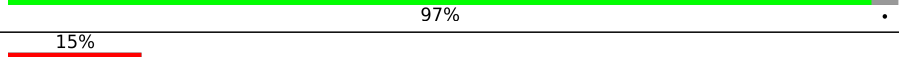
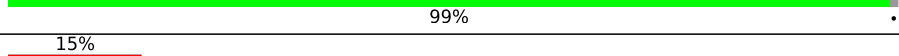
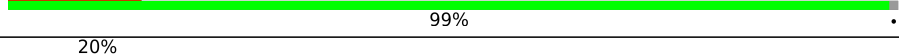
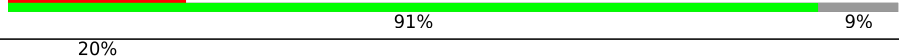
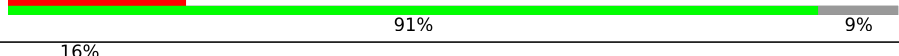
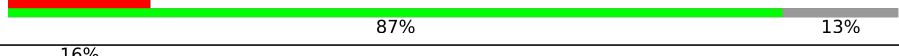

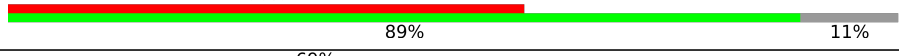

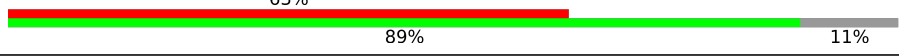
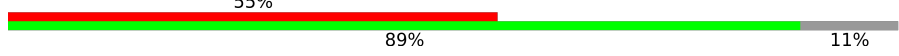
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Mol	Chain	Length	Quality of chain
5	g	112	 99%
6	H	476	 96%
6	h	476	 96%
7	I	98	 99%
7	i	98	 99%
8	J	104	 99%
8	j	104	 99%
9	K	113	 91% 9%
9	k	113	 91% 9%
10	L	57	 100%
10	l	57	 100%
11	M	169	 98%
11	m	169	 98%
12	N	137	 96%
12	n	137	 96%
13	O	116	 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%

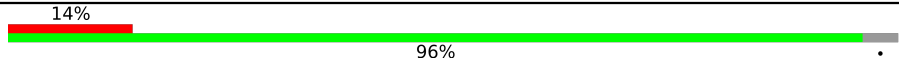
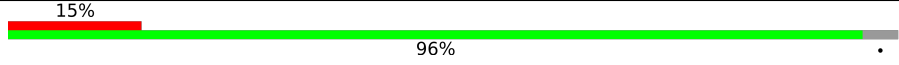
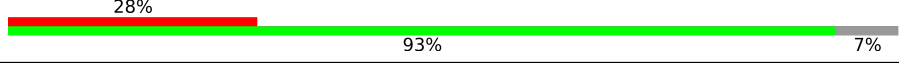
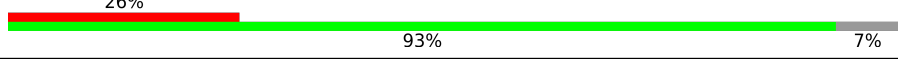
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Mol	Chain	Length	Quality of chain		
24	BL	192	61%	89%	11%
25	AM	267	53%	90%	9%
25	BM	267	52%	90%	9%
26	AN	103	31%	48%	52%
26	BN	103	31%	48%	52%
27	AO	104	21%	78%	22%
27	AP	104	12%	78%	22%
27	AQ	104	16%	78%	22%
27	AR	104	22%	78%	22%
27	AS	104	26%	78%	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	7864	2525	3919	677	733	10	0	0
1	a	486	7864	2525	3919	677	733	10	0	0

- Molecule 2 is a protein called ATPTB6.

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

- Molecule 3 is a protein called ATPTB12.

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

- 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	4642	1566	2329	342	391	14	0	0
4	f	274	4642	1566	2329	342	391	14	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called ATPEG1.

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

- Molecule 12 is a protein called ATPEG2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			
12	N	131	2168	714	1071	198	182	3	0	0
12	n	131	2168	714	1071	198	182	3	0	0

- Molecule 13 is a protein called ATPEG3.

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

- Molecule 14 is a protein called ATPEG4.

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

- Molecule 15 is a protein called ATPEG5.

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

- 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.

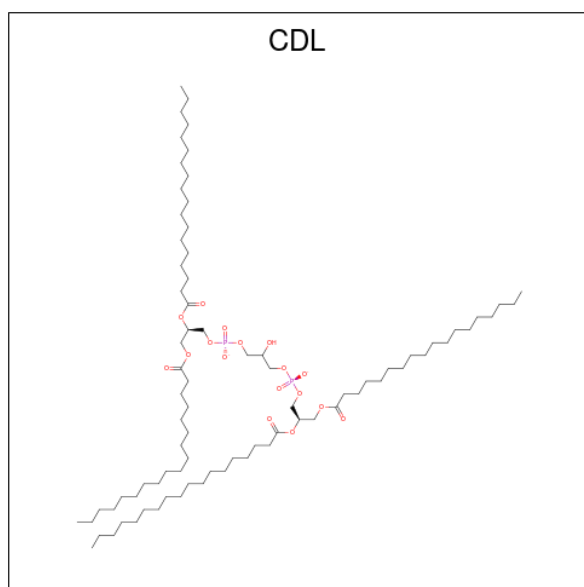
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	C	157	Total 2472	C 781	H 1241	N 211	O 237	S 2	0	0

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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).



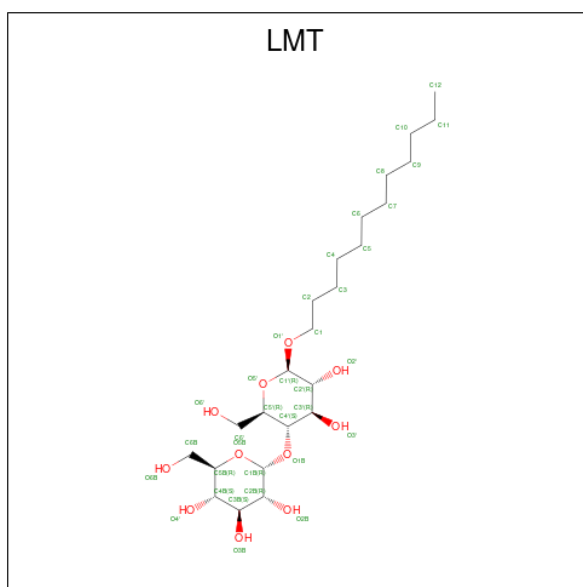
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
30	A	1	820	298	427	85	10	0
30	A	1	820	298	427	85	10	0
30	A	1	820	298	427	85	10	0
30	A	1	820	298	427	85	10	0
30	A	1	820	298	427	85	10	0
30	D	1	228	72	137	17	2	0
30	E	1	95	44	32	17	2	0
30	M	1	312	126	129	51	6	0
30	M	1	312	126	129	51	6	0
30	M	1	312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

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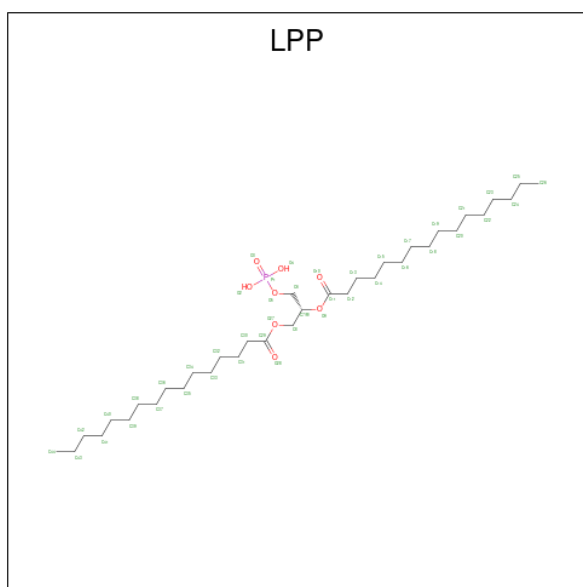
Mol	Chain	Residues	Atoms					AltConf
30	O	1	Total	C	H	O	P	0
			124	46	59	17	2	
30	P	1	Total	C	H	O	P	0
			319	108	173	34	4	
30	P	1	Total	C	H	O	P	0
			319	108	173	34	4	
30	R	1	Total	C	H	O	P	0
			150	57	74	17	2	
30	a	1	Total	C	H	O	P	0
			820	298	427	85	10	
30	a	1	Total	C	H	O	P	0
			820	298	427	85	10	
30	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: $C_{24}H_{46}O_{11}$).



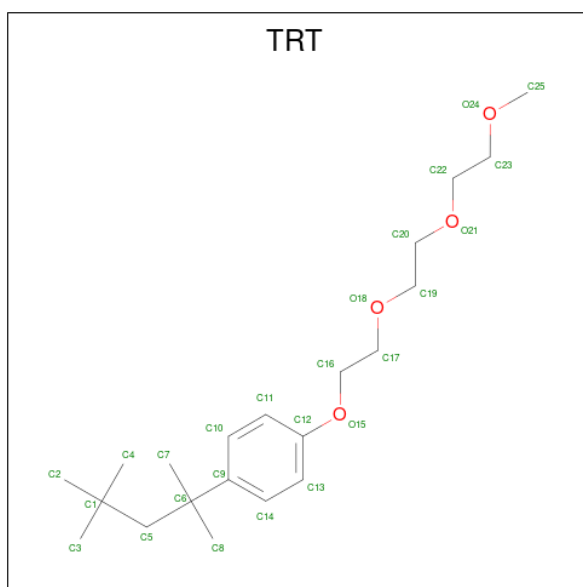
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
31	D	1	81	24	46	11	0
31	F	1	81	24	46	11	0
31	N	1	81	24	46	11	0
31	Q	1	81	24	46	11	0
31	d	1	81	24	46	11	0
31	g	1	81	24	46	11	0
31	n	1	81	24	46	11	0
31	q	1	81	24	46	11	0

- 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	41	15	17	8	1	0
32	I	1	111	35	67	8	1	0
32	K	1	48	22	17	8	1	0
32	N	1	43	17	17	8	1	0
32	O	1	114	37	59	16	2	0
32	O	1	114	37	59	16	2	0
32	f	1	41	15	17	8	1	0
32	i	1	111	35	67	8	1	0
32	k	1	48	22	17	8	1	0
32	n	1	43	17	17	8	1	0
32	o	1	114	37	59	16	2	0
32	o	1	114	37	59	16	2	0

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



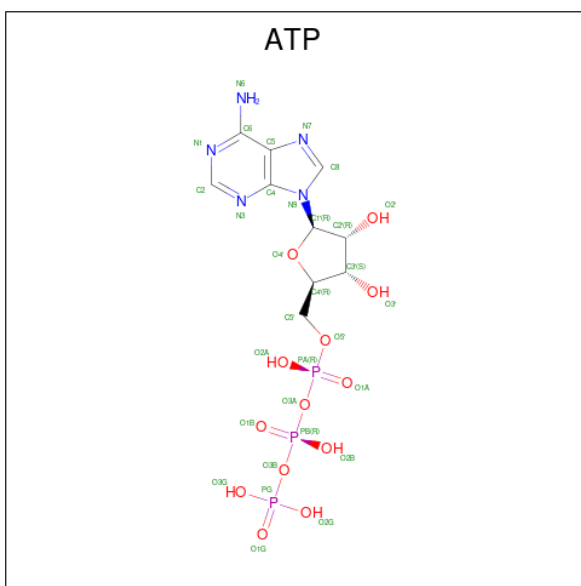
Mol	Chain	Residues	Atoms				AltConf
33	G	1	Total	C	H	O	0
			122	42	72	8	
33	G	1	Total	C	H	O	0
			122	42	72	8	
33	M	1	Total	C	H	O	0
			122	42	72	8	
33	M	1	Total	C	H	O	0
			122	42	72	8	
33	N	1	Total	C	H	O	0
			122	42	72	8	
33	N	1	Total	C	H	O	0
			122	42	72	8	
33	P	1	Total	C	H	O	0
			61	21	36	4	
33	g	1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

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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
			Total	C	H	N	O	P	
34	BF	1	35	10	4	5	13	3	0

- 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).



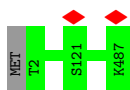
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
36	AD	1	34	10	7	5	10	2	0
36	BD	1	35	10	8	5	10	2	0

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.

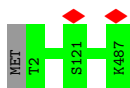
- Molecule 1: ATPTB1

Chain A:  100%



- Molecule 1: ATPTB1

Chain a:  100%



- Molecule 2: ATPTB6

Chain D:  99%



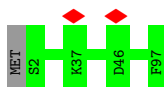
- Molecule 2: ATPTB6

Chain d:  99%

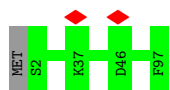


- Molecule 3: ATPTB12

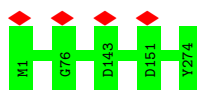
Chain E:  99%



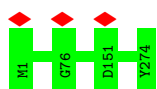
- Molecule 3: ATPTB12



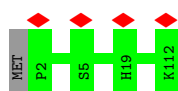
• Molecule 4: ATP synthase subunit a



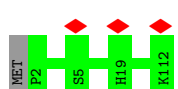
• Molecule 4: ATP synthase subunit a



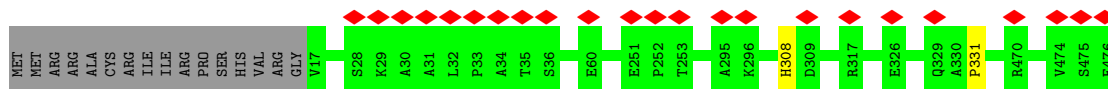
• Molecule 5: ATP synthase subunit b



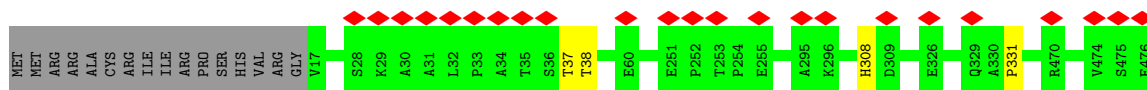
• Molecule 5: ATP synthase subunit b



• Molecule 6: ATP synthase subunit d



• Molecule 6: ATP synthase subunit d



- Molecule 7: ATP synthase subunit f

Chain I:  99%



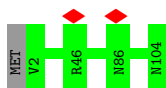
- Molecule 7: ATP synthase subunit f

Chain i:  99%



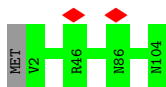
- Molecule 8: ATP synthase subunit i/j

Chain J:  99%

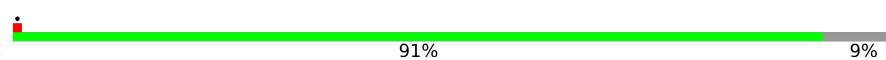


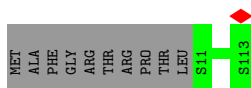
- Molecule 8: ATP synthase subunit i/j

Chain j:  99%

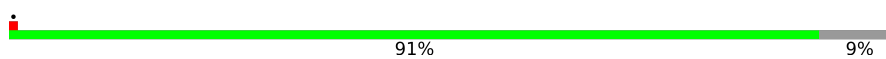


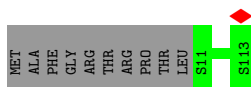
- Molecule 9: ATP synthase subunit k

Chain K:  91%



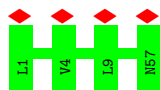
- Molecule 9: ATP synthase subunit k

Chain k:  91%

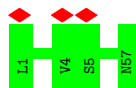


- Molecule 10: ATP synthase subunit 8

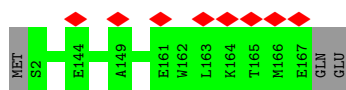
Chain L:  7%



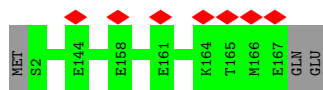
- Molecule 10: ATP synthase subunit 8



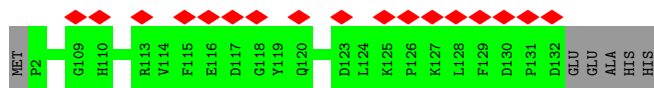
- Molecule 11: ATPEG1



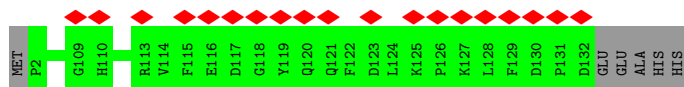
- Molecule 11: ATPEG1



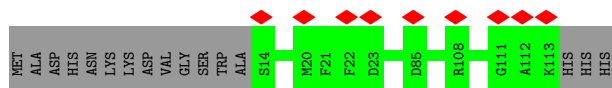
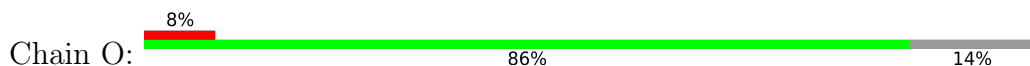
- Molecule 12: ATPEG2



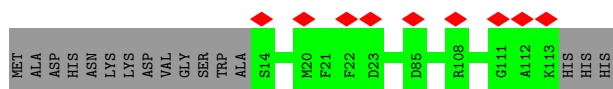
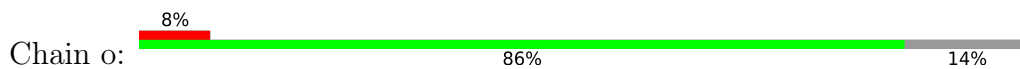
- Molecule 12: ATPEG2



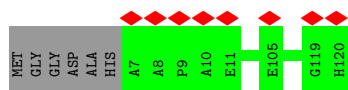
- Molecule 13: ATPEG3



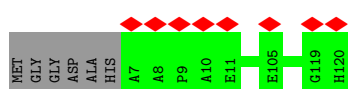
- Molecule 13: ATPEG3



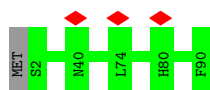
• Molecule 14: ATPEG4



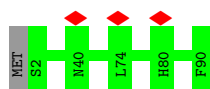
• Molecule 14: ATPEG4



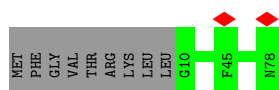
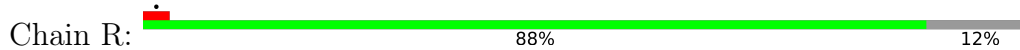
• Molecule 15: ATPEG5



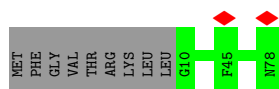
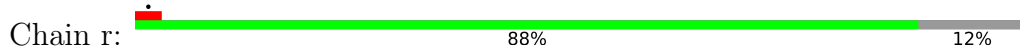
• Molecule 15: ATPEG5



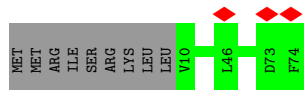
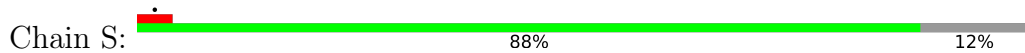
• Molecule 16: ATPEG6



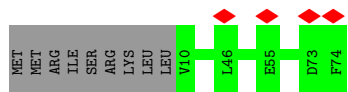
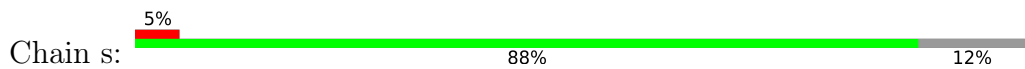
• Molecule 16: ATPEG6



• Molecule 17: ATPEG7



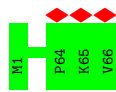
• Molecule 17: ATPEG7



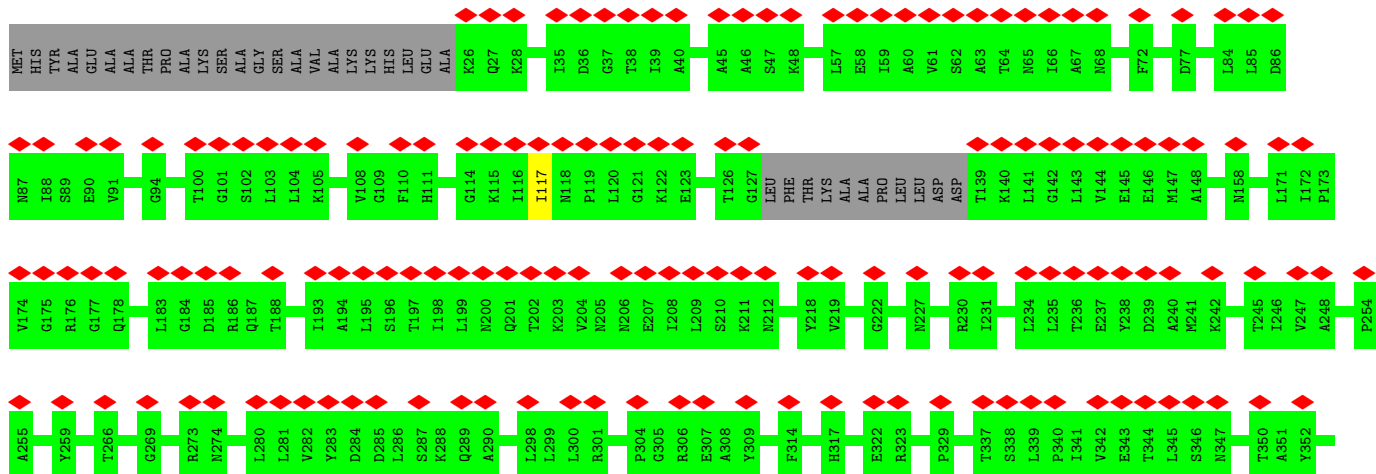
• Molecule 18: ATPEG8

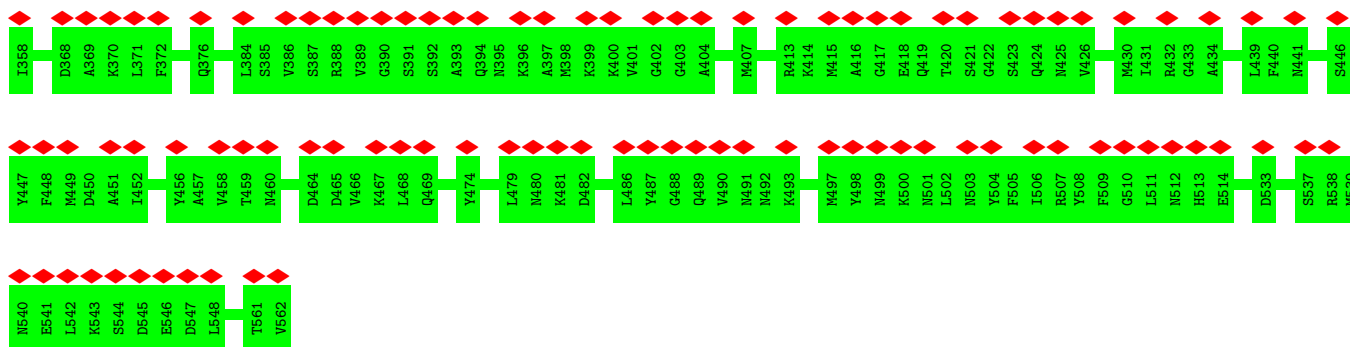


• Molecule 18: ATPEG8

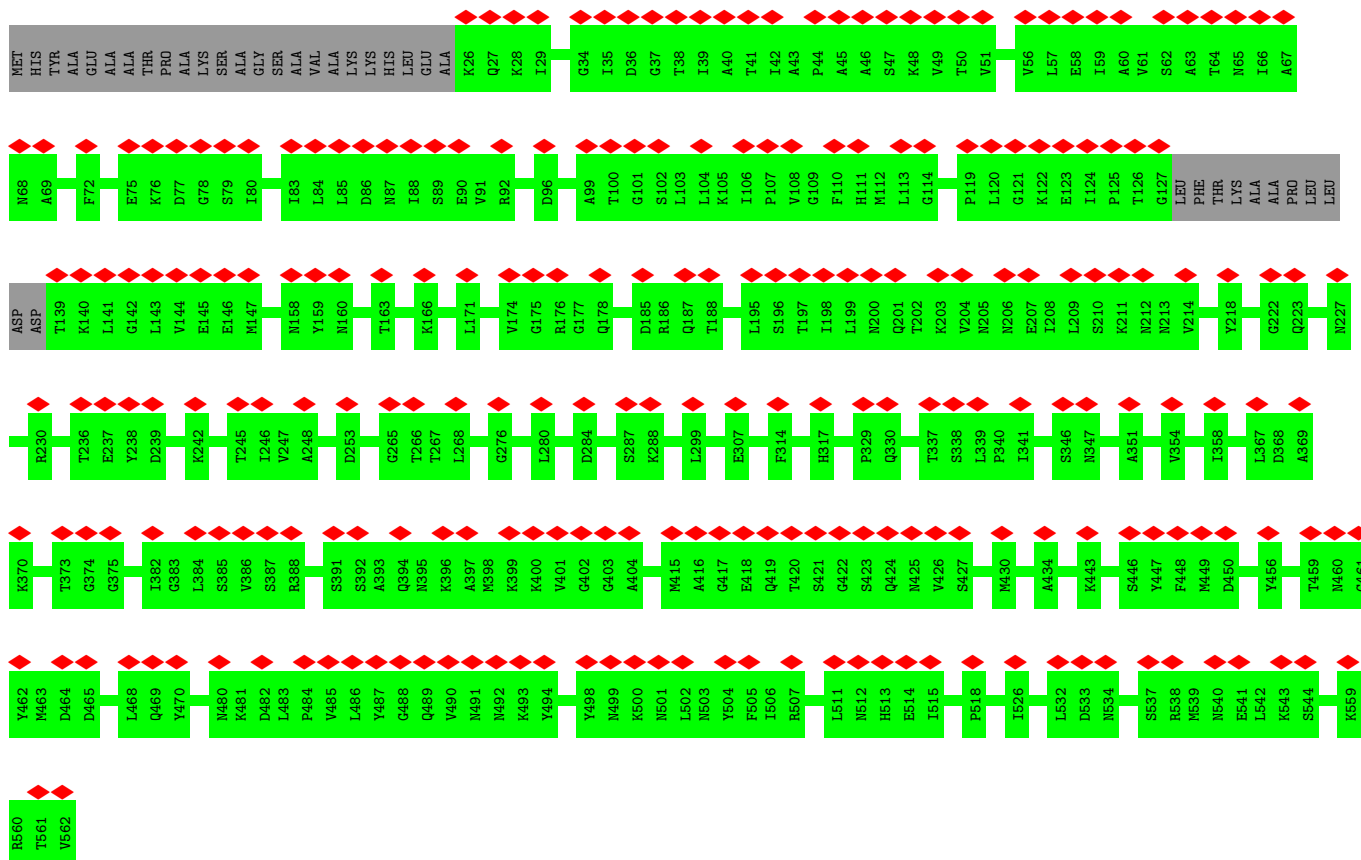


• Molecule 19: ATP synthase subunit alpha

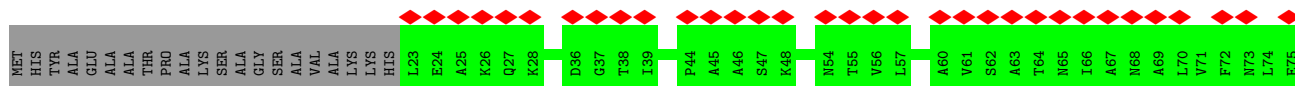


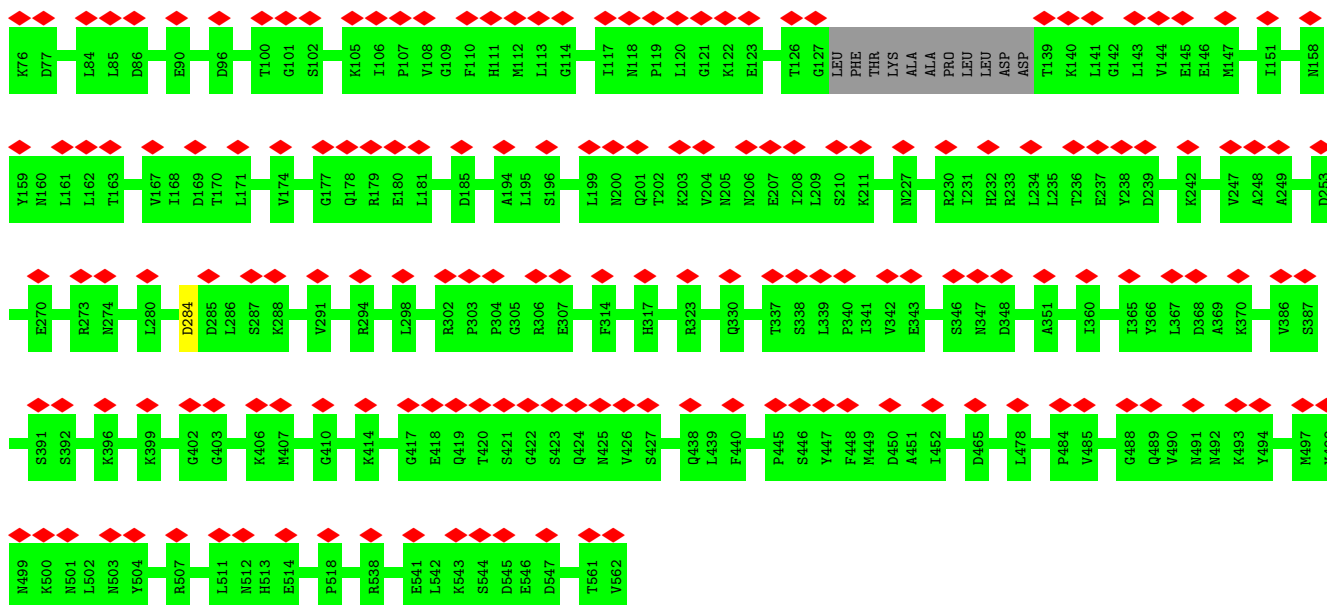


• Molecule 19: ATP synthase subunit alpha

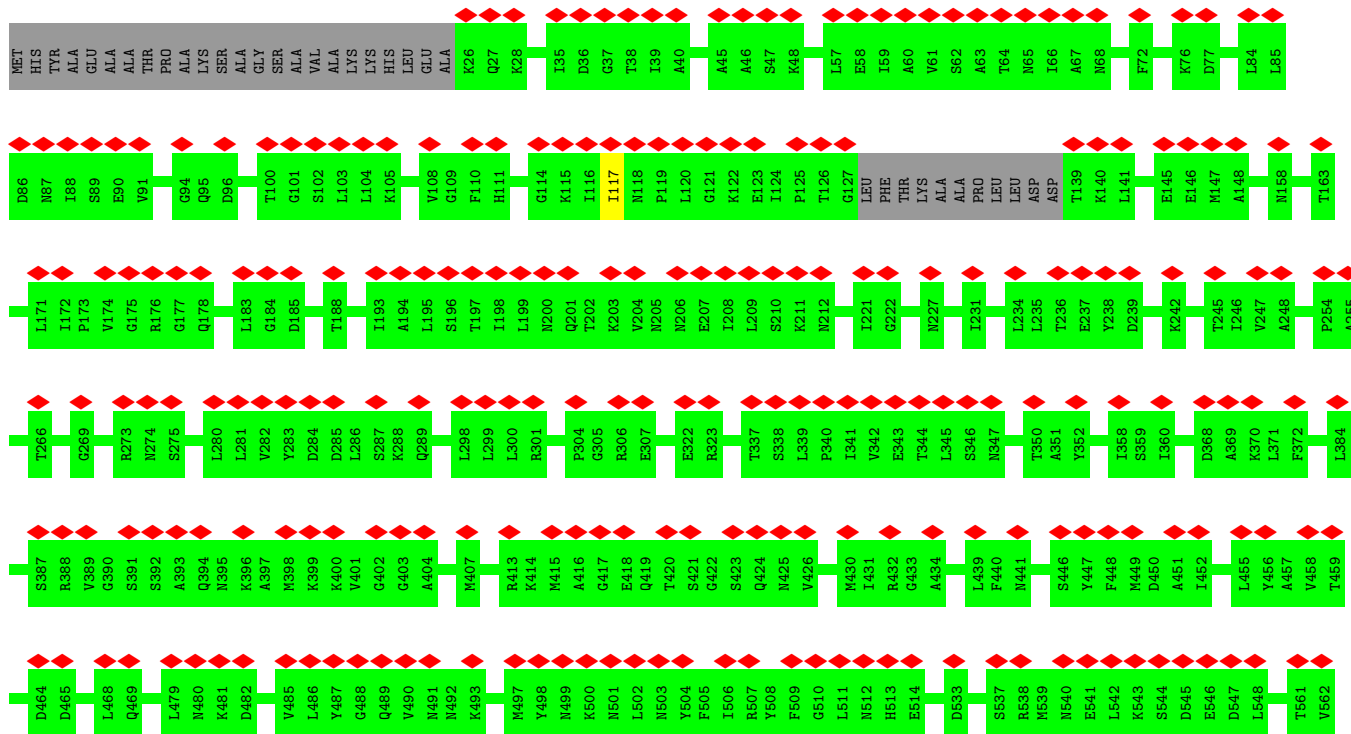
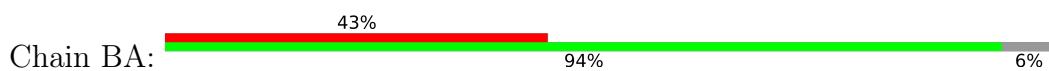


• Molecule 19: ATP synthase subunit alpha

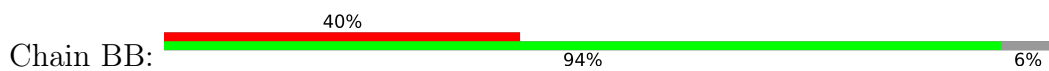


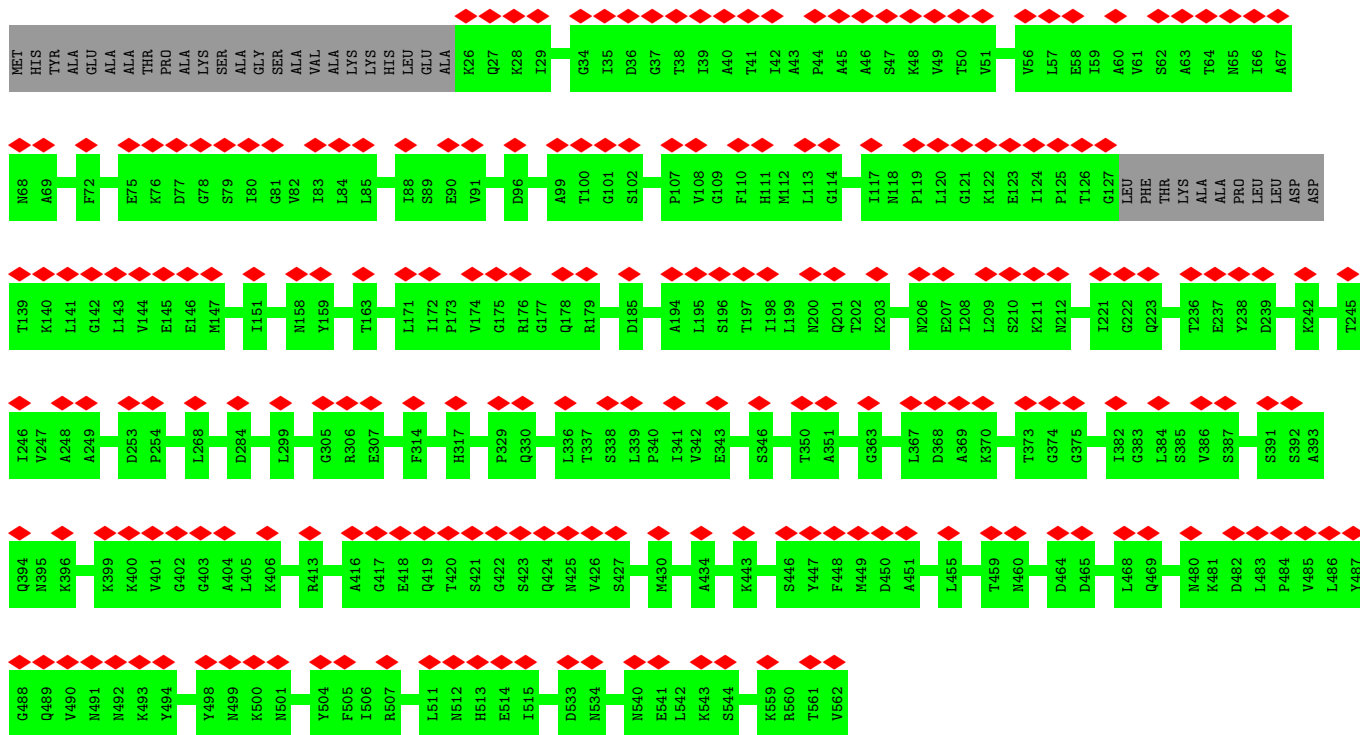


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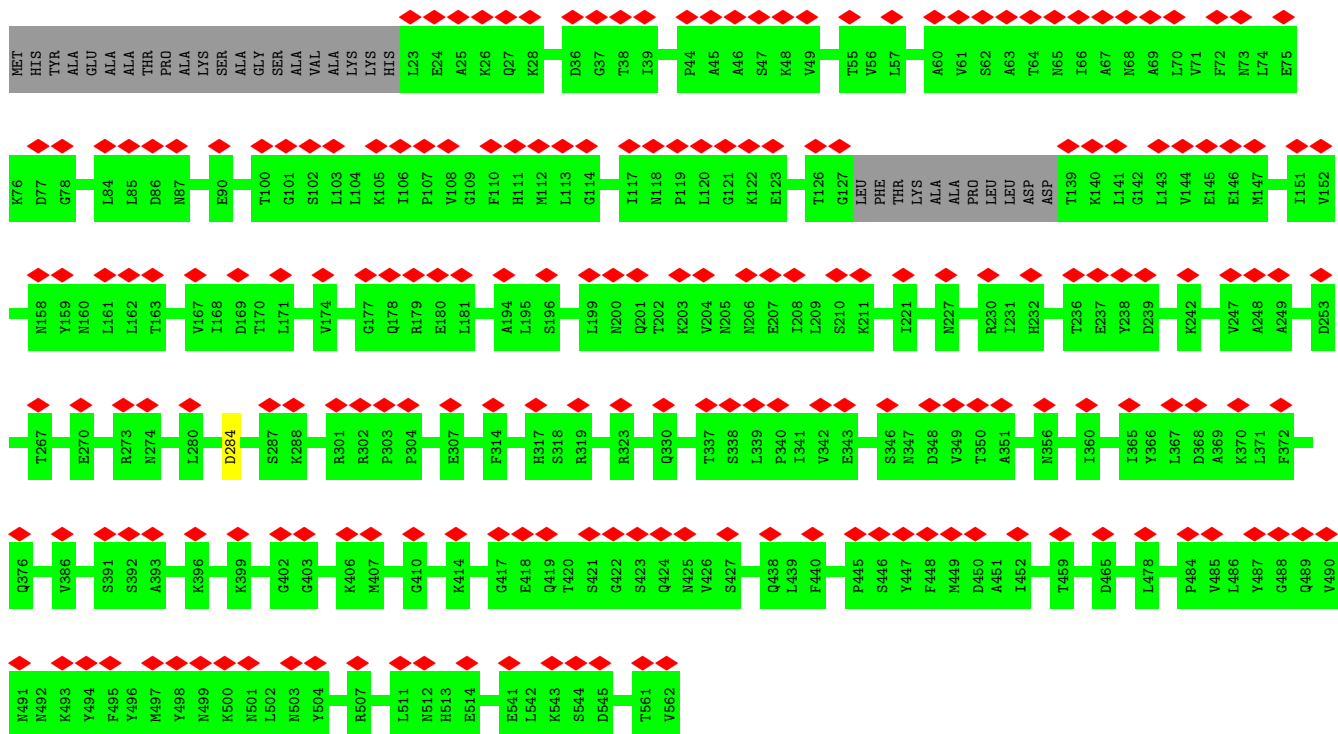
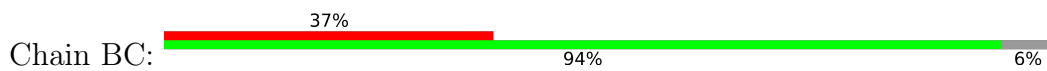


• Molecule 19: ATP synthase subunit alpha

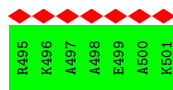




• Molecule 19: ATP synthase subunit alpha

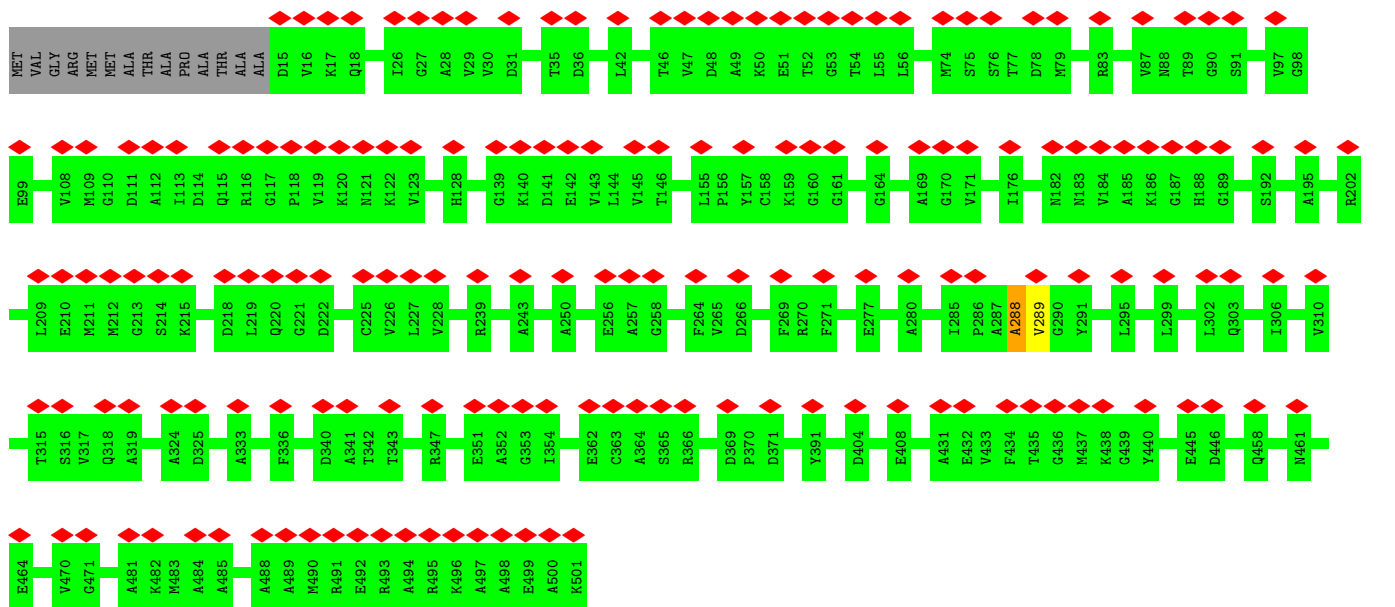


• Molecule 20: ATP synthase subunit beta



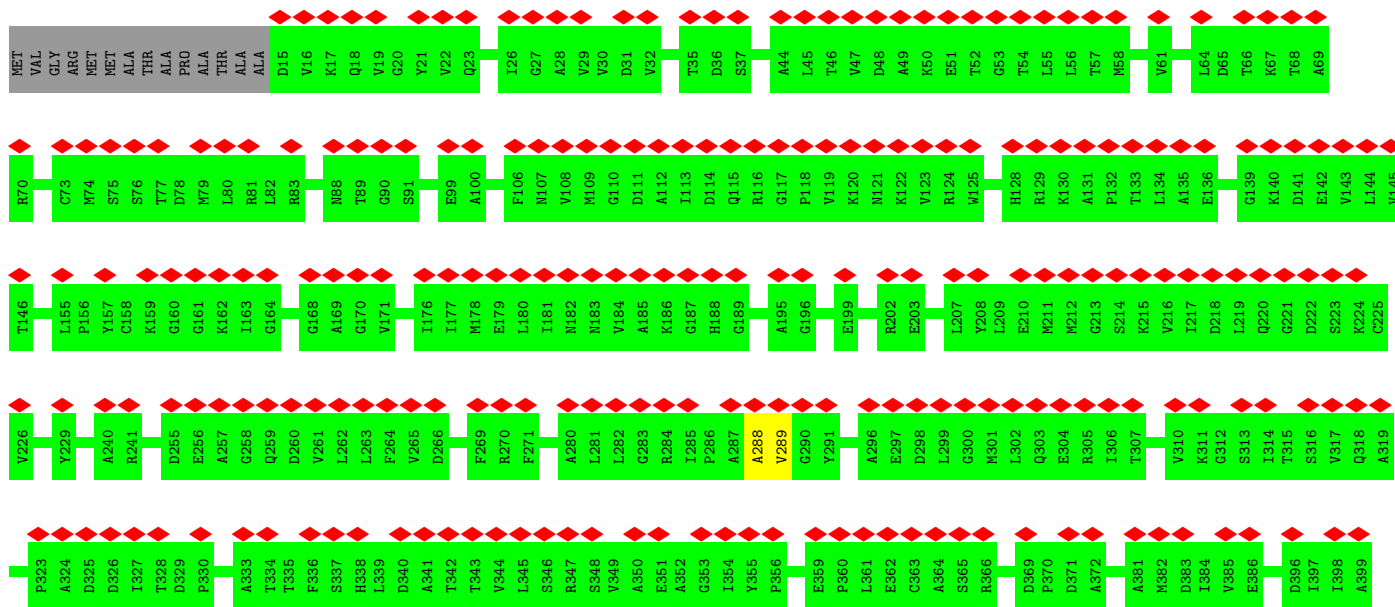
- Molecule 20: ATP synthase subunit beta

