



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 11:21 AM UTC

PDB ID : 9GRX / pdb_00009grx
EMDB ID : EMD-51527
Title : NDH-PSI-LHCI supercomplex from *S. oleracea*
Authors : Introini, B.; Hahn, A.; Kuehlbrandt, W.
Deposited on : 2024-09-13
Resolution : 3.19 Å (reported)
Based on initial models : 4y28, 6khj, .

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:

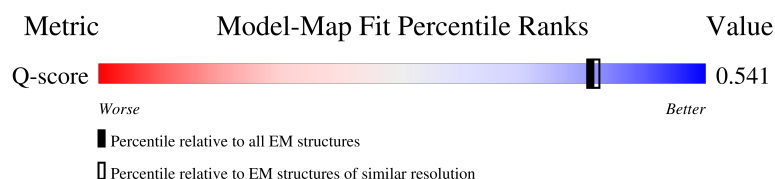
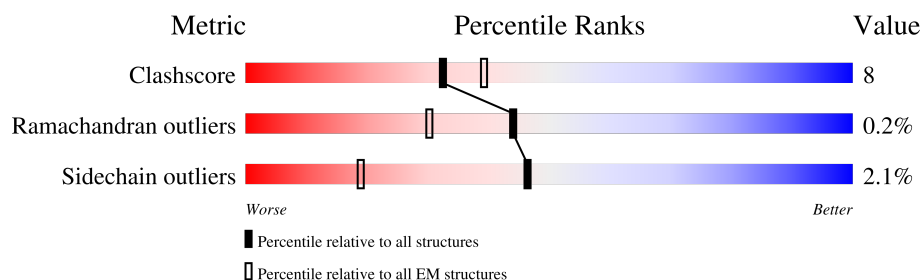
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.19 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.



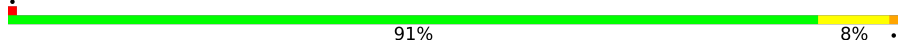
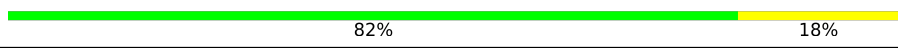
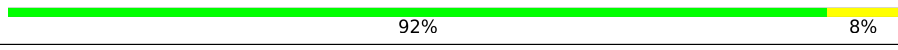
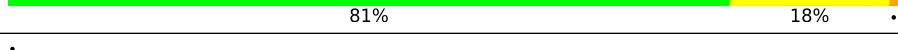
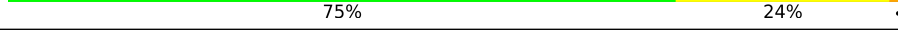
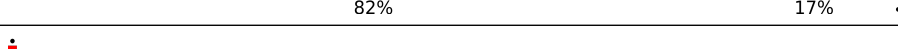
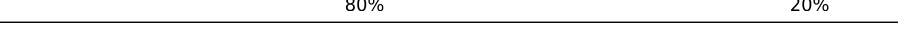
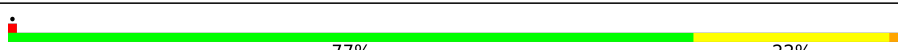
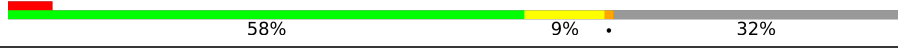
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14455 (2.69 - 3.69)

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

Mol	Chain	Length	Quality of chain
1	0	157	
2	1	403	
3	2	372	
4	3	139	

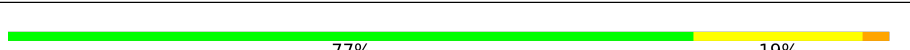
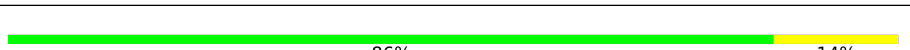
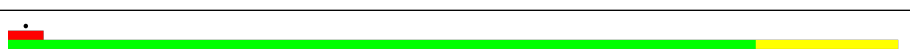
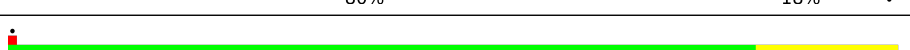
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Mol	Chain	Length	Quality of chain
5	4	93	
6	5	154	
7	6	125	
8	7	144	
9	8	143	
10	9	174	
11	A	350	
12	B	488	
13	C	115	
14	D	498	
15	E	100	
16	F	742	
17	G	176	
18	H	389	
19	I	163	
20	J	158	
21	K	202	
22	L	109	
23	M	141	
24	N	165	
25	O	95	
26	U	240	
27	a	742	
28	b	733	
29	c	81	

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Mol	Chain	Length	Quality of chain
30	d	143	
31	e	68	
32	f	153	
33	g	97	
34	h	95	
35	i	31	
36	j	42	
37	k	130	
38	l	160	
39	w	215	
40	x	198	
41	y	221	
42	z	193	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	a	801	X	-	-	-
50	CLA	a	802	X	-	-	-
50	CLA	a	809	X	-	-	-
50	CLA	a	811	X	-	-	-
50	CLA	a	812	X	-	-	-
50	CLA	a	813	X	-	-	-
50	CLA	a	814	X	-	-	-
50	CLA	a	815	X	-	-	-
50	CLA	a	816	X	-	-	-
50	CLA	a	817	X	-	-	-
50	CLA	a	818	X	-	-	-
50	CLA	a	819	X	-	-	-
50	CLA	a	820	X	-	-	-
50	CLA	a	821	X	-	-	-
50	CLA	a	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	a	823	X	-	-	-
50	CLA	a	824	X	-	-	-
50	CLA	a	826	X	-	-	-
50	CLA	a	833	X	-	-	-
50	CLA	a	834	X	-	-	-
50	CLA	a	835	X	-	-	-
50	CLA	a	836	X	-	-	-
50	CLA	a	837	X	-	-	-
50	CLA	a	838	X	-	-	-
50	CLA	a	839	X	-	-	-
50	CLA	a	840	X	-	-	-
50	CLA	a	841	X	-	-	-
50	CLA	a	842	X	-	-	-
50	CLA	a	843	X	-	-	-
50	CLA	a	844	X	-	-	-
50	CLA	a	845	X	-	-	-
50	CLA	a	846	X	-	-	-
50	CLA	a	847	X	-	-	-
50	CLA	a	848	X	-	-	-
50	CLA	a	849	X	-	-	-
50	CLA	a	850	X	-	-	-
50	CLA	a	851	X	-	-	-
50	CLA	a	852	X	-	-	-
50	CLA	a	853	X	-	-	-
50	CLA	a	854	X	-	-	-
50	CLA	a	855	X	-	-	-
50	CLA	a	856	X	-	-	-
50	CLA	a	857	X	-	-	-
50	CLA	a	858	X	-	-	-
50	CLA	b	801	X	-	-	-
50	CLA	b	802	X	-	-	-
50	CLA	b	803	X	-	-	-
50	CLA	b	804	X	-	-	-
50	CLA	b	805	X	-	-	-
50	CLA	b	806	X	-	-	-
50	CLA	b	807	X	-	-	-
50	CLA	b	808	X	-	-	-
50	CLA	b	809	X	-	-	-
50	CLA	b	810	X	-	-	-
50	CLA	b	811	X	-	-	-
50	CLA	b	812	X	-	-	-
50	CLA	b	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	b	814	X	-	-	-
50	CLA	b	815	X	-	-	-
50	CLA	b	822	X	-	-	-
50	CLA	b	823	X	-	-	-
50	CLA	b	824	X	-	-	-
50	CLA	b	825	X	-	-	-
50	CLA	b	826	X	-	-	-
50	CLA	b	828	X	-	-	-
50	CLA	b	832	X	-	-	-
50	CLA	b	833	X	-	-	-
50	CLA	b	834	X	-	-	-
50	CLA	b	835	X	-	-	-
50	CLA	b	836	X	-	-	-
50	CLA	b	837	X	-	-	-
50	CLA	b	838	X	-	-	-
50	CLA	b	839	X	-	-	-
50	CLA	b	840	X	-	-	-
50	CLA	b	841	X	-	-	-
50	CLA	b	842	X	-	-	-
50	CLA	b	843	X	-	-	-
50	CLA	b	844	X	-	-	-
50	CLA	b	845	X	-	-	-
50	CLA	b	846	X	-	-	-
50	CLA	b	847	X	-	-	-
50	CLA	b	848	X	-	-	-
50	CLA	b	849	X	-	-	-
50	CLA	b	851	X	-	-	-
50	CLA	f	301	X	-	-	-
50	CLA	f	302	X	-	-	-
50	CLA	f	303	X	-	-	-
50	CLA	g	201	X	-	-	-
50	CLA	g	203	X	-	-	-
50	CLA	g	204	X	-	-	-
50	CLA	h	201	X	-	-	-
50	CLA	j	102	X	-	-	-
50	CLA	k	203	X	-	-	-
50	CLA	k	204	X	-	-	-
50	CLA	k	205	X	-	-	-
50	CLA	l	301	X	-	-	-
50	CLA	l	305	X	-	-	-
50	CLA	l	306	X	-	-	-
50	CLA	w	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	w	303	X	-	-	-
50	CLA	w	305	X	-	-	-
50	CLA	w	306	X	-	-	-
50	CLA	w	307	X	-	-	-
50	CLA	w	308	X	-	-	-
50	CLA	w	310	X	-	-	-
50	CLA	w	314	X	-	-	-
50	CLA	w	315	X	-	-	-
50	CLA	w	316	X	-	-	-
50	CLA	x	302	X	-	-	-
50	CLA	x	303	X	-	-	-
50	CLA	x	304	X	-	-	-
50	CLA	x	306	X	-	-	-
50	CLA	x	307	X	-	-	-
50	CLA	x	308	X	-	-	-
50	CLA	x	309	X	-	-	-
50	CLA	x	310	X	-	-	-
50	CLA	x	312	X	-	-	-
50	CLA	x	313	X	-	-	-
50	CLA	x	316	X	-	-	-
50	CLA	x	318	X	-	-	-
50	CLA	y	302	X	-	-	-
50	CLA	y	303	X	-	-	-
50	CLA	y	304	X	-	-	-
50	CLA	y	305	X	-	-	-
50	CLA	y	306	X	-	-	-
50	CLA	y	307	X	-	-	-
50	CLA	y	308	X	-	-	-
50	CLA	y	309	X	-	-	-
50	CLA	y	310	X	-	-	-
50	CLA	y	311	X	-	-	-
50	CLA	y	312	X	-	-	-
50	CLA	y	313	X	-	-	-
50	CLA	y	314	X	-	-	-
50	CLA	z	302	X	-	-	-
50	CLA	z	303	X	-	-	-
50	CLA	z	305	X	-	-	-
50	CLA	z	306	X	-	-	-
50	CLA	z	307	X	-	-	-
50	CLA	z	308	X	-	-	-
50	CLA	z	309	X	-	-	-
50	CLA	z	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	z	311	X	-	-	-
50	CLA	z	316	X	-	-	-
50	CLA	z	319	X	-	-	-
52	CL0	a	808	X	-	-	-
54	CHL	w	304	X	-	-	-
54	CHL	w	309	X	-	-	-
54	CHL	w	311	X	-	-	-
54	CHL	x	301	X	-	-	-
54	CHL	x	305	X	-	-	-
54	CHL	x	311	X	-	-	-
54	CHL	x	319	X	-	-	-
54	CHL	z	304	X	-	-	-
54	CHL	z	312	X	-	-	-
55	LUT	w	320	-	-	X	-
55	LUT	y	315	-	-	X	-
55	LUT	y	316	-	-	X	-
55	LUT	z	320	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 83864 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosynthetic NDH subunit of lumenal location 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	157	Total	C	N	O	S	0	0
			1317	840	227	248	2		

- Molecule 2 is a protein called Photosynthetic NDH subunit of subcomplex B 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	403	Total	C	N	O	S	0	0
			3133	1994	515	607	17		

- Molecule 3 is a protein called Photosynthetic NDH subunit of subcomplex B 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	300	Total	C	N	O	S	0	0
			2305	1463	383	452	7		

- Molecule 4 is a protein called Photosynthetic NDH subunit of subcomplex B 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	139	Total	C	N	O	S	0	0
			1093	690	185	210	8		

- Molecule 5 is a protein called Photosynthetic NDH subunit of subcomplex B 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	93	Total	C	N	O	S	0	0
			756	482	125	143	6		

- Molecule 6 is a protein called Photosynthetic NDH subunit of subcomplex B 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	154	Total	C	N	O	S	0	0
			1258	816	194	242	6		

- Molecule 7 is a protein called Photosynthetic NDH subunit of luminal location 2, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	125	Total	C	N	O	S	0	0
			1048	675	174	193	6		

- Molecule 8 is a protein called Photosynthetic NDH subunit of luminal location 3, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	144	Total	C	N	O	S	0	0
			1156	739	198	213	6		

- Molecule 9 is a protein called peptidylprolyl isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	143	Total	C	N	O	S	0	0
			1075	680	187	201	7		

- Molecule 10 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	174	Total	C	N	O	S	0	0
			1326	836	233	251	6		

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit 1, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	350	Total	C	N	O	S	0	0
			2728	1821	420	482	5		

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit 2 A, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	488	Total	C	N	O	S	0	0
			3799	2506	583	683	27		

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloro-
plastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	115	Total	C	N	O	S	0	0
			944	653	133	155	3		

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	498	Total	C	N	O	S	0	0
			3955	2660	607	665	23		

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	100	Total	C	N	O	S	0	0
			780	509	133	135	3		

- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	722	Total	C	N	O	S	0	0
			5796	3885	889	990	32		

- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	176	Total	C	N	O	S	0	0
			1357	910	204	238	5		

- Molecule 18 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	371	Total	C	N	O	S	0	0
			3008	1948	506	535	19		

- Molecule 19 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	163	Total	C	N	O	S	0	0
			1329	845	226	246	12		

- Molecule 20 is a protein called NAD(P)H-quinone oxidoreductase subunit J, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	158	Total	C	N	O	S	0	0
			1324	864	224	231	5		

- Molecule 21 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	202	Total	C	N	O	S	0	0
			1597	1020	272	294	11		

- Molecule 22 is a protein called NAD(P)H-quinone oxidoreductase subunit L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	109	Total	C	N	O	S	0	0
			936	639	147	144	6		

- Molecule 23 is a protein called NAD(P)H-quinone oxidoreductase subunit M, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	141	Total	C	N	O	S	0	0
			1169	743	196	221	9		

- Molecule 24 is a protein called NAD(P)H-quinone oxidoreductase subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	165	Total	C	N	O	S	0	0
			1323	862	228	228	5		

- Molecule 25 is a protein called NAD(P)H-quinone oxidoreductase subunit O, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	95	Total	C	N	O	S	0	0
			786	515	127	142	2		

- Molecule 26 is a protein called NAD(P)H-quinone oxidoreductase subunit U, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	163	Total	C	N	O	S	0	0
			1266	802	218	243	3		

- Molecule 27 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	742	Total	C	N	O	S	0	0
			5827	3817	991	1001	18		

- Molecule 28 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	733	Total	C	N	O	S	0	0
			5855	3841	996	1003	15		

- Molecule 29 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	81	Total	C	N	O	S	0	0
			623	385	108	118	12		

- Molecule 30 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	143	Total	C	N	O	S	0	0
			1132	729	194	205	4		

- Molecule 31 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	68	Total	C	N	O	S	0	0
			546	348	98	99	1		

- Molecule 32 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	153	Total	C	N	O	S	0	0
			1211	785	206	217	3		

- Molecule 33 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	97	Total	C	N	O	S	0	0
			759	493	123	141	2		

- Molecule 34 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	h	95	Total	C	N	O	0	0
			737	479	120	138		

- Molecule 35 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	31	Total	C	N	O	S	0	0
			244	168	36	38	2		

- Molecule 36 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	42	Total	C	N	O	S	0	0
			345	236	51	57	1		

- Molecule 37 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	66	Total	C	N	O	S	0	0
			462	294	78	87	3		

- Molecule 38 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	160	Total	C	N	O	S	0	0
			1200	791	192	212	5		

- Molecule 39 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	w	215	Total	C	N	O	S	0	0
			1689	1096	281	300	12		

- Molecule 40 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	x	198	Total	C	N	O	S	0	0
			1568	1023	256	284	5		

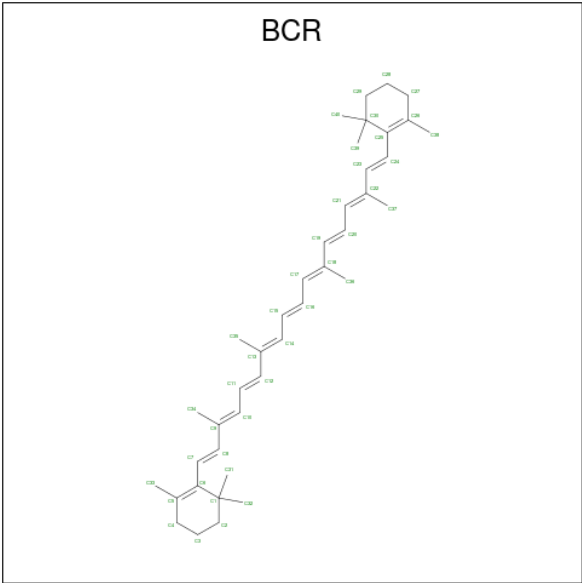
- Molecule 41 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	y	221	Total	C	N	O	S	0	0
			1713	1125	277	306	5		

- Molecule 42 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	z	193	Total	C	N	O	S	0	0
			1498	973	250	270	5		

- Molecule 43 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



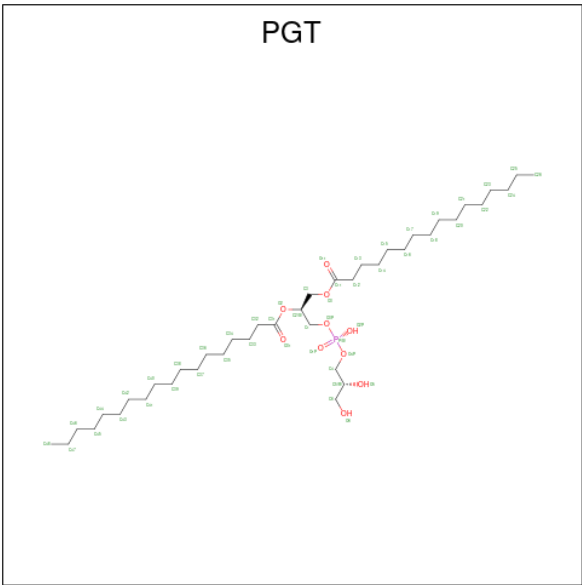
Mol	Chain	Residues	Atoms		AltConf
43	4	1	Total	C	0
			40	40	
43	a	1	Total	C	0
			27	27	
43	a	1	Total	C	0
			30	30	
43	a	1	Total	C	0
			39	39	
43	a	1	Total	C	0
			40	40	
43	a	1	Total	C	0
			40	40	
43	a	1	Total	C	0
			40	40	
43	a	1	Total	C	0
			39	39	
43	b	1	Total	C	0
			40	40	
43	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	f	1	Total C 40 40	0
43	g	1	Total C 40 40	0
43	i	1	Total C 40 40	0
43	j	1	Total C 40 40	0
43	j	1	Total C 40 40	0
43	k	1	Total C 40 40	0
43	k	1	Total C 40 40	0
43	l	1	Total C 40 40	0
43	l	1	Total C 40 40	0
43	l	1	Total C 40 40	0
43	w	1	Total C 40 40	0
43	x	1	Total C 40 40	0
43	y	1	Total C 40 40	0
43	z	1	Total C 40 40	0

- Molecule 44 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



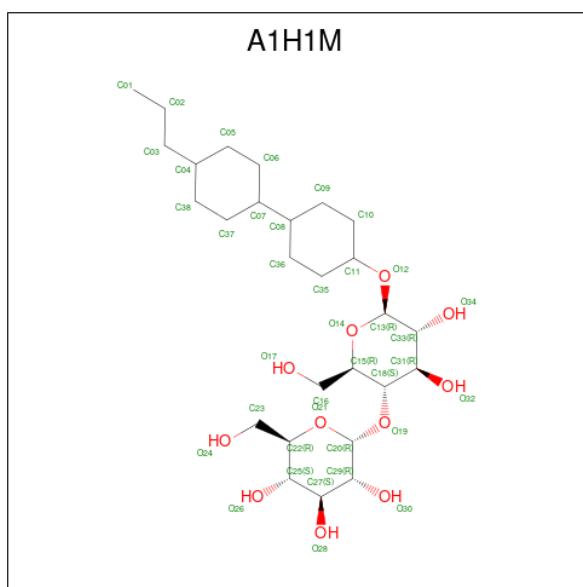
Mol	Chain	Residues	Atoms				AltConf
44	5	1	Total	C	O	P	0
			35	24	10	1	
44	A	1	Total	C	O	P	0
			32	21	10	1	
44	A	1	Total	C	O	P	0
			37	26	10	1	
44	A	1	Total	C	O	P	0
			38	27	10	1	
44	A	1	Total	C	O	P	0
			44	33	10	1	
44	B	1	Total	C	O	P	0
			34	23	10	1	
44	B	1	Total	C	O	P	0
			42	31	10	1	
44	B	1	Total	C	O	P	0
			46	35	10	1	
44	B	1	Total	C	O	P	0
			35	24	10	1	
44	D	1	Total	C	O	P	0
			34	23	10	1	
44	F	1	Total	C	O	P	0
			43	32	10	1	
44	I	1	Total	C	O	P	0
			44	33	10	1	
44	L	1	Total	C	O	P	0
			40	29	10	1	
44	N	1	Total	C	O	P	0
			26	15	10	1	

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Mol	Chain	Residues	Atoms				AltConf
44	a	1	Total	C	O	P	0
			32	21	10	1	
44	a	1	Total	C	O	P	0
			33	22	10	1	
44	a	1	Total	C	O	P	0
			46	35	10	1	
44	b	1	Total	C	O	P	0
			48	37	10	1	
44	b	1	Total	C	O	P	0
			39	28	10	1	
44	f	1	Total	C	O	P	0
			39	28	10	1	
44	w	1	Total	C	O	P	0
			40	29	10	1	
44	z	1	Total	C	O	P	0
			45	34	10	1	
44	z	1	Total	C	O	P	0
			33	22	10	1	
44	z	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 45 is 4-trans-(4-trans-Propylcyclohexyl)-cyclohexyl alpha-maltoside (CCD ID: A1H1M) (formula: C₂₇H₄₈O₁₁) (labeled as "Ligand of Interest" by depositor).



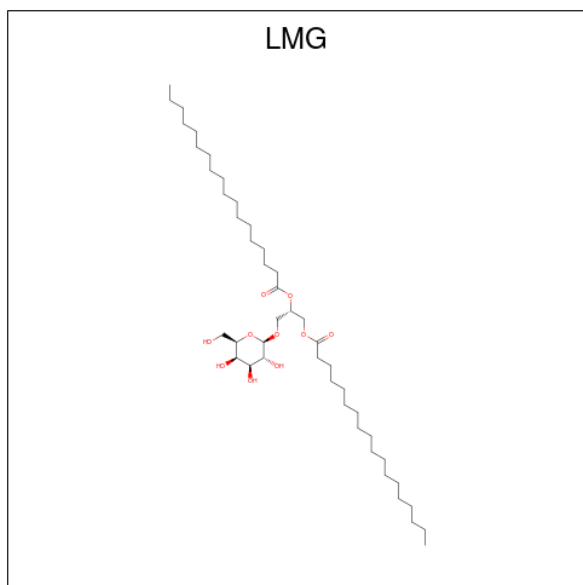
Mol	Chain	Residues	Atoms				AltConf
45	5	1	Total	C	O		0
			38	27	11		

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Mol	Chain	Residues	Atoms			AltConf
45	F	1	Total	C	O	0
			38	27	11	

- Molecule 46 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



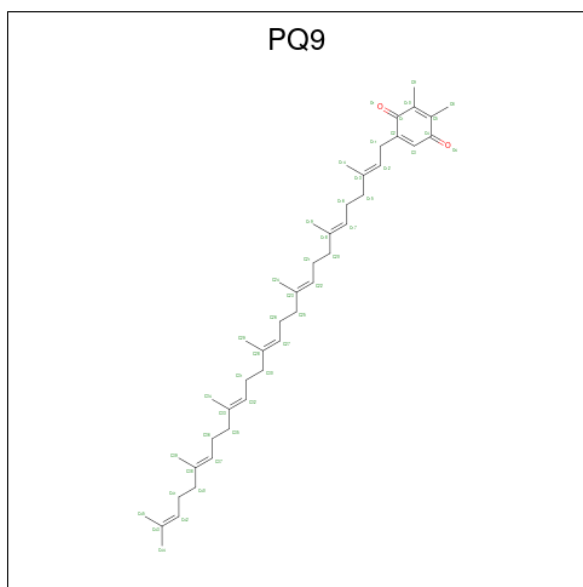
Mol	Chain	Residues	Atoms			AltConf
46	7	1	Total	C	O	0
			41	31	10	
46	B	1	Total	C	O	0
			37	27	10	
46	D	1	Total	C	O	0
			34	24	10	
46	F	1	Total	C	O	0
			28	18	10	
46	H	1	Total	C	O	0
			33	23	10	
46	f	1	Total	C	O	0
			34	24	10	
46	j	1	Total	C	O	0
			34	24	10	
46	j	1	Total	C	O	0
			37	27	10	
46	w	1	Total	C	O	0
			40	30	10	
46	x	1	Total	C	O	0
			48	38	10	

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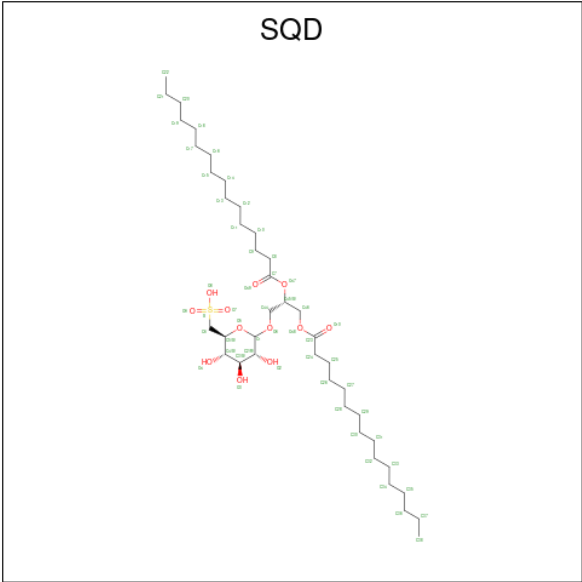
Mol	Chain	Residues	Atoms			AltConf
46	z	1	Total	C	O	0
			40	30	10	
46	z	1	Total	C	O	0
			36	26	10	

- Molecule 47 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: C₄₃H₆₄O₂) (labeled as "Ligand of Interest" by depositor).



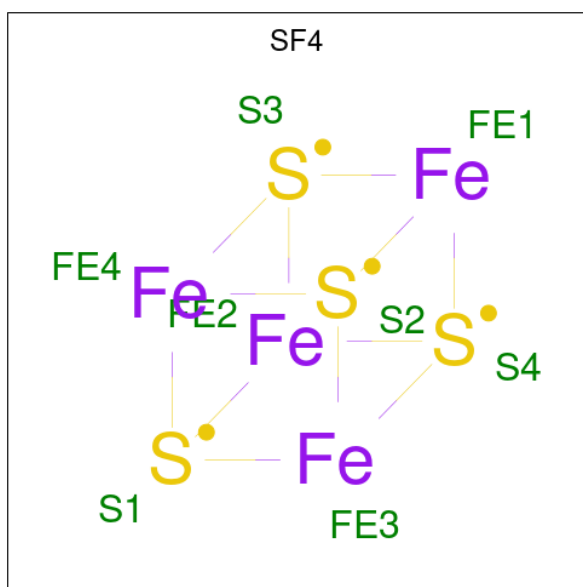
Mol	Chain	Residues	Atoms			AltConf
47	A	1	Total	C	O	0
			36	34	2	

- Molecule 48 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



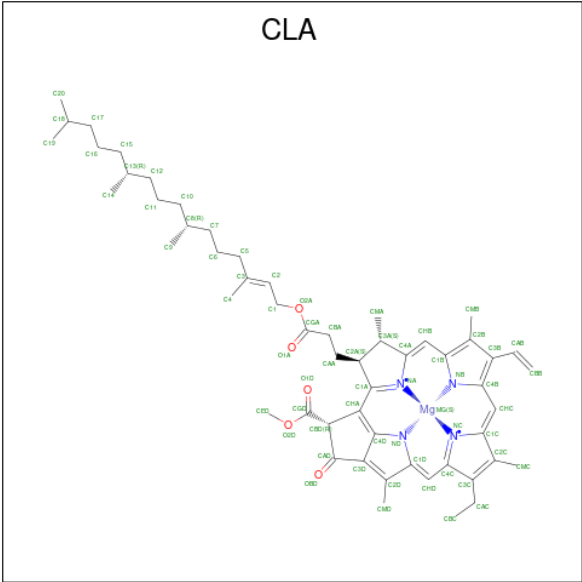
Mol	Chain	Residues	Atoms				AltConf
48	B	1	Total	C	O	S	0
			40	27	12	1	
48	F	1	Total	C	O	S	0
			41	28	12	1	
48	F	1	Total	C	O	S	0
			43	30	12	1	
48	a	1	Total	C	O	S	0
			36	23	12	1	
48	j	1	Total	C	O	S	0
			42	29	12	1	
48	w	1	Total	C	O	S	0
			31	18	12	1	
48	w	1	Total	C	O	S	0
			41	28	12	1	

- Molecule 49 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
49	I	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	
49	K	1	Total	Fe	S	0
			8	4	4	
49	a	1	Total	Fe	S	0
			8	4	4	
49	c	1	Total	Fe	S	0
			8	4	4	
49	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 50 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
50	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
50	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			63	53	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
50	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
50	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			42	35	1	3	3	
50	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
50	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
50	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
50	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	a	1	Total 42	C 34	Mg 1	N 4	O 3	0
50	a	1	Total 64	C 54	Mg 1	N 4	O 5	0
50	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
50	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
50	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 43	C 35	Mg 1	N 4	O 3	0
50	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
50	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
50	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
50	b	1	Total 62	C 52	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
50	b	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
50	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
50	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
50	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
50	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
50	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
50	f	1	Total 57	C 47	Mg 1	N 4	O 5	0
50	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
50	f	1	Total 41	C 33	Mg 1	N 4	O 3	0
50	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
50	g	1	Total 52	C 42	Mg 1	N 4	O 5	0
50	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
50	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
50	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
50	k	1	Total 41	C 33	Mg 1	N 4	O 3	0
50	k	1	Total 57	C 47	Mg 1	N 4	O 5	0
50	k	1	Total 42	C 34	Mg 1	N 4	O 3	0
50	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
50	l	1	Total 40	C 32	Mg 1	N 4	O 3	0
50	l	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
50	w	1	Total 50	C 40	Mg 1	N 4	O 5	0
50	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
50	w	1	Total 51	C 41	Mg 1	N 4	O 5	0
50	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
50	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	w	1	Total 44	C 35	Mg 1	N 4	O 4	0
50	w	1	Total 46	C 36	Mg 1	N 4	O 5	0
50	w	1	Total 50	C 40	Mg 1	N 4	O 5	0
50	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
50	x	1	Total 57	C 47	Mg 1	N 4	O 5	0
50	x	1	Total 47	C 37	Mg 1	N 4	O 5	0
50	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
50	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
50	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
50	x	1	Total 42	C 34	Mg 1	N 4	O 3	0
50	x	1	Total 43	C 35	Mg 1	N 4	O 3	0
50	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	x	1	Total 53	C 43	Mg 1	N 4	O 5	0
50	x	1	Total 45	C 35	Mg 1	N 4	O 5	0

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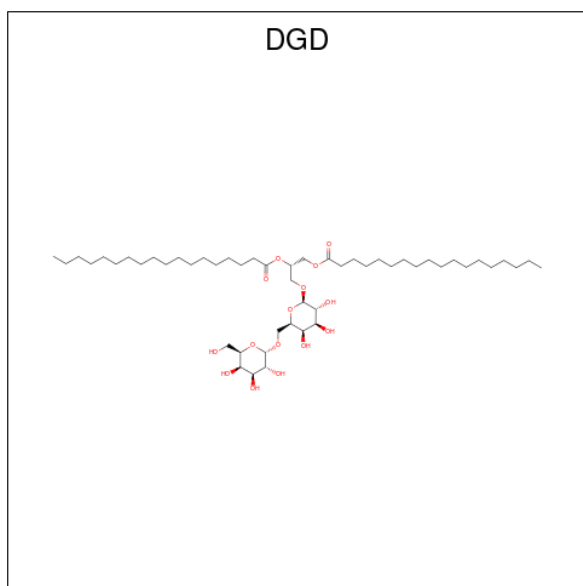
Mol	Chain	Residues	Atoms					AltConf
50	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
50	y	1	Total 52	C 42	Mg 1	N 4	O 5	0
50	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
50	y	1	Total 39	C 33	Mg 1	N 4	O 1	0
50	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
50	y	1	Total 40	C 32	Mg 1	N 4	O 3	0
50	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
50	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	y	1	Total 42	C 34	Mg 1	N 4	O 3	0
50	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	y	1	Total 51	C 41	Mg 1	N 4	O 5	0
50	y	1	Total 51	C 41	Mg 1	N 4	O 5	0
50	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
50	z	1	Total 55	C 45	Mg 1	N 4	O 5	0
50	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
50	z	1	Total 50	C 40	Mg 1	N 4	O 5	0
50	z	1	Total 56	C 46	Mg 1	N 4	O 5	0
50	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
50	z	1	Total 43	C 33	Mg 1	N 4	O 5	0
50	z	1	Total 42	C 34	Mg 1	N 4	O 3	0

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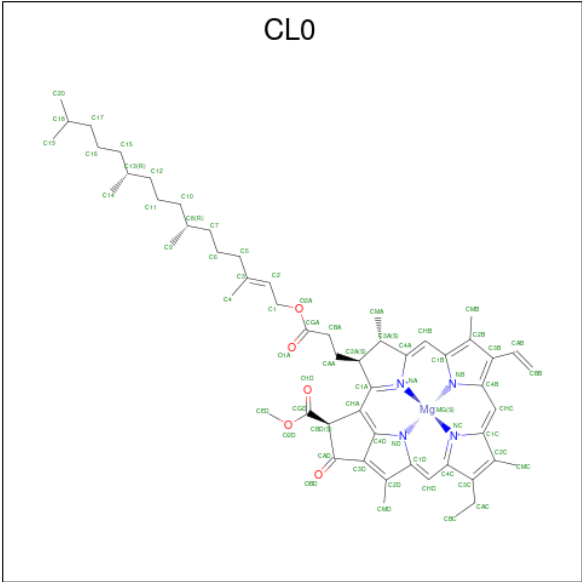
Mol	Chain	Residues	Atoms					AltConf
50	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
50	z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
50	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
50	z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 51 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



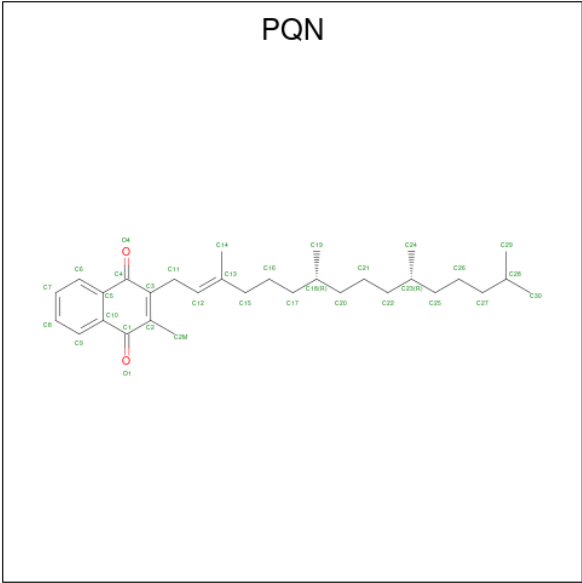
Mol	Chain	Residues	Atoms			AltConf
51	a	1	Total	C	O	0
			66	51	15	
51	b	1	Total	C	O	0
			59	44	15	
51	x	1	Total	C	O	0
			48	33	15	

- Molecule 52 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



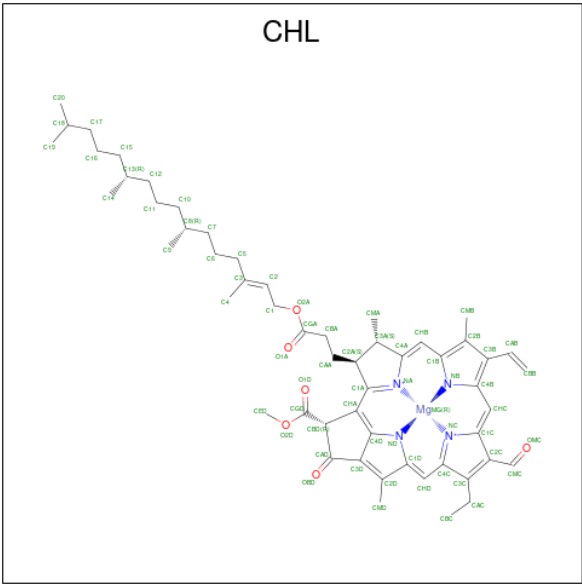
Mol	Chain	Residues	Atoms					AltConf
52	a	1	Total	C	Mg	N	O	0
			61	52	1	4	4	

- Molecule 53 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



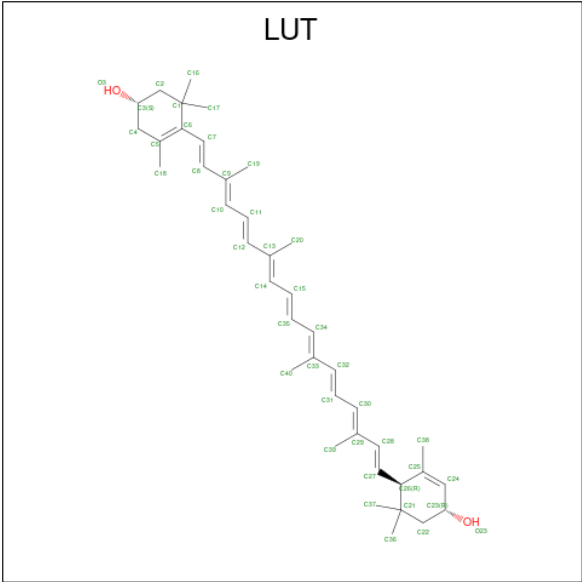
Mol	Chain	Residues	Atoms			AltConf
53	a	1	Total	C	O	0
			33	31	2	
53	b	1	Total	C	O	0
			33	31	2	

- Molecule 54 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
54	w	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
54	w	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	w	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
54	x	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	x	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	x	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
54	x	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
54	z	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	z	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 55 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).

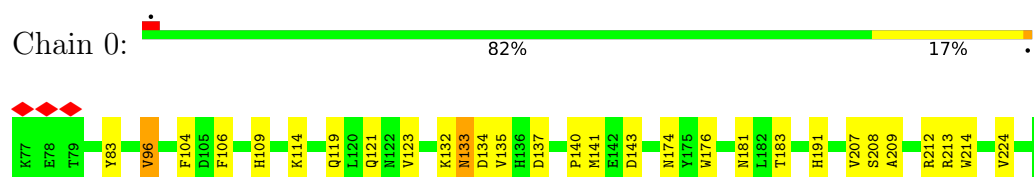


Mol	Chain	Residues	Atoms			AltConf
55	w	1	Total	C	O	0
			42	40	2	
55	w	1	Total	C	O	0
			42	40	2	
55	x	1	Total	C	O	0
			42	40	2	
55	x	1	Total	C	O	0
			42	40	2	
55	y	1	Total	C	O	0
			42	40	2	
55	y	1	Total	C	O	0
			42	40	2	
55	z	1	Total	C	O	0
			42	40	2	
55	z	1	Total	C	O	0
			42	40	2	

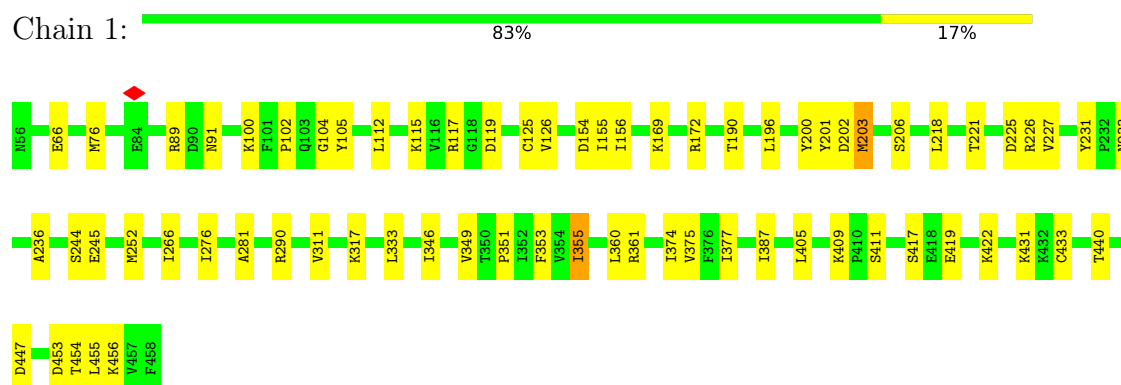
3 Residue-property plots

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.

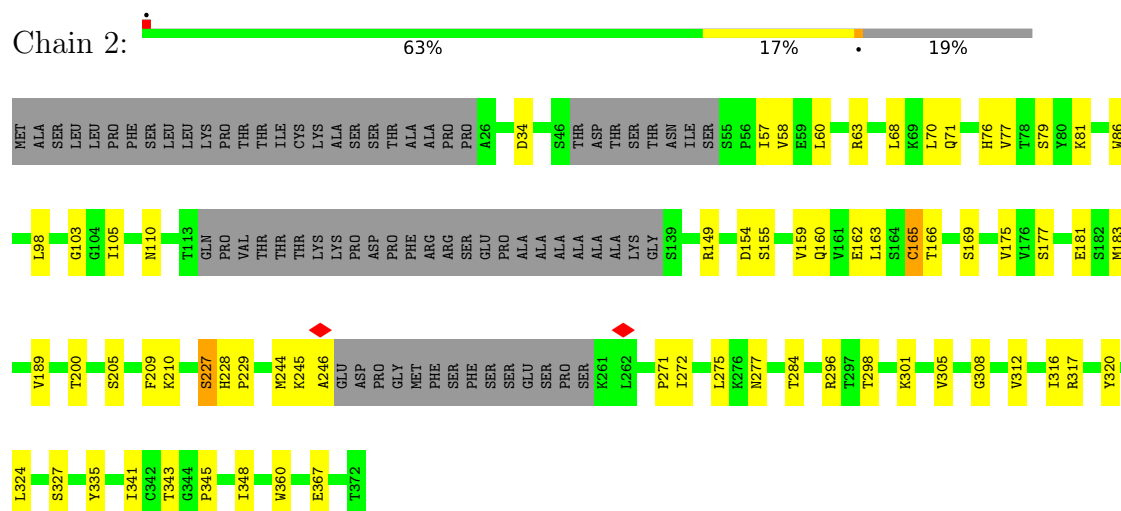
- Molecule 1: Photosynthetic NDH subunit of luminal location 1, chloroplastic



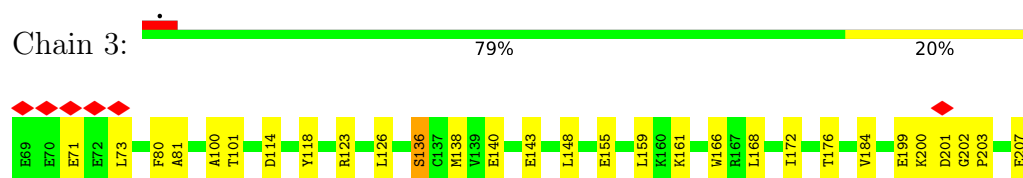
- Molecule 2: Photosynthetic NDH subunit of subcomplex B 1, chloroplastic



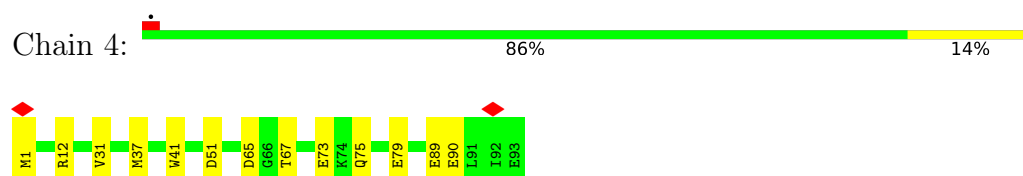
- Molecule 3: Photosynthetic NDH subunit of subcomplex B 2, chloroplastic



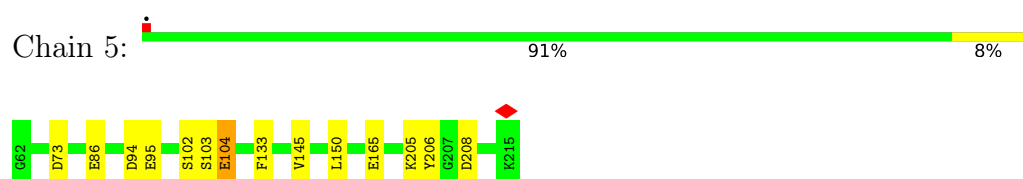
- Molecule 4: Photosynthetic NDH subunit of subcomplex B 3, chloroplastic



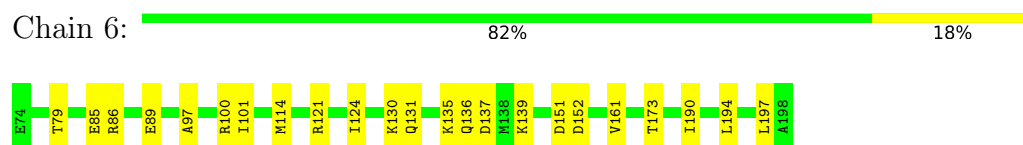
- Molecule 5: Photosynthetic NDH subunit of subcomplex B 4, chloroplastic



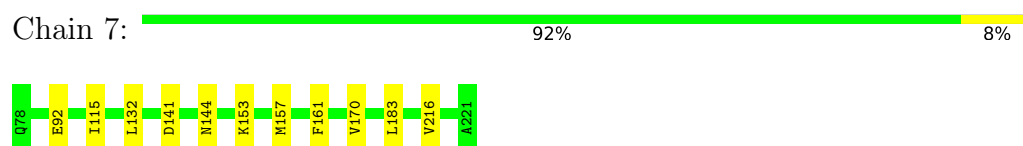
- Molecule 6: Photosynthetic NDH subunit of subcomplex B 5, chloroplastic



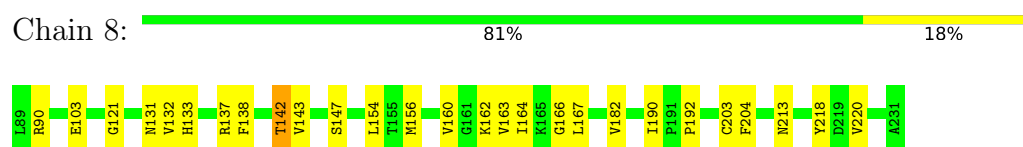
- Molecule 7: Photosynthetic NDH subunit of luminal location 2, chloroplastic



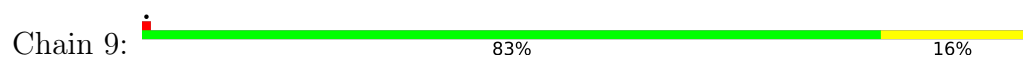
- Molecule 8: Photosynthetic NDH subunit of luminal location 3, chloroplastic



- Molecule 9: peptidylprolyl isomerase

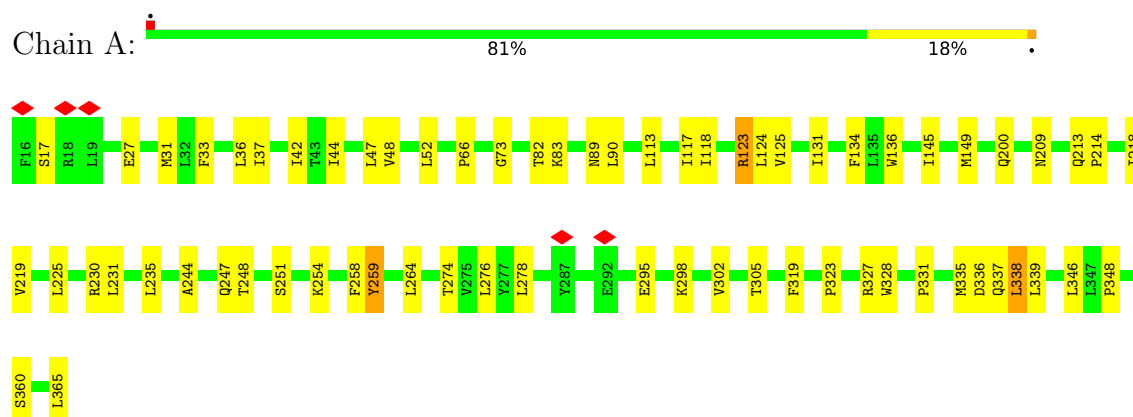


- Molecule 10: Peptidyl-prolyl cis-trans isomerase

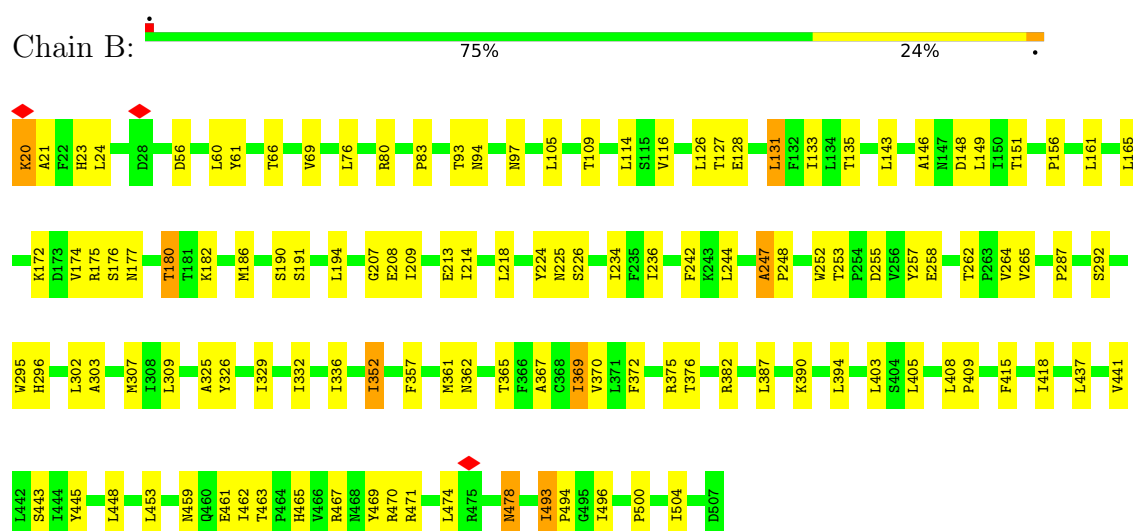




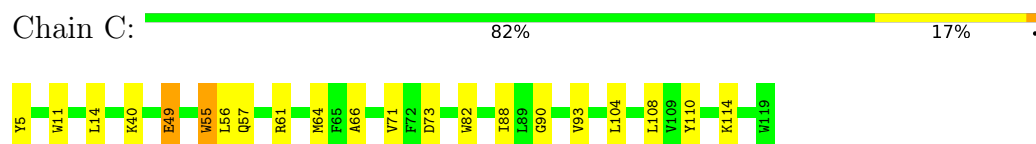
- Molecule 11: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic



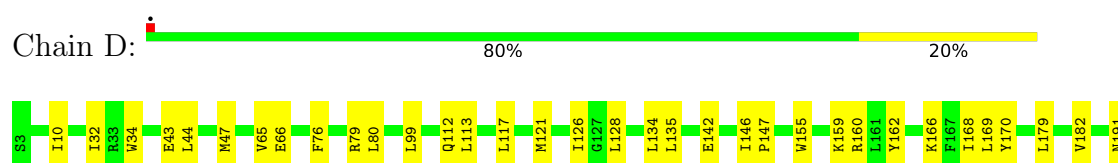
- Molecule 12: NAD(P)H-quinone oxidoreductase subunit 2 A, chloroplastic

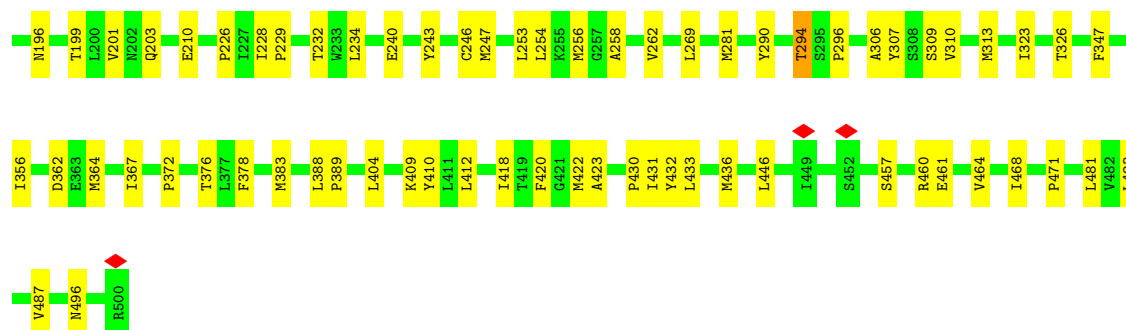


- Molecule 13: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic



- Molecule 14: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic





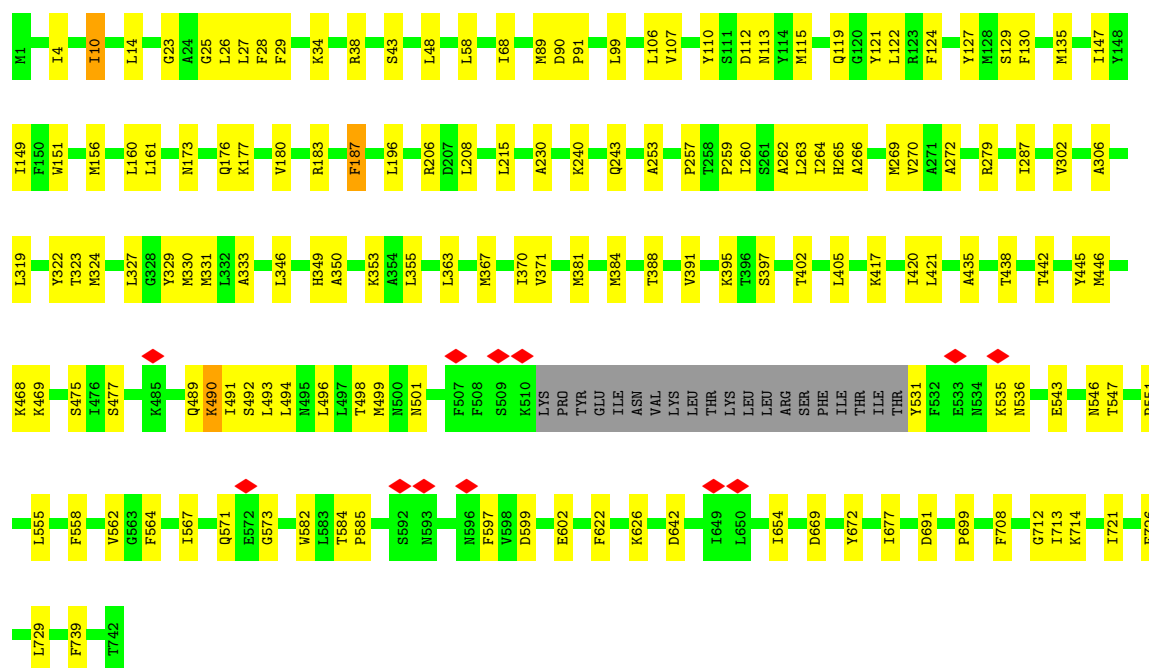
- Molecule 15: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic

Chain E: 81% 18% .



- Molecule 16: NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic

Chain F: 77% 20% .



- Molecule 17: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

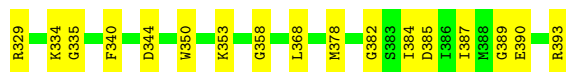
Chain G: 79% 19% .





- Molecule 18: NAD(P)H-quinone oxidoreductase subunit H, chloroplactic

Chain H: 77% 18% 5%



- Molecule 19: NAD(P)H-quinone oxidoreductase subunit I, chloroplactic

Chain I: 85% 15%



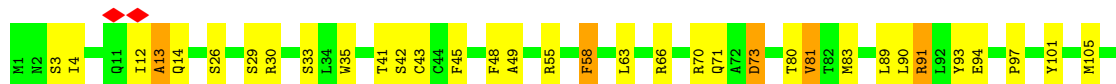
- Molecule 20: NAD(P)H-quinone oxidoreductase subunit J, chloroplactic

Chain J: 77% 22%



- Molecule 21: NAD(P)H-quinone oxidoreductase subunit K, chloroplactic

Chain K: 74% 23%

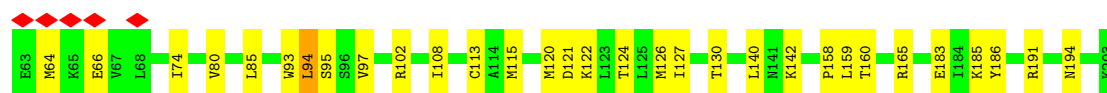
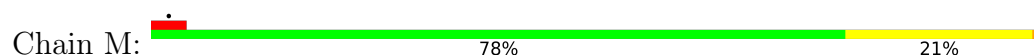


- Molecule 22: NAD(P)H-quinone oxidoreductase subunit L, chloroplactic

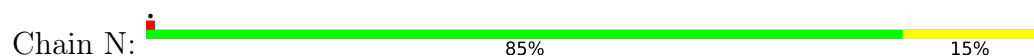
Chain L: 88% 11%



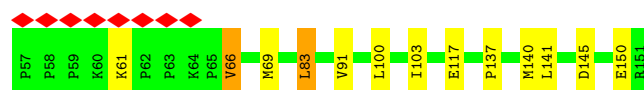
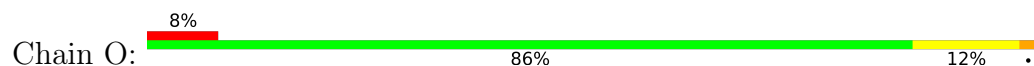
- Molecule 23: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic



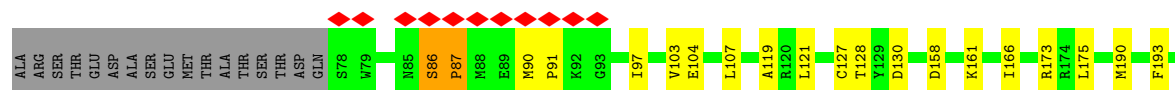
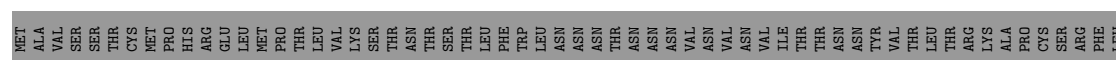
- Molecule 24: NAD(P)H-quinone oxidoreductase subunit N, chloroplastic



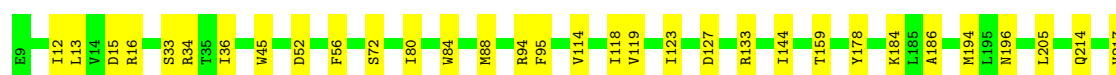
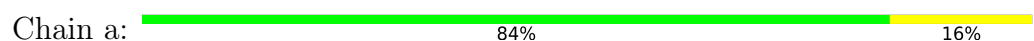
- Molecule 25: NAD(P)H-quinone oxidoreductase subunit O, chloroplastic

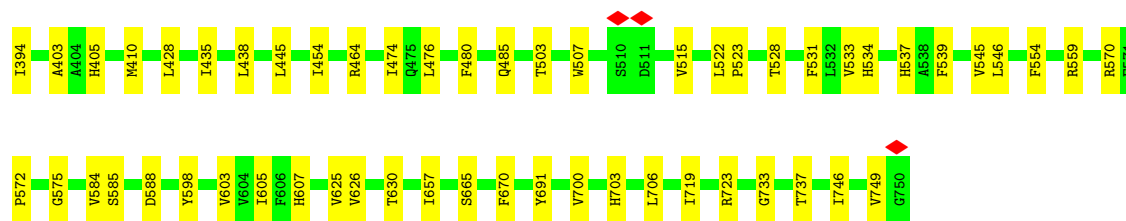


- Molecule 26: NAD(P)H-quinone oxidoreductase subunit U, chloroplastic



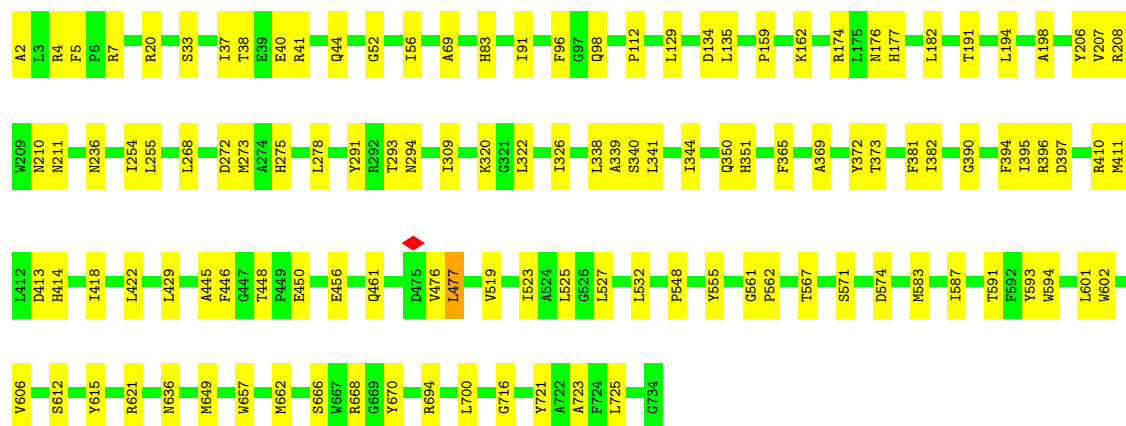
- Molecule 27: Photosystem I P700 chlorophyll a apoprotein A1





- Molecule 28: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 84% 16%



- Molecule 29: Photosystem I iron-sulfur center

Chain c: 85% 12%



- Molecule 30: Photosystem I reaction center subunit II, chloroplastic

Chain d: 83% 17%



- Molecule 31: Photosystem I reaction center subunit IV, chloroplastic

Chain e: 6% 87% 13%

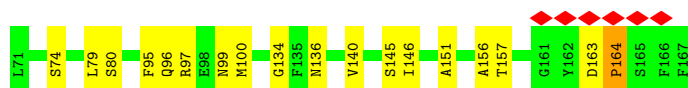
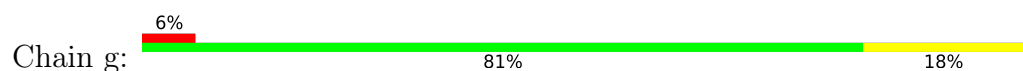


- Molecule 32: Photosystem I reaction center subunit III, chloroplastic

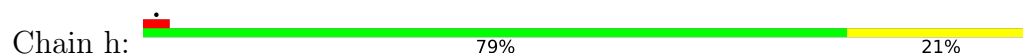
Chain f: 88% 12%



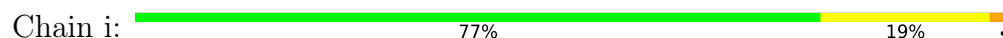
- Molecule 33: Photosystem I reaction center subunit V, chloroplastic



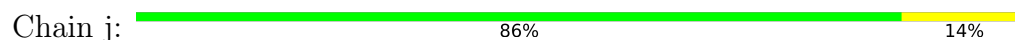
- Molecule 34: Photosystem I reaction center subunit VI, chloroplastic



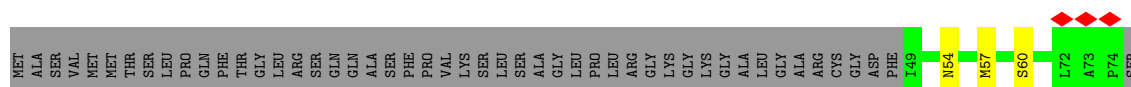
- Molecule 35: Photosystem I reaction center subunit VIII



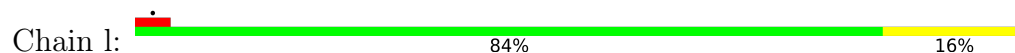
- Molecule 36: Photosystem I reaction center subunit IX

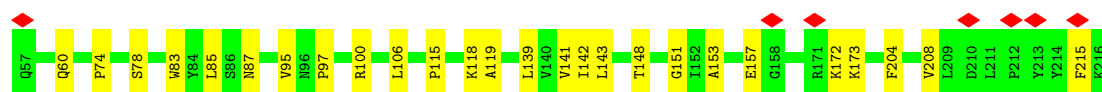


- Molecule 37: PSI-K

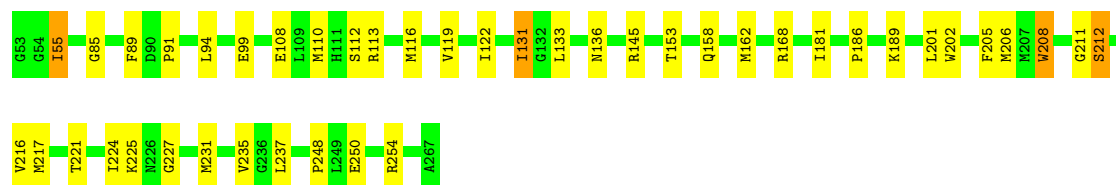
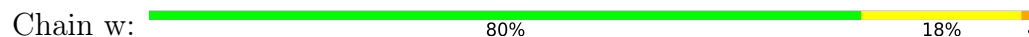


- Molecule 38: Photosystem I reaction center subunit XI, chloroplastic

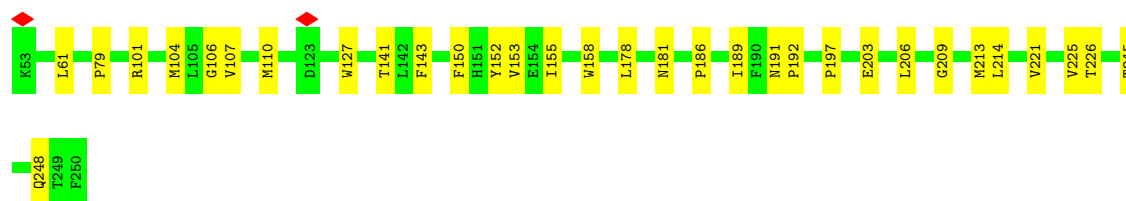
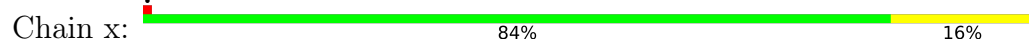




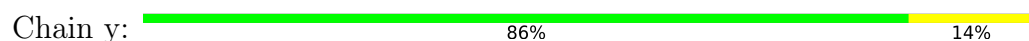
- Molecule 39: Chlorophyll a-b binding protein, chloroplastic



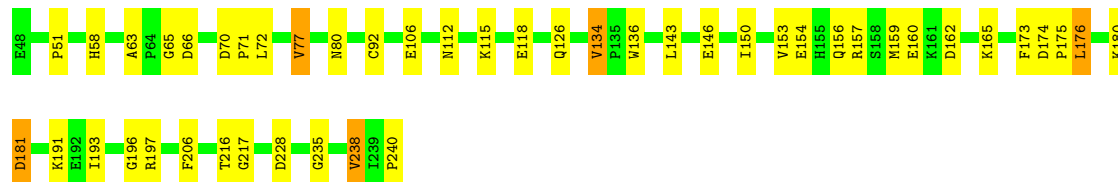
- Molecule 40: Chlorophyll a-b binding protein, chloroplastic



- Molecule 41: Chlorophyll a-b binding protein, chloroplastic



- Molecule 42: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38385	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.744	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, SQD, PGT, A1H1M, CHL, LUT, SF4, PQ9, CL0, LMG, DGD, CLA, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.15	0/1351	0.40	0/1831
2	1	0.13	0/3200	0.35	0/4340
3	2	0.13	0/2350	0.35	0/3186
4	3	0.15	0/1118	0.41	0/1512
5	4	0.17	0/777	0.38	0/1051
6	5	0.23	0/1301	0.44	0/1770
7	6	0.17	0/1075	0.40	0/1448
8	7	0.18	0/1178	0.38	0/1589
9	8	0.14	0/1101	0.34	0/1494
10	9	0.11	0/1352	0.35	1/1821 (0.1%)
11	A	0.21	0/2795	0.45	1/3810 (0.0%)
12	B	0.22	0/3890	0.48	0/5290
13	C	0.25	0/977	0.48	0/1333
14	D	0.16	0/4072	0.36	0/5535
15	E	0.18	0/791	0.42	0/1070
16	F	0.20	0/5965	0.43	1/8100 (0.0%)
17	G	0.17	0/1388	0.37	0/1893
18	H	0.17	0/3081	0.39	0/4170
19	I	0.15	0/1357	0.38	0/1839
20	J	0.13	0/1369	0.32	0/1862
21	K	0.18	0/1633	0.44	0/2212
22	L	0.17	0/975	0.43	0/1328
23	M	0.20	0/1193	0.46	0/1611
24	N	0.13	0/1363	0.33	0/1852
25	O	0.16	0/811	0.42	0/1100
26	U	0.22	0/1297	0.61	4/1764 (0.2%)
27	a	0.13	0/6024	0.31	0/8220
28	b	0.13	0/6067	0.31	0/8282
29	c	0.13	0/636	0.34	0/860
30	d	0.14	0/1162	0.37	0/1569
31	e	0.15	0/559	0.36	0/757
32	f	0.14	0/1239	0.30	0/1671

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.14	0/779	0.35	0/1055
34	h	0.13	0/758	0.32	0/1029
35	i	0.17	0/251	0.38	0/339
36	j	0.14	0/357	0.31	0/484
37	k	0.10	0/467	0.27	0/630
38	l	0.15	0/1235	0.35	0/1685
39	w	0.20	0/1750	0.45	0/2389
40	x	0.14	0/1619	0.32	0/2206
41	y	0.17	0/1768	0.39	0/2400
42	z	0.15	0/1546	0.35	1/2104 (0.0%)
All	All	0.17	0/73977	0.39	8/100491 (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
11	A	0	1
18	H	0	1
21	K	0	2
39	w	0	1
All	All	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U	91	PRO	N-CA-CB	13.58	110.53	102.92
26	U	87	PRO	N-CA-CB	8.01	111.67	103.25
10	9	80	PRO	N-CA-CB	6.78	110.46	103.00
11	A	258	PHE	CA-CB-CG	6.34	120.14	113.80
16	F	499	MET	CA-CB-CG	6.20	126.51	114.10
42	z	153	VAL	N-CA-C	-5.26	107.26	113.42
26	U	86	SER	CA-C-N	5.13	126.25	119.84
26	U	86	SER	C-N-CA	5.13	126.25	119.84