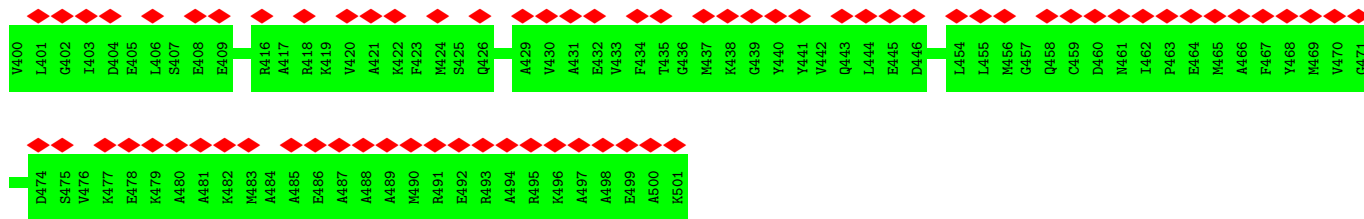
Chain AF: 35% 97%



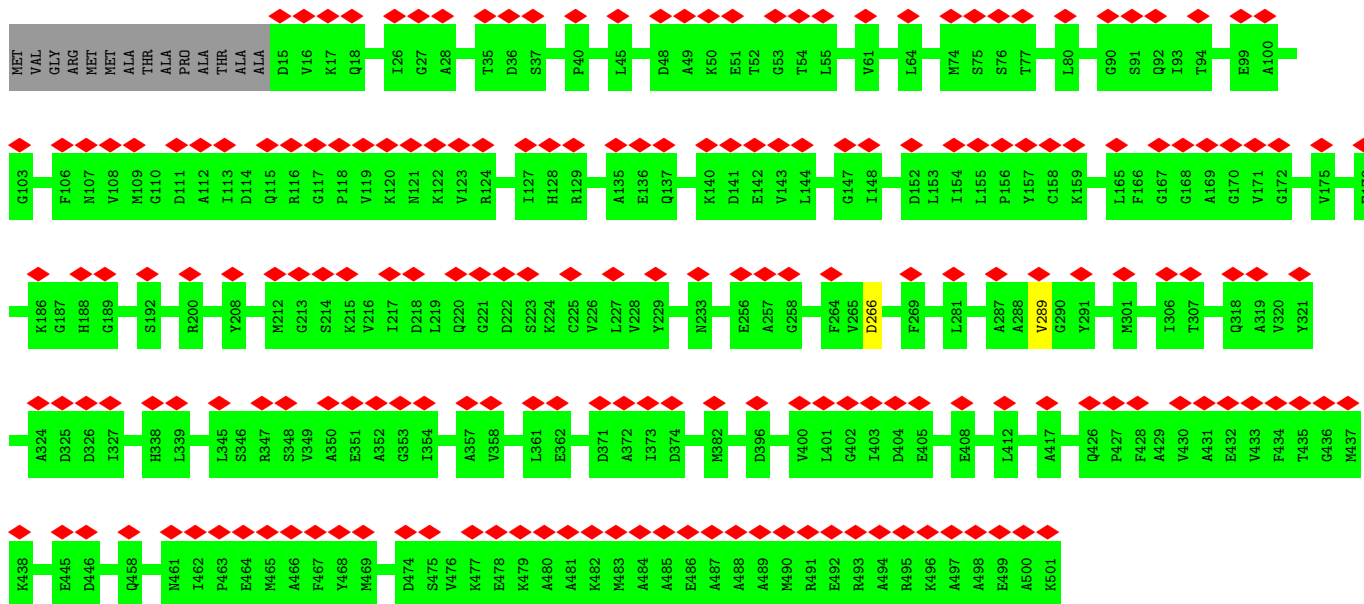
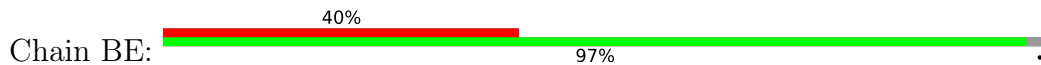
- Molecule 20: ATP synthase subunit beta

Chain BD: 61% 97%

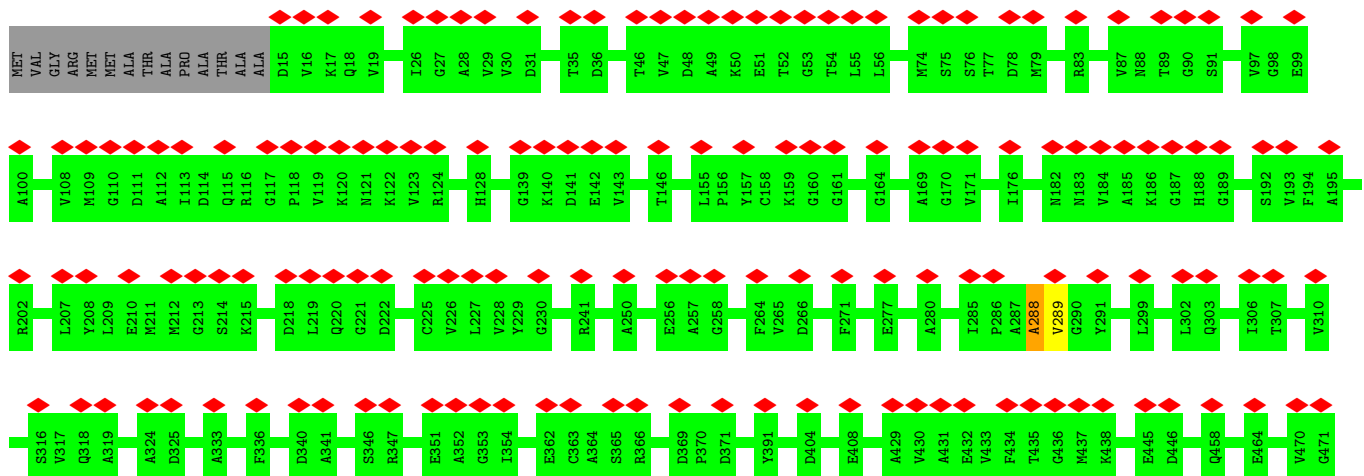




• Molecule 20: ATP synthase subunit beta



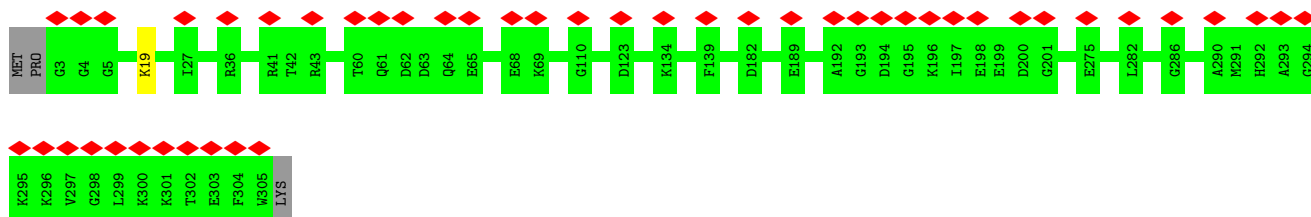
• Molecule 20: ATP synthase subunit beta





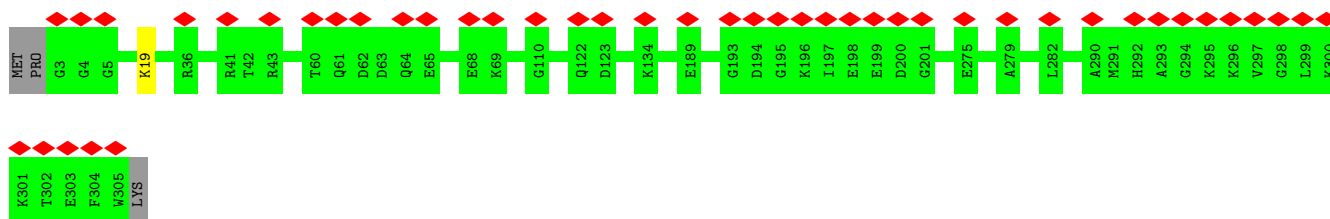
- Molecule 21: ATP synthase subunit gamma

Chain AG: 15% 99%



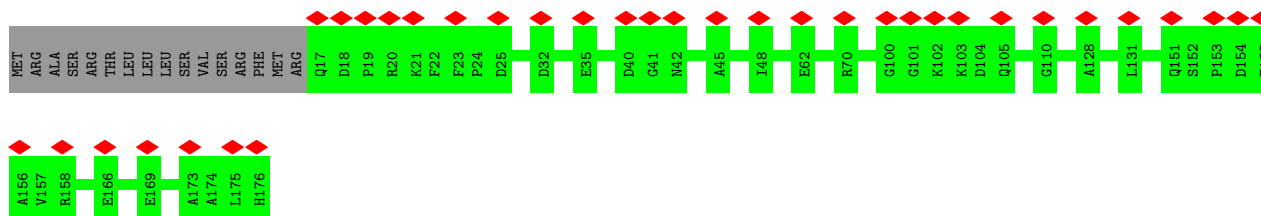
- Molecule 21: ATP synthase subunit gamma

Chain BG: 15% 99%



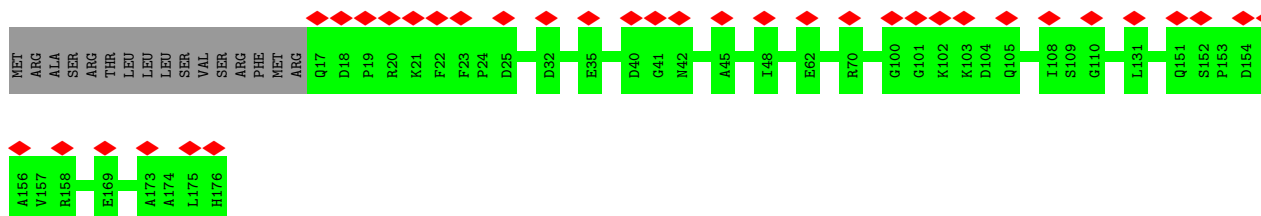
- Molecule 22: ATP synthase subunit delta

Chain AH: 20% 91% 9%

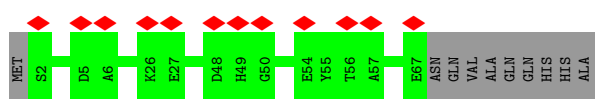
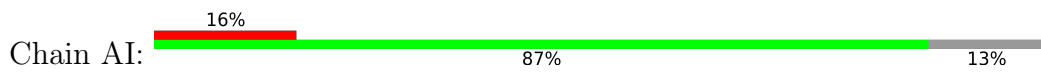


- Molecule 22: ATP synthase subunit delta

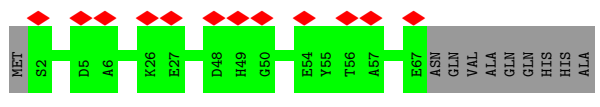
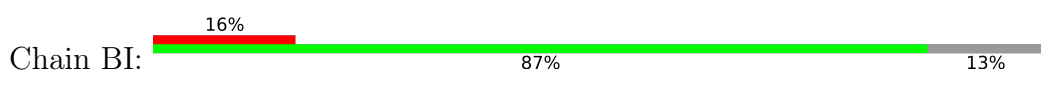
Chain BH: 20% 91% 9%



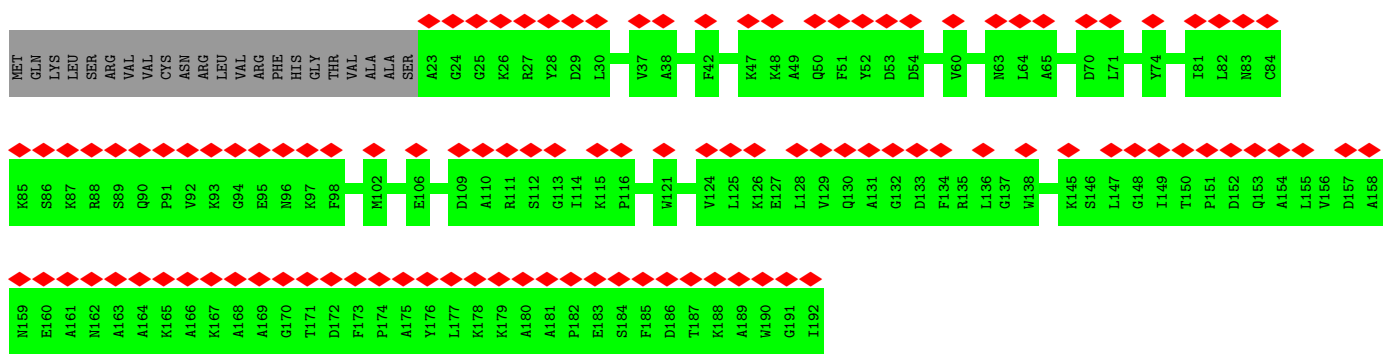
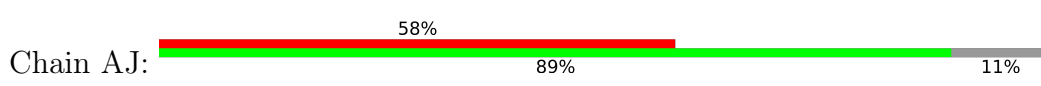
- Molecule 23: ATP synthase subunit epsilon



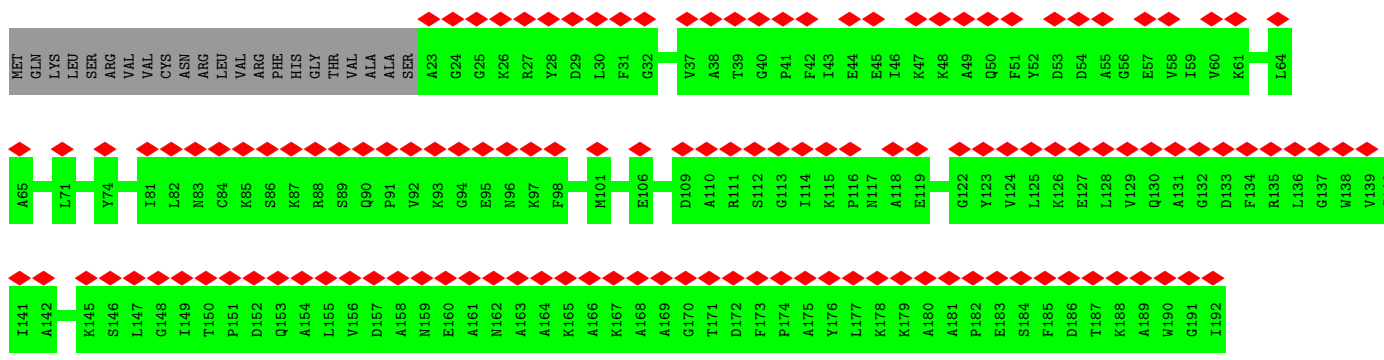
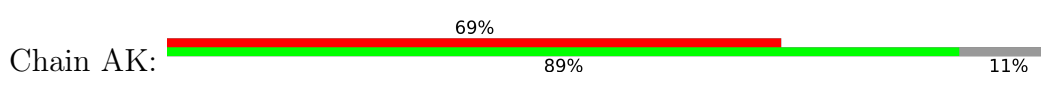
- Molecule 23: ATP synthase subunit epsilon



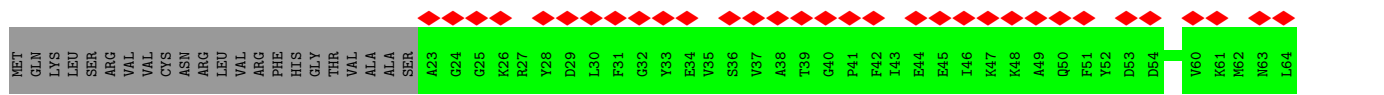
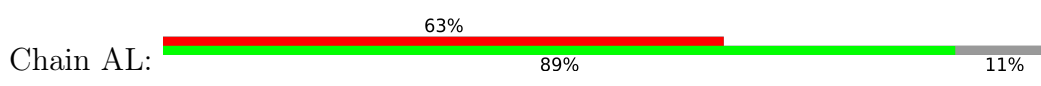
- Molecule 24: p18

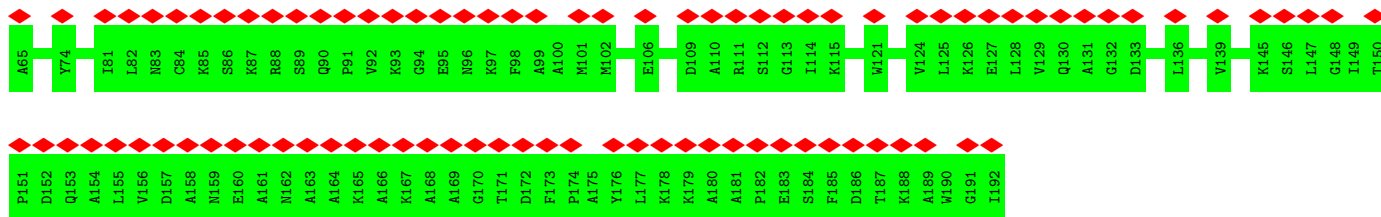


- Molecule 24: p18

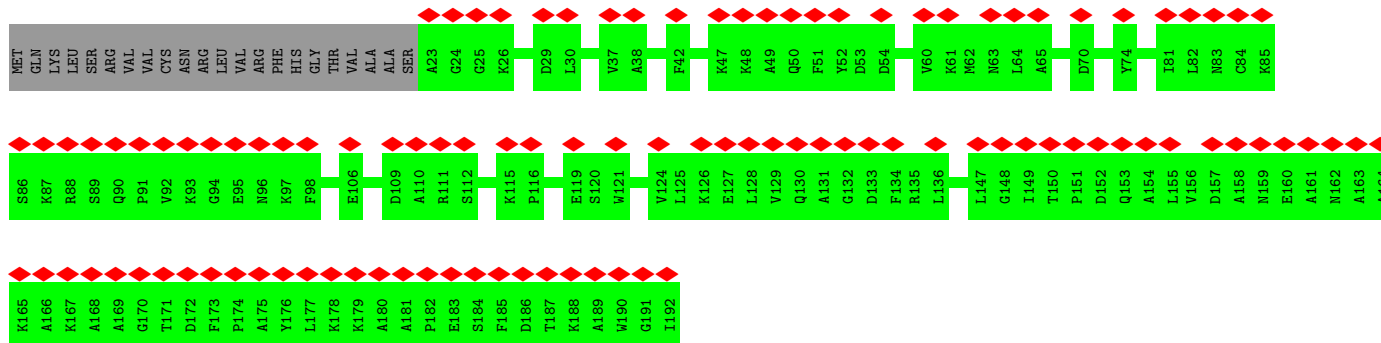
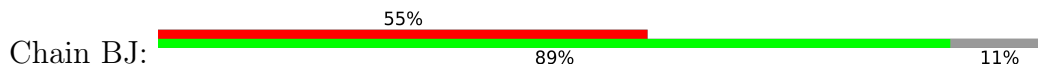


- Molecule 24: p18

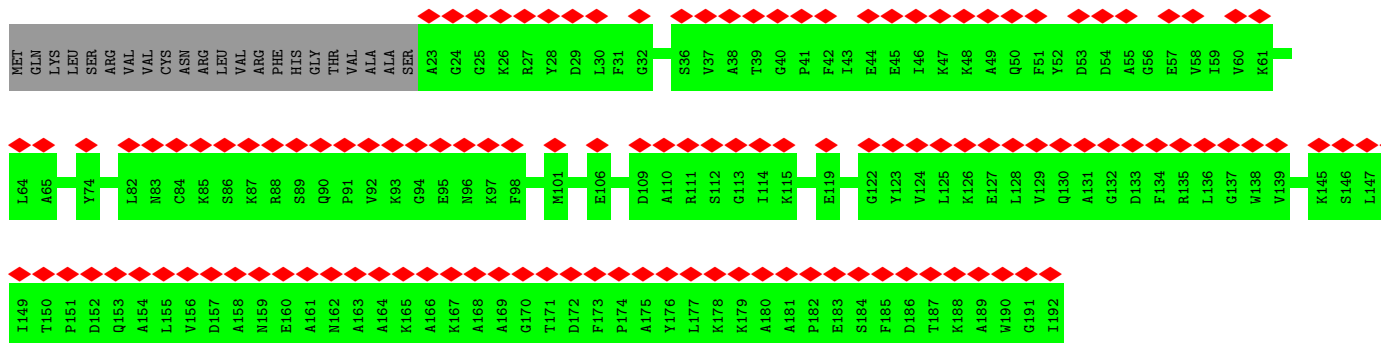
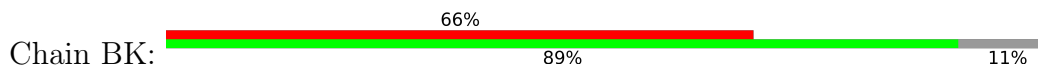




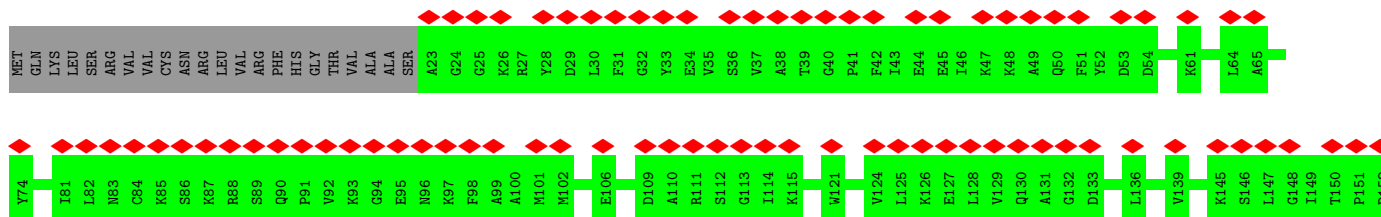
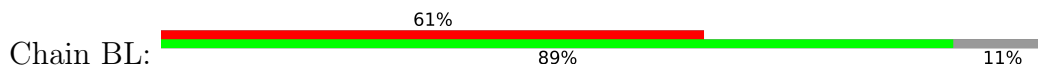
• Molecule 24: p18



• Molecule 24: p18

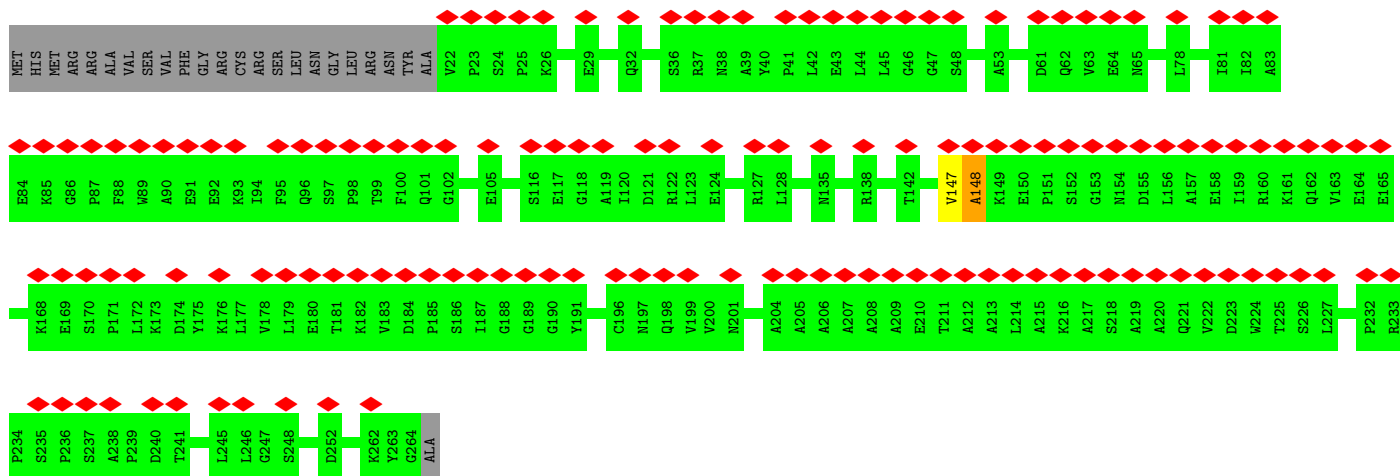


• Molecule 24: p18

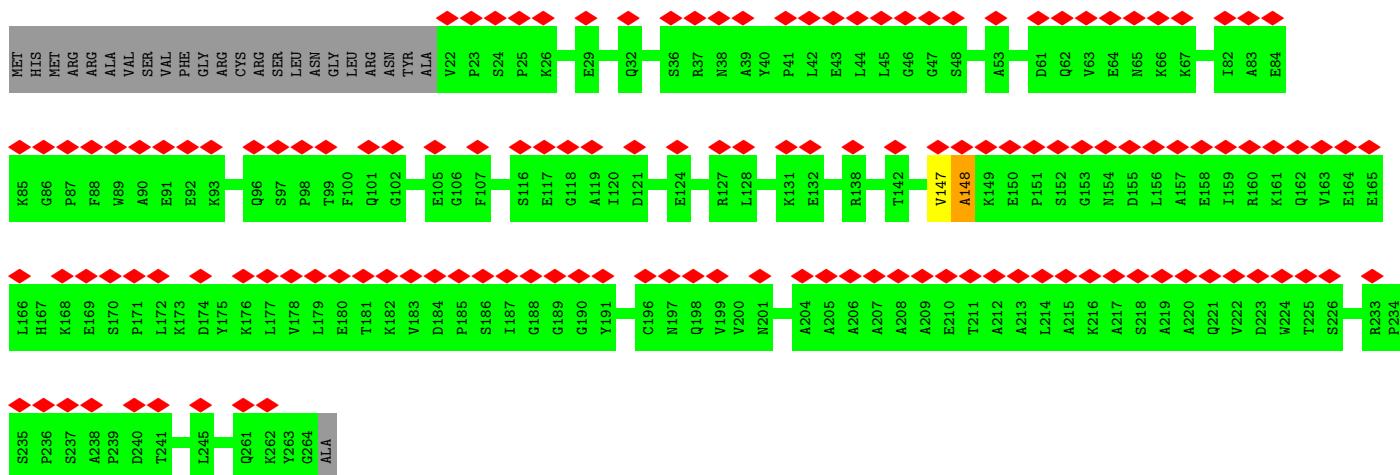




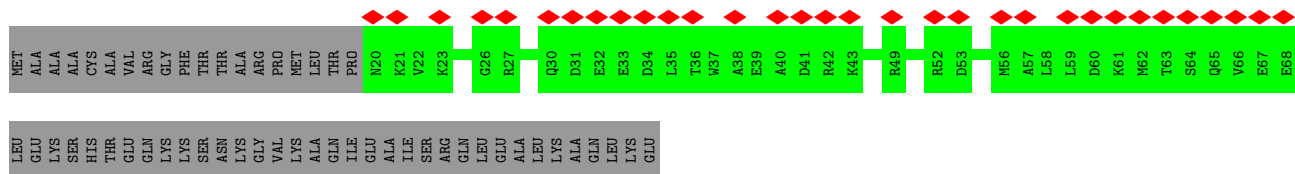
• Molecule 25: oligomycin sensitivity conferring protein (OSCP)



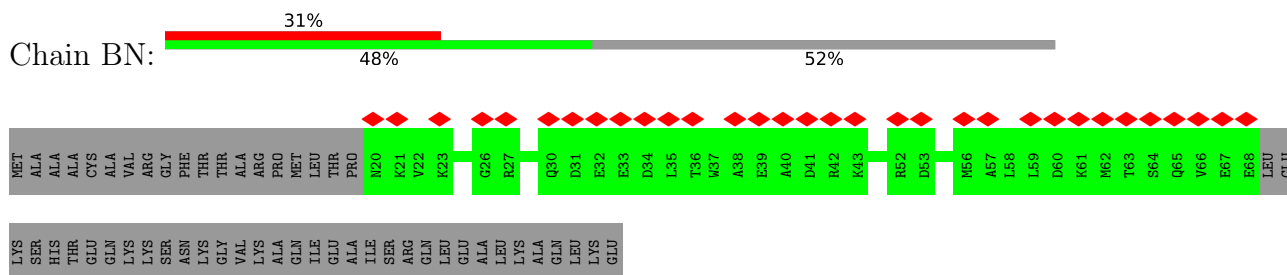
• Molecule 25: oligomycin sensitivity conferring protein (OSCP)



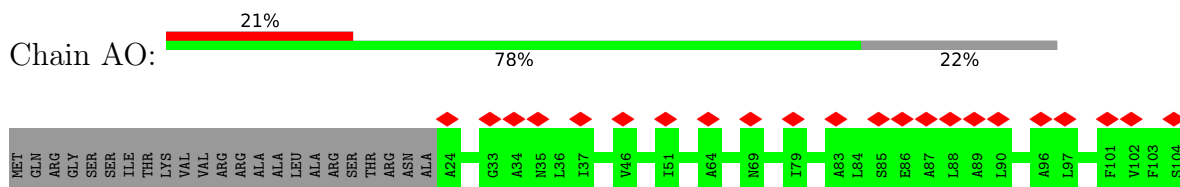
• Molecule 26: inhibitor of F1 (IF1)



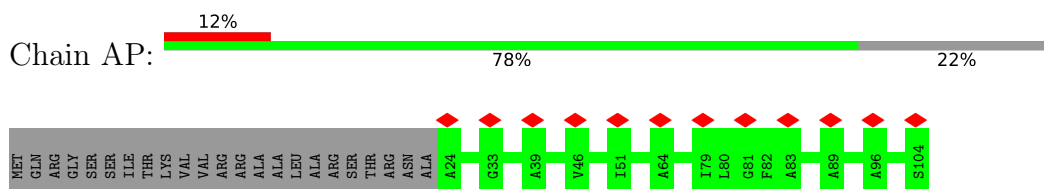
• Molecule 26: inhibitor of F1 (IF1)



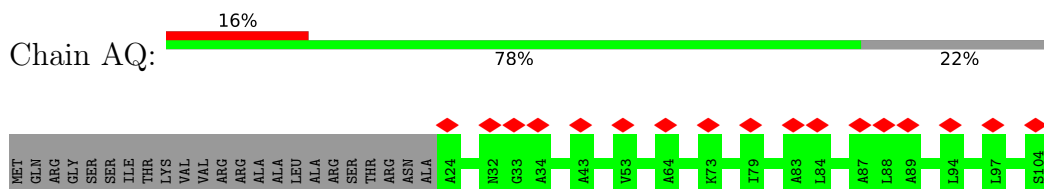
• Molecule 27: ATP synthase subunit c



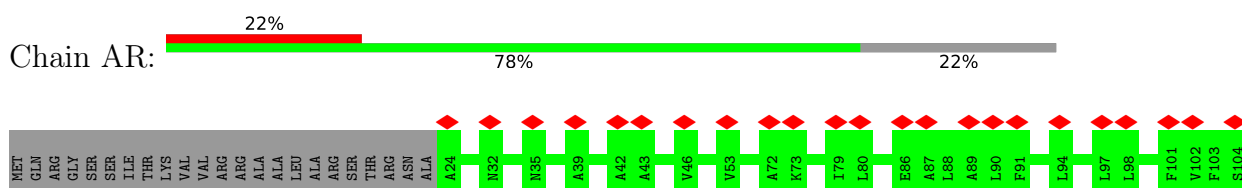
• Molecule 27: ATP synthase subunit c



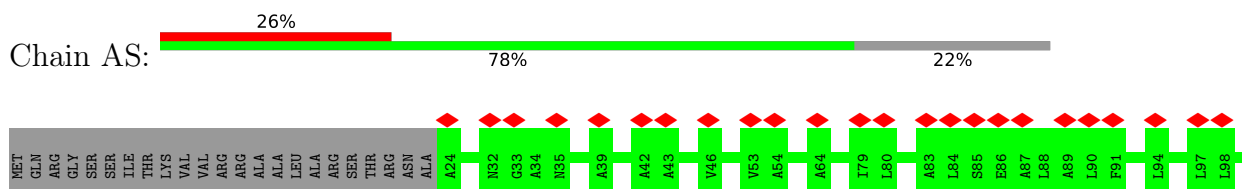
• Molecule 27: ATP synthase subunit c

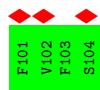


• Molecule 27: ATP synthase subunit c

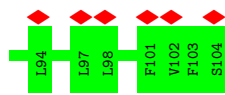
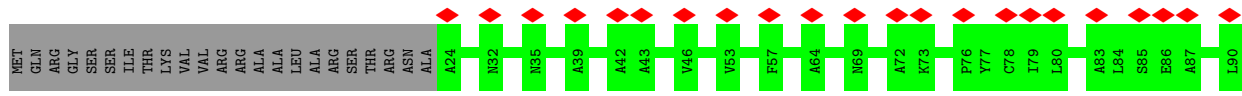
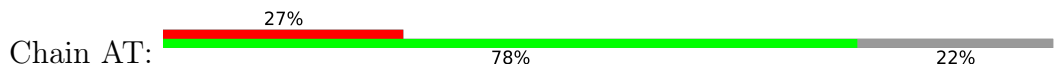


• Molecule 27: ATP synthase subunit c

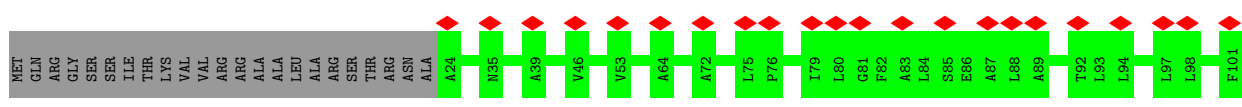
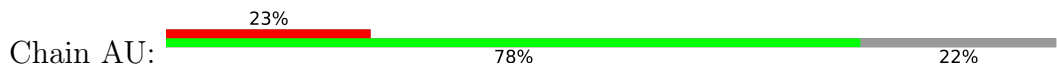




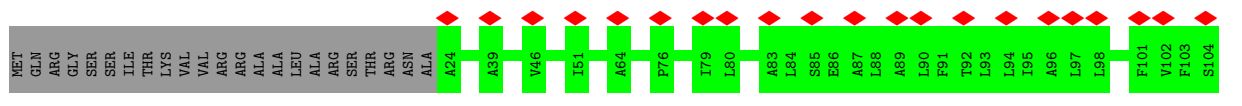
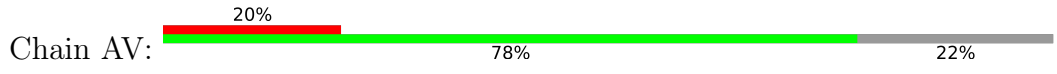
• Molecule 27: ATP synthase subunit c



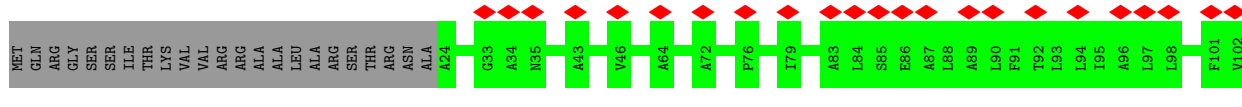
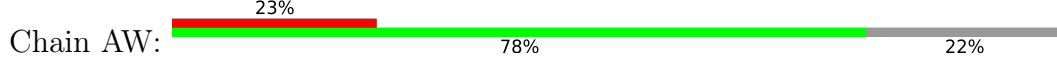
• Molecule 27: ATP synthase subunit c



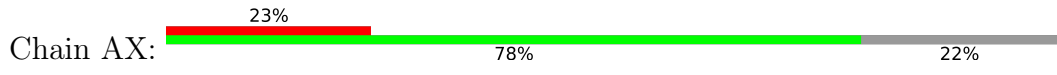
• Molecule 27: ATP synthase subunit c

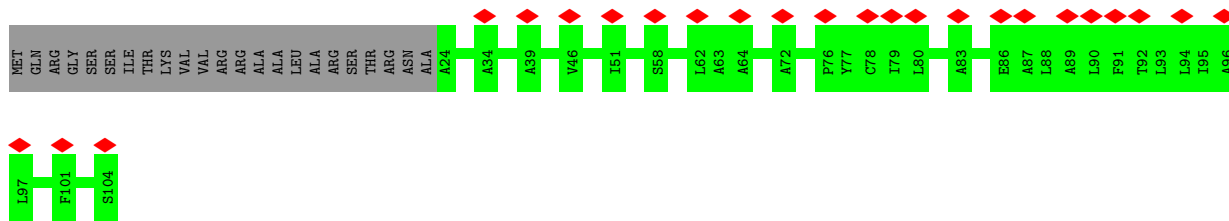


• Molecule 27: ATP synthase subunit c

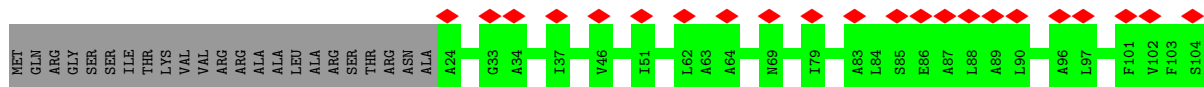
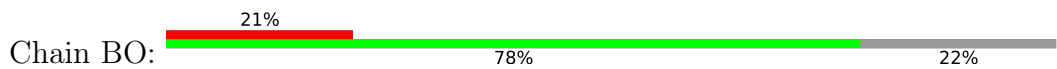


• Molecule 27: ATP synthase subunit c

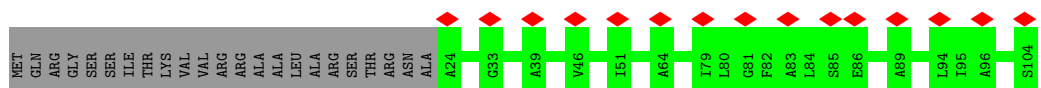
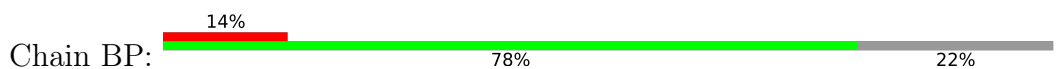




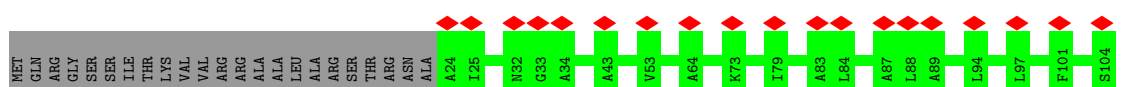
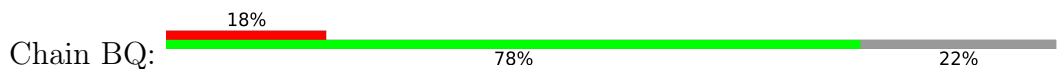
● Molecule 27: ATP synthase subunit c



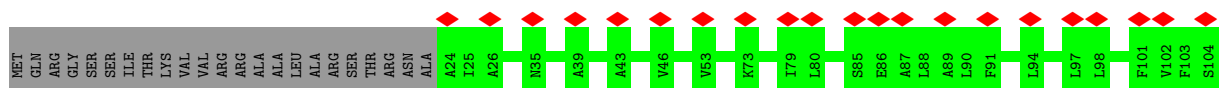
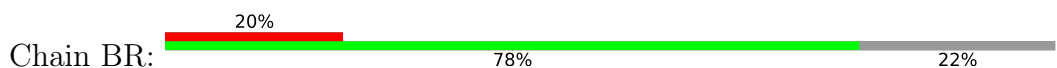
● Molecule 27: ATP synthase subunit c



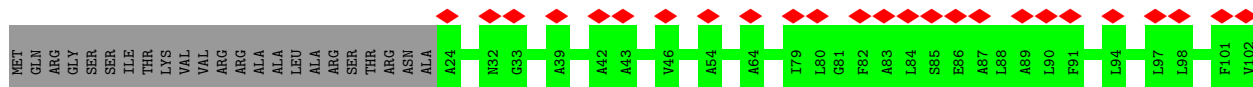
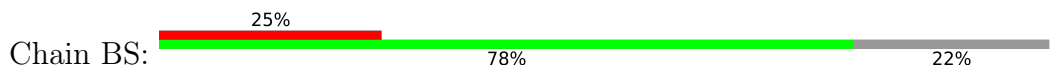
● Molecule 27: ATP synthase subunit c



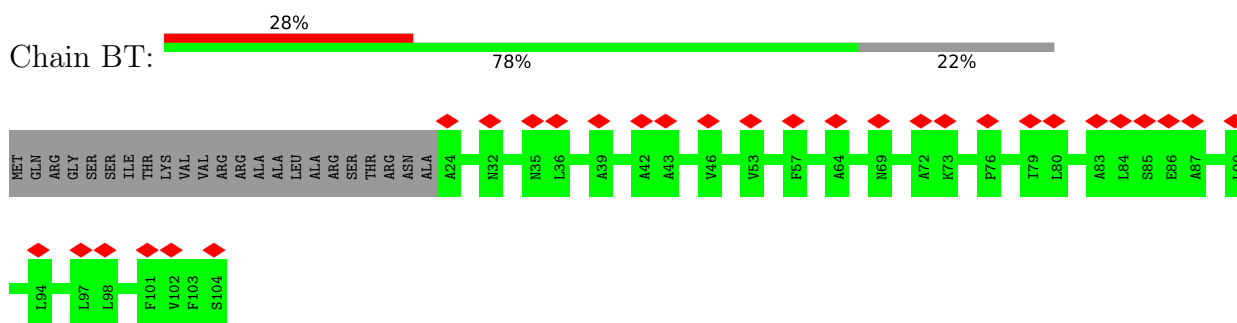
● Molecule 27: ATP synthase subunit c



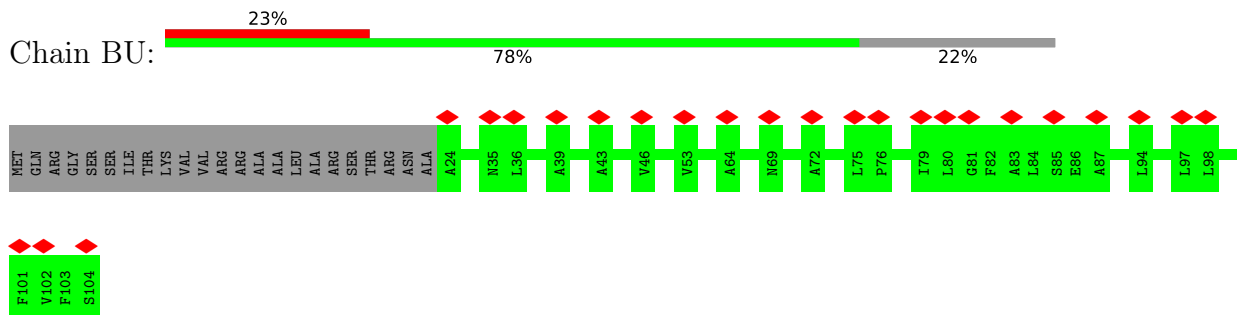
● Molecule 27: ATP synthase subunit c



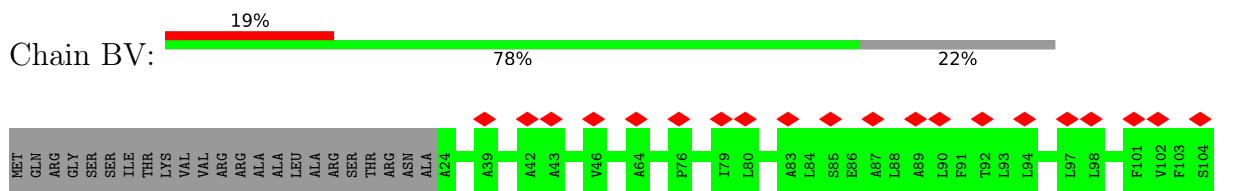
● Molecule 27: ATP synthase subunit c



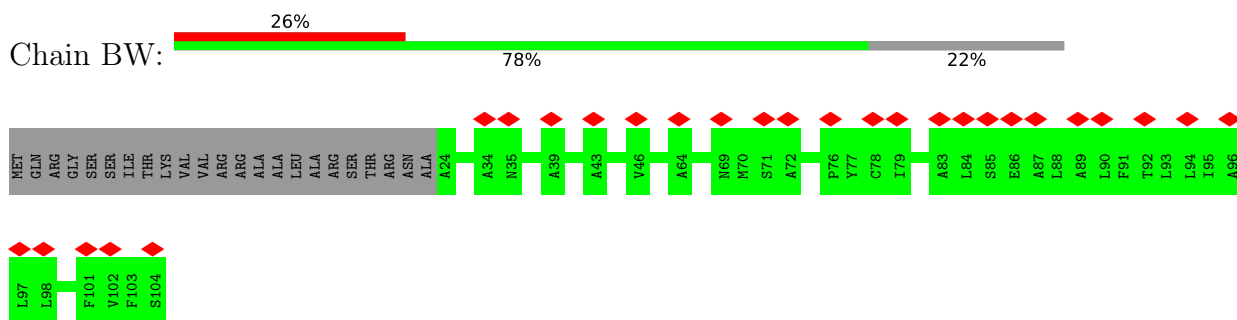
- Molecule 27: ATP synthase subunit c



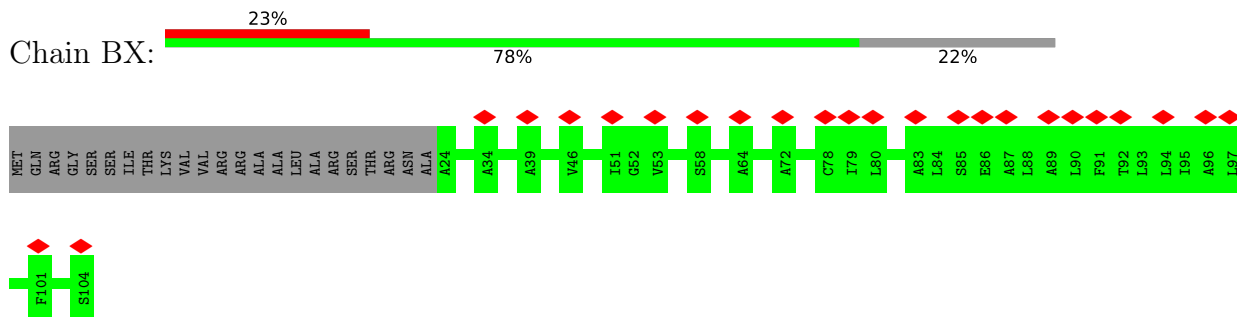
- Molecule 27: ATP synthase subunit c



- Molecule 27: ATP synthase subunit c



- Molecule 27: ATP synthase subunit c



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.