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	A	123	ARG	Sidechain
18	H	195	ARG	Sidechain
21	K	139	CYS	Peptide
21	K	91	ARG	Sidechain
39	w	212	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1317	0	1268	16	0
2	1	3133	0	3096	43	0
3	2	2305	0	2298	37	0
4	3	1093	0	1078	18	0
5	4	756	0	700	15	0
6	5	1258	0	1147	11	0
7	6	1048	0	1020	19	0
8	7	1156	0	1172	6	0
9	8	1075	0	1051	16	0
10	9	1326	0	1307	16	0
11	A	2728	0	2807	53	0
12	B	3799	0	3881	88	0
13	C	944	0	951	21	0
14	D	3955	0	4064	68	0
15	E	780	0	824	17	0
16	F	5796	0	5847	113	0
17	G	1357	0	1415	32	0
18	H	3008	0	3025	57	0
19	I	1329	0	1310	17	0
20	J	1324	0	1283	21	0
21	K	1597	0	1619	42	0
22	L	936	0	930	10	0
23	M	1169	0	1155	24	0
24	N	1323	0	1334	16	0
25	O	786	0	789	7	0
26	U	1266	0	1182	15	0
27	a	5827	0	5685	90	0
28	b	5855	0	5629	89	0
29	c	623	0	602	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	1132	0	1145	17	0
31	e	546	0	555	8	0
32	f	1211	0	1236	14	0
33	g	759	0	736	13	0
34	h	737	0	733	18	0
35	i	244	0	262	7	0
36	j	345	0	347	6	0
37	k	462	0	474	7	0
38	l	1200	0	1208	22	0
39	w	1689	0	1617	45	0
40	x	1568	0	1516	32	0
41	y	1713	0	1679	51	0
42	z	1498	0	1471	48	0
43	4	40	0	56	4	0
43	a	255	0	348	18	0
43	b	280	0	392	22	0
43	f	40	0	56	2	0
43	g	40	0	56	2	0
43	i	40	0	56	2	0
43	j	80	0	112	10	0
43	k	80	0	112	0	0
43	l	120	0	168	5	0
43	w	40	0	56	1	0
43	x	40	0	55	1	0
43	y	40	0	56	1	0
43	z	40	0	55	1	0
44	5	35	0	40	2	0
44	A	151	0	185	3	0
44	B	157	0	200	6	0
44	D	34	0	38	1	0
44	F	43	0	59	0	0
44	I	44	0	61	0	0
44	L	40	0	50	2	0
44	N	26	0	22	2	0
44	a	111	0	132	6	0
44	b	87	0	117	2	0
44	f	39	0	48	0	0
44	w	40	0	53	1	0
44	z	124	0	164	9	0
45	5	38	0	0	0	0
45	F	38	0	0	6	0
46	7	41	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	B	37	0	44	1	0
46	D	34	0	38	1	0
46	F	28	0	26	2	0
46	H	33	0	36	1	0
46	f	34	0	38	1	0
46	j	71	0	82	3	0
46	w	40	0	50	2	0
46	x	48	0	66	4	0
46	z	76	0	92	7	0
47	A	36	0	45	15	0
48	B	40	0	44	10	0
48	F	84	0	96	18	0
48	a	36	0	36	3	0
48	j	42	0	51	0	0
48	w	72	0	72	15	0
49	I	16	0	0	1	0
49	K	8	0	0	0	0
49	a	8	0	0	0	0
49	c	16	0	0	0	0
50	a	2583	0	2598	106	0
50	b	2314	0	2287	91	0
50	f	140	0	113	3	0
50	g	144	0	115	4	0
50	h	46	0	33	2	0
50	j	42	0	31	0	0
50	k	140	0	108	5	0
50	l	145	0	116	5	0
50	w	526	0	461	29	0
50	x	608	0	518	19	0
50	y	676	0	603	40	0
50	z	532	0	432	26	0
51	a	66	0	96	2	0
51	b	59	0	79	3	0
51	x	48	0	54	2	0
52	a	61	0	62	0	0
53	a	33	0	46	1	0
53	b	33	0	46	3	0
54	w	135	0	88	13	0
54	x	179	0	115	9	0
54	z	103	0	84	7	0
55	w	84	0	112	30	0
55	x	84	0	112	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	y	84	0	112	60	0
55	z	84	0	112	34	0
All	All	83864	0	83596	1415	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1415) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:y:302:CLA:H42	55:y:315:LUT:C37	1.52	1.37
41:y:240:TYR:CE1	55:y:315:LUT:H162	1.60	1.34
42:z:174:ASP:HA	55:z:320:LUT:O23	1.30	1.30
11:A:259:TYR:CE2	47:A:405:PQ9:H161	1.65	1.29
11:A:259:TYR:CD2	47:A:405:PQ9:H161	1.74	1.21
40:x:191:ASN:OD1	55:x:320:LUT:O23	1.58	1.19
50:y:303:CLA:C1B	55:y:315:LUT:H173	1.74	1.18
42:z:175:PRO:HD2	55:z:320:LUT:C23	1.81	1.11
50:y:302:CLA:H42	55:y:315:LUT:H373	1.18	1.07
11:A:259:TYR:HD2	47:A:405:PQ9:C18	1.70	1.05
39:w:205:PHE:CZ	55:w:320:LUT:H163	1.91	1.05
42:z:175:PRO:HD2	55:z:320:LUT:O23	1.56	1.05
41:y:240:TYR:CE1	55:y:315:LUT:C16	2.41	1.04
41:y:80:LEU:HD12	55:y:316:LUT:H24	1.41	1.00
41:y:240:TYR:HE1	55:y:315:LUT:H162	0.94	1.00
39:w:205:PHE:CE1	55:w:320:LUT:C16	2.45	0.99
41:y:115:ALA:HB2	55:y:316:LUT:C16	1.94	0.97
42:z:174:ASP:HA	55:z:320:LUT:H1	1.27	0.97
42:z:174:ASP:CA	55:z:320:LUT:O23	2.14	0.95
50:y:311:CLA:C1B	55:y:316:LUT:H173	1.96	0.95
50:y:302:CLA:C4	55:y:315:LUT:C37	2.44	0.95
16:F:712:GLY:HA3	45:F:804:A1H1M:C38	1.97	0.94
41:y:77:PHE:CD2	55:y:316:LUT:H373	2.05	0.91
41:y:209:PRO:HD2	55:y:315:LUT:C23	2.01	0.91
50:y:303:CLA:C2B	55:y:315:LUT:H173	2.02	0.90
11:A:259:TYR:CD2	47:A:405:PQ9:C16	2.56	0.89
42:z:173:PHE:O	55:z:320:LUT:H24	1.72	0.89
16:F:712:GLY:CA	45:F:804:A1H1M:C38	2.52	0.88
41:y:77:PHE:CE2	55:y:316:LUT:H373	2.08	0.88
39:w:205:PHE:CE1	55:w:320:LUT:H162	2.08	0.87
11:A:259:TYR:CE2	47:A:405:PQ9:C16	2.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:259:TYR:HE2	47:A:405:PQ9:H161	1.39	0.86
42:z:175:PRO:CD	55:z:320:LUT:O23	2.22	0.86
16:F:262:ALA:O	16:F:266:ALA:HB3	1.76	0.86
54:w:311:CHL:HBB2	48:w:318:SQD:C8	2.06	0.85
42:z:175:PRO:HD2	55:z:320:LUT:H23	1.58	0.84
16:F:23:GLY:HA2	48:F:805:SQD:H112	1.61	0.83
39:w:205:PHE:CZ	55:w:320:LUT:C16	2.62	0.82
41:y:209:PRO:HD2	55:y:315:LUT:H23	1.60	0.82
50:y:303:CLA:C1B	55:y:315:LUT:C17	2.57	0.81
50:y:310:CLA:H2	55:y:316:LUT:C36	2.11	0.81
50:z:309:CLA:O1D	55:z:321:LUT:H363	1.80	0.80
43:b:820:BCR:H17C	50:b:840:CLA:H143	1.61	0.80
50:y:302:CLA:C4	55:y:315:LUT:H373	2.08	0.80
50:y:302:CLA:H42	55:y:315:LUT:H371	1.59	0.79
42:z:176:LEU:HD23	55:z:320:LUT:H222	1.66	0.78
11:A:259:TYR:CD2	47:A:405:PQ9:C18	2.62	0.76
50:z:309:CLA:O1D	55:z:321:LUT:C36	2.33	0.76
39:w:94:LEU:HD12	55:w:319:LUT:H23	1.68	0.76
27:a:537:HIS:HB3	50:a:822:CLA:HBB1	1.67	0.76
9:8:133:HIS:HD1	9:8:147:SER:HG	1.32	0.76
12:B:20:LYS:HB2	13:C:90:GLY:HA3	1.69	0.75
54:w:311:CHL:HBB2	48:w:318:SQD:H82	1.67	0.74
54:x:319:CHL:HBB2	50:z:307:CLA:HAC1	1.70	0.74
17:G:43:LEU:HD13	17:G:66:TYR:HB3	1.69	0.74
41:y:240:TYR:CD1	55:y:315:LUT:C16	2.69	0.74
41:y:240:TYR:CD1	55:y:315:LUT:H162	2.22	0.73
2:1:227:VAL:HG13	2:1:245:GLU:HB3	1.69	0.73
54:w:311:CHL:HBB2	48:w:318:SQD:H81	1.69	0.73
16:F:564:PHE:HA	16:F:567:ILE:HG22	1.71	0.73
39:w:206:MET:HB2	55:w:320:LUT:O3	1.89	0.72
50:w:306:CLA:H2	55:w:319:LUT:C36	2.20	0.72
14:D:383:MET:HG3	48:F:805:SQD:C30	2.20	0.72
36:j:10:VAL:HG13	36:j:12:PRO:HD2	1.71	0.72
50:w:306:CLA:H2	55:w:319:LUT:H363	1.72	0.72
14:D:247:MET:HE2	14:D:347:PHE:HB2	1.72	0.71
21:K:4:ILE:HG22	23:M:186:TYR:HB2	1.72	0.71
43:b:816:BCR:HC7	33:g:146:ILE:HD11	1.72	0.71
43:a:830:BCR:H16C	50:a:844:CLA:H43	1.72	0.70
29:c:55:GLU:HB2	29:c:63:LEU:HD13	1.73	0.70
41:y:209:PRO:HD2	55:y:315:LUT:C24	2.21	0.70
50:z:306:CLA:C4D	55:z:320:LUT:H382	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:H:51:MET:HG2	18:H:70:TRP:HE1	1.57	0.70
50:w:308:CLA:CBB	55:w:320:LUT:H14	2.22	0.70
21:K:172:ASN:ND2	23:M:113:CYS:SG	2.64	0.70
41:y:234:MET:HB3	55:y:316:LUT:C35	2.22	0.70
3:2:160:GLN:HG3	3:2:177:SER:HB3	1.75	0.69
42:z:173:PHE:O	55:z:320:LUT:C24	2.39	0.69
2:1:290:ARG:HH22	5:4:89:GLU:HG3	1.57	0.69
24:N:105:GLY:O	24:N:109:ASN:HB2	1.92	0.69
41:y:77:PHE:HE2	55:y:316:LUT:H26	1.56	0.69
42:z:175:PRO:CD	55:z:320:LUT:C23	2.67	0.69
3:2:160:GLN:NE2	16:F:477:SER:O	2.24	0.69
20:J:147:ILE:HG21	25:O:103:ILE:HD11	1.74	0.69
41:y:115:ALA:CA	55:y:316:LUT:H163	2.23	0.68
16:F:672:TYR:CE2	48:F:801:SQD:H121	2.28	0.68
3:2:227:SER:HB3	3:2:246:ALA:HB1	1.75	0.68
13:C:66:ALA:HB1	17:G:72:VAL:HG22	1.76	0.68
16:F:490:LYS:HD2	16:F:492:SER:H	1.58	0.68
20:J:133:MET:HE3	20:J:134:PRO:HD2	1.74	0.68
12:B:247:ALA:HB3	12:B:302:LEU:HD13	1.76	0.67
27:a:531:PHE:HA	50:a:823:CLA:HED1	1.76	0.67
39:w:206:MET:CG	55:w:320:LUT:H22	2.24	0.67
13:C:55:TRP:HE1	13:C:57:GLN:HE21	1.40	0.67
43:b:819:BCR:H323	44:z:301:PGT:H381	1.75	0.67
50:w:307:CLA:HAA1	50:w:307:CLA:HBD	1.76	0.67
25:O:137:PRO:HD2	25:O:140:MET:HE3	1.77	0.67
50:y:303:CLA:C4B	55:y:315:LUT:C17	2.72	0.67
14:D:372:PRO:HB2	48:F:805:SQD:H442	1.75	0.67
50:w:306:CLA:C2	55:w:319:LUT:H363	2.24	0.66
12:B:177:ASN:HB3	15:E:84:ILE:HG12	1.77	0.66
19:I:20:ARG:HD2	26:U:216:PRO:HB2	1.78	0.66
50:y:303:CLA:NB	55:y:315:LUT:C17	2.59	0.66
4:3:81:ALA:HB3	4:3:184:VAL:HG22	1.77	0.66
39:w:205:PHE:CE1	55:w:320:LUT:H163	2.20	0.66
50:y:303:CLA:C2B	55:y:315:LUT:C17	2.73	0.66
14:D:431:ILE:HD11	48:F:801:SQD:C23	2.26	0.66
28:b:254:ILE:HG22	28:b:255:LEU:HG	1.78	0.66
42:z:175:PRO:CD	55:z:320:LUT:H23	2.26	0.65
28:b:418:ILE:HG23	50:b:851:CLA:HBB2	1.78	0.65
50:b:828:CLA:HBD	50:b:828:CLA:HBA2	1.77	0.65
16:F:712:GLY:HA2	45:F:804:A1H1M:C38	2.24	0.65
39:w:112:SER:HB3	39:w:227:GLY:HA3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:215:VAL:HG22	50:x:303:CLA:H2	1.77	0.65
41:y:262:PRO:O	41:y:266:ASN:ND2	2.30	0.65
1:0:121:GLN:HA	1:0:208:SER:O	1.97	0.65
41:y:237:ILE:HG21	55:y:316:LUT:H12	1.77	0.65
2:1:346:ILE:HD12	2:1:351:PRO:HB3	1.80	0.64
27:a:214:GLN:HA	27:a:218:SER:HB2	1.78	0.64
50:z:302:CLA:HBA1	50:z:302:CLA:HBD	1.80	0.64
50:a:824:CLA:HED3	50:a:824:CLA:H2A	1.79	0.64
2:1:361:ARG:HG3	2:1:374:ILE:HG21	1.79	0.64
50:y:310:CLA:H2	55:y:316:LUT:H362	1.80	0.63
50:z:306:CLA:CHA	55:z:320:LUT:H382	2.28	0.63
27:a:354:LEU:HD21	50:a:846:CLA:HBB1	1.79	0.63
11:A:42:ILE:HG23	11:A:264:LEU:HD21	1.80	0.63
18:H:172:ILE:HG23	18:H:279:LEU:HD22	1.80	0.63
50:w:307:CLA:HBB2	54:w:309:CHL:HAB	1.80	0.63
41:y:77:PHE:HD2	55:y:316:LUT:H373	1.60	0.63
41:y:115:ALA:HB2	55:y:316:LUT:H162	1.81	0.63
2:1:411:SER:OG	2:1:433:CYS:SG	2.57	0.63
14:D:226:PRO:HD2	14:D:313:MET:HG3	1.80	0.63
43:a:810:BCR:H323	50:a:823:CLA:HBC3	1.80	0.63
14:D:281:MET:HE1	14:D:404:LEU:HD13	1.80	0.62
14:D:372:PRO:HB2	48:F:805:SQD:C44	2.28	0.62
40:x:106:GLY:HA2	55:x:321:LUT:H181	1.81	0.62
16:F:468:LYS:O	16:F:536:ASN:ND2	2.32	0.62
50:y:311:CLA:C2B	55:y:316:LUT:H173	2.30	0.62
18:H:69:ARG:NH2	21:K:139:CYS:SG	2.69	0.62
16:F:38:ARG:NH1	39:w:212:SER:OG	2.33	0.62
43:a:827:BCR:H362	43:a:828:BCR:H21C	1.82	0.62
28:b:615:TYR:OH	28:b:621:ARG:NH2	2.31	0.62
50:b:847:CLA:H2	50:b:848:CLA:HMB1	1.79	0.62
34:h:99:ARG:NH1	38:l:151:GLY:O	2.32	0.62
40:x:79:PRO:HD2	55:x:321:LUT:H23	1.82	0.62
18:H:93:GLN:O	18:H:289:ASN:ND2	2.33	0.62
27:a:372:PRO:HG3	27:a:378:ALA:HB2	1.82	0.62
16:F:90:ASP:OD2	16:F:279:ARG:NH1	2.33	0.61
50:b:822:CLA:HBA2	50:b:822:CLA:HBD	1.81	0.61
54:w:304:CHL:CMC	55:w:319:LUT:H163	2.31	0.61
3:2:70:LEU:HD21	3:2:163:LEU:HD11	1.81	0.61
2:1:203:MET:HB2	2:1:225:ASP:HB2	1.81	0.61
41:y:77:PHE:CE2	55:y:316:LUT:H26	2.34	0.61
42:z:71:PRO:HD2	55:z:321:LUT:H3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:83:TRP:O	38:l:87:ASN:ND2	2.30	0.61
16:F:599:ASP:HB3	16:F:602:GLU:HB2	1.82	0.61
50:b:843:CLA:H91	50:b:844:CLA:H62	1.83	0.61
50:g:201:CLA:H2A	50:g:201:CLA:HED2	1.81	0.61
43:4:101:BCR:H23C	14:D:471:PRO:HB3	1.82	0.61
50:x:307:CLA:H52	55:x:321:LUT:H27	1.83	0.61
42:z:146:GLU:O	42:z:150:ILE:HB	2.01	0.61
41:y:115:ALA:CB	55:y:316:LUT:C16	2.77	0.61
11:A:247:GLN:O	21:K:71:GLN:NE2	2.33	0.60
11:A:259:TYR:HE2	47:A:405:PQ9:C12	2.13	0.60
23:M:108:ILE:HB	23:M:124:THR:HG21	1.83	0.60
10:9:87:ASN:HD22	10:9:123:ARG:HD3	1.66	0.60
41:y:77:PHE:HE2	55:y:316:LUT:H373	1.66	0.60
42:z:176:LEU:CD2	55:z:320:LUT:H222	2.31	0.60
50:a:857:CLA:H92	43:l:302:BCR:H21C	1.82	0.60
28:b:694:ARG:NH1	38:l:153:ALA:O	2.34	0.60
50:w:306:CLA:C2	55:w:319:LUT:C36	2.80	0.60
16:F:402:THR:HG23	16:F:446:MET:HB3	1.82	0.60
39:w:136:ASN:O	39:w:145:ARG:NH2	2.32	0.60
12:B:208:GLU:HB2	12:B:214:ILE:HG22	1.82	0.60
16:F:490:LYS:HB3	16:F:493:LEU:HG	1.82	0.60
3:2:63:ARG:NH2	3:2:155:SER:O	2.34	0.60
26:U:127:CYS:O	26:U:173:ARG:NH2	2.33	0.60
10:9:138:ALA:HB2	10:9:242:ARG:HH21	1.67	0.60
30:d:135:ARG:HB2	30:d:138:GLN:HG3	1.83	0.60
50:z:306:CLA:C4D	55:z:320:LUT:C38	2.80	0.60
18:H:84:ASN:HA	18:H:87:GLU:HG2	1.84	0.60
50:a:818:CLA:H91	43:a:830:BCR:H24C	1.82	0.60
14:D:32:ILE:HG12	14:D:112:GLN:HG2	1.83	0.59
50:b:839:CLA:H71	50:b:840:CLA:H42	1.83	0.59
13:C:114:LYS:O	17:G:175:ARG:NH2	2.32	0.59
27:a:194:MET:HB2	50:a:838:CLA:HBC2	1.83	0.59
27:a:474:ILE:HG12	43:a:810:BCR:H362	1.83	0.59
27:a:13:LEU:HB3	27:a:184:LYS:HD2	1.85	0.59
2:1:156:ILE:HD11	2:1:196:LEU:HD21	1.83	0.59
50:b:801:CLA:HAC1	53:b:827:PQN:H171	1.85	0.59
27:a:570:ARG:NH1	44:a:807:PGT:O11	2.35	0.59
50:a:815:CLA:HAB	43:j:101:BCR:H352	1.85	0.59
29:c:61:ASP:OD2	31:e:114:ASN:ND2	2.33	0.59
29:c:73:THR:H	29:c:76:SER:HB3	1.66	0.59
18:H:154:MET:SD	18:H:154:MET:N	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:97:PRO:HA	38:l:100:ARG:HD3	1.84	0.59
16:F:302:VAL:HG13	16:F:438:THR:HG21	1.83	0.59
50:a:853:CLA:H51	50:a:854:CLA:H171	1.84	0.59
40:x:101:ARG:HB3	50:x:312:CLA:HBC3	1.85	0.59
41:y:115:ALA:HB2	55:y:316:LUT:H163	1.83	0.59
41:y:208:ASN:HA	55:y:315:LUT:H24	1.84	0.59
44:z:301:PGT:H172	54:z:312:CHL:HBA1	1.84	0.59
48:B:604:SQD:H61	14:D:162:TYR:HB2	1.84	0.59
19:I:42:TYR:OH	19:I:126:GLU:OE1	2.20	0.58
24:N:94:ALA:HB2	24:N:217:LEU:HD13	1.85	0.58
32:f:199:ASP:HA	46:j:105:LMG:HC61	1.85	0.58
36:j:12:PRO:HB2	43:j:103:BCR:H291	1.84	0.58
40:x:192:PRO:HD2	55:x:320:LUT:H23	1.85	0.58
11:A:251:SER:HB2	21:K:70:ARG:HB3	1.84	0.58
16:F:10:ILE:HD12	16:F:14:LEU:HD22	1.84	0.58
3:2:60:LEU:HD12	3:2:68:LEU:HD23	1.85	0.58
15:E:16:ILE:HG21	17:G:23:ALA:HB1	1.85	0.58
25:O:100:LEU:HB3	25:O:103:ILE:HD12	1.85	0.58
50:b:845:CLA:H111	34:h:113:LEU:HD23	1.85	0.58
14:D:296:PRO:HG3	14:D:432:TYR:HB3	1.85	0.58
16:F:257:PRO:HG2	16:F:260:ILE:HG12	1.84	0.58
11:A:200:GLN:NE2	11:A:276:LEU:O	2.37	0.58
13:C:57:GLN:NE2	17:G:81:MET:O	2.35	0.58
20:J:73:ARG:NH2	20:J:75:GLU:OE1	2.37	0.58
27:a:585:SER:OG	27:a:588:ASP:OD1	2.22	0.58
43:b:819:BCR:H392	43:b:820:BCR:H23C	1.85	0.58
10:9:90:TYR:HB3	10:9:251:LEU:HD22	1.86	0.58
50:b:811:CLA:HAA1	43:b:819:BCR:H16C	1.86	0.58
10:9:173:ASN:ND2	10:9:175:ASN:OD1	2.37	0.58
10:9:184:VAL:HG22	10:9:200:ILE:HG12	1.86	0.58
50:y:310:CLA:HAB	50:y:310:CLA:H51	1.86	0.58
43:4:101:BCR:H373	14:D:481:LEU:HD13	1.85	0.58
12:B:60:LEU:HD12	12:B:126:LEU:HD23	1.85	0.58
28:b:369:ALA:HB1	28:b:725:LEU:HD11	1.84	0.57
42:z:92:CYS:HB3	42:z:196:GLY:HA3	1.85	0.57
5:4:51:ASP:OD2	14:D:460:ARG:NH1	2.36	0.57
12:B:114:LEU:HD11	12:B:367:ALA:HA	1.85	0.57
21:K:81:VAL:HG11	21:K:89:LEU:HD22	1.85	0.57
27:a:531:PHE:HE2	43:a:810:BCR:H313	1.69	0.57
50:x:312:CLA:HMC1	55:x:320:LUT:C31	2.34	0.57
15:E:13:LEU:HG	17:G:19:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:10:THR:HG21	31:e:74:ARG:HH22	1.68	0.57
12:B:176:SER:O	12:B:180:THR:OG1	2.22	0.57
30:d:115:GLU:O	30:d:145:ARG:NH1	2.38	0.57
30:d:172:ASP:N	30:d:172:ASP:OD1	2.37	0.57
1:0:119:GLN:NE2	17:G:142:GLN:OE1	2.38	0.57
11:A:83:LYS:NZ	21:K:73:ASP:OD1	2.36	0.57
14:D:323:ILE:HD12	14:D:409:LYS:HD2	1.87	0.57
42:z:77:VAL:HB	42:z:80:ASN:HB2	1.86	0.57
4:3:203:PRO:HA	16:F:490:LYS:HZ1	1.70	0.57
17:G:63:LEU:O	17:G:67:VAL:HB	2.04	0.57
39:w:108:GLU:O	39:w:112:SER:OG	2.22	0.57
50:y:303:CLA:C3B	55:y:315:LUT:C17	2.82	0.57
9:8:90:ARG:NH2	9:8:204:PHE:O	2.34	0.57
39:w:113:ARG:NH1	54:w:311:CHL:OBD	2.37	0.57
3:2:209:PHE:HE1	3:2:341:ILE:HG12	1.68	0.57
21:K:179:HIS:NE2	23:M:120:MET:O	2.30	0.57
28:b:174:ARG:HB2	50:b:833:CLA:HBC2	1.86	0.57
14:D:134:LEU:HD22	14:D:182:VAL:HG22	1.87	0.57
16:F:319:LEU:O	16:F:323:THR:OG1	2.22	0.57
12:B:148:ASP:HB3	12:B:151:THR:HG22	1.86	0.56
28:b:268:LEU:HB2	28:b:273:MET:HE3	1.87	0.56
42:z:126:GLN:NE2	42:z:134:VAL:O	2.37	0.56
42:z:156:GLN:HA	42:z:159:MET:HG3	1.87	0.56
12:B:149:LEU:HB2	12:B:209:ILE:HB	1.85	0.56
18:H:88:GLN:OE1	20:J:24:GLN:NE2	2.38	0.56
16:F:546:ASN:HB3	39:w:201:LEU:HA	1.85	0.56
50:a:824:CLA:H92	43:b:831:BCR:H15C	1.86	0.56
4:3:203:PRO:HA	16:F:490:LYS:NZ	2.20	0.56
30:d:191:ARG:NH2	30:d:212:LEU:OXT	2.39	0.56
24:N:131:THR:HA	24:N:135:LYS:HB2	1.87	0.56
12:B:390:LYS:HD2	12:B:469:TYR:HB3	1.86	0.56
14:D:210:GLU:HG3	14:D:269:LEU:HD23	1.88	0.56
50:w:310:CLA:H192	50:w:314:CLA:HAC2	1.87	0.56
2:1:202:ASP:OD1	12:B:382:ARG:NH1	2.38	0.56
18:H:271:SER:O	18:H:275:ILE:HD12	2.04	0.56
27:a:144:ILE:HD13	50:a:845:CLA:H11	1.87	0.56
39:w:217:MET:O	39:w:221:THR:HG23	2.06	0.56
46:x:315:LMG:H371	50:x:316:CLA:H3A	1.87	0.56
41:y:170:ARG:HB3	50:y:312:CLA:HMC2	1.86	0.56
2:1:196:LEU:HB3	2:1:221:THR:HG23	1.88	0.56
48:B:604:SQD:H121	16:F:699:PRO:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:66:GLU:O	14:D:79:ARG:HA	2.06	0.56
28:b:326:ILE:HG23	50:b:839:CLA:HBC3	1.87	0.56
1:0:134:ASP:OD2	1:0:174:ASN:ND2	2.38	0.56
7:6:161:VAL:HG12	11:A:17:SER:HB2	1.87	0.56
16:F:173:ASN:HB3	48:F:801:SQD:O8	2.06	0.56
27:a:670:PHE:HZ	50:a:820:CLA:H101	1.71	0.56
50:b:801:CLA:H143	50:b:825:CLA:H12	1.86	0.56
32:f:201:PRO:HD3	46:j:105:LMG:HC71	1.88	0.56
5:4:37:MET:HE1	6:5:150:LEU:HB3	1.88	0.56
9:8:121:GLY:HA3	9:8:182:VAL:HB	1.88	0.56
11:A:259:TYR:HE2	47:A:405:PQ9:C13	2.19	0.56
19:I:70:CYS:HB3	49:I:202:SF4:S1	2.46	0.56
28:b:422:LEU:HG	50:b:851:CLA:HAB	1.87	0.56
48:w:318:SQD:H81	48:w:318:SQD:H461	1.87	0.55
41:y:230:GLY:O	41:y:234:MET:HG3	2.07	0.55
3:2:296:ARG:NH2	4:3:114:ASP:OD2	2.40	0.55
27:a:194:MET:HE2	50:a:838:CLA:HHD	1.87	0.55
27:a:445:LEU:HB3	27:a:539:PHE:HB2	1.87	0.55
43:b:816:BCR:H342	33:g:146:ILE:HG13	1.89	0.55
39:w:110:MET:HA	39:w:110:MET:HE3	1.88	0.55
43:y:301:BCR:H391	50:y:311:CLA:H12	1.88	0.55
3:2:317:ARG:NH1	3:2:320:TYR:O	2.36	0.55
8:7:115:ILE:HA	16:F:215:LEU:HD21	1.87	0.55
12:B:372:PHE:O	12:B:376:THR:HB	2.07	0.55
16:F:370:ILE:HG13	16:F:371:VAL:HG13	1.88	0.55
41:y:221:GLU:HG3	41:y:225:LYS:HE3	1.88	0.55
50:z:309:CLA:CGD	55:z:321:LUT:H363	2.37	0.55
33:g:74:SER:HB3	50:g:203:CLA:HED2	1.87	0.55
39:w:250:GLU:O	39:w:254:ARG:HG3	2.06	0.55
3:2:301:LYS:HG2	3:2:316:ILE:HG12	1.87	0.55
9:8:103:GLU:OE2	9:8:103:GLU:N	2.39	0.55
14:D:423:ALA:HB1	16:F:187:PHE:HD1	1.71	0.55
16:F:388:THR:HG23	16:F:395:LYS:HE2	1.89	0.55
2:1:66:GLU:O	15:E:95:GLN:NE2	2.40	0.55
4:3:184:VAL:HG21	16:F:491:ILE:HD11	1.87	0.55
5:4:67:THR:HG23	14:D:155:TRP:HA	1.89	0.55
12:B:143:LEU:HD13	12:B:156:PRO:HD3	1.88	0.55
33:g:95:PHE:O	33:g:99:ASN:ND2	2.39	0.55
16:F:571:GLN:NE2	16:F:573:GLY:O	2.40	0.55
27:a:118:ILE:HB	43:j:103:BCR:H322	1.89	0.55
27:a:588:ASP:OD2	27:a:723:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:362:ILE:HG23	27:a:392:MET:HE1	1.89	0.55
28:b:429:LEU:HD11	50:b:815:CLA:HMB2	1.88	0.55
42:z:181:ASP:OD1	42:z:181:ASP:N	2.36	0.55
7:6:121:ARG:NH2	17:G:53:ALA:O	2.40	0.54
12:B:172:LYS:O	15:E:87:ASN:ND2	2.40	0.54
12:B:415:PHE:HB3	12:B:496:ILE:HD12	1.89	0.54
27:a:127:ASP:OD1	27:a:133:ARG:NH1	2.39	0.54
39:w:122:ILE:HG21	39:w:237:LEU:HD13	1.89	0.54
18:H:71:ASP:HA	18:H:387:ILE:HD11	1.89	0.54
28:b:159:PRO:HA	28:b:162:LYS:HE2	1.89	0.54
29:c:61:ASP:OD2	31:e:74:ARG:NH2	2.40	0.54
50:y:308:CLA:HAB	55:y:316:LUT:H403	1.90	0.54
42:z:65:GLY:HA3	42:z:193:ILE:HG21	1.88	0.54
10:9:141:ARG:NH1	10:9:149:GLN:OE1	2.40	0.54
16:F:322:TYR:CZ	16:F:353:LYS:HE2	2.42	0.54
27:a:244:ARG:NH1	41:y:272:LYS:O	2.39	0.54
50:a:848:CLA:H42	38:l:85:LEU:HD21	1.89	0.54
28:b:91:ILE:HB	28:b:112:PRO:HB2	1.89	0.54
50:y:312:CLA:HBA1	50:y:312:CLA:HBD	1.89	0.54
50:y:302:CLA:H42	55:y:315:LUT:H372	1.76	0.54
46:z:314:LMG:H132	46:z:314:LMG:H292	1.90	0.54
50:b:805:CLA:H151	50:b:836:CLA:HBB2	1.88	0.54
53:b:827:PQN:H172	43:b:850:BCR:H382	1.90	0.54
50:b:843:CLA:H142	50:b:843:CLA:HMB2	1.88	0.54
39:w:202:TRP:HB3	48:w:318:SQD:C32	2.36	0.54
41:y:140:VAL:HG21	55:y:316:LUT:H42	1.90	0.54
41:y:207:PHE:O	55:y:315:LUT:H24	2.08	0.54
11:A:44:ILE:O	11:A:48:VAL:HG23	2.07	0.54
15:E:100:ASN:ND2	45:F:804:A1H1M:O28	2.40	0.54
16:F:708:PHE:CE2	45:F:804:A1H1M:C02	2.90	0.54
10:9:101:LYS:NZ	14:D:203:GLN:OE1	2.36	0.54
12:B:357:PHE:O	12:B:361:MET:HG3	2.07	0.54
24:N:192:MET:O	24:N:195:SER:OG	2.25	0.54
44:z:301:PGT:H142	54:z:312:CHL:H3A	1.89	0.54
1:0:123:VAL:HG11	1:0:224:VAL:HG11	1.88	0.54
7:6:79:THR:HA	9:8:203:CYS:HB3	1.89	0.54
14:D:356:ILE:HG13	14:D:367:ILE:HD13	1.88	0.54
19:I:126:GLU:HG3	24:N:124:ARG:HH12	1.73	0.54
21:K:93:TYR:OH	23:M:191:ARG:NH1	2.41	0.54
28:b:338:LEU:HD21	50:b:842:CLA:HBB1	1.90	0.54
28:b:694:ARG:NH2	35:i:30:ASN:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:z:228:ASP:OD1	42:z:228:ASP:N	2.40	0.54
1:0:181:ASN:OD1	1:0:183:THR:OG1	2.26	0.54
43:a:828:BCR:H20C	50:a:839:CLA:H202	1.90	0.54
28:b:422:LEU:HD13	28:b:532:LEU:HA	1.90	0.54
28:b:670:TYR:OH	50:b:803:CLA:OBD	2.26	0.54
41:y:115:ALA:CB	55:y:316:LUT:H163	2.38	0.54
41:y:208:ASN:OD1	55:y:315:LUT:O23	2.26	0.54
14:D:281:MET:HE3	14:D:418:ILE:HD13	1.90	0.54
16:F:25:GLY:O	16:F:29:PHE:N	2.36	0.54
16:F:306:ALA:HB2	16:F:438:THR:HG23	1.89	0.54
9:8:162:LYS:NZ	12:B:213:GLU:OE2	2.35	0.53
28:b:410:ARG:O	28:b:414:HIS:ND1	2.35	0.53
39:w:85:GLY:H	39:w:221:THR:HG22	1.73	0.53
41:y:240:TYR:CD1	55:y:315:LUT:H163	2.43	0.53
12:B:361:MET:HE3	12:B:405:LEU:HA	1.90	0.53
32:f:93:LYS:O	32:f:97:GLN:HG3	2.08	0.53
34:h:106:LEU:HD22	38:l:141:VAL:HG13	1.90	0.53
7:6:173:THR:O	7:6:173:THR:OG1	2.23	0.53
12:B:80:ARG:NH1	44:B:603:PGT:O6	2.41	0.53
12:B:409:PRO:HG3	14:D:142:GLU:HB3	1.88	0.53
50:b:814:CLA:HAB	43:b:831:BCR:HC8	1.91	0.53
42:z:70:ASP:OD1	55:z:321:LUT:O3	2.27	0.53
27:a:205:LEU:HD22	43:a:827:BCR:H361	1.89	0.53
28:b:351:HIS:ND1	50:b:809:CLA:OBD	2.38	0.53
8:7:153:LYS:O	8:7:157:MET:HG3	2.09	0.53
12:B:207:GLY:O	15:E:58:LYS:NZ	2.33	0.53
12:B:441:VAL:HG12	48:B:604:SQD:H282	1.90	0.53
21:K:105:MET:HB2	21:K:136:LEU:HD23	1.89	0.53
24:N:96:TYR:O	24:N:212:VAL:HA	2.08	0.53
28:b:649:MET:HG2	28:b:723:ALA:HB2	1.89	0.53
50:b:804:CLA:HMA2	44:b:829:PGT:H332	1.91	0.53
50:b:840:CLA:ND	50:b:847:CLA:HMB1	2.23	0.53
30:d:135:ARG:NH2	30:d:137:GLU:OE1	2.41	0.53
54:w:311:CHL:CBB	48:w:318:SQD:H82	2.38	0.53
3:2:154:ASP:OD2	16:F:475:SER:OG	2.23	0.53
7:6:85:GLU:HA	7:6:89:GLU:HG3	1.91	0.53
23:M:127:ILE:HD11	23:M:140:LEU:HD22	1.90	0.53
24:N:87:VAL:HG11	24:N:111:LEU:HD21	1.90	0.53
50:a:858:CLA:H143	50:b:844:CLA:HAB	1.91	0.53
2:1:231:TYR:HB2	2:1:236:ALA:HB2	1.91	0.53
12:B:478:ASN:OD1	12:B:478:ASN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:445:TYR:HE1	48:B:604:SQD:O3	1.91	0.53
15:E:13:LEU:HB3	15:E:40:ALA:HB2	1.91	0.53
28:b:37:ILE:HG13	28:b:41:ARG:HD2	1.91	0.53
28:b:52:GLY:O	28:b:56:ILE:HD12	2.08	0.53
18:H:264:ARG:HH21	18:H:385:ASP:HB2	1.74	0.53
27:a:16:ARG:NH1	48:a:859:SQD:O7	2.42	0.53
28:b:373:THR:HG22	50:b:835:CLA:HAB	1.91	0.53
54:z:312:CHL:HBB1	54:z:312:CHL:HHC	1.91	0.53
39:w:119:VAL:HG11	55:w:320:LUT:H30	1.91	0.53
3:2:277:ASN:O	3:2:327:SER:OG	2.26	0.52
5:4:75:GLN:O	5:4:79:GLU:HG3	2.09	0.52
19:I:43:PRO:HG2	24:N:99:HIS:HB3	1.91	0.52
21:K:183:VAL:HG22	23:M:159:LEU:HD22	1.90	0.52
27:a:405:HIS:HE1	50:a:846:CLA:NA	2.07	0.52
27:a:706:LEU:O	32:f:179:ARG:NH1	2.42	0.52
39:w:181:ILE:HG23	48:w:318:SQD:C23	2.39	0.52
55:z:321:LUT:H181	55:z:321:LUT:C8	2.39	0.52
14:D:389:PRO:HB2	16:F:149:ILE:HG23	1.91	0.52
14:D:433:LEU:O	14:D:436:MET:HB3	2.09	0.52
27:a:394:ILE:HG21	50:a:845:CLA:HHC	1.91	0.52
50:a:811:CLA:H2A	50:a:811:CLA:HED3	1.91	0.52
42:z:143:LEU:HD23	46:z:315:LMG:H311	1.90	0.52
12:B:76:LEU:HD22	44:B:603:PGT:H132	1.91	0.52
16:F:496:LEU:HD12	16:F:498:THR:H	1.74	0.52
16:F:712:GLY:HA2	45:F:804:A1H1M:C37	2.39	0.52
18:H:58:ARG:HH22	21:K:117:THR:HB	1.73	0.52
18:H:223:MET:HE1	18:H:384:ILE:HG12	1.92	0.52
50:a:858:CLA:H91	50:b:803:CLA:H112	1.92	0.52
27:a:464:ARG:NH2	50:a:849:CLA:O1D	2.43	0.52
28:b:182:LEU:HD13	50:b:833:CLA:HHB	1.92	0.52
11:A:124:LEU:HD11	11:A:305:THR:HB	1.92	0.52
12:B:248:PRO:HB3	46:F:802:LMG:H121	1.90	0.52
16:F:113:ASN:HB2	16:F:547:THR:HB	1.91	0.52
50:x:303:CLA:HBA2	50:x:303:CLA:HBD	1.90	0.52
12:B:303:ALA:O	12:B:307:MET:HG3	2.09	0.52
18:H:67:VAL:HG21	18:H:82:THR:HG21	1.91	0.52
28:b:309:ILE:HD11	28:b:320:LYS:HG3	1.92	0.52
28:b:381:PHE:HB3	50:b:805:CLA:H112	1.91	0.52
50:b:822:CLA:H43	36:j:29:ILE:HG21	1.91	0.52
42:z:71:PRO:HA	46:z:314:LMG:HC3	1.91	0.52
42:z:115:LYS:HD2	42:z:118:GLU:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:a:833:CLA:HBC2	50:a:845:CLA:H91	1.91	0.52
28:b:4:ARG:NH1	35:i:29:LYS:O	2.43	0.52
2:1:453:ASP:O	2:1:456:LYS:NZ	2.37	0.52
3:2:275:LEU:HD13	3:2:341:ILE:HG21	1.91	0.52
50:b:801:CLA:H13	50:b:825:CLA:H142	1.92	0.52
44:z:301:PGT:H121	54:z:312:CHL:HAA2	1.92	0.52
16:F:107:VAL:HG21	16:F:263:LEU:HB2	1.91	0.52
18:H:254:GLU:HG2	18:H:259:ALA:HB2	1.92	0.52
19:I:153:TYR:HE1	22:L:166:VAL:HG21	1.74	0.52
42:z:72:LEU:HD12	55:z:321:LUT:H22	1.91	0.52
43:a:803:BCR:H353	50:a:835:CLA:H11	1.92	0.52
50:a:820:CLA:H111	50:a:856:CLA:H18	1.91	0.52
50:z:306:CLA:CBB	55:z:320:LUT:H34	2.40	0.52
16:F:349:HIS:O	16:F:353:LYS:HB2	2.10	0.51
50:b:833:CLA:HAB	50:b:834:CLA:HAC2	1.91	0.51
50:w:308:CLA:HBB2	55:w:320:LUT:H14	1.92	0.51
14:D:383:MET:HE3	16:F:156:MET:HG2	1.92	0.51
14:D:383:MET:CG	48:F:805:SQD:C30	2.88	0.51
28:b:429:LEU:HG	50:b:815:CLA:HBB1	1.93	0.51
50:b:833:CLA:HAA2	50:b:837:CLA:H112	1.92	0.51
11:A:348:PRO:HG3	13:C:108:LEU:HD21	1.92	0.51
12:B:375:ARG:NH1	12:B:471:ARG:O	2.44	0.51
22:L:145:ARG:NH2	44:N:301:PGT:O5	2.43	0.51
28:b:429:LEU:HB3	28:b:525:LEU:HB2	1.92	0.51
21:K:33:SER:OG	21:K:35:TRP:NE1	2.44	0.51
27:a:196:ASN:ND2	50:a:812:CLA:O1D	2.44	0.51
42:z:240:PRO:HD2	50:z:310:CLA:HMA3	1.91	0.51
14:D:65:VAL:HA	14:D:80:LEU:O	2.10	0.51
17:G:62:GLN:O	17:G:66:TYR:HB2	2.10	0.51
50:b:845:CLA:HBB2	35:i:12:GLY:HA3	1.92	0.51
50:y:303:CLA:NB	55:y:315:LUT:H172	2.25	0.51
8:7:92:GLU:OE2	8:7:92:GLU:N	2.43	0.51
40:x:106:GLY:HA2	55:x:321:LUT:C18	2.40	0.51
5:4:12:ARG:O	16:F:206:ARG:NH2	2.40	0.51
12:B:116:VAL:HA	12:B:126:LEU:HD11	1.91	0.51
18:H:344:ASP:HB2	18:H:350:TRP:HB2	1.93	0.51
50:a:815:CLA:HBB	50:a:835:CLA:HBB	1.92	0.51
14:D:196:ASN:HB3	14:D:199:THR:HG22	1.92	0.51
24:N:173:VAL:HG22	24:N:201:ARG:HB2	1.92	0.51
14:D:420:PHE:O	14:D:423:ALA:HB3	2.10	0.51
50:b:807:CLA:H112	50:b:836:CLA:H202	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:262:THR:HA	12:B:265:VAL:HG12	1.93	0.51
27:a:80:ILE:HD12	50:a:813:CLA:HAB	1.91	0.51
50:a:850:CLA:H11	50:k:204:CLA:H111	1.93	0.51
28:b:662:MET:O	28:b:666:SER:OG	2.25	0.51
28:b:721:TYR:HB2	50:b:802:CLA:HED3	1.92	0.51
34:h:76:ASP:OD1	38:l:173:LYS:NZ	2.41	0.51
27:a:13:LEU:HD12	27:a:186:ALA:HB3	1.93	0.50
50:a:838:CLA:H111	50:a:839:CLA:H191	1.93	0.50
41:y:122:GLY:O	41:y:129:GLN:NE2	2.43	0.50
42:z:191:LYS:HD3	50:z:319:CLA:HAA2	1.93	0.50
12:B:387:LEU:HD21	12:B:394:LEU:HD23	1.94	0.50
12:B:443:SER:O	12:B:443:SER:OG	2.23	0.50
22:L:117:ASN:OD1	22:L:117:ASN:N	2.44	0.50
43:a:828:BCR:H342	50:a:845:CLA:H2	1.92	0.50
39:w:227:GLY:O	39:w:231:MET:HG3	2.12	0.50
50:w:308:CLA:H41	55:w:320:LUT:H10	1.92	0.50
14:D:226:PRO:HD3	14:D:254:LEU:HD22	1.93	0.50
16:F:112:ASP:OD1	16:F:121:TYR:OH	2.21	0.50
28:b:98:GLN:OE1	34:h:130:ARG:NH1	2.44	0.50
33:g:157:THR:HG21	46:z:315:LMG:HC8	1.93	0.50
8:7:183:LEU:HD22	8:7:216:VAL:HG21	1.93	0.50
16:F:355:LEU:HB2	16:F:555:LEU:HB3	1.93	0.50
20:J:117:MET:HB3	20:J:142:LEU:HB2	1.92	0.50
27:a:733:GLY:O	27:a:737:THR:OG1	2.27	0.50
29:c:24:ASP:OD2	30:d:169:HIS:ND1	2.44	0.50
30:d:81:PRO:HB2	30:d:125:ARG:HD2	1.93	0.50
35:i:16:PRO:O	35:i:20:MET:HG3	2.11	0.50
12:B:56:ASP:N	12:B:56:ASP:OD1	2.40	0.50
12:B:165:LEU:HD21	15:E:76:ILE:HG12	1.94	0.50
12:B:445:TYR:HE1	48:B:604:SQD:HO3	1.53	0.50
16:F:672:TYR:CD2	48:F:801:SQD:H121	2.47	0.50
17:G:30:THR:OG1	17:G:91:GLN:N	2.44	0.50
18:H:47:LEU:HD13	21:K:41:THR:HG22	1.94	0.50
27:a:360:LEU:HD11	50:a:833:CLA:H61	1.94	0.50
50:y:311:CLA:HBD	50:y:311:CLA:HBA1	1.93	0.50
42:z:157:ARG:NH2	54:z:312:CHL:O1D	2.45	0.50
5:4:73:GLU:OE2	14:D:160:ARG:NH2	2.45	0.50
12:B:135:THR:HG21	17:G:165:VAL:HG21	1.94	0.50
28:b:129:LEU:HD23	28:b:134:ASP:HB3	1.94	0.50
28:b:339:ALA:HB2	43:b:820:BCR:H372	1.92	0.50
28:b:390:GLY:HA3	43:b:820:BCR:H382	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:169:SER:O	3:2:169:SER:OG	2.26	0.50
6:5:102:SER:HB3	6:5:104:GLU:HG2	1.94	0.50
11:A:131:ILE:HD11	11:A:134:PHE:HD2	1.76	0.50
27:a:545:VAL:HG21	50:a:852:CLA:HMA1	1.94	0.50
50:a:835:CLA:HAB	43:j:101:BCR:C5	2.41	0.50
28:b:350:GLN:OE1	28:b:372:TYR:OH	2.29	0.50
40:x:209:GLY:O	40:x:213:MET:HG3	2.11	0.50
12:B:80:ARG:HD3	44:B:603:PGT:H11	1.94	0.50
20:J:9:LEU:HD22	20:J:14:LEU:HD22	1.94	0.50
21:K:122:THR:O	21:K:124:ARG:NH1	2.35	0.50
27:a:274:THR:OG1	27:a:289:THR:OG1	2.25	0.50
27:a:353:ASN:ND2	50:a:801:CLA:OBD	2.33	0.50
39:w:89:PHE:CE2	55:w:319:LUT:H26	2.46	0.50
13:C:71:VAL:HG13	17:G:163:LEU:HB3	1.94	0.50
14:D:306:ALA:O	14:D:309:SER:OG	2.24	0.50
34:h:103:LEU:HB2	38:l:148:THR:HG21	1.94	0.50
11:A:235:LEU:HD12	11:A:338:LEU:HD22	1.93	0.49
11:A:244:ALA:HB3	11:A:248:THR:HA	1.93	0.49
14:D:117:LEU:HD22	14:D:147:PRO:HA	1.94	0.49
16:F:176:GLN:HE22	48:F:801:SQD:H4	1.76	0.49
31:e:104:ASN:OD1	31:e:104:ASN:N	2.42	0.49
40:x:178:LEU:HD21	40:x:189:ILE:HG22	1.94	0.49
40:x:225:VAL:HG23	40:x:226:THR:HG23	1.94	0.49
12:B:194:LEU:HD12	12:B:236:ILE:HA	1.94	0.49
20:J:107:ALA:HB1	20:J:111:GLU:HG3	1.93	0.49
21:K:187:ILE:H	21:K:187:ILE:HD12	1.76	0.49
40:x:101:ARG:NH1	54:x:305:CHL:OBD	2.45	0.49
14:D:234:LEU:HD22	14:D:310:VAL:HG23	1.94	0.49
23:M:142:LYS:NZ	23:M:183:GLU:OE1	2.44	0.49
32:f:206:LEU:HA	32:f:209:ARG:HG3	1.93	0.49
39:w:55:ILE:HG23	39:w:211:GLY:HA3	1.94	0.49
9:8:137:ARG:HA	9:8:143:VAL:HA	1.95	0.49
13:C:56:LEU:HD13	18:H:11:MET:HE2	1.94	0.49
16:F:58:LEU:HD13	16:F:89:MET:HE2	1.93	0.49
50:a:843:CLA:H72	50:a:844:CLA:H42	1.94	0.49
34:h:50:LYS:HG3	34:h:52:GLY:H	1.76	0.49
3:2:105:ILE:HG12	3:2:205:SER:HB3	1.94	0.49
4:3:161:LYS:HD3	6:5:86:GLU:HG3	1.95	0.49
9:8:166:GLY:HA3	9:8:190:ILE:HG12	1.93	0.49
28:b:83:HIS:H	34:h:144:ILE:HB	1.78	0.49
18:H:212:GLU:HB2	26:U:193:PHE:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:410:MET:HE1	27:a:428:LEU:HD11	1.93	0.49
50:b:801:CLA:H203	35:i:20:MET:HE3	1.95	0.49
2:1:102:PRO:HG2	2:1:105:TYR:HB2	1.94	0.49
17:G:139:ASN:HB3	17:G:142:GLN:HB2	1.95	0.49
19:I:124:GLU:OE2	24:N:124:ARG:NE	2.44	0.49
24:N:183:SER:OG	24:N:186:GLU:OE1	2.28	0.49
27:a:371:MET:SD	50:a:841:CLA:HBD	2.52	0.49
42:z:65:GLY:O	42:z:197:ARG:NH2	2.45	0.49
12:B:234:ILE:HD11	16:F:739:PHE:HB2	1.95	0.49
23:M:93:TRP:O	23:M:94:LEU:C	2.56	0.49
43:a:828:BCR:H372	50:a:839:CLA:H171	1.95	0.49
28:b:2:ALA:HB3	28:b:7:ARG:HA	1.93	0.49
39:w:231:MET:HB3	55:w:319:LUT:C35	2.43	0.49
18:H:58:ARG:NH1	21:K:118:ASP:OD2	2.46	0.49
25:O:145:ASP:OD1	25:O:145:ASP:N	2.36	0.49
50:a:811:CLA:HBB2	50:a:838:CLA:HMA3	1.94	0.49
42:z:160:GLU:HB2	50:z:305:CLA:HBC1	1.95	0.49
16:F:161:LEU:HB3	16:F:260:ILE:HG21	1.95	0.49
28:b:129:LEU:HD22	28:b:135:LEU:HD23	1.94	0.49
30:d:77:ASP:O	30:d:80:THR:OG1	2.29	0.49
41:y:115:ALA:HA	55:y:316:LUT:H163	1.93	0.49
17:G:146:ILE:O	17:G:150:THR:OG1	2.31	0.48
27:a:665:SER:HB2	28:b:445:ALA:HB1	1.95	0.48
50:a:857:CLA:H161	38:l:143:LEU:HD11	1.95	0.48
6:5:104:GLU:HG2	6:5:104:GLU:H	1.38	0.48
11:A:48:VAL:HG11	22:L:129:PHE:HA	1.95	0.48
14:D:376:THR:HA	48:F:805:SQD:H242	1.95	0.48
16:F:442:THR:HA	16:F:445:TYR:CZ	2.48	0.48
43:a:831:BCR:H23C	50:a:854:CLA:H111	1.95	0.48
50:b:811:CLA:HBC3	43:b:819:BCR:H372	1.94	0.48
44:D:602:PGT:H181	16:F:28:PHE:HE2	1.77	0.48
16:F:23:GLY:CA	48:F:805:SQD:H112	2.39	0.48
16:F:106:LEU:HB3	16:F:551:PRO:HB3	1.95	0.48
26:U:97:ILE:HD12	26:U:166:ILE:HD12	1.95	0.48
4:3:207:GLU:O	16:F:531:TYR:N	2.47	0.48
6:5:208:ASP:OD1	6:5:208:ASP:N	2.45	0.48
14:D:388:LEU:HD11	16:F:156:MET:HB2	1.94	0.48
16:F:322:TYR:CE2	16:F:405:LEU:HD23	2.48	0.48
18:H:152:ARG:O	18:H:155:HIS:NE2	2.46	0.48
53:a:825:PQN:H171	43:b:831:BCR:H382	1.95	0.48
50:x:308:CLA:C3B	55:x:321:LUT:H183	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:x:320:LUT:C8	55:x:320:LUT:H181	2.42	0.48
18:H:15:MET:HE1	18:H:378:MET:HE1	1.94	0.48
27:a:52:ASP:OD2	44:a:807:PGT:O6	2.31	0.48
50:b:807:CLA:HAB	50:b:836:CLA:H13	1.96	0.48
40:x:152:TYR:CE1	54:x:319:CHL:HBD	2.49	0.48
50:y:303:CLA:C4B	55:y:315:LUT:H172	2.43	0.48
4:3:143:GLU:HB2	4:3:184:VAL:HB	1.96	0.48
12:B:186:MET:HE3	12:B:242:PHE:HE1	1.79	0.48
20:J:14:LEU:HD23	20:J:39:ILE:HG12	1.96	0.48
26:U:97:ILE:HG23	26:U:175:LEU:HD23	1.96	0.48
50:a:835:CLA:HBA1	50:a:835:CLA:HBD	1.94	0.48
38:l:115:PRO:HG3	50:l:301:CLA:HBB1	1.96	0.48
55:y:316:LUT:H181	55:y:316:LUT:C8	2.42	0.48
5:4:12:ARG:HB2	16:F:585:PRO:HG3	1.96	0.48
21:K:164:ASP:HA	21:K:167:LYS:HG3	1.96	0.48
50:a:833:CLA:H3A	50:a:833:CLA:HBA2	1.54	0.48
50:a:857:CLA:H152	43:l:304:BCR:H15C	1.94	0.48
28:b:397:ASP:HA	30:d:200:ILE:HD13	1.95	0.48
43:b:831:BCR:H321	32:f:167:PHE:HB2	1.95	0.48
42:z:175:PRO:HG2	42:z:176:LEU:HD22	1.94	0.48
3:2:181:GLU:OE2	16:F:469:LYS:NZ	2.46	0.48
20:J:55:CYS:SG	20:J:56:ALA:N	2.86	0.48
21:K:30:ARG:NH1	21:K:101:TYR:OH	2.46	0.48
23:M:93:TRP:O	23:M:95:SER:N	2.46	0.48
26:U:158:ASP:HA	26:U:161:LYS:HB2	1.96	0.48
28:b:456:GLU:HG3	32:f:82:LEU:HD11	1.96	0.48
50:f:303:CLA:H3A	43:f:304:BCR:H382	1.95	0.48
54:w:311:CHL:CBB	48:w:318:SQD:C8	2.86	0.48
1:0:83:TYR:HB3	1:0:96:VAL:HG13	1.95	0.48
1:0:212:ARG:HH21	1:0:213:ARG:HH21	1.62	0.48
16:F:489:GLN:N	16:F:489:GLN:OE1	2.47	0.48
28:b:410:ARG:HA	28:b:413:ASP:HB2	1.96	0.48
50:b:845:CLA:H161	50:b:845:CLA:H122	1.74	0.48
37:k:114:HIS:CD2	50:k:205:CLA:NC	2.81	0.48
38:l:106:LEU:HD22	43:l:303:BCR:H10C	1.95	0.48
38:l:204:PHE:HA	38:l:208:VAL:HB	1.96	0.48
3:2:210:LYS:HB3	3:2:308:GLY:HA3	1.95	0.48
4:3:118:TYR:HD1	4:3:136:SER:HB2	1.79	0.48
27:a:84:TRP:O	27:a:88:MET:HG2	2.14	0.48
50:x:312:CLA:H41	55:x:320:LUT:H28	1.96	0.48
42:z:63:ALA:HB3	42:z:66:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:121:ARG:NH1	17:G:1:MET:O	2.47	0.47
10:9:160:GLY:O	10:9:197:GLN:NE2	2.48	0.47
11:A:90:LEU:HD11	13:C:40:LYS:HG2	1.96	0.47
16:F:381:MET:HA	16:F:384:MET:HB2	1.96	0.47
27:a:356:MET:HG3	50:a:842:CLA:HHB	1.94	0.47
27:a:379:THR:HG21	27:a:515:VAL:HB	1.96	0.47
27:a:559:ARG:NH2	30:d:89:THR:O	2.47	0.47
28:b:373:THR:HG23	28:b:591:THR:HG21	1.96	0.47
33:g:96:GLN:O	33:g:100:MET:HG3	2.14	0.47
40:x:104:MET:HG2	55:x:320:LUT:C35	2.44	0.47
41:y:225:LYS:HG2	50:y:314:CLA:HED3	1.96	0.47
12:B:182:LYS:HA	16:F:721:ILE:HD13	1.96	0.47
14:D:430:PRO:HG2	16:F:183:ARG:HG2	1.94	0.47
16:F:99:LEU:HD11	16:F:350:ALA:HB3	1.96	0.47
23:M:93:TRP:C	23:M:95:SER:N	2.72	0.47
27:a:118:ILE:HG13	27:a:119:VAL:HG13	1.95	0.47
50:a:858:CLA:H192	50:a:858:CLA:H162	1.79	0.47
31:e:63:GLY:HA2	31:e:118:LEU:HD11	1.96	0.47
33:g:97:ARG:NH2	33:g:134:GLY:O	2.47	0.47
40:x:106:GLY:O	40:x:110:MET:HG3	2.14	0.47
11:A:225:LEU:HD21	11:A:323:PRO:HB3	1.96	0.47
14:D:191:ASN:OD1	14:D:191:ASN:N	2.45	0.47
16:F:180:VAL:HG11	48:F:801:SQD:H45	1.96	0.47
16:F:355:LEU:HD11	16:F:397:SER:HB2	1.97	0.47
18:H:131:PHE:HZ	21:K:49:ALA:HB1	1.80	0.47
55:w:319:LUT:C8	55:w:319:LUT:H181	2.44	0.47
4:3:123:ARG:HB2	4:3:126:LEU:HD12	1.97	0.47
18:H:130:PRO:O	18:H:134:ILE:HG23	2.14	0.47
50:a:815:CLA:H202	50:a:834:CLA:H61	1.97	0.47
50:z:306:CLA:H42	50:z:319:CLA:H3A	1.96	0.47
2:1:104:GLY:HA3	12:B:172:LYS:HG3	1.95	0.47
4:3:140:GLU:HG3	4:3:166:TRP:CD1	2.50	0.47
14:D:243:TYR:HA	14:D:246:CYS:HB2	1.96	0.47
21:K:163:GLU:O	21:K:166:ILE:HG13	2.14	0.47
50:h:201:CLA:HBB2	43:l:303:BCR:H311	1.96	0.47
39:w:206:MET:HB2	55:w:320:LUT:H22	1.97	0.47
5:4:12:ARG:NH2	16:F:582:TRP:O	2.47	0.47
7:6:100:ARG:NH2	7:6:136:GLN:OE1	2.46	0.47
7:6:151:ASP:OD1	7:6:152:ASP:N	2.47	0.47
12:B:20:LYS:HA	12:B:20:LYS:HD3	1.50	0.47
14:D:159:LYS:HB2	14:D:240:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:10:ILE:O	16:F:14:LEU:HB2	2.14	0.47
23:M:121:ASP:OD1	23:M:122:LYS:NZ	2.36	0.47
51:b:821:DGD:HB81	50:b:842:CLA:HBC2	1.97	0.47
39:w:208:TRP:HB3	50:w:308:CLA:HBA1	1.97	0.47
55:w:320:LUT:C8	55:w:320:LUT:H181	2.45	0.47
2:1:117:ARG:NH2	2:1:119:ASP:OD2	2.43	0.47
3:2:79:SER:OG	3:2:81:LYS:NZ	2.47	0.47
11:A:200:GLN:NE2	11:A:209:ASN:OD1	2.30	0.47
12:B:114:LEU:HG	12:B:370:VAL:HG21	1.97	0.47
12:B:326:TYR:HA	12:B:329:ILE:HG12	1.97	0.47
16:F:330:MET:HE2	16:F:346:LEU:HA	1.96	0.47
26:U:210:GLU:H	26:U:210:GLU:HG3	1.43	0.47
27:a:123:ILE:HG21	28:b:446:PHE:HA	1.97	0.47
28:b:236:ASN:OD1	28:b:236:ASN:N	2.47	0.47
50:b:805:CLA:H193	50:b:805:CLA:H161	1.80	0.47
50:w:303:CLA:H3A	50:w:303:CLA:HBA2	1.53	0.47