All (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
19	BC	284	ASP	Peptide
20	BE	266	ASP	Peptide
20	BF	288	ALA	Peptide
25	BM	147	VAL	Peptide
25	BM	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
20	BD	289	VAL
20	BF	289	VAL
25	BM	148	ALA
6	h	37	THR
20	AD	288	ALA
20	AF	288	ALA
20	BD	288	ALA
20	BF	288	ALA
6	h	331	PRO
20	AE	289	VAL
20	BE	289	VAL
6	H	331	PRO

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
4	F	32	ASN
8	J	79	GLN
4	f	32	ASN
5	g	59	ASN
8	j	79	GLN
19	AB	356	ASN
19	AC	356	ASN
20	AE	303	GLN
20	AF	426	GLN
21	AG	162	ASN
19	BB	356	ASN
19	BC	356	ASN
20	BE	303	GLN
20	BF	426	GLN
21	BG	162	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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. '2' 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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
32	N	203	LPP	O9-C11	3.33	1.43	1.34
32	n	201	LPP	O9-C11	3.33	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	o	202	LPP	O9-C11	3.32	1.43	1.34
32	F	301	LPP	O9-C11	3.28	1.43	1.34
32	o	203	LPP	O9-C11	3.26	1.43	1.34
32	O	203	LPP	O9-C11	3.26	1.43	1.34
32	f	301	LPP	O9-C11	3.23	1.43	1.34
32	k	201	LPP	O9-C11	3.22	1.43	1.34
32	K	201	LPP	O9-C11	3.21	1.43	1.34
32	O	203	LPP	O27-C29	2.96	1.42	1.33
32	o	203	LPP	O27-C29	2.93	1.41	1.33
32	I	101	LPP	O27-C29	2.92	1.41	1.33
32	i	101	LPP	O27-C29	2.91	1.41	1.33
32	O	202	LPP	O27-C29	2.91	1.41	1.33
32	o	202	LPP	O27-C29	2.88	1.41	1.33
32	K	201	LPP	O27-C29	2.88	1.41	1.33
32	k	201	LPP	O27-C29	2.87	1.41	1.33
32	f	301	LPP	O27-C29	2.87	1.41	1.33
32	n	201	LPP	O27-C29	2.85	1.41	1.33
31	n	202	LMT	O3'-C3'	-2.83	1.36	1.43
31	N	204	LMT	O3'-C3'	-2.83	1.36	1.43
32	F	301	LPP	O27-C29	2.83	1.41	1.33
32	N	203	LPP	O27-C29	2.80	1.41	1.33
31	D	202	LMT	O3'-C3'	-2.78	1.36	1.43
30	A	505	CDL	OB6-CB4	-2.78	1.39	1.46
31	F	302	LMT	O3'-C3'	-2.76	1.36	1.43
31	Q	101	LMT	O3'-C3'	-2.76	1.36	1.43
31	d	202	LMT	O3'-C3'	-2.75	1.36	1.43
31	g	201	LMT	O3'-C3'	-2.74	1.36	1.43
30	a	505	CDL	OB6-CB4	-2.74	1.39	1.46
31	q	101	LMT	O3'-C3'	-2.74	1.36	1.43
30	D	201	CDL	OB6-CB4	-2.66	1.39	1.46
30	d	201	CDL	OB6-CB4	-2.64	1.40	1.46
30	A	504	CDL	OA8-CA7	2.63	1.41	1.33
30	a	504	CDL	OA8-CA7	2.62	1.41	1.33
30	M	205	CDL	OB6-CB4	-2.62	1.40	1.46
30	M	201	CDL	OA6-CA4	-2.62	1.40	1.46
30	M	201	CDL	OB6-CB4	-2.61	1.40	1.46
30	a	501	CDL	OB6-CB4	-2.60	1.40	1.46
30	P	202	CDL	OB6-CB4	-2.60	1.40	1.46
30	D	201	CDL	OB8-CB7	2.59	1.40	1.33
30	d	201	CDL	OB8-CB7	2.59	1.40	1.33
30	A	501	CDL	OB6-CB4	-2.58	1.40	1.46
31	D	202	LMT	O2B-C2B	-2.57	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	E	101	CDL	OB6-CB4	-2.57	1.40	1.46
30	P	201	CDL	OB6-CB4	-2.56	1.40	1.46
30	a	502	CDL	OB8-CB7	2.56	1.40	1.33
30	m	201	CDL	OA6-CA4	-2.55	1.40	1.46
31	g	201	LMT	O2'-C2'	-2.55	1.37	1.43
30	A	502	CDL	OB8-CB7	2.55	1.40	1.33
31	F	302	LMT	O2'-C2'	-2.54	1.37	1.43
30	p	201	CDL	OB6-CB4	-2.53	1.40	1.46
31	N	204	LMT	O2'-C2'	-2.52	1.37	1.43
31	g	201	LMT	O3B-C3B	-2.52	1.37	1.43
31	d	202	LMT	O2B-C2B	-2.51	1.37	1.43
30	A	503	CDL	OB6-CB4	-2.50	1.40	1.46
30	D	201	CDL	OA6-CA4	-2.50	1.40	1.46
30	a	503	CDL	OB6-CB4	-2.49	1.40	1.46
30	e	101	CDL	OB6-CB4	-2.49	1.40	1.46
30	a	501	CDL	OA6-CA4	-2.48	1.40	1.46
30	A	501	CDL	OA6-CA4	-2.48	1.40	1.46
30	M	205	CDL	OA6-CA4	-2.48	1.40	1.46
30	O	201	CDL	OA8-CA7	2.48	1.40	1.33
31	F	302	LMT	O3B-C3B	-2.48	1.37	1.43
30	E	101	CDL	OA8-CA7	2.47	1.40	1.33
30	R	101	CDL	OA8-CA7	2.47	1.40	1.33
30	o	201	CDL	OB8-CB7	2.47	1.40	1.33
30	d	201	CDL	OA6-CA4	-2.47	1.40	1.46
34	AB	601	ATP	C5-C4	2.47	1.47	1.40
30	M	204	CDL	OA6-CA4	-2.46	1.40	1.46
30	P	202	CDL	OA6-CA4	-2.46	1.40	1.46
30	e	101	CDL	OA8-CA7	2.46	1.40	1.33
30	a	505	CDL	OA8-CA7	2.46	1.40	1.33
30	A	502	CDL	OB6-CB4	-2.46	1.40	1.46
30	P	201	CDL	OA8-CA7	2.46	1.40	1.33
34	BF	601	ATP	C5-C4	2.46	1.47	1.40
30	M	201	CDL	OB8-CB7	2.45	1.40	1.33
31	n	202	LMT	O3B-C3B	-2.45	1.37	1.43
31	N	204	LMT	O3B-C3B	-2.45	1.37	1.43
30	M	205	CDL	OB8-CB7	2.45	1.40	1.33
30	p	201	CDL	OA8-CA7	2.45	1.40	1.33
30	A	505	CDL	OA8-CA7	2.45	1.40	1.33
34	BB	601	ATP	C5-C4	2.45	1.47	1.40
30	O	201	CDL	OB8-CB7	2.45	1.40	1.33
30	m	201	CDL	OB6-CB4	-2.45	1.40	1.46
34	AF	601	ATP	C5-C4	2.44	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AA	601	ATP	C5-C4	2.44	1.47	1.40
30	r	101	CDL	OA8-CA7	2.44	1.40	1.33
30	a	502	CDL	OB6-CB4	-2.43	1.40	1.46
31	D	202	LMT	O2'-C2'	-2.43	1.37	1.43
30	M	205	CDL	OA8-CA7	2.42	1.40	1.33
30	o	201	CDL	OA8-CA7	2.42	1.40	1.33
30	M	204	CDL	OB6-CB4	-2.41	1.40	1.46
31	D	202	LMT	O3B-C3B	-2.41	1.37	1.43
31	d	202	LMT	O2'-C2'	-2.41	1.37	1.43
34	BA	601	ATP	C5-C4	2.41	1.47	1.40
30	E	101	CDL	OB8-CB7	2.41	1.40	1.33
30	a	504	CDL	OA6-CA4	-2.41	1.40	1.46
30	P	202	CDL	OA8-CA6	-2.41	1.39	1.45
30	e	101	CDL	OB8-CB7	2.40	1.40	1.33
31	n	202	LMT	O2'-C2'	-2.40	1.37	1.43
30	a	504	CDL	OB6-CB4	-2.40	1.40	1.46
31	d	202	LMT	O3B-C3B	-2.40	1.37	1.43
30	O	201	CDL	OB6-CB4	-2.40	1.40	1.46
30	a	504	CDL	OB8-CB7	2.39	1.40	1.33
30	A	501	CDL	OB8-CB7	2.39	1.40	1.33
30	r	101	CDL	OB6-CB4	-2.39	1.40	1.46
30	A	504	CDL	OB6-CB4	-2.39	1.40	1.46
30	R	101	CDL	OA6-CA4	-2.39	1.40	1.46
30	r	101	CDL	OA6-CA4	-2.38	1.40	1.46
36	BD	601	ADP	C5-C4	2.38	1.47	1.40
30	A	501	CDL	OA8-CA7	2.38	1.40	1.33
34	AC	601	ATP	C5-C4	2.38	1.47	1.40
31	N	204	LMT	O2B-C2B	-2.38	1.37	1.43
30	a	505	CDL	OB8-CB7	2.38	1.40	1.33
30	p	201	CDL	OB8-CB7	2.38	1.40	1.33
30	o	201	CDL	OB6-CB4	-2.38	1.40	1.46
31	Q	101	LMT	O3B-C3B	-2.38	1.37	1.43
31	Q	101	LMT	O2B-C2B	-2.37	1.37	1.43
34	BC	601	ATP	C5-C4	2.37	1.47	1.40
30	M	201	CDL	OA8-CA7	2.37	1.40	1.33
30	P	201	CDL	OB8-CB7	2.37	1.40	1.33
36	AD	601	ADP	C5-C4	2.37	1.47	1.40
30	m	201	CDL	OB8-CB7	2.37	1.40	1.33
30	a	501	CDL	OB8-CB7	2.37	1.40	1.33
30	R	101	CDL	OB6-CB4	-2.37	1.40	1.46
30	A	504	CDL	OB8-CB7	2.37	1.40	1.33
30	A	502	CDL	OA8-CA7	2.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	204	CDL	OB8-CB7	2.37	1.40	1.33
30	a	501	CDL	OA8-CA7	2.37	1.40	1.33
30	A	505	CDL	OB8-CB7	2.36	1.40	1.33
30	R	101	CDL	OB8-CB7	2.36	1.40	1.33
30	r	101	CDL	OB8-CB7	2.36	1.40	1.33
31	q	101	LMT	O3B-C3B	-2.36	1.37	1.43
30	O	201	CDL	OA6-CA4	-2.35	1.40	1.46
31	Q	101	LMT	O2'-C2'	-2.35	1.37	1.43
30	A	504	CDL	OA6-CA4	-2.35	1.40	1.46
30	m	201	CDL	OA8-CA7	2.35	1.40	1.33
30	o	201	CDL	OB6-CB5	2.35	1.40	1.34
31	q	101	LMT	O2B-C2B	-2.35	1.37	1.43
30	a	502	CDL	OA8-CA7	2.34	1.40	1.33
30	P	201	CDL	OB6-CB5	2.34	1.40	1.35
30	r	101	CDL	OB6-CB5	2.34	1.40	1.34
30	a	503	CDL	OB8-CB7	2.34	1.40	1.33
30	R	101	CDL	OB6-CB5	2.34	1.40	1.34
31	N	204	LMT	O1'-C1'	-2.33	1.36	1.40
30	M	204	CDL	OA8-CA6	-2.33	1.39	1.45
30	M	205	CDL	OA6-CA5	2.33	1.40	1.34
30	d	201	CDL	OA8-CA7	2.32	1.40	1.33
31	n	202	LMT	O2B-C2B	-2.32	1.37	1.43
30	A	503	CDL	OB8-CB7	2.32	1.40	1.33
30	M	204	CDL	OA8-CA7	2.32	1.40	1.33
31	q	101	LMT	O2'-C2'	-2.32	1.37	1.43
30	O	201	CDL	OB6-CB5	2.31	1.40	1.34
30	m	201	CDL	OB6-CB5	2.31	1.40	1.34
30	A	504	CDL	OA6-CA5	2.31	1.40	1.34
30	A	504	CDL	OB6-CB5	2.31	1.40	1.34
30	m	201	CDL	OA8-CA6	-2.31	1.39	1.45
30	o	201	CDL	OA6-CA4	-2.30	1.40	1.46
30	p	201	CDL	OB6-CB5	2.30	1.40	1.35
30	P	202	CDL	OA8-CA7	2.30	1.40	1.33
30	p	201	CDL	OA6-CA4	-2.30	1.40	1.46
30	D	201	CDL	OA8-CA7	2.30	1.40	1.33
30	P	202	CDL	OB8-CB7	2.30	1.40	1.33
33	P	203	TRT	C8-C6	2.30	1.60	1.53
30	a	502	CDL	OA6-CA4	-2.30	1.40	1.46
30	A	503	CDL	OA8-CA7	2.30	1.40	1.33
30	a	504	CDL	OB6-CB5	2.29	1.40	1.34
30	e	101	CDL	OA6-CA5	2.29	1.40	1.34
30	E	101	CDL	OA6-CA5	2.29	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	504	CDL	OA6-CA5	2.29	1.40	1.34
30	A	502	CDL	OB6-CB5	2.29	1.40	1.34
30	a	505	CDL	OA6-CA5	2.29	1.40	1.34
30	a	503	CDL	OA8-CA7	2.28	1.40	1.33
30	A	505	CDL	OA6-CA5	2.28	1.40	1.34
30	a	503	CDL	OA8-CA6	-2.28	1.39	1.45
30	A	502	CDL	OA6-CA4	-2.28	1.40	1.46
30	P	201	CDL	OA6-CA4	-2.28	1.40	1.46
31	Q	101	LMT	O4'-C4B	-2.27	1.37	1.43
30	A	505	CDL	OA6-CA4	-2.27	1.40	1.46
30	A	503	CDL	OB6-CB5	2.27	1.40	1.34
30	A	502	CDL	OA8-CA6	-2.27	1.40	1.45
30	a	502	CDL	OB6-CB5	2.27	1.40	1.34
30	A	503	CDL	OA8-CA6	-2.26	1.40	1.45
33	p	202	TRT	C8-C6	2.26	1.60	1.53
30	a	502	CDL	OA8-CA6	-2.26	1.40	1.45
30	a	503	CDL	OB6-CB5	2.26	1.40	1.34
30	e	101	CDL	OB6-CB5	2.26	1.40	1.34
30	A	505	CDL	OB8-CB6	-2.25	1.40	1.45
30	M	204	CDL	OB6-CB5	2.25	1.40	1.34
30	p	201	CDL	OA6-CA5	2.25	1.40	1.34
30	a	505	CDL	OA6-CA4	-2.25	1.41	1.46
31	D	202	LMT	O4'-C4B	-2.25	1.37	1.43
31	n	202	LMT	O1'-C1'	-2.24	1.36	1.40
30	D	201	CDL	OA6-CA5	2.24	1.40	1.34
30	d	201	CDL	OA6-CA5	2.24	1.40	1.34
30	D	201	CDL	OA8-CA6	-2.23	1.40	1.45
31	q	101	LMT	O4'-C4B	-2.23	1.37	1.43
31	F	302	LMT	O2B-C2B	-2.23	1.37	1.43
30	M	201	CDL	OA8-CA6	-2.23	1.40	1.45
31	d	202	LMT	O4'-C4B	-2.22	1.37	1.43
30	M	205	CDL	OA8-CA6	-2.22	1.40	1.45
30	M	201	CDL	OA6-CA5	2.22	1.40	1.34
30	d	201	CDL	OA8-CA6	-2.21	1.40	1.45
31	g	201	LMT	O2B-C2B	-2.21	1.37	1.43
30	P	202	CDL	OB8-CB6	-2.21	1.40	1.45
30	a	505	CDL	OB8-CB6	-2.21	1.40	1.45
31	N	204	LMT	O4'-C4B	-2.21	1.37	1.43
30	R	101	CDL	OA6-CA5	2.21	1.40	1.34
30	P	201	CDL	OA6-CA5	2.20	1.40	1.34
30	A	503	CDL	OA6-CA4	-2.20	1.41	1.46
30	P	201	CDL	OA8-CA6	-2.20	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	r	101	CDL	OA6-CA5	2.20	1.40	1.34
30	m	201	CDL	OA6-CA5	2.19	1.40	1.34
30	a	503	CDL	OA6-CA4	-2.19	1.41	1.46
30	A	501	CDL	OA6-CA5	2.19	1.40	1.34
30	a	503	CDL	OB8-CB6	-2.18	1.40	1.45
33	BE	600	TRT	O15-C12	2.18	1.42	1.37
31	n	202	LMT	O4'-C4B	-2.18	1.37	1.43
30	a	501	CDL	OA6-CA5	2.18	1.40	1.34
30	e	101	CDL	OA6-CA4	-2.17	1.41	1.46
30	E	101	CDL	OB6-CB5	2.17	1.40	1.34
30	M	205	CDL	OB6-CB5	2.17	1.40	1.34
33	AE	600	TRT	O15-C12	2.17	1.42	1.37
30	A	505	CDL	OA8-CA6	-2.16	1.40	1.45
30	E	101	CDL	OA6-CA4	-2.16	1.41	1.46
30	o	201	CDL	OA6-CA5	2.16	1.40	1.34
33	p	202	TRT	C7-C6	2.16	1.59	1.53
30	a	503	CDL	OA6-CA5	2.16	1.40	1.34
31	g	201	LMT	O4'-C4B	-2.16	1.37	1.43
30	P	202	CDL	OA6-CA5	2.16	1.40	1.34
30	a	501	CDL	OA8-CA6	-2.15	1.40	1.45
30	M	201	CDL	OB6-CB5	2.15	1.40	1.34
30	A	503	CDL	OA6-CA5	2.15	1.40	1.34
30	p	201	CDL	OA8-CA6	-2.14	1.40	1.45
30	O	201	CDL	OA6-CA5	2.14	1.40	1.34
30	a	502	CDL	OA6-CA5	2.14	1.40	1.34
30	A	502	CDL	OA6-CA5	2.13	1.40	1.34
30	A	503	CDL	OB8-CB6	-2.13	1.40	1.45
30	o	201	CDL	OA8-CA6	-2.13	1.40	1.45
30	R	101	CDL	OB8-CB6	-2.13	1.40	1.45
30	A	501	CDL	OA8-CA6	-2.13	1.40	1.45
33	P	203	TRT	C7-C6	2.13	1.59	1.53
30	A	504	CDL	OB8-CB6	-2.12	1.40	1.45
30	a	504	CDL	OB8-CB6	-2.11	1.40	1.45
30	P	202	CDL	OB6-CB5	2.11	1.40	1.34
30	r	101	CDL	OA8-CA6	-2.11	1.40	1.45
32	n	201	LPP	P1-O5	2.11	1.67	1.60
30	O	201	CDL	OA8-CA6	-2.11	1.40	1.45
30	M	204	CDL	OA6-CA5	2.11	1.40	1.34
31	F	302	LMT	O4'-C4B	-2.10	1.38	1.43
30	a	505	CDL	OA8-CA6	-2.10	1.40	1.45
32	i	101	LPP	C12-C11	2.10	1.56	1.50
30	P	201	CDL	OB8-CB6	-2.10	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	o	202	LPP	C12-C11	2.10	1.56	1.50
30	m	201	CDL	OB8-CB6	-2.09	1.40	1.45
30	p	201	CDL	OB8-CB6	-2.09	1.40	1.45
30	r	101	CDL	OB8-CB6	-2.09	1.40	1.45
30	R	101	CDL	OA8-CA6	-2.08	1.40	1.45
32	I	101	LPP	C12-C11	2.08	1.56	1.50
32	O	202	LPP	C12-C11	2.08	1.56	1.50
30	E	101	CDL	OA8-CA6	-2.08	1.40	1.45
32	N	203	LPP	P1-O5	2.08	1.66	1.60
30	e	101	CDL	OA8-CA6	-2.08	1.40	1.45
30	d	201	CDL	OB6-CB5	2.08	1.40	1.34
30	a	501	CDL	OB8-CB6	-2.07	1.40	1.45
31	D	202	LMT	O1'-C1'	-2.07	1.36	1.40
32	f	301	LPP	P1-O5	2.06	1.66	1.60
30	A	501	CDL	OB8-CB6	-2.06	1.40	1.45
32	k	201	LPP	C12-C11	2.06	1.56	1.50
32	F	301	LPP	P1-O5	2.06	1.66	1.60
30	M	201	CDL	OB8-CB6	-2.06	1.40	1.45
32	K	201	LPP	C12-C11	2.05	1.56	1.50
31	d	202	LMT	O1'-C1'	-2.05	1.36	1.40
30	D	201	CDL	OB6-CB5	2.05	1.40	1.34
30	M	205	CDL	OB8-CB6	-2.04	1.40	1.45
32	o	203	LPP	P1-O5	2.04	1.66	1.60
30	e	101	CDL	OB8-CB6	-2.04	1.40	1.45
30	M	204	CDL	OB8-CB6	-2.03	1.40	1.45
30	O	201	CDL	OB8-CB6	-2.02	1.40	1.45
32	o	202	LPP	P1-O5	2.02	1.66	1.60
32	O	202	LPP	P1-O5	2.02	1.66	1.60
30	E	101	CDL	OB8-CB6	-2.01	1.40	1.45
30	A	505	CDL	OB6-CB5	2.01	1.40	1.34
32	O	203	LPP	P1-O5	2.00	1.66	1.60
30	a	502	CDL	OB8-CB6	-2.00	1.40	1.45
32	O	203	LPP	C12-C11	2.00	1.56	1.50
32	o	203	LPP	C12-C11	2.00	1.56	1.50

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	P	203	TRT	C8-C6-C9	-11.41	81.58	110.20
33	p	202	TRT	C8-C6-C9	-11.31	81.84	110.20
33	p	202	TRT	C7-C6-C9	-10.97	82.69	110.20
33	P	203	TRT	C7-C6-C9	-10.91	82.85	110.20
34	BF	601	ATP	PA-O3A-PB	-5.08	115.41	132.83
30	p	201	CDL	OB6-CB5-C51	4.92	120.13	111.09
30	P	201	CDL	OB6-CB5-C51	4.88	120.07	111.09
34	AF	601	ATP	PA-O3A-PB	-4.86	116.16	132.83
30	M	205	CDL	OA6-CA5-C11	4.66	121.54	111.50
30	a	504	CDL	OA6-CA5-C11	4.62	121.46	111.50
33	P	203	TRT	C8-C6-C5	-4.61	87.51	109.08
33	p	202	TRT	C8-C6-C5	-4.59	87.58	109.08
30	A	504	CDL	OA6-CA5-C11	4.57	121.34	111.50
30	M	201	CDL	OA6-CA5-C11	4.48	121.15	111.50
34	BF	601	ATP	PB-O3B-PG	-4.45	117.56	132.83
34	AF	601	ATP	PB-O3B-PG	-4.43	117.62	132.83
36	AD	601	ADP	PA-O3A-PB	-4.39	117.77	132.83
36	BD	601	ADP	PA-O3A-PB	-4.39	117.78	132.83
33	p	202	TRT	C7-C6-C5	-4.32	88.84	109.08
32	k	201	LPP	O9-C11-C12	4.30	120.77	111.50
33	P	203	TRT	C7-C6-C5	-4.28	89.04	109.08
30	E	101	CDL	OA6-CA5-C11	4.28	120.72	111.50
30	e	101	CDL	OA6-CA5-C11	4.27	120.70	111.50
32	K	201	LPP	O9-C11-C12	4.25	120.66	111.50
30	a	502	CDL	OB6-CB5-C51	4.22	120.60	111.50
30	A	502	CDL	OB6-CB5-C51	4.20	120.56	111.50
30	R	101	CDL	OA6-CA5-C11	4.20	120.56	111.50
30	r	101	CDL	OA6-CA5-C11	4.17	120.48	111.50
36	BD	601	ADP	C3'-C2'-C1'	4.11	107.17	100.98
30	A	503	CDL	OA6-CA5-C11	4.11	120.36	111.50
30	a	503	CDL	OA6-CA5-C11	4.08	120.30	111.50
32	N	203	LPP	O9-C11-C12	4.07	120.28	111.50
32	n	201	LPP	O9-C11-C12	4.07	120.27	111.50
30	R	101	CDL	OB6-CB5-C51	4.06	120.25	111.50
30	r	101	CDL	OB6-CB5-C51	4.06	120.25	111.50
30	o	201	CDL	OB6-CB5-C51	4.04	120.21	111.50
30	O	201	CDL	OB6-CB5-C51	4.03	120.19	111.50
30	A	501	CDL	OA6-CA5-C11	4.02	120.17	111.50
30	M	201	CDL	OB6-CB5-C51	4.01	120.13	111.50
30	a	501	CDL	OA6-CA5-C11	4.00	120.12	111.50
36	AD	601	ADP	C3'-C2'-C1'	4.00	106.99	100.98
30	d	201	CDL	OA6-CA5-C11	3.96	120.05	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	201	CDL	OA6-CA5-C11	3.92	119.96	111.50
32	o	202	LPP	O9-C11-C12	3.89	119.89	111.50
30	a	503	CDL	OB6-CB5-C51	3.88	119.86	111.50
30	M	205	CDL	OB6-CB5-C51	3.87	119.84	111.50
34	BC	601	ATP	PB-O3B-PG	-3.83	119.68	132.83
32	O	202	LPP	O9-C11-C12	3.80	119.68	111.50
34	AC	601	ATP	PB-O3B-PG	-3.77	119.89	132.83
30	A	503	CDL	OB6-CB5-C51	3.76	119.61	111.50
30	M	204	CDL	OA6-CA5-C11	3.74	119.56	111.50
33	BE	600	TRT	C7-C6-C9	-3.73	100.86	110.20
33	AE	600	TRT	C7-C6-C9	-3.69	100.94	110.20
34	BB	601	ATP	PB-O3B-PG	-3.68	120.19	132.83
30	A	504	CDL	OB6-CB5-C51	3.68	119.43	111.50
36	BD	601	ADP	N3-C2-N1	-3.68	122.93	128.68
30	a	504	CDL	OB6-CB5-C51	3.67	119.41	111.50
34	AB	601	ATP	PB-O3B-PG	-3.67	120.24	132.83
34	BA	601	ATP	PB-O3B-PG	-3.66	120.28	132.83
36	AD	601	ADP	N3-C2-N1	-3.66	122.97	128.68
34	AA	601	ATP	PB-O3B-PG	-3.65	120.30	132.83
34	AA	601	ATP	N3-C2-N1	-3.65	122.97	128.68
30	M	204	CDL	OB6-CB5-C51	3.64	119.35	111.50
34	BA	601	ATP	N3-C2-N1	-3.64	122.98	128.68
34	AC	601	ATP	N3-C2-N1	-3.61	123.03	128.68
30	m	201	CDL	OB6-CB5-C51	3.61	119.28	111.50
33	n	204	TRT	C7-C6-C9	-3.61	101.16	110.20
34	AF	601	ATP	N3-C2-N1	-3.60	123.06	128.68
33	p	202	TRT	C1-C5-C6	-3.59	110.97	123.91
34	BC	601	ATP	N3-C2-N1	-3.59	123.07	128.68
34	BF	601	ATP	N3-C2-N1	-3.59	123.07	128.68
34	BB	601	ATP	N3-C2-N1	-3.58	123.08	128.68
33	P	203	TRT	C1-C5-C6	-3.57	111.07	123.91
34	AB	601	ATP	N3-C2-N1	-3.56	123.11	128.68
30	e	101	CDL	OB6-CB5-C51	3.55	119.15	111.50
34	BC	601	ATP	PA-O3A-PB	-3.52	120.73	132.83
30	m	201	CDL	OA6-CA5-C11	3.52	119.08	111.50
34	AC	601	ATP	PA-O3A-PB	-3.51	120.79	132.83
34	BA	601	ATP	PA-O3A-PB	-3.49	120.84	132.83
34	AA	601	ATP	PA-O3A-PB	-3.49	120.86	132.83
30	P	202	CDL	OB6-CB5-C51	3.48	119.01	111.50
32	f	301	LPP	O9-C11-C12	3.47	118.99	111.50
30	A	502	CDL	OA6-CA5-C11	3.45	118.93	111.50
32	F	301	LPP	O9-C11-C12	3.45	118.93	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	201	CDL	OB6-CB5-C51	3.45	118.93	111.50
32	O	203	LPP	O9-C11-C12	3.43	118.90	111.50
30	A	504	CDL	OA8-CA7-C31	3.42	122.64	111.91
32	I	101	LPP	O9-C11-C12	3.42	118.87	111.50
32	o	203	LPP	O9-C11-C12	3.42	118.86	111.50
30	a	504	CDL	OA8-CA7-C31	3.41	122.61	111.91
33	N	202	TRT	C7-C6-C9	-3.41	101.66	110.20
32	i	101	LPP	O9-C11-C12	3.40	118.83	111.50
30	D	201	CDL	OB6-CB5-C51	3.39	118.81	111.50
30	E	101	CDL	OB6-CB5-C51	3.38	118.79	111.50
30	a	502	CDL	OA6-CA5-C11	3.38	118.79	111.50
30	o	201	CDL	OA8-CA7-C31	3.38	120.24	111.38
34	AB	601	ATP	PA-O3A-PB	-3.35	121.35	132.83
30	M	204	CDL	OA8-CA7-C31	3.33	122.35	111.91
30	a	501	CDL	OB6-CB5-C51	3.32	118.66	111.50
34	BB	601	ATP	PA-O3A-PB	-3.32	121.45	132.83
30	O	201	CDL	OA8-CA7-C31	3.28	119.99	111.38
30	m	201	CDL	OA8-CA7-C31	3.28	122.21	111.91
30	o	201	CDL	OA6-CA5-C11	3.27	118.55	111.50
30	A	501	CDL	OB6-CB5-C51	3.27	118.54	111.50
30	R	101	CDL	OA8-CA7-C31	3.26	122.14	111.91
30	P	202	CDL	OA6-CA5-C11	3.22	118.43	111.50
30	a	505	CDL	OB6-CB5-C51	3.21	118.43	111.50
30	r	101	CDL	OA8-CA7-C31	3.21	121.97	111.91
30	O	201	CDL	OA6-CA5-C11	3.20	118.40	111.50
30	P	201	CDL	OA6-CA5-C11	3.15	118.29	111.50
30	A	505	CDL	OB6-CB5-C51	3.13	118.25	111.50
30	p	201	CDL	OA6-CA5-C11	3.08	118.14	111.50
33	G	202	TRT	C8-C6-C9	-3.06	102.53	110.20
30	M	205	CDL	OA8-CA7-C31	3.04	121.46	111.91
30	A	505	CDL	OA6-CA5-C11	3.04	118.05	111.50
33	g	203	TRT	C8-C6-C9	-3.02	102.64	110.20
30	M	201	CDL	OA8-CA7-C31	2.99	121.30	111.91
30	a	501	CDL	CB4-OB6-CB5	-2.99	110.42	117.79
30	D	201	CDL	OA8-CA7-C31	2.99	121.30	111.91
30	P	202	CDL	OB8-CB7-C71	2.97	121.23	111.91
30	A	501	CDL	CB4-OB6-CB5	-2.97	110.48	117.79
30	p	201	CDL	OA8-CA7-C31	2.96	121.21	111.91
30	a	505	CDL	OA6-CA5-C11	2.96	117.88	111.50
30	P	201	CDL	OA8-CA7-C31	2.96	121.18	111.91
30	d	201	CDL	OA8-CA7-C31	2.94	121.12	111.91
30	a	501	CDL	OA8-CA7-C31	2.90	121.01	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	n	203	TRT	C5-C6-C9	-2.88	105.56	111.93
30	a	502	CDL	OA8-CA7-C31	2.87	120.92	111.91
30	A	502	CDL	OA8-CA7-C31	2.87	120.90	111.91
33	n	203	TRT	C7-C6-C9	-2.85	103.06	110.20
33	p	202	TRT	C14-C9-C6	2.81	126.70	121.53
33	BR	201	TRT	C7-C6-C9	-2.81	103.15	110.20
30	a	503	CDL	OB8-CB7-C71	2.80	120.70	111.91
33	N	201	TRT	C5-C6-C9	-2.79	105.76	111.93
33	N	201	TRT	C7-C6-C9	-2.79	103.22	110.20
30	A	501	CDL	OA8-CA7-C31	2.76	120.58	111.91
33	AR	201	TRT	C5-C6-C9	-2.76	105.83	111.93
33	M	203	TRT	C7-C6-C9	-2.76	103.29	110.20
33	P	203	TRT	C14-C9-C6	2.75	126.58	121.53
30	A	503	CDL	OB8-CB7-C71	2.74	120.52	111.91
30	E	101	CDL	OB8-CB7-C71	2.74	120.50	111.91
30	e	101	CDL	OB8-CB7-C71	2.74	120.49	111.91
32	n	201	LPP	O27-C29-C30	2.71	120.40	111.91
34	AA	601	ATP	C4-C5-N7	-2.70	106.58	109.40
36	BD	601	ADP	C4-C5-N7	-2.70	106.58	109.40
30	m	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
32	N	203	LPP	O27-C29-C30	2.69	120.36	111.91
30	a	504	CDL	OB8-CB7-C71	2.69	120.36	111.91
30	A	504	CDL	OB8-CB7-C71	2.69	120.35	111.91
30	M	204	CDL	OB8-CB7-C71	2.69	120.34	111.91
34	BA	601	ATP	C4-C5-N7	-2.69	106.60	109.40
33	M	203	TRT	C5-C6-C9	-2.68	106.00	111.93
36	AD	601	ADP	C4-C5-N7	-2.68	106.60	109.40
34	AB	601	ATP	C4-C5-N7	-2.68	106.61	109.40
33	m	203	TRT	C5-C6-C9	-2.67	106.04	111.93
34	AF	601	ATP	C4-C5-N7	-2.65	106.64	109.40
36	AD	601	ADP	C5'-C4'-C3'	2.63	125.04	115.18
34	BF	601	ATP	C4-C5-N7	-2.63	106.66	109.40
33	AR	201	TRT	C7-C6-C9	-2.62	103.62	110.20
34	BB	601	ATP	C4-C5-N7	-2.62	106.67	109.40
33	m	203	TRT	C7-C6-C9	-2.60	103.69	110.20
30	r	101	CDL	OB8-CB7-C71	2.60	120.05	111.91
34	AC	601	ATP	C4-C5-N7	-2.59	106.70	109.40
30	P	202	CDL	OA8-CA7-C31	2.59	120.03	111.91
30	R	101	CDL	OB8-CB7-C71	2.58	120.02	111.91
33	BR	201	TRT	C5-C6-C9	-2.58	106.24	111.93
30	p	201	CDL	OB8-CB7-C71	2.58	119.99	111.91
30	P	201	CDL	OB8-CB7-C71	2.57	119.98	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	502	CDL	OB8-CB7-C71	2.57	119.97	111.91
30	a	502	CDL	OB8-CB7-C71	2.56	119.94	111.91
34	BC	601	ATP	C4-C5-N7	-2.55	106.74	109.40
32	F	301	LPP	O27-C29-C30	2.55	119.91	111.91
30	M	201	CDL	OB8-CB7-C71	2.54	119.88	111.91
36	BD	601	ADP	C5'-C4'-C3'	2.53	124.66	115.18
30	O	201	CDL	OB8-CB7-C71	2.50	119.76	111.91
32	o	202	LPP	O27-C29-C30	2.50	119.76	111.91
30	M	205	CDL	OB8-CB7-C71	2.50	119.76	111.91
31	Q	101	LMT	C3B-C4B-C5B	-2.50	105.78	110.24
32	f	301	LPP	O27-C29-C30	2.49	119.71	111.91
30	p	201	CDL	CB4-OB6-CB5	-2.49	113.27	117.90
33	G	201	TRT	C5-C6-C9	-2.48	106.44	111.93
32	O	202	LPP	O27-C29-C30	2.48	119.70	111.91
30	P	201	CDL	CB4-OB6-CB5	-2.48	113.28	117.90
30	o	201	CDL	OB8-CB7-C71	2.47	119.67	111.91
31	q	101	LMT	C3B-C4B-C5B	-2.47	105.84	110.24
30	A	505	CDL	OB8-CB7-C71	2.46	119.63	111.91
30	a	505	CDL	OB8-CB7-C71	2.44	119.58	111.91
30	A	505	CDL	OA8-CA7-C31	2.44	119.56	111.91
30	A	503	CDL	OA8-CA7-C31	2.44	119.55	111.91
30	a	501	CDL	OB8-CB7-C71	2.43	119.54	111.91
33	g	202	TRT	C5-C6-C9	-2.42	106.58	111.93
30	D	201	CDL	OB8-CB7-C71	2.42	119.49	111.91
30	d	201	CDL	OB8-CB7-C71	2.41	119.49	111.91
30	a	503	CDL	OA8-CA7-C31	2.41	119.45	111.91
30	A	501	CDL	OB8-CB7-C71	2.38	119.36	111.91
32	O	203	LPP	O27-C29-C30	2.36	119.32	111.91
30	E	101	CDL	OA8-CA7-C31	2.34	119.27	111.91
30	a	505	CDL	OA8-CA7-C31	2.34	119.25	111.91
30	e	101	CDL	OA8-CA7-C31	2.33	119.22	111.91
31	q	101	LMT	C3'-C4'-C5'	-2.32	105.61	110.93
31	Q	101	LMT	C3'-C4'-C5'	-2.30	105.64	110.93
33	N	201	TRT	C16-O15-C12	-2.30	111.90	117.93
32	K	201	LPP	O27-C29-C30	2.30	119.13	111.91
31	n	202	LMT	C3'-C4'-C5'	-2.30	105.65	110.93
32	k	201	LPP	O27-C29-C30	2.30	119.12	111.91
31	g	201	LMT	C3B-C4B-C5B	-2.28	106.17	110.24
31	N	204	LMT	C3'-C4'-C5'	-2.26	105.73	110.93
32	o	203	LPP	O27-C29-C30	2.25	118.98	111.91
33	n	203	TRT	C16-O15-C12	-2.25	112.04	117.93
31	F	302	LMT	C3B-C4B-C5B	-2.25	106.23	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	p	202	TRT	C10-C9-C6	-2.18	117.53	121.53
32	i	101	LPP	O27-C29-C30	2.15	118.66	111.91
32	I	101	LPP	O27-C29-C30	2.13	118.59	111.91
31	g	201	LMT	C3'-C4'-C5'	-2.09	106.13	110.93
31	N	204	LMT	C3B-C4B-C5B	-2.09	106.51	110.24
31	F	302	LMT	C3'-C4'-C5'	-2.08	106.15	110.93
31	n	202	LMT	C3B-C4B-C5B	-2.06	106.56	110.24
33	P	203	TRT	C10-C9-C6	-2.03	117.81	121.53
36	AD	601	ADP	C2-N1-C6	2.03	122.23	118.75
36	BD	601	ADP	C2-N1-C6	2.03	122.23	118.75
31	Q	101	LMT	C1B-C2B-C3B	2.02	114.19	110.00
34	BF	601	ATP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (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
30	A	503	CDL	CB2-C1-CA2-OA2
30	A	503	CDL	CA2-OA2-PA1-OA3
30	A	503	CDL	CA3-OA5-PA1-OA3
30	A	503	CDL	CA3-OA5-PA1-OA4
30	A	503	CDL	CB3-OB5-PB2-OB2
30	A	503	CDL	CB3-OB5-PB2-OB3
30	A	504	CDL	O1-C1-CB2-OB2
30	A	504	CDL	CA2-C1-CB2-OB2
30	A	504	CDL	OA6-CA4-CA6-OA8
30	A	504	CDL	OA7-CA5-OA6-CA4
30	A	505	CDL	O1-C1-CA2-OA2
30	A	505	CDL	CA2-OA2-PA1-OA3
30	A	505	CDL	CA3-OA5-PA1-OA3
30	A	505	CDL	CA3-OA5-PA1-OA4
30	A	505	CDL	CB2-OB2-PB2-OB3
30	A	505	CDL	C51-CB5-OB6-CB4
30	D	201	CDL	CA2-OA2-PA1-OA3
30	D	201	CDL	CA2-OA2-PA1-OA4
30	D	201	CDL	CB2-OB2-PB2-OB3
30	E	101	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
30	E	101	CDL	CA2-OA2-PA1-OA4
30	E	101	CDL	CA3-OA5-PA1-OA2
30	E	101	CDL	CA3-OA5-PA1-OA3
30	E	101	CDL	CA3-OA5-PA1-OA4
30	E	101	CDL	CB2-OB2-PB2-OB3
30	M	201	CDL	CB2-OB2-PB2-OB3
30	M	204	CDL	CA2-OA2-PA1-OA3
30	M	204	CDL	CA2-OA2-PA1-OA4
30	M	205	CDL	CB2-OB2-PB2-OB3
30	O	201	CDL	CA3-OA5-PA1-OA2
30	O	201	CDL	CA3-OA5-PA1-OA3
30	O	201	CDL	CA3-OA5-PA1-OA4
30	O	201	CDL	CB2-OB2-PB2-OB3
30	O	201	CDL	CB3-OB5-PB2-OB2
30	O	201	CDL	CB3-OB5-PB2-OB3
30	O	201	CDL	CB3-OB5-PB2-OB4
30	P	201	CDL	CA2-OA2-PA1-OA3
30	P	201	CDL	CA3-OA5-PA1-OA3
30	P	201	CDL	CB2-OB2-PB2-OB3
30	P	202	CDL	OA5-CA3-CA4-OA6
30	P	202	CDL	CB3-OB5-PB2-OB3
30	P	202	CDL	CB3-OB5-PB2-OB4
30	R	101	CDL	CB2-OB2-PB2-OB5
30	a	501	CDL	CB2-OB2-PB2-OB3
30	a	501	CDL	C51-CB5-OB6-CB4
30	a	502	CDL	OA7-CA5-OA6-CA4
30	a	502	CDL	C11-CA5-OA6-CA4
30	a	502	CDL	CB2-OB2-PB2-OB3
30	a	502	CDL	CB3-OB5-PB2-OB3
30	a	502	CDL	OB7-CB5-OB6-CB4
30	a	503	CDL	CB2-C1-CA2-OA2
30	a	503	CDL	CA2-OA2-PA1-OA3
30	a	503	CDL	CA3-OA5-PA1-OA3
30	a	503	CDL	CA3-OA5-PA1-OA4
30	a	503	CDL	CB3-OB5-PB2-OB2
30	a	503	CDL	CB3-OB5-PB2-OB3
30	a	504	CDL	O1-C1-CB2-OB2
30	a	504	CDL	CA2-C1-CB2-OB2
30	a	504	CDL	OA6-CA4-CA6-OA8
30	a	504	CDL	OA7-CA5-OA6-CA4
30	a	504	CDL	CB3-OB5-PB2-OB4
30	a	505	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
30	a	505	CDL	CA2-OA2-PA1-OA3
30	a	505	CDL	CA3-OA5-PA1-OA3
30	a	505	CDL	CA3-OA5-PA1-OA4
30	a	505	CDL	CB2-OB2-PB2-OB3
30	a	505	CDL	C51-CB5-OB6-CB4
30	d	201	CDL	CA2-OA2-PA1-OA3
30	d	201	CDL	CA2-OA2-PA1-OA4
30	d	201	CDL	CB2-OB2-PB2-OB3
30	e	101	CDL	O1-C1-CB2-OB2
30	e	101	CDL	CA3-OA5-PA1-OA2
30	e	101	CDL	CA3-OA5-PA1-OA3
30	e	101	CDL	CA3-OA5-PA1-OA4
30	e	101	CDL	CB2-OB2-PB2-OB3
30	m	201	CDL	CA2-OA2-PA1-OA3
30	m	201	CDL	CA2-OA2-PA1-OA4
30	m	201	CDL	OA5-CA3-CA4-OA6
30	o	201	CDL	CA3-OA5-PA1-OA2
30	o	201	CDL	CA3-OA5-PA1-OA3
30	o	201	CDL	CA3-OA5-PA1-OA4
30	o	201	CDL	CB2-OB2-PB2-OB3
30	o	201	CDL	CB3-OB5-PB2-OB2
30	o	201	CDL	CB3-OB5-PB2-OB3
30	o	201	CDL	CB3-OB5-PB2-OB4
30	p	201	CDL	CA2-OA2-PA1-OA3
30	p	201	CDL	CA3-OA5-PA1-OA3
30	p	201	CDL	CB2-OB2-PB2-OB3
30	r	101	CDL	CB2-OB2-PB2-OB5
31	N	204	LMT	C2'-C1'-O1'-C1
31	N	204	LMT	O5'-C1'-O1'-C1
31	n	202	LMT	C2'-C1'-O1'-C1
31	n	202	LMT	O5'-C1'-O1'-C1
32	I	101	LPP	C6-O5-P1-O2
32	I	101	LPP	C6-O5-P1-O4
32	K	201	LPP	O10-C11-O9-C7
32	N	203	LPP	C6-O5-P1-O2
32	N	203	LPP	C6-O5-P1-O3
32	N	203	LPP	C6-O5-P1-O4
32	O	202	LPP	C6-O5-P1-O2
32	O	202	LPP	C6-O5-P1-O3
32	O	202	LPP	C6-O5-P1-O4
32	i	101	LPP	C6-O5-P1-O2
32	i	101	LPP	C6-O5-P1-O3

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Mol	Chain	Res	Type	Atoms
32	i	101	LPP	C6-O5-P1-O4
32	k	201	LPP	O10-C11-O9-C7
32	n	201	LPP	C6-O5-P1-O2
32	n	201	LPP	C6-O5-P1-O3
32	n	201	LPP	C6-O5-P1-O4
32	o	202	LPP	C6-O5-P1-O2
32	o	202	LPP	C6-O5-P1-O3
32	o	202	LPP	C6-O5-P1-O4
34	AF	601	ATP	C5'-O5'-PA-O1A
34	AF	601	ATP	C5'-O5'-PA-O3A
34	BF	601	ATP	C5'-O5'-PA-O1A
34	BF	601	ATP	C5'-O5'-PA-O3A
30	P	201	CDL	OB7-CB5-OB6-CB4
30	P	201	CDL	C51-CB5-OB6-CB4
30	p	201	CDL	OB7-CB5-OB6-CB4
30	p	201	CDL	C51-CB5-OB6-CB4
30	P	201	CDL	OA9-CA7-OA8-CA6
32	K	201	LPP	O28-C29-O27-C8
32	k	201	LPP	O28-C29-O27-C8
30	M	201	CDL	C31-CA7-OA8-CA6
30	M	205	CDL	C31-CA7-OA8-CA6
30	d	201	CDL	C31-CA7-OA8-CA6
30	p	201	CDL	C31-CA7-OA8-CA6
30	A	501	CDL	OA9-CA7-OA8-CA6
30	D	201	CDL	OA9-CA7-OA8-CA6
30	M	201	CDL	OA9-CA7-OA8-CA6
30	M	204	CDL	OA9-CA7-OA8-CA6
30	M	205	CDL	OA9-CA7-OA8-CA6
30	P	202	CDL	OB9-CB7-OB8-CB6
30	a	501	CDL	OA9-CA7-OA8-CA6
30	d	201	CDL	OA9-CA7-OA8-CA6
30	m	201	CDL	OA9-CA7-OA8-CA6
30	p	201	CDL	OA9-CA7-OA8-CA6
30	A	501	CDL	OB7-CB5-OB6-CB4
30	A	502	CDL	OA7-CA5-OA6-CA4
30	A	505	CDL	OB7-CB5-OB6-CB4
30	a	501	CDL	OB7-CB5-OB6-CB4
30	a	505	CDL	OB7-CB5-OB6-CB4
30	A	501	CDL	C31-CA7-OA8-CA6
30	D	201	CDL	C31-CA7-OA8-CA6
30	M	204	CDL	C31-CA7-OA8-CA6
30	P	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
30	P	202	CDL	C71-CB7-OB8-CB6
30	a	501	CDL	C31-CA7-OA8-CA6
30	m	201	CDL	C31-CA7-OA8-CA6
32	K	201	LPP	C30-C29-O27-C8
32	k	201	LPP	C30-C29-O27-C8
30	A	502	CDL	C11-CA5-OA6-CA4
30	A	502	CDL	C51-CB5-OB6-CB4
30	A	504	CDL	C11-CA5-OA6-CA4
30	a	502	CDL	C51-CB5-OB6-CB4
30	a	504	CDL	C11-CA5-OA6-CA4
32	K	201	LPP	C12-C11-O9-C7
32	k	201	LPP	C12-C11-O9-C7
33	P	203	TRT	C4-C1-C5-C6
33	p	202	TRT	C4-C1-C5-C6
30	P	201	CDL	C71-CB7-OB8-CB6
30	p	201	CDL	C71-CB7-OB8-CB6
31	F	302	LMT	C4B-C5B-C6B-O6B
31	g	201	LMT	C4B-C5B-C6B-O6B
30	P	201	CDL	OB9-CB7-OB8-CB6
30	P	202	CDL	OA9-CA7-OA8-CA6
30	p	201	CDL	OB9-CB7-OB8-CB6
32	N	203	LPP	O28-C29-O27-C8
32	n	201	LPP	O28-C29-O27-C8
31	d	202	LMT	O5B-C5B-C6B-O6B
30	A	503	CDL	O1-C1-CA2-OA2
30	O	201	CDL	O1-C1-CA2-OA2
30	a	503	CDL	O1-C1-CA2-OA2
30	o	201	CDL	O1-C1-CA2-OA2
30	R	101	CDL	C31-CA7-OA8-CA6
30	M	204	CDL	C11-CA5-OA6-CA4
31	D	202	LMT	O5B-C5B-C6B-O6B
31	Q	101	LMT	C4B-C5B-C6B-O6B
33	P	203	TRT	C2-C1-C5-C6
33	p	202	TRT	C2-C1-C5-C6
32	K	201	LPP	C37-C38-C39-C40
32	k	201	LPP	C37-C38-C39-C40
31	N	204	LMT	C4'-C5'-C6'-O6'
31	q	101	LMT	C4B-C5B-C6B-O6B
30	A	502	CDL	C74-C75-C76-C77
30	a	502	CDL	C74-C75-C76-C77
30	P	202	CDL	C31-CA7-OA8-CA6
30	r	101	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
32	N	203	LPP	C30-C29-O27-C8
32	n	201	LPP	C30-C29-O27-C8
33	P	203	TRT	O21-C22-C23-O24
33	g	203	TRT	O21-C22-C23-O24
33	p	202	TRT	O21-C22-C23-O24
33	G	202	TRT	O21-C22-C23-O24
33	P	203	TRT	O15-C16-C17-O18
33	p	202	TRT	O15-C16-C17-O18
31	N	204	LMT	O5'-C5'-C6'-O6'
31	g	201	LMT	O5B-C5B-C6B-O6B
30	M	201	CDL	C71-C72-C73-C74
30	M	205	CDL	C71-C72-C73-C74
31	F	302	LMT	O5B-C5B-C6B-O6B
30	R	101	CDL	OA9-CA7-OA8-CA6
30	a	505	CDL	C75-C76-C77-C78
33	BR	201	TRT	C13-C12-O15-C16
30	A	505	CDL	C75-C76-C77-C78
33	AR	201	TRT	C13-C12-O15-C16
33	AR	201	TRT	C11-C12-O15-C16
33	BR	201	TRT	C11-C12-O15-C16
30	r	101	CDL	OA9-CA7-OA8-CA6
30	m	201	CDL	C11-CA5-OA6-CA4
33	G	201	TRT	O18-C19-C20-O21
33	g	202	TRT	O18-C19-C20-O21
30	A	505	CDL	CB2-C1-CA2-OA2
30	a	505	CDL	CB2-C1-CA2-OA2
31	n	202	LMT	O5B-C5B-C6B-O6B
33	P	203	TRT	C3-C1-C5-C6
33	p	202	TRT	C3-C1-C5-C6
30	A	503	CDL	C71-CB7-OB8-CB6
30	A	505	CDL	C71-CB7-OB8-CB6
30	E	101	CDL	C71-CB7-OB8-CB6
30	a	503	CDL	C71-CB7-OB8-CB6
30	a	505	CDL	C71-CB7-OB8-CB6
30	e	101	CDL	C71-CB7-OB8-CB6
31	d	202	LMT	C4B-C5B-C6B-O6B
30	P	202	CDL	C57-C58-C59-C60
33	N	201	TRT	C13-C12-O15-C16
33	N	201	TRT	C11-C12-O15-C16
33	n	203	TRT	C13-C12-O15-C16
33	n	203	TRT	C11-C12-O15-C16
33	AR	201	TRT	O21-C22-C23-O24

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Mol	Chain	Res	Type	Atoms
33	BR	201	TRT	O21-C22-C23-O24
33	P	203	TRT	C1-C5-C6-C7
33	p	202	TRT	C1-C5-C6-C7
31	N	204	LMT	O5B-C5B-C6B-O6B
30	M	204	CDL	OA5-CA3-CA4-OA6
33	P	203	TRT	C13-C12-O15-C16
33	p	202	TRT	C13-C12-O15-C16
33	AE	600	TRT	O15-C16-C17-O18
33	BE	600	TRT	O15-C16-C17-O18
30	A	502	CDL	O1-C1-CB2-OB2
30	A	504	CDL	CB5-C51-C52-C53
30	E	101	CDL	OB6-CB4-CB6-OB8
30	e	101	CDL	OB6-CB4-CB6-OB8
33	P	203	TRT	C11-C12-O15-C16
33	g	202	TRT	C11-C12-O15-C16
33	p	202	TRT	C11-C12-O15-C16
30	E	101	CDL	OB9-CB7-OB8-CB6
30	e	101	CDL	OB9-CB7-OB8-CB6
33	G	201	TRT	C11-C12-O15-C16
31	D	202	LMT	C4B-C5B-C6B-O6B
31	n	202	LMT	C4'-C5'-C6'-O6'
30	P	202	CDL	CB5-C51-C52-C53
30	a	504	CDL	CB5-C51-C52-C53
30	A	505	CDL	OB9-CB7-OB8-CB6
30	a	505	CDL	OB9-CB7-OB8-CB6
30	a	501	CDL	C72-C73-C74-C75
33	G	201	TRT	C13-C12-O15-C16
30	A	501	CDL	C72-C73-C74-C75
33	g	202	TRT	C13-C12-O15-C16
33	G	202	TRT	C11-C12-O15-C16
33	g	203	TRT	C11-C12-O15-C16
30	A	504	CDL	CA5-C11-C12-C13
30	A	503	CDL	CB5-C51-C52-C53
30	A	504	CDL	CA7-C31-C32-C33
30	a	503	CDL	CB5-C51-C52-C53
30	a	504	CDL	CA7-C31-C32-C33
32	N	203	LPP	C29-C30-C31-C32
32	n	201	LPP	C29-C30-C31-C32
31	Q	101	LMT	O5B-C5B-C6B-O6B
30	A	502	CDL	C31-CA7-OA8-CA6
33	N	202	TRT	O18-C19-C20-O21
33	n	204	TRT	O18-C19-C20-O21

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Mol	Chain	Res	Type	Atoms
33	P	203	TRT	C5-C6-C9-C14
33	p	202	TRT	C5-C6-C9-C14
31	q	101	LMT	O5B-C5B-C6B-O6B
30	M	204	CDL	OA7-CA5-OA6-CA4
33	G	202	TRT	C13-C12-O15-C16
33	g	203	TRT	C13-C12-O15-C16
33	BR	201	TRT	O18-C19-C20-O21
30	P	202	CDL	CA5-C11-C12-C13
30	R	101	CDL	CA5-C11-C12-C13
33	AR	201	TRT	O18-C19-C20-O21
30	a	505	CDL	C78-C79-C80-C81
33	P	203	TRT	C1-C5-C6-C8
33	p	202	TRT	C1-C5-C6-C8
33	AR	201	TRT	C1-C5-C6-C8
33	BR	201	TRT	C1-C5-C6-C8
30	A	503	CDL	OB9-CB7-OB8-CB6
30	A	503	CDL	C31-CA7-OA8-CA6
30	A	505	CDL	C78-C79-C80-C81
31	Q	101	LMT	O5'-C5'-C6'-O6'
30	m	201	CDL	OA7-CA5-OA6-CA4
30	a	503	CDL	C31-CA7-OA8-CA6
30	a	503	CDL	OB9-CB7-OB8-CB6
33	P	203	TRT	C5-C6-C9-C10
33	p	202	TRT	C5-C6-C9-C10
30	A	502	CDL	CA3-OA5-PA1-OA2
30	A	503	CDL	CA3-OA5-PA1-OA2
30	A	504	CDL	CB3-OB5-PB2-OB2
30	A	505	CDL	CA3-OA5-PA1-OA2
30	A	505	CDL	CB2-OB2-PB2-OB5
30	A	505	CDL	CB3-OB5-PB2-OB2
30	D	201	CDL	CA2-OA2-PA1-OA5
30	D	201	CDL	CA3-OA5-PA1-OA2
30	D	201	CDL	CB2-OB2-PB2-OB5
30	E	101	CDL	CB2-OB2-PB2-OB5
30	M	201	CDL	CA2-OA2-PA1-OA5
30	M	201	CDL	CA3-OA5-PA1-OA2
30	M	201	CDL	CB3-OB5-PB2-OB2
30	M	204	CDL	CA2-OA2-PA1-OA5
30	M	205	CDL	CA2-OA2-PA1-OA5
30	M	205	CDL	CA3-OA5-PA1-OA2
30	M	205	CDL	CB3-OB5-PB2-OB2
30	O	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
30	O	201	CDL	CB2-OB2-PB2-OB5
30	P	201	CDL	CA3-OA5-PA1-OA2
30	P	201	CDL	CB2-OB2-PB2-OB5
30	P	202	CDL	CB2-OB2-PB2-OB5
30	P	202	CDL	CB3-OB5-PB2-OB2
30	a	502	CDL	CA3-OA5-PA1-OA2
30	a	503	CDL	CA3-OA5-PA1-OA2
30	a	504	CDL	CB3-OB5-PB2-OB2
30	a	505	CDL	CA3-OA5-PA1-OA2
30	a	505	CDL	CB2-OB2-PB2-OB5
30	a	505	CDL	CB3-OB5-PB2-OB2
30	d	201	CDL	CA2-OA2-PA1-OA5
30	d	201	CDL	CA3-OA5-PA1-OA2
30	d	201	CDL	CB2-OB2-PB2-OB5
30	e	101	CDL	CB2-OB2-PB2-OB5
30	m	201	CDL	CA2-OA2-PA1-OA5
30	o	201	CDL	CA2-OA2-PA1-OA5
30	o	201	CDL	CB2-OB2-PB2-OB5
30	p	201	CDL	CA3-OA5-PA1-OA2
30	p	201	CDL	CB2-OB2-PB2-OB5
31	d	202	LMT	O5'-C5'-C6'-O6'
31	q	101	LMT	O5'-C5'-C6'-O6'
30	a	502	CDL	C31-CA7-OA8-CA6
31	n	202	LMT	C4B-C5B-C6B-O6B
30	r	101	CDL	CA5-C11-C12-C13
30	E	101	CDL	CA2-C1-CB2-OB2
30	e	101	CDL	CA2-C1-CB2-OB2
33	M	202	TRT	O15-C16-C17-O18
33	m	202	TRT	O15-C16-C17-O18
31	g	201	LMT	O1'-C1-C2-C3
31	F	302	LMT	O1'-C1-C2-C3
30	E	101	CDL	C72-C73-C74-C75
30	A	502	CDL	C13-C14-C15-C16
30	A	503	CDL	C72-C73-C74-C75
30	D	201	CDL	C17-C18-C19-C20
30	M	204	CDL	C13-C14-C15-C16
30	M	204	CDL	C71-C72-C73-C74
30	M	204	CDL	C73-C74-C75-C76
30	a	502	CDL	C13-C14-C15-C16
30	m	201	CDL	C13-C14-C15-C16
30	m	201	CDL	C71-C72-C73-C74
30	m	201	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
32	I	101	LPP	C21-C22-C23-C24
32	O	203	LPP	C17-C18-C19-C20
32	i	101	LPP	C21-C22-C23-C24
32	o	203	LPP	C17-C18-C19-C20
30	A	501	CDL	C17-C18-C19-C20
30	A	503	CDL	C74-C75-C76-C77
30	a	501	CDL	C17-C18-C19-C20
30	d	201	CDL	C17-C18-C19-C20
30	e	101	CDL	C72-C73-C74-C75
32	O	203	LPP	C18-C19-C20-C21
32	o	203	LPP	C18-C19-C20-C21
33	N	202	TRT	C13-C12-O15-C16
30	R	101	CDL	OB7-CB5-OB6-CB4
30	A	505	CDL	CA5-C11-C12-C13
30	M	204	CDL	C32-C33-C34-C35
33	n	204	TRT	C13-C12-O15-C16
30	a	503	CDL	C74-C75-C76-C77
30	a	505	CDL	C37-C38-C39-C40
30	m	201	CDL	C32-C33-C34-C35
30	r	101	CDL	C55-C56-C57-C58
33	N	202	TRT	C11-C12-O15-C16
30	M	204	CDL	O1-C1-CB2-OB2
30	a	502	CDL	O1-C1-CB2-OB2
30	m	201	CDL	O1-C1-CB2-OB2
30	A	505	CDL	C37-C38-C39-C40
30	A	505	CDL	C77-C78-C79-C80
30	R	101	CDL	C55-C56-C57-C58
30	a	505	CDL	C77-C78-C79-C80
31	n	202	LMT	C11-C10-C9-C8
32	I	101	LPP	C35-C36-C37-C38
32	i	101	LPP	C35-C36-C37-C38
30	A	503	CDL	OA9-CA7-OA8-CA6
30	A	502	CDL	C60-C61-C62-C63
30	A	505	CDL	C72-C73-C74-C75
30	D	201	CDL	C42-C43-C44-C45
30	a	502	CDL	C60-C61-C62-C63
30	a	503	CDL	C72-C73-C74-C75
30	a	505	CDL	C72-C73-C74-C75
30	d	201	CDL	C42-C43-C44-C45
30	e	101	CDL	C71-C72-C73-C74
31	N	204	LMT	C11-C10-C9-C8
32	K	201	LPP	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
32	k	201	LPP	C30-C31-C32-C33
30	a	501	CDL	CB7-C71-C72-C73
30	O	201	CDL	C71-C72-C73-C74
30	P	202	CDL	C18-C19-C20-C21
30	R	101	CDL	C57-C58-C59-C60
30	r	101	CDL	C57-C58-C59-C60
33	m	203	TRT	C13-C12-O15-C16
30	A	502	CDL	OA9-CA7-OA8-CA6
30	a	503	CDL	OA9-CA7-OA8-CA6
30	E	101	CDL	C71-C72-C73-C74
30	M	204	CDL	C79-C80-C81-C82
30	P	202	CDL	C15-C16-C17-C18
30	o	201	CDL	C71-C72-C73-C74
33	M	203	TRT	C13-C12-O15-C16
33	n	204	TRT	C11-C12-O15-C16
30	P	201	CDL	OA7-CA5-OA6-CA4
30	r	101	CDL	OB7-CB5-OB6-CB4
30	R	101	CDL	C51-CB5-OB6-CB4
30	r	101	CDL	C51-CB5-OB6-CB4
30	m	201	CDL	C79-C80-C81-C82
32	K	201	LPP	C32-C33-C34-C35
31	N	204	LMT	C4B-C5B-C6B-O6B
30	A	505	CDL	C34-C35-C36-C37
30	A	505	CDL	C74-C75-C76-C77
30	a	505	CDL	C74-C75-C76-C77
32	k	201	LPP	C32-C33-C34-C35
30	A	502	CDL	C72-C73-C74-C75
30	a	505	CDL	C34-C35-C36-C37
30	A	503	CDL	C33-C34-C35-C36
30	a	502	CDL	C72-C73-C74-C75
30	a	503	CDL	C33-C34-C35-C36
30	A	501	CDL	CB7-C71-C72-C73
30	M	201	CDL	CA5-C11-C12-C13
30	M	205	CDL	CA5-C11-C12-C13
30	a	505	CDL	CA5-C11-C12-C13
30	P	202	CDL	C55-C56-C57-C58
33	G	202	TRT	C5-C6-C9-C10
33	M	202	TRT	C5-C6-C9-C14
33	M	202	TRT	C5-C6-C9-C10
33	g	203	TRT	C5-C6-C9-C10
33	m	202	TRT	C5-C6-C9-C14
33	m	202	TRT	C5-C6-C9-C10

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Mol	Chain	Res	Type	Atoms
30	P	202	CDL	C31-C32-C33-C34
33	G	201	TRT	O21-C22-C23-O24
33	g	202	TRT	O21-C22-C23-O24
33	m	203	TRT	C11-C12-O15-C16
30	a	502	CDL	OA9-CA7-OA8-CA6
30	P	201	CDL	C72-C73-C74-C75
30	p	201	CDL	C72-C73-C74-C75
30	r	101	CDL	C36-C37-C38-C39
31	n	202	LMT	C3-C4-C5-C6
33	M	203	TRT	C11-C12-O15-C16
30	e	101	CDL	OA7-CA5-OA6-CA4
30	R	101	CDL	C36-C37-C38-C39
31	N	204	LMT	C3-C4-C5-C6
30	D	201	CDL	C11-CA5-OA6-CA4
30	D	201	CDL	C51-CB5-OB6-CB4
30	P	201	CDL	C11-CA5-OA6-CA4
30	d	201	CDL	C11-CA5-OA6-CA4
30	d	201	CDL	C51-CB5-OB6-CB4
30	e	101	CDL	C11-CA5-OA6-CA4
30	p	201	CDL	C11-CA5-OA6-CA4
32	o	203	LPP	C19-C20-C21-C22
32	O	203	LPP	C19-C20-C21-C22
30	a	504	CDL	CA5-C11-C12-C13
31	D	202	LMT	C3-C4-C5-C6
30	D	201	CDL	O1-C1-CB2-OB2
30	d	201	CDL	O1-C1-CB2-OB2
31	n	202	LMT	O5'-C5'-C6'-O6'
31	d	202	LMT	C3-C4-C5-C6
33	n	204	TRT	C5-C6-C9-C10
30	m	201	CDL	CB7-C71-C72-C73
30	D	201	CDL	OA7-CA5-OA6-CA4
30	E	101	CDL	OA7-CA5-OA6-CA4
30	d	201	CDL	OA7-CA5-OA6-CA4
30	d	201	CDL	OB7-CB5-OB6-CB4
30	p	201	CDL	OA7-CA5-OA6-CA4
30	A	504	CDL	C74-C75-C76-C77
30	a	503	CDL	C21-C22-C23-C24
30	a	504	CDL	C74-C75-C76-C77
32	K	201	LPP	C36-C37-C38-C39
32	k	201	LPP	C36-C37-C38-C39
30	R	101	CDL	C74-C75-C76-C77
30	a	502	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	r	101	CDL	C74-C75-C76-C77
30	M	204	CDL	CB7-C71-C72-C73
30	A	503	CDL	C21-C22-C23-C24
30	M	204	CDL	C74-C75-C76-C77
30	E	101	CDL	C11-CA5-OA6-CA4
30	M	201	CDL	C11-CA5-OA6-CA4
30	M	204	CDL	C51-CB5-OB6-CB4
30	P	202	CDL	C51-CB5-OB6-CB4
30	m	201	CDL	C51-CB5-OB6-CB4
30	m	201	CDL	C74-C75-C76-C77
30	A	502	CDL	C11-C12-C13-C14
30	A	503	CDL	OA7-CA5-OA6-CA4
30	A	503	CDL	OB7-CB5-OB6-CB4
30	a	503	CDL	OA7-CA5-OA6-CA4
30	a	503	CDL	OB7-CB5-OB6-CB4
30	o	201	CDL	OB7-CB5-OB6-CB4
30	D	201	CDL	CB5-C51-C52-C53
30	d	201	CDL	CB5-C51-C52-C53
33	G	202	TRT	C5-C6-C9-C14
33	N	202	TRT	C5-C6-C9-C14
33	N	202	TRT	C5-C6-C9-C10
33	g	203	TRT	C5-C6-C9-C14
33	n	204	TRT	C5-C6-C9-C14
30	M	204	CDL	C77-C78-C79-C80
30	m	201	CDL	C82-C83-C84-C85
30	A	503	CDL	C31-C32-C33-C34
30	M	204	CDL	C82-C83-C84-C85
30	M	205	CDL	C53-C54-C55-C56
30	m	201	CDL	C77-C78-C79-C80
30	a	503	CDL	C31-C32-C33-C34
30	R	101	CDL	C62-C63-C64-C65
30	E	101	CDL	C56-C57-C58-C59
30	A	503	CDL	C11-CA5-OA6-CA4
30	A	503	CDL	C51-CB5-OB6-CB4
30	A	505	CDL	C11-CA5-OA6-CA4
30	M	201	CDL	C51-CB5-OB6-CB4
30	M	205	CDL	C11-CA5-OA6-CA4
30	M	205	CDL	C51-CB5-OB6-CB4
30	O	201	CDL	C51-CB5-OB6-CB4
30	a	503	CDL	C11-CA5-OA6-CA4
30	a	503	CDL	C51-CB5-OB6-CB4
30	a	505	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
30	o	201	CDL	C51-CB5-OB6-CB4
32	N	203	LPP	C12-C11-O9-C7
32	n	201	LPP	C12-C11-O9-C7
30	r	101	CDL	C62-C63-C64-C65
30	O	201	CDL	C55-C56-C57-C58
30	o	201	CDL	C55-C56-C57-C58
30	A	505	CDL	OA7-CA5-OA6-CA4
30	D	201	CDL	OB7-CB5-OB6-CB4
30	M	205	CDL	OB7-CB5-OB6-CB4
30	O	201	CDL	OB7-CB5-OB6-CB4
32	K	201	LPP	C34-C35-C36-C37
32	k	201	LPP	C34-C35-C36-C37
30	e	101	CDL	C56-C57-C58-C59
30	A	502	CDL	C20-C21-C22-C23
30	a	502	CDL	C20-C21-C22-C23
31	Q	101	LMT	C1-C2-C3-C4
31	q	101	LMT	C1-C2-C3-C4
30	M	201	CDL	OB7-CB5-OB6-CB4
30	M	204	CDL	OB7-CB5-OB6-CB4
30	M	205	CDL	OA7-CA5-OA6-CA4
30	P	202	CDL	OB7-CB5-OB6-CB4
30	a	505	CDL	OA7-CA5-OA6-CA4
30	m	201	CDL	OB7-CB5-OB6-CB4
30	M	201	CDL	C53-C54-C55-C56
30	A	502	CDL	CB3-OB5-PB2-OB2
30	A	505	CDL	CA2-OA2-PA1-OA5
30	M	205	CDL	CB2-OB2-PB2-OB5
30	a	502	CDL	CB3-OB5-PB2-OB2
30	a	505	CDL	CA2-OA2-PA1-OA5
30	p	201	CDL	CA2-OA2-PA1-OA5
30	A	502	CDL	C23-C24-C25-C26
30	a	502	CDL	C23-C24-C25-C26
32	K	201	LPP	C11-C12-C13-C14
30	M	205	CDL	C1-CA2-OA2-PA1
30	A	503	CDL	OB5-CB3-CB4-CB6
30	A	505	CDL	OA5-CA3-CA4-CA6
30	E	101	CDL	OA5-CA3-CA4-CA6
30	P	202	CDL	OA5-CA3-CA4-CA6
30	a	503	CDL	OB5-CB3-CB4-CB6
30	a	505	CDL	OA5-CA3-CA4-CA6
30	e	101	CDL	OA5-CA3-CA4-CA6
32	k	201	LPP	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	D	202	LMT	O5'-C5'-C6'-O6'
30	a	501	CDL	C34-C35-C36-C37
30	E	101	CDL	C63-C64-C65-C66
30	A	501	CDL	C34-C35-C36-C37
30	P	202	CDL	C41-C42-C43-C44
30	e	101	CDL	C63-C64-C65-C66
30	e	101	CDL	CB3-CB4-CB6-OB8
30	M	205	CDL	C51-C52-C53-C54
31	d	202	LMT	O1'-C1-C2-C3
30	O	201	CDL	C15-C16-C17-C18
31	D	202	LMT	O1'-C1-C2-C3
30	E	101	CDL	C53-C54-C55-C56
30	O	201	CDL	C20-C21-C22-C23
30	P	202	CDL	C79-C80-C81-C82
30	a	505	CDL	C43-C44-C45-C46
30	o	201	CDL	C15-C16-C17-C18
30	o	201	CDL	C20-C21-C22-C23
30	A	505	CDL	C43-C44-C45-C46
30	A	502	CDL	C75-C76-C77-C78
30	a	502	CDL	C75-C76-C77-C78
32	N	203	LPP	C32-C33-C34-C35
32	n	201	LPP	C32-C33-C34-C35
32	I	101	LPP	C30-C29-O27-C8
32	i	101	LPP	C30-C29-O27-C8
30	P	201	CDL	CA6-CA4-OA6-CA5
30	p	201	CDL	CA6-CA4-OA6-CA5
30	e	101	CDL	C53-C54-C55-C56
30	M	201	CDL	C1-CA2-OA2-PA1
32	f	301	LPP	C6-O5-P1-O3
30	A	501	CDL	C55-C56-C57-C58
30	P	202	CDL	C37-C38-C39-C40
30	a	501	CDL	C55-C56-C57-C58
30	m	201	CDL	C72-C73-C74-C75
30	M	204	CDL	OB5-CB3-CB4-OB6
30	m	201	CDL	OB5-CB3-CB4-OB6
30	P	202	CDL	CA7-C31-C32-C33
30	M	204	CDL	C72-C73-C74-C75
30	M	205	CDL	C73-C74-C75-C76
30	A	502	CDL	C73-C74-C75-C76
31	F	302	LMT	C5-C6-C7-C8
30	R	101	CDL	OB6-CB4-CB6-OB8
30	o	201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
30	r	101	CDL	OB6-CB4-CB6-OB8
30	P	202	CDL	C81-C82-C83-C84
30	a	503	CDL	C52-C53-C54-C55
31	g	201	LMT	C5-C6-C7-C8
32	K	201	LPP	C38-C39-C40-C41
32	k	201	LPP	C38-C39-C40-C41
30	M	201	CDL	OA7-CA5-OA6-CA4
32	N	203	LPP	O10-C11-O9-C7
32	n	201	LPP	O10-C11-O9-C7
30	M	201	CDL	C73-C74-C75-C76
30	a	502	CDL	C73-C74-C75-C76
33	g	202	TRT	O15-C16-C17-O18
33	G	201	TRT	O15-C16-C17-O18
34	AB	601	ATP	PG-O3B-PB-O1B
34	AC	601	ATP	PG-O3B-PB-O1B
34	BB	601	ATP	PG-O3B-PB-O1B
34	BC	601	ATP	PG-O3B-PB-O1B
33	M	202	TRT	O18-C19-C20-O21
33	m	202	TRT	O18-C19-C20-O21
30	r	101	CDL	C59-C60-C61-C62
30	M	204	CDL	C71-CB7-OB8-CB6
30	m	201	CDL	C71-CB7-OB8-CB6
30	R	101	CDL	C59-C60-C61-C62
30	A	501	CDL	OB5-CB3-CB4-CB6
30	D	201	CDL	OB5-CB3-CB4-CB6
30	M	204	CDL	OA5-CA3-CA4-CA6
30	P	201	CDL	OA5-CA3-CA4-CA6
30	d	201	CDL	OB5-CB3-CB4-CB6
30	m	201	CDL	OA5-CA3-CA4-CA6
32	I	101	LPP	O28-C29-O27-C8
32	N	203	LPP	C13-C14-C15-C16
32	n	201	LPP	C13-C14-C15-C16
32	i	101	LPP	O28-C29-O27-C8
30	P	202	CDL	C59-C60-C61-C62
33	AR	201	TRT	O15-C16-C17-O18
33	BR	201	TRT	O15-C16-C17-O18
30	A	503	CDL	C52-C53-C54-C55
33	AR	201	TRT	C22-C23-O24-C25
33	BR	201	TRT	C22-C23-O24-C25
33	P	203	TRT	C17-C16-O15-C12
31	F	302	LMT	C2-C1-O1'-C1'
31	g	201	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
30	D	201	CDL	C71-CB7-OB8-CB6
30	d	201	CDL	C71-CB7-OB8-CB6
30	A	502	CDL	C31-C32-C33-C34
33	p	202	TRT	C17-C16-O15-C12
30	E	101	CDL	CB3-CB4-CB6-OB8
30	M	201	CDL	CB3-CB4-CB6-OB8
30	M	205	CDL	CB3-CB4-CB6-OB8
30	R	101	CDL	CA3-CA4-CA6-OA8
30	R	101	CDL	CB3-CB4-CB6-OB8
30	o	201	CDL	CA3-CA4-CA6-OA8
30	r	101	CDL	CA3-CA4-CA6-OA8
30	r	101	CDL	CB3-CB4-CB6-OB8
32	f	301	LPP	C6-C7-C8-O27
30	A	503	CDL	C71-C72-C73-C74
30	P	201	CDL	CA2-OA2-PA1-OA5
30	a	502	CDL	C31-C32-C33-C34
33	P	203	TRT	C22-C23-O24-C25
33	p	202	TRT	C22-C23-O24-C25
30	E	101	CDL	OB5-CB3-CB4-OB6
30	d	201	CDL	OA5-CA3-CA4-OA6
30	e	101	CDL	OB5-CB3-CB4-OB6
32	F	301	LPP	C12-C13-C14-C15
32	f	301	LPP	C12-C13-C14-C15
30	A	501	CDL	C15-C16-C17-C18
30	a	503	CDL	C71-C72-C73-C74
30	e	101	CDL	C51-C52-C53-C54
30	M	205	CDL	OB6-CB4-CB6-OB8
30	O	201	CDL	OA6-CA4-CA6-OA8
30	P	202	CDL	OB6-CB4-CB6-OB8
32	F	301	LPP	O9-C7-C8-O27
32	f	301	LPP	O9-C7-C8-O27
31	D	202	LMT	C6-C7-C8-C9
30	O	201	CDL	CB2-C1-CA2-OA2
30	o	201	CDL	CB2-C1-CA2-OA2
31	d	202	LMT	C6-C7-C8-C9
30	A	505	CDL	C53-C54-C55-C56
30	D	201	CDL	C12-C13-C14-C15
30	P	202	CDL	C38-C39-C40-C41
30	e	101	CDL	C62-C63-C64-C65
30	P	202	CDL	C72-C73-C74-C75
30	d	201	CDL	C12-C13-C14-C15
33	m	203	TRT	O18-C19-C20-O21

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Mol	Chain	Res	Type	Atoms
30	A	504	CDL	CA4-CA3-OA5-PA1
30	A	505	CDL	C1-CA2-OA2-PA1
30	A	505	CDL	CB4-CB3-OB5-PB2
30	M	201	CDL	CB4-CB3-OB5-PB2
30	M	205	CDL	CB4-CB3-OB5-PB2
30	a	504	CDL	C1-CA2-OA2-PA1
30	a	504	CDL	CA4-CA3-OA5-PA1
30	a	505	CDL	C1-CA2-OA2-PA1
30	a	505	CDL	CB4-CB3-OB5-PB2
30	o	201	CDL	C1-CB2-OB2-PB2
30	E	101	CDL	C62-C63-C64-C65
33	M	203	TRT	O18-C19-C20-O21
30	p	201	CDL	C32-C33-C34-C35
31	q	101	LMT	C3-C4-C5-C6
30	E	101	CDL	C12-C11-CA5-OA6
30	e	101	CDL	C12-C11-CA5-OA6
30	a	505	CDL	C53-C54-C55-C56
31	Q	101	LMT	C3-C4-C5-C6
33	AE	600	TRT	C5-C6-C9-C10
33	BE	600	TRT	C5-C6-C9-C10
30	A	504	CDL	C53-C54-C55-C56
30	r	101	CDL	CA7-C31-C32-C33
33	M	203	TRT	C1-C5-C6-C8
33	m	203	TRT	C1-C5-C6-C8
33	BE	600	TRT	C1-C5-C6-C8
30	M	204	CDL	OB9-CB7-OB8-CB6
30	a	501	CDL	OB5-CB3-CB4-CB6
30	o	201	CDL	OB5-CB3-CB4-CB6
30	p	201	CDL	OA5-CA3-CA4-CA6
30	a	501	CDL	C15-C16-C17-C18
30	a	504	CDL	C53-C54-C55-C56
30	E	101	CDL	C51-C52-C53-C54
30	a	505	CDL	C39-C40-C41-C42
33	N	202	TRT	C22-C23-O24-C25
33	n	204	TRT	C22-C23-O24-C25
30	A	505	CDL	C39-C40-C41-C42
30	A	505	CDL	C13-C14-C15-C16
30	M	201	CDL	C51-C52-C53-C54
30	P	202	CDL	C74-C75-C76-C77
30	R	101	CDL	C75-C76-C77-C78
30	r	101	CDL	C75-C76-C77-C78
31	F	302	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
30	a	505	CDL	CA6-CA4-OA6-CA5
31	g	201	LMT	C11-C10-C9-C8
30	D	201	CDL	C11-C12-C13-C14
30	m	201	CDL	OB9-CB7-OB8-CB6
30	a	505	CDL	C13-C14-C15-C16
30	r	101	CDL	C72-C73-C74-C75
30	R	101	CDL	C72-C73-C74-C75
30	e	101	CDL	CA7-C31-C32-C33
30	A	504	CDL	CA3-CA4-CA6-OA8
30	A	505	CDL	CB3-CB4-CB6-OB8
30	P	202	CDL	CB3-CB4-CB6-OB8
30	a	501	CDL	CB4-CB3-OB5-PB2
30	a	504	CDL	CA3-CA4-CA6-OA8
30	a	505	CDL	CB3-CB4-CB6-OB8
30	o	201	CDL	C1-CA2-OA2-PA1
32	F	301	LPP	C6-C7-C8-O27
30	A	501	CDL	C11-CA5-OA6-CA4
30	a	501	CDL	C11-CA5-OA6-CA4
30	R	101	CDL	C31-C32-C33-C34
33	AE	600	TRT	C1-C5-C6-C8
30	A	505	CDL	OA5-CA3-CA4-OA6
30	D	201	CDL	OA5-CA3-CA4-OA6
30	D	201	CDL	OB5-CB3-CB4-OB6
30	a	505	CDL	OA5-CA3-CA4-OA6
30	d	201	CDL	OB5-CB3-CB4-OB6
30	e	101	CDL	OA5-CA3-CA4-OA6
30	o	201	CDL	OB5-CB3-CB4-OB6
32	N	203	LPP	O5-C6-C7-O9
32	n	201	LPP	O5-C6-C7-O9
31	g	201	LMT	O5'-C5'-C6'-O6'
30	P	201	CDL	C32-C33-C34-C35
30	r	101	CDL	C31-C32-C33-C34
33	AR	201	TRT	C17-C16-O15-C12
30	d	201	CDL	C11-C12-C13-C14
32	k	201	LPP	C35-C36-C37-C38
33	G	202	TRT	C17-C16-O15-C12
33	g	203	TRT	C17-C16-O15-C12
30	A	502	CDL	CA2-C1-CB2-OB2
30	A	502	CDL	C76-C77-C78-C79
30	d	201	CDL	OB9-CB7-OB8-CB6
33	N	202	TRT	C16-C17-O18-C19
30	P	202	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
32	K	201	LPP	C35-C36-C37-C38
33	g	202	TRT	C16-C17-O18-C19
33	n	204	TRT	C16-C17-O18-C19
30	R	101	CDL	OA6-CA4-CA6-OA8
30	r	101	CDL	OA6-CA4-CA6-OA8
33	G	201	TRT	C16-C17-O18-C19
33	M	203	TRT	C16-C17-O18-C19
33	m	203	TRT	C16-C17-O18-C19
30	D	201	CDL	OB9-CB7-OB8-CB6
30	a	501	CDL	C51-C52-C53-C54
30	a	501	CDL	CA7-C31-C32-C33
30	A	501	CDL	OA7-CA5-OA6-CA4
30	a	501	CDL	OA7-CA5-OA6-CA4
30	A	501	CDL	C51-C52-C53-C54
30	A	503	CDL	C18-C19-C20-C21
30	A	505	CDL	C31-C32-C33-C34
30	A	501	CDL	CA7-C31-C32-C33
30	M	205	CDL	C12-C11-CA5-OA6
30	a	501	CDL	C58-C59-C60-C61
33	AR	201	TRT	C1-C5-C6-C9
33	BR	201	TRT	C1-C5-C6-C9
30	A	501	CDL	C58-C59-C60-C61
30	A	502	CDL	CB2-OB2-PB2-OB5
30	E	101	CDL	CA2-OA2-PA1-OA5
30	M	201	CDL	CB2-OB2-PB2-OB5
30	a	502	CDL	CB2-OB2-PB2-OB5
30	e	101	CDL	CA2-OA2-PA1-OA5
30	a	502	CDL	C76-C77-C78-C79
30	a	503	CDL	C18-C19-C20-C21
30	m	201	CDL	C17-C18-C19-C20
33	n	203	TRT	C17-C16-O15-C12
30	O	201	CDL	C72-C71-CB7-OB8
30	A	501	CDL	CB4-CB3-OB5-PB2
30	A	504	CDL	C1-CA2-OA2-PA1
30	O	201	CDL	C1-CA2-OA2-PA1
30	O	201	CDL	C1-CB2-OB2-PB2
30	P	202	CDL	C1-CA2-OA2-PA1
30	d	201	CDL	C53-C54-C55-C56
30	A	502	CDL	CA3-OA5-PA1-OA3
30	A	502	CDL	CA3-OA5-PA1-OA4
30	A	504	CDL	CB3-OB5-PB2-OB4
30	A	505	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
30	D	201	CDL	CA3-OA5-PA1-OA4
30	D	201	CDL	CB2-OB2-PB2-OB4
30	E	101	CDL	CA2-OA2-PA1-OA3
30	E	101	CDL	CB2-OB2-PB2-OB4
30	E	101	CDL	CB3-OB5-PB2-OB4
30	M	201	CDL	CA2-OA2-PA1-OA3
30	M	201	CDL	CA3-OA5-PA1-OA3
30	M	201	CDL	CA3-OA5-PA1-OA4
30	M	201	CDL	CB3-OB5-PB2-OB3
30	M	201	CDL	CB3-OB5-PB2-OB4
30	M	205	CDL	CA2-OA2-PA1-OA3
30	M	205	CDL	CA3-OA5-PA1-OA3
30	M	205	CDL	CA3-OA5-PA1-OA4
30	M	205	CDL	CB3-OB5-PB2-OB3
30	M	205	CDL	CB3-OB5-PB2-OB4
30	O	201	CDL	CA2-OA2-PA1-OA4
30	O	201	CDL	CB2-OB2-PB2-OB4
30	P	201	CDL	CA2-OA2-PA1-OA4
30	P	201	CDL	CB2-OB2-PB2-OB4
30	P	202	CDL	CA3-OA5-PA1-OA3
30	P	202	CDL	CB2-OB2-PB2-OB4
30	a	502	CDL	CA3-OA5-PA1-OA3
30	a	502	CDL	CA3-OA5-PA1-OA4
30	a	505	CDL	CB3-OB5-PB2-OB4
30	d	201	CDL	CA3-OA5-PA1-OA4
30	d	201	CDL	CB2-OB2-PB2-OB4
30	e	101	CDL	CA2-OA2-PA1-OA3
30	e	101	CDL	CA2-OA2-PA1-OA4
30	e	101	CDL	CB2-OB2-PB2-OB4
30	o	201	CDL	CA2-OA2-PA1-OA4
30	o	201	CDL	CB2-OB2-PB2-OB4
30	p	201	CDL	CA2-OA2-PA1-OA4
30	p	201	CDL	CB2-OB2-PB2-OB4
34	AF	601	ATP	C5'-O5'-PA-O2A
34	BF	601	ATP	C5'-O5'-PA-O2A
30	R	101	CDL	CA7-C31-C32-C33
30	O	201	CDL	OB5-CB3-CB4-CB6
30	m	201	CDL	OB5-CB3-CB4-CB6
32	N	203	LPP	O5-C6-C7-C8
32	n	201	LPP	O5-C6-C7-C8
30	M	204	CDL	C81-C82-C83-C84
33	AE	600	TRT	C5-C6-C9-C14

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Mol	Chain	Res	Type	Atoms
30	M	204	CDL	C17-C18-C19-C20
30	P	202	CDL	C53-C54-C55-C56
30	r	101	CDL	C63-C64-C65-C66
32	O	202	LPP	C13-C14-C15-C16
33	N	201	TRT	O21-C22-C23-O24
30	o	201	CDL	C72-C71-CB7-OB8
30	D	201	CDL	C53-C54-C55-C56
33	n	203	TRT	O21-C22-C23-O24
30	R	101	CDL	C63-C64-C65-C66
30	m	201	CDL	C81-C82-C83-C84
32	o	202	LPP	C13-C14-C15-C16
30	A	503	CDL	OB5-CB3-CB4-OB6
30	E	101	CDL	OA5-CA3-CA4-OA6
30	O	201	CDL	OB5-CB3-CB4-OB6
30	a	503	CDL	OB5-CB3-CB4-OB6
30	m	201	CDL	C16-C17-C18-C19
33	BE	600	TRT	C5-C6-C9-C14
30	M	204	CDL	C80-C81-C82-C83
30	E	101	CDL	CA7-C31-C32-C33
30	M	204	CDL	C16-C17-C18-C19
30	a	505	CDL	C31-C32-C33-C34
32	o	203	LPP	C12-C13-C14-C15
32	O	203	LPP	C12-C13-C14-C15
30	P	202	CDL	C76-C77-C78-C79
30	M	201	CDL	OB6-CB4-CB6-OB8
30	a	505	CDL	OA6-CA4-CA6-OA8
32	I	101	LPP	C18-C19-C20-C21
30	M	201	CDL	C12-C11-CA5-OA6
33	n	203	TRT	C1-C5-C6-C8
32	I	101	LPP	C31-C32-C33-C34
32	i	101	LPP	C31-C32-C33-C34
33	AE	600	TRT	C1-C5-C6-C9
33	BE	600	TRT	C1-C5-C6-C9
30	E	101	CDL	C73-C74-C75-C76
31	q	101	LMT	C7-C8-C9-C10
30	m	201	CDL	C21-C22-C23-C24
31	Q	101	LMT	C7-C8-C9-C10
30	A	501	CDL	C12-C11-CA5-OA6
30	a	501	CDL	C12-C11-CA5-OA6
30	M	204	CDL	C21-C22-C23-C24
32	i	101	LPP	C18-C19-C20-C21
30	m	201	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
33	N	201	TRT	C17-C16-O15-C12
30	a	505	CDL	C73-C74-C75-C76
30	e	101	CDL	C73-C74-C75-C76
30	P	201	CDL	C71-C72-C73-C74
32	N	203	LPP	O9-C11-C12-C13
32	n	201	LPP	O9-C11-C12-C13
30	a	501	CDL	C20-C21-C22-C23
30	A	503	CDL	C55-C56-C57-C58
30	a	503	CDL	C55-C56-C57-C58
30	E	101	CDL	C32-C33-C34-C35
30	A	502	CDL	CA6-CA4-OA6-CA5
30	A	503	CDL	CA6-CA4-OA6-CA5
30	A	505	CDL	CA6-CA4-OA6-CA5
30	E	101	CDL	CA6-CA4-OA6-CA5
30	a	502	CDL	CA6-CA4-OA6-CA5
30	a	503	CDL	CA6-CA4-OA6-CA5
30	e	101	CDL	CA6-CA4-OA6-CA5
30	M	204	CDL	OB5-CB3-CB4-CB6
33	n	203	TRT	O15-C16-C17-O18
33	N	201	TRT	C1-C5-C6-C8
33	N	201	TRT	O15-C16-C17-O18
30	A	504	CDL	C32-C31-CA7-OA8
30	A	501	CDL	C13-C14-C15-C16
30	A	503	CDL	C51-C52-C53-C54
30	M	201	CDL	C1-CB2-OB2-PB2
32	F	301	LPP	C6-O5-P1-O3
30	A	501	CDL	OB5-CB3-CB4-OB6
30	p	201	CDL	OA5-CA3-CA4-OA6
32	I	101	LPP	C39-C40-C41-C42
30	e	101	CDL	C32-C33-C34-C35
33	AE	600	TRT	C7-C6-C9-C10
30	o	201	CDL	C17-C18-C19-C20
32	i	101	LPP	C39-C40-C41-C42
30	A	505	CDL	C32-C31-CA7-OA8
30	a	504	CDL	C32-C31-CA7-OA8
33	BE	600	TRT	C7-C6-C9-C10
30	O	201	CDL	C17-C18-C19-C20
32	K	201	LPP	C39-C40-C41-C42
30	A	504	CDL	C75-C76-C77-C78
30	a	504	CDL	C75-C76-C77-C78
32	k	201	LPP	C39-C40-C41-C42
33	G	202	TRT	O15-C16-C17-O18