12:B:20:LYS:HB2	13:C:90:GLY:CA	2.43	0.47
13:C:82:TRP:HD1	13:C:93:VAL:HB	1.80	0.47
15:E:22:VAL:HG11	17:G:100:THR:HG21	1.97	0.47
18:H:154:MET:HG2	21:K:140:PRO:HG2	1.95	0.47
27:a:271:ASP:OD1	27:a:271:ASP:N	2.40	0.47
44:a:805:PGT:H322	39:w:91:PRO:HB3	1.96	0.47
50:a:834:CLA:H112	43:j:103:BCR:H19C	1.97	0.47
50:w:310:CLA:HHB	55:w:320:LUT:H362	1.95	0.47
50:z:319:CLA:CHC	55:z:320:LUT:H203	2.45	0.47
3:2:244:MET:HE3	3:2:244:MET:HA	1.95	0.47
7:6:114:MET:HE3	17:G:128:LYS:HB3	1.97	0.47
11:A:214:PRO:O	11:A:218:ILE:HG13	2.15	0.47
12:B:247:ALA:HB1	12:B:248:PRO:HD2	1.97	0.47
16:F:243:GLN:HE22	16:F:331:MET:HG2	1.80	0.47
18:H:117:TRP:NE1	18:H:382:GLY:O	2.45	0.47
50:b:815:CLA:H18	43:f:304:BCR:H272	1.97	0.47
50:h:201:CLA:HBA1	50:h:201:CLA:H3A	1.48	0.47
39:w:237:LEU:HD22	39:w:248:PRO:HB3	1.97	0.47
4:3:201:ASP:CG	4:3:202:GLY:H	2.23	0.47
12:B:146:ALA:HB1	12:B:151:THR:HG23	1.97	0.47
21:K:12:ILE:HG22	21:K:163:GLU:HG3	1.97	0.47
27:a:12:ILE:HD13	50:a:811:CLA:HAA2	1.97	0.47
50:a:856:CLA:H101	50:a:856:CLA:H62	1.74	0.47
28:b:657:TRP:HB2	28:b:716:GLY:HA3	1.96	0.47
32:f:112:ASP:OD1	32:f:112:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:87:LYS:O	34:h:91:THR:HG23	2.15	0.47
37:k:54:ASN:ND2	50:k:205:CLA:OBD	2.48	0.47
41:y:251:PRO:O	55:y:315:LUT:O3	2.32	0.47
2:1:422:LYS:HB3	2:1:422:LYS:HE2	1.67	0.46
10:9:144:LYS:HA	10:9:229:GLU:HG3	1.96	0.46
47:A:405:PQ9:H311	47:A:405:PQ9:H291	1.73	0.46
12:B:146:ALA:O	12:B:148:ASP:N	2.47	0.46
19:I:68:GLU:OE1	19:I:83:TRP:NE1	2.42	0.46
39:w:235:VAL:HG12	50:w:310:CLA:HBC3	1.96	0.46
50:w:303:CLA:HBA1	48:w:317:SQD:O7	2.15	0.46
42:z:197:ARG:HB3	50:z:307:CLA:HBC3	1.96	0.46
12:B:474:LEU:HD23	12:B:474:LEU:HA	1.78	0.46
17:G:85:GLU:HB3	17:G:88:LYS:HG2	1.96	0.46
20:J:50:TYR:HB3	20:J:72:THR:HG23	1.98	0.46
26:U:104:GLU:HA	26:U:107:LEU:HD12	1.97	0.46
50:a:849:CLA:H2A	38:l:119:ALA:O	2.15	0.46
41:y:140:VAL:HG21	55:y:316:LUT:C4	2.45	0.46
42:z:106:GLU:HG3	42:z:112:ASN:HB3	1.96	0.46
42:z:174:ASP:C	55:z:320:LUT:O23	2.58	0.46
1:0:140:PRO:HG2	1:0:143:ASP:HB3	1.98	0.46
5:4:1:MET:HE2	5:4:1:MET:HB2	1.81	0.46
7:6:131:GLN:O	7:6:135:LYS:HG2	2.16	0.46
11:A:52:LEU:HD11	22:L:129:PHE:HB2	1.96	0.46
13:C:114:LYS:HD3	13:C:114:LYS:HA	1.71	0.46
16:F:391:VAL:HG12	16:F:543:GLU:HA	1.97	0.46
19:I:46:LYS:HG3	19:I:155:ILE:HD12	1.97	0.46
21:K:83:MET:O	23:M:165:ARG:NH1	2.39	0.46
22:L:140:PRO:HB3	44:N:301:PGT:H2	1.98	0.46
50:f:301:CLA:H42	36:j:15:SER:HA	1.96	0.46
42:z:162:ASP:HB3	42:z:165:LYS:HB2	1.98	0.46
9:8:160:VAL:HG23	9:8:162:LYS:HG2	1.96	0.46
9:8:192:PRO:HB3	9:8:213:ASN:HA	1.98	0.46
50:a:809:CLA:H93	50:y:310:CLA:H111	1.97	0.46
28:b:207:VAL:O	28:b:208:ARG:NH1	2.48	0.46
39:w:206:MET:HB2	55:w:320:LUT:C2	2.45	0.46
2:1:172:ARG:NH1	12:B:461:GLU:OE1	2.49	0.46
11:A:231:LEU:HB3	11:A:327:ARG:HA	1.98	0.46
12:B:445:TYR:CE1	48:B:604:SQD:O3	2.64	0.46
14:D:10:ILE:HG22	14:D:126:ILE:HG21	1.97	0.46
16:F:160:LEU:HD11	48:F:805:SQD:H292	1.96	0.46
27:a:319:LEU:HD23	50:a:843:CLA:HED2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:a:859:SQD:H3	41:y:91:PHE:CE1	2.51	0.46
50:b:841:CLA:HAA1	50:b:841:CLA:HBD	1.96	0.46
11:A:328:TRP:O	18:H:129:THR:OG1	2.26	0.46
18:H:65:PRO:O	18:H:69:ARG:NH1	2.48	0.46
19:I:165:LYS:HD2	19:I:165:LYS:HA	1.76	0.46
27:a:296:LEU:O	27:a:300:ILE:HG12	2.15	0.46
27:a:480:PHE:HB3	50:a:822:CLA:H11	1.98	0.46
27:a:691:TYR:OH	50:a:854:CLA:OBD	2.31	0.46
50:a:824:CLA:HHC	50:a:824:CLA:H111	1.98	0.46
28:b:69:ALA:HB2	28:b:135:LEU:HB2	1.97	0.46
12:B:83:PRO:HA	12:B:93:THR:O	2.15	0.46
12:B:500:PRO:O	12:B:504:ILE:HG13	2.16	0.46
14:D:43:GLU:O	14:D:47:MET:HG3	2.16	0.46
17:G:55:SER:HB3	17:G:58:VAL:HB	1.96	0.46
39:w:206:MET:HG2	55:w:320:LUT:H22	1.97	0.46
50:z:306:CLA:ND	55:z:320:LUT:C38	2.79	0.46
12:B:128:GLU:OE2	13:C:110:TYR:OH	2.31	0.46
18:H:221:GLY:HA3	18:H:335:GLY:HA2	1.97	0.46
18:H:358:GLY:N	18:H:390:GLU:OE2	2.43	0.46
21:K:105:MET:HA	21:K:136:LEU:HB3	1.97	0.46
50:b:844:CLA:H112	50:b:844:CLA:H151	1.80	0.46
50:w:307:CLA:HBA2	50:w:307:CLA:H3A	1.68	0.46
5:4:65:ASP:N	5:4:65:ASP:OD1	2.48	0.46
19:I:156:ARG:HA	22:L:149:ARG:HD3	1.97	0.46
50:b:807:CLA:H161	50:b:807:CLA:H141	1.82	0.46
16:F:642:ASP:N	16:F:642:ASP:OD1	2.49	0.46
18:H:51:MET:N	18:H:393:ARG:OXT	2.43	0.46
18:H:73:LEU:HD22	18:H:116:LEU:HD23	1.98	0.46
27:a:454:ILE:HG22	50:a:849:CLA:HBC2	1.98	0.46
50:a:809:CLA:HBA1	41:y:80:LEU:HB3	1.98	0.46
46:z:314:LMG:O10	46:z:314:LMG:O2	2.31	0.46
4:3:155:GLU:O	4:3:159:LEU:HB2	2.16	0.45
12:B:253:THR:HG22	12:B:325:ALA:HB1	1.97	0.45
12:B:258:GLU:HB3	15:E:99:LEU:HD22	1.98	0.45
14:D:44:LEU:HD12	14:D:47:MET:HE2	1.98	0.45
16:F:230:ALA:HB2	16:F:287:ILE:HD12	1.98	0.45
28:b:273:MET:HE2	50:b:846:CLA:HMA2	1.98	0.45
51:x:317:DGD:HD5	51:x:317:DGD:HE1	1.66	0.45
7:6:97:ALA:O	7:6:101:ILE:HG12	2.16	0.45
11:A:302:VAL:HG22	44:L:201:PGT:H381	1.97	0.45
11:A:360:SER:O	26:U:239:ASN:ND2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:2:ASP:OD2	17:G:8:HIS:ND1	2.49	0.45
18:H:135:LEU:HD23	18:H:135:LEU:HA	1.83	0.45
27:a:95:PHE:HB3	27:a:114:VAL:HG22	1.97	0.45
50:a:801:CLA:H143	43:a:827:BCR:HC41	1.98	0.45
48:a:859:SQD:H3	41:y:91:PHE:CZ	2.52	0.45
29:c:60:THR:OG1	29:c:62:PHE:O	2.21	0.45
50:y:314:CLA:H152	50:y:314:CLA:H111	1.71	0.45
2:1:353:PHE:HB2	2:1:374:ILE:HD12	1.97	0.45
6:5:95:GLU:HB3	16:F:119:GLN:HG3	1.98	0.45
11:A:27:GLU:O	11:A:31:MET:HE3	2.16	0.45
11:A:113:LEU:HD11	13:C:14:LEU:HD13	1.98	0.45
12:B:463:THR:HG22	12:B:465:HIS:H	1.82	0.45
16:F:367:MET:HE3	16:F:367:MET:HB3	1.88	0.45
20:J:102:TRP:HE1	20:J:124:ASN:HB3	1.81	0.45
3:2:305:VAL:HG22	3:2:312:VAL:HG22	1.97	0.45
18:H:219:LEU:HD13	18:H:223:MET:HG2	1.97	0.45
28:b:206:TYR:O	28:b:211:ASN:ND2	2.50	0.45
50:b:813:CLA:HBB1	50:b:851:CLA:CBB	2.46	0.45
38:l:215:PHE:HA	50:l:301:CLA:HAA2	1.98	0.45
48:w:318:SQD:C32	48:w:318:SQD:H282	2.46	0.45
50:y:313:CLA:H41	50:y:313:CLA:H61	1.53	0.45
2:1:196:LEU:HD22	2:1:201:TYR:HE2	1.81	0.45
3:2:86:TRP:HB3	39:w:186:PRO:HB3	1.98	0.45
7:6:190:ILE:O	7:6:194:LEU:HD23	2.17	0.45
14:D:307:TYR:OH	16:F:691:ASP:OD1	2.30	0.45
16:F:417:LYS:O	16:F:421:LEU:HG	2.17	0.45
20:J:49:ASN:OD1	26:U:199:GLN:NE2	2.43	0.45
23:M:85:LEU:CD2	23:M:120:MET:HE2	2.46	0.45
25:O:91:VAL:HG11	25:O:100:LEU:HD11	1.99	0.45
50:a:809:CLA:H92	50:a:809:CLA:H62	1.79	0.45
50:a:814:CLA:H72	50:a:846:CLA:HBC3	1.98	0.45
50:a:820:CLA:H152	43:j:101:BCR:H351	1.97	0.45
42:z:154:GLU:OE2	42:z:157:ARG:NH1	2.50	0.45
9:8:131:ASN:HA	9:8:154:LEU:O	2.17	0.45
16:F:26:LEU:HD13	48:F:805:SQD:H2	1.98	0.45
27:a:435:ILE:HG13	27:a:554:PHE:HE2	1.80	0.45
28:b:456:GLU:OE1	28:b:461:GLN:NE2	2.49	0.45
3:2:110:ASN:OD1	3:2:200:THR:OG1	2.35	0.45
12:B:352:ILE:H	12:B:352:ILE:HG12	1.60	0.45
12:B:462:ILE:O	12:B:467:ARG:NH2	2.49	0.45
13:C:49:GLU:OE1	21:K:91:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:450:GLU:OE2	32:f:129:ARG:NE	2.48	0.45
32:f:136:TYR:CZ	36:j:40:PRO:HG3	2.52	0.45
37:k:96:GLY:HA3	50:k:203:CLA:HMA3	1.99	0.45
50:l:306:CLA:H92	50:l:306:CLA:H61	1.87	0.45
3:2:271:PRO:HG2	3:2:272:ILE:HD12	1.97	0.45
44:B:606:PGT:H62	14:D:113:LEU:HD13	1.97	0.45
15:E:53:ASP:OD2	15:E:58:LYS:NZ	2.50	0.45
15:E:60:ASN:ND2	17:G:55:SER:OG	2.50	0.45
19:I:127:LEU:HD23	24:N:124:ARG:HD3	1.98	0.45
27:a:657:ILE:HD12	28:b:621:ARG:HG3	1.99	0.45
50:a:858:CLA:HBB1	50:b:803:CLA:C1B	2.47	0.45
38:l:172:LYS:NZ	38:l:173:LYS:O	2.48	0.45
2:1:112:LEU:HD11	12:B:174:VAL:HG12	1.98	0.45
16:F:177:LYS:NZ	16:F:669:ASP:OD2	2.39	0.45
17:G:39:LEU:O	17:G:43:LEU:HG	2.17	0.45
18:H:47:LEU:HD23	18:H:389:GLY:HA2	1.99	0.45
24:N:104:GLU:N	24:N:104:GLU:OE1	2.50	0.45
27:a:36:ILE:HG13	27:a:45:TRP:NE1	2.32	0.45
27:a:324:GLU:HG2	27:a:336:LYS:HG3	1.99	0.45
50:a:801:CLA:H111	50:a:838:CLA:H42	1.97	0.45
50:a:857:CLA:H13	50:a:857:CLA:H102	1.86	0.45
28:b:448:THR:O	28:b:448:THR:OG1	2.30	0.45
50:b:806:CLA:HBA1	35:i:11:VAL:HG11	1.99	0.45
50:b:810:CLA:H3A	50:b:810:CLA:HBA2	1.62	0.45
33:g:145:SER:HA	43:g:202:BCR:H20C	1.99	0.45
41:y:104:ASN:ND2	50:y:313:CLA:OBD	2.50	0.45
50:z:302:CLA:C4B	55:z:320:LUT:H173	2.47	0.45
2:1:190:THR:CG2	48:B:604:SQD:H441	2.47	0.45
7:6:100:ARG:HE	7:6:137:ASP:CG	2.25	0.45
47:A:405:PQ9:H311	47:A:405:PQ9:H351	1.44	0.45
16:F:558:PHE:O	16:F:562:VAL:HB	2.17	0.45
28:b:5:PHE:O	28:b:20:ARG:NH1	2.37	0.45
51:b:821:DGD:HB92	51:b:821:DGD:HBW1	1.74	0.45
40:x:214:LEU:HD11	46:x:315:LMG:H162	1.98	0.45
41:y:109:MET:HB3	55:y:315:LUT:C35	2.46	0.45
2:1:89:ARG:HG3	2:1:100:LYS:HB3	1.99	0.44
12:B:218:LEU:HD22	12:B:224:TYR:HA	1.99	0.44
13:C:82:TRP:CD1	13:C:93:VAL:HB	2.52	0.44
16:F:319:LEU:HD23	16:F:322:TYR:HE1	1.83	0.44
16:F:322:TYR:HE2	16:F:405:LEU:HD23	1.82	0.44
21:K:35:TRP:N	21:K:73:ASP:OD2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:522:LEU:HD23	27:a:523:PRO:HD2	1.98	0.44
50:a:838:CLA:HBA1	50:a:838:CLA:H3A	1.66	0.44
28:b:56:ILE:HD13	50:b:804:CLA:HAB	1.99	0.44
28:b:322:LEU:HD12	28:b:322:LEU:HA	1.87	0.44
28:b:341:LEU:HD23	28:b:382:ILE:HD13	1.98	0.44
34:h:99:ARG:NH2	38:l:157:GLU:OE2	2.49	0.44
34:h:130:ARG:HB2	34:h:133:GLN:HE21	1.82	0.44
39:w:131:ILE:HG22	39:w:133:LEU:HG	1.99	0.44
2:1:115:LYS:HE2	15:E:99:LEU:HD23	1.99	0.44
2:1:266:ILE:HD12	2:1:281:ALA:HB2	1.99	0.44
2:1:317:LYS:HA	2:1:333:LEU:HD13	1.99	0.44
14:D:99:LEU:HD23	14:D:99:LEU:HA	1.87	0.44
18:H:74:ALA:HB1	18:H:77:PHE:HD2	1.82	0.44
55:x:321:LUT:H181	55:x:321:LUT:C8	2.47	0.44
42:z:72:LEU:HD21	44:z:313:PGT:H151	1.99	0.44
42:z:216:THR:OG1	42:z:217:GLY:N	2.50	0.44
5:4:12:ARG:HD2	16:F:68:ILE:HG13	1.99	0.44
5:4:31:VAL:HG22	44:5:301:PGT:H331	1.99	0.44
6:5:205:LYS:HE2	6:5:206:TYR:CZ	2.51	0.44
7:6:173:THR:HG22	13:C:5:TYR:HB2	1.99	0.44
16:F:130:PHE:HE2	16:F:156:MET:HE1	1.82	0.44
20:J:42:ILE:HG13	26:U:103:VAL:HG21	1.99	0.44
27:a:56:PHE:HE1	50:a:813:CLA:HED1	1.82	0.44
38:l:118:LYS:HG2	50:l:301:CLA:HMA1	1.98	0.44
39:w:162:MET:HE3	39:w:162:MET:HB3	1.91	0.44
40:x:150:PHE:HA	40:x:153:VAL:HG22	1.99	0.44
50:y:311:CLA:NB	55:y:316:LUT:H173	2.31	0.44
1:0:209:ALA:HB3	1:0:214:TRP:HE3	1.82	0.44
3:2:284:THR:HA	3:2:298:THR:HG23	2.00	0.44
11:A:33:PHE:O	11:A:37:ILE:HG22	2.16	0.44
50:a:802:CLA:H92	50:a:802:CLA:H61	1.83	0.44
50:b:803:CLA:H111	43:b:850:BCR:H362	1.99	0.44
50:b:845:CLA:H102	50:b:845:CLA:H13	1.59	0.44
30:d:116:MET:HE3	30:d:116:MET:HB3	1.84	0.44
50:x:312:CLA:C4D	55:x:320:LUT:H382	2.47	0.44
50:z:302:CLA:C3B	55:z:320:LUT:H173	2.47	0.44
46:z:315:LMG:H112	46:z:315:LMG:H141	1.79	0.44
2:1:447:ASP:OD1	2:1:447:ASP:N	2.40	0.44
11:A:295:GLU:OE2	11:A:298:LYS:NZ	2.45	0.44
12:B:257:TYR:HA	12:B:265:VAL:HG21	1.99	0.44
14:D:457:SER:HB2	14:D:461:GLU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:491:ILE:HA	16:F:494:LEU:HD12	1.98	0.44
18:H:66:TYR:OH	21:K:114:MET:O	2.33	0.44
27:a:257:GLY:HA3	41:y:272:LYS:HA	2.00	0.44
44:a:805:PGT:H322	44:a:805:PGT:H352	1.82	0.44
50:a:836:CLA:HAB	43:j:101:BCR:H392	2.00	0.44
50:a:858:CLA:H93	50:b:801:CLA:HAB	1.98	0.44
30:d:147:ARG:NH1	30:d:177:GLU:OE1	2.50	0.44
2:1:126:VAL:HG13	2:1:156:ILE:HB	1.99	0.44
10:9:114:ASP:HB3	10:9:175:ASN:HD21	1.83	0.44
20:J:140:TRP:HB2	20:J:143:ARG:HD3	1.99	0.44
38:l:118:LYS:HA	38:l:118:LYS:HD2	1.73	0.44
50:w:308:CLA:H41	50:w:308:CLA:H62	1.62	0.44
40:x:203:GLU:O	46:x:315:LMG:O5	2.30	0.44
1:0:106:PHE:HB3	1:0:109:HIS:HB2	1.99	0.44
1:0:133:ASN:OD1	1:0:133:ASN:N	2.51	0.44
3:2:60:LEU:HB3	3:2:159:VAL:HG21	1.98	0.44
17:G:67:VAL:HA	17:G:70:ILE:HG22	2.00	0.44
20:J:136:SER:HB2	23:M:160:THR:HB	2.00	0.44
23:M:194:ASN:OD1	23:M:194:ASN:N	2.50	0.44
28:b:411:MET:HE2	43:b:819:BCR:H292	1.99	0.44
41:y:266:ASN:O	41:y:270:SER:OG	2.32	0.44
50:z:306:CLA:HBB2	55:z:320:LUT:H34	1.98	0.44
1:0:141:MET:HG3	1:0:176:TRP:CE2	2.53	0.44
7:6:130:LYS:HD3	7:6:130:LYS:HA	1.75	0.44
44:B:602:PGT:H151	44:B:602:PGT:H121	1.74	0.44
14:D:290:TYR:O	14:D:294:THR:OG1	2.30	0.44
18:H:71:ASP:H	18:H:390:GLU:HB2	1.83	0.44
18:H:136:ARG:NH1	18:H:181:TYR:OH	2.44	0.44
50:a:846:CLA:H62	50:a:846:CLA:H41	1.80	0.44
28:b:527:LEU:HD12	50:b:851:CLA:HED3	1.99	0.44
50:b:802:CLA:H121	50:b:802:CLA:H161	1.78	0.44
50:b:805:CLA:H52	51:b:821:DGD:HB72	2.00	0.44
50:b:812:CLA:HBD	50:b:849:CLA:HMB1	2.00	0.44
41:y:115:ALA:N	55:y:316:LUT:H163	2.32	0.44
4:3:148:LEU:HD13	4:3:172:ILE:HD13	1.98	0.44
14:D:258:ALA:O	14:D:262:VAL:HG23	2.17	0.44
27:a:364:VAL:O	27:a:368:MET:HG3	2.16	0.44
50:a:836:CLA:H143	43:j:101:BCR:HC31	2.00	0.44
3:2:165:CYS:SG	3:2:166:THR:N	2.91	0.43
12:B:448:LEU:HD11	14:D:168:ILE:HD13	1.99	0.43
21:K:90:LEU:HD23	23:M:97:VAL:HG23	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:571:SER:OG	28:b:574:ASP:OD2	2.36	0.43
50:b:840:CLA:H192	50:b:840:CLA:H161	1.77	0.43
39:w:189:LYS:HE3	39:w:189:LYS:HB2	1.67	0.43
50:y:303:CLA:C3B	55:y:315:LUT:H171	2.47	0.43
44:5:301:PGT:H361	44:5:301:PGT:H332	1.89	0.43
27:a:72:SER:OG	27:a:178:TYR:HB2	2.18	0.43
50:a:814:CLA:H102	50:a:820:CLA:HBC1	2.00	0.43
50:a:826:CLA:HAB	50:a:844:CLA:HMB1	2.00	0.43
43:b:831:BCR:H381	50:f:301:CLA:HMC1	2.00	0.43
30:d:169:HIS:HB3	30:d:170:PRO:HD3	1.99	0.43
37:k:60:SER:OG	37:k:113:GLY:O	2.37	0.43
40:x:110:MET:HE3	40:x:127:TRP:CD2	2.53	0.43
50:y:314:CLA:H193	50:y:314:CLA:H162	1.88	0.43
50:z:306:CLA:H3A	50:z:306:CLA:HBA2	1.63	0.43
3:2:189:VAL:HG12	3:2:360:TRP:HE3	1.84	0.43
7:6:86:ARG:HA	7:6:86:ARG:HD2	1.77	0.43
7:6:197:LEU:HD23	7:6:197:LEU:HA	1.87	0.43
11:A:259:TYR:OH	47:A:405:PQ9:O1	2.32	0.43
12:B:415:PHE:HA	12:B:418:ILE:HG12	2.01	0.43
13:C:110:TYR:CZ	17:G:168:ILE:HG23	2.53	0.43
28:b:583:MET:HE3	28:b:583:MET:HB3	1.78	0.43
43:b:850:BCR:H20C	43:b:850:BCR:H361	1.83	0.43
54:w:309:CHL:HHC	54:w:309:CHL:HBB1	2.00	0.43
40:x:213:MET:HB3	55:x:321:LUT:C35	2.49	0.43
41:y:261:ASP:HA	41:y:262:PRO:HD3	1.91	0.43
3:2:183:MET:HB3	3:2:183:MET:HE3	1.75	0.43
12:B:242:PHE:O	12:B:252:TRP:NE1	2.51	0.43
14:D:253:LEU:HA	14:D:256:MET:HG3	2.00	0.43
23:M:158:PRO:HB2	23:M:160:THR:HG23	1.99	0.43
24:N:219:GLU:HG2	24:N:226:LEU:HA	2.00	0.43
50:a:801:CLA:H161	50:a:801:CLA:H202	1.79	0.43
50:b:825:CLA:H2A	35:i:24:PHE:HE1	1.83	0.43
12:B:365:THR:O	12:B:369:ILE:HG12	2.18	0.43
14:D:160:ARG:HG2	14:D:160:ARG:HH11	1.82	0.43
21:K:110:ILE:HG22	21:K:111:THR:HG23	2.01	0.43
27:a:503:THR:HG21	50:a:850:CLA:HMA2	2.00	0.43
50:a:856:CLA:HAB	28:b:525:LEU:HD21	2.00	0.43
28:b:594:TRP:HD1	50:b:849:CLA:HMC1	1.83	0.43
2:1:252:MET:HE3	2:1:252:MET:HB3	1.91	0.43
3:2:98:LEU:HD11	3:2:335:TYR:HB3	2.00	0.43
11:A:48:VAL:HG22	22:L:132:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:292:SER:HA	12:B:295:TRP:NE1	2.34	0.43
13:C:11:TRP:CD1	17:G:3:LEU:HD11	2.53	0.43
14:D:281:MET:HE2	14:D:410:TYR:CE2	2.54	0.43
50:a:836:CLA:HAB	43:j:101:BCR:H24C	2.01	0.43
50:b:805:CLA:H72	50:b:805:CLA:H111	1.87	0.43
53:b:827:PQN:H252	53:b:827:PQN:H212	1.67	0.43
37:k:57:MET:HE3	37:k:57:MET:HB3	1.80	0.43
50:x:312:CLA:H3A	50:x:312:CLA:HBA2	1.59	0.43
50:x:318:CLA:HED1	44:z:317:PGT:H401	1.99	0.43
3:2:57:ILE:HG22	3:2:71:GLN:HA	2.00	0.43
3:2:317:ARG:HB2	3:2:345:PRO:HG3	2.00	0.43
12:B:94:ASN:OD1	12:B:97:ASN:ND2	2.52	0.43
25:O:69:MET:HE1	25:O:141:LEU:HB2	2.00	0.43
28:b:636:ASN:OD1	28:b:636:ASN:N	2.52	0.43
50:b:828:CLA:H62	50:b:828:CLA:H41	1.77	0.43
32:f:96:LYS:HD3	32:f:96:LYS:HA	1.65	0.43
50:g:203:CLA:H41	50:g:203:CLA:H61	1.87	0.43
54:w:311:CHL:HAB	48:w:318:SQD:H92	2.01	0.43
54:z:304:CHL:HBB2	54:z:312:CHL:HBC1	2.01	0.43
2:1:226:ARG:O	2:1:244:SER:N	2.52	0.43
4:3:71:GLU:C	4:3:73:LEU:H	2.26	0.43
16:F:260:ILE:O	16:F:264:ILE:HB	2.18	0.43
50:b:801:CLA:H152	43:l:302:BCR:H15C	2.01	0.43
50:b:812:CLA:H3A	50:b:851:CLA:O1A	2.19	0.43
50:x:312:CLA:C4	55:x:320:LUT:H28	2.48	0.43
54:x:319:CHL:HED3	42:z:51:PRO:HD2	2.01	0.43
42:z:143:LEU:HD12	42:z:143:LEU:HA	1.88	0.43
54:z:312:CHL:H93	54:z:312:CHL:H111	1.89	0.43
11:A:66:PRO:HB2	11:A:73:GLY:HA3	2.00	0.43
12:B:105:LEU:O	12:B:109:THR:OG1	2.30	0.43
18:H:66:TYR:CE2	21:K:114:MET:HB2	2.54	0.43
27:a:410:MET:HE3	27:a:410:MET:HB3	1.79	0.43
27:a:438:LEU:HD21	27:a:545:VAL:HG12	1.99	0.43
27:a:746:ILE:HD12	27:a:746:ILE:HA	1.91	0.43
50:a:846:CLA:H192	50:a:846:CLA:H161	1.76	0.43
48:w:318:SQD:H81	48:w:318:SQD:C46	2.47	0.43
40:x:79:PRO:HD2	55:x:321:LUT:C23	2.46	0.43
6:5:94:ASP:OD1	6:5:94:ASP:N	2.43	0.43
12:B:214:ILE:HD11	12:B:287:PRO:HB2	2.01	0.43
46:D:601:LMG:HC92	46:D:601:LMG:H291	1.81	0.43
16:F:353:LYS:HD2	16:F:353:LYS:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:24:LEU:O	17:G:28:LEU:HB2	2.19	0.43
21:K:70:ARG:HA	21:K:97:PRO:HD3	2.01	0.43
27:a:485:GLN:HG2	27:a:507:TRP:HE3	1.84	0.43
27:a:575:GLY:HA2	28:b:562:PRO:HD3	2.00	0.43
44:a:805:PGT:H341	44:a:805:PGT:H32	2.00	0.43
50:a:839:CLA:H152	50:a:839:CLA:H18	1.66	0.43
50:b:826:CLA:H51	50:b:826:CLA:H8	1.94	0.43
50:w:310:CLA:H141	50:w:310:CLA:H162	1.87	0.43
54:x:301:CHL:CBB	54:x:311:CHL:HBB2	2.49	0.43
2:1:125:CYS:HB2	2:1:155:ILE:HD13	2.00	0.42
2:1:375:VAL:HG12	2:1:377:ILE:HG12	2.01	0.42
12:B:21:ALA:C	12:B:23:HIS:N	2.76	0.42
15:E:49:SER:HB2	15:E:59:GLY:HA3	2.00	0.42
19:I:76:ILE:HG13	19:I:78:LEU:HB2	2.01	0.42
21:K:58:PHE:CE1	21:K:63:LEU:HD23	2.54	0.42
27:a:94:ARG:HE	27:a:94:ARG:HB3	1.61	0.42
27:a:438:LEU:HG	27:a:546:LEU:HB2	2.01	0.42
50:b:804:CLA:H3A	44:b:829:PGT:H381	2.00	0.42
32:f:148:LEU:HD22	32:f:159:GLU:HG2	2.01	0.42
40:x:158:TRP:HH2	46:z:314:LMG:HC8	1.84	0.42
40:x:221:VAL:O	40:x:225:VAL:HG22	2.19	0.42
2:1:405:LEU:HD22	2:1:431:LYS:HB3	2.01	0.42
47:A:405:PQ9:H162	47:A:405:PQ9:H143	1.93	0.42
47:A:405:PQ9:H261	47:A:405:PQ9:H242	1.85	0.42
48:B:604:SQD:H251	14:D:169:LEU:HD13	2.00	0.42
14:D:76:PHE:CD1	14:D:135:LEU:HB3	2.54	0.42
16:F:34:LYS:HG2	16:F:122:LEU:HD13	2.01	0.42
23:M:130:THR:O	23:M:130:THR:OG1	2.37	0.42
27:a:343:THR:HA	50:a:842:CLA:H193	1.96	0.42
27:a:572:PRO:HB3	27:a:719:ILE:HB	2.01	0.42
50:a:836:CLA:H62	43:j:103:BCR:H363	2.01	0.42
40:x:143:PHE:CE2	50:z:310:CLA:HHC	2.54	0.42
41:y:186:PHE:CE2	50:y:312:CLA:HBB2	2.54	0.42
50:y:308:CLA:H101	50:y:313:CLA:H43	2.00	0.42
12:B:131:LEU:HD11	17:G:165:VAL:HG22	2.00	0.42
48:B:604:SQD:H81	14:D:166:LYS:HG3	2.00	0.42
19:I:80:VAL:HG22	24:N:143:HIS:CD2	2.54	0.42
27:a:703:HIS:HE1	50:a:824:CLA:ND	2.17	0.42
28:b:476:VAL:HG22	28:b:477:LEU:H	1.85	0.42
50:b:840:CLA:C4D	50:b:847:CLA:HMB1	2.49	0.42
34:h:138:LEU:HD23	34:h:138:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:x:155:ILE:HD13	40:x:155:ILE:HA	1.81	0.42
2:l:154:ASP:OD2	2:l:172:ARG:NH2	2.41	0.42
44:A:403:PGT:H131	44:A:403:PGT:H161	1.66	0.42
14:D:128:LEU:HD22	14:D:256:MET:SD	2.59	0.42
16:F:183:ARG:HD3	16:F:183:ARG:HA	1.78	0.42
18:H:329:ARG:NH2	20:J:83:GLU:OE1	2.39	0.42
28:b:561:GLY:O	28:b:567:THR:OG1	2.37	0.42
39:w:225:LYS:HB2	39:w:225:LYS:HE3	1.69	0.42
50:w:303:CLA:HAA1	50:w:307:CLA:HMA2	2.00	0.42
40:x:107:VAL:HG11	55:x:320:LUT:H12	2.01	0.42
6:5:165:GLU:HG3	14:D:34:TRP:CZ2	2.54	0.42
12:B:493:ILE:HD12	12:B:493:ILE:HA	1.79	0.42
44:B:602:PGT:H161	44:B:602:PGT:H321	2.01	0.42
16:F:91:PRO:HB3	16:F:582:TRP:CD1	2.54	0.42
16:F:147:ILE:O	16:F:151:TRP:HB2	2.18	0.42
27:a:393:TRP:HZ3	27:a:598:TYR:HA	1.85	0.42
50:a:814:CLA:H152	50:a:845:CLA:HBB2	2.01	0.42
28:b:33:SER:OG	28:b:396:ARG:NH2	2.52	0.42
50:b:844:CLA:H41	50:b:844:CLA:H61	1.57	0.42
34:h:79:SER:HB2	38:l:95:VAL:HG13	2.00	0.42
37:k:102:THR:OG1	37:k:105:ASP:OD1	2.33	0.42
50:w:308:CLA:HBB1	55:w:320:LUT:H14	2.00	0.42
10:9:175:ASN:OD1	10:9:175:ASN:N	2.46	0.42
11:A:47:LEU:HD21	47:A:405:PQ9:H292	2.02	0.42
12:B:244:LEU:HD22	12:B:332:ILE:HD11	2.02	0.42
14:D:362:ASP:OD1	14:D:362:ASP:N	2.52	0.42
22:L:101:MET:HE2	22:L:101:MET:HB2	1.89	0.42
27:a:13:LEU:HA	41:y:87:GLY:HA3	2.01	0.42
27:a:476:LEU:HB2	27:a:528:THR:HG23	2.01	0.42
50:a:854:CLA:H93	50:a:854:CLA:H61	1.86	0.42
30:d:93:LEU:HD23	30:d:93:LEU:HA	1.93	0.42
42:z:136:TRP:NE1	50:z:309:CLA:HAC2	2.34	0.42
9:8:132:VAL:HG22	9:8:156:MET:HE1	2.02	0.42
46:B:605:LMG:H112	46:B:605:LMG:HC8	1.65	0.42
14:D:464:VAL:O	14:D:468:ILE:HG13	2.20	0.42
16:F:110:TYR:HD1	16:F:259:PRO:HG3	1.84	0.42
16:F:270:VAL:HB	16:F:327:LEU:HD11	2.00	0.42
27:a:218:SER:O	27:a:222:ASN:HB2	2.19	0.42
50:a:802:CLA:C1D	50:a:841:CLA:HBB2	2.50	0.42
51:a:804:DGD:HA92	50:a:839:CLA:H51	2.02	0.42
50:a:857:CLA:H141	38:l:139:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:b:823:CLA:H41	50:b:823:CLA:H62	1.73	0.42
42:z:180:LYS:HA	42:z:180:LYS:HD2	1.88	0.42
2:1:169:LYS:HD2	5:4:90:GLU:HG3	2.02	0.42
2:1:233:ASN:OD1	2:1:233:ASN:N	2.52	0.42
3:2:77:VAL:HB	3:2:105:ILE:HB	2.01	0.42
3:2:162:GLU:HG2	3:2:175:VAL:HG22	2.01	0.42
13:C:88:ILE:HD12	17:G:146:ILE:HD11	2.00	0.42
16:F:571:GLN:HE22	16:F:597:PHE:HB2	1.85	0.42
18:H:192:LEU:HB2	19:I:28:ILE:HG21	2.02	0.42
23:M:74:ILE:HD12	23:M:74:ILE:HA	1.88	0.42
27:a:217:VAL:HG13	27:a:237:PRO:HB3	2.02	0.42
28:b:601:LEU:HA	28:b:606:VAL:HG12	2.01	0.42
50:b:809:CLA:HBA2	50:b:809:CLA:H3A	1.70	0.42
50:b:822:CLA:H92	50:b:822:CLA:H62	1.84	0.42
29:c:5:VAL:HG11	29:c:26:LEU:HD21	2.02	0.42
50:x:306:CLA:HAA1	50:x:306:CLA:HBD	2.02	0.42
54:x:311:CHL:HHC	54:x:311:CHL:HBB1	2.02	0.42
54:x:319:CHL:HBA1	54:x:319:CHL:H3A	1.49	0.42
2:1:311:VAL:HG13	2:1:349:VAL:HG11	2.01	0.42
2:1:387:ILE:O	2:1:409:LYS:NZ	2.52	0.42
3:2:228:HIS:ND1	3:2:229:PRO:HD2	2.35	0.42
9:8:164:ILE:HG13	9:8:167:LEU:HB2	2.01	0.42
12:B:493:ILE:HG22	12:B:494:PRO:HD3	2.01	0.42
16:F:196:LEU:HB3	16:F:208:LEU:HD11	2.02	0.42
26:U:119:ALA:C	26:U:121:LEU:H	2.28	0.42
27:a:315:ILE:HG13	50:a:812:CLA:HED1	2.02	0.42
51:a:804:DGD:HBG1	51:a:804:DGD:HA81	2.02	0.42
50:b:847:CLA:H92	50:b:847:CLA:H61	1.82	0.42
36:j:32:PHE:O	46:j:104:LMG:O4	2.35	0.42
39:w:168:ARG:NE	50:x:316:CLA:OBD	2.48	0.42
42:z:235:GLY:HA2	42:z:238:VAL:HG12	2.01	0.42
2:1:91:ASN:O	12:B:470:ARG:NH2	2.52	0.42
7:6:124:ILE:HD12	7:6:124:ILE:HA	1.90	0.42
10:9:107:VAL:HG13	10:9:251:LEU:HD21	2.02	0.42
14:D:146:ILE:HD13	14:D:146:ILE:HA	1.86	0.42
16:F:622:PHE:O	16:F:626:LYS:HB2	2.19	0.42
18:H:209:ILE:HG12	18:H:368:LEU:HD21	2.02	0.42
20:J:106:SER:OG	20:J:110:GLN:NE2	2.52	0.42
26:U:190:MET:HE3	26:U:190:MET:HB2	1.90	0.42
50:a:801:CLA:H93	50:a:838:CLA:H42	2.01	0.42
28:b:40:GLU:OE1	28:b:44:GLN:NE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:519:VAL:HG21	28:b:593:TYR:HB2	2.02	0.42
28:b:612:SER:HA	28:b:615:TYR:HE1	1.85	0.42
34:h:50:LYS:N	34:h:53:ASP:OD2	2.52	0.42
48:w:318:SQD:C8	48:w:318:SQD:H461	2.50	0.42
50:x:307:CLA:H61	50:x:307:CLA:H92	1.80	0.42
9:8:138:PHE:HB2	9:8:142:THR:HG23	2.01	0.41
9:8:218:TYR:HB3	9:8:220:VAL:HG13	2.02	0.41
10:9:196:SER:O	10:9:196:SER:OG	2.38	0.41
12:B:362:ASN:HA	12:B:365:THR:HG22	2.02	0.41
12:B:437:LEU:HD21	14:D:179:LEU:HD23	2.02	0.41
48:B:604:SQD:O2	48:B:604:SQD:H442	2.20	0.41
18:H:378:MET:N	18:H:378:MET:SD	2.92	0.41
21:K:45:PHE:O	21:K:48:PHE:HB3	2.20	0.41
27:a:389:THR:CG2	50:a:820:CLA:HAB	2.50	0.41
43:b:818:BCR:H392	50:b:836:CLA:H51	2.02	0.41
34:h:135:PRO:HA	34:h:136:PRO:HD3	1.96	0.41
37:k:57:MET:HE2	50:k:205:CLA:C1D	2.50	0.41
39:w:116:MET:HB3	55:w:320:LUT:C15	2.50	0.41
2:1:206:SER:HB2	2:1:218:LEU:HD11	2.02	0.41
3:2:162:GLU:HG3	3:2:175:VAL:HG13	2.02	0.41
14:D:121:MET:HE1	14:D:253:LEU:HD11	2.02	0.41
16:F:323:THR:OG1	16:F:353:LYS:HE3	2.20	0.41
20:J:51:LEU:HA	20:J:71:LEU:HD23	2.01	0.41
27:a:312:ASN:OD1	27:a:312:ASN:N	2.53	0.41
43:a:831:BCR:H342	50:a:846:CLA:H162	2.02	0.41
28:b:662:MET:HB2	50:b:803:CLA:C4C	2.50	0.41
33:g:79:LEU:HD23	33:g:79:LEU:HA	1.95	0.41
39:w:168:ARG:HH12	39:w:181:ILE:HD11	1.85	0.41
39:w:206:MET:CB	55:w:320:LUT:H22	2.50	0.41
44:w:313:PGT:H2	50:w:316:CLA:HMC2	2.02	0.41
42:z:175:PRO:N	55:z:320:LUT:O23	2.53	0.41
1:0:104:PHE:CE1	1:0:114:LYS:HB3	2.55	0.41
10:9:93:ILE:HG21	10:9:228:ILE:HD11	2.02	0.41
11:A:219:VAL:HG13	11:A:346:LEU:HD22	2.02	0.41
44:A:402:PGT:O5	17:G:89:LYS:NZ	2.43	0.41
16:F:127:TYR:OH	48:F:805:SQD:H252	2.20	0.41
48:F:805:SQD:H4	48:F:805:SQD:O7	2.20	0.41
18:H:47:LEU:HD11	21:K:42:SER:HB2	2.02	0.41
18:H:131:PHE:O	18:H:134:ILE:HG12	2.21	0.41
50:b:845:CLA:H62	50:b:845:CLA:H41	1.89	0.41
30:d:156:PHE:CZ	30:d:169:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:187:ASP:OD1	32:f:187:ASP:N	2.52	0.41
43:w:301:BCR:H332	46:x:315:LMG:H302	2.02	0.41
40:x:152:TYR:HE1	54:x:319:CHL:HBD	1.85	0.41
40:x:245:THR:N	40:x:248:GLN:OE1	2.47	0.41
50:x:310:CLA:HBA2	50:x:310:CLA:H3A	1.70	0.41
50:z:306:CLA:CBB	55:z:320:LUT:H32	2.50	0.41
10:9:238:ARG:HE	10:9:238:ARG:HB3	1.52	0.41
11:A:145:ILE:HD11	17:G:67:VAL:HG13	2.02	0.41
11:A:274:THR:HA	11:A:278:LEU:HB2	2.03	0.41
16:F:329:TYR:OH	16:F:435:ALA:O	2.39	0.41
16:F:333:ALA:HB2	16:F:420:ILE:HG12	2.02	0.41
18:H:289:ASN:HB3	18:H:292:ILE:HG22	2.02	0.41
21:K:66:ARG:HE	21:K:66:ARG:HB3	1.65	0.41
23:M:64:MET:HG2	23:M:66:GLU:HG2	2.02	0.41
44:a:806:PGT:O1P	50:a:826:CLA:NB	2.53	0.41
50:a:814:CLA:H121	50:a:814:CLA:H162	1.75	0.41
28:b:194:LEU:HA	28:b:198:ALA:HB3	2.02	0.41
50:b:802:CLA:H192	50:b:802:CLA:H162	1.87	0.41
31:e:119:ASP:OD1	31:e:119:ASP:N	2.48	0.41
38:l:74:PRO:O	38:l:78:SER:HB2	2.21	0.41
50:w:308:CLA:H3A	50:w:308:CLA:HBA2	1.63	0.41
46:w:312:LMG:H192	46:w:312:LMG:H162	1.87	0.41
50:y:308:CLA:H93	50:y:313:CLA:H43	2.02	0.41
50:y:310:CLA:H2	55:y:316:LUT:H363	2.00	0.41
50:z:316:CLA:NC	44:z:317:PGT:H11	2.35	0.41
11:A:225:LEU:HD22	11:A:230:ARG:HB2	2.02	0.41
21:K:155:LYS:HB3	24:N:175:TRP:HH2	1.86	0.41
27:a:403:ALA:HB2	43:a:830:BCR:H323	2.01	0.41
27:a:533:VAL:HG11	27:a:607:HIS:CG	2.55	0.41
27:a:534:HIS:ND1	50:a:823:CLA:HED2	2.36	0.41
28:b:395:ILE:HD13	28:b:555:TYR:HA	2.02	0.41
28:b:523:ILE:HG23	50:b:849:CLA:HBB1	2.03	0.41
40:x:206:LEU:HA	40:x:206:LEU:HD23	1.86	0.41
50:y:302:CLA:C4	55:y:315:LUT:H372	2.44	0.41
8:7:132:LEU:HA	8:7:132:LEU:HD23	1.86	0.41
18:H:195:ARG:O	18:H:196:ASN:C	2.64	0.41
43:a:810:BCR:H11C	43:a:810:BCR:H341	1.78	0.41
28:b:275:HIS:HE1	50:b:841:CLA:C4D	2.34	0.41
50:b:837:CLA:HBA1	50:b:837:CLA:H3A	1.71	0.41
33:g:136:ASN:O	33:g:140:VAL:HG23	2.21	0.41
46:w:312:LMG:H302	46:w:312:LMG:H331	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:x:308:CLA:H42	43:x:314:BCR:H402	2.02	0.41
21:K:94:GLU:OE2	23:M:102:ARG:NH2	2.54	0.41
27:a:33:SER:OG	27:a:34:ARG:N	2.54	0.41
34:h:60:LEU:HD23	34:h:60:LEU:HA	1.84	0.41
34:h:106:LEU:HD23	34:h:106:LEU:HA	1.94	0.41
50:w:308:CLA:CBB	55:w:320:LUT:H12	2.50	0.41
50:w:316:CLA:HED3	50:w:316:CLA:HBD	1.68	0.41
40:x:214:LEU:HD23	40:x:214:LEU:HA	1.89	0.41
50:z:306:CLA:C1A	55:z:320:LUT:H382	2.51	0.41
2:1:200:TYR:CE2	12:B:453:LEU:HD11	2.55	0.41
4:3:199:GLU:O	4:3:200:LYS:HG2	2.21	0.41
5:4:41:TRP:HB2	6:5:133:PHE:HD2	1.85	0.41
12:B:255:ASP:OD1	12:B:255:ASP:N	2.54	0.41
12:B:332:ILE:O	12:B:336:ILE:HG12	2.21	0.41
18:H:143:ASP:OD2	21:K:55:ARG:NH2	2.54	0.41
18:H:334:LYS:HZ2	18:H:334:LYS:HG3	1.58	0.41
46:H:401:LMG:O5	46:H:401:LMG:O4	2.27	0.41
19:I:76:ILE:HD12	19:I:103:ILE:HG22	2.01	0.41
21:K:3:SER:HB3	23:M:185:LYS:HD3	2.02	0.41
50:a:842:CLA:H92	50:a:842:CLA:H61	1.87	0.41
28:b:129:LEU:HD11	50:b:807:CLA:HMA2	2.02	0.41
28:b:340:SER:O	28:b:344:ILE:HG23	2.21	0.41
30:d:111:GLU:HG2	30:d:125:ARG:HA	2.01	0.41
46:f:306:LMG:H292	50:z:310:CLA:H3A	2.02	0.41
50:w:306:CLA:HED2	50:w:306:CLA:H2A	2.01	0.41
51:x:317:DGD:HG31	51:x:317:DGD:HD2	1.82	0.41
1:0:123:VAL:HG12	1:0:207:VAL:HG22	2.02	0.41
1:0:191:HIS:HA	1:0:207:VAL:O	2.21	0.41
2:1:276:ILE:HD13	2:1:276:ILE:HA	1.86	0.41
2:1:355:ILE:HG22	2:1:360:LEU:HD23	2.02	0.41
3:2:76:HIS:NE2	3:2:103:GLY:O	2.38	0.41
6:5:102:SER:HB3	6:5:104:GLU:CG	2.50	0.41
10:9:90:TYR:OH	10:9:247:GLU:OE2	2.30	0.41
11:A:335:MET:O	11:A:339:LEU:HG	2.21	0.41
11:A:336:ASP:OD1	11:A:337:GLN:N	2.53	0.41
12:B:161:LEU:HD21	15:E:73:GLU:HG2	2.02	0.41
14:D:483:LEU:O	14:D:487:VAL:HG13	2.21	0.41
16:F:253:ALA:HB1	16:F:265:HIS:NE2	2.36	0.41
18:H:209:ILE:HD11	18:H:368:LEU:HD11	2.01	0.41
19:I:41:GLN:O	19:I:45:GLU:N	2.52	0.41
21:K:12:ILE:HG13	21:K:13:ALA:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:108:ILE:HG12	23:M:115:MET:HB2	2.03	0.41
25:O:83:LEU:HD13	25:O:83:LEU:HA	1.88	0.41
26:U:213:ASP:OD1	26:U:213:ASP:N	2.54	0.41
27:a:302:PHE:CE1	50:a:843:CLA:HBB1	2.56	0.41
27:a:537:HIS:CE1	27:a:603:VAL:HG12	2.56	0.41
27:a:537:HIS:HE1	27:a:603:VAL:HG12	1.85	0.41
27:a:539:PHE:CE2	50:a:858:CLA:HAB	2.56	0.41
50:a:814:CLA:H111	50:a:814:CLA:H71	1.53	0.41
50:a:849:CLA:H41	50:a:849:CLA:H62	1.83	0.41
28:b:191:THR:HG21	28:b:278:LEU:HB2	2.03	0.41
28:b:365:PHE:HB3	28:b:602:TRP:CZ3	2.56	0.41
43:b:816:BCR:H313	50:b:828:CLA:H111	2.02	0.41
43:b:819:BCR:H363	50:b:838:CLA:H12	2.03	0.41
50:b:828:CLA:H62	50:b:828:CLA:H92	1.81	0.41
50:b:828:CLA:H42	44:z:301:PGT:H181	2.03	0.41
50:b:840:CLA:H62	50:b:840:CLA:H41	1.82	0.41
31:e:65:LYS:HB2	31:e:65:LYS:HE3	1.93	0.41
34:h:88:PHE:O	34:h:92:PHE:HB2	2.21	0.41
38:l:139:LEU:HA	38:l:142:ILE:HD12	2.03	0.41
50:l:305:CLA:HMB2	50:l:306:CLA:HMA2	2.02	0.41
50:w:306:CLA:H71	50:w:306:CLA:H112	1.78	0.41
50:w:307:CLA:HBB2	54:w:309:CHL:CAB	2.48	0.41
54:w:311:CHL:CBB	48:w:318:SQD:H81	2.46	0.41
54:x:311:CHL:HBB1	55:x:321:LUT:H161	2.02	0.41
11:A:82:THR:HB	21:K:29:SER:OG	2.21	0.41
11:A:264:LEU:HD23	11:A:264:LEU:HA	1.78	0.41
12:B:175:ARG:HE	12:B:175:ARG:HB2	1.71	0.41
12:B:403:LEU:HD22	12:B:408:LEU:HG	2.03	0.41
16:F:135:MET:HE1	16:F:272:ALA:HB2	2.02	0.41
18:H:19:HIS:HB3	18:H:22:MET:HG2	2.02	0.41
18:H:51:MET:HE3	18:H:70:TRP:CD1	2.56	0.41
27:a:12:ILE:HG21	50:a:811:CLA:HAA2	2.03	0.41
27:a:389:THR:HG23	27:a:605:ILE:HG21	2.03	0.41
43:a:827:BCR:H11C	43:a:827:BCR:H341	1.96	0.41
43:b:817:BCR:H15C	43:b:817:BCR:H351	1.91	0.41
50:y:303:CLA:CHB	55:y:315:LUT:H173	2.40	0.41
8:7:144:ASN:OD1	8:7:144:ASN:N	2.52	0.40
15:E:92:ARG:H	15:E:92:ARG:HG2	1.48	0.40
16:F:48:LEU:HD12	16:F:48:LEU:HA	1.84	0.40
16:F:677:ILE:HG23	48:F:801:SQD:H1	2.03	0.40
31:e:71:ARG:HB2	31:e:122:GLN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:w:110:MET:HE1	54:w:311:CHL:CAD	2.52	0.40
50:w:306:CLA:H92	50:w:306:CLA:H62	1.88	0.40
50:w:308:CLA:HAA1	55:w:320:LUT:H41	2.02	0.40
50:x:307:CLA:HMC2	55:x:321:LUT:C31	2.52	0.40
3:2:324:LEU:O	3:2:343:THR:HA	2.21	0.40
11:A:149:MET:HE2	11:A:149:MET:HB2	1.96	0.40
12:B:66:THR:HA	12:B:69:VAL:HG22	2.03	0.40
12:B:190:SER:OG	12:B:191:SER:N	2.54	0.40
16:F:714:LYS:O	46:F:802:LMG:O2	2.35	0.40
16:F:726:PHE:CD1	17:G:100:THR:HG22	2.56	0.40
18:H:340:PHE:HB3	18:H:353:LYS:HB3	2.04	0.40
43:a:829:BCR:H24C	43:a:829:BCR:H371	1.83	0.40
43:g:202:BCR:H11C	43:g:202:BCR:H341	1.94	0.40
41:y:141:ILE:HG22	41:y:143:PRO:HG2	2.03	0.40
44:z:317:PGT:H352	44:z:317:PGT:H322	1.94	0.40
2:1:417:SER:OG	2:1:419:GLU:OE1	2.39	0.40
4:3:80:PHE:HE2	4:3:100:ALA:HB3	1.86	0.40
11:A:89:ASN:OD1	11:A:254:LYS:NZ	2.54	0.40
11:A:278:LEU:HD11	11:A:319:PHE:HE2	1.86	0.40
12:B:309:LEU:HD22	16:F:713:ILE:HG21	2.04	0.40
13:C:61:ARG:HA	13:C:64:MET:HE2	2.03	0.40
20:J:109:PHE:O	20:J:112:ARG:HB2	2.21	0.40
28:b:177:HIS:HB3	50:b:833:CLA:HHC	2.03	0.40
28:b:583:MET:O	28:b:587:ILE:HG12	2.21	0.40
50:b:805:CLA:H2	50:b:805:CLA:H62	1.90	0.40
29:c:41:SER:HG	30:d:186:VAL:H	1.69	0.40
33:g:80:SER:HB3	33:g:151:ALA:HB2	2.02	0.40
33:g:164:PRO:HB2	50:g:201:CLA:C4C	2.51	0.40
43:i:101:BCR:H24C	43:i:101:BCR:H392	1.82	0.40
39:w:224:ILE:HD13	39:w:224:ILE:HA	1.98	0.40
40:x:213:MET:HB3	55:x:321:LUT:C34	2.51	0.40
41:y:135:TRP:HB2	55:y:316:LUT:H3	2.02	0.40
50:y:308:CLA:CHB	50:y:313:CLA:H111	2.52	0.40
43:4:101:BCR:H15C	43:4:101:BCR:H351	1.84	0.40
43:4:101:BCR:H361	43:4:101:BCR:H20C	1.81	0.40
7:6:139:LYS:HB2	7:6:139:LYS:NZ	2.36	0.40
11:A:117:ILE:HD11	11:A:136:TRP:HB2	2.03	0.40
11:A:118:ILE:HD13	11:A:118:ILE:HA	1.90	0.40
44:A:403:PGT:H362	44:A:403:PGT:H391	1.65	0.40
14:D:364:MET:HB3	14:D:367:ILE:HD11	2.02	0.40
14:D:423:ALA:HB1	16:F:187:PHE:CD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:567:ILE:HD12	16:F:567:ILE:HA	1.98	0.40
18:H:212:GLU:HB3	26:U:199:GLN:HB3	2.02	0.40
18:H:353:LYS:HG2	20:J:55:CYS:HB2	2.03	0.40
22:L:83:LEU:HD13	44:L:201:PGT:H41	2.03	0.40
50:a:834:CLA:HBB2	50:a:837:CLA:H72	2.03	0.40
50:a:838:CLA:H62	50:a:838:CLA:H92	1.80	0.40
28:b:33:SER:HG	28:b:396:ARG:HH22	1.69	0.40
28:b:668:ARG:HG3	28:b:700:LEU:O	2.21	0.40
40:x:181:ASN:ND2	40:x:186:PRO:HA	2.37	0.40
40:x:191:ASN:HA	55:x:320:LUT:O23	2.20	0.40
42:z:206:PHE:CE1	55:z:320:LUT:C16	3.05	0.40
43:z:318:BCR:H20C	43:z:318:BCR:H361	1.81	0.40
1:0:132:LYS:HB3	1:0:137:ASP:HB2	2.04	0.40
4:3:155:GLU:HG2	4:3:168:LEU:HB2	2.03	0.40
9:8:167:LEU:HA	9:8:167:LEU:HD23	1.87	0.40
11:A:331:PRO:HB3	18:H:125:ILE:HG22	2.03	0.40
14:D:228:ILE:HA	14:D:229:PRO:HA	1.94	0.40
16:F:115:MET:HG3	16:F:124:PHE:CD2	2.57	0.40
16:F:161:LEU:HD22	16:F:260:ILE:HG13	2.04	0.40
16:F:240:LYS:NZ	16:F:269:MET:HE3	2.37	0.40
18:H:16:GLY:HA2	18:H:27:ARG:HG3	2.03	0.40
20:J:5:LEU:HD23	20:J:84:VAL:HG21	2.04	0.40
50:a:835:CLA:H62	50:a:835:CLA:H41	1.91	0.40
50:a:853:CLA:H3A	50:a:853:CLA:HBA2	1.93	0.40
28:b:176:ASN:ND2	28:b:291:TYR:O	2.53	0.40
28:b:523:ILE:CG2	50:b:849:CLA:HBB1	2.51	0.40
28:b:548:PRO:HD2	29:c:62:PHE:CZ	2.57	0.40
50:b:841:CLA:H43	33:g:156:ALA:HB3	2.04	0.40
43:i:101:BCR:H20C	43:i:101:BCR:H361	1.91	0.40
39:w:99:GLU:OE1	48:w:317:SQD:O2	2.39	0.40
40:x:197:PRO:HG3	50:x:312:CLA:HED3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	155/157 (99%)	152 (98%)	3 (2%)	0	100	100
2	1	401/403 (100%)	393 (98%)	8 (2%)	0	100	100
3	2	292/372 (78%)	286 (98%)	5 (2%)	1 (0%)	36	68
4	3	137/139 (99%)	129 (94%)	8 (6%)	0	100	100
5	4	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
6	5	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
7	6	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
8	7	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
9	8	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
10	9	172/174 (99%)	167 (97%)	5 (3%)	0	100	100
11	A	348/350 (99%)	340 (98%)	8 (2%)	0	100	100
12	B	486/488 (100%)	453 (93%)	32 (7%)	1 (0%)	43	73
13	C	113/115 (98%)	103 (91%)	9 (8%)	1 (1%)	14	47
14	D	496/498 (100%)	483 (97%)	12 (2%)	1 (0%)	43	73
15	E	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
16	F	718/742 (97%)	683 (95%)	33 (5%)	2 (0%)	36	68
17	G	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
18	H	367/389 (94%)	352 (96%)	15 (4%)	0	100	100
19	I	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
20	J	156/158 (99%)	152 (97%)	4 (3%)	0	100	100
21	K	200/202 (99%)	189 (94%)	8 (4%)	3 (2%)	8	37
22	L	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
23	M	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	52
24	N	163/165 (99%)	156 (96%)	6 (4%)	1 (1%)	21	56
25	O	93/95 (98%)	90 (97%)	1 (1%)	2 (2%)	5	29
26	U	161/240 (67%)	151 (94%)	7 (4%)	3 (2%)	6	33
27	a	740/742 (100%)	721 (97%)	19 (3%)	0	100	100
28	b	731/733 (100%)	716 (98%)	15 (2%)	0	100	100
29	c	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
30	d	141/143 (99%)	135 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	e	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
32	f	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
33	g	95/97 (98%)	91 (96%)	2 (2%)	2 (2%)	5	31
34	h	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
35	i	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
36	j	40/42 (95%)	40 (100%)	0	0	100	100
37	k	62/130 (48%)	61 (98%)	1 (2%)	0	100	100
38	l	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
39	w	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
40	x	196/198 (99%)	194 (99%)	2 (1%)	0	100	100
41	y	219/221 (99%)	214 (98%)	5 (2%)	0	100	100
42	z	191/193 (99%)	188 (98%)	3 (2%)	0	100	100
All	All	8990/9337 (96%)	8691 (97%)	281 (3%)	18 (0%)	44	73