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Mol	Chain	Res	Type	Atoms
30	m	201	CDL	C75-C76-C77-C78
33	g	203	TRT	O15-C16-C17-O18
30	A	501	CDL	CB3-OB5-PB2-OB2
30	A	503	CDL	CA2-OA2-PA1-OA5
30	A	504	CDL	CA2-OA2-PA1-OA5
30	M	204	CDL	CB2-OB2-PB2-OB5
30	R	101	CDL	CA3-OA5-PA1-OA2
30	a	501	CDL	CB3-OB5-PB2-OB2
30	a	503	CDL	CA2-OA2-PA1-OA5
30	a	504	CDL	CA2-OA2-PA1-OA5
30	m	201	CDL	CB2-OB2-PB2-OB5
30	r	101	CDL	CA2-OA2-PA1-OA5
30	r	101	CDL	CA3-OA5-PA1-OA2
31	n	202	LMT	C5'-C4'-O1B-C1B
30	a	505	CDL	C81-C82-C83-C84
33	BR	201	TRT	C1-C5-C6-C7
33	M	203	TRT	C1-C5-C6-C9
33	m	203	TRT	C1-C5-C6-C9
33	BE	600	TRT	O21-C22-C23-O24
33	AE	600	TRT	O21-C22-C23-O24
30	A	505	CDL	C73-C74-C75-C76
34	AB	601	ATP	PG-O3B-PB-O2B
34	AC	601	ATP	PG-O3B-PB-O2B
34	BB	601	ATP	PG-O3B-PB-O2B
34	BC	601	ATP	PG-O3B-PB-O2B
33	AE	600	TRT	C7-C6-C9-C14
31	N	204	LMT	C5'-C4'-O1B-C1B
33	m	202	TRT	C20-C19-O18-C17
30	a	502	CDL	C32-C33-C34-C35
30	A	505	CDL	C81-C82-C83-C84
31	N	204	LMT	C2-C3-C4-C5
30	M	205	CDL	C1-CB2-OB2-PB2
30	r	101	CDL	C1-CB2-OB2-PB2
30	M	204	CDL	C75-C76-C77-C78
31	n	202	LMT	C2-C3-C4-C5
30	a	501	CDL	C13-C14-C15-C16
33	BE	600	TRT	C7-C6-C9-C14
33	AR	201	TRT	C1-C5-C6-C7
33	BR	201	TRT	C17-C16-O15-C12
32	I	101	LPP	C12-C13-C14-C15
33	m	203	TRT	O21-C22-C23-O24
32	i	101	LPP	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	d	201	CDL	OA5-CA3-CA4-CA6
31	g	201	LMT	C4'-C5'-C6'-O6'
30	a	504	CDL	C54-C55-C56-C57
33	M	203	TRT	O21-C22-C23-O24
30	a	501	CDL	C40-C41-C42-C43
33	G	202	TRT	C4-C1-C5-C6
30	A	504	CDL	C54-C55-C56-C57
33	G	201	TRT	C1-C5-C6-C9
33	N	201	TRT	C1-C5-C6-C9
33	N	202	TRT	C1-C5-C6-C9
33	g	202	TRT	C1-C5-C6-C9
33	n	203	TRT	C1-C5-C6-C9
33	n	204	TRT	C1-C5-C6-C9
30	A	501	CDL	C40-C41-C42-C43
32	o	203	LPP	C23-C24-C25-C26
30	P	201	CDL	CA4-CA3-OA5-PA1
30	R	101	CDL	C1-CB2-OB2-PB2
30	p	201	CDL	CA4-CA3-OA5-PA1
30	a	503	CDL	C51-C52-C53-C54
32	O	203	LPP	C23-C24-C25-C26
33	g	203	TRT	C4-C1-C5-C6
31	F	302	LMT	O5'-C5'-C6'-O6'
30	O	201	CDL	CA3-CA4-CA6-OA8
30	d	201	CDL	CB2-C1-CA2-OA2
30	P	202	CDL	C73-C74-C75-C76
30	A	502	CDL	C24-C25-C26-C27
30	a	504	CDL	C71-C72-C73-C74
33	M	202	TRT	C11-C12-O15-C16
30	O	201	CDL	CA3-CA4-OA6-CA5
32	N	203	LPP	C8-C7-O9-C11
32	n	201	LPP	C8-C7-O9-C11
30	a	502	CDL	C24-C25-C26-C27
32	i	101	LPP	C23-C24-C25-C26
30	O	201	CDL	C52-C51-CB5-OB6
30	a	505	CDL	C32-C31-CA7-OA8
30	O	201	CDL	C18-C19-C20-C21
32	I	101	LPP	C23-C24-C25-C26
30	a	505	CDL	C15-C16-C17-C18
30	P	202	CDL	CA3-OA5-PA1-OA2
30	R	101	CDL	CA2-OA2-PA1-OA5
30	o	201	CDL	C52-C51-CB5-OB6
30	o	201	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
33	M	202	TRT	C20-C19-O18-C17
33	m	203	TRT	C23-C22-O21-C20
30	D	201	CDL	OA5-CA3-CA4-CA6
30	P	202	CDL	C42-C43-C44-C45
30	A	505	CDL	C40-C41-C42-C43
31	F	302	LMT	C1-C2-C3-C4
31	g	201	LMT	C1-C2-C3-C4
30	a	505	CDL	C40-C41-C42-C43
32	F	301	LPP	C29-C30-C31-C32
32	f	301	LPP	C29-C30-C31-C32
30	P	202	CDL	C83-C84-C85-C86
33	P	203	TRT	C1-C5-C6-C9
33	p	202	TRT	C1-C5-C6-C9
30	d	201	CDL	C34-C35-C36-C37
30	A	505	CDL	OA6-CA4-CA6-OA8
30	A	504	CDL	C71-C72-C73-C74
30	D	201	CDL	C55-C56-C57-C58
30	R	101	CDL	C13-C14-C15-C16
33	N	202	TRT	C7-C6-C9-C10
33	BR	201	TRT	C23-C22-O21-C20
30	D	201	CDL	CB2-C1-CA2-OA2
30	A	505	CDL	C15-C16-C17-C18
33	M	202	TRT	C13-C12-O15-C16
30	d	201	CDL	C55-C56-C57-C58
33	n	204	TRT	C1-C5-C6-C8
30	D	201	CDL	C34-C35-C36-C37
33	m	202	TRT	C13-C12-O15-C16
33	G	202	TRT	O18-C19-C20-O21
33	g	203	TRT	O18-C19-C20-O21
33	m	202	TRT	C11-C12-O15-C16
30	R	101	CDL	C60-C61-C62-C63
30	r	101	CDL	C60-C61-C62-C63
32	N	203	LPP	C31-C32-C33-C34
32	n	201	LPP	C31-C32-C33-C34
31	g	201	LMT	C7-C8-C9-C10
30	E	101	CDL	C60-C61-C62-C63
30	e	101	CDL	C60-C61-C62-C63
30	E	101	CDL	C72-C71-CB7-OB8
31	F	302	LMT	C7-C8-C9-C10
31	D	202	LMT	C1-C2-C3-C4
30	P	201	CDL	OA5-CA3-CA4-OA6
30	a	501	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
31	d	202	LMT	C1-C2-C3-C4
33	M	203	TRT	C23-C22-O21-C20
33	n	204	TRT	C7-C6-C9-C10
30	E	101	CDL	OB5-CB3-CB4-CB6
32	O	202	LPP	O5-C6-C7-C8
30	R	101	CDL	C37-C38-C39-C40
30	p	201	CDL	OA6-CA4-CA6-OA8
32	o	202	LPP	C30-C29-O27-C8
30	e	101	CDL	C72-C71-CB7-OB8
30	m	201	CDL	C72-C71-CB7-OB8
30	A	504	CDL	C31-CA7-OA8-CA6
30	e	101	CDL	C31-CA7-OA8-CA6
32	O	202	LPP	C30-C29-O27-C8
33	G	202	TRT	C7-C6-C9-C14
30	P	202	CDL	C61-C62-C63-C64
30	p	201	CDL	C71-C72-C73-C74
30	M	204	CDL	C72-C71-CB7-OB8
30	R	101	CDL	C32-C31-CA7-OA8
33	P	203	TRT	O18-C19-C20-O21
32	O	203	LPP	C21-C22-C23-C24
33	p	202	TRT	O18-C19-C20-O21
30	A	501	CDL	CB2-OB2-PB2-OB5
30	a	501	CDL	CB2-OB2-PB2-OB5
32	o	203	LPP	C21-C22-C23-C24
33	M	202	TRT	O21-C22-C23-O24
33	N	201	TRT	C16-C17-O18-C19
33	m	202	TRT	O21-C22-C23-O24
33	g	203	TRT	C23-C22-O21-C20
32	O	202	LPP	O28-C29-O27-C8
32	o	202	LPP	O28-C29-O27-C8
33	g	203	TRT	C7-C6-C9-C14
33	n	203	TRT	C16-C17-O18-C19
30	o	201	CDL	CA3-CA4-OA6-CA5
30	r	101	CDL	C35-C36-C37-C38
30	M	205	CDL	C52-C51-CB5-OB6
30	r	101	CDL	C32-C31-CA7-OA8
32	O	203	LPP	C15-C16-C17-C18
30	d	201	CDL	C40-C41-C42-C43
32	I	101	LPP	C6-O5-P1-O3
30	r	101	CDL	C13-C14-C15-C16
30	E	101	CDL	C12-C11-CA5-OA7
30	a	504	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
32	O	202	LPP	O5-C6-C7-O9
33	N	202	TRT	C7-C6-C9-C14
33	N	202	TRT	C8-C6-C9-C10
33	n	204	TRT	C7-C6-C9-C14
33	n	204	TRT	C8-C6-C9-C10
30	M	201	CDL	C52-C51-CB5-OB6
32	o	203	LPP	C15-C16-C17-C18
33	G	202	TRT	C1-C5-C6-C9
33	g	203	TRT	C1-C5-C6-C9
30	A	504	CDL	C73-C74-C75-C76
30	r	101	CDL	C32-C33-C34-C35
30	a	504	CDL	OB9-CB7-OB8-CB6
33	G	202	TRT	C2-C1-C5-C6
33	n	203	TRT	O18-C19-C20-O21
33	M	202	TRT	C7-C6-C9-C10
30	e	101	CDL	C12-C11-CA5-OA7
30	e	101	CDL	OA9-CA7-OA8-CA6
30	A	502	CDL	C32-C33-C34-C35
33	N	201	TRT	O18-C19-C20-O21
33	G	202	TRT	C7-C6-C9-C10
33	m	202	TRT	C7-C6-C9-C10
30	M	204	CDL	C33-C34-C35-C36
30	d	201	CDL	C33-C34-C35-C36
30	e	101	CDL	OB5-CB3-CB4-CB6
33	N	202	TRT	C8-C6-C9-C14
33	n	204	TRT	C8-C6-C9-C14
33	m	203	TRT	O15-C16-C17-O18
30	a	505	CDL	OB6-CB4-CB6-OB8
30	A	504	CDL	OB9-CB7-OB8-CB6
33	g	203	TRT	C2-C1-C5-C6
33	M	203	TRT	O15-C16-C17-O18
33	N	202	TRT	C1-C5-C6-C8
33	BE	600	TRT	C1-C5-C6-C7
30	r	101	CDL	C77-C78-C79-C80
33	g	203	TRT	C7-C6-C9-C10
30	D	201	CDL	CB7-C71-C72-C73
30	a	504	CDL	C72-C73-C74-C75
30	P	202	CDL	OA7-CA5-OA6-CA4
30	R	101	CDL	C77-C78-C79-C80
30	m	201	CDL	C72-C71-CB7-OB9
31	Q	101	LMT	C4'-C5'-C6'-O6'
30	A	504	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
33	M	202	TRT	C8-C6-C9-C10
33	m	202	TRT	C8-C6-C9-C10
30	d	201	CDL	CA7-C31-C32-C33
30	A	504	CDL	C72-C73-C74-C75
33	G	202	TRT	C23-C22-O21-C20
32	f	301	LPP	O28-C29-O27-C8
32	o	203	LPP	C14-C15-C16-C17
32	o	202	LPP	C14-C15-C16-C17
30	m	201	CDL	C33-C34-C35-C36
32	O	203	LPP	C14-C15-C16-C17
30	O	201	CDL	C13-C14-C15-C16
32	O	202	LPP	C14-C15-C16-C17
30	D	201	CDL	C33-C34-C35-C36
30	o	201	CDL	C13-C14-C15-C16
33	M	202	TRT	C7-C6-C9-C14
33	m	202	TRT	C7-C6-C9-C14
30	o	201	CDL	OA9-CA7-OA8-CA6
30	M	204	CDL	C72-C71-CB7-OB9
30	D	201	CDL	C40-C41-C42-C43
32	F	301	LPP	O28-C29-O27-C8
30	o	201	CDL	C31-CA7-OA8-CA6
32	F	301	LPP	C30-C29-O27-C8
32	f	301	LPP	C30-C29-O27-C8
30	a	504	CDL	C60-C61-C62-C63
30	A	501	CDL	C54-C55-C56-C57
30	d	201	CDL	C59-C60-C61-C62
30	o	201	CDL	C72-C73-C74-C75
30	D	201	CDL	C22-C23-C24-C25
30	R	101	CDL	C35-C36-C37-C38
30	M	201	CDL	C52-C51-CB5-OB7
30	M	205	CDL	C52-C51-CB5-OB7
30	R	101	CDL	C32-C31-CA7-OA9
30	r	101	CDL	C32-C31-CA7-OA9
30	R	101	CDL	C53-C54-C55-C56
30	A	501	CDL	CB3-OB5-PB2-OB3
30	A	502	CDL	CA2-OA2-PA1-OA3
30	A	503	CDL	CB2-OB2-PB2-OB3
30	A	504	CDL	CB2-OB2-PB2-OB3
30	M	204	CDL	CB2-OB2-PB2-OB3
30	P	202	CDL	CB2-OB2-PB2-OB3
30	a	501	CDL	CB3-OB5-PB2-OB3
30	a	503	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
30	a	504	CDL	CB2-OB2-PB2-OB3
30	e	101	CDL	CB3-OB5-PB2-OB4
30	m	201	CDL	CB2-OB2-PB2-OB3
30	D	201	CDL	C59-C60-C61-C62
30	a	501	CDL	C54-C55-C56-C57
30	d	201	CDL	C22-C23-C24-C25
30	r	101	CDL	C52-C51-CB5-OB6
33	AE	600	TRT	C1-C5-C6-C7
31	D	202	LMT	O5'-C1'-O1'-C1
33	N	202	TRT	O21-C22-C23-O24
33	n	204	TRT	O21-C22-C23-O24
30	O	201	CDL	C72-C73-C74-C75
33	N	202	TRT	O15-C16-C17-O18
30	r	101	CDL	C53-C54-C55-C56
30	M	204	CDL	C52-C51-CB5-OB6
32	i	101	LPP	O9-C11-C12-C13
33	n	204	TRT	O15-C16-C17-O18
30	R	101	CDL	C76-C77-C78-C79
30	R	101	CDL	C52-C51-CB5-OB6
30	m	201	CDL	C52-C51-CB5-OB6
32	I	101	LPP	O9-C11-C12-C13
30	D	201	CDL	CA7-C31-C32-C33
33	M	202	TRT	C8-C6-C9-C14
30	O	201	CDL	C12-C13-C14-C15
30	A	504	CDL	C52-C51-CB5-OB6
30	P	201	CDL	C72-C71-CB7-OB8
30	O	201	CDL	C12-C11-CA5-OA6
30	a	504	CDL	C52-C51-CB5-OB6
30	d	201	CDL	C52-C51-CB5-OB6
30	E	101	CDL	C59-C60-C61-C62
30	m	201	CDL	C12-C13-C14-C15
32	f	301	LPP	C14-C15-C16-C17
30	r	101	CDL	C76-C77-C78-C79
30	p	201	CDL	C11-C12-C13-C14
30	e	101	CDL	C59-C60-C61-C62
30	a	504	CDL	C31-CA7-OA8-CA6
30	D	201	CDL	C52-C51-CB5-OB6
30	d	201	CDL	C12-C11-CA5-OA6
30	p	201	CDL	C12-C11-CA5-OA6
32	I	101	LPP	O27-C29-C30-C31
32	i	101	LPP	O27-C29-C30-C31
30	M	204	CDL	CA2-C1-CB2-OB2

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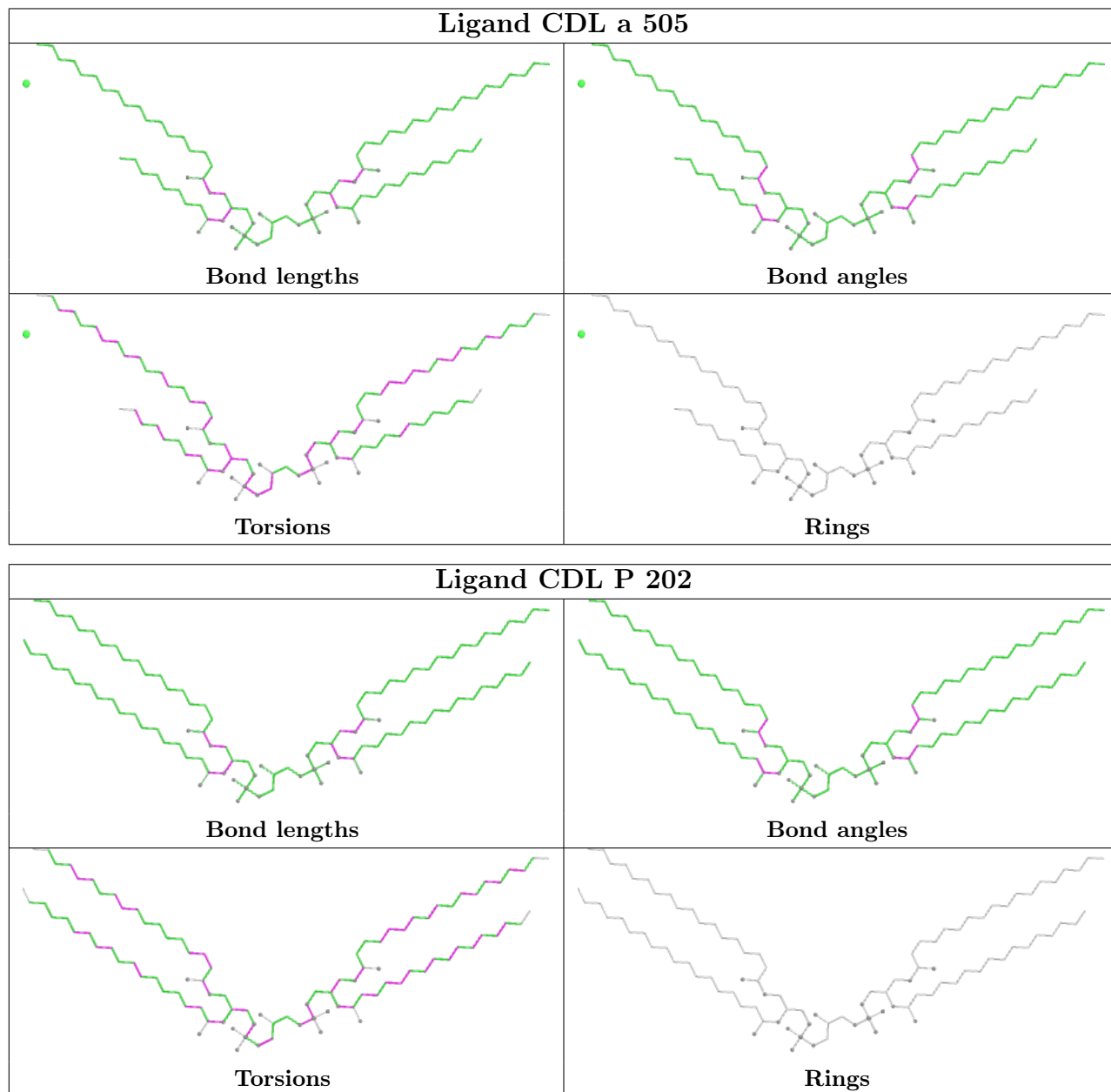
Mol	Chain	Res	Type	Atoms
30	A	504	CDL	C52-C51-CB5-OB7
33	g	203	TRT	C8-C6-C9-C14
33	m	202	TRT	C8-C6-C9-C14
32	F	301	LPP	C14-C15-C16-C17
30	O	201	CDL	C72-C71-CB7-OB9
30	a	504	CDL	C52-C51-CB5-OB7
30	D	201	CDL	C12-C11-CA5-OA6
30	M	205	CDL	C32-C31-CA7-OA8
30	P	201	CDL	C12-C11-CA5-OA6
30	o	201	CDL	C12-C11-CA5-OA6
30	p	201	CDL	C72-C71-CB7-OB8
30	R	101	CDL	C51-C52-C53-C54
30	r	101	CDL	C33-C34-C35-C36
30	D	201	CDL	C52-C51-CB5-OB7
30	P	201	CDL	C12-C11-CA5-OA7
30	p	201	CDL	C72-C71-CB7-OB9
31	D	202	LMT	C2-C1-O1'-C1'
31	d	202	LMT	C2-C1-O1'-C1'
30	M	201	CDL	C32-C31-CA7-OA8
30	P	202	CDL	C52-C53-C54-C55
31	d	202	LMT	O5'-C1'-O1'-C1
30	O	201	CDL	C12-C11-CA5-OA7
30	P	201	CDL	C72-C71-CB7-OB9
30	d	201	CDL	C52-C51-CB5-OB7
30	o	201	CDL	C72-C71-CB7-OB9
30	o	201	CDL	C12-C13-C14-C15
31	q	101	LMT	C4'-C5'-C6'-O6'
30	p	201	CDL	C12-C11-CA5-OA7
30	r	101	CDL	C52-C51-CB5-OB7
30	d	201	CDL	CB7-C71-C72-C73
30	R	101	CDL	C52-C51-CB5-OB7
30	o	201	CDL	C12-C11-CA5-OA7
33	G	202	TRT	C8-C6-C9-C14

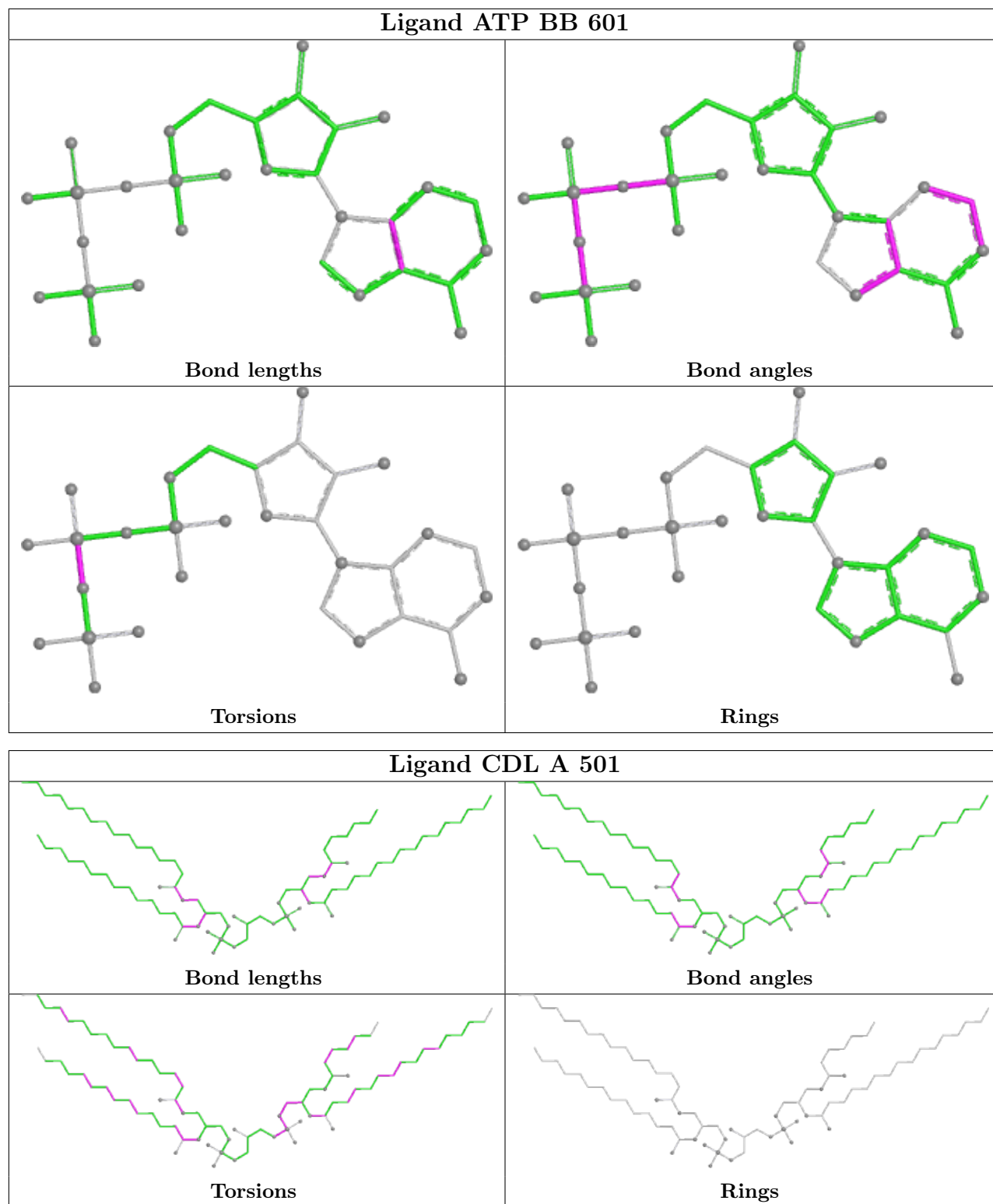
There are no ring outliers.

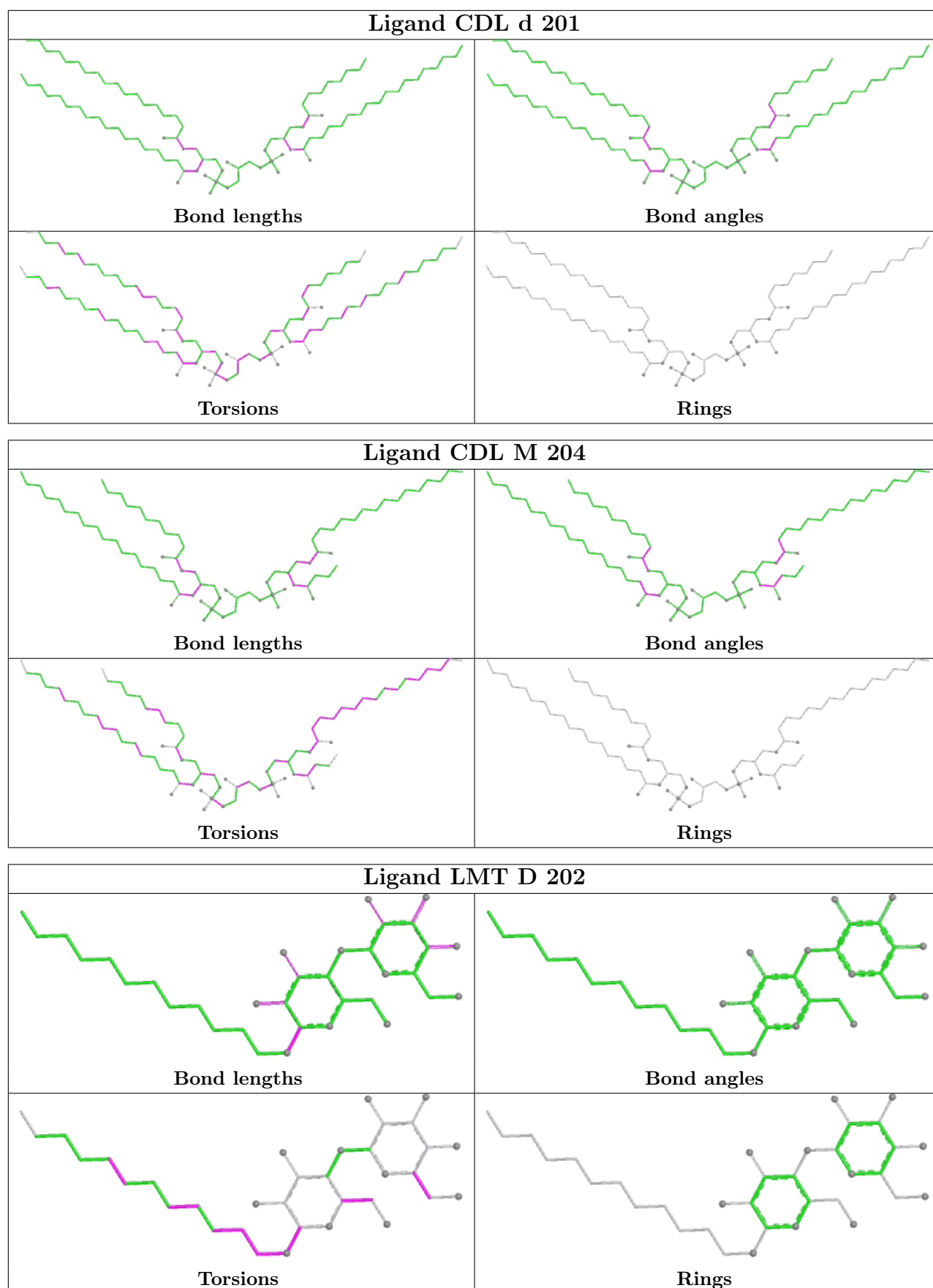
No monomer is involved in short contacts.

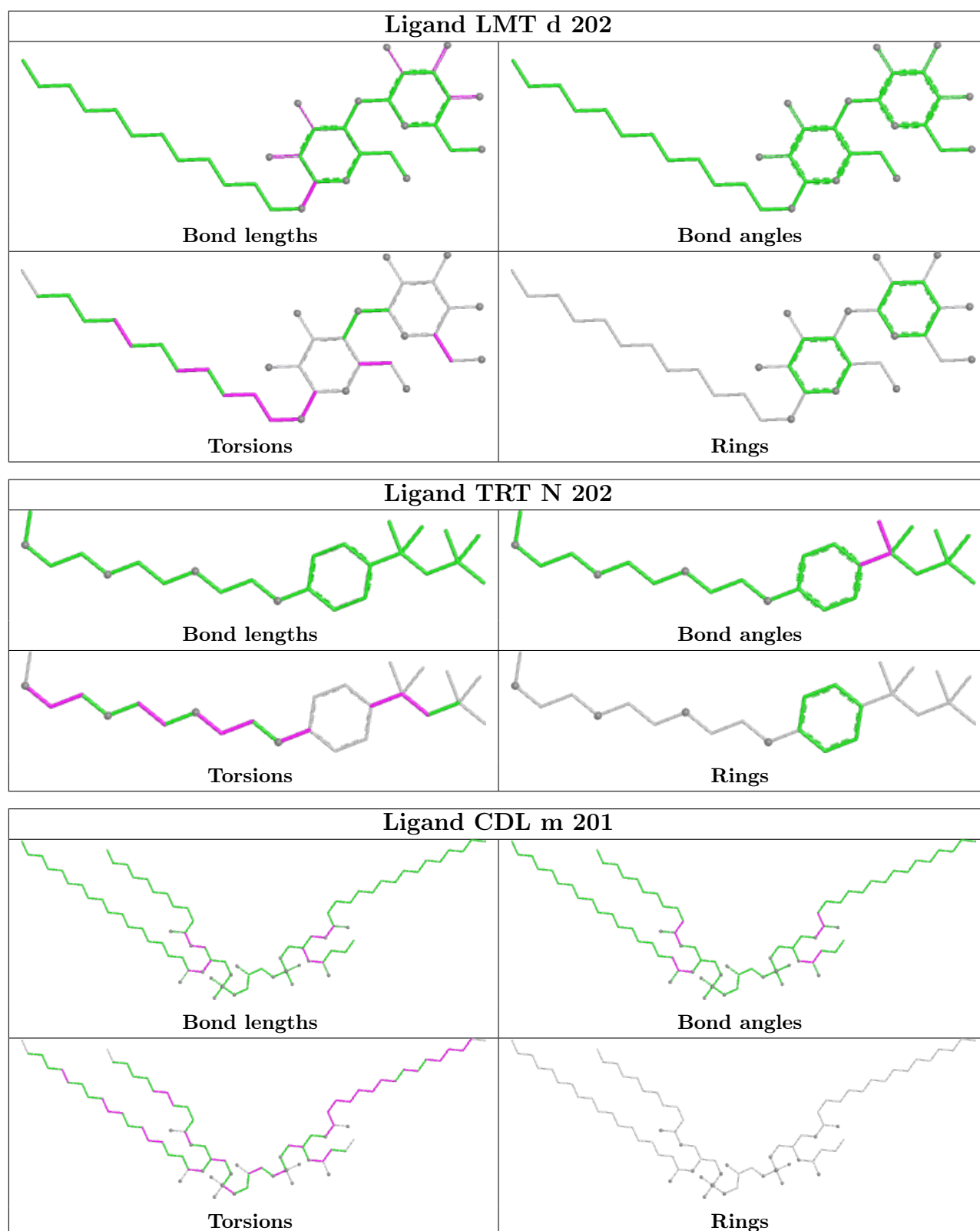
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

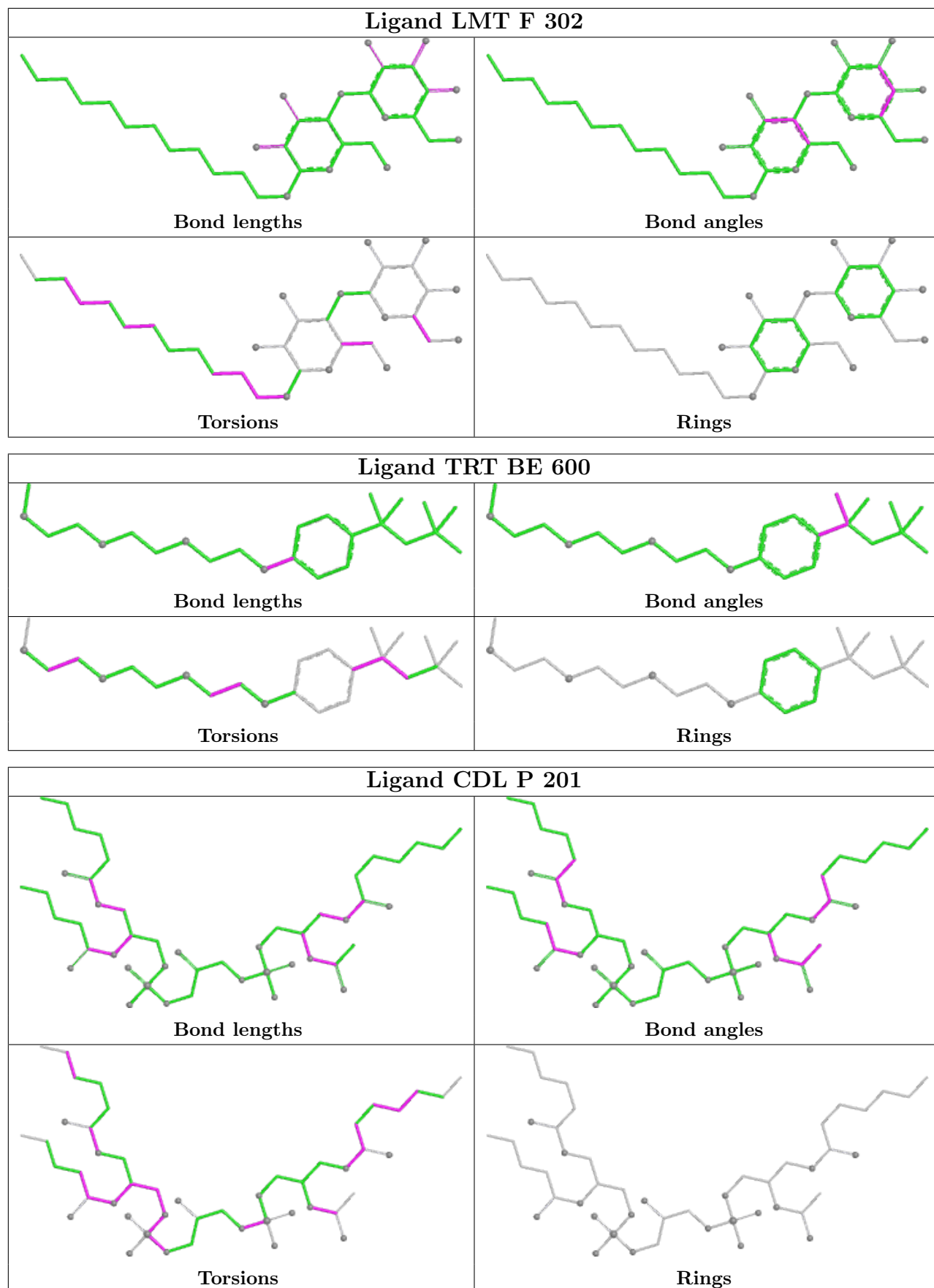
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