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	F	501	ASN
21	K	140	PRO
23	M	94	LEU
25	O	61	LYS
26	U	86	SER
26	U	87	PRO
33	g	164	PRO
12	B	247	ALA
21	K	13	ALA
24	N	67	ILE
25	O	66	VAL
3	2	245	LYS
16	F	535	LYS
21	K	14	GLN
26	U	90	MET
13	C	55	TRP
14	D	412	LEU
33	g	163	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	143/143 (100%)	140 (98%)	3 (2%)	47	71
2	1	340/340 (100%)	334 (98%)	6 (2%)	51	74
3	2	260/321 (81%)	253 (97%)	7 (3%)	39	68
4	3	120/120 (100%)	116 (97%)	4 (3%)	33	65
5	4	76/76 (100%)	76 (100%)	0	100	100
6	5	131/131 (100%)	127 (97%)	4 (3%)	35	66
7	6	112/112 (100%)	112 (100%)	0	100	100
8	7	123/123 (100%)	120 (98%)	3 (2%)	43	70
9	8	114/115 (99%)	112 (98%)	2 (2%)	51	74
10	9	143/144 (99%)	138 (96%)	5 (4%)	32	64
11	A	296/304 (97%)	289 (98%)	7 (2%)	43	70
12	B	424/424 (100%)	408 (96%)	16 (4%)	29	62
13	C	99/99 (100%)	96 (97%)	3 (3%)	36	66
14	D	430/430 (100%)	421 (98%)	9 (2%)	47	71
15	E	86/86 (100%)	83 (96%)	3 (4%)	32	64
16	F	626/652 (96%)	614 (98%)	12 (2%)	50	73
17	G	153/153 (100%)	148 (97%)	5 (3%)	33	65
18	H	321/339 (95%)	318 (99%)	3 (1%)	70	81
19	I	150/150 (100%)	147 (98%)	3 (2%)	48	72
20	J	140/140 (100%)	135 (96%)	5 (4%)	31	63
21	K	180/180 (100%)	173 (96%)	7 (4%)	28	62
22	L	99/99 (100%)	94 (95%)	5 (5%)	21	54
23	M	129/129 (100%)	127 (98%)	2 (2%)	55	75
24	N	139/139 (100%)	138 (99%)	1 (1%)	76	83
25	O	87/87 (100%)	83 (95%)	4 (5%)	24	58
26	U	127/212 (60%)	124 (98%)	3 (2%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	a	598/598 (100%)	586 (98%)	12 (2%)	48	72
28	b	599/599 (100%)	591 (99%)	8 (1%)	61	78
29	c	71/71 (100%)	69 (97%)	2 (3%)	38	68
30	d	122/122 (100%)	119 (98%)	3 (2%)	42	69
31	e	60/60 (100%)	60 (100%)	0	100	100
32	f	126/126 (100%)	125 (99%)	1 (1%)	73	82
33	g	82/82 (100%)	82 (100%)	0	100	100
34	h	79/79 (100%)	79 (100%)	0	100	100
35	i	27/27 (100%)	26 (96%)	1 (4%)	30	63
36	j	37/37 (100%)	37 (100%)	0	100	100
37	k	49/97 (50%)	48 (98%)	1 (2%)	48	72
38	l	123/123 (100%)	122 (99%)	1 (1%)	73	82
39	w	177/177 (100%)	171 (97%)	6 (3%)	32	64
40	x	166/166 (100%)	164 (99%)	2 (1%)	63	79
41	y	173/173 (100%)	173 (100%)	0	100	100
42	z	154/154 (100%)	148 (96%)	6 (4%)	28	62
All	All	7691/7939 (97%)	7526 (98%)	165 (2%)	46	71

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	96	VAL
1	0	133	ASN
1	0	135	VAL
2	1	76	MET
2	1	203	MET
2	1	355	ILE
2	1	440	THR
2	1	454	THR
2	1	455	LEU
3	2	34	ASP
3	2	58	VAL
3	2	149	ARG
3	2	165	CYS
3	2	227	SER
3	2	348	ILE

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Mol	Chain	Res	Type
3	2	367	GLU
4	3	101	THR
4	3	136	SER
4	3	138	MET
4	3	176	THR
6	5	73	ASP
6	5	103	SER
6	5	104	GLU
6	5	145	VAL
8	7	141	ASP
8	7	161	PHE
8	7	170	VAL
9	8	142	THR
9	8	163	VAL
10	9	115	VAL
10	9	129	GLU
10	9	167	ARG
10	9	193	THR
10	9	196	SER
11	A	36	LEU
11	A	123	ARG
11	A	125	VAL
11	A	213	GLN
11	A	259	TYR
11	A	338	LEU
11	A	365	LEU
12	B	20	LYS
12	B	24	LEU
12	B	61	TYR
12	B	127	THR
12	B	131	LEU
12	B	133	ILE
12	B	180	THR
12	B	225	ASN
12	B	226	SER
12	B	264	VAL
12	B	296	HIS
12	B	352	ILE
12	B	369	ILE
12	B	459	ASN
12	B	478	ASN
12	B	493	ILE

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Mol	Chain	Res	Type
13	C	49	GLU
13	C	73	ASP
13	C	104	LEU
14	D	170	TYR
14	D	201	VAL
14	D	232	THR
14	D	294	THR
14	D	326	THR
14	D	378	PHE
14	D	422	MET
14	D	446	LEU
14	D	496	ASN
15	E	13	LEU
15	E	44	ASN
15	E	63	SER
16	F	4	ILE
16	F	10	ILE
16	F	27	LEU
16	F	43	SER
16	F	129	SER
16	F	187	PHE
16	F	324	MET
16	F	363	LEU
16	F	490	LYS
16	F	584	THR
16	F	654	ILE
16	F	729	LEU
17	G	67	VAL
17	G	70	ILE
17	G	92	LEU
17	G	138	ILE
17	G	150	THR
18	H	40	CYS
18	H	70	TRP
18	H	263	ILE
19	I	50	SER
19	I	87	THR
19	I	160	ASN
20	J	35	ASP
20	J	58	ASP
20	J	75	GLU
20	J	143	ARG