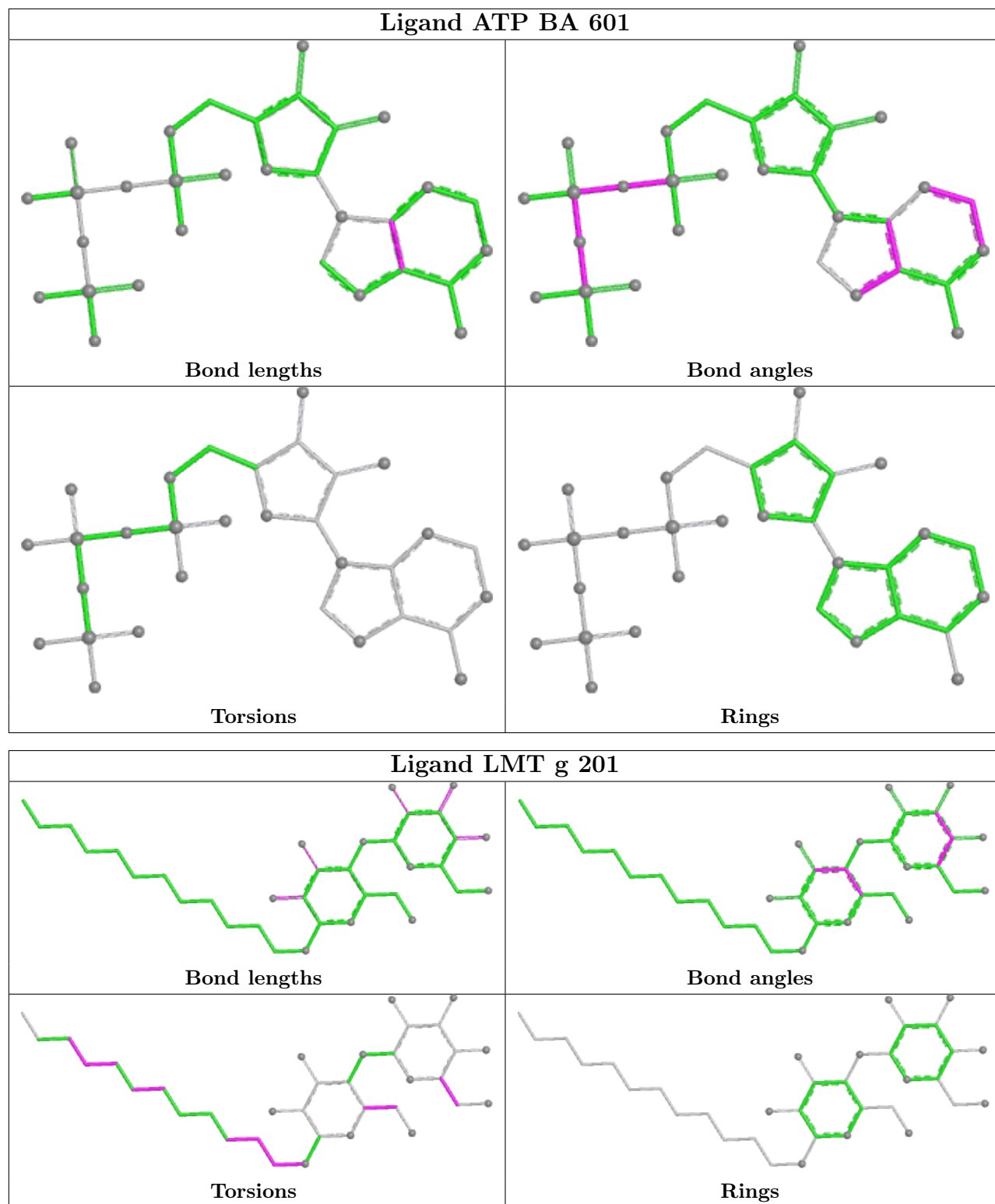


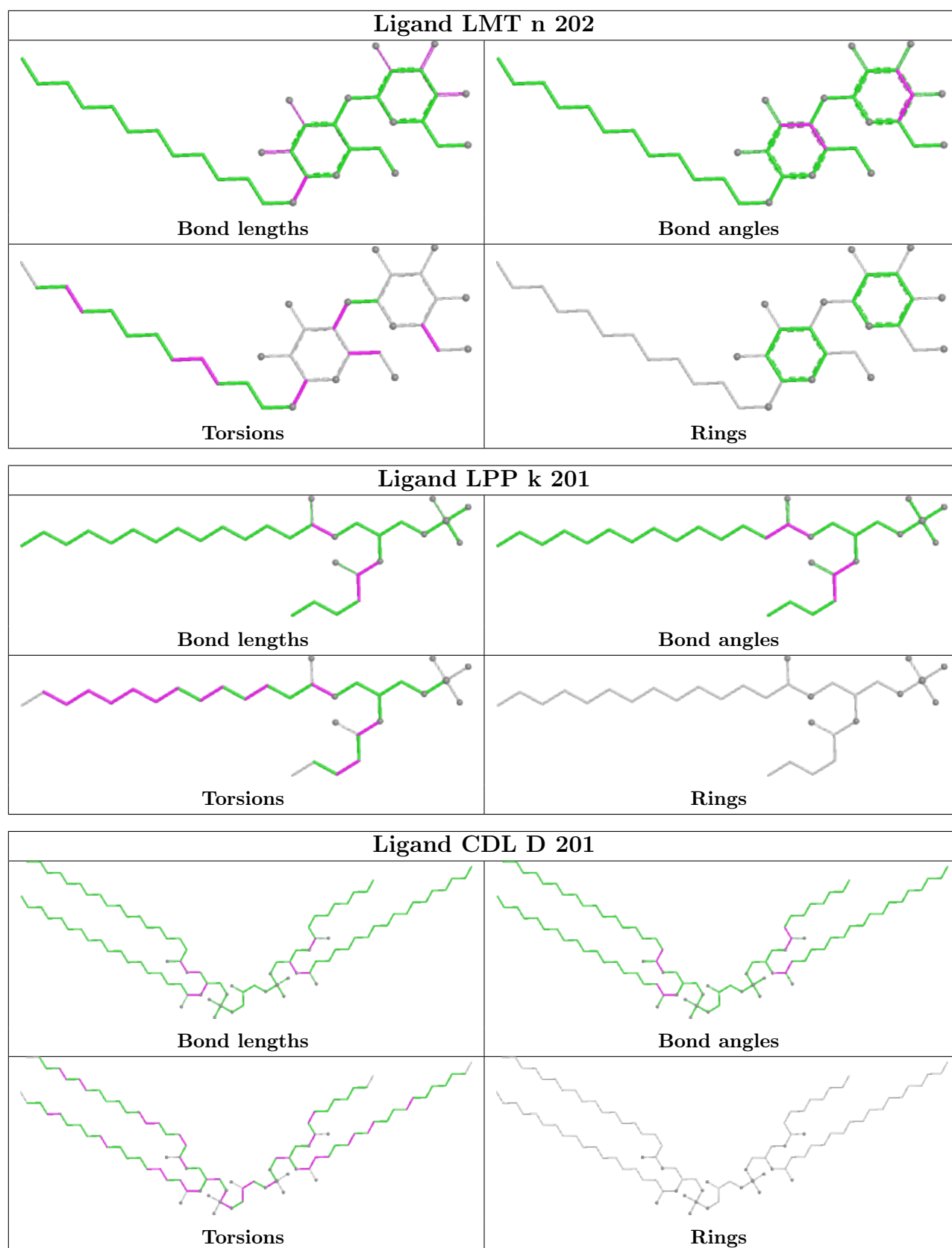


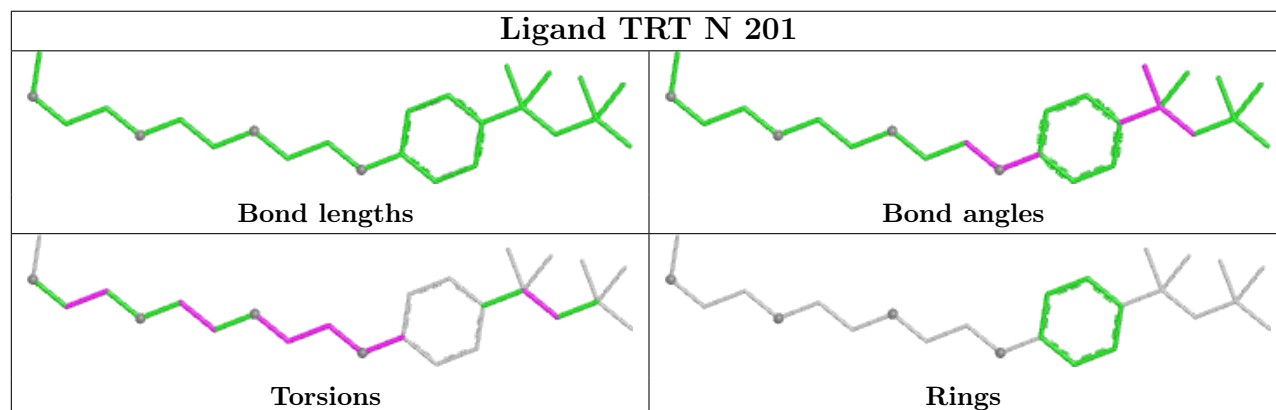
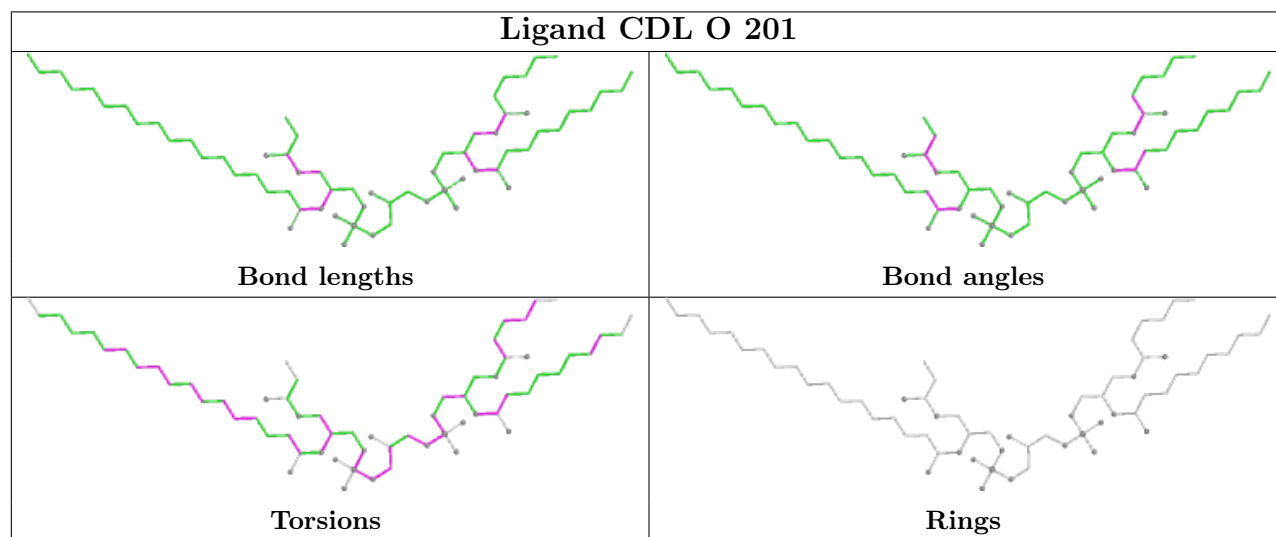
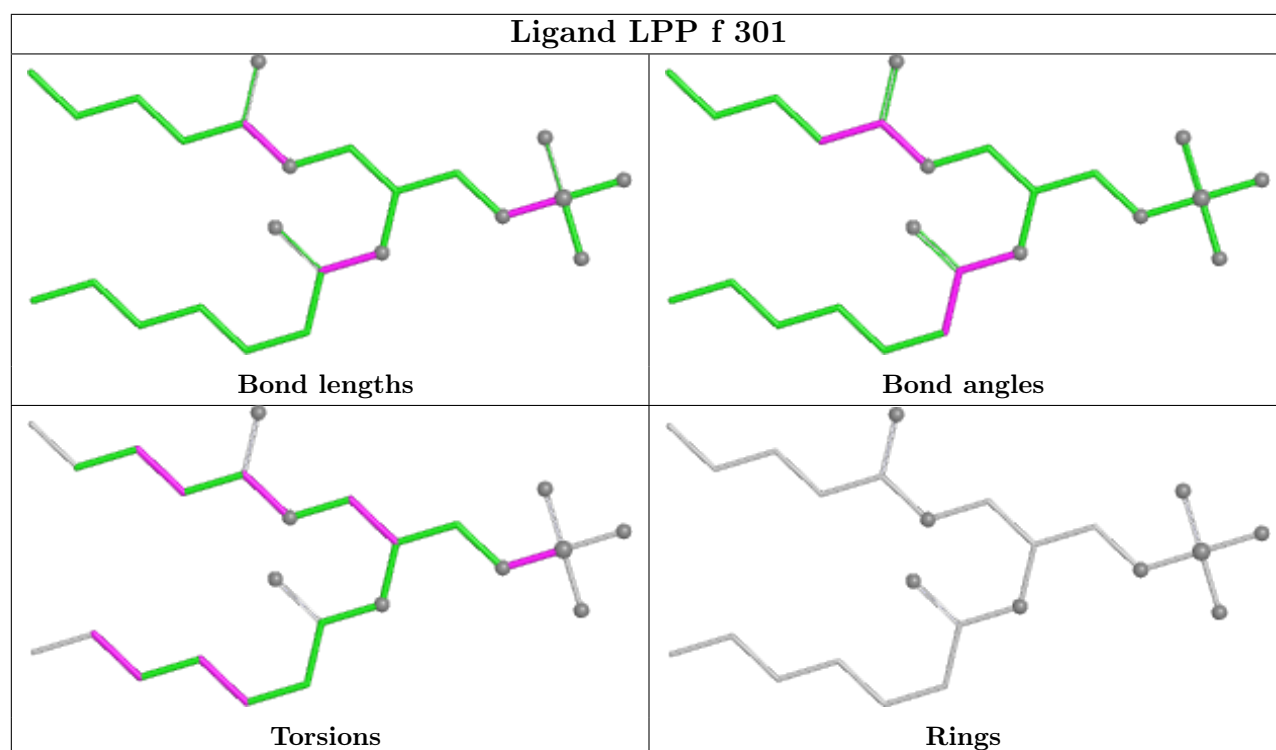


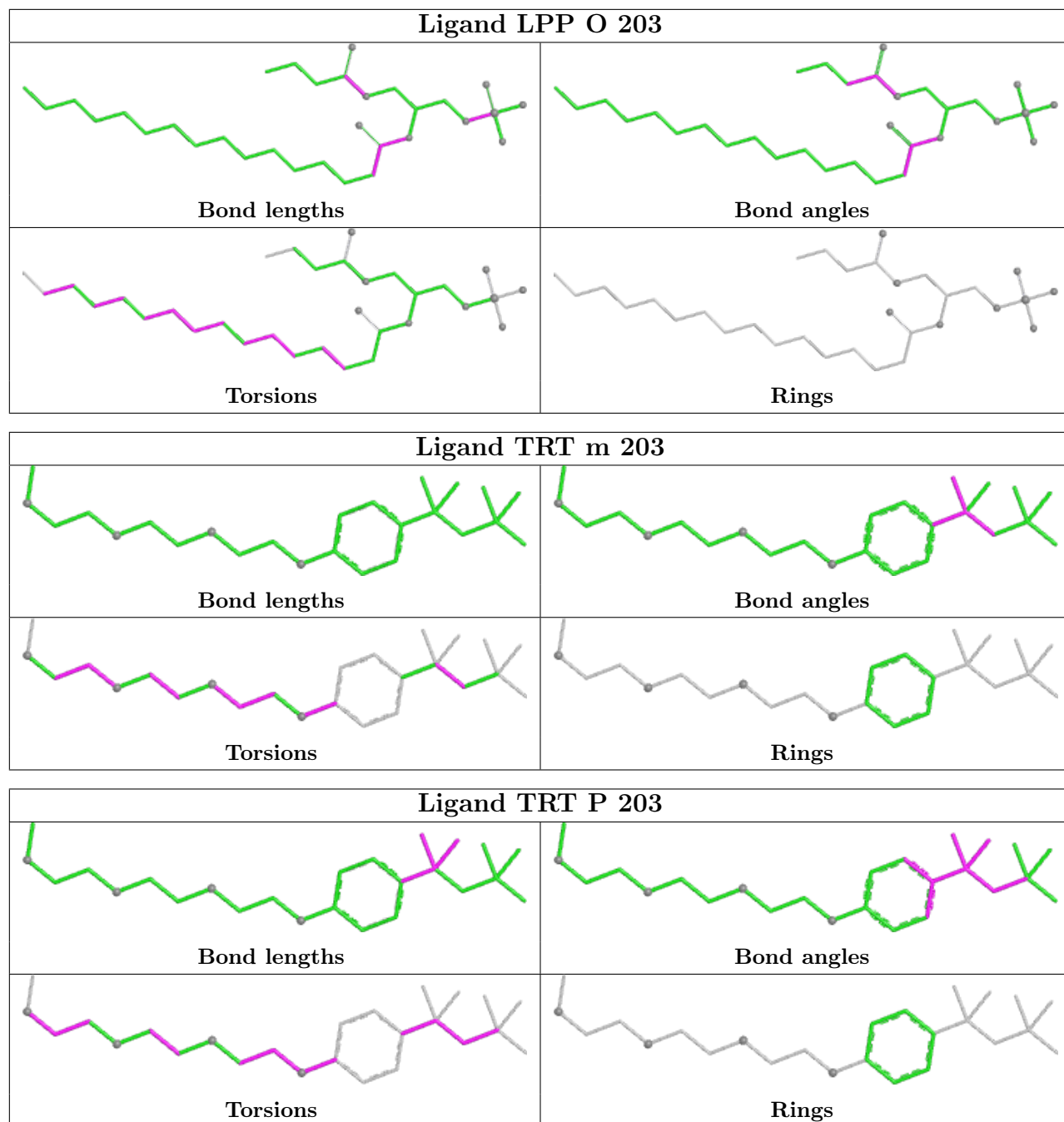


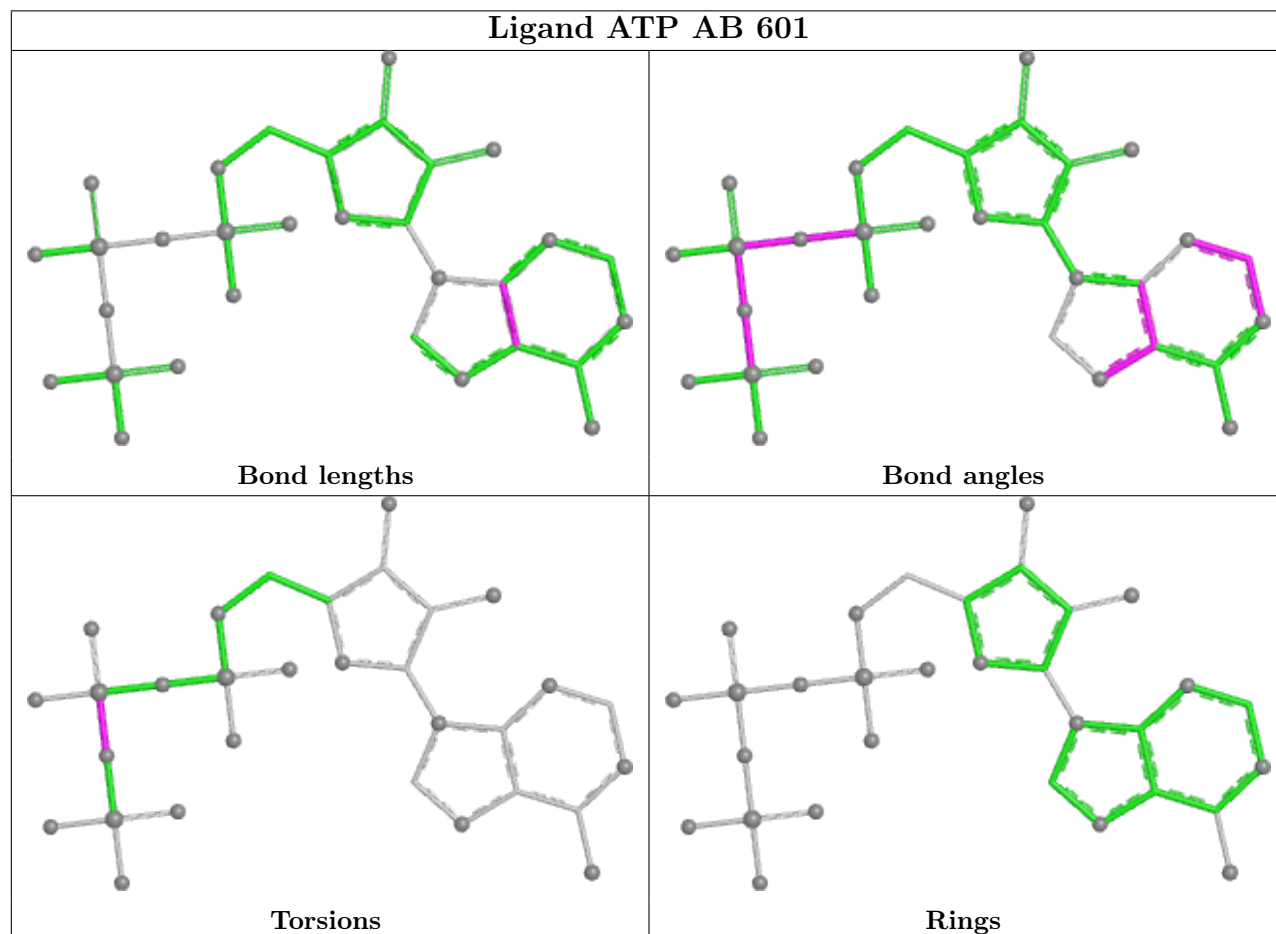
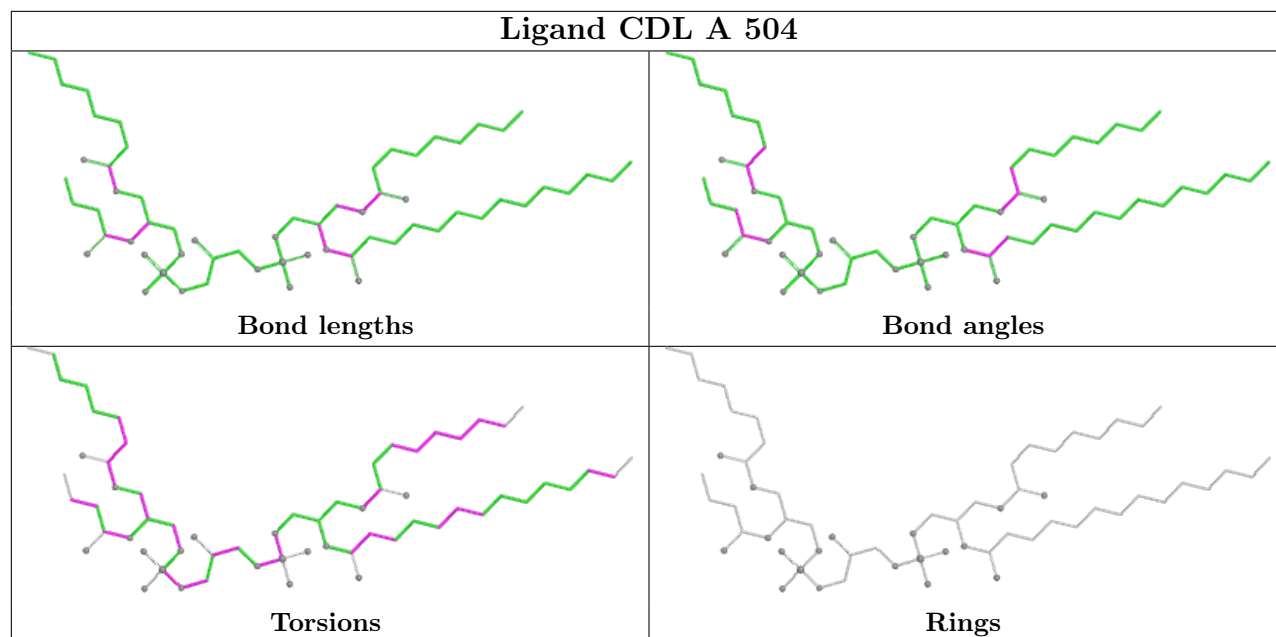


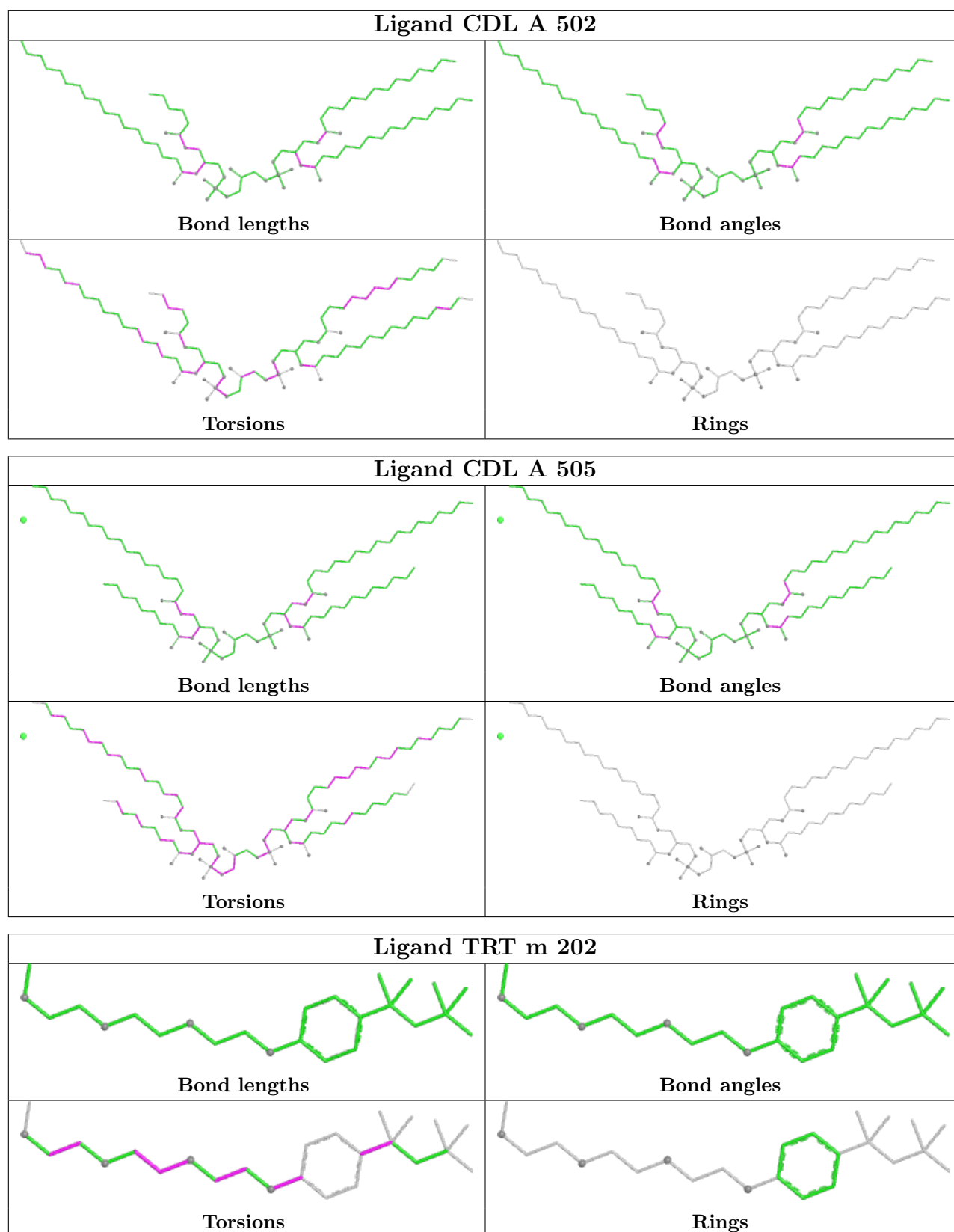


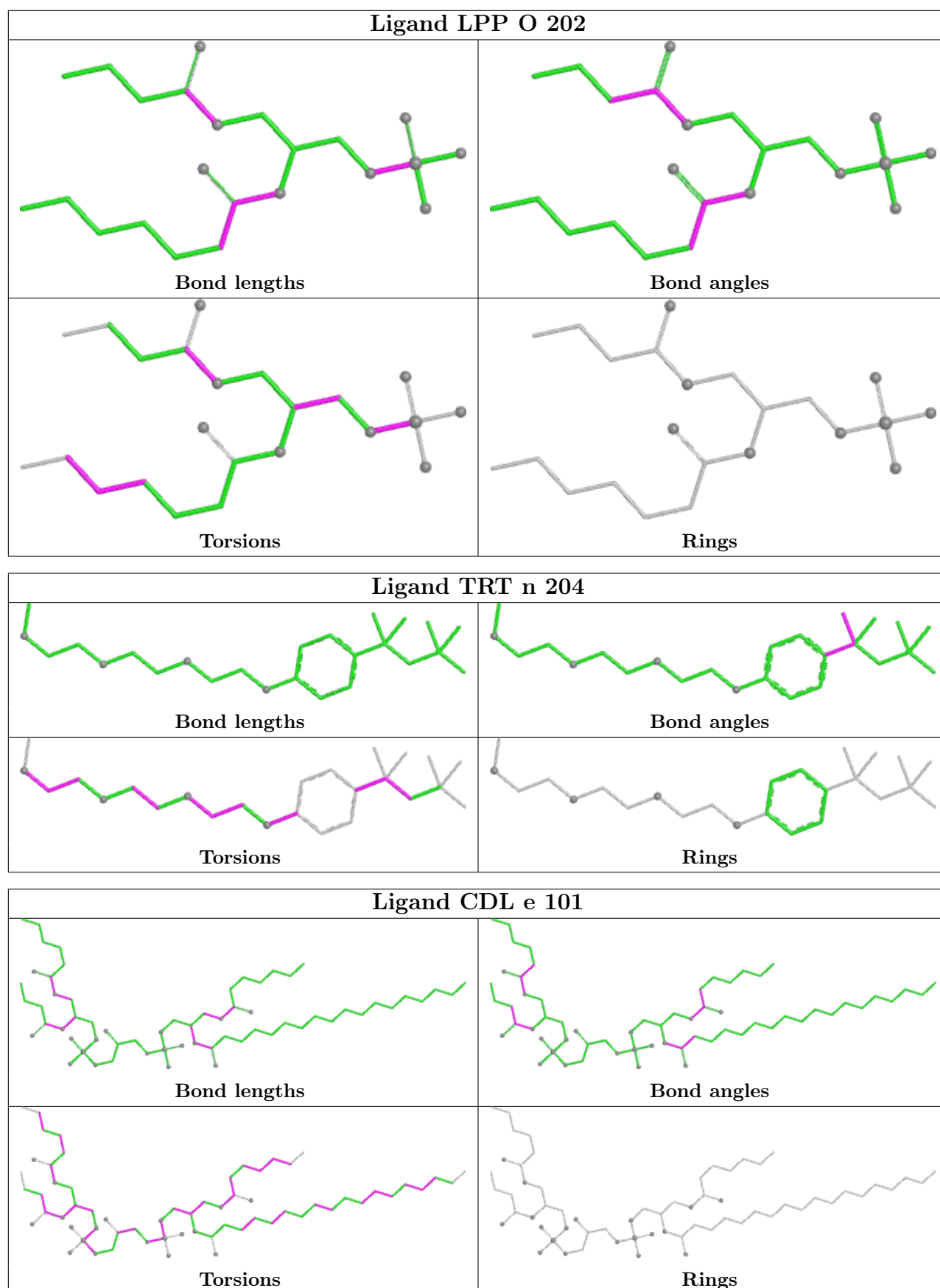


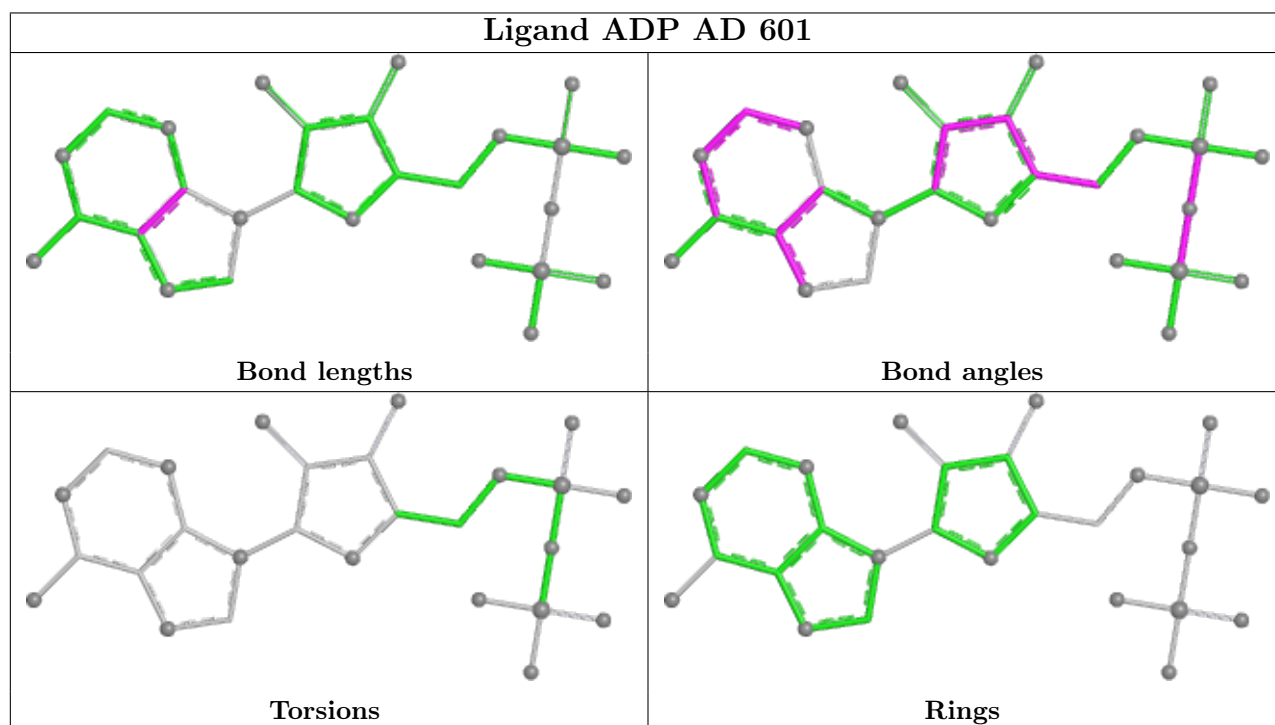
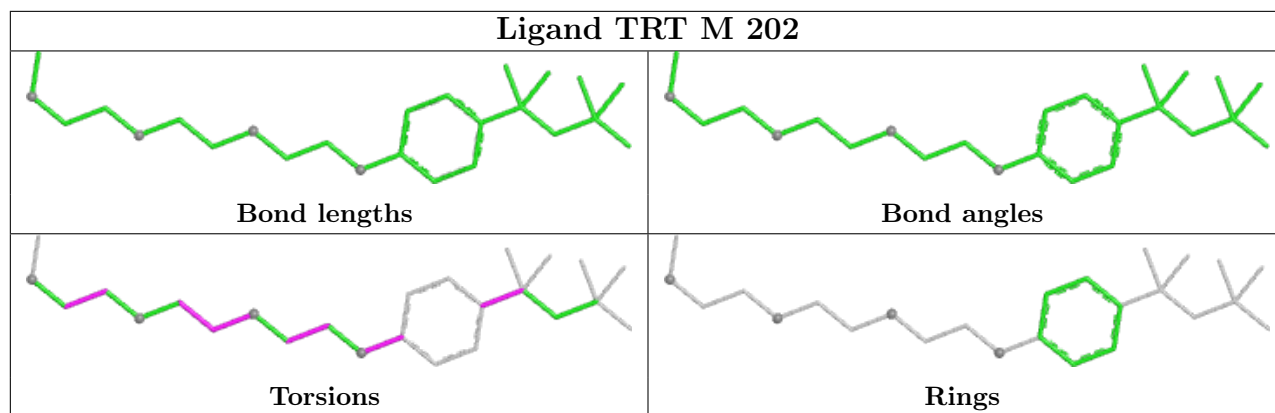


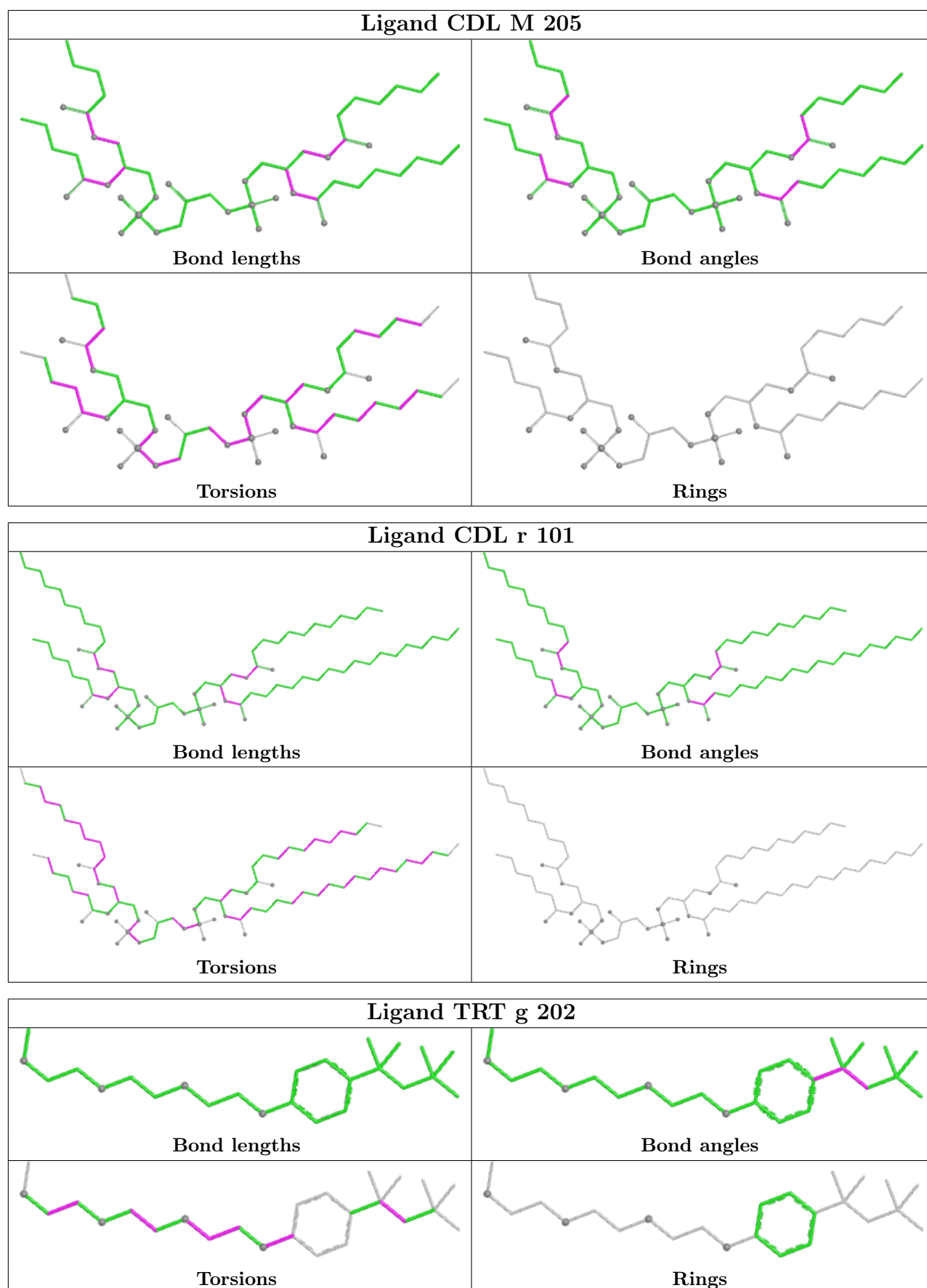


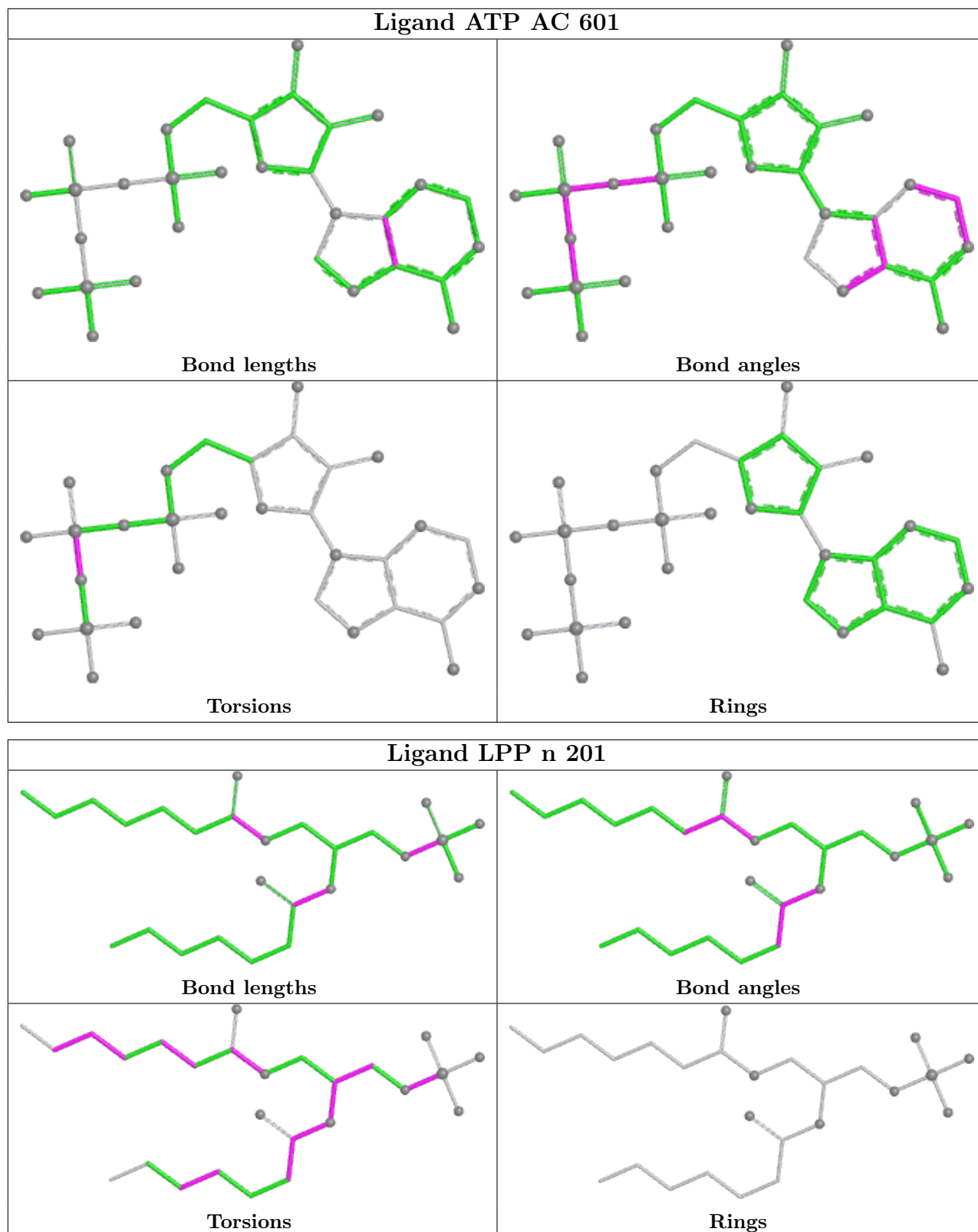


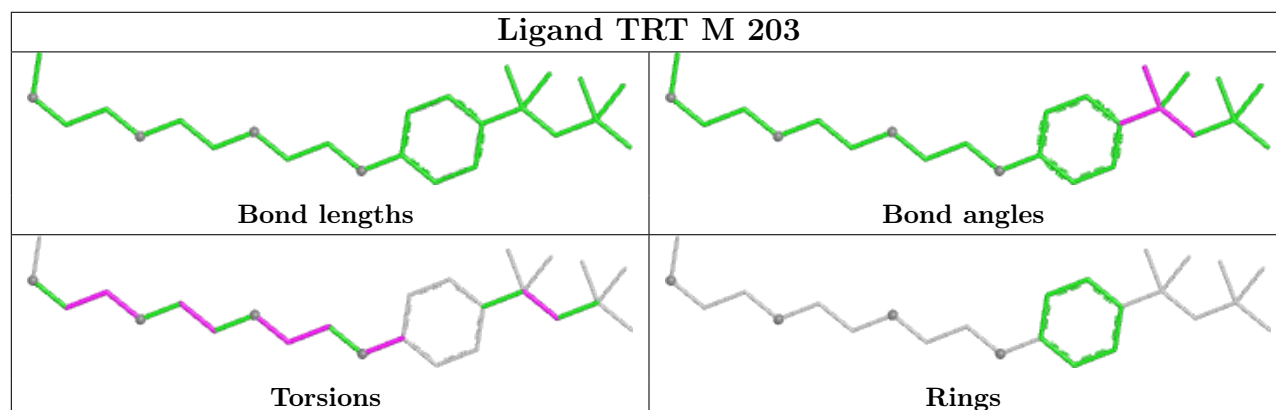
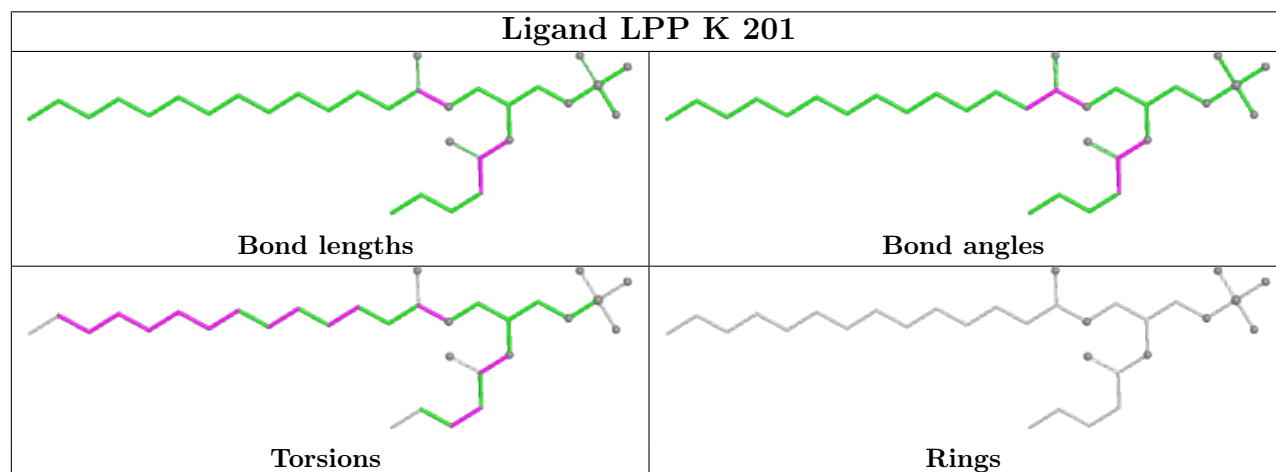
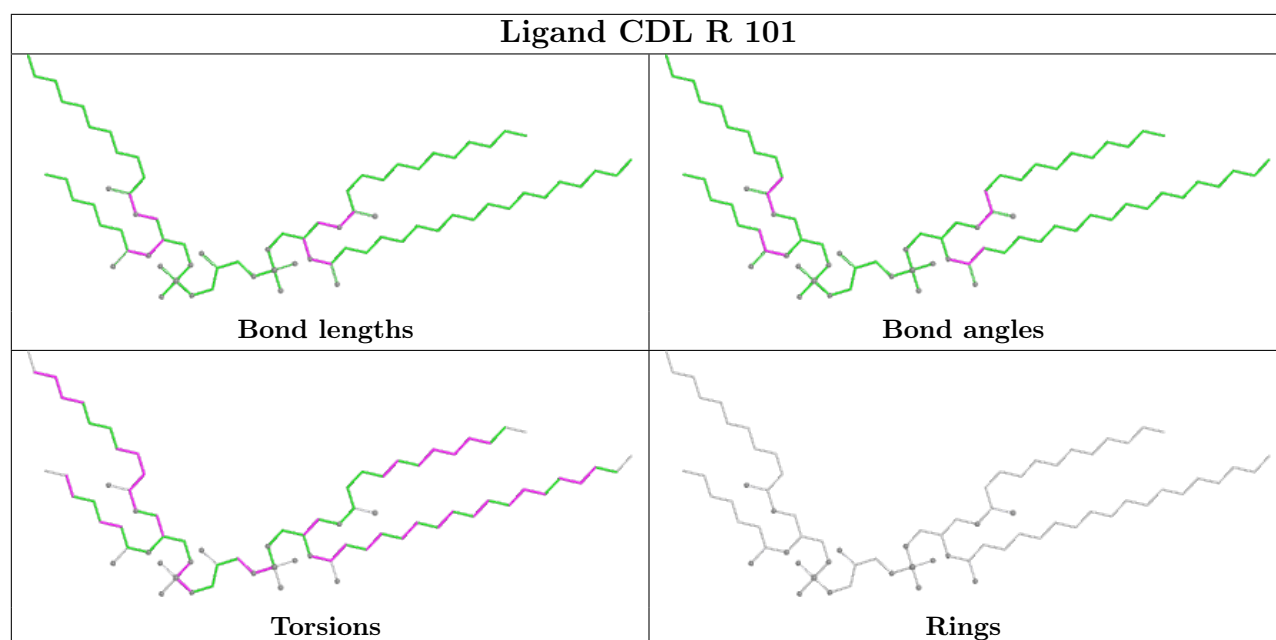


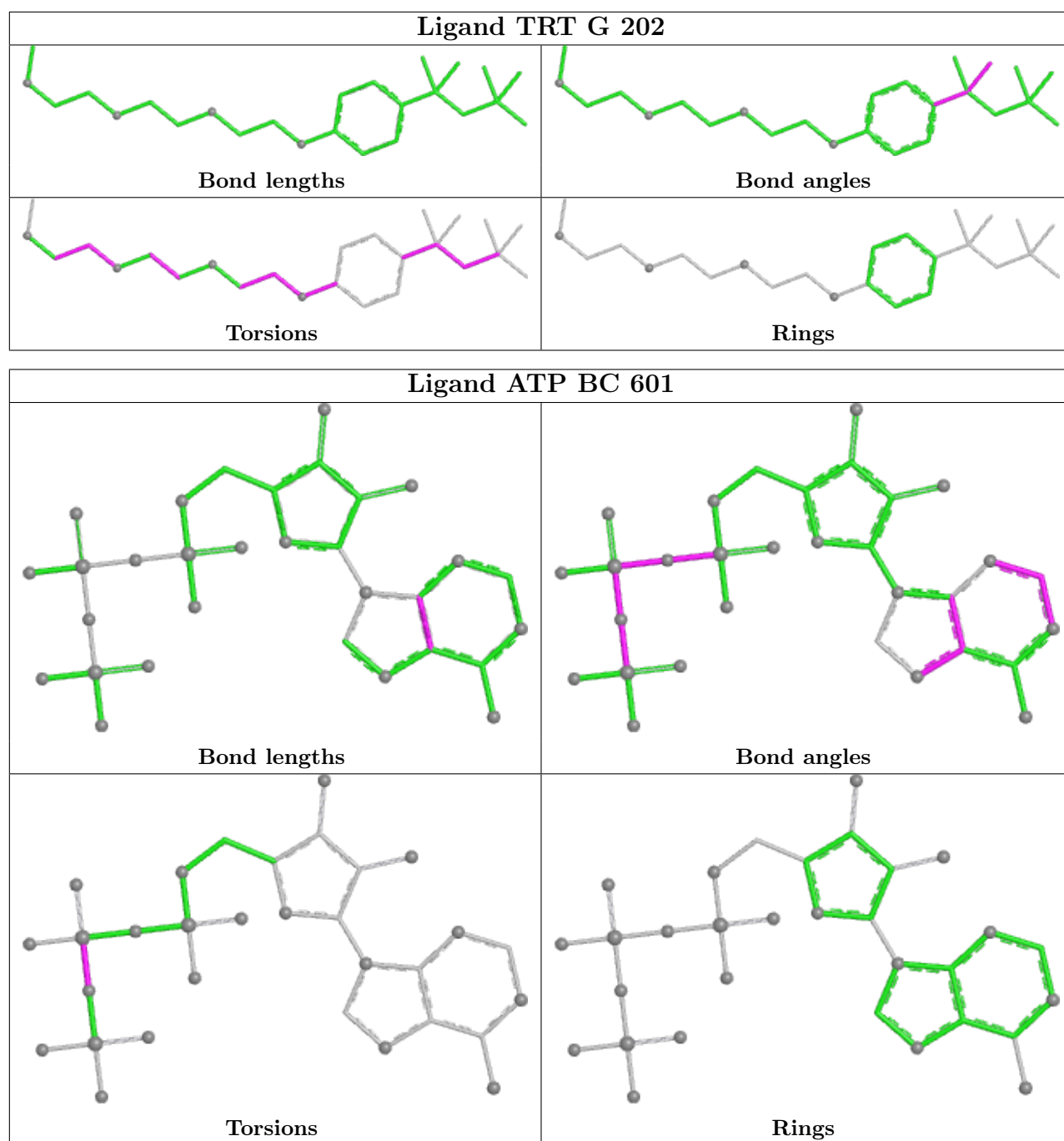


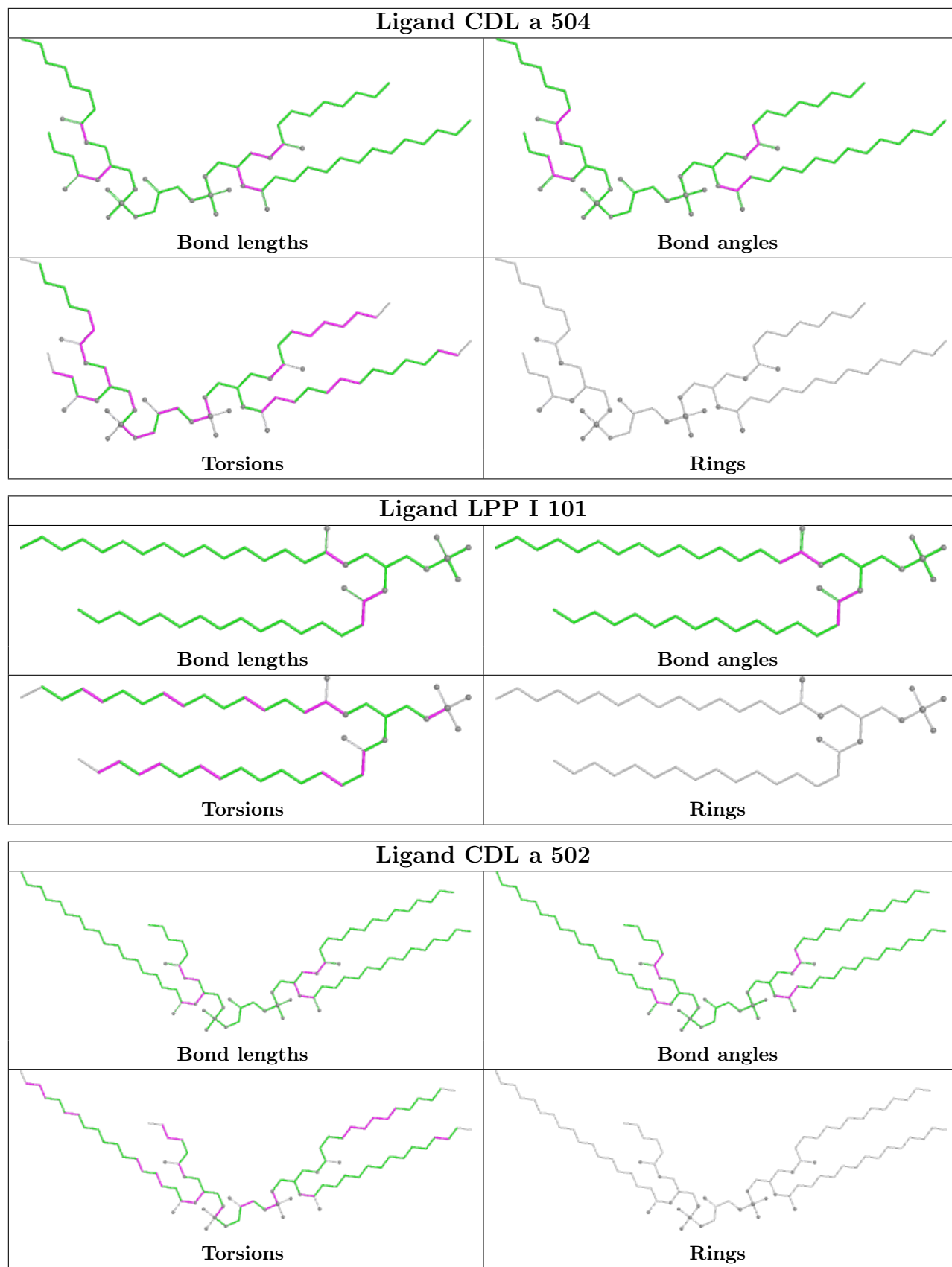


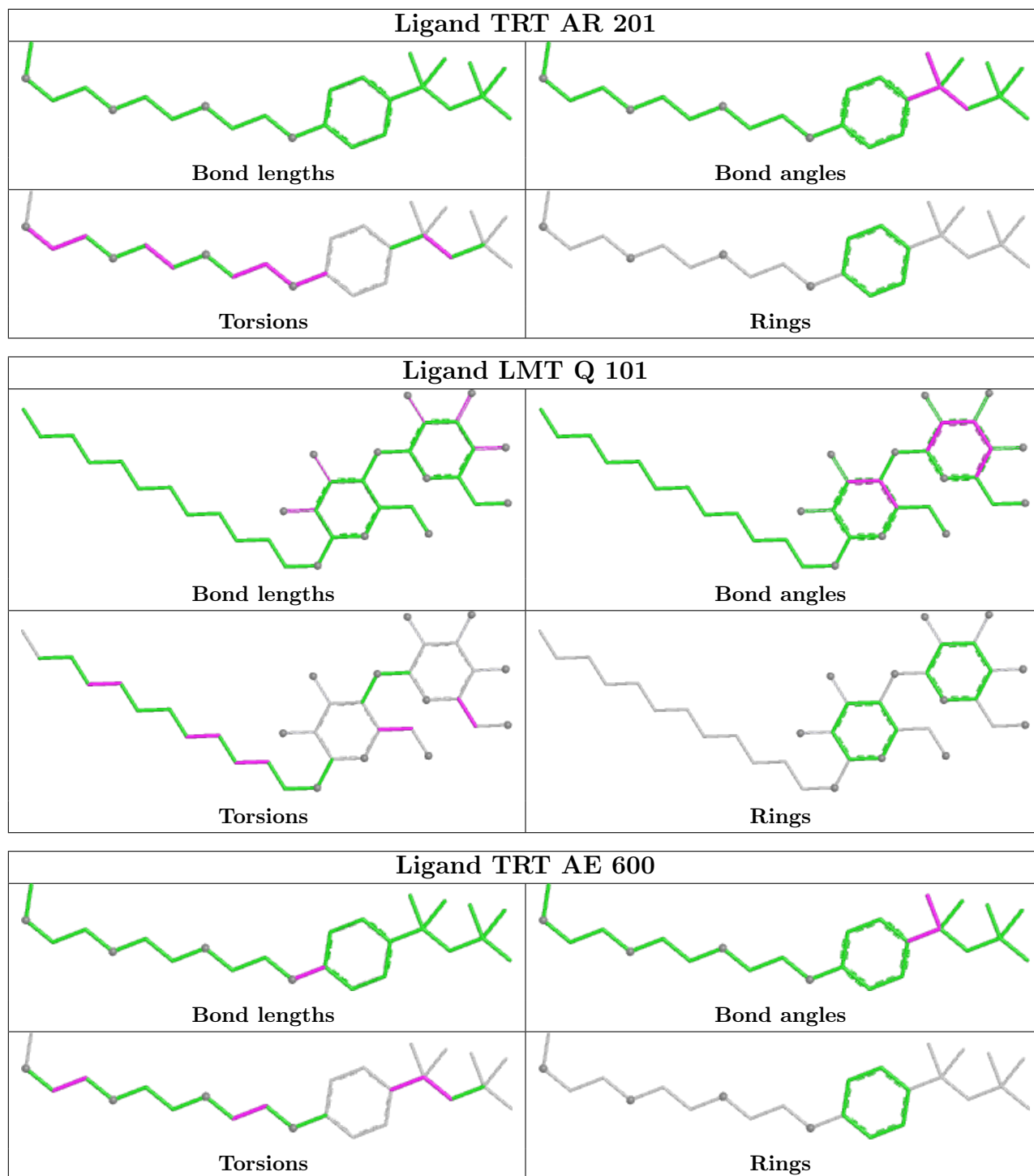


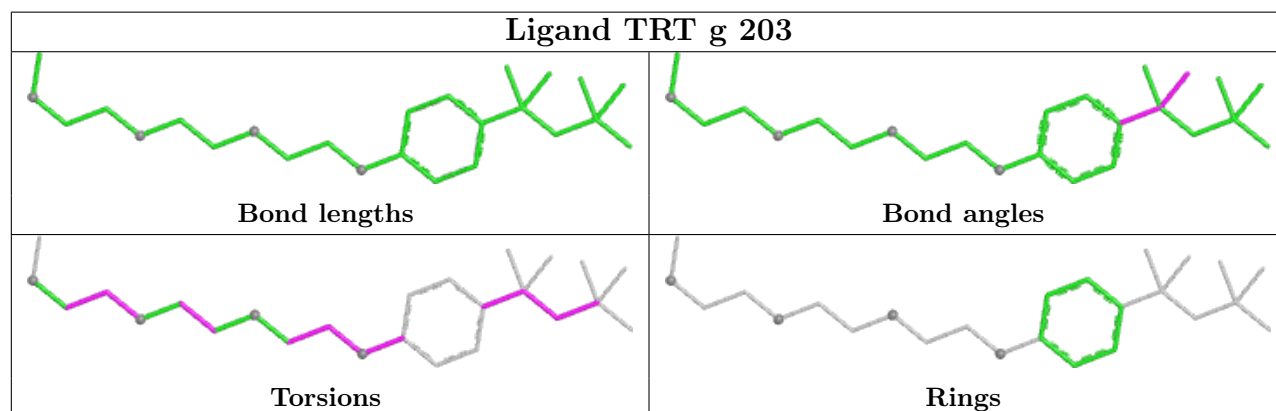
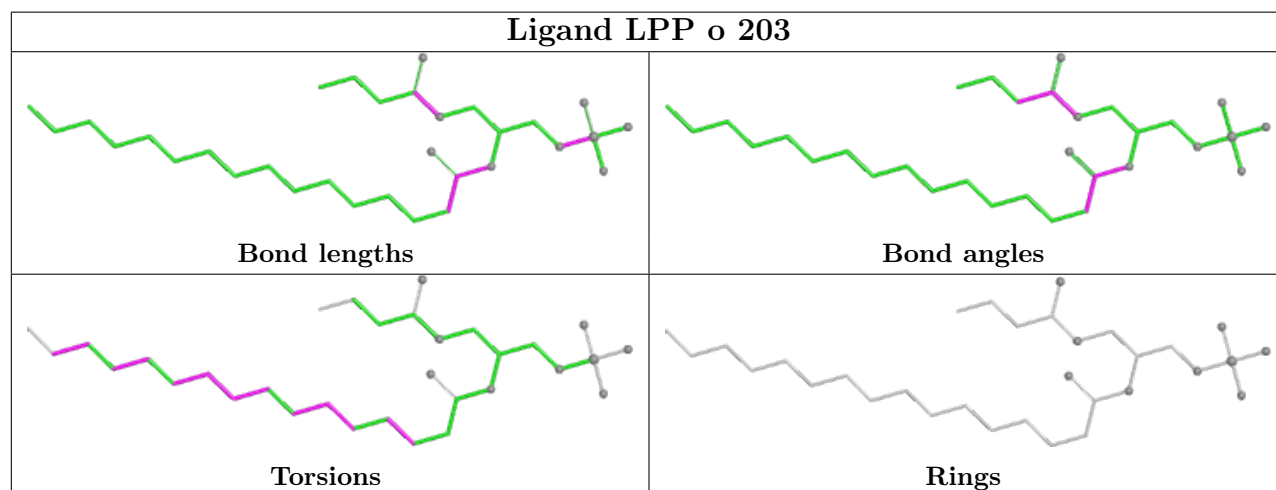
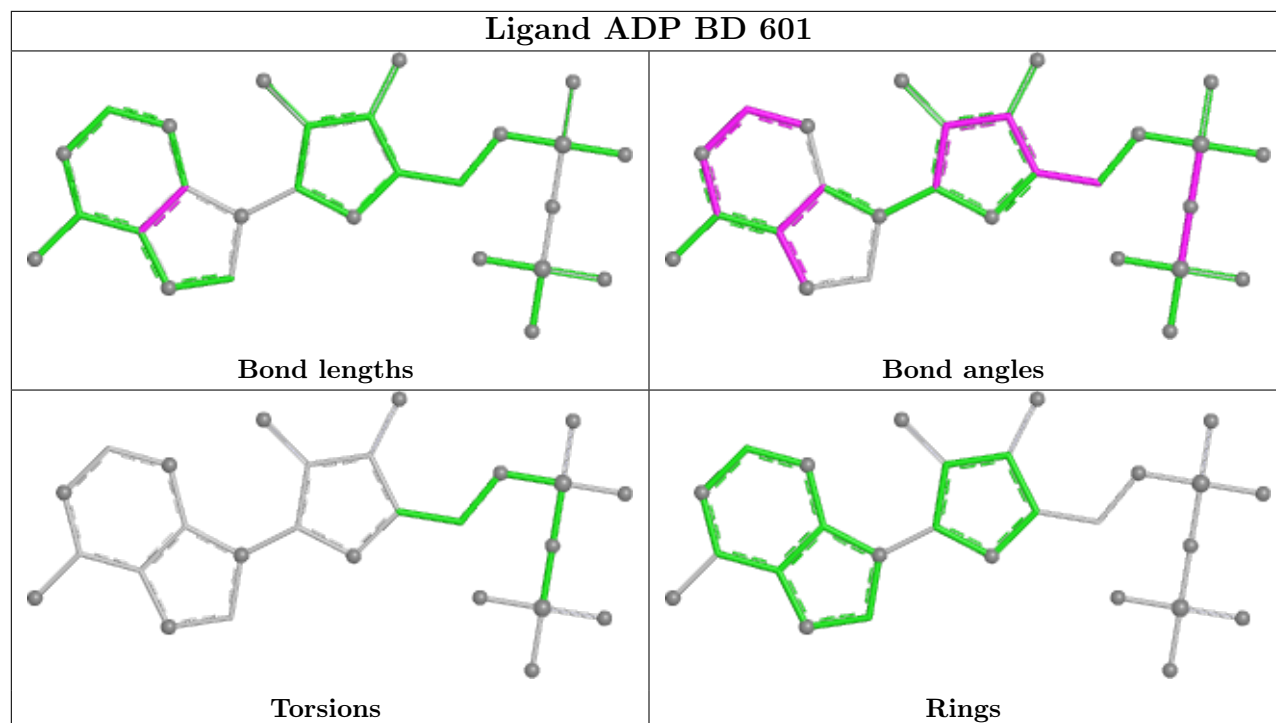


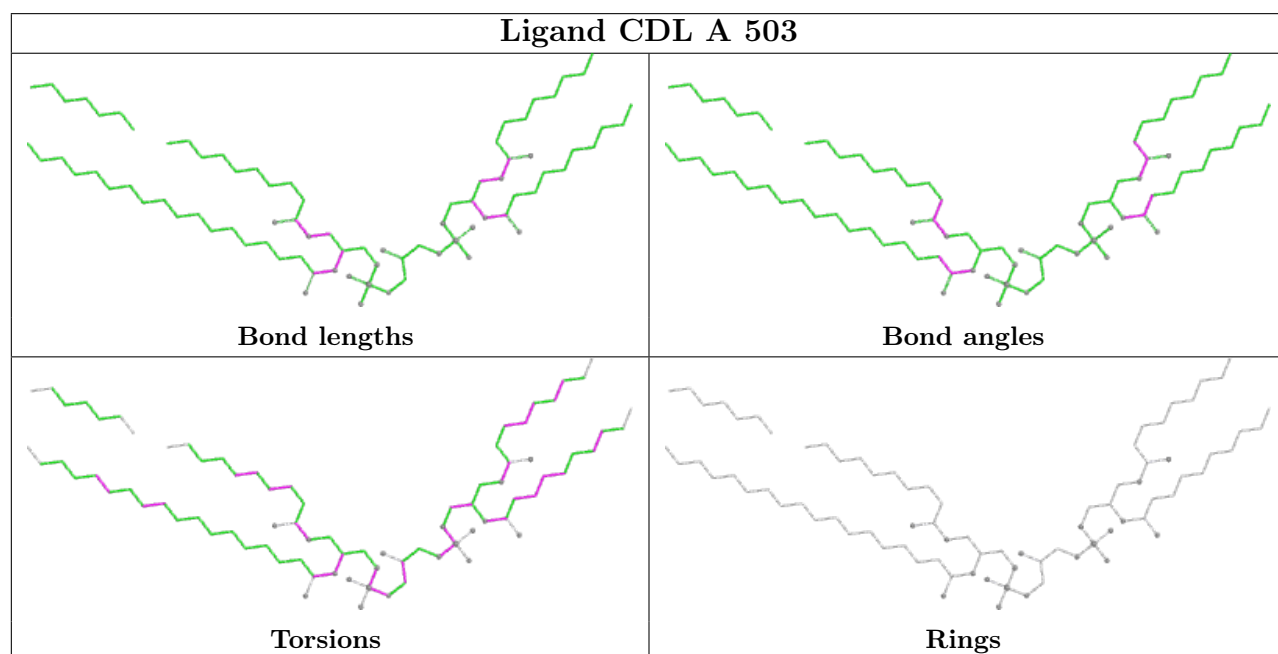
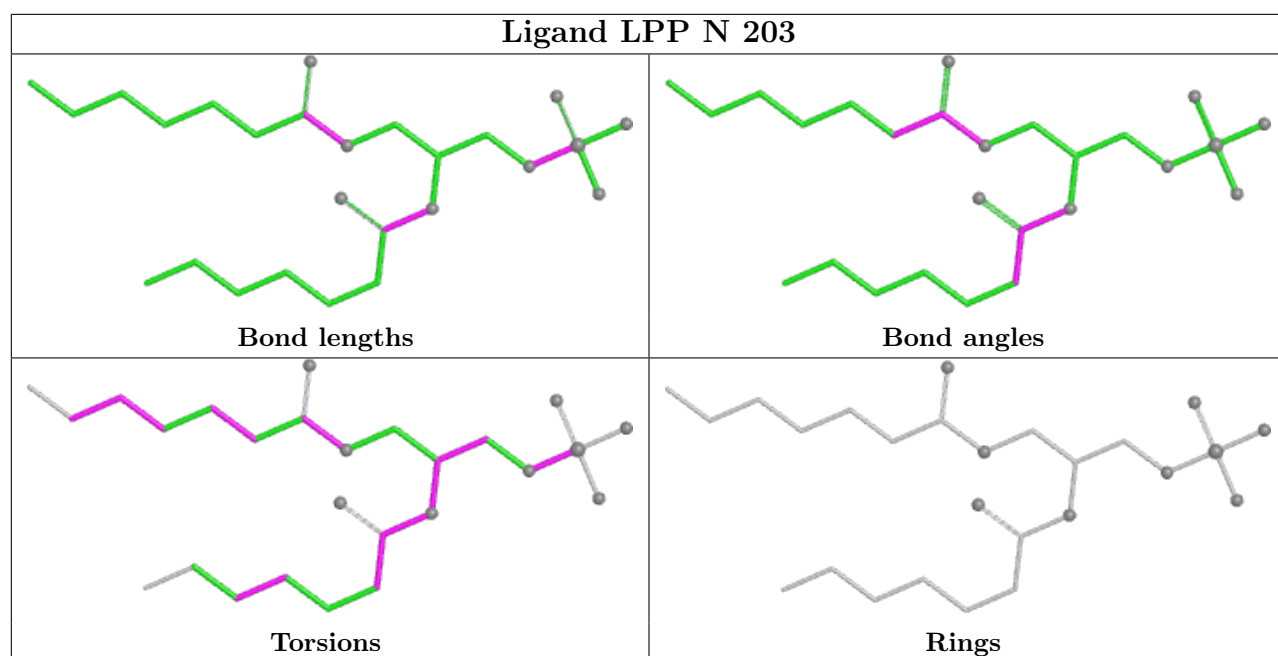


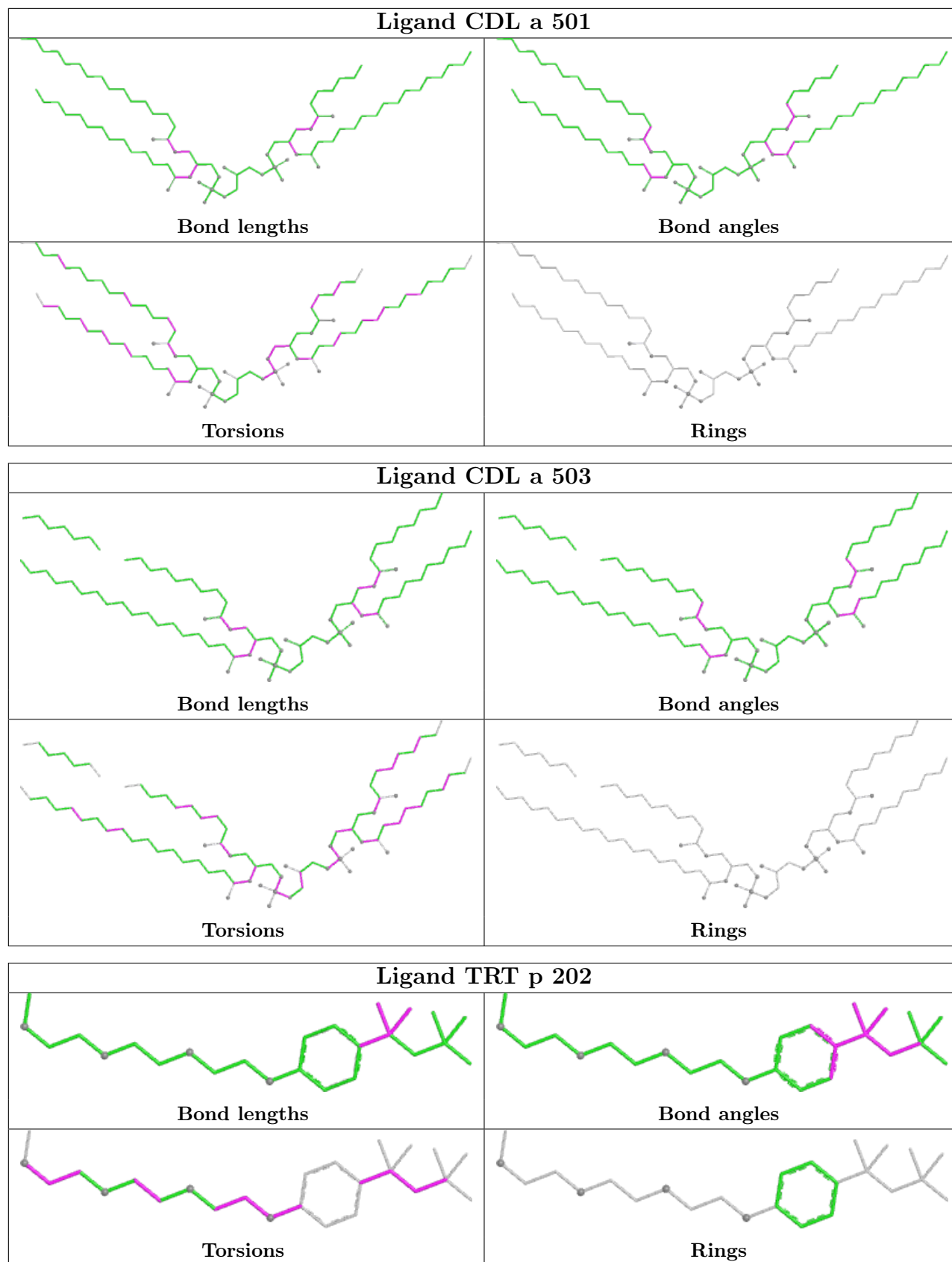


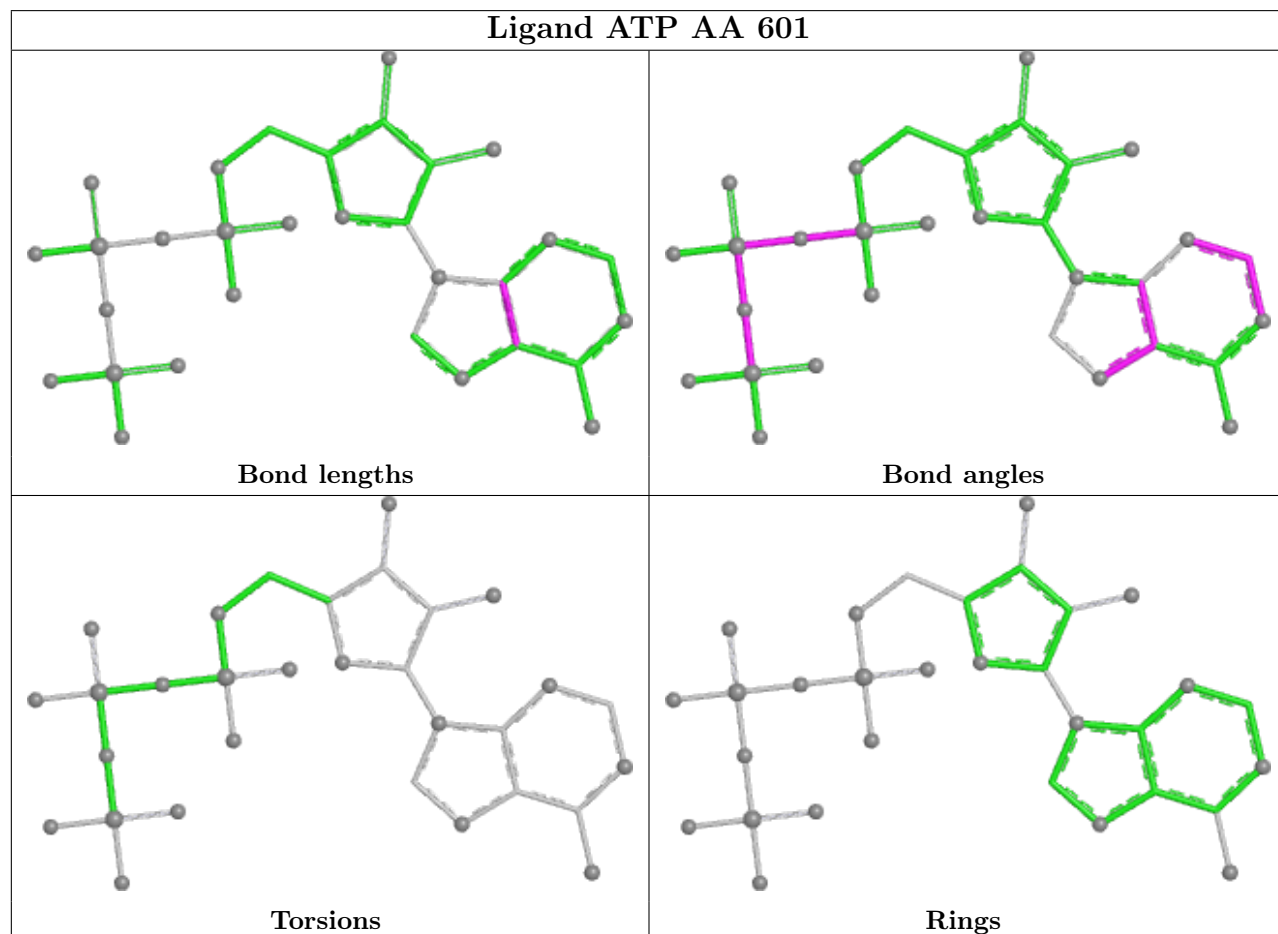
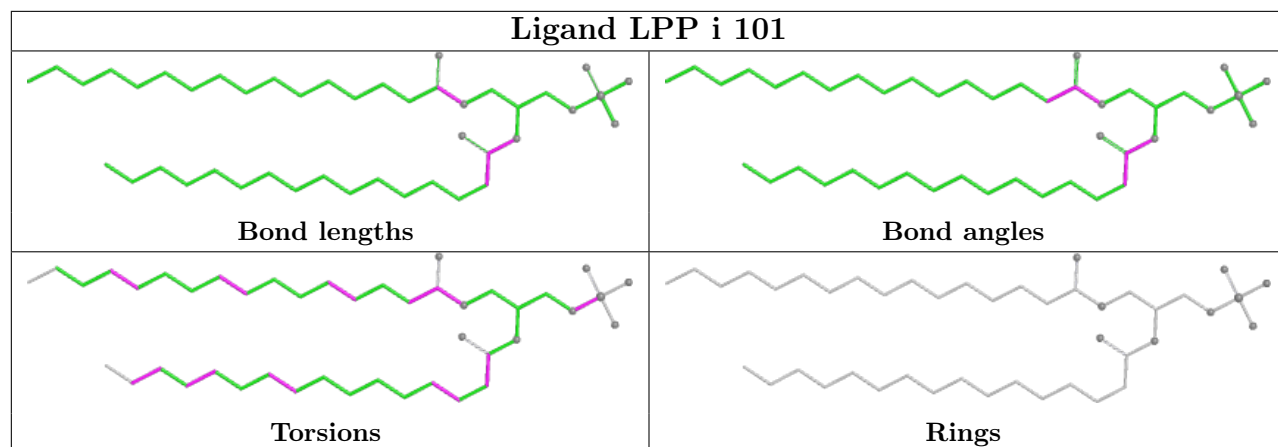