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Mol	Chain	Res	Type
20	J	145	ASP
21	K	26	SER
21	K	43	CYS
21	K	58	PHE
21	K	73	ASP
21	K	80	THR
21	K	81	VAL
21	K	139	CYS
22	L	92	VAL
22	L	117	ASN
22	L	152	THR
22	L	165	GLU
22	L	175	TRP
23	M	80	VAL
23	M	126	MET
24	N	75	LEU
25	O	66	VAL
25	O	83	LEU
25	O	117	GLU
25	O	150	GLU
26	U	128	THR
26	U	130	ASP
26	U	210	GLU
27	a	15	ASP
27	a	159	THR
27	a	259	THR
27	a	312	ASN
27	a	363	VAL
27	a	369	TYR
27	a	584	VAL
27	a	625	VAL
27	a	626	VAL
27	a	630	THR
27	a	700	VAL
27	a	749	VAL
28	b	38	THR
28	b	96	PHE
28	b	210	ASN
28	b	272	ASP
28	b	293	THR
28	b	294	ASN
28	b	394	PHE

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Mol	Chain	Res	Type
28	b	477	LEU
29	c	10	THR
29	c	73	THR
30	d	113	ILE
30	d	125	ARG
30	d	155	GLN
32	f	105	SER
35	i	11	VAL
37	k	97	ASP
38	l	60	GLN
39	w	55	ILE
39	w	131	ILE
39	w	153	THR
39	w	158	GLN
39	w	208	TRP
39	w	216	VAL
40	x	61	LEU
40	x	141	THR
42	z	58	HIS
42	z	77	VAL
42	z	134	VAL
42	z	176	LEU
42	z	181	ASP
42	z	238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	119	GLN
1	0	199	ASN
2	1	142	GLN
2	1	170	ASN
4	3	96	HIS
10	9	173	ASN
10	9	188	ASN
11	A	213	GLN
11	A	361	GLN
12	B	147	ASN
12	B	468	ASN
13	C	57	GLN
14	D	110	ASN
15	E	44	ASN

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Mol	Chain	Res	Type
16	F	176	GLN
16	F	390	HIS
16	F	459	ASN
16	F	534	ASN
16	F	571	GLN
17	G	142	GLN
18	H	18	HIS
19	I	96	ASN
20	J	12	HIS
20	J	24	GLN
20	J	124	ASN
21	K	23	ASN
21	K	172	ASN
23	M	117	GLN
27	a	214	GLN
27	a	721	GLN
28	b	10	GLN
28	b	156	HIS
28	b	333	GLN
28	b	506	ASN
28	b	704	GLN
30	d	112	GLN
32	f	223	ASN
33	g	107	GLN
39	w	240	GLN
40	x	99	ASN
41	y	254	ASN
42	z	209	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

248 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	LUT	y	316	-	42,43,43	0.87	0	51,60,60	0.77	1 (1%)
43	BCR	l	302	-	41,41,41	0.66	0	56,56,56	1.04	3 (5%)
54	CHL	z	312	42	55,69,74	2.04	12 (21%)	52,108,114	2.66	19 (36%)
50	CLA	a	856	-	68,72,73	1.20	7 (10%)	80,111,113	1.46	9 (11%)
46	LMG	f	306	-	34,34,55	1.01	1 (2%)	42,42,63	1.15	2 (4%)
51	DGD	a	804	-	67,67,67	1.01	2 (2%)	81,81,81	1.00	1 (1%)
50	CLA	a	824	-	69,73,73	1.23	6 (8%)	82,113,113	1.68	9 (10%)
44	PGT	B	602	-	41,41,50	0.53	0	44,47,56	0.45	0
50	CLA	x	306	-	64,68,73	1.28	7 (10%)	76,107,113	1.66	9 (11%)
43	BCR	b	816	-	41,41,41	0.69	0	56,56,56	1.17	6 (10%)
43	BCR	y	301	-	41,41,41	0.67	0	56,56,56	1.06	3 (5%)
50	CLA	w	302	-	54,58,73	1.40	8 (14%)	64,95,113	1.78	7 (10%)
44	PGT	a	805	-	31,31,50	0.60	0	34,37,56	0.57	0
50	CLA	y	302	41	56,60,73	1.44	11 (19%)	69,97,113	2.09	13 (18%)
50	CLA	a	815	27	69,73,73	1.23	9 (13%)	82,113,113	1.65	8 (9%)
50	CLA	b	811	-	49,53,73	1.41	7 (14%)	58,89,113	1.77	7 (12%)
50	CLA	a	834	-	69,73,73	1.23	7 (10%)	82,113,113	1.60	6 (7%)
51	DGD	x	317	-	49,49,67	1.11	0	63,63,81	1.04	1 (1%)
50	CLA	g	203	-	56,60,73	1.36	7 (12%)	65,97,113	1.66	8 (12%)
44	PGT	5	301	-	34,34,50	0.58	0	37,40,56	0.59	0
46	LMG	j	105	-	37,37,55	0.95	1 (2%)	45,45,63	1.07	1 (2%)
43	BCR	w	301	-	41,41,41	0.64	0	56,56,56	1.06	4 (7%)
43	BCR	a	810	-	30,30,41	0.88	1 (3%)	39,39,56	1.34	5 (12%)
50	CLA	b	807	-	69,73,73	1.22	6 (8%)	82,113,113	1.66	8 (9%)
50	CLA	b	810	-	54,58,73	1.39	6 (11%)	64,95,113	1.74	6 (9%)
50	CLA	y	310	41	69,73,73	1.22	6 (8%)	82,113,113	1.66	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	LMG	H	401	-	33,33,55	1.06	2 (6%)	41,41,63	1.26	4 (9%)
50	CLA	a	823	-	59,63,73	1.32	7 (11%)	70,101,113	1.68	7 (10%)
43	BCR	a	827	-	40,40,41	0.69	0	54,54,56	1.14	5 (9%)
50	CLA	b	823	-	59,63,73	1.33	7 (11%)	70,101,113	1.68	8 (11%)
50	CLA	b	849	-	54,58,73	1.40	8 (14%)	64,95,113	1.75	7 (10%)
43	BCR	a	829	-	41,41,41	0.76	0	56,56,56	1.17	6 (10%)
50	CLA	z	307	42	64,68,73	1.29	8 (12%)	76,107,113	1.67	7 (9%)
50	CLA	x	308	-	54,58,73	1.38	6 (11%)	64,95,113	1.80	9 (14%)
50	CLA	y	308	-	69,73,73	1.24	7 (10%)	82,113,113	1.65	7 (8%)
49	SF4	K	301	21	0,12,12	-	-	-	-	-
50	CLA	b	808	-	47,51,73	1.39	7 (14%)	55,86,113	1.78	5 (9%)
43	BCR	b	820	-	41,41,41	0.70	0	56,56,56	1.15	6 (10%)
46	LMG	F	802	-	28,28,55	1.09	2 (7%)	36,36,63	1.16	2 (5%)
50	CLA	y	307	-	45,49,73	1.44	8 (17%)	54,84,113	2.06	6 (11%)
50	CLA	b	838	-	56,60,73	1.37	7 (12%)	65,97,113	1.79	8 (12%)
50	CLA	b	848	-	46,50,73	1.42	7 (15%)	53,85,113	1.88	6 (11%)
50	CLA	a	846	-	69,73,73	1.24	7 (10%)	82,113,113	1.68	9 (10%)
50	CLA	y	314	41	69,73,73	1.24	8 (11%)	82,113,113	1.58	10 (12%)
50	CLA	z	316	44	51,55,73	1.38	7 (13%)	60,91,113	1.73	6 (10%)
50	CLA	a	812	-	60,66,73	1.79	9 (15%)	69,101,113	2.08	11 (15%)
44	PGT	B	606	-	34,34,50	0.54	0	37,40,56	0.74	1 (2%)
50	CLA	l	301	-	49,53,73	1.42	7 (14%)	58,89,113	1.79	6 (10%)
50	CLA	w	308	39	69,73,73	1.23	5 (7%)	82,113,113	1.69	11 (13%)
50	CLA	b	805	28	69,73,73	1.23	6 (8%)	82,113,113	1.69	10 (12%)
45	A1H1M	5	302	-	41,41,41	1.07	3 (7%)	58,58,58	1.91	13 (22%)
44	PGT	b	830	50	38,38,50	0.55	0	41,44,56	0.51	0
50	CLA	b	847	-	64,68,73	1.28	6 (9%)	76,107,113	1.74	9 (11%)
50	CLA	b	851	-	51,55,73	1.38	7 (13%)	60,91,113	1.77	7 (11%)
50	CLA	f	301	-	61,65,73	1.30	6 (9%)	72,103,113	1.78	9 (12%)
50	CLA	f	303	-	45,49,73	1.44	8 (17%)	54,84,113	1.83	7 (12%)
50	CLA	x	312	40	69,73,73	1.23	7 (10%)	82,113,113	1.60	9 (10%)
46	LMG	w	312	-	40,40,55	0.94	1 (2%)	48,48,63	1.11	2 (4%)
50	CLA	a	842	-	69,73,73	1.23	6 (8%)	82,113,113	1.57	9 (10%)
49	SF4	I	202	19	0,12,12	-	-	-	-	-
50	CLA	b	814	-	69,73,73	1.25	7 (10%)	82,113,113	1.73	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	CLA	z	308	-	44,50,73	1.54	9 (20%)	47,82,113	2.12	7 (14%)
50	CLA	a	849	-	69,73,73	1.24	6 (8%)	82,113,113	1.56	10 (12%)
54	CHL	w	311	-	41,55,74	2.14	10 (24%)	34,90,114	3.29	15 (44%)
50	CLA	f	302	-	46,50,73	1.41	6 (13%)	53,85,113	1.90	5 (9%)
44	PGT	D	602	-	33,33,50	0.57	0	36,39,56	0.62	0
50	CLA	b	826	-	59,63,73	1.33	7 (11%)	70,101,113	1.75	8 (11%)
50	CLA	a	826	44	49,53,73	1.40	7 (14%)	58,89,113	1.75	6 (10%)
54	CHL	x	305	-	40,54,74	2.26	11 (27%)	34,90,114	3.26	17 (50%)
50	CLA	a	848	-	56,60,73	1.36	6 (10%)	65,97,113	1.70	9 (13%)
50	CLA	z	309	-	46,50,73	1.41	7 (15%)	53,85,113	1.79	4 (7%)
50	CLA	w	303	39	49,53,73	1.41	8 (16%)	58,89,113	1.81	7 (12%)
50	CLA	x	316	-	49,53,73	1.41	6 (12%)	58,89,113	1.77	5 (8%)
50	CLA	a	801	-	69,73,73	1.23	6 (8%)	82,113,113	1.63	7 (8%)
46	LMG	x	315	-	48,48,55	0.83	2 (4%)	56,56,63	1.10	2 (3%)
50	CLA	a	811	-	69,73,73	1.23	6 (8%)	82,113,113	1.66	9 (10%)
46	LMG	z	314	-	40,40,55	1.11	4 (10%)	48,48,63	1.07	1 (2%)
55	LUT	x	320	-	42,43,43	0.86	0	51,60,60	0.56	0
55	LUT	x	321	-	42,43,43	0.87	0	51,60,60	0.86	2 (3%)
50	CLA	b	844	28	69,73,73	1.23	7 (10%)	82,113,113	1.63	9 (10%)
44	PGT	z	301	-	44,44,50	0.51	0	47,50,56	0.51	0
50	CLA	y	305	41	49,53,73	1.41	6 (12%)	58,89,113	1.76	5 (8%)
43	BCR	b	819	-	41,41,41	0.75	1 (2%)	56,56,56	1.26	6 (10%)
43	BCR	g	202	-	41,41,41	0.72	0	56,56,56	1.01	3 (5%)
43	BCR	f	304	-	41,41,41	0.69	1 (2%)	56,56,56	1.05	5 (8%)
50	CLA	x	302	-	45,49,73	1.44	8 (17%)	54,84,113	1.94	9 (16%)
50	CLA	z	306	42	60,64,73	1.30	6 (10%)	71,102,113	1.78	12 (16%)
50	CLA	x	318	-	47,53,73	1.34	5 (10%)	54,88,113	1.86	6 (11%)
50	CLA	z	310	42	45,49,73	1.42	7 (15%)	54,84,113	1.94	9 (16%)
50	CLA	k	205	-	46,50,73	1.40	6 (13%)	53,85,113	1.84	7 (13%)
43	BCR	j	101	-	41,41,41	0.73	0	56,56,56	1.17	3 (5%)
43	BCR	a	830	-	41,41,41	0.70	0	56,56,56	1.04	4 (7%)
50	CLA	x	304	40	51,55,73	1.37	5 (9%)	60,91,113	1.73	6 (10%)
50	CLA	a	858	-	69,73,73	1.22	6 (8%)	82,113,113	1.49	8 (9%)
44	PGT	b	829	-	47,47,50	0.50	0	50,53,56	0.45	0
50	CLA	b	837	-	69,73,73	1.23	7 (10%)	82,113,113	1.66	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
43	BCR	4	101	-	41,41,41	0.66	0	56,56,56	1.21	4 (7%)
43	BCR	b	817	-	41,41,41	0.69	0	56,56,56	1.19	6 (10%)
50	CLA	b	828	-	64,68,73	1.29	7 (10%)	76,107,113	1.59	8 (10%)
50	CLA	b	840	-	69,73,73	1.22	6 (8%)	82,113,113	1.62	7 (8%)
50	CLA	w	306	39	69,73,73	1.24	8 (11%)	82,113,113	1.60	9 (10%)
44	PGT	z	317	50	45,45,50	0.51	0	48,51,56	0.48	0
49	SF4	I	201	19	0,12,12	-	-	-	-	-
50	CLA	a	819	-	64,68,73	1.28	7 (10%)	76,107,113	1.65	8 (10%)
50	CLA	a	841	-	59,63,73	1.33	6 (10%)	70,101,113	1.69	7 (10%)
43	BCR	b	831	-	41,41,41	0.65	0	56,56,56	1.35	8 (14%)
47	PQ9	A	405	-	36,36,45	2.92	20 (55%)	44,46,57	10.90	22 (50%)
50	CLA	b	841	-	59,63,73	1.33	8 (13%)	70,101,113	1.76	7 (10%)
54	CHL	w	304	-	40,53,74	2.39	12 (30%)	35,89,114	3.21	17 (48%)
49	SF4	c	101	29	0,12,12	-	-	-	-	-
50	CLA	x	307	40	64,68,73	1.27	8 (12%)	76,107,113	1.72	9 (11%)
53	PQN	a	825	-	34,34,34	1.02	3 (8%)	43,45,45	1.76	10 (23%)
50	CLA	a	821	-	67,71,73	1.27	8 (11%)	81,110,113	1.88	10 (12%)
50	CLA	a	814	-	69,73,73	1.23	6 (8%)	82,113,113	1.67	8 (9%)
50	CLA	w	316	39	54,58,73	1.37	6 (11%)	64,95,113	1.88	9 (14%)
50	CLA	z	302	-	59,63,73	1.33	7 (11%)	70,101,113	1.68	8 (11%)
54	CHL	x	311	-	34,48,74	2.39	9 (26%)	32,82,114	2.95	12 (37%)
55	LUT	y	315	-	42,43,43	0.89	0	51,60,60	0.62	0
50	CLA	z	303	-	45,49,73	1.45	8 (17%)	54,84,113	1.76	8 (14%)
44	PGT	I	203	-	43,43,50	0.52	0	46,49,56	0.48	0
50	CLA	w	307	-	49,53,73	1.44	7 (14%)	58,89,113	1.71	6 (10%)
50	CLA	a	852	-	55,59,73	1.36	6 (10%)	64,96,113	1.77	8 (12%)
50	CLA	a	843	-	69,73,73	1.24	7 (10%)	82,113,113	1.66	9 (10%)
50	CLA	b	839	-	69,73,73	1.23	7 (10%)	82,113,113	1.63	9 (10%)
43	BCR	l	303	-	41,41,41	0.65	0	56,56,56	1.22	5 (8%)
50	CLA	a	844	-	61,65,73	1.30	6 (9%)	72,103,113	1.64	10 (13%)
50	CLA	b	803	-	69,73,73	1.23	6 (8%)	82,113,113	1.78	10 (12%)
44	PGT	f	305	-	38,38,50	0.54	0	41,44,56	0.51	0
50	CLA	b	822	-	62,66,73	1.30	7 (11%)	73,104,113	1.72	8 (10%)
50	CLA	a	833	-	69,73,73	1.23	7 (10%)	82,113,113	1.58	11 (13%)
50	CLA	a	820	-	69,73,73	1.21	7 (10%)	82,113,113	1.59	10 (12%)
50	CLA	b	804	-	45,49,73	1.43	7 (15%)	54,84,113	1.81	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	CLA	b	832	-	58,62,73	1.34	6 (10%)	68,99,113	1.72	8 (11%)
44	PGT	a	806	50	32,32,50	0.60	0	35,38,56	0.54	0
55	LUT	w	319	-	42,43,43	0.83	0	51,60,60	0.94	2 (3%)
44	PGT	A	403	-	37,37,50	0.32	0	40,43,56	0.38	0
44	PGT	w	313	50	39,39,50	0.54	0	42,45,56	0.51	0
55	LUT	w	320	-	42,43,43	0.78	0	51,60,60	0.69	1 (1%)
46	LMG	D	601	-	34,34,55	1.00	1 (2%)	42,42,63	1.14	3 (7%)
53	PQN	b	827	-	34,34,34	1.03	3 (8%)	43,45,45	1.82	10 (23%)
50	CLA	b	836	-	69,73,73	1.23	7 (10%)	82,113,113	1.62	9 (10%)
49	SF4	c	102	29	0,12,12	-	-	-	-	-
50	CLA	w	310	-	69,73,73	1.24	6 (8%)	82,113,113	1.72	15 (18%)
50	CLA	a	851	27	50,54,73	1.40	7 (14%)	59,90,113	1.78	6 (10%)
43	BCR	b	818	-	41,41,41	0.68	0	56,56,56	1.04	3 (5%)
50	CLA	a	850	-	69,73,73	1.22	6 (8%)	82,113,113	1.55	9 (10%)
50	CLA	w	305	-	55,59,73	1.37	7 (12%)	64,96,113	1.88	7 (10%)
50	CLA	a	816	-	46,50,73	1.40	6 (13%)	53,85,113	1.72	4 (7%)
43	BCR	a	803	-	27,27,41	0.70	0	34,35,56	1.23	2 (5%)
49	SF4	a	832	28,27	0,12,12	-	-	-	-	-
50	CLA	a	838	-	69,73,73	1.22	6 (8%)	82,113,113	1.69	10 (12%)
43	BCR	a	831	-	40,40,41	0.66	0	54,54,56	1.16	5 (9%)
50	CLA	w	314	44	47,52,73	1.41	7 (14%)	55,87,113	1.88	7 (12%)
44	PGT	z	313	-	32,32,50	0.58	0	35,38,56	0.54	0
44	PGT	a	807	-	45,45,50	0.51	0	48,51,56	0.51	0
50	CLA	a	854	-	69,73,73	1.22	6 (8%)	82,113,113	1.54	10 (12%)
50	CLA	a	809	-	61,65,73	1.30	7 (11%)	72,103,113	1.73	10 (13%)
50	CLA	a	817	-	45,49,73	1.45	7 (15%)	54,84,113	1.75	5 (9%)
50	CLA	b	824	44	69,73,73	1.23	6 (8%)	82,113,113	1.70	8 (9%)
44	PGT	B	603	-	45,45,50	0.51	0	48,51,56	0.46	0
50	CLA	b	801	-	69,73,73	1.23	6 (8%)	82,113,113	1.60	8 (9%)
50	CLA	b	812	-	66,70,73	1.25	7 (10%)	78,109,113	1.63	11 (14%)
50	CLA	y	309	-	46,50,73	1.44	7 (15%)	53,85,113	1.64	4 (7%)
50	CLA	a	818	-	63,67,73	1.28	7 (11%)	74,105,113	1.62	10 (13%)
50	CLA	a	853	-	69,73,73	1.23	6 (8%)	82,113,113	1.64	9 (10%)
44	PGT	A	404	-	43,43,50	0.52	0	46,49,56	0.47	0
50	CLA	y	306	-	42,48,73	1.38	8 (19%)	49,82,113	1.92	7 (14%)
46	LMG	B	605	-	37,37,55	0.98	2 (5%)	45,45,63	1.05	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	CL0	a	808	-	55,69,73	3.19	17 (30%)	58,107,113	2.17	14 (24%)
46	LMG	z	315	-	36,36,55	0.97	1 (2%)	44,44,63	1.13	2 (4%)
50	CLA	a	847	-	40,48,73	1.63	4 (10%)	48,76,113	1.41	8 (16%)
46	LMG	7	301	-	41,41,55	0.99	1 (2%)	49,49,63	1.23	4 (8%)
50	CLA	x	310	-	47,51,73	1.39	6 (12%)	55,86,113	1.71	5 (9%)
54	CHL	x	301	-	37,51,74	2.31	11 (29%)	30,86,114	3.27	14 (46%)
48	SQD	w	317	-	29,31,54	0.54	1 (3%)	39,42,65	0.58	0
50	CLA	b	835	-	63,67,73	1.28	6 (9%)	74,105,113	1.63	7 (9%)
50	CLA	b	809	-	63,67,73	1.28	7 (11%)	74,105,113	1.65	9 (12%)
44	PGT	L	201	-	39,39,50	0.55	0	42,45,56	0.55	0
44	PGT	B	601	-	33,33,50	0.58	0	36,39,56	0.57	0
45	A1H1M	F	804	-	41,41,41	1.27	5 (12%)	58,58,58	1.83	16 (27%)
50	CLA	a	840	-	46,50,73	1.40	7 (15%)	53,85,113	1.77	5 (9%)
50	CLA	a	855	-	46,50,73	1.41	6 (13%)	53,85,113	1.85	6 (11%)
50	CLA	l	306	-	64,68,73	1.30	9 (14%)	76,107,113	1.67	10 (13%)
50	CLA	k	204	-	61,65,73	1.31	6 (9%)	72,103,113	1.76	8 (11%)
48	SQD	a	859	-	34,36,54	0.51	1 (2%)	44,47,65	0.83	1 (2%)
50	CLA	b	842	-	61,65,73	1.30	6 (9%)	72,103,113	1.60	8 (11%)
50	CLA	x	313	40	57,61,73	1.38	8 (14%)	67,98,113	1.66	9 (13%)
50	CLA	g	201	-	53,57,73	1.37	7 (13%)	61,93,113	1.60	6 (9%)
55	LUT	z	320	-	42,43,43	0.96	1 (2%)	51,60,60	0.67	0
50	CLA	b	802	-	69,73,73	1.21	6 (8%)	82,113,113	1.54	8 (9%)
50	CLA	a	802	-	64,68,73	1.29	7 (10%)	76,107,113	1.63	9 (11%)
50	CLA	b	815	-	69,73,73	1.23	8 (11%)	82,113,113	1.68	9 (10%)
50	CLA	h	201	34	50,54,73	1.40	6 (12%)	59,90,113	1.83	5 (8%)
50	CLA	b	833	-	69,73,73	1.22	7 (10%)	82,113,113	1.67	9 (10%)
48	SQD	B	604	-	38,40,54	0.52	1 (2%)	48,51,65	0.62	0
43	BCR	i	101	-	41,41,41	0.66	0	56,56,56	1.14	3 (5%)
48	SQD	w	318	-	39,41,54	0.44	1 (2%)	49,52,65	0.92	3 (6%)
50	CLA	b	813	-	47,51,73	1.40	7 (14%)	55,86,113	1.65	6 (10%)
50	CLA	y	304	-	41,47,73	1.49	8 (19%)	51,81,113	1.82	4 (7%)
44	PGT	F	803	-	42,42,50	0.52	0	45,48,56	0.48	0
51	DGD	b	821	-	60,60,67	1.01	1 (1%)	74,74,81	1.02	3 (4%)
50	CLA	a	822	-	55,59,73	1.37	7 (12%)	64,96,113	1.92	9 (14%)
50	CLA	x	303	40	61,65,73	1.34	6 (9%)	72,103,113	1.63	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	CLA	b	834	-	49,53,73	1.41	7 (14%)	58,89,113	1.69	6 (10%)
50	CLA	a	857	-	69,73,73	1.23	6 (8%)	82,113,113	1.65	8 (9%)
50	CLA	b	845	-	69,73,73	1.25	6 (8%)	82,113,113	1.43	8 (9%)
50	CLA	y	313	41	69,73,73	1.23	8 (11%)	82,113,113	1.75	8 (9%)
50	CLA	a	839	-	69,73,73	1.22	7 (10%)	82,113,113	1.55	9 (10%)
50	CLA	j	102	36	46,50,73	1.41	6 (13%)	53,85,113	1.88	6 (11%)
50	CLA	a	836	27	69,73,73	1.22	5 (7%)	82,113,113	1.58	8 (9%)
54	CHL	x	319	42	44,58,74	2.21	11 (25%)	37,94,114	3.10	17 (45%)
50	CLA	a	835	-	62,66,73	1.30	6 (9%)	73,104,113	1.71	9 (12%)
48	SQD	F	801	-	39,41,54	0.45	1 (2%)	49,52,65	1.05	2 (4%)
43	BCR	j	103	-	41,41,41	0.71	0	56,56,56	1.16	4 (7%)
50	CLA	g	204	33	47,51,73	1.41	7 (14%)	55,86,113	1.71	5 (9%)
48	SQD	j	106	-	40,42,54	0.45	1 (2%)	50,53,65	0.57	1 (2%)
54	CHL	w	309	-	37,51,74	2.31	10 (27%)	30,86,114	3.27	13 (43%)
44	PGT	A	401	-	31,31,50	0.59	0	34,37,56	0.61	0
50	CLA	b	846	-	69,73,73	1.22	6 (8%)	82,113,113	1.61	8 (9%)
50	CLA	l	305	38	44,48,73	1.46	7 (15%)	53,83,113	1.77	7 (13%)
50	CLA	b	806	-	56,60,73	1.36	6 (10%)	65,97,113	1.79	8 (12%)
43	BCR	z	318	-	41,41,41	0.71	0	56,56,56	1.40	5 (8%)
43	BCR	k	201	-	41,41,41	0.70	0	56,56,56	1.48	10 (17%)
44	PGT	N	301	-	25,25,50	0.65	0	28,31,56	0.60	0
43	BCR	a	828	-	41,41,41	0.70	0	56,56,56	1.10	3 (5%)
46	LMG	j	104	-	34,34,55	1.02	1 (2%)	42,42,63	1.15	2 (4%)
43	BCR	b	850	-	41,41,41	0.72	0	56,56,56	1.18	5 (8%)
50	CLA	k	203	-	45,49,73	1.47	8 (17%)	54,84,113	1.81	6 (11%)
50	CLA	x	309	-	46,50,73	1.41	7 (15%)	53,85,113	1.83	5 (9%)
54	CHL	z	304	42	36,50,74	2.36	10 (27%)	29,85,114	3.50	15 (51%)
50	CLA	y	311	-	55,59,73	1.38	9 (16%)	64,96,113	1.87	8 (12%)
48	SQD	F	805	-	41,43,54	0.46	0	51,54,65	0.79	2 (3%)
50	CLA	w	315	39	50,54,73	1.41	6 (12%)	59,90,113	1.80	6 (10%)
43	BCR	k	202	-	41,41,41	0.72	1 (2%)	56,56,56	1.14	3 (5%)
43	BCR	x	314	-	41,41,41	0.62	0	56,56,56	1.18	4 (7%)
50	CLA	a	813	-	56,60,73	1.35	7 (12%)	65,97,113	1.67	8 (12%)
50	CLA	z	305	-	54,58,73	1.38	6 (11%)	64,95,113	1.73	7 (10%)
50	CLA	b	825	-	69,73,73	1.24	6 (8%)	82,113,113	1.58	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	CLA	y	312	-	55,59,73	1.35	6 (10%)	64,96,113	1.74	8 (12%)
50	CLA	y	303	-	59,63,73	1.33	6 (10%)	70,101,113	1.75	7 (10%)
55	LUT	z	321	-	42,43,43	0.86	0	51,60,60	0.73	1 (1%)
50	CLA	z	311	-	59,63,73	1.32	6 (10%)	70,101,113	1.59	6 (8%)
50	CLA	b	843	-	69,73,73	1.22	7 (10%)	82,113,113	1.68	8 (9%)
44	PGT	A	402	-	36,36,50	0.57	0	39,42,56	0.52	0
50	CLA	a	845	-	69,73,73	1.24	6 (8%)	82,113,113	1.62	8 (9%)
50	CLA	z	319	-	46,50,73	1.44	6 (13%)	53,85,113	1.75	4 (7%)
43	BCR	l	304	-	41,41,41	0.68	0	56,56,56	1.09	4 (7%)
50	CLA	a	837	-	69,73,73	1.24	6 (8%)	82,113,113	1.61	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	LUT	y	316	-	-	4/29/67/67	0/2/2/2
43	BCR	l	302	-	-	8/29/63/63	0/2/2/2
54	CHL	z	312	42	3/3/19/26	12/33/131/137	-
50	CLA	a	856	-	1/1/14/20	8/37/113/115	-
46	LMG	f	306	-	-	12/29/49/70	0/1/1/1
51	DGD	a	804	-	-	32/55/95/95	0/2/2/2
50	CLA	a	824	-	1/1/15/20	15/39/115/115	-
50	CLA	x	306	-	1/1/14/20	12/33/109/115	-
44	PGT	B	602	-	-	10/46/46/55	-
43	BCR	b	816	-	-	6/29/63/63	0/2/2/2
43	BCR	y	301	-	-	5/29/63/63	0/2/2/2
50	CLA	w	302	-	1/1/12/20	12/21/97/115	-
50	CLA	y	302	41	1/1/13/20	5/23/99/115	-
44	PGT	a	805	-	-	14/36/36/55	-
50	CLA	a	815	27	1/1/15/20	16/39/115/115	-
50	CLA	b	811	-	1/1/11/20	4/15/91/115	-
50	CLA	a	834	-	1/1/15/20	11/39/115/115	-
51	DGD	x	317	-	-	24/37/77/95	0/2/2/2
50	CLA	g	203	-	1/1/12/20	4/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	b	807	-	1/1/15/20	19/39/115/115	-
50	CLA	z	308	-	1/1/11/20	6/15/88/115	-
43	BCR	w	301	-	-	3/29/63/63	0/2/2/2
43	BCR	a	810	-	-	11/24/41/63	0/1/1/2
50	CLA	b	810	-	1/1/12/20	4/21/97/115	-
50	CLA	y	310	41	1/1/15/20	11/39/115/115	-
50	CLA	z	307	42	1/1/14/20	11/33/109/115	-
50	CLA	b	823	-	1/1/13/20	10/27/103/115	-
50	CLA	a	823	-	1/1/13/20	7/27/103/115	-
50	CLA	b	849	-	1/1/12/20	8/21/97/115	-
43	BCR	a	827	-	-	3/27/61/63	0/2/2/2
46	LMG	H	401	-	-	10/28/48/70	0/1/1/1
43	BCR	a	829	-	-	2/29/63/63	0/2/2/2
50	CLA	x	308	-	1/1/12/20	9/21/97/115	-
50	CLA	y	308	-	1/1/15/20	15/39/115/115	-
50	CLA	b	808	-	1/1/10/20	7/13/89/115	-
50	CLA	y	307	-	1/1/10/20	4/10/86/115	-
50	CLA	z	316	44	1/1/11/20	3/18/94/115	-
50	CLA	y	314	41	1/1/15/20	18/39/115/115	-
43	BCR	b	820	-	-	2/29/63/63	0/2/2/2
50	CLA	b	838	-	1/1/12/20	9/24/100/115	-
50	CLA	b	848	-	1/1/10/20	3/12/88/115	-
50	CLA	a	846	-	1/1/15/20	15/39/115/115	-
46	LMG	F	802	-	-	5/23/43/70	0/1/1/1
49	SF4	K	301	21	-	-	0/6/5/5
50	CLA	a	812	-	1/1/14/20	17/36/109/115	-
50	CLA	l	301	-	1/1/11/20	5/15/91/115	-
50	CLA	w	308	39	1/1/15/20	19/39/115/115	-
44	PGT	B	606	-	-	24/39/39/55	-
50	CLA	b	805	28	1/1/15/20	23/39/115/115	-
45	A1H1M	5	302	-	-	10/19/79/79	0/4/4/4
44	PGT	b	830	50	-	16/43/43/55	-
50	CLA	b	847	-	1/1/14/20	11/33/109/115	-
50	CLA	b	851	-	1/1/11/20	3/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	f	301	-	1/1/13/20	11/30/106/115	-
50	CLA	f	303	-	1/1/10/20	2/10/86/115	-
50	CLA	x	312	40	1/1/15/20	20/39/115/115	-
50	CLA	a	842	-	1/1/15/20	24/39/115/115	-
46	LMG	w	312	-	-	15/35/55/70	0/1/1/1
50	CLA	b	814	-	1/1/15/20	13/39/115/115	-
49	SF4	I	202	19	-	-	0/6/5/5
50	CLA	a	849	-	1/1/15/20	17/39/115/115	-
54	CHL	w	311	-	3/3/15/26	5/16/114/137	-
50	CLA	f	302	-	1/1/10/20	1/12/88/115	-
44	PGT	D	602	-	-	10/38/38/55	-
50	CLA	b	826	-	1/1/13/20	12/27/103/115	-
50	CLA	a	826	44	1/1/11/20	11/15/91/115	-
54	CHL	x	305	-	3/3/16/26	4/15/113/137	-
50	CLA	a	848	-	1/1/12/20	6/24/100/115	-
50	CLA	z	309	-	1/1/10/20	2/12/88/115	-
50	CLA	w	303	39	1/1/11/20	3/15/91/115	-
50	CLA	x	316	-	1/1/11/20	4/15/91/115	-
50	CLA	a	801	-	1/1/15/20	13/39/115/115	-
50	CLA	a	811	-	1/1/15/20	21/39/115/115	-
46	LMG	x	315	-	-	16/43/63/70	0/1/1/1
46	LMG	z	314	-	-	13/35/55/70	0/1/1/1
55	LUT	x	320	-	-	1/29/67/67	0/2/2/2
55	LUT	x	321	-	-	6/29/67/67	0/2/2/2
50	CLA	b	844	28	1/1/15/20	22/39/115/115	-
44	PGT	z	301	-	-	18/49/49/55	-
50	CLA	y	305	41	1/1/11/20	2/15/91/115	-
43	BCR	b	819	-	-	5/29/63/63	0/2/2/2
43	BCR	g	202	-	-	6/29/63/63	0/2/2/2
50	CLA	x	302	-	1/1/10/20	2/10/86/115	-
43	BCR	f	304	-	-	2/29/63/63	0/2/2/2
50	CLA	z	306	42	1/1/13/20	8/29/105/115	-
50	CLA	x	318	-	1/1/11/20	6/17/93/115	-
50	CLA	z	310	42	1/1/10/20	4/10/86/115	-
50	CLA	k	205	-	1/1/10/20	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	BCR	j	101	-	-	10/29/63/63	0/2/2/2
43	BCR	a	830	-	-	7/29/63/63	0/2/2/2
50	CLA	x	304	40	1/1/11/20	3/18/94/115	-
50	CLA	a	858	-	1/1/15/20	14/39/115/115	-
44	PGT	b	829	-	-	19/52/52/55	-
50	CLA	b	837	-	1/1/15/20	17/39/115/115	-
43	BCR	4	101	-	-	8/29/63/63	0/2/2/2
50	CLA	b	828	-	1/1/14/20	14/33/109/115	-
43	BCR	b	817	-	-	3/29/63/63	0/2/2/2
50	CLA	b	840	-	1/1/15/20	16/39/115/115	-
50	CLA	w	306	39	1/1/15/20	17/39/115/115	-
50	CLA	a	819	-	1/1/14/20	13/33/109/115	-
50	CLA	a	841	-	1/1/13/20	9/27/103/115	-
50	CLA	b	841	-	1/1/13/20	9/27/103/115	-
44	PGT	z	317	50	-	16/50/50/55	-
54	CHL	w	304	-	3/3/16/26	7/15/111/137	-
43	BCR	b	831	-	-	4/29/63/63	0/2/2/2
47	PQ9	A	405	-	-	4/31/51/61	0/1/1/1
49	SF4	I	201	19	-	-	0/6/5/5
49	SF4	c	101	29	-	-	0/6/5/5
50	CLA	x	307	40	1/1/14/20	13/33/109/115	-
53	PQN	a	825	-	-	8/23/43/43	0/2/2/2
50	CLA	a	821	-	1/1/14/20	12/35/111/115	-
50	CLA	a	814	-	1/1/15/20	20/39/115/115	-
50	CLA	w	316	39	1/1/12/20	8/21/97/115	-
50	CLA	z	302	-	1/1/13/20	8/27/103/115	-
54	CHL	x	311	-	3/3/14/26	5/8/102/137	-
55	LUT	y	315	-	-	0/29/67/67	0/2/2/2
50	CLA	z	303	-	1/1/10/20	2/10/86/115	-
44	PGT	I	203	-	-	14/48/48/55	-
50	CLA	w	307	-	1/1/11/20	6/15/91/115	-
50	CLA	a	852	-	1/1/12/20	5/23/99/115	-
50	CLA	a	843	-	1/1/15/20	17/39/115/115	-
50	CLA	b	839	-	1/1/15/20	21/39/115/115	-
43	BCR	l	303	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	a	844	-	1/1/13/20	8/30/106/115	-
50	CLA	b	803	-	1/1/15/20	16/39/115/115	-
44	PGT	f	305	-	-	10/43/43/55	-
50	CLA	b	822	-	1/1/13/20	10/31/107/115	-
50	CLA	a	833	-	1/1/15/20	18/39/115/115	-
50	CLA	a	820	-	1/1/15/20	17/39/115/115	-
50	CLA	b	804	-	1/1/10/20	0/10/86/115	-
50	CLA	b	832	-	1/1/12/20	12/26/102/115	-
44	PGT	a	806	50	-	14/37/37/55	-
55	LUT	w	319	-	-	6/29/67/67	0/2/2/2
44	PGT	A	403	-	-	18/42/42/55	-
44	PGT	w	313	50	-	10/44/44/55	-
55	LUT	w	320	-	-	1/29/67/67	0/2/2/2
46	LMG	D	601	-	-	13/29/49/70	0/1/1/1
53	PQN	b	827	-	-	8/23/43/43	0/2/2/2
50	CLA	b	836	-	1/1/15/20	11/39/115/115	-
49	SF4	c	102	29	-	-	0/6/5/5
50	CLA	w	310	-	1/1/15/20	18/39/115/115	-
50	CLA	a	851	27	1/1/11/20	4/17/93/115	-
50	CLA	a	850	-	1/1/15/20	14/39/115/115	-
43	BCR	b	818	-	-	6/29/63/63	0/2/2/2
50	CLA	w	305	-	1/1/12/20	4/23/99/115	-
50	CLA	a	816	-	1/1/10/20	3/12/88/115	-
43	BCR	a	803	-	-	5/21/38/63	0/1/1/2
49	SF4	a	832	28,27	-	-	0/6/5/5
50	CLA	a	838	-	1/1/15/20	14/39/115/115	-
43	BCR	a	831	-	-	8/27/61/63	0/2/2/2
50	CLA	w	314	44	1/1/10/20	8/14/90/115	-
44	PGT	z	313	-	-	13/37/37/55	-
50	CLA	a	854	-	1/1/15/20	15/39/115/115	-
44	PGT	a	807	-	-	15/50/50/55	-
50	CLA	a	809	-	1/1/13/20	5/30/106/115	-
50	CLA	a	817	-	1/1/10/20	0/10/86/115	-
50	CLA	b	824	44	1/1/15/20	17/39/115/115	-
44	PGT	B	603	-	-	19/50/50/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	b	801	-	1/1/15/20	17/39/115/115	-
50	CLA	b	812	-	1/1/14/20	9/36/112/115	-
50	CLA	y	309	-	1/1/10/20	3/12/88/115	-
50	CLA	a	818	-	1/1/13/20	12/32/108/115	-
50	CLA	a	853	-	1/1/15/20	11/39/115/115	-
50	CLA	y	306	-	1/1/10/20	2/10/86/115	-
44	PGT	A	404	-	-	15/48/48/55	-
46	LMG	B	605	-	-	17/32/52/70	0/1/1/1
52	CL0	a	808	-	3/3/18/25	5/33/125/135	-
46	LMG	z	315	-	-	8/31/51/70	0/1/1/1
50	CLA	a	847	-	1/1/7/20	11/26/62/115	-
46	LMG	7	301	-	-	14/36/56/70	0/1/1/1
50	CLA	x	310	-	1/1/10/20	3/13/89/115	-
54	CHL	x	301	-	3/3/15/26	4/12/110/137	-
48	SQD	w	317	-	-	5/26/46/69	0/1/1/1
50	CLA	b	835	-	1/1/13/20	9/32/108/115	-
50	CLA	b	809	-	1/1/13/20	12/32/108/115	-
44	PGT	L	201	-	-	12/44/44/55	-
50	CLA	a	855	-	1/1/10/20	2/12/88/115	-
50	CLA	a	840	-	1/1/10/20	2/12/88/115	-
50	CLA	l	306	-	1/1/14/20	19/33/109/115	-
44	PGT	B	601	-	-	15/38/38/55	-
45	A1H1M	F	804	-	-	13/19/79/79	0/4/4/4
50	CLA	k	204	-	1/1/13/20	7/30/106/115	-
50	CLA	b	842	-	1/1/13/20	22/30/106/115	-
44	PGT	5	301	-	-	16/39/39/55	-
48	SQD	a	859	-	-	6/31/51/69	0/1/1/1
50	CLA	x	313	40	1/1/12/20	6/25/101/115	-
50	CLA	g	201	-	1/1/11/20	10/20/96/115	-
55	LUT	z	320	-	-	6/29/67/67	0/2/2/2
50	CLA	b	802	-	1/1/15/20	20/39/115/115	-
50	CLA	a	802	-	1/1/14/20	8/33/109/115	-
50	CLA	b	815	-	1/1/15/20	11/39/115/115	-
50	CLA	h	201	34	1/1/11/20	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	b	833	-	1/1/15/20	16/39/115/115	-
50	CLA	y	304	-	1/1/9/20	0/6/82/115	-
50	CLA	b	813	-	1/1/10/20	4/13/89/115	-
43	BCR	i	101	-	-	6/29/63/63	0/2/2/2
48	SQD	B	604	-	-	6/35/55/69	0/1/1/1
48	SQD	w	318	-	-	8/36/56/69	0/1/1/1
44	PGT	F	803	-	-	12/47/47/55	-
51	DGD	b	821	-	-	22/48/88/95	0/2/2/2
50	CLA	a	822	-	1/1/12/20	8/23/99/115	-
50	CLA	x	303	40	1/1/13/20	9/30/106/115	-
50	CLA	b	834	-	1/1/11/20	4/15/91/115	-
50	CLA	a	857	-	1/1/15/20	12/39/115/115	-
50	CLA	b	845	-	1/1/15/20	18/39/115/115	-
50	CLA	y	313	41	1/1/15/20	18/39/115/115	-
50	CLA	a	839	-	1/1/15/20	16/39/115/115	-
50	CLA	j	102	36	1/1/10/20	2/12/88/115	-
50	CLA	a	836	27	1/1/15/20	15/39/115/115	-
54	CHL	x	319	42	3/3/16/26	7/20/118/137	-
50	CLA	a	835	-	1/1/13/20	15/31/107/115	-
48	SQD	F	801	-	-	2/36/56/69	0/1/1/1
50	CLA	g	204	33	1/1/10/20	5/13/89/115	-
43	BCR	j	103	-	-	8/29/63/63	0/2/2/2
48	SQD	j	106	-	-	8/37/57/69	0/1/1/1
54	CHL	w	309	-	3/3/15/26	5/12/110/137	-
50	CLA	b	846	-	1/1/15/20	16/39/115/115	-
44	PGT	A	401	-	-	9/36/36/55	-
50	CLA	l	305	38	1/1/10/20	0/8/84/115	-
50	CLA	b	806	-	1/1/12/20	5/24/100/115	-
43	BCR	z	318	-	-	8/29/63/63	0/2/2/2
54	CHL	z	304	42	3/3/15/26	6/10/108/137	-
50	CLA	k	203	-	1/1/10/20	2/10/86/115	-
43	BCR	a	828	-	-	0/29/63/63	0/2/2/2
43	BCR	k	201	-	-	5/29/63/63	0/2/2/2
43	BCR	b	850	-	-	2/29/63/63	0/2/2/2
44	PGT	N	301	-	-	15/30/30/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	x	309	-	1/1/10/20	2/12/88/115	-
46	LMG	j	104	-	-	10/29/49/70	0/1/1/1
50	CLA	y	311	-	1/1/12/20	7/23/99/115	-
48	SQD	F	805	-	-	7/38/58/69	0/1/1/1
50	CLA	w	315	39	1/1/11/20	4/17/93/115	-
50	CLA	a	813	-	1/1/12/20	8/24/100/115	-
50	CLA	z	305	-	1/1/12/20	5/21/97/115	-
43	BCR	k	202	-	-	4/29/63/63	0/2/2/2
43	BCR	x	314	-	-	11/29/63/63	0/2/2/2
50	CLA	b	825	-	1/1/15/20	16/39/115/115	-
50	CLA	y	312	-	1/1/12/20	6/23/99/115	-
46	LMG	j	105	-	-	18/32/52/70	0/1/1/1
50	CLA	y	303	-	1/1/13/20	8/27/103/115	-
55	LUT	z	321	-	-	0/29/67/67	0/2/2/2
50	CLA	z	311	-	1/1/13/20	10/27/103/115	-
50	CLA	b	843	-	1/1/15/20	19/39/115/115	-
44	PGT	A	402	-	-	11/41/41/55	-
50	CLA	a	845	-	1/1/15/20	15/39/115/115	-
50	CLA	z	319	-	1/1/10/20	3/12/88/115	-
43	BCR	l	304	-	-	7/29/63/63	0/2/2/2
50	CLA	a	837	-	1/1/15/20	10/39/115/115	-

All (1152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	808	CL0	C1A-CHA	9.95	1.51	1.40
52	a	808	CL0	C1B-C2B	8.55	1.49	1.39
52	a	808	CL0	C1D-C2D	8.41	1.49	1.39
47	A	405	PQ9	C3-C2	8.05	1.54	1.34
52	a	808	CL0	C4B-C3B	7.70	1.48	1.39
54	w	304	CHL	C4B-C3B	6.30	1.46	1.39
50	a	812	CLA	C3B-C4B	6.30	1.48	1.41
50	a	812	CLA	CHB-C4A	6.21	1.39	1.33
54	z	312	CHL	C3B-C4B	5.94	1.47	1.41
54	w	309	CHL	C3B-C4B	5.91	1.47	1.41
54	x	319	CHL	C3B-C4B	5.88	1.47	1.41
54	z	304	CHL	C3B-C4B	5.79	1.47	1.41
54	z	312	CHL	CMC-C2C	5.79	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	w	309	CHL	CMC-C2C	5.79	1.56	1.44
50	a	847	CLA	CHA-C4D	5.73	1.39	1.34
54	x	319	CHL	CMC-C2C	5.72	1.56	1.44
54	w	304	CHL	CMC-C2C	5.72	1.56	1.44
54	x	301	CHL	CMC-C2C	5.71	1.56	1.44
54	x	311	CHL	CMC-C2C	5.70	1.56	1.44
54	z	304	CHL	CMC-C2C	5.69	1.56	1.44
54	x	305	CHL	CMC-C2C	5.67	1.56	1.44
54	x	301	CHL	C3B-C4B	5.64	1.46	1.41
54	x	311	CHL	C3B-C4B	5.64	1.46	1.41
54	w	311	CHL	CMC-C2C	5.51	1.56	1.44
50	x	303	CLA	MG-NA	5.40	2.19	2.06
54	w	311	CHL	C3B-C4B	5.40	1.46	1.41
54	x	305	CHL	C3B-C4B	5.33	1.46	1.41
50	z	319	CLA	MG-NA	5.29	2.18	2.06
47	A	405	PQ9	C11-C2	5.25	1.58	1.51
50	w	307	CLA	MG-NA	5.24	2.18	2.06
50	k	203	CLA	MG-NA	5.21	2.18	2.06
50	x	313	CLA	MG-NA	5.19	2.18	2.06
50	y	309	CLA	MG-NA	5.18	2.18	2.06
50	b	849	CLA	MG-NA	5.16	2.18	2.06
50	g	204	CLA	MG-NA	5.13	2.18	2.06
50	a	812	CLA	MG-NA	5.13	2.18	2.06
52	a	808	CL0	CHB-C1B	5.13	1.47	1.39
50	w	315	CLA	MG-NA	5.13	2.18	2.06
50	z	309	CLA	MG-NA	5.12	2.18	2.06
54	x	301	CHL	C1D-C2D	5.11	1.45	1.39
54	w	304	CHL	C1D-C2D	5.10	1.45	1.39
50	a	819	CLA	MG-NA	5.09	2.18	2.06
50	g	203	CLA	MG-NA	5.09	2.18	2.06
50	a	847	CLA	CHB-C1B	-5.08	1.34	1.44
50	b	848	CLA	MG-NA	5.07	2.18	2.06
50	a	822	CLA	MG-NA	5.06	2.18	2.06
50	z	311	CLA	MG-NA	5.06	2.18	2.06
50	a	853	CLA	MG-NA	5.06	2.18	2.06
50	f	302	CLA	MG-NA	5.05	2.18	2.06
50	b	814	CLA	MG-NA	5.05	2.18	2.06
50	l	301	CLA	MG-NA	5.04	2.18	2.06
50	z	308	CLA	MG-NA	5.04	2.18	2.06
50	y	307	CLA	MG-NA	5.03	2.18	2.06
50	a	821	CLA	MG-NA	5.03	2.18	2.06
50	y	314	CLA	MG-NA	5.03	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	j	102	CLA	MG-NA	5.03	2.18	2.06
50	a	846	CLA	MG-NA	5.02	2.18	2.06
50	b	805	CLA	MG-NA	5.02	2.18	2.06
50	k	204	CLA	MG-NA	5.02	2.18	2.06
50	h	201	CLA	MG-NA	5.02	2.18	2.06
50	x	308	CLA	MG-NA	5.02	2.18	2.06
50	y	304	CLA	MG-NA	5.01	2.18	2.06
50	a	837	CLA	MG-NA	5.01	2.18	2.06
50	l	305	CLA	MG-NA	5.01	2.18	2.06
50	x	302	CLA	MG-NA	5.01	2.18	2.06
50	a	855	CLA	MG-NA	5.00	2.18	2.06
50	b	841	CLA	MG-NA	5.00	2.18	2.06
50	a	845	CLA	MG-NA	5.00	2.18	2.06
50	w	314	CLA	MG-NA	5.00	2.18	2.06
50	a	851	CLA	MG-NA	5.00	2.18	2.06
50	a	802	CLA	MG-NA	5.00	2.18	2.06
50	g	201	CLA	MG-NA	5.00	2.18	2.06
50	x	316	CLA	MG-NA	4.99	2.18	2.06
50	y	303	CLA	MG-NA	4.99	2.18	2.06
50	x	309	CLA	MG-NA	4.99	2.18	2.06
50	b	825	CLA	MG-NA	4.99	2.18	2.06
50	b	826	CLA	MG-NA	4.99	2.18	2.06
54	z	312	CHL	C1D-C2D	4.99	1.45	1.39
50	w	302	CLA	MG-NA	4.98	2.18	2.06
50	b	844	CLA	MG-NA	4.98	2.18	2.06
50	x	310	CLA	MG-NA	4.98	2.18	2.06
50	a	814	CLA	MG-NA	4.97	2.18	2.06
50	w	305	CLA	MG-NA	4.97	2.18	2.06
50	a	823	CLA	MG-NA	4.97	2.18	2.06
50	a	849	CLA	MG-NA	4.97	2.18	2.06
54	w	309	CHL	C1D-C2D	4.97	1.45	1.39
50	b	851	CLA	MG-NA	4.96	2.18	2.06
50	a	801	CLA	MG-NA	4.96	2.18	2.06
50	b	810	CLA	MG-NA	4.96	2.18	2.06
50	b	836	CLA	MG-NA	4.96	2.18	2.06
50	a	842	CLA	MG-NA	4.96	2.18	2.06
50	y	311	CLA	MG-NA	4.96	2.18	2.06
50	z	303	CLA	MG-NA	4.96	2.18	2.06
50	b	835	CLA	MG-NA	4.96	2.18	2.06
52	a	808	CL0	CHC-C4B	4.96	1.47	1.39
50	a	852	CLA	MG-NA	4.96	2.18	2.06
50	b	801	CLA	MG-NA	4.96	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	b	832	CLA	MG-NA	4.95	2.18	2.06
50	b	806	CLA	MG-NA	4.95	2.18	2.06
50	y	305	CLA	MG-NA	4.95	2.18	2.06
50	f	301	CLA	MG-NA	4.95	2.18	2.06
50	a	841	CLA	MG-NA	4.95	2.18	2.06
50	a	817	CLA	MG-NA	4.95	2.18	2.06
50	b	823	CLA	MG-NA	4.94	2.18	2.06
50	a	857	CLA	MG-NA	4.94	2.18	2.06
54	z	304	CHL	C1D-C2D	4.94	1.45	1.39
50	y	308	CLA	MG-NA	4.94	2.18	2.06
50	b	838	CLA	MG-NA	4.93	2.18	2.06
54	x	305	CHL	C1D-C2D	4.93	1.45	1.39
50	l	306	CLA	MG-NA	4.93	2.18	2.06
50	b	828	CLA	MG-NA	4.92	2.18	2.06
50	y	306	CLA	MG-NA	4.92	2.18	2.06
50	f	303	CLA	MG-NA	4.92	2.18	2.06
52	a	808	CL0	OBD-CAD	4.92	1.28	1.22
50	z	316	CLA	MG-NA	4.92	2.18	2.06
50	a	811	CLA	MG-NA	4.92	2.18	2.06
50	x	306	CLA	MG-NA	4.92	2.18	2.06
50	x	318	CLA	MG-NA	4.92	2.17	2.06
50	a	824	CLA	MG-NA	4.92	2.17	2.06
50	b	808	CLA	MG-NA	4.91	2.17	2.06
50	w	306	CLA	MG-NA	4.91	2.17	2.06
50	b	845	CLA	MG-NA	4.91	2.17	2.06
50	z	310	CLA	MG-NA	4.91	2.17	2.06
50	z	302	CLA	MG-NA	4.91	2.17	2.06
50	b	839	CLA	MG-NA	4.91	2.17	2.06
50	a	809	CLA	MG-NA	4.91	2.17	2.06
50	a	848	CLA	MG-NA	4.90	2.17	2.06
54	x	311	CHL	C1D-C2D	4.90	1.45	1.39
50	a	840	CLA	MG-NA	4.90	2.17	2.06
50	b	833	CLA	MG-NA	4.90	2.17	2.06
50	b	843	CLA	MG-NA	4.89	2.17	2.06
50	a	834	CLA	MG-NA	4.89	2.17	2.06
50	b	834	CLA	MG-NA	4.89	2.17	2.06
50	b	846	CLA	MG-NA	4.89	2.17	2.06
50	k	205	CLA	MG-NA	4.89	2.17	2.06
50	a	843	CLA	MG-NA	4.89	2.17	2.06
50	b	804	CLA	MG-NA	4.89	2.17	2.06
50	a	816	CLA	MG-NA	4.89	2.17	2.06
50	b	807	CLA	MG-NA	4.88	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	y	312	CLA	MG-NA	4.88	2.17	2.06
50	a	826	CLA	MG-NA	4.88	2.17	2.06
50	x	304	CLA	MG-NA	4.88	2.17	2.06
50	b	842	CLA	MG-NA	4.88	2.17	2.06
50	a	838	CLA	MG-NA	4.88	2.17	2.06
50	b	824	CLA	MG-NA	4.88	2.17	2.06
50	b	809	CLA	MG-NA	4.87	2.17	2.06
50	b	815	CLA	MG-NA	4.87	2.17	2.06
50	b	822	CLA	MG-NA	4.87	2.17	2.06
50	b	837	CLA	MG-NA	4.86	2.17	2.06
54	x	319	CHL	C1D-C2D	4.86	1.45	1.39
50	b	840	CLA	MG-NA	4.86	2.17	2.06
50	b	813	CLA	MG-NA	4.85	2.17	2.06
50	a	833	CLA	MG-NA	4.84	2.17	2.06
50	a	835	CLA	MG-NA	4.84	2.17	2.06
50	a	844	CLA	MG-NA	4.84	2.17	2.06
50	a	836	CLA	MG-NA	4.84	2.17	2.06
54	w	311	CHL	C1B-C2B	4.84	1.45	1.39
50	x	312	CLA	MG-NA	4.84	2.17	2.06
50	z	305	CLA	MG-NA	4.83	2.17	2.06
50	y	313	CLA	MG-NA	4.83	2.17	2.06
50	z	307	CLA	MG-NA	4.83	2.17	2.06
50	w	316	CLA	MG-NA	4.83	2.17	2.06
50	w	310	CLA	MG-NA	4.82	2.17	2.06
50	a	856	CLA	MG-NA	4.82	2.17	2.06
50	b	803	CLA	MG-NA	4.81	2.17	2.06
50	a	858	CLA	MG-NA	4.81	2.17	2.06
54	w	311	CHL	C1D-C2D	4.80	1.45	1.39
50	a	839	CLA	MG-NA	4.79	2.17	2.06
50	b	847	CLA	MG-NA	4.79	2.17	2.06
50	b	802	CLA	MG-NA	4.79	2.17	2.06
54	w	304	CHL	C1B-C2B	4.79	1.45	1.39
47	A	405	PQ9	C15-C13	4.78	1.61	1.51
50	w	303	CLA	MG-NA	4.78	2.17	2.06
50	a	813	CLA	MG-NA	4.78	2.17	2.06
50	a	820	CLA	MG-NA	4.78	2.17	2.06
50	a	850	CLA	MG-NA	4.78	2.17	2.06
54	x	301	CHL	C1B-C2B	4.77	1.45	1.39
54	z	312	CHL	C1B-C2B	4.77	1.45	1.39
50	a	854	CLA	MG-NA	4.76	2.17	2.06
50	y	310	CLA	MG-NA	4.76	2.17	2.06
50	y	302	CLA	MG-NA	4.75	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	b	811	CLA	MG-NA	4.75	2.17	2.06
50	b	812	CLA	MG-NA	4.74	2.17	2.06
52	a	808	CL0	O2D-CGD	4.74	1.45	1.30
50	a	818	CLA	MG-NA	4.74	2.17	2.06
50	w	308	CLA	MG-NA	4.73	2.17	2.06
54	z	304	CHL	C1B-C2B	4.71	1.44	1.39
50	a	815	CLA	MG-NA	4.71	2.17	2.06
54	x	311	CHL	C1B-C2B	4.71	1.44	1.39
50	x	307	CLA	MG-NA	4.70	2.17	2.06
54	x	305	CHL	C1B-C2B	4.67	1.44	1.39
50	z	306	CLA	MG-NA	4.66	2.17	2.06
52	a	808	CL0	O2A-C1	4.64	1.60	1.42
54	x	319	CHL	C1B-C2B	4.58	1.44	1.39
54	w	309	CHL	C1B-C2B	4.58	1.44	1.39
52	a	808	CL0	C3D-C4D	-4.56	1.34	1.41
52	a	808	CL0	CHD-C1D	4.54	1.47	1.39
52	a	808	CL0	C3D-C2D	4.39	1.47	1.39
50	a	812	CLA	C1B-CHB	-4.36	1.34	1.48
52	a	808	CL0	CHC-C1C	4.32	1.47	1.39
47	A	405	PQ9	C20-C18	4.31	1.60	1.51
52	a	808	CL0	C3A-C4A	-4.25	1.48	1.50
52	a	808	CL0	CHD-C4C	4.15	1.47	1.39
54	w	304	CHL	CAB-C3B	-3.89	1.43	1.51
47	A	405	PQ9	C25-C23	3.88	1.59	1.51
47	A	405	PQ9	C10-C5	3.77	1.53	1.35
54	x	311	CHL	C3B-C2B	-3.73	1.35	1.40
54	x	319	CHL	CHA-CBD	3.73	1.56	1.51
54	z	304	CHL	CHA-CBD	3.64	1.55	1.51
54	x	311	CHL	CHA-CBD	3.63	1.55	1.51
54	x	319	CHL	C3B-C2B	-3.62	1.35	1.40
47	A	405	PQ9	C35-C33	3.62	1.61	1.51
54	w	311	CHL	C3B-C2B	-3.57	1.35	1.40
54	w	309	CHL	CHA-CBD	3.55	1.55	1.51
54	x	305	CHL	C3B-C2B	-3.55	1.35	1.40
54	w	309	CHL	C3B-C2B	-3.55	1.35	1.40
54	x	301	CHL	CHA-CBD	3.50	1.55	1.51
54	x	301	CHL	O2D-CGD	3.46	1.41	1.33
54	x	301	CHL	C3B-C2B	-3.46	1.35	1.40
54	z	304	CHL	O2D-CGD	3.45	1.41	1.33
54	z	304	CHL	C3B-C2B	-3.42	1.35	1.40
45	F	804	A1H1M	O12-C11	-3.42	1.40	1.44
54	w	309	CHL	O2D-CGD	3.41	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	w	304	CHL	CHA-CBD	3.41	1.55	1.51
54	w	304	CHL	O2D-CGD	3.41	1.41	1.33
54	x	311	CHL	O2D-CGD	3.41	1.41	1.33
54	w	311	CHL	O2D-CGD	3.40	1.41	1.33
54	z	312	CHL	O2D-CGD	3.40	1.41	1.33
54	x	305	CHL	O2A-CGA	3.40	1.42	1.30
54	w	304	CHL	O2A-CGA	3.37	1.41	1.30
54	w	311	CHL	CHA-CBD	3.36	1.55	1.51
47	A	405	PQ9	C9-C10	3.36	1.57	1.50
47	A	405	PQ9	C3-C4	3.34	1.53	1.44
54	x	319	CHL	O2D-CGD	3.34	1.41	1.33
50	a	847	CLA	CHB-C4A	3.32	1.39	1.32
54	z	312	CHL	CHA-CBD	3.32	1.55	1.51
47	A	405	PQ9	C11-C12	3.29	1.55	1.50
47	A	405	PQ9	C5-C4	3.28	1.54	1.48
54	x	305	CHL	CHA-CBD	3.26	1.55	1.51
54	x	305	CHL	O2D-CGD	3.25	1.41	1.33
54	z	312	CHL	C3B-C2B	-3.22	1.36	1.40
54	z	312	CHL	O2A-CGA	3.01	1.42	1.33
45	F	804	A1H1M	O21-C22	-3.01	1.37	1.44
54	z	312	CHL	C1A-CHA	3.01	1.43	1.40
53	b	827	PQN	C10-C5	-2.95	1.35	1.40
54	x	319	CHL	O2A-CGA	2.94	1.41	1.33
47	A	405	PQ9	C24-C23	2.89	1.57	1.50
50	z	308	CLA	C1D-CHD	2.88	1.41	1.35
53	a	825	PQN	C10-C5	-2.88	1.36	1.40
50	w	308	CLA	C1D-ND	-2.88	1.34	1.37
54	x	319	CHL	C1A-CHA	2.87	1.43	1.40
50	a	854	CLA	C1D-ND	-2.86	1.34	1.37
50	a	836	CLA	C1D-ND	-2.82	1.34	1.37
47	A	405	PQ9	C2-C1	2.82	1.54	1.49
47	A	405	PQ9	C30-C28	2.81	1.57	1.51
54	x	311	CHL	C1A-CHA	2.80	1.43	1.40
54	z	304	CHL	C1A-CHA	2.80	1.43	1.40
54	z	312	CHL	C2C-C3C	2.78	1.39	1.36
50	l	306	CLA	C1D-ND	-2.76	1.34	1.37
50	y	302	CLA	C2C-C1C	2.76	1.46	1.40
50	b	803	CLA	C1D-ND	-2.75	1.34	1.37
50	b	845	CLA	C1D-ND	-2.75	1.34	1.37
50	y	302	CLA	C4C-C3C	2.74	1.47	1.42
54	z	304	CHL	C2C-C3C	2.74	1.39	1.36
50	b	811	CLA	C1D-ND	-2.73	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	x	305	CHL	C1A-CHA	2.72	1.43	1.40
54	x	301	CHL	C1A-CHA	2.71	1.43	1.40
50	b	839	CLA	C1D-ND	-2.71	1.34	1.37
50	a	856	CLA	C1D-ND	-2.70	1.34	1.37
50	x	303	CLA	MG-NB	2.70	2.11	2.05
45	F	804	A1H1M	O14-C15	-2.70	1.37	1.44
43	a	810	BCR	C1-C6	-2.69	1.50	1.53
50	a	801	CLA	C1D-ND	-2.68	1.34	1.37
50	x	307	CLA	C1D-ND	-2.68	1.34	1.37
46	z	314	LMG	C4-C5	2.68	1.58	1.53
50	a	858	CLA	C1D-ND	-2.68	1.34	1.37
50	x	304	CLA	C1D-ND	-2.68	1.34	1.37
50	b	847	CLA	CHC-C1C	2.66	1.43	1.38
50	z	302	CLA	C1D-ND	-2.66	1.34	1.37
50	y	313	CLA	C1D-ND	-2.65	1.34	1.37
50	y	308	CLA	C1D-ND	-2.65	1.34	1.37
50	a	845	CLA	C1D-ND	-2.65	1.34	1.37
50	b	845	CLA	CHC-C1C	2.64	1.43	1.38
54	w	309	CHL	C1A-CHA	2.64	1.43	1.40
54	w	304	CHL	C1A-CHA	2.64	1.43	1.40
50	a	841	CLA	C1D-ND	-2.63	1.34	1.37
50	b	847	CLA	C1D-ND	-2.63	1.34	1.37
54	z	312	CHL	C2-C3	2.63	1.39	1.33
50	a	835	CLA	C1D-ND	-2.63	1.34	1.37
50	a	850	CLA	C1D-ND	-2.63	1.34	1.37
50	z	316	CLA	C1D-ND	-2.63	1.34	1.37
50	w	316	CLA	C1D-ND	-2.62	1.34	1.37
50	w	308	CLA	CHC-C1C	2.62	1.43	1.38
54	w	304	CHL	C2C-C3C	2.62	1.38	1.36
50	a	811	CLA	C1D-ND	-2.62	1.34	1.37
50	b	813	CLA	C1D-ND	-2.61	1.34	1.37
50	z	306	CLA	C1D-ND	-2.61	1.34	1.37
50	a	824	CLA	C1D-ND	-2.61	1.34	1.37
50	b	838	CLA	C1D-ND	-2.60	1.34	1.37
50	y	312	CLA	C1D-ND	-2.60	1.34	1.37
50	a	838	CLA	C1D-ND	-2.59	1.34	1.37
53	a	825	PQN	C2M-C2	-2.59	1.45	1.50
50	a	857	CLA	C1D-ND	-2.59	1.34	1.37
50	b	825	CLA	C1D-ND	-2.59	1.34	1.37
50	b	806	CLA	C1D-ND	-2.59	1.34	1.37
50	b	842	CLA	C1D-ND	-2.59	1.34	1.37
50	a	843	CLA	C1D-ND	-2.59	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	w	309	CHL	MG-NB	2.58	2.10	2.05
50	a	816	CLA	C1D-ND	-2.58	1.34	1.37
50	b	815	CLA	C1D-ND	-2.58	1.34	1.37
50	y	310	CLA	C1D-ND	-2.58	1.34	1.37
50	a	809	CLA	C1D-ND	-2.58	1.34	1.37
50	a	849	CLA	MG-NB	2.57	2.10	2.05
50	a	818	CLA	C1D-ND	-2.57	1.34	1.37
50	a	813	CLA	C1D-ND	-2.57	1.34	1.37
50	a	813	CLA	CHC-C1C	2.57	1.43	1.38
54	x	311	CHL	MG-NB	2.57	2.10	2.05
50	b	826	CLA	C1D-ND	-2.57	1.34	1.37
46	z	314	LMG	C3-C2	2.57	1.59	1.52
50	b	802	CLA	C1D-ND	-2.57	1.34	1.37
50	b	812	CLA	CHC-C1C	2.57	1.43	1.38
50	b	811	CLA	CHC-C1C	2.57	1.43	1.38
50	w	303	CLA	CHC-C1C	2.56	1.43	1.38
50	z	307	CLA	C1D-ND	-2.56	1.34	1.37
54	w	304	CHL	MG-NB	2.56	2.10	2.05
50	a	848	CLA	C1D-ND	-2.56	1.34	1.37
50	b	836	CLA	C1D-ND	-2.56	1.34	1.37
46	z	314	LMG	C4-C3	2.56	1.59	1.52
50	a	815	CLA	C1D-ND	-2.56	1.34	1.37
50	b	844	CLA	C1D-ND	-2.56	1.34	1.37
50	y	308	CLA	CHC-C1C	2.55	1.43	1.38
50	z	306	CLA	CHC-C1C	2.55	1.43	1.38
50	y	307	CLA	C1D-ND	-2.54	1.34	1.37
50	x	306	CLA	C1D-ND	-2.54	1.34	1.37
50	w	307	CLA	C1D-ND	-2.54	1.34	1.37
50	y	309	CLA	MG-NB	2.54	2.10	2.05
50	b	814	CLA	C1D-ND	-2.54	1.34	1.37
50	f	301	CLA	C1D-ND	-2.54	1.34	1.37
50	z	310	CLA	C1D-ND	-2.53	1.34	1.37
50	y	311	CLA	C1D-ND	-2.53	1.34	1.37
54	x	301	CHL	MG-NB	2.53	2.10	2.05
50	a	817	CLA	C1D-ND	-2.53	1.34	1.37
50	a	840	CLA	C1D-ND	-2.53	1.34	1.37
50	b	804	CLA	C1D-ND	-2.53	1.34	1.37
50	b	822	CLA	C1D-ND	-2.53	1.34	1.37
50	a	826	CLA	C1D-ND	-2.53	1.34	1.37
50	a	853	CLA	C1D-ND	-2.53	1.34	1.37
50	b	810	CLA	C1D-ND	-2.53	1.34	1.37
54	w	311	CHL	C1A-CHA	2.53	1.42	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	g	203	CLA	MG-NB	2.52	2.10	2.05
50	b	837	CLA	C1D-ND	-2.52	1.34	1.37
50	z	319	CLA	MG-NB	2.52	2.10	2.05
50	b	851	CLA	C1D-ND	-2.52	1.34	1.37
50	w	307	CLA	CHB-C1B	-2.52	1.33	1.39
50	b	812	CLA	C1D-ND	-2.52	1.34	1.37
50	b	813	CLA	CHC-C1C	2.52	1.43	1.38
50	w	310	CLA	C1D-ND	-2.51	1.34	1.37
50	a	818	CLA	CHC-C1C	2.51	1.43	1.38
50	a	835	CLA	CHC-C1C	2.51	1.43	1.38
50	b	841	CLA	C1D-ND	-2.51	1.34	1.37
50	b	843	CLA	C1D-ND	-2.51	1.34	1.37
50	w	303	CLA	C1D-ND	-2.51	1.34	1.37
50	a	839	CLA	C1D-ND	-2.51	1.34	1.37
50	a	839	CLA	CHC-C1C	2.51	1.43	1.38
50	b	809	CLA	C1D-ND	-2.50	1.34	1.37
50	z	308	CLA	C4D-CHA	2.50	1.39	1.35
50	a	842	CLA	C1D-ND	-2.50	1.34	1.37
50	b	803	CLA	CHC-C1C	2.50	1.43	1.38
50	x	307	CLA	CHC-C1C	2.50	1.43	1.38
50	z	307	CLA	CHC-C1C	2.50	1.43	1.38
50	b	834	CLA	C1D-ND	-2.50	1.34	1.37
50	l	306	CLA	CHC-C1C	2.50	1.43	1.38
50	a	814	CLA	C1D-ND	-2.50	1.34	1.37
50	x	303	CLA	MG-NC	2.50	2.12	2.06
50	b	849	CLA	MG-NB	2.49	2.10	2.05
50	w	314	CLA	C1D-ND	-2.49	1.34	1.37
54	w	311	CHL	MG-NB	2.49	2.10	2.05
50	b	839	CLA	CHC-C1C	2.49	1.43	1.38
50	a	815	CLA	CHC-C1C	2.49	1.43	1.38
54	x	319	CHL	MG-NB	2.49	2.10	2.05
50	z	303	CLA	C1D-ND	-2.49	1.34	1.37
53	b	827	PQN	C2M-C2	-2.49	1.45	1.50
50	a	802	CLA	C1D-ND	-2.49	1.34	1.37
50	a	823	CLA	C1D-ND	-2.49	1.34	1.37
50	k	203	CLA	MG-NB	2.49	2.10	2.05
50	z	311	CLA	MG-NB	2.49	2.10	2.05
50	a	821	CLA	C1D-ND	-2.48	1.34	1.37
50	y	304	CLA	C1D-ND	-2.48	1.34	1.37
50	b	801	CLA	MG-NB	2.48	2.10	2.05
50	a	846	CLA	C1D-ND	-2.48	1.34	1.37
50	f	302	CLA	C1D-ND	-2.48	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	w	302	CLA	C1D-ND	-2.48	1.34	1.37
50	y	313	CLA	CHC-C1C	2.48	1.43	1.38
54	x	305	CHL	MG-NB	2.48	2.10	2.05
50	b	804	CLA	CHC-C1C	2.48	1.43	1.38
50	l	305	CLA	C1D-ND	-2.48	1.34	1.37
50	y	302	CLA	C1D-ND	-2.48	1.34	1.37
50	a	822	CLA	C1D-ND	-2.48	1.34	1.37
50	b	822	CLA	CHC-C1C	2.48	1.43	1.38
50	b	814	CLA	CHC-C1C	2.48	1.43	1.38
50	x	313	CLA	C1D-ND	-2.48	1.34	1.37
50	w	306	CLA	CHC-C1C	2.48	1.43	1.38
50	b	808	CLA	C1D-ND	-2.48	1.34	1.37
50	b	823	CLA	C1D-ND	-2.48	1.34	1.37
50	x	313	CLA	MG-NB	2.48	2.10	2.05
50	k	205	CLA	C1D-ND	-2.47	1.34	1.37
50	l	301	CLA	C1D-ND	-2.47	1.34	1.37
50	a	826	CLA	CHC-C1C	2.47	1.43	1.38
50	f	301	CLA	CHC-C1C	2.47	1.43	1.38
50	y	305	CLA	C1D-ND	-2.47	1.34	1.37
50	a	801	CLA	CHC-C1C	2.47	1.43	1.38
50	a	843	CLA	CHC-C1C	2.47	1.43	1.38
50	y	310	CLA	CHC-C1C	2.47	1.43	1.38
54	z	304	CHL	MG-NB	2.47	2.10	2.05
50	k	204	CLA	C1D-ND	-2.47	1.34	1.37
50	a	834	CLA	MG-NB	2.47	2.10	2.05
50	g	204	CLA	C1D-ND	-2.47	1.34	1.37
50	l	301	CLA	CHC-C1C	2.47	1.43	1.38
50	z	308	CLA	MG-NB	2.47	2.10	2.05
50	x	312	CLA	C1D-ND	-2.47	1.34	1.37
50	b	848	CLA	C1D-ND	-2.47	1.34	1.37
50	z	319	CLA	CHB-C1B	-2.47	1.33	1.39
50	x	303	CLA	CHB-C1B	-2.47	1.33	1.39
50	b	837	CLA	CHC-C1C	2.46	1.43	1.38
50	f	303	CLA	CHC-C1C	2.46	1.43	1.38
50	a	833	CLA	C1D-ND	-2.46	1.34	1.37
50	a	855	CLA	C1D-ND	-2.46	1.34	1.37
50	a	814	CLA	CHC-C1C	2.46	1.43	1.38
50	b	815	CLA	CHC-C1C	2.46	1.43	1.38
50	b	828	CLA	C1D-ND	-2.46	1.34	1.37
50	a	851	CLA	C1D-ND	-2.46	1.34	1.37
50	a	837	CLA	C1D-ND	-2.46	1.34	1.37
50	w	306	CLA	C1D-ND	-2.46	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	x	310	CLA	MG-NB	2.46	2.10	2.05
50	a	850	CLA	CHC-C1C	2.46	1.43	1.38
50	b	835	CLA	C1D-ND	-2.46	1.34	1.37
50	w	316	CLA	CHC-C1C	2.46	1.43	1.38
50	w	315	CLA	CHB-C1B	-2.45	1.33	1.39
51	a	804	DGD	C1D-C2D	2.45	1.59	1.52
50	g	201	CLA	C1D-ND	-2.45	1.34	1.37
50	b	832	CLA	MG-NB	2.45	2.10	2.05
50	x	309	CLA	C1D-ND	-2.45	1.34	1.37
50	b	833	CLA	C1D-ND	-2.45	1.34	1.37
50	a	841	CLA	CHC-C1C	2.45	1.43	1.38
50	b	809	CLA	CHC-C1C	2.45	1.43	1.38
50	x	316	CLA	C1D-ND	-2.45	1.34	1.37
50	a	812	CLA	C1D-ND	-2.45	1.34	1.37
50	z	305	CLA	C1D-ND	-2.45	1.34	1.37
50	y	314	CLA	MG-NB	2.45	2.10	2.05
50	a	849	CLA	C1D-ND	-2.45	1.34	1.37
50	f	303	CLA	C1D-ND	-2.45	1.34	1.37
50	b	814	CLA	MG-NB	2.44	2.10	2.05
50	b	807	CLA	C1D-ND	-2.44	1.34	1.37
50	a	821	CLA	MG-NB	2.44	2.10	2.05
50	a	856	CLA	CHC-C1C	2.44	1.43	1.38
50	b	828	CLA	CHC-C1C	2.44	1.43	1.38
50	z	316	CLA	CHC-C1C	2.44	1.43	1.38
50	b	824	CLA	C1D-ND	-2.44	1.34	1.37
50	y	314	CLA	C1D-ND	-2.44	1.34	1.37
50	g	204	CLA	MG-NB	2.44	2.10	2.05
50	b	832	CLA	C1D-ND	-2.44	1.34	1.37
50	a	844	CLA	C1D-ND	-2.43	1.34	1.37
50	z	309	CLA	C1D-ND	-2.43	1.34	1.37
50	z	305	CLA	MG-NB	2.43	2.10	2.05
50	a	848	CLA	CHC-C1C	2.43	1.43	1.38
50	a	845	CLA	CHC-C1C	2.43	1.43	1.38
50	w	315	CLA	MG-NB	2.43	2.10	2.05
50	a	820	CLA	C1D-ND	-2.43	1.34	1.37
50	w	302	CLA	CHC-C1C	2.43	1.43	1.38
50	y	303	CLA	C1D-ND	-2.43	1.34	1.37
50	b	845	CLA	C1B-NB	-2.42	1.34	1.37
54	x	305	CHL	CBA-CGA	2.42	1.56	1.50
50	a	820	CLA	CHC-C1C	2.42	1.43	1.38
50	x	313	CLA	MG-NC	2.42	2.12	2.06
54	w	304	CHL	CBA-CGA	2.42	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	b	846	CLA	C1D-ND	-2.42	1.34	1.37
50	w	305	CLA	C1D-ND	-2.42	1.34	1.37
50	a	802	CLA	MG-NB	2.42	2.10	2.05
50	y	309	CLA	CHB-C1B	-2.42	1.34	1.39
50	b	805	CLA	C1D-ND	-2.42	1.34	1.37
50	z	303	CLA	MG-NB	2.42	2.10	2.05
50	a	851	CLA	CHC-C1C	2.42	1.43	1.38
50	b	842	CLA	CHC-C1C	2.42	1.43	1.38
50	z	305	CLA	CHC-C1C	2.41	1.43	1.38
50	b	849	CLA	C1D-ND	-2.41	1.34	1.37
50	l	305	CLA	CHC-C1C	2.41	1.43	1.38
50	a	809	CLA	CHC-C1C	2.41	1.43	1.38
50	b	826	CLA	CHC-C1C	2.41	1.43	1.38
50	a	820	CLA	MG-NB	2.41	2.10	2.05
50	y	304	CLA	CHC-C1C	2.41	1.43	1.38
50	b	840	CLA	C1D-ND	-2.41	1.34	1.37
50	b	825	CLA	CHC-C1C	2.41	1.43	1.38
50	b	851	CLA	CHC-C1C	2.41	1.43	1.38
50	b	835	CLA	MG-NB	2.41	2.10	2.05
50	b	834	CLA	CHC-C1C	2.41	1.43	1.38
50	y	305	CLA	CHC-C1C	2.41	1.43	1.38
46	f	306	LMG	O8-C28	2.41	1.40	1.33
50	a	852	CLA	C1D-ND	-2.41	1.34	1.37
50	g	201	CLA	MG-NB	2.40	2.10	2.05
50	b	849	CLA	CHB-C1B	-2.40	1.34	1.39
50	z	309	CLA	CHB-C1B	-2.40	1.34	1.39
50	b	801	CLA	C1D-ND	-2.40	1.34	1.37
50	a	858	CLA	CHC-C1C	2.40	1.43	1.38
50	x	312	CLA	CHC-C1C	2.40	1.43	1.38
50	a	842	CLA	CHC-C1C	2.40	1.43	1.38
50	x	316	CLA	CHC-C1C	2.39	1.43	1.38
50	x	313	CLA	CHB-C1B	-2.39	1.34	1.39
50	a	837	CLA	MG-NB	2.39	2.10	2.05
46	j	104	LMG	O8-C28	2.39	1.40	1.33
50	a	854	CLA	CHC-C1C	2.39	1.43	1.38
50	b	848	CLA	CHC-C1C	2.39	1.43	1.38
50	h	201	CLA	C1D-ND	-2.39	1.34	1.37
50	f	302	CLA	CHC-C1C	2.39	1.43	1.38
50	b	843	CLA	MG-NB	2.39	2.10	2.05
50	w	315	CLA	C1D-ND	-2.39	1.34	1.37
50	a	834	CLA	CHB-C1B	-2.39	1.34	1.39
50	j	102	CLA	C1D-ND	-2.39	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	y	302	CLA	CHC-C1C	2.38	1.43	1.38
50	b	810	CLA	CHC-C1C	2.38	1.43	1.38
50	b	836	CLA	MG-NB	2.38	2.10	2.05
50	b	808	CLA	CHC-C1C	2.38	1.43	1.38
50	g	203	CLA	C1D-ND	-2.38	1.34	1.37
50	z	310	CLA	CHC-C1C	2.38	1.43	1.38
50	l	306	CLA	CHB-C1B	-2.38	1.34	1.39
50	a	840	CLA	CHC-C1C	2.38	1.43	1.38
50	z	319	CLA	MG-NC	2.38	2.11	2.06
50	w	314	CLA	CHC-C1C	2.38	1.43	1.38
50	y	303	CLA	MG-NB	2.38	2.10	2.05
50	a	845	CLA	MG-NB	2.37	2.10	2.05
50	k	204	CLA	MG-NB	2.37	2.10	2.05
50	a	817	CLA	MG-NB	2.37	2.10	2.05
50	g	204	CLA	CHB-C1B	-2.37	1.34	1.39
50	k	204	CLA	CHC-C1C	2.37	1.43	1.38
50	a	816	CLA	CHC-C1C	2.37	1.43	1.38
50	j	102	CLA	CHC-C1C	2.37	1.43	1.38
50	k	203	CLA	MG-NC	2.37	2.11	2.06
50	x	308	CLA	C1D-ND	-2.37	1.34	1.37
50	a	819	CLA	MG-NB	2.37	2.10	2.05
50	b	828	CLA	MG-NB	2.37	2.10	2.05
50	a	802	CLA	CHC-C1C	2.37	1.43	1.38
50	a	819	CLA	C1D-ND	-2.37	1.34	1.37
50	a	852	CLA	MG-NB	2.37	2.10	2.05
50	w	305	CLA	MG-NB	2.37	2.10	2.05
50	a	845	CLA	CHB-C1B	-2.37	1.34	1.39
50	x	310	CLA	C1D-ND	-2.37	1.34	1.37
50	a	823	CLA	CHC-C1C	2.37	1.43	1.38
50	a	824	CLA	CHC-C1C	2.37	1.43	1.38
50	b	807	CLA	CHC-C1C	2.36	1.43	1.38
50	b	808	CLA	MG-NB	2.36	2.10	2.05
50	x	309	CLA	MG-NB	2.36	2.10	2.05
50	b	802	CLA	MG-NB	2.36	2.10	2.05
50	g	201	CLA	CHC-C1C	2.36	1.43	1.38
50	w	315	CLA	MG-NC	2.36	2.11	2.06
50	z	311	CLA	C1D-ND	-2.36	1.34	1.37
50	b	805	CLA	CHC-C1C	2.36	1.43	1.38
50	x	306	CLA	CHC-C1C	2.36	1.43	1.38
50	x	304	CLA	CHC-C1C	2.36	1.43	1.38
50	a	819	CLA	CHB-C1B	-2.36	1.34	1.39
50	y	307	CLA	MG-NB	2.36	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	a	833	CLA	CHC-C1C	2.36	1.43	1.38
50	a	849	CLA	CHB-C1B	-2.36	1.34	1.39
50	h	201	CLA	CHC-C1C	2.35	1.43	1.38
50	w	310	CLA	CHC-C1C	2.35	1.43	1.38
50	y	312	CLA	CHC-C1C	2.35	1.43	1.38
50	z	308	CLA	MG-NC	2.35	2.11	2.06
54	x	301	CHL	C2C-C3C	2.35	1.38	1.36
50	b	814	CLA	CHB-C1B	-2.35	1.34	1.39
46	7	301	LMG	O8-C28	2.35	1.40	1.33
50	b	846	CLA	MG-NB	2.35	2.10	2.05
50	b	824	CLA	MG-NB	2.35	2.10	2.05
50	a	834	CLA	C1D-ND	-2.35	1.34	1.37
50	y	311	CLA	CHC-C1C	2.35	1.43	1.38
50	a	856	CLA	MG-NB	2.35	2.10	2.05
50	z	308	CLA	C4D-ND	2.35	1.38	1.34
50	b	838	CLA	CHC-C1C	2.35	1.43	1.38
50	a	820	CLA	CHB-C1B	-2.35	1.34	1.39
50	b	823	CLA	CHC-C1C	2.35	1.43	1.38
50	b	823	CLA	MG-NB	2.35	2.10	2.05
46	B	605	LMG	O8-C28	2.35	1.40	1.33
50	a	852	CLA	CHB-C1B	-2.35	1.34	1.39
50	z	308	CLA	CHB-C1B	-2.34	1.34	1.39
50	j	102	CLA	MG-NB	2.34	2.10	2.05
50	k	203	CLA	CHB-C1B	-2.34	1.34	1.39
54	x	319	CHL	C2C-C3C	2.34	1.38	1.36
50	a	853	CLA	MG-NB	2.34	2.10	2.05
50	w	307	CLA	MG-NC	2.34	2.11	2.06
50	a	836	CLA	CHC-C1C	2.34	1.43	1.38
50	z	319	CLA	C1D-ND	-2.34	1.34	1.37
50	y	306	CLA	CHC-C1C	2.34	1.43	1.38
50	g	201	CLA	CHB-C1B	-2.34	1.34	1.39
50	b	805	CLA	CHB-C1B	-2.34	1.34	1.39
50	a	843	CLA	CHB-C1B	-2.34	1.34	1.39
50	b	836	CLA	CHC-C1C	2.33	1.43	1.38
50	y	311	CLA	CHB-C1B	-2.33	1.34	1.39
50	z	311	CLA	CHB-C1B	-2.33	1.34	1.39
50	y	307	CLA	CHC-C1C	2.33	1.43	1.38
50	a	844	CLA	MG-NB	2.33	2.10	2.05
50	y	314	CLA	CHC-C1C	2.33	1.43	1.38
50	x	302	CLA	CHB-C1B	-2.33	1.34	1.39
50	x	303	CLA	C1D-ND	-2.33	1.34	1.37
50	z	303	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	x	308	CLA	CHC-C1C	2.33	1.43	1.38
50	b	825	CLA	CHB-C1B	-2.33	1.34	1.39
52	a	808	CL0	CHB-C4A	-2.33	1.34	1.38
50	b	841	CLA	MG-NB	2.33	2.10	2.05
50	a	817	CLA	CHC-C1C	2.33	1.43	1.38
50	b	840	CLA	CHC-C1C	2.33	1.43	1.38
50	b	849	CLA	MG-NC	2.33	2.11	2.06
50	x	310	CLA	CHC-C1C	2.32	1.43	1.38
50	a	811	CLA	CHC-C1C	2.32	1.43	1.38
50	a	813	CLA	CHB-C1B	-2.32	1.34	1.39
50	g	203	CLA	CHB-C1B	-2.32	1.34	1.39
50	x	312	CLA	CHB-C1B	-2.32	1.34	1.39
50	w	305	CLA	CHC-C1C	2.32	1.43	1.38
50	a	823	CLA	MG-NB	2.32	2.10	2.05
50	b	805	CLA	MG-NB	2.32	2.10	2.05
50	a	833	CLA	MG-NB	2.32	2.10	2.05
50	b	851	CLA	MG-NB	2.32	2.10	2.05
50	x	318	CLA	MG-NB	2.32	2.10	2.05
50	y	307	CLA	CHB-C1B	-2.32	1.34	1.39
50	b	848	CLA	CHB-C1B	-2.32	1.34	1.39
50	a	855	CLA	CHC-C1C	2.32	1.43	1.38
50	l	305	CLA	MG-NB	2.32	2.10	2.05
50	y	309	CLA	CHC-C1C	2.32	1.43	1.38
46	D	601	LMG	O8-C28	2.31	1.40	1.33
50	a	837	CLA	CHB-C1B	-2.31	1.34	1.39
50	b	841	CLA	CHC-C1C	2.31	1.43	1.38
50	a	850	CLA	CHB-C1B	-2.31	1.34	1.39
50	a	819	CLA	CHC-C1C	2.31	1.43	1.38
50	a	834	CLA	CHC-C1C	2.31	1.43	1.38
50	k	205	CLA	CHC-C1C	2.31	1.43	1.38
50	y	314	CLA	CHB-C1B	-2.31	1.34	1.39
50	a	851	CLA	MG-NB	2.31	2.10	2.05
50	x	302	CLA	MG-NB	2.31	2.10	2.05
50	a	852	CLA	CHC-C1C	2.31	1.43	1.38
50	b	849	CLA	CHC-C1C	2.31	1.43	1.38
50	a	814	CLA	CHB-C1B	-2.31	1.34	1.39
50	a	837	CLA	CHC-C1C	2.31	1.43	1.38
50	k	205	CLA	MG-NB	2.31	2.10	2.05
50	b	832	CLA	MG-NC	2.31	2.11	2.06
50	f	302	CLA	MG-NB	2.31	2.10	2.05
50	y	307	CLA	C4B-C3B	2.31	1.48	1.43
50	a	822	CLA	CHB-C1B	-2.31	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	x	309	CLA	CHC-C1C	2.30	1.43	1.38
50	x	316	CLA	MG-NB	2.30	2.10	2.05
50	b	851	CLA	CHB-C1B	-2.30	1.34	1.39
50	w	307	CLA	MG-NB	2.30	2.10	2.05
50	k	203	CLA	C1D-ND	-2.30	1.34	1.37
50	y	309	CLA	C1D-ND	-2.30	1.34	1.37
50	b	824	CLA	CHB-C1B	-2.30	1.34	1.39
50	y	304	CLA	CHB-C1B	-2.30	1.34	1.39
50	a	811	CLA	MG-NB	2.30	2.10	2.05
50	x	310	CLA	CHB-C1B	-2.30	1.34	1.39
46	z	314	LMG	O8-C28	2.30	1.40	1.33
50	b	833	CLA	CHB-C1B	-2.30	1.34	1.39
50	a	817	CLA	CHB-C1B	-2.30	1.34	1.39
50	a	814	CLA	MG-NB	2.30	2.10	2.05
50	b	834	CLA	MG-NB	2.30	2.10	2.05
50	b	848	CLA	MG-NB	2.30	2.10	2.05
50	l	301	CLA	MG-NB	2.30	2.10	2.05
50	b	836	CLA	CHB-C1B	-2.30	1.34	1.39
50	a	853	CLA	CHB-C1B	-2.30	1.34	1.39
50	w	314	CLA	MG-NB	2.30	2.10	2.05
50	y	302	CLA	C4B-C3B	2.29	1.48	1.43
50	b	806	CLA	CHC-C1C	2.29	1.43	1.38
50	z	302	CLA	CHC-C1C	2.29	1.43	1.38
50	b	810	CLA	MG-NB	2.29	2.10	2.05
50	b	840	CLA	MG-NB	2.29	2.10	2.05
50	w	305	CLA	CHB-C1B	-2.29	1.34	1.39
50	z	302	CLA	MG-NB	2.29	2.10	2.05
50	a	857	CLA	MG-NB	2.29	2.10	2.05
50	a	844	CLA	CHC-C1C	2.29	1.43	1.38
50	b	802	CLA	CHC-C1C	2.29	1.43	1.38
50	f	302	CLA	CHB-C1B	-2.29	1.34	1.39
50	b	801	CLA	MG-NC	2.29	2.11	2.06
47	A	405	PQ9	C21-C22	2.29	1.57	1.50
50	k	204	CLA	CHB-C1B	-2.29	1.34	1.39
50	x	302	CLA	CHC-C1C	2.29	1.43	1.38
50	a	833	CLA	CHB-C1B	-2.29	1.34	1.39
50	b	837	CLA	MG-NB	2.29	2.10	2.05
50	h	201	CLA	MG-NB	2.28	2.10	2.05
50	a	809	CLA	CHB-C1B	-2.28	1.34	1.39
50	b	846	CLA	CHB-C1B	-2.28	1.34	1.39
50	z	309	CLA	MG-NB	2.28	2.10	2.05
50	b	810	CLA	CHB-C1B	-2.28	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	x	302	CLA	C1D-ND	-2.28	1.34	1.37
50	b	822	CLA	MG-NB	2.28	2.10	2.05
50	g	204	CLA	MG-NC	2.28	2.11	2.06
50	b	823	CLA	CHB-C1B	-2.28	1.34	1.39
50	l	305	CLA	CHB-C1B	-2.28	1.34	1.39
50	x	309	CLA	CHB-C1B	-2.28	1.34	1.39
50	y	309	CLA	MG-NC	2.28	2.11	2.06
50	z	302	CLA	MG-NC	2.28	2.11	2.06
50	a	840	CLA	MG-NB	2.28	2.10	2.05
50	b	835	CLA	CHB-C1B	-2.28	1.34	1.39
50	h	201	CLA	CHB-C1B	-2.28	1.34	1.39
50	l	301	CLA	CHB-C1B	-2.28	1.34	1.39
50	a	838	CLA	CHC-C1C	2.28	1.43	1.38
50	x	308	CLA	MG-NC	2.28	2.11	2.06
50	a	802	CLA	CHB-C1B	-2.28	1.34	1.39
50	j	102	CLA	CHB-C1B	-2.27	1.34	1.39
50	z	310	CLA	MG-NB	2.27	2.10	2.05
50	a	853	CLA	CHC-C1C	2.27	1.43	1.38
50	w	302	CLA	CHB-C1B	-2.27	1.34	1.39
50	a	842	CLA	MG-NB	2.27	2.10	2.05
50	b	824	CLA	CHC-C1C	2.27	1.43	1.38
50	b	826	CLA	CHB-C1B	-2.27	1.34	1.39
50	y	303	CLA	CHB-C1B	-2.27	1.34	1.39
43	b	819	BCR	C30-C25	-2.27	1.50	1.53
52	a	808	CL0	O2A-CGA	-2.27	1.32	1.42
50	a	824	CLA	CHB-C1B	-2.27	1.34	1.39
50	a	841	CLA	CHB-C1B	-2.27	1.34	1.39
50	a	822	CLA	CHC-C1C	2.27	1.43	1.38
50	z	309	CLA	MG-NC	2.27	2.11	2.06
50	b	801	CLA	CHB-C1B	-2.27	1.34	1.39
50	a	849	CLA	MG-NC	2.26	2.11	2.06
50	b	843	CLA	CHB-C1B	-2.26	1.34	1.39
50	a	823	CLA	CHB-C1B	-2.26	1.34	1.39
50	b	841	CLA	CHB-C1B	-2.26	1.34	1.39
50	b	809	CLA	CHB-C1B	-2.26	1.34	1.39
50	y	305	CLA	MG-NB	2.26	2.10	2.05
50	y	314	CLA	MG-NC	2.26	2.11	2.06
50	a	824	CLA	MG-NB	2.26	2.10	2.05
50	b	828	CLA	CHB-C1B	-2.26	1.34	1.39
50	x	308	CLA	MG-NB	2.26	2.10	2.05
50	a	851	CLA	CHB-C1B	-2.26	1.34	1.39
50	z	306	CLA	CHB-C1B	-2.26	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	b	839	CLA	CHB-C1B	-2.26	1.34	1.39
46	x	315	LMG	O8-C28	2.26	1.39	1.33
50	a	838	CLA	CHB-C1B	-2.26	1.34	1.39
50	w	310	CLA	MG-NB	2.26	2.10	2.05
50	a	812	CLA	MG-NB	2.26	2.10	2.05
53	b	827	PQN	C11-C12	-2.26	1.47	1.50
50	a	815	CLA	CHB-C1B	-2.25	1.34	1.39
50	b	808	CLA	CHB-C1B	-2.25	1.34	1.39
50	k	203	CLA	CHC-C1C	2.25	1.43	1.38
50	b	804	CLA	CHB-C1B	-2.25	1.34	1.39
50	z	303	CLA	CHB-C1B	-2.25	1.34	1.39
50	a	846	CLA	CHC-C1C	2.25	1.43	1.38
50	x	313	CLA	CHC-C1C	2.25	1.43	1.38
50	a	840	CLA	CHB-C1B	-2.25	1.34	1.39
50	a	855	CLA	MG-NB	2.25	2.10	2.05
50	a	802	CLA	MG-NC	2.25	2.11	2.06
50	b	813	CLA	CHB-C1B	-2.25	1.34	1.39
50	b	832	CLA	CHC-C1C	2.25	1.43	1.38
50	a	821	CLA	CHB-C1B	-2.25	1.34	1.39
50	a	813	CLA	MG-NB	2.25	2.10	2.05
50	w	306	CLA	CHB-C1B	-2.25	1.34	1.39
50	a	812	CLA	MG-NC	2.25	2.11	2.06
50	x	318	CLA	CHB-C1B	-2.25	1.34	1.39
50	b	826	CLA	MG-NB	2.25	2.10	2.05
50	a	801	CLA	CHB-C1B	-2.25	1.34	1.39
50	a	816	CLA	CHB-C1B	-2.25	1.34	1.39
50	z	308	CLA	CHC-C1C	2.25	1.43	1.38
50	z	307	CLA	CHB-C1B	-2.25	1.34	1.39
50	a	809	CLA	MG-NB	2.25	2.10	2.05
50	a	822	CLA	MG-NB	2.25	2.10	2.05
50	k	205	CLA	CHB-C1B	-2.25	1.34	1.39
50	y	306	CLA	CHB-C1B	-2.25	1.34	1.39
50	x	316	CLA	MG-NC	2.25	2.11	2.06
54	z	312	CHL	MG-NB	2.25	2.10	2.05
50	a	821	CLA	CHC-C1C	2.25	1.43	1.38
50	a	847	CLA	CHC-C1C	2.25	1.43	1.38
50	a	842	CLA	CHB-C1B	-2.24	1.34	1.39
50	b	809	CLA	MG-NB	2.24	2.10	2.05
46	w	312	LMG	O8-C28	2.24	1.39	1.33
50	b	837	CLA	CHB-C1B	-2.24	1.34	1.39
45	5	302	A1H1M	C10-C11	2.24	1.57	1.51
46	H	401	LMG	O8-C28	2.24	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	b	836	CLA	MG-NC	2.24	2.11	2.06
50	a	816	CLA	MG-NB	2.24	2.10	2.05
50	b	844	CLA	CHB-C1B	-2.24	1.34	1.39
50	b	841	CLA	MG-NC	2.24	2.11	2.06
50	a	811	CLA	CHB-C1B	-2.24	1.34	1.39
50	y	304	CLA	MG-NB	2.24	2.10	2.05
50	b	846	CLA	CHC-C1C	2.24	1.43	1.38
50	b	834	CLA	CHB-C1B	-2.24	1.34	1.39
50	x	302	CLA	MG-NC	2.24	2.11	2.06
50	y	312	CLA	MG-NB	2.24	2.10	2.05
50	w	316	CLA	CHB-C1B	-2.24	1.34	1.39
50	a	842	CLA	MG-NC	2.23	2.11	2.06
50	a	854	CLA	CHB-C1B	-2.23	1.34	1.39
50	b	812	CLA	CHB-C1B	-2.23	1.34	1.39
50	b	802	CLA	CHB-C1B	-2.23	1.34	1.39
50	k	204	CLA	MG-NC	2.23	2.11	2.06
50	a	821	CLA	MG-NC	2.23	2.11	2.06
46	F	802	LMG	O8-C28	2.23	1.39	1.33
50	a	821	CLA	C4B-C3B	2.23	1.48	1.43
50	b	842	CLA	MG-NB	2.23	2.10	2.05
50	y	306	CLA	MG-NB	2.23	2.10	2.05
50	b	840	CLA	CHB-C1B	-2.23	1.34	1.39
50	f	303	CLA	CHB-C1B	-2.23	1.34	1.39
50	b	848	CLA	MG-NC	2.23	2.11	2.06
50	a	858	CLA	CHB-C1B	-2.23	1.34	1.39
50	a	801	CLA	MG-NB	2.23	2.10	2.05
50	x	306	CLA	MG-NB	2.23	2.10	2.05
50	w	302	CLA	MG-NB	2.23	2.10	2.05
50	b	815	CLA	CHB-C1B	-2.23	1.34	1.39
50	a	824	CLA	MG-NC	2.23	2.11	2.06
50	z	309	CLA	CHC-C1C	2.23	1.42	1.38
50	b	833	CLA	CHC-C1C	2.22	1.42	1.38
50	y	303	CLA	CHC-C1C	2.22	1.42	1.38
50	a	846	CLA	CHB-C1B	-2.22	1.34	1.39
50	y	307	CLA	MG-NC	2.22	2.11	2.06
50	a	834	CLA	MG-NC	2.22	2.11	2.06
50	a	855	CLA	CHB-C1B	-2.22	1.34	1.39
50	b	838	CLA	CHB-C1B	-2.22	1.34	1.39
50	l	306	CLA	MG-NB	2.22	2.10	2.05
50	x	316	CLA	CHB-C1B	-2.22	1.34	1.39
50	f	302	CLA	MG-NC	2.22	2.11	2.06
50	z	316	CLA	MG-NB	2.22	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	g	201	CLA	MG-NC	2.22	2.11	2.06
50	w	307	CLA	CHC-C1C	2.22	1.42	1.38
50	w	310	CLA	CHB-C1B	-2.22	1.34	1.39
50	z	302	CLA	CAA-C2A	2.22	1.58	1.54
50	a	836	CLA	CHB-C1B	-2.22	1.34	1.39
50	a	856	CLA	CHB-C1B	-2.21	1.34	1.39
50	a	852	CLA	MG-NC	2.21	2.11	2.06
50	w	306	CLA	MG-NB	2.21	2.10	2.05
50	z	303	CLA	MG-NC	2.21	2.11	2.06
50	g	203	CLA	MG-NC	2.21	2.11	2.06
50	b	835	CLA	CHC-C1C	2.21	1.42	1.38
50	g	204	CLA	CHC-C1C	2.21	1.42	1.38
50	z	306	CLA	C3B-C4B	2.21	1.49	1.42
50	b	806	CLA	MG-NB	2.21	2.10	2.05
50	a	846	CLA	MG-NC	2.21	2.11	2.06
50	x	306	CLA	MG-NC	2.21	2.11	2.06
50	a	857	CLA	CHC-C1C	2.21	1.42	1.38
50	f	303	CLA	MG-NB	2.21	2.10	2.05
50	w	315	CLA	CHC-C1C	2.21	1.42	1.38
50	b	822	CLA	CHB-C1B	-2.21	1.34	1.39
50	x	309	CLA	MG-NC	2.21	2.11	2.06
50	z	302	CLA	CHB-C1B	-2.21	1.34	1.39
50	z	311	CLA	MG-NC	2.21	2.11	2.06
50	f	301	CLA	CHB-C1B	-2.21	1.34	1.39
54	w	309	CHL	C2C-C3C	2.21	1.38	1.36
50	b	806	CLA	MG-NC	2.20	2.11	2.06
50	y	303	CLA	MG-NC	2.20	2.11	2.06
50	b	813	CLA	MG-NB	2.20	2.10	2.05
50	b	842	CLA	CHB-C1B	-2.20	1.34	1.39
50	w	303	CLA	CHB-C1B	-2.20	1.34	1.39
50	a	853	CLA	MG-NC	2.20	2.11	2.06
50	x	318	CLA	MG-NC	2.20	2.11	2.06
50	y	305	CLA	CHB-C1B	-2.20	1.34	1.39
50	b	832	CLA	CHB-C1B	-2.20	1.34	1.39
50	b	823	CLA	MG-NC	2.20	2.11	2.06
50	b	835	CLA	MG-NC	2.20	2.11	2.06
50	a	838	CLA	MG-NB	2.20	2.10	2.05
50	l	301	CLA	MG-NC	2.20	2.11	2.06
50	b	807	CLA	CHB-C1B	-2.20	1.34	1.39
50	w	314	CLA	CHB-C1B	-2.20	1.34	1.39
50	a	845	CLA	MG-NC	2.20	2.11	2.06
50	a	837	CLA	MG-NC	2.20	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	a	815	CLA	MG-NB	2.20	2.10	2.05
50	y	312	CLA	CHB-C1B	-2.20	1.34	1.39
50	a	822	CLA	MG-NC	2.20	2.11	2.06
50	w	314	CLA	MG-NC	2.20	2.11	2.06
50	b	814	CLA	C3B-C4B	2.20	1.49	1.42
50	y	304	CLA	MG-NC	2.20	2.11	2.06
50	z	305	CLA	MG-NC	2.19	2.11	2.06
50	a	839	CLA	MG-NB	2.19	2.10	2.05
50	a	817	CLA	MG-NC	2.19	2.11	2.06
50	b	805	CLA	MG-NC	2.19	2.11	2.06
50	a	857	CLA	CHB-C1B	-2.19	1.34	1.39
50	b	833	CLA	MG-NC	2.19	2.11	2.06
50	b	807	CLA	MG-NB	2.19	2.10	2.05
50	b	825	CLA	MG-NC	2.19	2.11	2.06
50	a	835	CLA	CHB-C1B	-2.19	1.34	1.39
50	a	856	CLA	MG-NC	2.19	2.11	2.06
50	b	802	CLA	MG-NC	2.19	2.11	2.06
50	l	305	CLA	MG-NC	2.19	2.11	2.06
50	a	812	CLA	CHC-C1C	2.19	1.42	1.38
50	b	851	CLA	MG-NC	2.19	2.11	2.06
50	k	205	CLA	MG-NC	2.19	2.11	2.06
50	f	303	CLA	MG-NC	2.19	2.11	2.06
50	h	201	CLA	MG-NC	2.19	2.11	2.06
50	a	819	CLA	MG-NC	2.19	2.11	2.06
50	a	814	CLA	MG-NC	2.18	2.11	2.06
50	z	310	CLA	CHB-C1B	-2.18	1.34	1.39
47	A	405	PQ9	C29-C28	2.18	1.56	1.50
50	b	806	CLA	CHB-C1B	-2.18	1.34	1.39
50	x	306	CLA	CHB-C1B	-2.18	1.34	1.39
50	b	838	CLA	MG-NB	2.18	2.10	2.05
50	y	302	CLA	CHB-C1B	-2.18	1.34	1.39
50	a	844	CLA	CHB-C1B	-2.18	1.34	1.39
50	a	835	CLA	MG-NB	2.18	2.10	2.05
50	b	815	CLA	MG-NB	2.18	2.10	2.05
50	w	305	CLA	MG-NC	2.18	2.11	2.06
50	y	302	CLA	CAA-C2A	2.18	1.58	1.54
50	w	302	CLA	MG-NC	2.18	2.11	2.06
50	j	102	CLA	MG-NC	2.18	2.11	2.06
50	a	839	CLA	CHB-C1B	-2.18	1.34	1.39
50	b	825	CLA	MG-NB	2.18	2.10	2.05
50	b	833	CLA	MG-NB	2.17	2.10	2.05
50	z	316	CLA	CHB-C1B	-2.17	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	b	810	CLA	MG-NC	2.17	2.11	2.06
50	y	305	CLA	MG-NC	2.17	2.11	2.06
50	a	843	CLA	MG-NB	2.17	2.10	2.05
50	a	849	CLA	CHC-C1C	2.17	1.42	1.38
50	a	811	CLA	MG-NC	2.17	2.11	2.06
50	a	801	CLA	MG-NC	2.17	2.11	2.06
50	a	848	CLA	CHB-C1B	-2.17	1.34	1.39
50	a	857	CLA	MG-NC	2.17	2.11	2.06
50	b	847	CLA	CHB-C1B	-2.17	1.34	1.39
50	b	842	CLA	MG-NC	2.17	2.11	2.06
50	z	311	CLA	CHC-C1C	2.17	1.42	1.38
50	b	837	CLA	MG-NC	2.17	2.11	2.06
50	w	306	CLA	MG-NC	2.17	2.11	2.06
50	x	307	CLA	CHB-C1B	-2.17	1.34	1.39
50	b	803	CLA	CHB-C1B	-2.17	1.34	1.39
50	a	854	CLA	C1B-NB	-2.17	1.35	1.37
50	x	318	CLA	CHC-C1C	2.16	1.42	1.38
50	b	814	CLA	MG-NC	2.16	2.11	2.06
50	a	818	CLA	CHB-C1B	-2.16	1.34	1.39
46	j	105	LMG	O8-C28	2.16	1.39	1.33
50	b	804	CLA	MG-NB	2.16	2.10	2.05
50	b	844	CLA	C1B-NB	-2.16	1.35	1.37
50	b	843	CLA	MG-NC	2.16	2.11	2.06
50	b	840	CLA	MG-NC	2.16	2.11	2.06
50	b	839	CLA	MG-NC	2.16	2.11	2.06
50	a	841	CLA	MG-NC	2.16	2.11	2.06
50	a	818	CLA	MG-NB	2.16	2.10	2.05
50	a	851	CLA	MG-NC	2.16	2.11	2.06
50	b	826	CLA	MG-NC	2.16	2.11	2.06
50	z	307	CLA	MG-NB	2.16	2.10	2.05
50	a	823	CLA	MG-NC	2.15	2.11	2.06
50	b	846	CLA	MG-NC	2.15	2.11	2.06
50	x	310	CLA	MG-NC	2.15	2.11	2.06
50	b	843	CLA	CHC-C1C	2.15	1.42	1.38
50	z	319	CLA	CHC-C1C	2.15	1.42	1.38
50	b	834	CLA	MG-NC	2.15	2.11	2.06
50	a	826	CLA	CHB-C1B	-2.15	1.34	1.39
46	z	315	LMG	O8-C28	2.15	1.39	1.33
50	a	841	CLA	MG-NB	2.15	2.10	2.05
50	a	858	CLA	MG-NC	2.15	2.11	2.06
50	b	803	CLA	MG-NB	2.15	2.10	2.05
50	g	203	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	b	839	CLA	MG-NB	2.14	2.10	2.05
47	A	405	PQ9	C10-C1	2.14	1.54	1.47
50	a	855	CLA	MG-NC	2.14	2.11	2.06
50	a	848	CLA	MG-NB	2.14	2.10	2.05
50	b	811	CLA	CHB-C1B	-2.14	1.34	1.39
50	a	850	CLA	MG-NB	2.14	2.10	2.05
50	y	313	CLA	CHB-C1B	-2.14	1.34	1.39
50	a	838	CLA	MG-NC	2.14	2.11	2.06
50	b	807	CLA	MG-NC	2.14	2.11	2.06
50	b	813	CLA	MG-NC	2.14	2.11	2.06
50	b	828	CLA	MG-NC	2.14	2.11	2.06
50	a	820	CLA	MG-NC	2.14	2.11	2.06
50	l	306	CLA	MG-NC	2.14	2.11	2.06
50	a	846	CLA	MG-NB	2.14	2.10	2.05
50	w	310	CLA	MG-NC	2.14	2.11	2.06
50	y	308	CLA	MG-NC	2.14	2.11	2.06
50	x	308	CLA	CHB-C1B	-2.14	1.34	1.39
50	z	316	CLA	MG-NC	2.14	2.11	2.06
50	b	808	CLA	MG-NC	2.14	2.11	2.06
50	z	305	CLA	CHB-C1B	-2.13	1.34	1.39
50	b	844	CLA	MG-NB	2.13	2.10	2.05
50	b	804	CLA	MG-NC	2.13	2.11	2.06
50	y	308	CLA	CHB-C1B	-2.13	1.34	1.39
50	b	845	CLA	CHB-C1B	-2.13	1.34	1.39
50	y	310	CLA	CHB-C1B	-2.13	1.34	1.39
50	a	858	CLA	MG-NB	2.13	2.10	2.05
50	w	316	CLA	MG-NB	2.13	2.10	2.05
50	b	809	CLA	MG-NC	2.13	2.11	2.06
50	f	301	CLA	MG-NC	2.13	2.11	2.06
50	w	303	CLA	MG-NB	2.13	2.10	2.05
50	b	812	CLA	MG-NB	2.13	2.10	2.05
50	z	310	CLA	MG-NC	2.13	2.11	2.06
50	b	811	CLA	MG-NB	2.13	2.10	2.05
50	w	303	CLA	MG-NC	2.13	2.11	2.06
50	b	847	CLA	C1B-NB	-2.13	1.35	1.37
50	a	835	CLA	MG-NC	2.12	2.11	2.06
50	y	311	CLA	C1B-NB	-2.12	1.35	1.37
45	F	804	A1H1M	O19-C18	-2.12	1.38	1.43
50	x	312	CLA	MG-NB	2.12	2.10	2.05
50	b	838	CLA	MG-NC	2.12	2.11	2.06
50	x	313	CLA	CAA-C2A	2.12	1.57	1.54
45	5	302	A1H1M	C35-C11	2.12	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	F	801	SQD	O8-S	2.12	1.55	1.47
50	a	821	CLA	C3B-C2B	-2.12	1.36	1.44
50	y	307	CLA	C3B-C2B	-2.12	1.36	1.44
50	x	306	CLA	CAA-C2A	2.12	1.57	1.54
50	a	836	CLA	MG-NC	2.12	2.11	2.06
50	y	311	CLA	MG-NC	2.11	2.11	2.06
50	w	308	CLA	CHB-C1B	-2.11	1.34	1.39
50	a	833	CLA	MG-NC	2.11	2.11	2.06
50	b	841	CLA	CAA-C2A	2.11	1.57	1.54
48	a	859	SQD	O8-S	2.11	1.55	1.47
50	x	304	CLA	CHB-C1B	-2.11	1.34	1.39
50	b	822	CLA	MG-NC	2.11	2.11	2.06
50	z	307	CLA	MG-NC	2.11	2.11	2.06
51	b	821	DGD	O2G-C2G	-2.11	1.41	1.46
50	w	308	CLA	C3B-C4B	2.11	1.48	1.42
50	a	815	CLA	CAA-C2A	2.11	1.57	1.54
50	y	302	CLA	C1B-NB	-2.10	1.35	1.37
50	z	306	CLA	MG-NB	2.10	2.10	2.05
46	x	315	LMG	O7-C8	-2.10	1.41	1.46
45	F	804	A1H1M	C13-C33	2.10	1.58	1.52
50	a	812	CLA	CBB-CAB	-2.10	1.27	1.32
50	a	843	CLA	MG-NC	2.10	2.11	2.06
54	w	311	CHL	C3D-C2D	-2.10	1.36	1.39
50	a	826	CLA	MG-NC	2.10	2.11	2.06
50	b	847	CLA	C3B-C4B	2.10	1.48	1.42
50	a	840	CLA	MG-NC	2.09	2.11	2.06
50	a	844	CLA	MG-NC	2.09	2.11	2.06
53	a	825	PQN	C11-C12	-2.09	1.47	1.50
50	a	826	CLA	MG-NB	2.09	2.09	2.05
50	f	301	CLA	MG-NB	2.09	2.09	2.05
50	a	848	CLA	MG-NC	2.09	2.11	2.06
47	A	405	PQ9	C31-C32	2.09	1.56	1.50
50	l	306	CLA	C3B-C4B	2.09	1.48	1.42
50	a	843	CLA	C3B-C4B	2.09	1.48	1.42
50	b	849	CLA	C3B-C4B	2.09	1.48	1.42
50	a	818	CLA	MG-NC	2.09	2.11	2.06
50	y	306	CLA	MG-NC	2.09	2.11	2.06
50	b	811	CLA	C3B-C4B	2.09	1.48	1.42
50	a	839	CLA	MG-NC	2.09	2.11	2.06
48	w	318	SQD	O8-S	2.09	1.55	1.47
47	A	405	PQ9	C22-C23	2.08	1.37	1.33
50	x	312	CLA	MG-NC	2.08	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	y	308	CLA	C3B-C4B	2.08	1.48	1.42
50	a	816	CLA	MG-NC	2.08	2.11	2.06
50	x	304	CLA	MG-NC	2.08	2.11	2.06
50	b	849	CLA	C1B-NB	-2.08	1.35	1.37
50	l	306	CLA	C1B-NB	-2.08	1.35	1.37
50	k	203	CLA	CAA-C2A	2.08	1.57	1.53
50	x	312	CLA	C3B-C4B	2.08	1.48	1.42
50	b	812	CLA	C3B-C4B	2.08	1.48	1.42
50	y	310	CLA	C3B-C4B	2.08	1.48	1.42
50	b	844	CLA	CHC-C1C	2.08	1.42	1.38
50	a	840	CLA	C3B-C4B	2.08	1.48	1.42
50	a	822	CLA	C1B-NB	-2.08	1.35	1.37
50	w	303	CLA	C3B-C4B	2.08	1.48	1.42
50	b	844	CLA	MG-NC	2.07	2.11	2.06
50	a	809	CLA	MG-NC	2.07	2.11	2.06
50	y	302	CLA	C3B-C2B	-2.07	1.36	1.44
50	a	813	CLA	MG-NC	2.07	2.11	2.06
45	5	302	A1H1M	O12-C11	-2.07	1.42	1.44
50	y	312	CLA	MG-NC	2.07	2.11	2.06
47	A	405	PQ9	O4-C4	-2.07	1.19	1.24
50	b	823	CLA	CAA-C2A	2.07	1.57	1.54
50	b	803	CLA	C1B-NB	-2.07	1.35	1.37
50	b	843	CLA	CAA-C2A	2.07	1.57	1.54
50	a	818	CLA	C3B-C4B	2.06	1.48	1.42
50	w	306	CLA	C3B-C4B	2.06	1.48	1.42
48	w	317	SQD	O8-S	2.06	1.54	1.47
50	a	851	CLA	C3B-C4B	2.06	1.48	1.42
46	F	802	LMG	O7-C8	-2.06	1.41	1.46
50	b	828	CLA	C3B-C4B	2.06	1.48	1.42
50	y	313	CLA	MG-NC	2.06	2.11	2.06
48	j	106	SQD	O8-S	2.06	1.54	1.47
50	y	313	CLA	MG-NB	2.06	2.09	2.05
55	z	320	LUT	C22-C23	2.06	1.55	1.52
46	B	605	LMG	O7-C10	2.06	1.40	1.34
50	l	306	CLA	CAA-C2A	2.06	1.57	1.54
50	b	824	CLA	MG-NC	2.06	2.11	2.06
50	w	307	CLA	C1B-NB	-2.06	1.35	1.37
50	l	301	CLA	C3B-C4B	2.05	1.48	1.42
50	b	812	CLA	MG-NC	2.05	2.11	2.06
50	a	826	CLA	C1B-NB	-2.05	1.35	1.37
50	z	309	CLA	C1B-NB	-2.05	1.35	1.37
50	x	307	CLA	MG-NB	2.05	2.09	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	y	306	CLA	CAA-C2A	2.05	1.57	1.53
50	b	851	CLA	C3B-C4B	2.05	1.48	1.42
48	B	604	SQD	O8-S	2.05	1.54	1.47
50	a	813	CLA	C3B-C4B	2.05	1.48	1.42
50	b	815	CLA	C3B-C4B	2.05	1.48	1.42
50	y	311	CLA	CAA-C2A	2.05	1.57	1.54
50	z	307	CLA	CAA-C2A	2.05	1.57	1.54
50	b	804	CLA	CAA-C2A	2.05	1.57	1.53
50	y	306	CLA	C1B-NB	-2.05	1.35	1.37
50	y	308	CLA	C1B-NB	-2.05	1.35	1.37
50	x	307	CLA	MG-NC	2.05	2.11	2.06
50	y	311	CLA	MG-NB	2.04	2.09	2.05
50	z	307	CLA	C3B-C4B	2.04	1.48	1.42
50	b	813	CLA	C3B-C4B	2.04	1.48	1.42
50	y	313	CLA	CAA-C2A	2.04	1.57	1.54
50	z	303	CLA	CAA-C2A	2.04	1.57	1.53
50	a	854	CLA	MG-NC	2.04	2.11	2.06
50	b	811	CLA	MG-NC	2.04	2.11	2.06
50	z	316	CLA	C3B-C4B	2.04	1.48	1.42
51	a	804	DGD	O1G-C1A	2.04	1.39	1.33
50	x	303	CLA	CHC-C1C	2.04	1.42	1.38
50	w	316	CLA	MG-NC	2.04	2.11	2.06
50	b	838	CLA	C1B-NB	-2.04	1.35	1.37
50	w	303	CLA	CHD-C1D	2.04	1.42	1.38
50	b	809	CLA	C3B-C4B	2.04	1.48	1.42
50	x	302	CLA	C1B-NB	-2.04	1.35	1.37
50	b	815	CLA	MG-NC	2.03	2.11	2.06
50	z	303	CLA	C3B-C4B	2.03	1.48	1.42
50	b	841	CLA	C3B-C4B	2.03	1.48	1.42
50	b	848	CLA	C3B-C4B	2.03	1.48	1.42
50	f	303	CLA	C3B-C4B	2.03	1.48	1.42
50	x	309	CLA	C3B-C4B	2.03	1.48	1.42
50	b	826	CLA	C3B-C4B	2.03	1.48	1.42
50	y	304	CLA	C3B-C4B	2.03	1.48	1.42
50	a	839	CLA	C3B-C4B	2.03	1.48	1.42
50	b	822	CLA	C3B-C4B	2.03	1.48	1.42
50	f	303	CLA	CAA-C2A	2.03	1.57	1.53
50	g	201	CLA	C3B-C4B	2.03	1.48	1.42
50	w	306	CLA	C1B-NB	-2.03	1.35	1.37
50	a	846	CLA	C1B-NB	-2.02	1.35	1.37
50	b	815	CLA	C1B-NB	-2.02	1.35	1.37
50	a	856	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	a	817	CLA	CAA-C2A	2.02	1.57	1.53
43	f	304	BCR	C1-C6	-2.02	1.51	1.53
50	b	839	CLA	C3B-C4B	2.02	1.48	1.42
50	a	834	CLA	C3B-C4B	2.02	1.48	1.42
50	y	310	CLA	MG-NC	2.02	2.11	2.06
50	a	820	CLA	C3B-C4B	2.02	1.48	1.42
50	w	302	CLA	CAA-C2A	2.02	1.57	1.54
50	b	845	CLA	MG-NC	2.02	2.11	2.06
50	a	819	CLA	C3B-C4B	2.02	1.48	1.42
50	a	833	CLA	C3B-C4B	2.01	1.48	1.42
50	y	314	CLA	C3B-C4B	2.01	1.48	1.42
50	y	313	CLA	C3B-C4B	2.01	1.48	1.42
50	a	823	CLA	C3B-C4B	2.01	1.48	1.42
50	w	314	CLA	C3B-C4B	2.01	1.48	1.42
50	a	815	CLA	C3B-C4B	2.01	1.48	1.42
50	y	309	CLA	C3B-C4B	2.01	1.48	1.42
50	y	302	CLA	MG-NC	2.01	2.11	2.06
46	H	401	LMG	O6-C1	2.01	1.47	1.41
50	b	808	CLA	C3B-C4B	2.01	1.48	1.42
50	x	307	CLA	CAA-C2A	2.01	1.57	1.54
50	y	311	CLA	C3B-C4B	2.01	1.48	1.42
50	a	802	CLA	C3B-C4B	2.01	1.48	1.42
43	k	202	BCR	C1-C6	-2.01	1.51	1.53
54	x	301	CHL	O1D-CGD	2.01	1.26	1.21
50	b	837	CLA	C3B-C4B	2.01	1.48	1.42
50	x	302	CLA	CAA-C2A	2.01	1.57	1.53
50	b	801	CLA	CHC-C1C	2.01	1.42	1.38
50	z	310	CLA	C3B-C4B	2.01	1.48	1.42
50	a	815	CLA	C1B-NB	-2.01	1.35	1.37
50	g	203	CLA	C3B-C4B	2.00	1.48	1.42
50	k	203	CLA	C3B-C4B	2.00	1.48	1.42
50	x	307	CLA	C3B-C4B	2.00	1.48	1.42
50	a	850	CLA	C3B-C4B	2.00	1.48	1.42
50	b	833	CLA	C1B-NB	-2.00	1.35	1.37
50	w	305	CLA	C3B-C4B	2.00	1.48	1.42
50	y	306	CLA	C3B-C4B	2.00	1.48	1.42
50	y	314	CLA	CAA-C2A	2.00	1.57	1.54
50	b	834	CLA	C3B-C4B	2.00	1.48	1.42
50	g	204	CLA	C3B-C4B	2.00	1.48	1.42
50	x	313	CLA	C3B-C4B	2.00	1.48	1.42
50	l	305	CLA	CAA-C2A	2.00	1.57	1.53
50	y	304	CLA	CAA-C2A	2.00	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	a	815	CLA	MG-NC	2.00	2.11	2.06
50	w	302	CLA	C3B-C4B	2.00	1.48	1.42
50	z	308	CLA	C3B-C4B	2.00	1.48	1.42
50	a	809	CLA	C3B-C4B	2.00	1.48	1.42
50	b	836	CLA	C3B-C4B	2.00	1.48	1.42