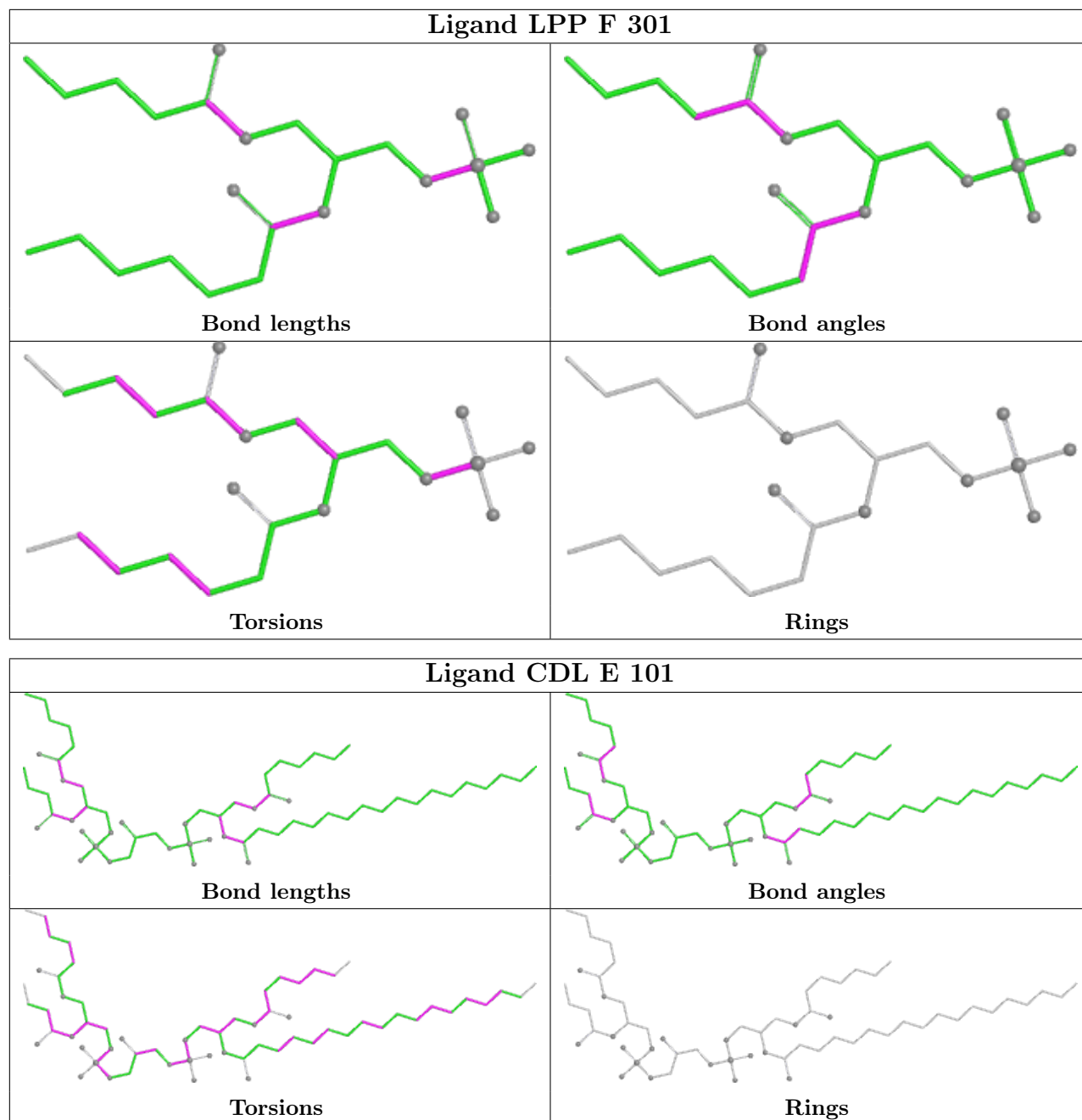


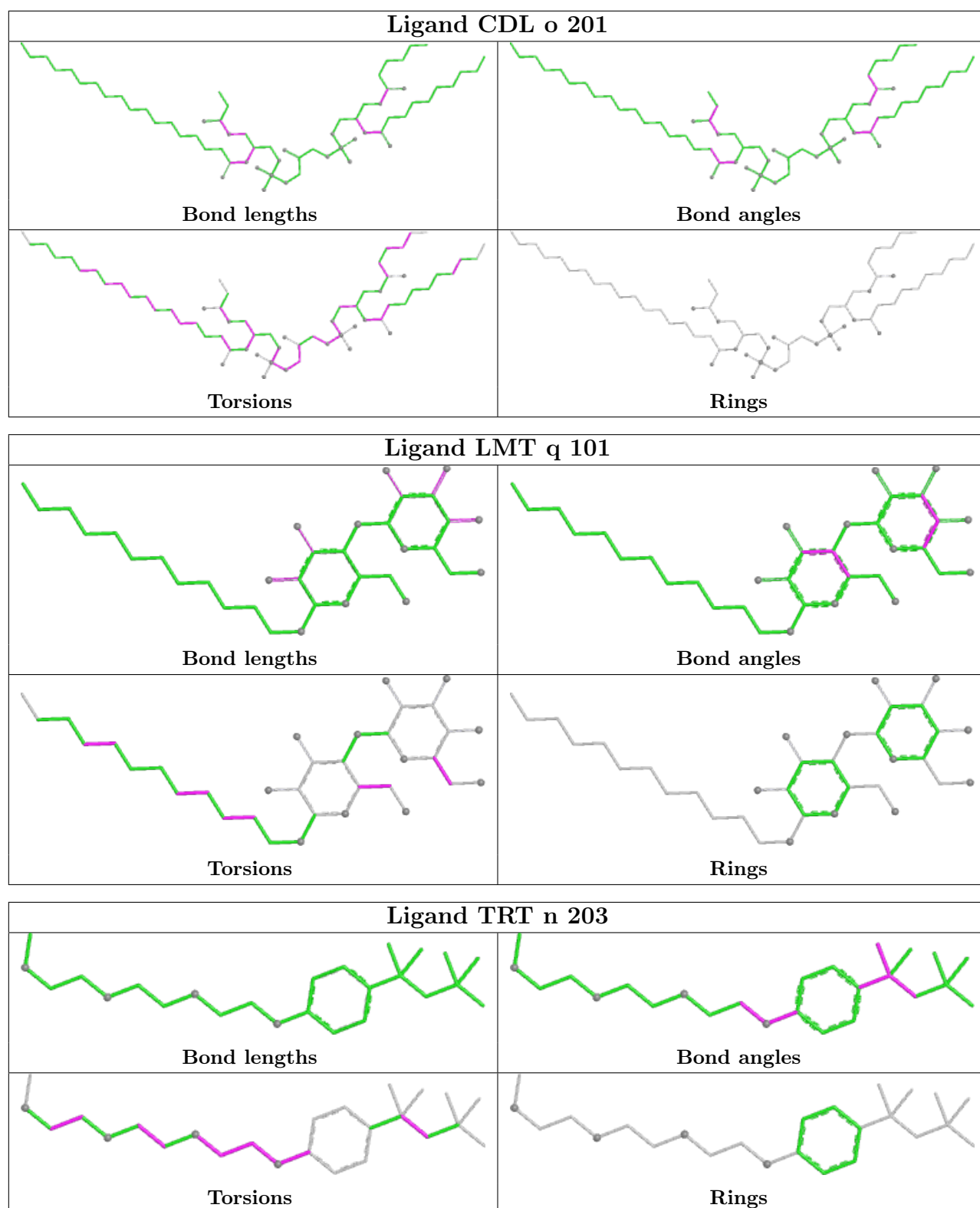


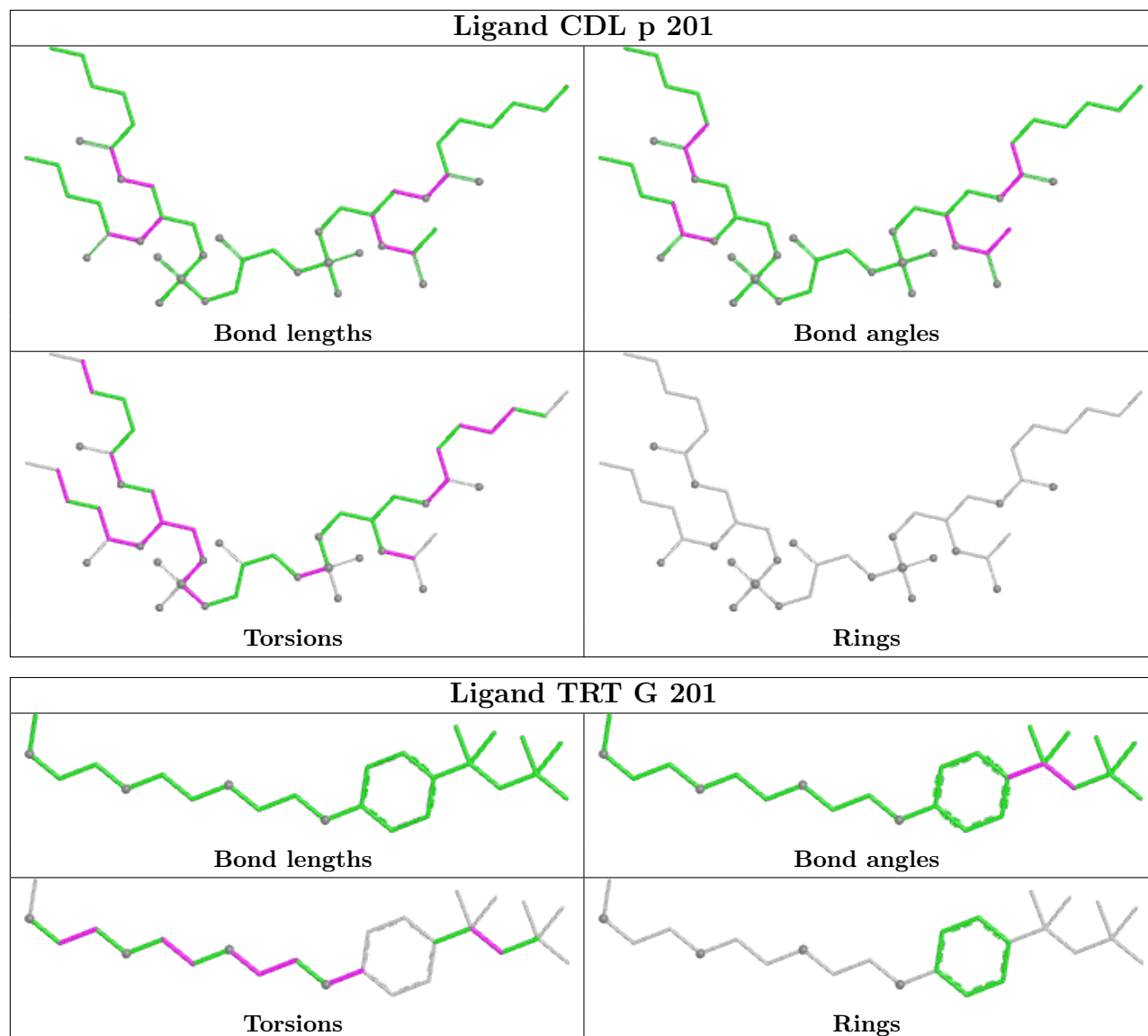


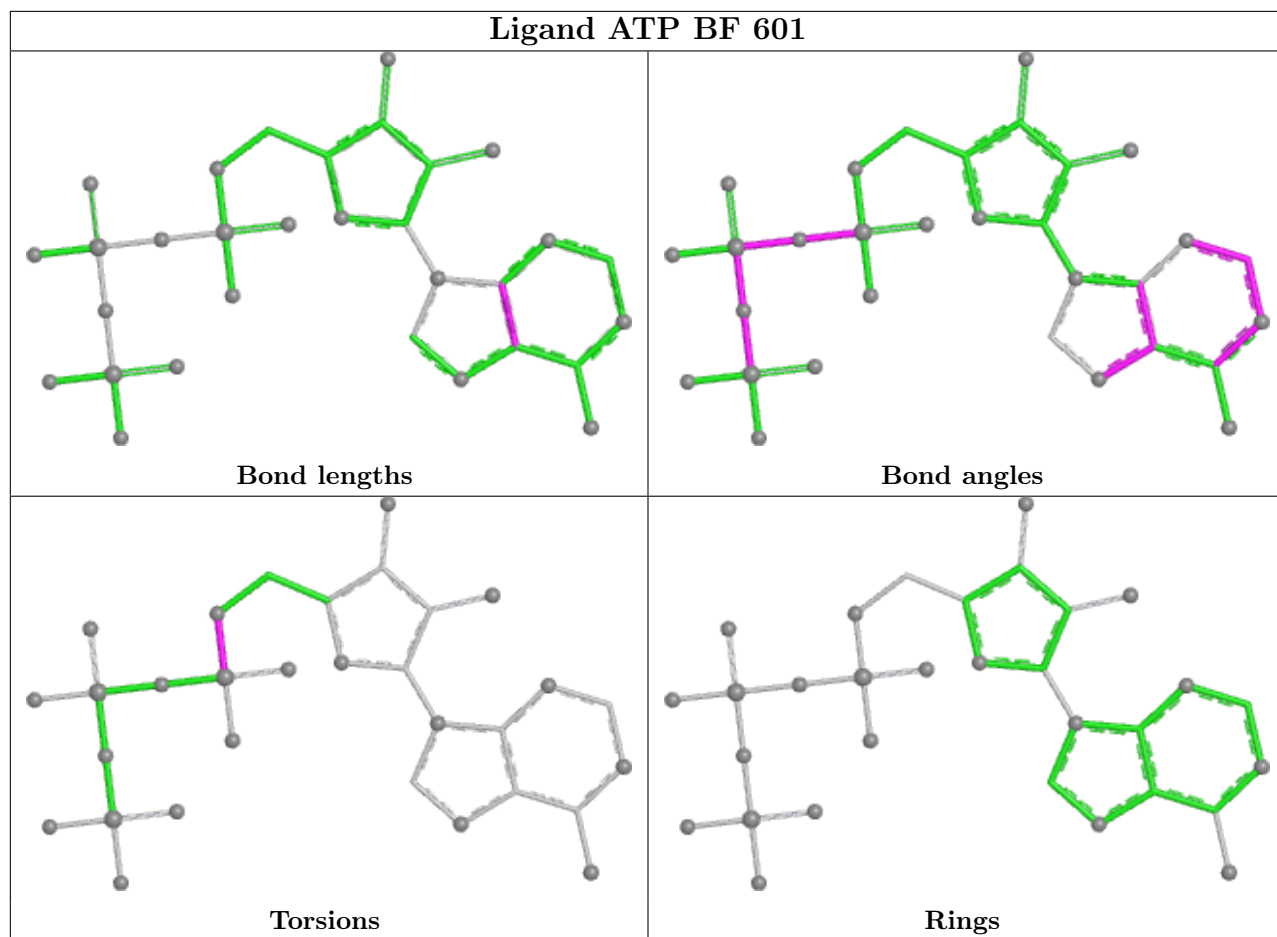


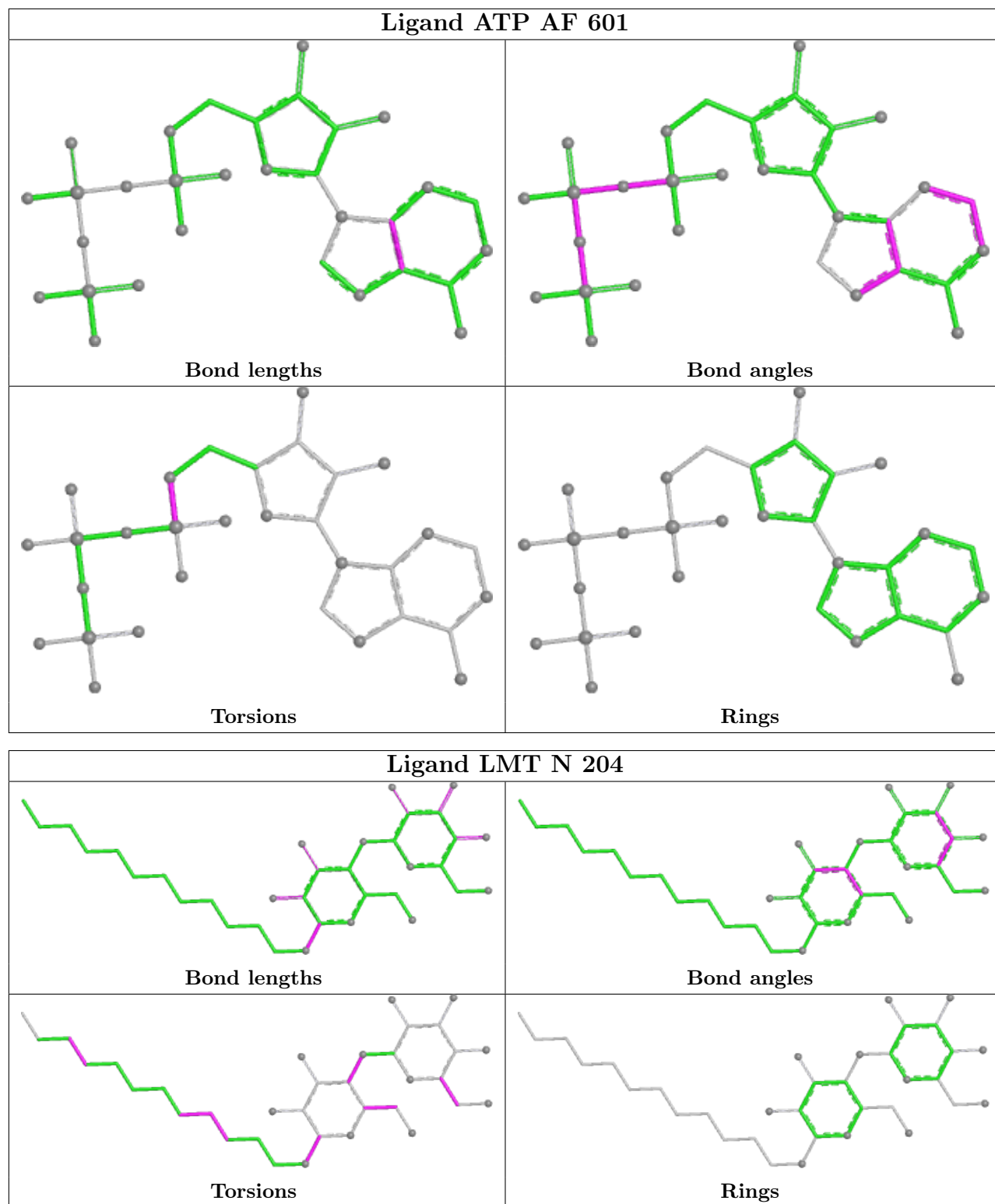


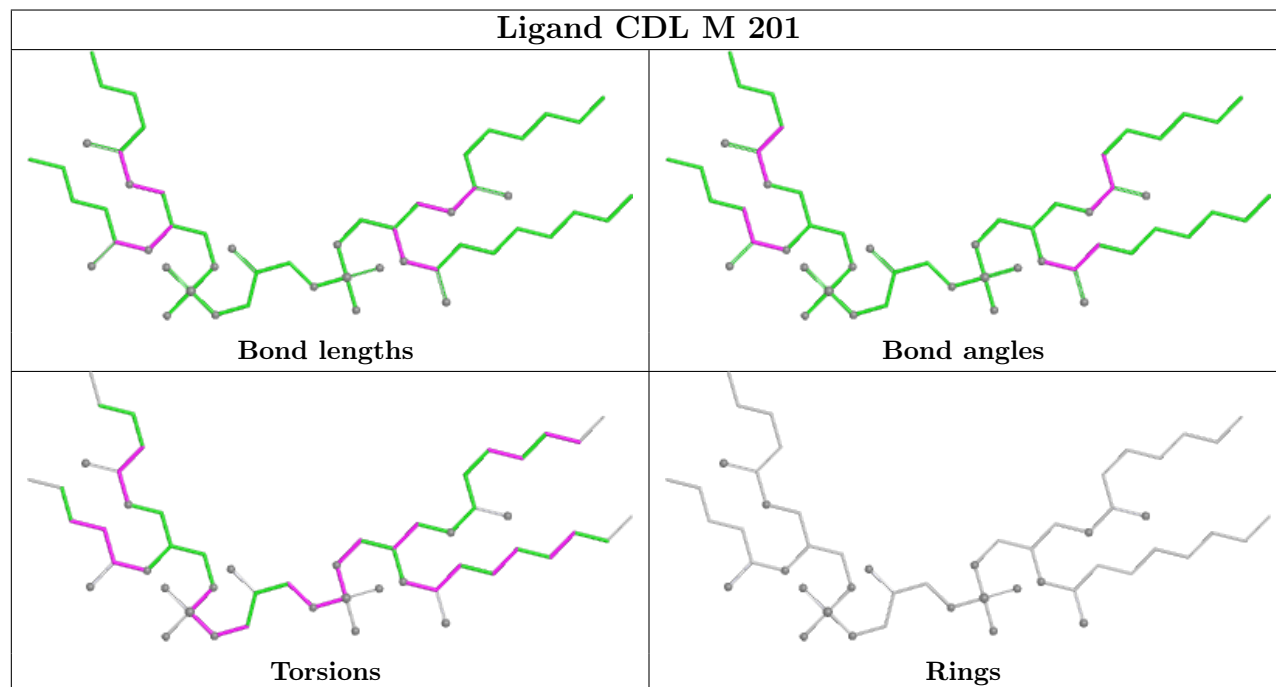
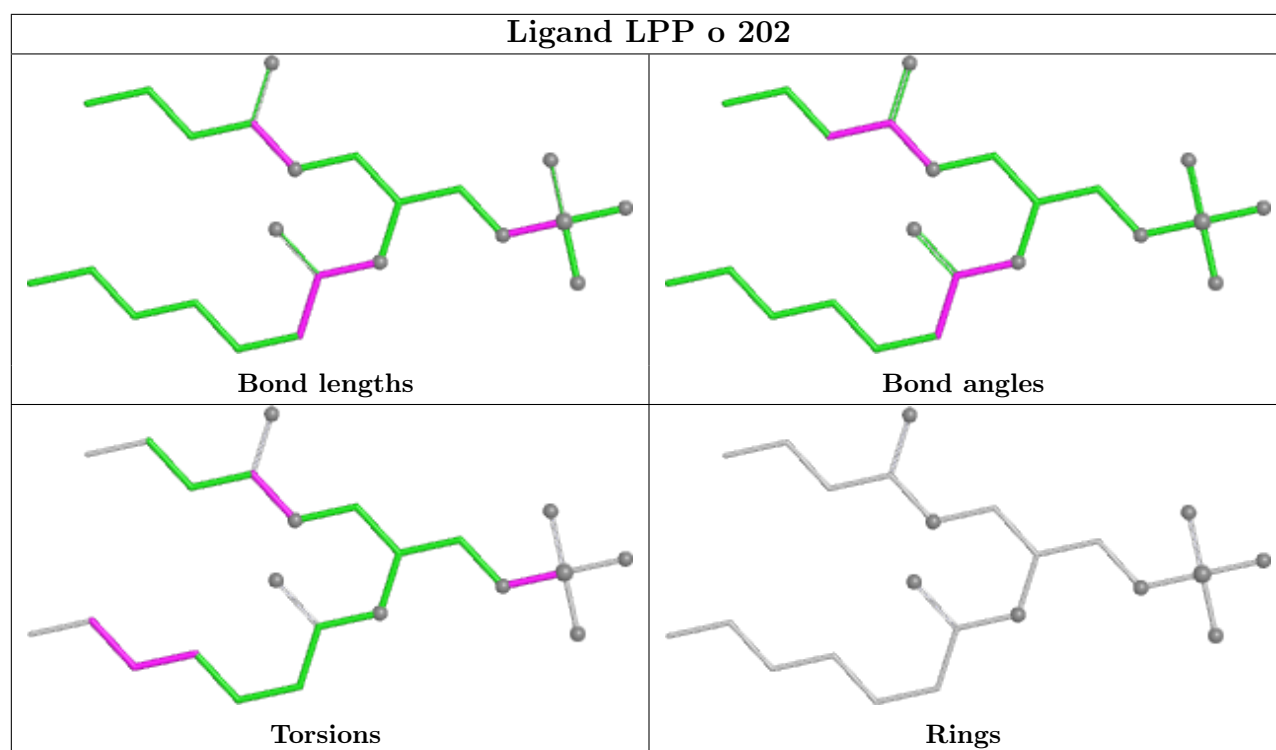


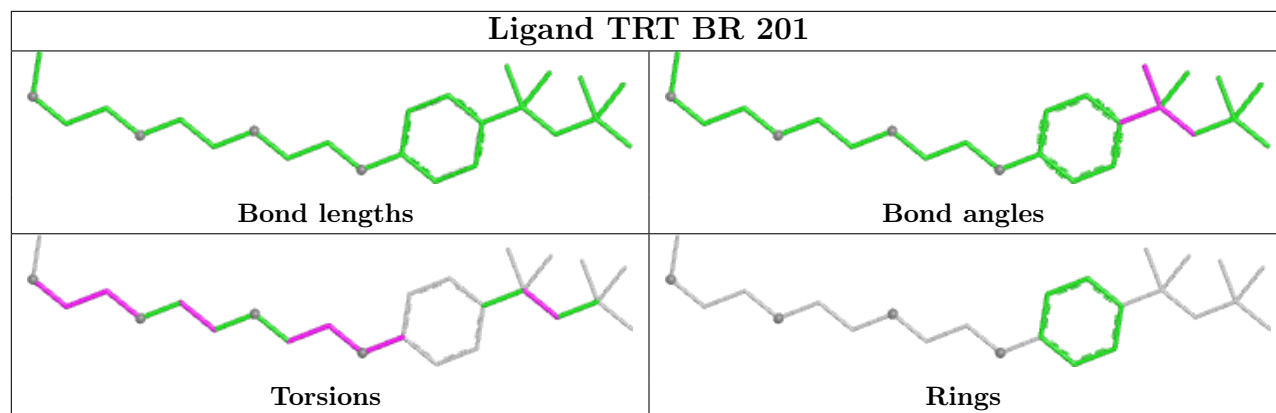












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

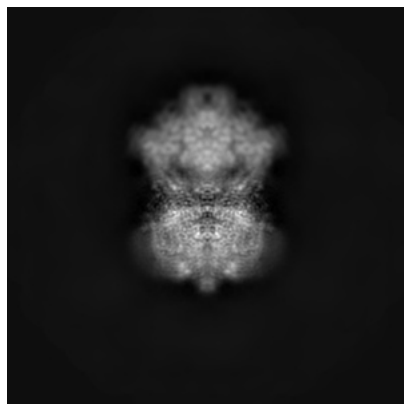
6 Map visualisation [i](#)

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.

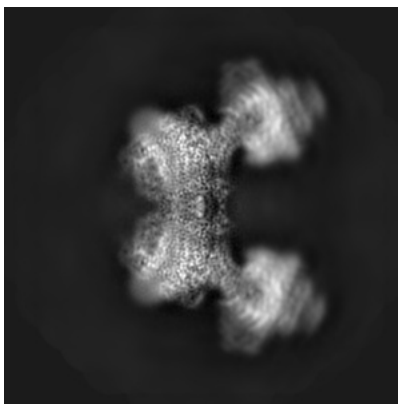
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

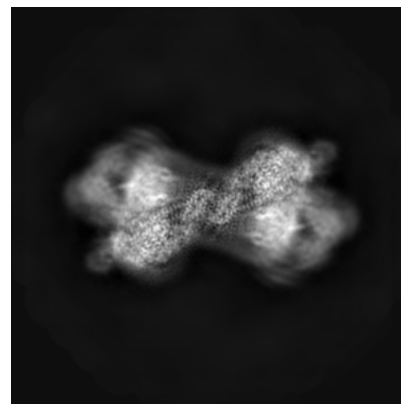
6.1.1 Primary map



X

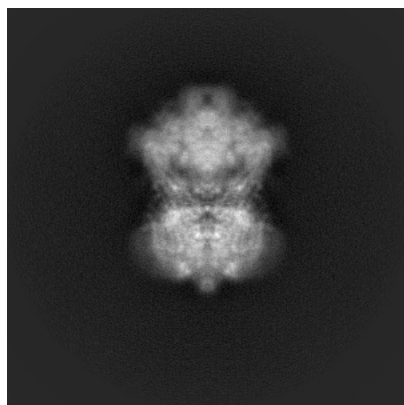


Y

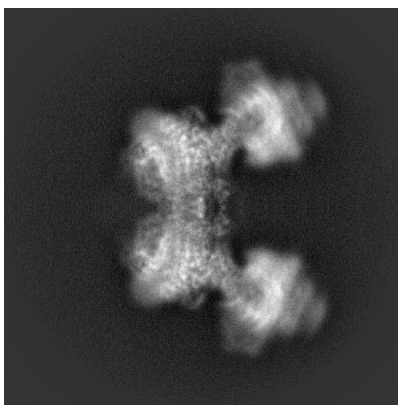


Z

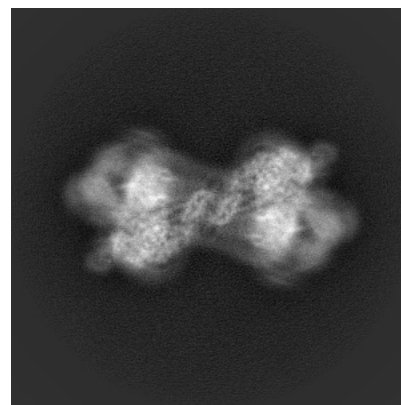
6.1.2 Raw map



X



Y

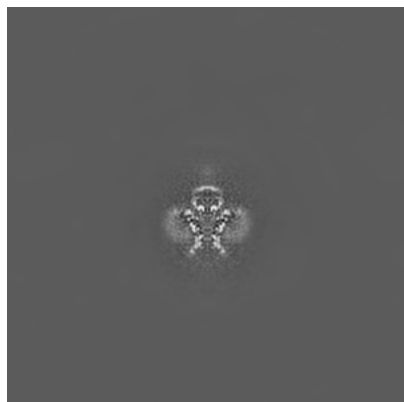


Z

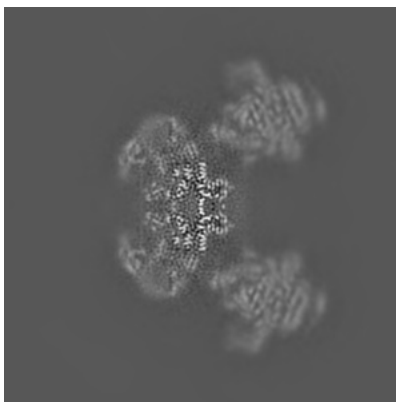
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 220

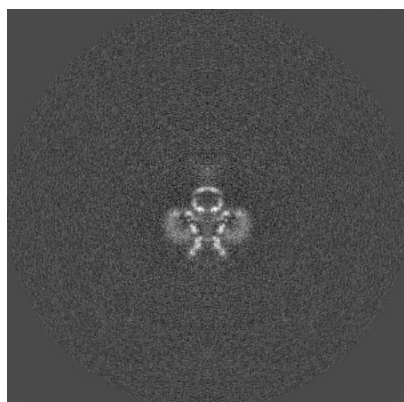


Y Index: 220

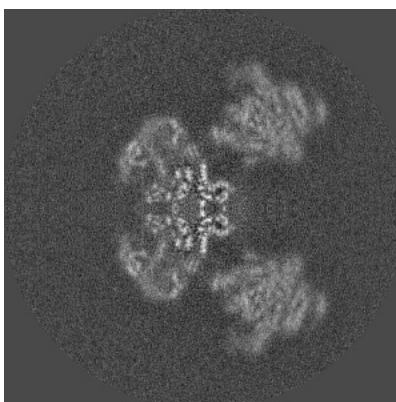


Z Index: 220

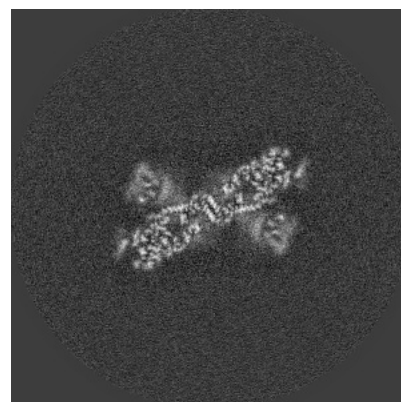
6.2.2 Raw map



X Index: 220



Y Index: 220

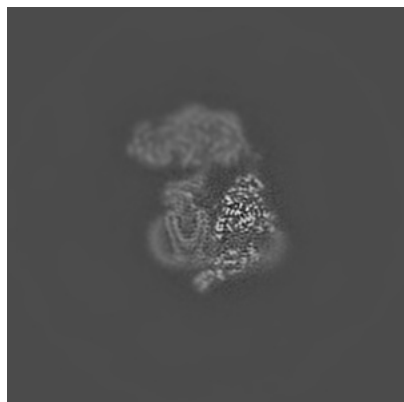


Z Index: 220

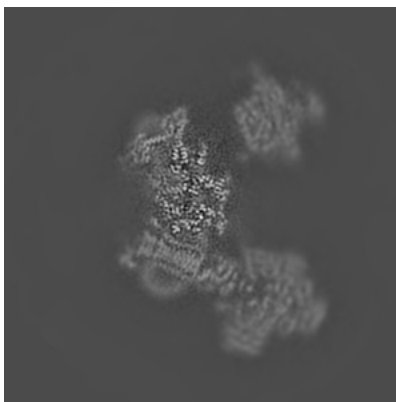
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

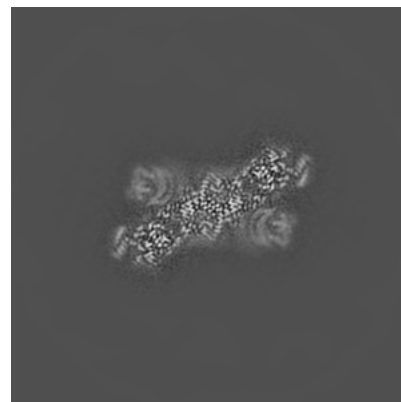
6.3.1 Primary map



X Index: 283

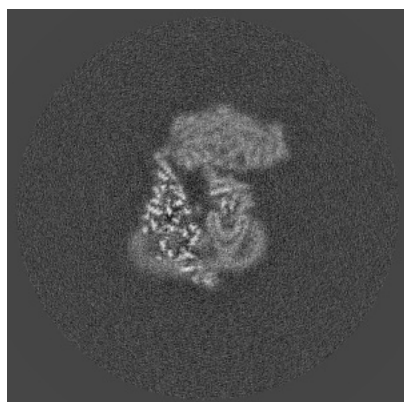


Y Index: 230

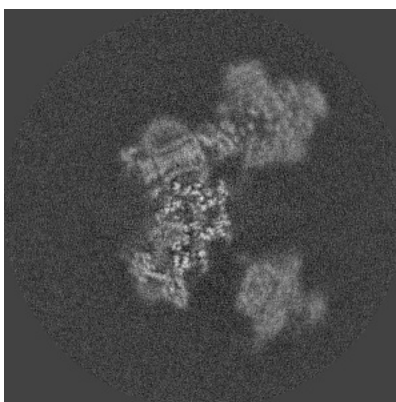


Z Index: 215

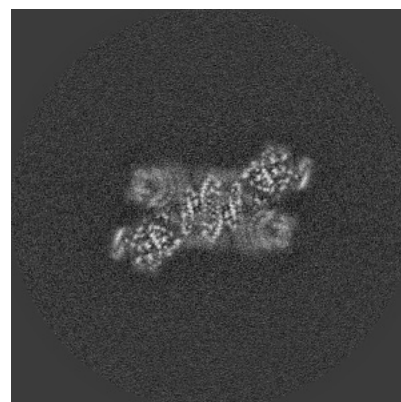
6.3.2 Raw map



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



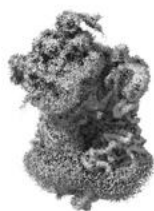
Y



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.

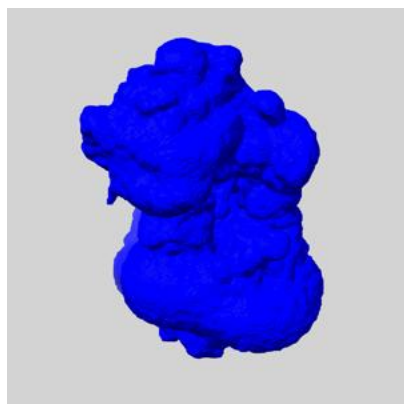
6.5 Mask visualisation [i](#)

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

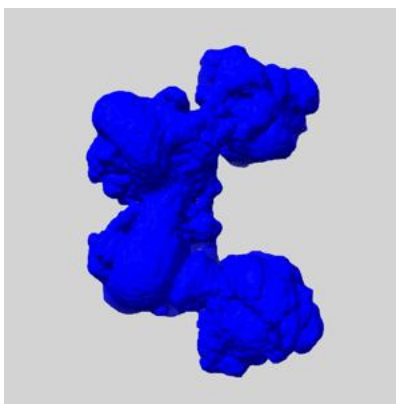
A mask typically either:

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

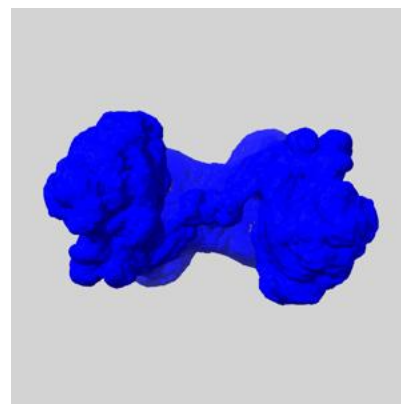
6.5.1 emd_10467_msk_1.map [i](#)



X



Y

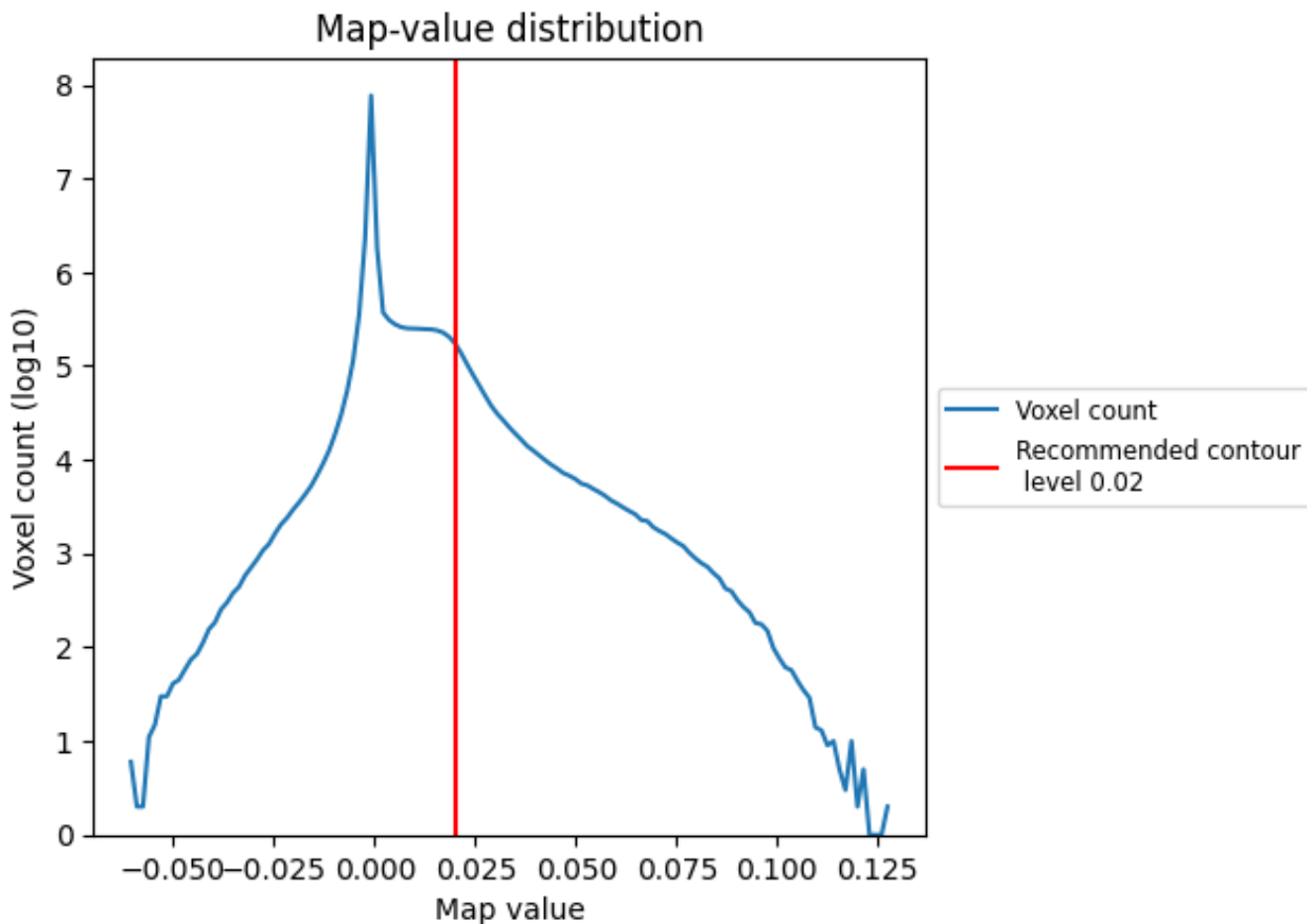


Z

7 Map analysis [i](#)

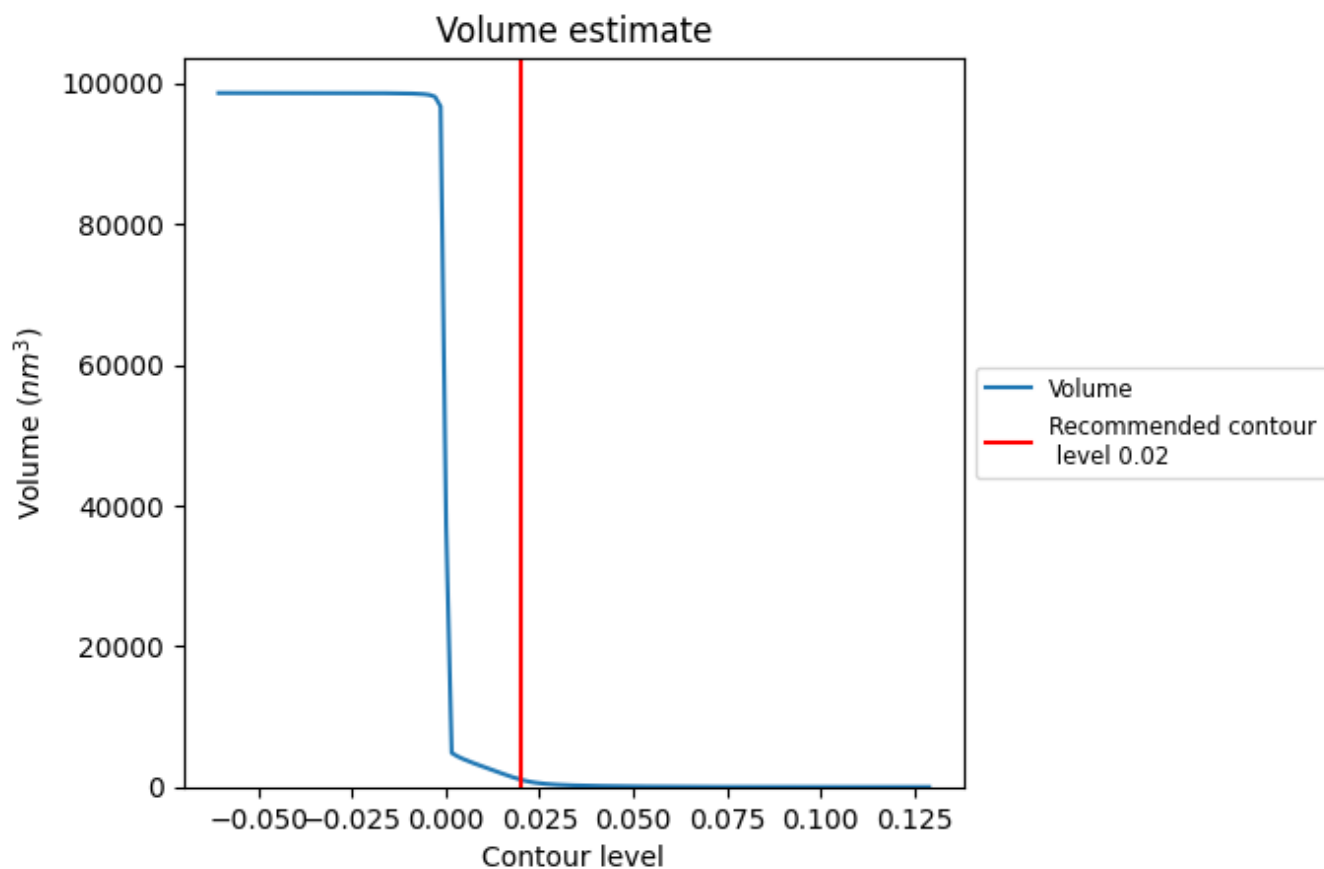
This section contains the results of statistical analysis of the map.

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.

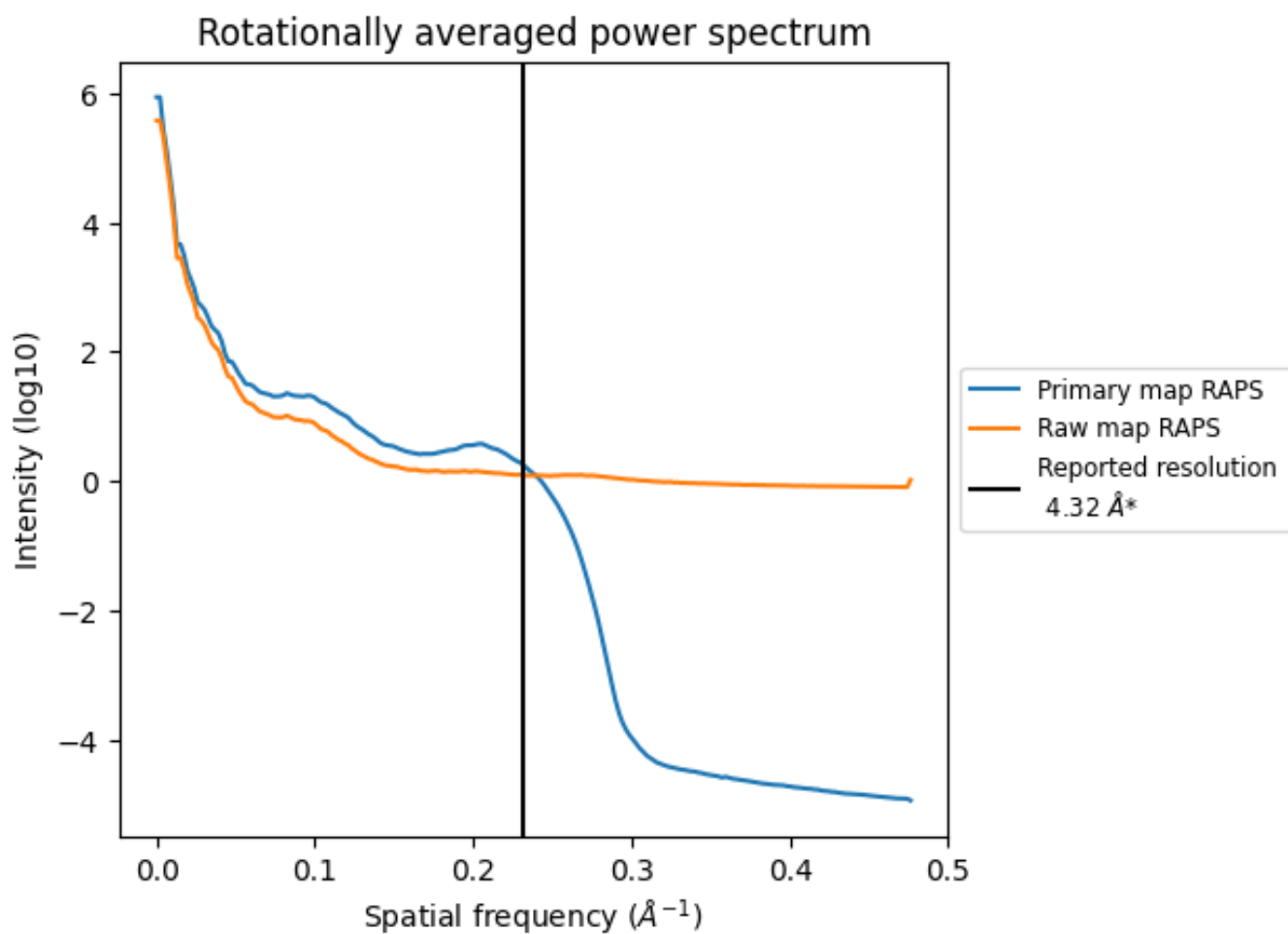
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1048 nm^3 ; 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

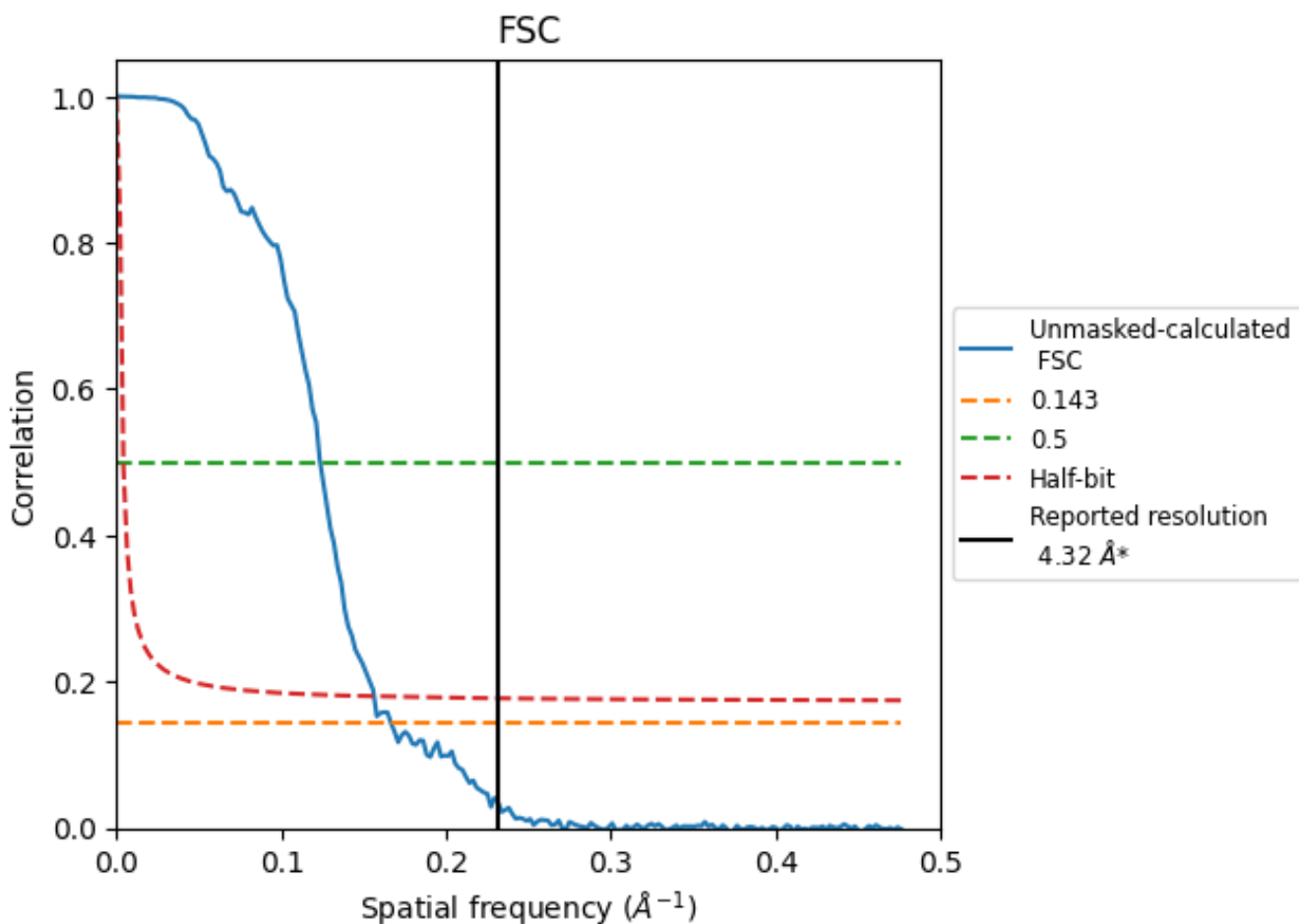


*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

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](#)

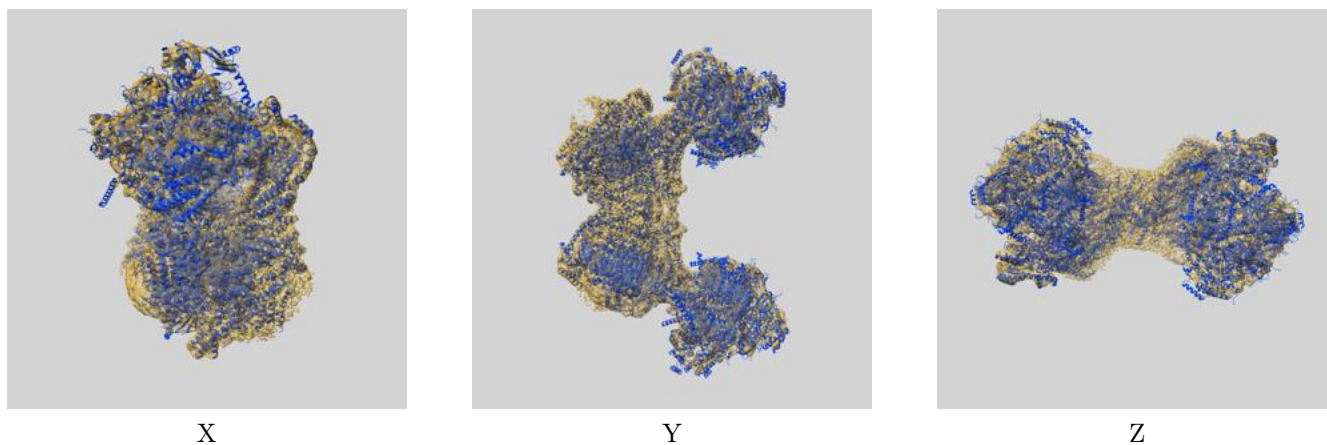
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.00	8.09	6.39

*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](#)

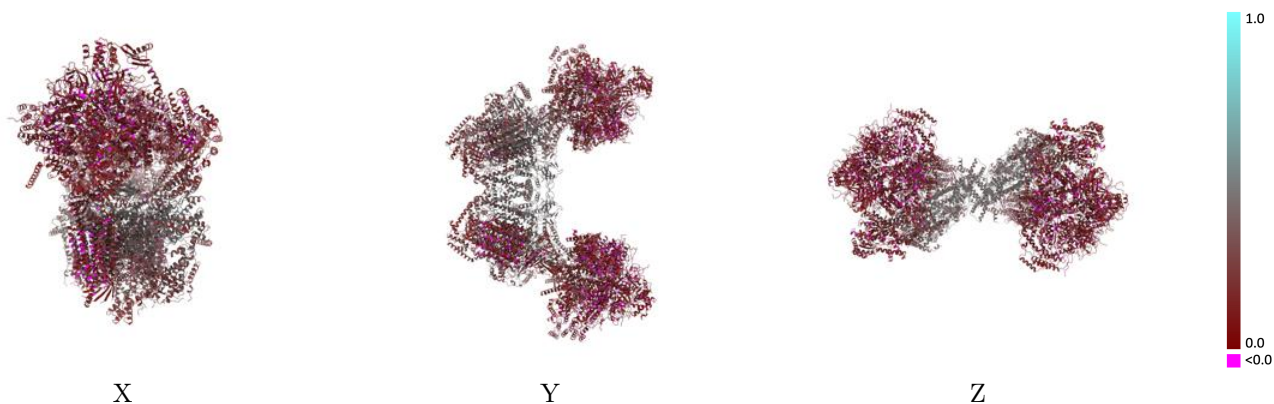
This section contains information regarding the fit between EMDB map EMD-10467 and PDB model 6TDU. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



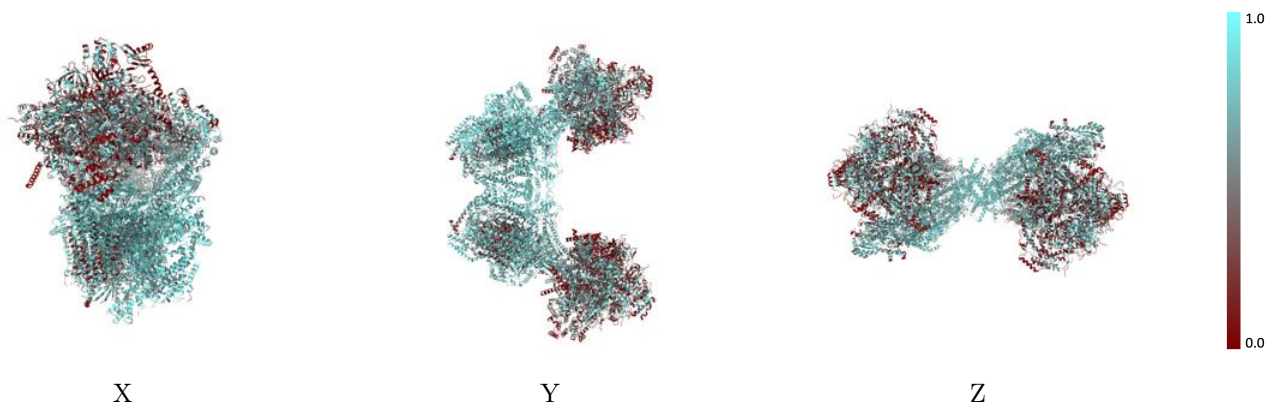
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



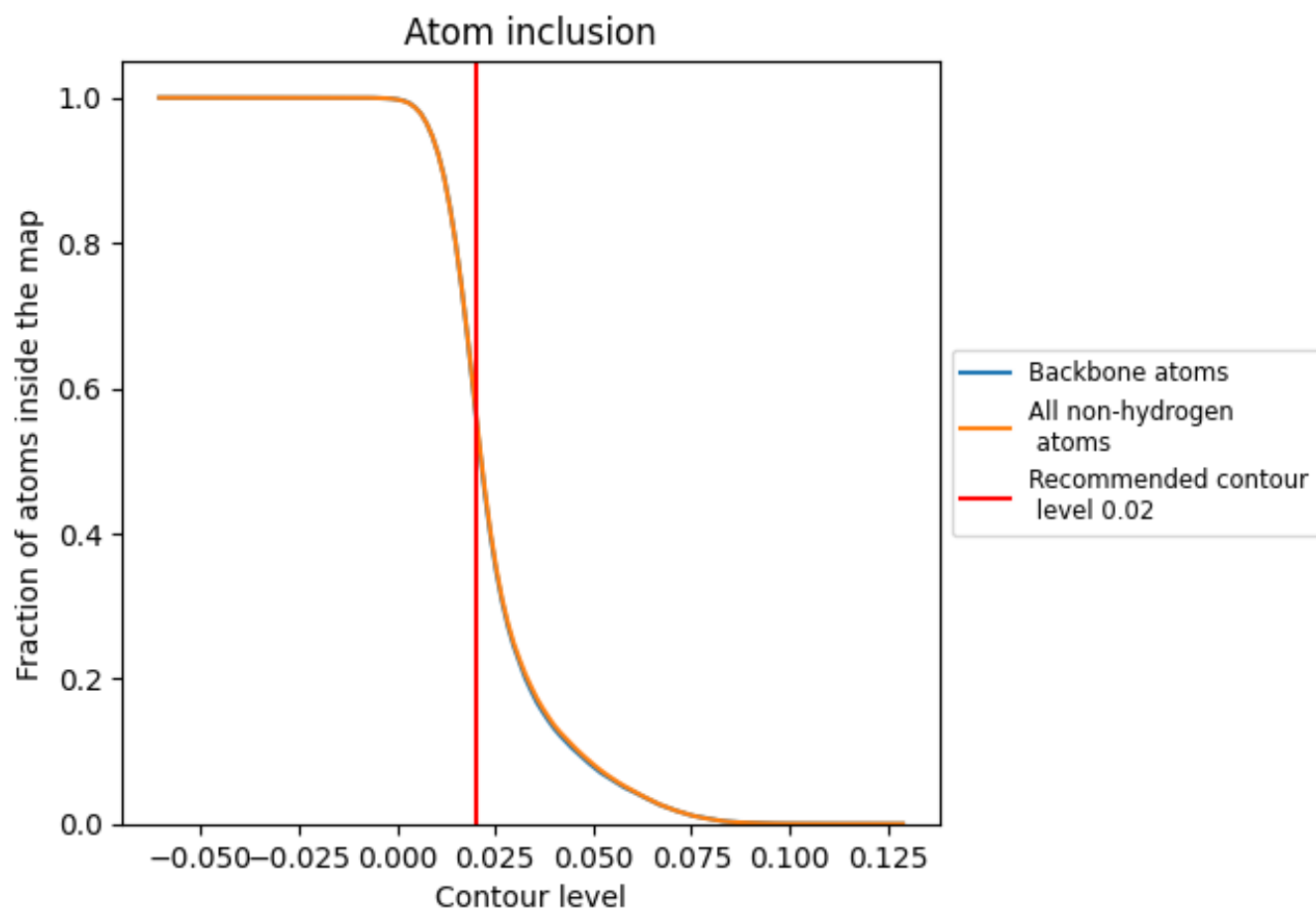
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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