All (1538) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	405	PQ9	C34-C33-C35	-27.40	83.87	116.13
47	A	405	PQ9	C19-C18-C20	-26.51	69.21	115.23
47	A	405	PQ9	C24-C23-C25	-26.42	69.37	115.23
47	A	405	PQ9	C14-C13-C15	-26.12	69.88	115.23
47	A	405	PQ9	C29-C28-C27	17.84	169.45	123.63
47	A	405	PQ9	C34-C33-C32	16.62	166.31	123.63
47	A	405	PQ9	C29-C28-C30	-16.21	87.09	115.23
47	A	405	PQ9	C15-C13-C12	-16.08	85.07	121.17
47	A	405	PQ9	C25-C23-C22	-15.89	85.50	121.17
47	A	405	PQ9	C20-C18-C17	-15.56	86.25	121.17
47	A	405	PQ9	C19-C18-C17	12.39	155.44	123.63
54	w	304	CHL	C1B-CHB-C4A	12.28	129.22	121.32
54	w	311	CHL	C1B-CHB-C4A	12.21	129.18	121.32
47	A	405	PQ9	C14-C13-C12	12.20	154.95	123.63
47	A	405	PQ9	C24-C23-C22	12.16	154.86	123.63
54	x	319	CHL	C1B-CHB-C4A	11.99	129.03	121.32
54	x	301	CHL	C1B-CHB-C4A	11.82	128.93	121.32
54	x	305	CHL	C1B-CHB-C4A	11.74	128.87	121.32
54	z	304	CHL	C1B-CHB-C4A	11.73	128.87	121.32
54	w	309	CHL	C1B-CHB-C4A	11.67	128.83	121.32
54	z	312	CHL	C1B-CHB-C4A	11.45	128.69	121.32
50	y	313	CLA	C4A-NA-C1A	11.13	111.76	106.68
50	b	803	CLA	C4A-NA-C1A	11.05	111.72	106.68
50	b	824	CLA	C4A-NA-C1A	10.88	111.64	106.68
50	a	822	CLA	C4A-NA-C1A	10.84	111.62	106.68
50	a	838	CLA	C4A-NA-C1A	10.84	111.62	106.68
50	a	846	CLA	C4A-NA-C1A	10.76	111.59	106.68
50	w	316	CLA	C4A-NA-C1A	10.75	111.58	106.68
50	b	843	CLA	C4A-NA-C1A	10.63	111.53	106.68
50	b	833	CLA	C4A-NA-C1A	10.63	111.53	106.68
50	a	814	CLA	C4A-NA-C1A	10.52	111.48	106.68
50	b	805	CLA	C4A-NA-C1A	10.50	111.47	106.68
50	k	204	CLA	C4A-NA-C1A	10.50	111.47	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	f	302	CLA	C4A-NA-C1A	10.50	111.47	106.68
50	b	814	CLA	C4A-NA-C1A	10.45	111.45	106.68
50	w	305	CLA	C4A-NA-C1A	10.40	111.42	106.68
50	a	824	CLA	C4A-NA-C1A	10.39	111.42	106.68
50	b	807	CLA	C4A-NA-C1A	10.38	111.41	106.68
50	w	314	CLA	C4A-NA-C1A	10.35	111.40	106.68
50	j	102	CLA	C4A-NA-C1A	10.30	111.38	106.68
50	h	201	CLA	C4A-NA-C1A	10.30	111.38	106.68
50	f	301	CLA	C4A-NA-C1A	10.29	111.37	106.68
50	z	310	CLA	C4A-NA-C1A	10.26	111.36	106.68
50	x	308	CLA	C4A-NA-C1A	10.22	111.34	106.68
50	w	308	CLA	C4A-NA-C1A	10.20	111.33	106.68
50	a	811	CLA	C4A-NA-C1A	10.19	111.33	106.68
50	y	304	CLA	C4A-NA-C1A	10.19	111.33	106.68
50	y	308	CLA	C4A-NA-C1A	10.18	111.33	106.68
50	y	303	CLA	C4A-NA-C1A	10.18	111.32	106.68
50	a	853	CLA	C4A-NA-C1A	10.16	111.31	106.68
50	b	841	CLA	C4A-NA-C1A	10.15	111.31	106.68
50	y	311	CLA	C4A-NA-C1A	10.14	111.31	106.68
50	b	837	CLA	C4A-NA-C1A	10.14	111.31	106.68
50	a	857	CLA	C4A-NA-C1A	10.13	111.30	106.68
50	b	826	CLA	C4A-NA-C1A	10.10	111.29	106.68
50	b	848	CLA	C4A-NA-C1A	10.08	111.28	106.68
50	b	815	CLA	C4A-NA-C1A	10.05	111.26	106.68
50	y	310	CLA	C4A-NA-C1A	10.02	111.25	106.68
50	x	306	CLA	C4A-NA-C1A	10.00	111.24	106.68
50	b	806	CLA	C4A-NA-C1A	10.00	111.24	106.68
50	w	315	CLA	C4A-NA-C1A	9.98	111.23	106.68
50	x	307	CLA	C4A-NA-C1A	9.97	111.23	106.68
50	x	318	CLA	C4A-NA-C1A	9.97	111.23	106.68
50	x	302	CLA	C4A-NA-C1A	9.96	111.22	106.68
50	w	302	CLA	C4A-NA-C1A	9.94	111.21	106.68
50	x	309	CLA	C4A-NA-C1A	9.91	111.20	106.68
50	a	821	CLA	C4A-NA-C1A	9.90	111.20	106.68
50	b	801	CLA	C4A-NA-C1A	9.90	111.20	106.68
50	a	855	CLA	C4A-NA-C1A	9.88	111.19	106.68
50	b	822	CLA	C4A-NA-C1A	9.88	111.19	106.68
50	a	801	CLA	C4A-NA-C1A	9.87	111.18	106.68
50	a	815	CLA	C4A-NA-C1A	9.86	111.18	106.68
50	b	840	CLA	C4A-NA-C1A	9.84	111.17	106.68
50	a	834	CLA	C4A-NA-C1A	9.83	111.16	106.68
50	b	838	CLA	C4A-NA-C1A	9.77	111.14	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	808	CLA	C4A-NA-C1A	9.69	111.10	106.68
50	a	843	CLA	C4A-NA-C1A	9.69	111.10	106.68
50	b	836	CLA	C4A-NA-C1A	9.69	111.10	106.68
50	a	851	CLA	C4A-NA-C1A	9.67	111.09	106.68
50	z	302	CLA	C4A-NA-C1A	9.67	111.09	106.68
50	a	837	CLA	C4A-NA-C1A	9.67	111.09	106.68
50	z	309	CLA	C4A-NA-C1A	9.66	111.08	106.68
50	a	809	CLA	C4A-NA-C1A	9.65	111.08	106.68
50	y	306	CLA	C4A-NA-C1A	9.65	111.08	106.68
50	z	305	CLA	C4A-NA-C1A	9.64	111.08	106.68
50	b	846	CLA	C4A-NA-C1A	9.62	111.07	106.68
50	l	301	CLA	C4A-NA-C1A	9.60	111.06	106.68
50	z	307	CLA	C4A-NA-C1A	9.57	111.05	106.68
50	f	303	CLA	C4A-NA-C1A	9.57	111.04	106.68
50	k	205	CLA	C4A-NA-C1A	9.56	111.04	106.68
50	y	305	CLA	C4A-NA-C1A	9.54	111.03	106.68
50	a	819	CLA	C4A-NA-C1A	9.54	111.03	106.68
50	x	316	CLA	C4A-NA-C1A	9.53	111.03	106.68
50	b	844	CLA	C4A-NA-C1A	9.53	111.03	106.68
50	a	823	CLA	C4A-NA-C1A	9.52	111.02	106.68
50	b	847	CLA	C4A-NA-C1A	9.52	111.02	106.68
50	a	845	CLA	C4A-NA-C1A	9.51	111.02	106.68
50	b	810	CLA	C4A-NA-C1A	9.51	111.02	106.68
50	b	832	CLA	C4A-NA-C1A	9.49	111.01	106.68
50	l	306	CLA	C4A-NA-C1A	9.47	111.00	106.68
50	a	835	CLA	C4A-NA-C1A	9.46	111.00	106.68
50	k	203	CLA	C4A-NA-C1A	9.46	110.99	106.68
50	z	306	CLA	C4A-NA-C1A	9.44	110.98	106.68
50	y	302	CLA	C4A-NA-C1A	9.43	110.98	106.68
50	a	841	CLA	C4A-NA-C1A	9.43	110.98	106.68
50	b	823	CLA	C4A-NA-C1A	9.41	110.97	106.68
50	w	306	CLA	C4A-NA-C1A	9.41	110.97	106.68
50	w	303	CLA	C4A-NA-C1A	9.38	110.96	106.68
50	a	826	CLA	C4A-NA-C1A	9.33	110.94	106.68
50	g	204	CLA	C4A-NA-C1A	9.32	110.93	106.68
50	a	802	CLA	C4A-NA-C1A	9.31	110.92	106.68
50	b	839	CLA	C4A-NA-C1A	9.26	110.91	106.68
50	b	849	CLA	C4A-NA-C1A	9.24	110.90	106.68
50	z	319	CLA	C4A-NA-C1A	9.22	110.88	106.68
50	a	812	CLA	C4A-NA-C1A	9.21	110.88	106.68
50	x	310	CLA	C4A-NA-C1A	9.20	110.88	106.68
50	z	316	CLA	C4A-NA-C1A	9.16	110.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	851	CLA	C4A-NA-C1A	9.14	110.85	106.68
50	a	836	CLA	C4A-NA-C1A	9.13	110.85	106.68
50	y	307	CLA	C4A-NA-C1A	9.12	110.84	106.68
50	a	840	CLA	C4A-NA-C1A	9.07	110.82	106.68
50	a	842	CLA	C4A-NA-C1A	9.06	110.81	106.68
50	a	852	CLA	C4A-NA-C1A	9.05	110.81	106.68
50	a	817	CLA	C4A-NA-C1A	9.01	110.79	106.68
50	b	804	CLA	C4A-NA-C1A	9.01	110.79	106.68
50	a	833	CLA	C4A-NA-C1A	9.00	110.78	106.68
50	z	308	CLA	C4A-NA-C1A	8.99	110.78	106.68
50	b	812	CLA	C4A-NA-C1A	8.99	110.78	106.68
50	b	811	CLA	C4A-NA-C1A	8.96	110.77	106.68
50	a	849	CLA	C4A-NA-C1A	8.91	110.74	106.68
50	y	314	CLA	C4A-NA-C1A	8.89	110.74	106.68
50	b	825	CLA	C4A-NA-C1A	8.88	110.73	106.68
50	w	310	CLA	C4A-NA-C1A	8.87	110.73	106.68
54	x	311	CHL	C1B-CHB-C4A	8.86	128.89	120.23
50	b	835	CLA	C4A-NA-C1A	8.84	110.71	106.68
50	x	312	CLA	C4A-NA-C1A	8.82	110.70	106.68
50	z	303	CLA	C4A-NA-C1A	8.81	110.70	106.68
50	x	304	CLA	C4A-NA-C1A	8.78	110.68	106.68
50	a	820	CLA	C4A-NA-C1A	8.75	110.67	106.68
50	y	312	CLA	C4A-NA-C1A	8.73	110.66	106.68
50	b	834	CLA	C4A-NA-C1A	8.72	110.66	106.68
50	a	844	CLA	C4A-NA-C1A	8.71	110.65	106.68
50	a	848	CLA	C4A-NA-C1A	8.71	110.65	106.68
50	b	828	CLA	C4A-NA-C1A	8.71	110.65	106.68
50	b	809	CLA	C4A-NA-C1A	8.68	110.64	106.68
50	a	816	CLA	C4A-NA-C1A	8.67	110.64	106.68
50	l	305	CLA	C4A-NA-C1A	8.64	110.62	106.68
50	x	313	CLA	C4A-NA-C1A	8.59	110.60	106.68
50	a	812	CLA	CAB-C3B-C4B	8.59	136.42	124.33
50	a	839	CLA	C4A-NA-C1A	8.52	110.56	106.68
50	g	203	CLA	C4A-NA-C1A	8.46	110.54	106.68
50	b	802	CLA	C4A-NA-C1A	8.46	110.54	106.68
50	w	307	CLA	C4A-NA-C1A	8.46	110.54	106.68
50	z	311	CLA	C4A-NA-C1A	8.42	110.52	106.68
50	a	854	CLA	C4A-NA-C1A	8.41	110.52	106.68
50	a	850	CLA	C4A-NA-C1A	8.39	110.51	106.68
50	x	303	CLA	C4A-NA-C1A	8.36	110.50	106.68
50	y	309	CLA	C4A-NA-C1A	8.13	110.39	106.68
50	a	818	CLA	C4A-NA-C1A	8.10	110.38	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	a	808	CL0	C1B-CHB-C4A	8.05	128.10	120.23
50	b	842	CLA	C4A-NA-C1A	8.04	110.35	106.68
50	b	813	CLA	C4A-NA-C1A	8.01	110.33	106.68
47	A	405	PQ9	C30-C28-C27	-7.94	103.34	121.17
47	A	405	PQ9	C16-C17-C18	-7.88	109.58	127.62
47	A	405	PQ9	C11-C12-C13	-7.87	113.28	126.83
50	y	307	CLA	CAB-C3B-C4B	7.84	137.36	125.42
50	a	856	CLA	C4A-NA-C1A	7.78	110.23	106.68
50	y	302	CLA	CAB-C3B-C4B	7.77	137.25	125.42
50	a	858	CLA	C4A-NA-C1A	7.76	110.22	106.68
50	a	813	CLA	C4A-NA-C1A	7.74	110.21	106.68
50	a	821	CLA	CAB-C3B-C4B	7.74	137.20	125.42
50	g	201	CLA	C4A-NA-C1A	7.70	110.19	106.68
54	z	304	CHL	O2D-CGD-CBD	7.24	118.90	110.95
54	x	319	CHL	O2D-CGD-CBD	7.08	118.73	110.95
54	w	311	CHL	O2D-CGD-CBD	6.94	118.58	110.95
54	w	309	CHL	O2D-CGD-CBD	6.81	118.43	110.95
47	A	405	PQ9	C21-C22-C23	-6.77	112.13	127.62
52	a	808	CL0	CHB-C4A-NA	6.57	128.68	121.83
53	b	827	PQN	C14-C13-C15	6.52	126.55	115.23
54	x	311	CHL	O2D-CGD-CBD	6.51	118.10	110.95
47	A	405	PQ9	C26-C27-C28	-6.46	112.85	127.62
54	x	301	CHL	O2D-CGD-CBD	6.36	117.93	110.95
53	a	825	PQN	C14-C13-C15	6.29	126.14	115.23
54	x	305	CHL	O2D-CGD-CBD	6.18	117.74	110.95
54	w	304	CHL	O2D-CGD-CBD	6.18	117.73	110.95
54	x	305	CHL	CBC-CAC-C3C	-5.96	104.34	112.87
52	a	808	CL0	CHA-C1A-C2A	-5.93	125.06	133.83
54	z	312	CHL	O2D-CGD-CBD	5.84	117.36	110.95
50	b	845	CLA	C4A-NA-C1A	5.82	109.33	106.68
43	z	318	BCR	C16-C17-C18	-5.78	119.18	127.28
54	x	311	CHL	CHA-C1A-C2A	-5.65	125.48	133.83
54	x	311	CHL	C4D-CHA-CBD	-5.52	103.40	108.97
50	y	302	CLA	C1C-NC-C4C	5.41	109.15	106.68
54	z	304	CHL	CAA-C2A-C3A	-5.37	103.91	116.23
50	z	308	CLA	C1D-CHD-C4C	5.25	126.38	120.72
50	a	812	CLA	CHC-C4B-C3B	5.15	124.87	122.09
54	w	311	CHL	CBC-CAC-C3C	-4.95	105.79	112.87
45	5	302	A1H1M	C36-C08-C07	4.92	123.32	112.46
50	a	852	CLA	O2D-CGD-CBD	4.90	119.80	111.23
45	5	302	A1H1M	C13-O14-C15	4.88	123.24	113.72
54	z	312	CHL	C3D-C4D-CHA	4.85	115.91	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	5	302	A1H1M	C06-C07-C08	4.77	122.99	112.46
54	x	319	CHL	C3D-C4D-CHA	4.60	115.54	108.54
54	z	304	CHL	C4D-CHA-CBD	-4.58	104.35	108.97
54	z	312	CHL	C4D-CHA-CBD	-4.56	104.37	108.97
54	x	305	CHL	C3D-C4D-CHA	4.56	115.47	108.54
45	F	804	A1H1M	C13-O14-C15	4.54	122.59	113.72
54	x	301	CHL	C3D-C4D-CHA	4.53	115.42	108.54
54	x	305	CHL	C4D-CHA-CBD	-4.50	104.43	108.97
54	w	309	CHL	C3D-C4D-CHA	4.49	115.36	108.54
54	w	311	CHL	C3D-C4D-CHA	4.48	115.36	108.54
54	x	319	CHL	C4D-CHA-CBD	-4.46	104.47	108.97
50	b	839	CLA	O2D-CGD-CBD	4.45	119.02	111.23
48	F	801	SQD	O47-C7-C8	-4.45	101.86	111.48
45	F	804	A1H1M	C06-C07-C08	4.44	122.27	112.46
54	w	304	CHL	C4D-CHA-CBD	-4.43	104.50	108.97
50	y	309	CLA	O2D-CGD-CBD	4.42	118.96	111.23
54	z	304	CHL	C3D-C4D-CHA	4.41	115.25	108.54
50	a	847	CLA	O2D-CGD-CBD	4.39	118.90	111.23
50	b	845	CLA	C3B-C4B-NB	-4.39	106.61	110.53
43	4	101	BCR	C16-C17-C18	-4.38	121.14	127.28
53	b	827	PQN	C15-C13-C12	-4.35	111.40	121.17
50	a	818	CLA	O2D-CGD-CBD	4.34	118.82	111.23
54	x	311	CHL	C3D-C4D-CHA	4.34	115.14	108.54
54	w	304	CHL	C3D-C4D-CHA	4.32	115.10	108.54
47	A	405	PQ9	C11-C2-C1	4.31	120.46	116.91
50	b	810	CLA	O2D-CGD-CBD	4.29	118.74	111.23
54	w	311	CHL	C4D-CHA-CBD	-4.25	104.68	108.97
50	x	312	CLA	O2D-CGD-CBD	4.22	118.61	111.23
50	b	837	CLA	O2D-CGD-CBD	4.21	118.59	111.23
50	z	308	CLA	OBD-CAD-CBD	-4.21	120.97	124.94
50	b	840	CLA	O2D-CGD-CBD	4.20	118.58	111.23
54	w	309	CHL	C4D-CHA-CBD	-4.20	104.73	108.97
50	b	843	CLA	O2D-CGD-CBD	4.18	118.53	111.23
50	a	812	CLA	O2D-CGD-CBD	4.17	118.53	111.23
50	a	813	CLA	O2D-CGD-CBD	4.16	118.51	111.23
50	b	815	CLA	O2D-CGD-CBD	4.16	118.50	111.23
50	h	201	CLA	O2D-CGD-CBD	4.15	118.48	111.23
54	x	301	CHL	C4D-CHA-CBD	-4.14	104.79	108.97
54	x	301	CHL	CBC-CAC-C3C	-4.14	106.94	112.87
50	a	819	CLA	O2D-CGD-CBD	4.13	118.46	111.23
50	w	314	CLA	O2D-CGD-CBD	4.13	118.46	111.23
50	a	834	CLA	O2D-CGD-CBD	4.13	118.45	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	x	304	CLA	O2D-CGD-CBD	4.12	118.44	111.23
50	f	301	CLA	O2D-CGD-CBD	4.12	118.43	111.23
50	a	801	CLA	O2D-CGD-CBD	4.12	118.43	111.23
50	b	847	CLA	O2D-CGD-CBD	4.11	118.42	111.23
50	b	849	CLA	O2D-CGD-CBD	4.11	118.41	111.23
50	b	847	CLA	C3B-C4B-NB	-4.11	106.86	110.53
43	a	803	BCR	C21-C20-C19	-4.10	117.03	125.28
50	a	845	CLA	O2D-CGD-CBD	4.10	118.39	111.23
50	z	319	CLA	O2D-CGD-CBD	4.10	118.39	111.23
50	y	303	CLA	O2D-CGD-CBD	4.09	118.38	111.23
50	b	836	CLA	O2D-CGD-CBD	4.09	118.38	111.23
50	b	809	CLA	O2D-CGD-CBD	4.08	118.36	111.23
50	z	308	CLA	O2D-CGD-CBD	4.08	118.36	111.23
50	z	310	CLA	O2D-CGD-CBD	4.07	118.35	111.23
50	a	817	CLA	O2D-CGD-CBD	4.07	118.34	111.23
43	k	201	BCR	C15-C14-C13	-4.06	121.58	127.28
50	b	845	CLA	O2D-CGD-CBD	4.06	118.32	111.23
50	a	826	CLA	O2D-CGD-CBD	4.05	118.31	111.23
50	x	313	CLA	O2D-CGD-CBD	4.04	118.29	111.23
50	x	303	CLA	O2D-CGD-CBD	4.04	118.29	111.23
50	z	311	CLA	O2D-CGD-CBD	4.02	118.25	111.23
50	a	809	CLA	O2D-CGD-CBD	4.02	118.25	111.23
50	y	313	CLA	O2D-CGD-CBD	4.01	118.25	111.23
50	a	822	CLA	O2D-CGD-CBD	4.01	118.24	111.23
50	x	308	CLA	O2D-CGD-CBD	4.01	118.24	111.23
53	a	825	PQN	C15-C13-C12	-4.00	112.18	121.17
50	w	308	CLA	C3B-C4B-NB	-4.00	106.96	110.53
50	b	832	CLA	O2D-CGD-CBD	4.00	118.22	111.23
50	g	201	CLA	O2D-CGD-CBD	4.00	118.22	111.23
45	5	302	A1H1M	C09-C10-C11	3.98	117.36	110.96
50	a	858	CLA	C3B-C4B-NB	-3.98	106.98	110.53
50	g	203	CLA	O2D-CGD-CBD	3.97	118.18	111.23
50	w	303	CLA	O2D-CGD-CBD	3.97	118.18	111.23
50	x	310	CLA	O2D-CGD-CBD	3.97	118.18	111.23
50	l	305	CLA	O2D-CGD-CBD	3.97	118.17	111.23
50	b	834	CLA	O2D-CGD-CBD	3.97	118.17	111.23
50	z	306	CLA	C3B-C4B-NB	-3.96	107.00	110.53
50	a	836	CLA	O2D-CGD-CBD	3.96	118.15	111.23
50	j	102	CLA	O2D-CGD-CBD	3.95	118.14	111.23
50	w	302	CLA	O2D-CGD-CBD	3.94	118.12	111.23
50	f	302	CLA	O2D-CGD-CBD	3.94	118.12	111.23
50	b	805	CLA	O2D-CGD-CBD	3.94	118.12	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	816	CLA	O2D-CGD-CBD	3.94	118.11	111.23
50	a	824	CLA	O2D-CGD-CBD	3.93	118.11	111.23
50	z	302	CLA	O2D-CGD-CBD	3.93	118.11	111.23
50	b	842	CLA	O2D-CGD-CBD	3.93	118.10	111.23
50	a	835	CLA	O2D-CGD-CBD	3.93	118.09	111.23
50	a	814	CLA	O2D-CGD-CBD	3.92	118.09	111.23
50	b	826	CLA	O2D-CGD-CBD	3.92	118.08	111.23
50	b	822	CLA	O2D-CGD-CBD	3.91	118.06	111.23
50	y	313	CLA	C3B-C4B-NB	-3.91	107.04	110.53
50	b	828	CLA	O2D-CGD-CBD	3.90	118.06	111.23
50	a	842	CLA	O2D-CGD-CBD	3.90	118.05	111.23
50	b	802	CLA	O2D-CGD-CBD	3.90	118.05	111.23
50	k	203	CLA	O2D-CGD-CBD	3.89	118.04	111.23
50	a	853	CLA	O2D-CGD-CBD	3.89	118.04	111.23
50	a	854	CLA	O2D-CGD-CBD	3.89	118.04	111.23
50	w	310	CLA	O2D-CGD-CBD	3.89	118.04	111.23
50	a	815	CLA	O2D-CGD-CBD	3.89	118.03	111.23
50	b	812	CLA	C3B-C4B-NB	-3.89	107.06	110.53
50	b	851	CLA	O2D-CGD-CBD	3.89	118.02	111.23
43	j	101	BCR	C2-C1-C6	3.88	116.08	110.44
50	y	314	CLA	O2D-CGD-CBD	3.88	118.01	111.23
50	k	205	CLA	O2D-CGD-CBD	3.88	118.01	111.23
50	b	838	CLA	O2D-CGD-CBD	3.88	118.01	111.23
50	a	813	CLA	C3B-C4B-NB	-3.87	107.07	110.53
50	b	824	CLA	O2D-CGD-CBD	3.87	118.00	111.23
50	y	306	CLA	O2D-CGD-CBD	3.86	117.99	111.23
50	a	836	CLA	C3B-C4B-NB	-3.85	107.09	110.53
50	y	305	CLA	O2D-CGD-CBD	3.85	117.97	111.23
50	b	844	CLA	O2D-CGD-CBD	3.85	117.96	111.23
50	a	854	CLA	C3B-C4B-NB	-3.85	107.09	110.53
50	b	833	CLA	O2D-CGD-CBD	3.84	117.95	111.23
50	a	821	CLA	O2D-CGD-CBD	3.84	117.94	111.23
50	x	302	CLA	O2D-CGD-CBD	3.84	117.94	111.23
50	y	308	CLA	C3B-C4B-NB	-3.84	107.11	110.53
50	l	301	CLA	O2D-CGD-CBD	3.83	117.93	111.23
50	b	823	CLA	O2D-CGD-CBD	3.83	117.93	111.23
50	y	307	CLA	O2D-CGD-CBD	3.83	117.93	111.23
50	x	316	CLA	O2D-CGD-CBD	3.83	117.93	111.23
50	z	316	CLA	O2D-CGD-CBD	3.83	117.92	111.23
50	a	846	CLA	O2D-CGD-CBD	3.83	117.92	111.23
50	b	811	CLA	C3B-C4B-NB	-3.83	107.11	110.53
50	b	814	CLA	O2D-CGD-CBD	3.83	117.92	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	w	309	CHL	CBC-CAC-C3C	-3.82	107.40	112.87
50	w	303	CLA	C3B-C4B-NB	-3.82	107.12	110.53
50	a	855	CLA	O2D-CGD-CBD	3.82	117.91	111.23
50	a	848	CLA	O2D-CGD-CBD	3.82	117.91	111.23
50	y	311	CLA	O2D-CGD-CBD	3.82	117.91	111.23
50	w	305	CLA	C4-C3-C5	-3.81	111.64	116.13
50	z	306	CLA	O2D-CGD-CBD	3.81	117.89	111.23
50	b	846	CLA	O2D-CGD-CBD	3.80	117.88	111.23
50	x	307	CLA	O2D-CGD-CBD	3.80	117.88	111.23
50	w	315	CLA	O2D-CGD-CBD	3.80	117.88	111.23
50	x	318	CLA	O2D-CGD-CBD	3.80	117.88	111.23
50	b	813	CLA	C3B-C4B-NB	-3.80	107.14	110.53
50	w	310	CLA	CAC-C3C-C4C	-3.80	119.85	124.79
50	w	310	CLA	CAC-C3C-C2C	3.79	134.52	127.56
50	a	850	CLA	O2D-CGD-CBD	3.79	117.85	111.23
50	a	843	CLA	C3B-C4B-NB	-3.78	107.15	110.53
50	b	806	CLA	O2D-CGD-CBD	3.78	117.84	111.23
50	b	804	CLA	O2D-CGD-CBD	3.77	117.83	111.23
50	a	857	CLA	O2D-CGD-CBD	3.77	117.82	111.23
50	a	840	CLA	O2D-CGD-CBD	3.77	117.81	111.23
50	b	804	CLA	C3B-C4B-NB	-3.77	107.17	110.53
50	b	825	CLA	O2D-CGD-CBD	3.76	117.81	111.23
50	b	803	CLA	C3B-C4B-NB	-3.76	107.17	110.53
50	b	835	CLA	O2D-CGD-CBD	3.76	117.80	111.23
50	y	312	CLA	O2D-CGD-CBD	3.76	117.80	111.23
50	z	307	CLA	O2D-CGD-CBD	3.76	117.80	111.23
50	a	841	CLA	O2D-CGD-CBD	3.75	117.79	111.23
50	x	309	CLA	O2D-CGD-CBD	3.75	117.79	111.23
50	w	307	CLA	O2D-CGD-CBD	3.75	117.78	111.23
50	k	204	CLA	O2D-CGD-CBD	3.75	117.78	111.23
50	y	302	CLA	O2D-CGD-CBD	3.74	117.77	111.23
50	w	316	CLA	C3B-C4B-NB	-3.74	107.19	110.53
54	w	304	CHL	CBC-CAC-C3C	-3.73	107.53	112.87
50	b	808	CLA	O2D-CGD-CBD	3.73	117.75	111.23
50	a	858	CLA	O2D-CGD-CBD	3.73	117.75	111.23
50	w	305	CLA	O2D-CGD-CBD	3.73	117.75	111.23
50	b	807	CLA	O2D-CGD-CBD	3.72	117.74	111.23
50	a	837	CLA	O2D-CGD-CBD	3.71	117.72	111.23
50	f	303	CLA	O2D-CGD-CBD	3.70	117.69	111.23
54	z	312	CHL	O1D-CGD-CBD	-3.70	119.12	124.72
45	5	302	A1H1M	O14-C15-C18	3.69	117.36	109.72
50	y	308	CLA	O2D-CGD-CBD	3.69	117.68	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	848	CLA	O2D-CGD-CBD	3.69	117.68	111.23
50	a	856	CLA	O2D-CGD-CBD	3.69	117.68	111.23
43	l	303	BCR	C37-C22-C23	3.69	123.72	118.09
50	y	312	CLA	C4-C3-C5	-3.69	111.79	116.13
50	b	803	CLA	O2D-CGD-CBD	3.68	117.67	111.23
50	a	839	CLA	C3B-C4B-NB	-3.68	107.25	110.53
50	a	839	CLA	O2D-CGD-CBD	3.68	117.66	111.23
54	w	311	CHL	CMA-C3A-C4A	-3.67	106.71	114.61
54	w	309	CHL	CMA-C3A-C4A	-3.67	106.71	114.61
50	a	820	CLA	O2D-CGD-CBD	3.66	117.63	111.23
50	z	305	CLA	O2D-CGD-CBD	3.66	117.63	111.23
43	4	101	BCR	C15-C14-C13	-3.66	122.14	127.28
50	a	849	CLA	O2D-CGD-CBD	3.66	117.63	111.23
50	f	301	CLA	C3B-C4B-NB	-3.65	107.27	110.53
50	x	304	CLA	C3B-C4B-NB	-3.65	107.27	110.53
50	a	820	CLA	C3B-C4B-NB	-3.64	107.28	110.53
50	y	310	CLA	C3B-C4B-NB	-3.64	107.28	110.53
50	b	801	CLA	O2D-CGD-CBD	3.64	117.60	111.23
50	a	833	CLA	O2D-CGD-CBD	3.64	117.59	111.23
50	a	848	CLA	C3B-C4B-NB	-3.64	107.28	110.53
50	b	813	CLA	O2D-CGD-CBD	3.63	117.58	111.23
50	w	306	CLA	C3B-C4B-NB	-3.63	107.29	110.53
54	z	312	CHL	CMA-C3A-C4A	-3.63	106.80	114.61
51	a	804	DGD	O6D-C1D-O3G	-3.62	101.48	110.04
50	x	306	CLA	O2D-CGD-CBD	3.61	117.54	111.23
50	x	302	CLA	CAA-C2A-C3A	-3.61	107.95	116.23
50	a	818	CLA	C3B-C4B-NB	-3.61	107.31	110.53
43	a	831	BCR	C19-C18-C17	-3.61	116.38	124.72
50	w	306	CLA	O2D-CGD-CBD	3.61	117.54	111.23
50	a	851	CLA	O2D-CGD-CBD	3.60	117.53	111.23
50	b	815	CLA	C3B-C4B-NB	-3.60	107.31	110.53
50	f	303	CLA	C3B-C4B-NB	-3.60	107.31	110.53
50	b	809	CLA	C3B-C4B-NB	-3.60	107.31	110.53
50	a	802	CLA	O2D-CGD-CBD	3.60	117.52	111.23
50	a	843	CLA	O2D-CGD-CBD	3.60	117.52	111.23
50	a	838	CLA	O2D-CGD-CBD	3.60	117.52	111.23
50	a	815	CLA	C3B-C4B-NB	-3.59	107.32	110.53
53	a	825	PQN	C9-C10-C5	3.59	123.29	119.26
45	5	302	A1H1M	C36-C35-C11	3.59	116.73	110.96
50	a	856	CLA	C3B-C4B-NB	-3.58	107.33	110.53
50	a	841	CLA	C3B-C4B-NB	-3.58	107.33	110.53
50	b	825	CLA	C3B-C4B-NB	-3.58	107.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	827	PQN	C9-C10-C5	3.57	123.26	119.26
50	a	850	CLA	C3B-C4B-NB	-3.56	107.35	110.53
50	a	844	CLA	O2D-CGD-CBD	3.56	117.46	111.23
50	l	306	CLA	O2D-CGD-CBD	3.56	117.46	111.23
43	j	101	BCR	C16-C17-C18	-3.56	122.28	127.28
54	x	311	CHL	CHB-C4A-NA	3.56	125.54	121.83
43	a	827	BCR	C16-C17-C18	-3.56	122.29	127.28
45	5	302	A1H1M	C09-C08-C07	-3.55	104.61	112.46
50	a	837	CLA	O2A-CGA-CBA	3.55	122.67	111.83
50	a	823	CLA	O2D-CGD-CBD	3.55	117.44	111.23
50	x	307	CLA	C3B-C4B-NB	-3.55	107.36	110.53
45	F	804	A1H1M	C36-C08-C07	3.55	120.29	112.46
43	k	201	BCR	C2-C1-C6	3.54	115.59	110.44
50	a	824	CLA	C3B-C4B-NB	-3.54	107.37	110.53
50	y	311	CLA	C3B-C4B-NB	-3.54	107.37	110.53
50	a	835	CLA	C3B-C4B-NB	-3.54	107.37	110.53
50	z	316	CLA	C3B-C4B-NB	-3.54	107.37	110.53
54	w	311	CHL	OBD-CAD-CBD	-3.53	120.64	125.82
54	x	305	CHL	CMA-C3A-C4A	-3.53	107.01	114.61
50	b	842	CLA	C3B-C4B-NB	-3.53	107.38	110.53
52	a	808	CL0	C1C-CHC-C4B	3.52	128.68	116.07
50	z	307	CLA	C3B-C4B-NB	-3.52	107.39	110.53
50	z	303	CLA	O2D-CGD-CBD	3.52	117.38	111.23
43	x	314	BCR	C21-C20-C19	-3.51	113.02	123.20
54	x	319	CHL	CMA-C3A-C4A	-3.51	107.04	114.61
50	b	807	CLA	C3B-C4B-NB	-3.51	107.40	110.53
50	l	306	CLA	C3B-C4B-NB	-3.50	107.40	110.53
50	a	801	CLA	C3B-C4B-NB	-3.49	107.41	110.53
48	w	318	SQD	O47-C7-C8	3.49	119.04	111.48
54	w	304	CHL	CMA-C3A-C4A	-3.49	107.09	114.61
43	b	831	BCR	C2-C1-C6	3.49	115.50	110.44
50	w	308	CLA	O2D-CGD-CBD	3.48	117.32	111.23
43	j	103	BCR	C20-C21-C22	-3.48	122.40	127.28
45	F	804	A1H1M	O19-C20-O21	-3.47	101.55	110.69
50	y	310	CLA	O2D-CGD-CBD	3.47	117.29	111.23
54	x	301	CHL	CMA-C3A-C4A	-3.47	107.14	114.61
50	b	837	CLA	C3B-C4B-NB	-3.46	107.44	110.53
54	z	304	CHL	CMA-C3A-C4A	-3.46	107.16	114.61
54	z	312	CHL	C1-C2-C3	3.46	131.86	126.20
50	y	312	CLA	C3B-C4B-NB	-3.45	107.45	110.53
50	z	310	CLA	C3B-C4B-NB	-3.45	107.45	110.53
50	y	304	CLA	C3B-C4B-NB	-3.45	107.45	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	841	CLA	O2D-CGD-CBD	3.45	117.25	111.23
50	b	839	CLA	C3B-C4B-NB	-3.44	107.46	110.53
50	b	848	CLA	C3B-C4B-NB	-3.44	107.46	110.53
50	y	302	CLA	O2A-CGA-CBA	3.44	122.32	111.83
50	a	840	CLA	C3B-C4B-NB	-3.44	107.46	110.53
50	x	312	CLA	C3B-C4B-NB	-3.44	107.46	110.53
54	z	312	CHL	OBD-CAD-CBD	-3.43	120.79	125.82
45	F	804	A1H1M	C09-C08-C07	-3.43	104.90	112.46
50	h	201	CLA	C3B-C4B-NB	-3.42	107.47	110.53
52	a	808	CL0	CBC-CAC-C3C	-3.42	107.98	112.87
50	z	309	CLA	O2D-CGD-CBD	3.41	117.20	111.23
50	z	308	CLA	OBD-CAD-C3D	3.41	130.43	125.89
50	a	826	CLA	C3B-C4B-NB	-3.41	107.48	110.53
50	g	204	CLA	O2D-CGD-CBD	3.41	117.20	111.23
54	x	319	CHL	CBC-CAC-C3C	-3.41	108.00	112.87
50	b	822	CLA	C3B-C4B-NB	-3.41	107.49	110.53
43	b	819	BCR	C11-C10-C9	3.40	132.05	127.28
50	a	822	CLA	C4-C3-C5	-3.39	112.13	116.13
50	a	816	CLA	C3B-C4B-NB	-3.39	107.50	110.53
50	b	806	CLA	C3B-C4B-NB	-3.39	107.50	110.53
50	x	316	CLA	C3B-C4B-NB	-3.39	107.50	110.53
50	b	828	CLA	C3B-C4B-NB	-3.39	107.51	110.53
50	a	851	CLA	C3B-C4B-NB	-3.38	107.52	110.53
50	b	811	CLA	O2D-CGD-CBD	3.38	117.13	111.23
50	w	302	CLA	C3B-C4B-NB	-3.38	107.52	110.53
50	a	855	CLA	C3B-C4B-NB	-3.37	107.52	110.53
43	b	831	BCR	C29-C30-C25	3.37	115.34	110.44
50	b	832	CLA	O2A-CGA-CBA	3.36	122.09	111.83
50	a	811	CLA	C3B-C4B-NB	-3.36	107.53	110.53
50	a	843	CLA	O2A-CGA-CBA	3.36	122.08	111.83
50	b	838	CLA	C3B-C4B-NB	-3.36	107.53	110.53
43	b	850	BCR	C16-C17-C18	-3.36	122.57	127.28
50	y	305	CLA	C3B-C4B-NB	-3.35	107.54	110.53
50	l	301	CLA	C3B-C4B-NB	-3.34	107.55	110.53
50	a	809	CLA	C3B-C4B-NB	-3.34	107.55	110.53
50	b	843	CLA	O2A-CGA-CBA	3.34	122.00	111.83
54	w	304	CHL	CAB-C3B-C2B	-3.33	117.71	124.69
50	b	808	CLA	C3B-C4B-NB	-3.33	107.55	110.53
50	b	834	CLA	C3B-C4B-NB	-3.33	107.55	110.53
43	k	201	BCR	C29-C30-C25	3.33	115.28	110.44
50	b	826	CLA	C3B-C4B-NB	-3.33	107.56	110.53
50	y	306	CLA	C3B-C4B-NB	-3.32	107.56	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	304	CHL	CBC-CAC-C3C	-3.32	108.11	112.87
50	a	811	CLA	O2D-CGD-CBD	3.32	117.04	111.23
43	z	318	BCR	C20-C21-C22	-3.32	122.62	127.28
50	b	846	CLA	O2A-CGA-CBA	3.32	121.95	111.83
50	l	305	CLA	C3B-C4B-NB	-3.31	107.58	110.53
43	a	831	BCR	C19-C20-C21	-3.31	116.75	123.52
50	g	201	CLA	O2A-CGA-CBA	3.31	121.92	111.83
50	f	302	CLA	C3B-C4B-NB	-3.30	107.58	110.53
50	x	306	CLA	C3B-C4B-NB	-3.30	107.59	110.53
50	a	833	CLA	C3B-C4B-NB	-3.29	107.59	110.53
50	b	802	CLA	O2A-CGA-CBA	3.29	121.86	111.83
50	b	842	CLA	O2A-CGA-CBA	3.29	121.86	111.83
50	w	314	CLA	C3B-C4B-NB	-3.29	107.60	110.53
50	a	823	CLA	C3B-C4B-NB	-3.28	107.60	110.53
54	x	305	CHL	CAA-C2A-C3A	-3.28	104.14	113.00
50	a	814	CLA	C3B-C4B-NB	-3.27	107.61	110.53
50	b	851	CLA	C3B-C4B-NB	-3.27	107.61	110.53
50	x	307	CLA	O2A-CGA-CBA	3.26	121.78	111.83
43	b	831	BCR	C20-C21-C22	-3.26	122.71	127.28
50	b	810	CLA	C3B-C4B-NB	-3.26	107.62	110.53
50	b	812	CLA	O2D-CGD-CBD	3.26	116.92	111.23
50	a	857	CLA	O2A-CGA-CBA	3.26	121.76	111.83
45	F	804	A1H1M	C36-C35-C11	3.26	116.19	110.96
50	b	809	CLA	O2A-CGA-CBA	3.25	121.76	111.83
50	a	845	CLA	C3B-C4B-NB	-3.25	107.63	110.53
50	z	306	CLA	O2A-CGA-CBA	3.25	121.74	111.83
50	b	851	CLA	O2A-CGA-CBA	3.24	121.72	111.83
50	y	311	CLA	C4-C3-C5	-3.24	112.32	116.13
50	a	842	CLA	C3B-C4B-NB	-3.24	107.64	110.53
50	a	839	CLA	O2A-CGA-CBA	3.23	121.70	111.83
50	b	802	CLA	C3B-C4B-NB	-3.23	107.64	110.53
50	b	823	CLA	C3B-C4B-NB	-3.23	107.64	110.53
50	y	303	CLA	O2A-CGA-CBA	3.23	121.69	111.83
50	k	204	CLA	C3B-C4B-NB	-3.23	107.65	110.53
50	a	853	CLA	C3B-C4B-NB	-3.23	107.65	110.53
50	a	802	CLA	O2A-CGA-CBA	3.22	121.66	111.83
50	j	102	CLA	C3B-C4B-NB	-3.22	107.65	110.53
50	b	840	CLA	C3B-C4B-NB	-3.22	107.66	110.53
50	l	306	CLA	O2A-CGA-CBA	3.21	121.64	111.83
50	w	310	CLA	C3B-C4B-NB	-3.21	107.66	110.53
50	a	802	CLA	C3B-C4B-NB	-3.21	107.66	110.53
50	b	805	CLA	C3B-C4B-NB	-3.21	107.66	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	z	316	CLA	O2A-CGA-CBA	3.21	121.63	111.83
50	x	309	CLA	C3B-C4B-NB	-3.21	107.67	110.53
43	b	817	BCR	C2-C1-C6	3.21	115.10	110.44
50	b	814	CLA	O2A-CGA-CBA	3.21	121.61	111.83
50	b	839	CLA	O2A-CGA-CBA	3.21	121.61	111.83
50	a	845	CLA	O2A-CGA-CBA	3.20	121.60	111.83
50	b	837	CLA	O2A-CGA-CBA	3.20	121.59	111.83
50	y	313	CLA	O2A-CGA-CBA	3.20	121.59	111.83
50	a	819	CLA	O2A-CGA-CBA	3.20	121.59	111.83
50	b	815	CLA	O2A-CGA-CBA	3.20	121.59	111.83
50	a	844	CLA	C3B-C4B-NB	-3.20	107.68	110.53
50	y	310	CLA	O2A-CGA-CBA	3.20	121.58	111.83
50	a	838	CLA	C3B-C4B-NB	-3.19	107.68	110.53
50	a	852	CLA	C3B-C4B-NB	-3.19	107.68	110.53
50	b	841	CLA	C3B-C4B-NB	-3.19	107.68	110.53
50	w	305	CLA	O2A-CGA-CBA	3.18	121.55	111.83
50	y	314	CLA	O2A-CGA-CBA	3.18	121.55	111.83
50	a	856	CLA	O2A-CGA-CBA	3.18	121.54	111.83
50	g	203	CLA	O2A-CGA-CBA	3.18	121.53	111.83
50	z	305	CLA	C3B-C4B-NB	-3.18	107.69	110.53
50	k	204	CLA	O2A-CGA-CBA	3.18	121.53	111.83
50	b	806	CLA	O2A-CGA-CBA	3.18	121.53	111.83
50	a	811	CLA	O2A-CGA-CBA	3.18	121.52	111.83
50	a	857	CLA	C3B-C4B-NB	-3.18	107.69	110.53
50	a	801	CLA	C1-C2-C3	3.17	131.40	126.20
50	x	308	CLA	C3B-C4B-NB	-3.17	107.70	110.53
50	a	824	CLA	O2A-CGA-CBA	3.17	121.50	111.83
50	b	849	CLA	O2A-CGA-CBA	3.17	121.50	111.83
50	b	810	CLA	O2A-CGA-CBA	3.17	121.49	111.83
50	b	836	CLA	C3B-C4B-NB	-3.16	107.71	110.53
50	a	850	CLA	O2A-CGA-CBA	3.16	121.48	111.83
50	z	302	CLA	O2A-CGA-CBA	3.16	121.46	111.83
50	x	304	CLA	O2A-CGA-CBA	3.16	121.46	111.83
50	a	847	CLA	C2A-C3A-C4A	-3.16	104.31	110.51
50	a	818	CLA	O2A-CGA-CBA	3.15	121.44	111.83
50	b	822	CLA	O2A-CGA-CBA	3.15	121.44	111.83
50	z	307	CLA	O2A-CGA-CBA	3.15	121.44	111.83
50	a	817	CLA	C3B-C4B-NB	-3.15	107.72	110.53
50	w	316	CLA	O2A-CGA-CBA	3.14	121.42	111.83
50	z	303	CLA	C3B-C4B-NB	-3.14	107.72	110.53
50	a	834	CLA	O2A-CGA-CBA	3.14	121.42	111.83
50	a	815	CLA	O2A-CGA-CBA	3.14	121.42	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	w	304	CHL	CAA-C2A-C3A	-3.14	104.51	113.00
50	b	841	CLA	O2A-CGA-CBA	3.14	121.40	111.83
50	b	825	CLA	C1-C2-C3	3.13	131.33	126.20
50	b	843	CLA	C3B-C4B-NB	-3.13	107.73	110.53
50	k	205	CLA	C3B-C4B-NB	-3.13	107.73	110.53
54	w	311	CHL	CAA-C2A-C3A	-3.13	104.54	113.00
50	a	822	CLA	O2A-CGA-CBA	3.13	121.37	111.83
50	w	302	CLA	O2A-CGA-CBA	3.13	121.37	111.83
50	a	847	CLA	C3B-C4B-NB	-3.13	107.74	110.53
50	g	201	CLA	C3B-C4B-NB	-3.13	107.74	110.53
50	z	311	CLA	O2A-CGA-CBA	3.13	121.37	111.83
50	b	846	CLA	C3B-C4B-NB	-3.13	107.74	110.53
50	a	852	CLA	C4-C3-C5	-3.12	112.45	116.13
50	x	303	CLA	O2A-CGA-CBA	3.12	121.35	111.83
50	a	846	CLA	C3B-C4B-NB	-3.12	107.75	110.53
50	z	302	CLA	C3B-C4B-NB	-3.11	107.75	110.53
50	b	845	CLA	O2A-CGA-CBA	3.11	121.33	111.83
43	a	810	BCR	C37-C22-C23	3.11	121.75	114.59
54	x	305	CHL	OBD-CAD-CBD	-3.11	121.26	125.82
50	b	814	CLA	C3B-C4B-NB	-3.11	107.75	110.53
50	b	805	CLA	O2A-CGA-CBA	3.11	121.31	111.83
50	b	844	CLA	C3B-C4B-NB	-3.11	107.76	110.53
50	a	813	CLA	O2A-CGA-CBA	3.11	121.31	111.83
50	a	852	CLA	O2A-CGA-CBA	3.10	121.29	111.83
50	y	312	CLA	O2A-CGA-CBA	3.10	121.29	111.83
43	b	817	BCR	C15-C14-C13	-3.10	122.94	127.28
50	b	832	CLA	C3B-C4B-NB	-3.10	107.77	110.53
50	z	303	CLA	CMA-C3A-C2A	-3.09	109.14	116.23
50	w	305	CLA	C3B-C4B-NB	-3.09	107.77	110.53
50	b	824	CLA	C3B-C4B-NB	-3.09	107.77	110.53
50	a	809	CLA	O2A-CGA-CBA	3.09	121.25	111.83
43	l	303	BCR	C24-C23-C22	3.08	130.80	126.23
50	w	306	CLA	O2A-CGA-CBA	3.08	121.24	111.83
50	b	809	CLA	C12-C11-C10	-3.08	102.00	113.62
50	a	848	CLA	O2A-CGA-CBA	3.08	121.23	111.83
50	b	833	CLA	C3B-C4B-NB	-3.08	107.78	110.53
50	x	313	CLA	O2A-CGA-CBA	3.08	121.22	111.83
50	a	837	CLA	C3B-C4B-NB	-3.08	107.78	110.53
54	w	304	CHL	O1D-CGD-CBD	-3.08	120.06	124.72
50	a	821	CLA	O2A-CGA-CBA	3.07	121.21	111.83
50	a	834	CLA	C3B-C4B-NB	-3.07	107.79	110.53
50	a	836	CLA	O2A-CGA-CBA	3.07	121.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	823	CLA	O2A-CGA-CBA	3.07	121.19	111.83
50	b	801	CLA	O2A-CGA-CBA	3.07	121.19	111.83
50	b	812	CLA	C1-C2-C3	3.06	131.21	126.20
50	y	303	CLA	C3B-C4B-NB	-3.06	107.80	110.53
50	x	302	CLA	C3B-C4B-NB	-3.06	107.80	110.53
50	z	308	CLA	C3B-C4B-NB	-3.06	107.80	110.53
50	a	842	CLA	O2A-CGA-CBA	3.06	121.15	111.83
50	b	844	CLA	O2A-CGA-CBA	3.05	121.14	111.83
50	b	835	CLA	C3B-C4B-NB	-3.05	107.81	110.53
50	a	819	CLA	C3B-C4B-NB	-3.05	107.81	110.53
50	f	301	CLA	O2A-CGA-CBA	3.04	121.10	111.83
50	a	833	CLA	C1-C2-C3	3.03	131.16	126.20
54	z	312	CHL	C1A-CHA-C4D	3.03	124.04	118.98
50	y	314	CLA	C3B-C4B-NB	-3.03	107.83	110.53
43	j	103	BCR	C16-C17-C18	-3.02	123.04	127.28
50	a	835	CLA	O2A-CGA-CBA	3.02	121.05	111.83
54	z	312	CHL	C1C-CHC-C4B	3.02	126.87	116.07
50	z	309	CLA	C3B-C4B-NB	-3.01	107.84	110.53
50	b	838	CLA	O2A-CGA-CBA	3.01	121.00	111.83
50	x	313	CLA	C3B-C4B-NB	-3.01	107.85	110.53
50	z	305	CLA	O2A-CGA-CBA	3.01	121.00	111.83
52	a	808	CL0	O2D-CGD-O1D	-3.01	117.26	124.08
50	x	308	CLA	O2A-CGA-CBA	3.01	121.00	111.83
43	4	101	BCR	C29-C30-C25	3.01	114.81	110.44
50	a	841	CLA	O2A-CGA-CBA	3.00	120.99	111.83
50	b	826	CLA	O2A-CGA-CBA	3.00	120.99	111.83
50	a	818	CLA	C12-C11-C10	-3.00	102.30	113.62
50	y	311	CLA	O2A-CGA-CBA	3.00	120.99	111.83
50	b	835	CLA	O2A-CGA-CBA	3.00	120.98	111.83
43	a	810	BCR	C11-C12-C13	2.99	134.57	126.36
50	b	807	CLA	O2A-CGA-CBA	2.99	120.96	111.83
50	b	803	CLA	O2A-CGA-CBA	2.99	120.96	111.83
50	x	302	CLA	C2A-C1A-CHA	2.99	129.05	123.86
50	x	312	CLA	O2A-CGA-CBA	2.99	120.96	111.83
50	a	814	CLA	O2A-CGA-CBA	2.99	120.96	111.83
50	a	849	CLA	O2A-CGA-CBA	2.99	120.95	111.83
43	a	810	BCR	C2-C1-C6	2.99	114.78	110.44
50	y	308	CLA	O2A-CGA-CBA	2.99	120.94	111.83
50	w	316	CLA	O1D-CGD-CBD	-2.99	118.63	124.52
50	a	858	CLA	O2A-CGA-CBA	2.99	120.94	111.83
50	a	846	CLA	O2A-CGA-CBA	2.98	120.93	111.83
50	b	836	CLA	O2A-CGA-CBA	2.98	120.93	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	823	CLA	O2A-CGA-CBA	2.98	120.93	111.83
50	x	310	CLA	C3B-C4B-NB	-2.98	107.87	110.53
50	a	820	CLA	O2A-CGA-CBA	2.98	120.92	111.83
50	b	847	CLA	O2A-CGA-CBA	2.98	120.91	111.83
50	w	307	CLA	C3B-C4B-NB	-2.98	107.87	110.53
50	w	310	CLA	O2A-CGA-CBA	2.97	120.90	111.83
50	b	824	CLA	O2A-CGA-CBA	2.97	120.90	111.83
50	b	803	CLA	C1-C2-C3	2.97	131.06	126.20
54	z	312	CHL	CBC-CAC-C3C	-2.96	108.63	112.87
43	b	818	BCR	C2-C1-C6	2.96	114.74	110.44
50	a	853	CLA	O2A-CGA-CBA	2.96	120.86	111.83
50	w	315	CLA	C3B-C4B-NB	-2.96	107.89	110.53
50	a	838	CLA	O2A-CGA-CBA	2.96	120.84	111.83
50	b	840	CLA	O2A-CGA-CBA	2.95	120.84	111.83
53	b	827	PQN	C2M-C2-C1	-2.95	111.24	116.68
50	w	308	CLA	O2A-CGA-CBA	2.95	120.84	111.83
47	A	405	PQ9	C11-C2-C3	-2.95	119.91	123.39
50	b	833	CLA	O2A-CGA-CBA	2.95	120.82	111.83
55	x	321	LUT	C28-C29-C30	2.95	123.64	119.01
50	a	801	CLA	O2A-CGA-CBA	2.95	120.82	111.83
50	y	310	CLA	C1-C2-C3	2.95	131.02	126.20
50	x	318	CLA	C3B-C4B-NB	-2.93	107.91	110.53
50	b	828	CLA	O2A-CGA-CBA	2.93	120.78	111.83
43	b	850	BCR	C2-C1-C6	2.93	114.70	110.44
53	b	827	PQN	C11-C3-C4	-2.93	115.49	118.58
50	b	825	CLA	O2A-CGA-CBA	2.93	120.78	111.83
43	k	202	BCR	C2-C1-C6	2.93	114.70	110.44
50	a	821	CLA	C12-C11-C10	-2.93	102.58	113.62
54	z	312	CHL	CAA-C2A-C3A	-2.93	105.09	113.00
43	b	819	BCR	C15-C14-C13	-2.92	123.18	127.28
43	b	816	BCR	C2-C1-C6	2.92	114.69	110.44
54	x	319	CHL	C1C-CHC-C4B	2.92	126.51	116.07
54	x	305	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
54	x	305	CHL	C1A-CHA-C4D	2.91	123.84	118.98
50	a	817	CLA	CMA-C3A-C2A	-2.91	109.56	116.23
50	b	835	CLA	C12-C11-C10	-2.91	102.67	113.62
50	g	204	CLA	C3B-C4B-NB	-2.90	107.94	110.53
50	a	844	CLA	O2A-CGA-CBA	2.90	120.68	111.83
54	w	309	CHL	OBD-CAD-CBD	-2.90	121.57	125.82
43	b	820	BCR	C15-C14-C13	-2.90	123.21	127.28
50	y	303	CLA	C1-C2-C3	2.90	130.94	126.20
54	z	304	CHL	CMA-C3A-C2A	-2.89	109.59	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	y	309	CLA	C3B-C4B-NB	-2.89	107.95	110.53
54	w	309	CHL	C1C-CHC-C4B	2.88	126.38	116.07
50	a	857	CLA	C1-C2-C3	2.88	130.91	126.20
43	b	816	BCR	C29-C30-C25	2.87	114.61	110.44
43	x	314	BCR	C29-C30-C25	2.87	114.61	110.44
50	w	310	CLA	O1D-CGD-CBD	-2.87	118.86	124.52
51	b	821	DGD	O6D-C1D-O3G	-2.87	103.26	110.04
43	j	103	BCR	C2-C1-C6	2.87	114.61	110.44
54	x	319	CHL	OBD-CAD-CBD	-2.87	121.61	125.82
50	a	812	CLA	O2A-CGA-CBA	2.87	120.58	111.83
54	w	304	CHL	C1A-CHA-C4D	2.87	123.77	118.98
50	g	203	CLA	C3B-C4B-NB	-2.87	107.97	110.53
50	b	802	CLA	C1-C2-C3	2.86	130.89	126.20
43	k	202	BCR	C29-C30-C25	2.86	114.59	110.44
45	F	804	A1H1M	O14-C13-C33	2.86	116.24	110.37
43	z	318	BCR	C15-C14-C13	-2.86	123.27	127.28
54	x	301	CHL	O1D-CGD-CBD	-2.86	120.39	124.72
52	a	808	CL0	O2D-CGD-CBD	2.85	120.90	113.90
50	a	849	CLA	C3B-C4B-NB	-2.85	107.98	110.53
43	i	101	BCR	C16-C17-C18	-2.85	123.28	127.28
50	k	203	CLA	C3B-C4B-NB	-2.85	107.99	110.53
50	x	307	CLA	C1-C2-C3	2.85	130.86	126.20
50	b	841	CLA	O1D-CGD-CBD	-2.84	118.91	124.52
50	w	316	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
43	a	829	BCR	C29-C30-C25	2.84	114.57	110.44
54	w	304	CHL	OBD-CAD-CBD	-2.84	121.65	125.82
43	k	201	BCR	C16-C15-C14	-2.84	117.72	123.52
50	f	303	CLA	CMA-C3A-C2A	-2.83	109.74	116.23
52	a	808	CL0	C4D-ND-C1D	-2.83	103.07	105.22
43	i	101	BCR	C2-C1-C6	2.83	114.55	110.44
50	z	307	CLA	C1-C2-C3	2.83	130.83	126.20
50	a	809	CLA	C1-C2-C3	2.82	130.82	126.20
50	w	310	CLA	CMC-C2C-C1C	-2.82	120.62	125.03
54	z	304	CHL	C1C-CHC-C4B	2.82	126.15	116.07
50	y	307	CLA	CAB-C3B-C2B	-2.82	116.05	123.53
50	a	833	CLA	O2A-CGA-CBA	2.82	120.42	111.83
50	a	822	CLA	C3B-C4B-NB	-2.82	108.02	110.53
54	x	301	CHL	C1C-CHC-C4B	2.82	126.14	116.07
54	x	301	CHL	C1A-CHA-C4D	2.81	123.68	118.98
43	y	301	BCR	C37-C22-C23	2.81	122.37	118.09
50	b	832	CLA	C1-C2-C3	2.80	130.78	126.20
50	b	847	CLA	C1-C2-C3	2.79	130.77	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	850	CLA	C1-C2-C3	2.79	130.77	126.20
46	7	301	LMG	C1-O6-C5	2.79	119.17	113.72
50	y	302	CLA	C1-C2-C3	2.78	130.75	126.20
50	z	310	CLA	C2A-C1A-CHA	2.78	128.68	123.86
50	g	204	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
50	b	840	CLA	C1-C2-C3	2.78	130.75	126.20
50	b	812	CLA	O2A-CGA-CBA	2.77	120.29	111.83
50	z	311	CLA	C3B-C4B-NB	-2.77	108.06	110.53
50	b	814	CLA	CHD-C1D-ND	-2.77	120.90	124.80
50	x	303	CLA	C1-C2-C3	2.77	130.74	126.20
43	a	829	BCR	C2-C1-C6	2.77	114.46	110.44
54	w	311	CHL	O1D-CGD-CBD	-2.77	120.53	124.72
50	a	815	CLA	C1-C2-C3	2.76	130.73	126.20
54	x	319	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
50	g	203	CLA	C1-C2-C3	2.76	130.72	126.20
53	b	827	PQN	C9-C10-C1	-2.76	116.07	120.10
43	z	318	BCR	C2-C1-C6	2.76	114.44	110.44
54	x	319	CHL	O2A-CGA-CBA	2.75	120.22	111.83
50	a	821	CLA	CAB-C3B-C2B	-2.75	116.23	123.53
50	l	305	CLA	CMA-C3A-C2A	-2.75	109.93	116.23
54	w	309	CHL	C1A-CHA-C4D	2.75	123.56	118.98
46	H	401	LMG	C4-C3-C2	-2.75	106.01	110.83
54	x	319	CHL	CAA-C2A-C3A	-2.75	105.58	113.00
50	a	854	CLA	O2A-CGA-CBA	2.74	120.20	111.83
43	a	810	BCR	C11-C10-C9	-2.74	123.44	127.28
50	b	836	CLA	C1-C2-C3	2.74	130.68	126.20
48	F	801	SQD	O47-C45-C46	-2.73	98.54	108.34
54	x	311	CHL	O1D-CGD-CBD	-2.73	120.58	124.72
43	w	301	BCR	C2-C1-C6	2.73	114.41	110.44
52	a	808	CL0	CMC-C2C-C1C	2.73	129.65	124.73
50	a	845	CLA	C1-C2-C3	2.73	130.66	126.20
43	b	850	BCR	C20-C21-C22	-2.73	123.45	127.28
43	g	202	BCR	C29-C30-C25	2.73	114.40	110.44
50	b	849	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
53	a	825	PQN	C6-C5-C4	-2.72	116.12	120.10
43	b	820	BCR	C15-C16-C17	-2.72	117.95	123.52
50	a	812	CLA	CHB-C1B-NB	2.72	127.40	112.89
50	x	313	CLA	C2A-C1A-CHA	2.72	128.59	123.87
54	z	304	CHL	C1A-CHA-C4D	2.72	123.52	118.98
48	a	859	SQD	O47-C7-C8	2.72	117.36	111.48
52	a	808	CL0	O2A-CGA-CBA	2.72	124.59	110.32
54	z	312	CHL	O2A-CGA-CBA	2.72	120.12	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	x	305	CHL	C1C-CHC-C4B	2.72	125.79	116.07
53	b	827	PQN	C6-C5-C4	-2.71	116.13	120.10
54	x	311	CHL	OBD-CAD-CBD	-2.71	121.84	125.82
50	z	306	CLA	C2A-C1A-CHA	2.71	128.57	123.87
51	x	317	DGD	O6D-C1D-O3G	-2.71	103.64	110.04
46	H	401	LMG	C1-O6-C5	2.71	119.01	113.72
50	w	305	CLA	C1-C2-C3	2.71	130.64	126.20
50	a	837	CLA	C1-C2-C3	2.71	130.63	126.20
50	a	812	CLA	C1-C2-C3	2.71	130.63	126.20
50	a	835	CLA	C1-C2-C3	2.70	130.63	126.20
50	b	804	CLA	CMA-C3A-C2A	-2.70	110.03	116.23
50	z	306	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
43	l	302	BCR	C29-C30-C25	2.70	114.36	110.44
43	4	101	BCR	C2-C1-C6	2.69	114.35	110.44
50	y	314	CLA	C1-C2-C3	2.69	130.60	126.20
50	w	316	CLA	CHD-C1D-ND	-2.69	121.02	124.80
54	x	311	CHL	C1C-CHC-C4B	2.68	125.67	116.07
54	w	304	CHL	C4C-CHD-C1D	2.68	125.66	116.07
43	l	304	BCR	C29-C30-C25	2.68	114.33	110.44
50	b	847	CLA	CHD-C1D-ND	-2.68	121.03	124.80
50	b	807	CLA	C1-C2-C3	2.68	130.58	126.20
50	b	842	CLA	C1-C2-C3	2.67	130.58	126.20
43	g	202	BCR	C16-C17-C18	-2.67	123.53	127.28
50	a	849	CLA	C1-C2-C3	2.66	130.56	126.20
46	7	301	LMG	C1-C2-C3	-2.66	104.40	110.01
50	a	820	CLA	C1-C2-C3	2.66	130.56	126.20
46	D	601	LMG	O1-C7-C8	-2.66	104.35	110.82
54	x	319	CHL	C1A-CHA-C4D	2.66	123.42	118.98
50	k	203	CLA	CAA-C2A-C3A	-2.66	110.14	116.23
54	w	304	CHL	C1C-CHC-C4B	2.66	125.58	116.07
43	l	302	BCR	C2-C1-C6	2.66	114.30	110.44
46	j	104	LMG	O1-C7-C8	-2.66	104.36	110.82
50	b	803	CLA	CHD-C1D-ND	-2.66	121.06	124.80
50	y	302	CLA	CAB-C3B-C2B	-2.65	116.49	123.53
54	w	311	CHL	C1C-CHC-C4B	2.65	125.55	116.07
50	l	306	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
50	b	835	CLA	C1-C2-C3	2.65	130.54	126.20
50	k	204	CLA	C1-C2-C3	2.65	130.53	126.20
50	w	307	CLA	C2A-C1A-CHA	2.65	128.46	123.87
50	x	312	CLA	C1-C2-C3	2.65	130.53	126.20
50	w	310	CLA	CBC-CAC-C3C	2.64	119.59	112.42
50	a	843	CLA	C1-C2-C3	2.64	130.52	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	x	313	CLA	C1-C2-C3	2.64	130.52	126.20
54	z	304	CHL	O1D-CGD-CBD	-2.63	120.73	124.72
50	b	811	CLA	CHD-C1D-ND	-2.63	121.10	124.80
45	F	804	A1H1M	C09-C10-C11	2.63	115.19	110.96
50	z	319	CLA	C3B-C4B-NB	-2.62	108.19	110.53
50	b	841	CLA	C1-C2-C3	2.62	130.49	126.20
50	a	846	CLA	C1-C2-C3	2.62	130.49	126.20
50	y	306	CLA	CMA-C3A-C2A	-2.62	110.23	116.23
54	x	305	CHL	C3C-C4C-NC	-2.62	108.25	114.65
54	w	309	CHL	O1D-CGD-CBD	-2.62	120.76	124.72
50	x	318	CLA	O2A-CGA-CBA	2.61	122.02	112.14
54	x	301	CHL	OBD-CAD-CBD	-2.61	121.99	125.82
54	x	305	CHL	CHA-C1A-C2A	-2.61	127.17	133.31
50	b	815	CLA	C1-C2-C3	2.61	130.47	126.20
43	b	831	BCR	C24-C23-C22	-2.60	122.38	126.23
50	a	858	CLA	C1-C2-C3	2.60	130.46	126.20
43	b	819	BCR	C21-C20-C19	-2.60	115.66	123.20
54	x	319	CHL	C4C-CHD-C1D	2.60	125.37	116.07
43	a	827	BCR	C2-C1-C6	2.60	114.22	110.44
44	B	606	PGT	C2-O2-C31	2.60	124.02	117.80
50	a	813	CLA	C1-C2-C3	2.60	130.45	126.20
50	y	308	CLA	C1-C2-C3	2.60	130.45	126.20
53	a	825	PQN	C9-C10-C1	-2.60	116.31	120.10
50	b	845	CLA	C1-C2-C3	2.60	130.45	126.20
43	b	817	BCR	C15-C16-C17	-2.60	118.21	123.52
43	b	819	BCR	C37-C22-C23	2.59	122.05	118.09
50	w	306	CLA	C1-C2-C3	2.59	130.44	126.20
50	k	203	CLA	CMA-C3A-C2A	-2.59	110.29	116.23
46	z	315	LMG	O1-C7-C8	-2.59	104.52	110.82
47	A	405	PQ9	C31-C32-C33	-2.59	121.70	127.62
43	l	303	BCR	C29-C30-C25	2.58	114.19	110.44
50	b	849	CLA	C3B-C4B-NB	-2.58	108.23	110.53
54	w	309	CHL	C4C-CHD-C1D	2.58	125.30	116.07
43	g	202	BCR	C2-C1-C6	2.58	114.19	110.44
54	z	312	CHL	C3C-C4C-NC	-2.58	108.35	114.65
54	x	311	CHL	C1A-CHA-C4D	2.58	123.28	118.98
54	w	304	CHL	CHA-C1A-C2A	-2.57	127.26	133.31
50	y	307	CLA	C3B-C4B-NB	-2.57	107.66	110.33
43	w	301	BCR	C37-C22-C23	2.57	122.02	118.09
50	a	802	CLA	C1-C2-C3	2.57	130.41	126.20
43	a	827	BCR	C23-C22-C21	-2.57	118.78	124.72
50	y	313	CLA	C1-C2-C3	2.57	130.41	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	a	830	BCR	C2-C1-C6	2.57	114.17	110.44
50	z	303	CLA	O1D-CGD-CBD	-2.57	119.46	124.52
43	a	829	BCR	C28-C27-C26	-2.56	109.48	114.06
43	l	303	BCR	C2-C1-C6	2.56	114.16	110.44
45	F	804	A1H1M	C37-C07-C08	-2.56	106.81	112.46
53	a	825	PQN	C10-C5-C4	2.56	123.46	120.71
54	w	311	CHL	C4C-CHD-C1D	2.56	125.22	116.07
50	w	303	CLA	CHD-C1D-ND	-2.55	121.22	124.80
54	z	304	CHL	OBD-CAD-CBD	-2.55	122.08	125.82
50	a	833	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
50	a	839	CLA	C1-C2-C3	2.54	130.37	126.20
43	b	850	BCR	C29-C30-C25	2.54	114.14	110.44
50	a	856	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
54	x	311	CHL	C4C-CHD-C1D	2.54	125.17	116.07
54	w	311	CHL	C3C-C4C-NC	-2.54	108.43	114.65
50	a	802	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
50	y	304	CLA	CHD-C1D-ND	-2.54	121.23	124.80
50	a	857	CLA	C12-C11-C10	-2.54	101.89	113.28
50	y	311	CLA	C1-C2-C3	2.54	130.36	126.20
50	a	851	CLA	O2A-CGA-CBA	2.54	121.73	112.14
43	k	201	BCR	C21-C20-C19	-2.54	115.85	123.20
54	x	305	CHL	C4C-CHD-C1D	2.54	125.15	116.07
43	b	820	BCR	C2-C1-C6	2.54	114.12	110.44
50	z	306	CLA	C1-C2-C3	2.54	130.35	126.20
43	j	103	BCR	C29-C30-C25	2.54	114.12	110.44
50	a	847	CLA	CHB-C1B-NB	2.53	126.64	120.96
43	y	301	BCR	C21-C20-C19	-2.53	115.87	123.20
43	a	803	BCR	C2-C1-C6	2.53	114.11	110.44
50	b	815	CLA	CHD-C1D-ND	-2.53	121.25	124.80
50	y	302	CLA	C3B-C4B-NB	-2.52	107.71	110.33
50	a	843	CLA	C12-C11-C10	-2.52	101.97	113.28
50	y	312	CLA	C1-C2-C3	2.52	130.33	126.20
50	a	824	CLA	C12-C11-C10	-2.52	101.99	113.28
50	b	835	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
45	F	804	A1H1M	O12-C13-O14	-2.52	104.07	110.69
46	w	312	LMG	O1-C7-C8	-2.52	104.70	110.82
50	w	308	CLA	CHD-C1D-ND	-2.52	121.26	124.80
50	b	833	CLA	O1D-CGD-CBD	-2.52	119.56	124.52
53	a	825	PQN	C2M-C2-C1	-2.51	112.05	116.68
50	a	848	CLA	C1-C2-C3	2.51	130.32	126.20
50	w	315	CLA	O2A-CGA-CBA	2.51	121.63	112.14
54	z	312	CHL	O2A-CGA-O1A	-2.51	117.35	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	304	CHL	C4C-CHD-C1D	2.51	125.05	116.07
43	a	831	BCR	C2-C1-C6	2.51	114.09	110.44
50	a	835	CLA	CHD-C1D-ND	-2.51	121.27	124.80
54	w	311	CHL	C1A-CHA-C4D	2.51	123.17	118.98
50	b	814	CLA	C12-C11-C10	-2.51	102.05	113.28
53	a	825	PQN	C11-C3-C4	-2.50	115.94	118.58
43	k	201	BCR	C24-C25-C26	2.50	127.32	121.56
50	z	306	CLA	CHD-C1D-ND	-2.50	121.28	124.80
50	a	811	CLA	C1-C2-C3	2.50	130.29	126.20
52	a	808	CL0	C1-O2A-CGA	2.50	122.56	112.40
50	b	801	CLA	C3B-C4B-NB	-2.50	108.30	110.53
50	a	824	CLA	C4-C3-C5	-2.50	110.90	115.23
54	x	301	CHL	C3C-C4C-NC	-2.50	108.55	114.65
50	b	839	CLA	C1-C2-C3	2.49	130.28	126.20
50	z	311	CLA	C1-C2-C3	2.49	130.28	126.20
50	x	313	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
50	a	834	CLA	C1-C2-C3	2.49	130.28	126.20
43	a	828	BCR	C29-C30-C25	2.49	114.06	110.44
50	b	814	CLA	C1-C2-C3	2.49	130.28	126.20
50	a	844	CLA	CHD-C1D-ND	-2.49	121.30	124.80
43	l	304	BCR	C2-C1-C6	2.49	114.05	110.44
50	b	851	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
43	b	816	BCR	C15-C14-C13	-2.48	123.79	127.28
50	b	837	CLA	C1-C2-C3	2.48	130.27	126.20
54	w	309	CHL	CHA-C1A-C2A	-2.48	127.47	133.31
50	a	836	CLA	C12-C11-C10	-2.48	102.16	113.28
50	a	844	CLA	C1-C2-C3	2.48	130.26	126.20
50	b	823	CLA	C1-C2-C3	2.48	130.26	126.20
50	b	846	CLA	C1-C2-C3	2.48	130.26	126.20
50	a	819	CLA	C1-C2-C3	2.48	130.25	126.20
53	b	827	PQN	C10-C5-C4	2.48	123.37	120.71
50	l	301	CLA	CED-O2D-CGD	2.47	121.53	115.92
43	b	820	BCR	C29-C30-C25	2.47	114.03	110.44
50	a	850	CLA	C12-C11-C10	-2.47	102.20	113.28
50	b	802	CLA	C12-C11-C10	-2.47	102.20	113.28
50	w	310	CLA	C12-C11-C10	-2.47	102.20	113.28
50	a	821	CLA	C3B-C4B-NB	-2.47	107.76	110.33
50	a	820	CLA	CHD-C1D-ND	-2.47	121.33	124.80
50	b	844	CLA	C1-C2-C3	2.47	130.24	126.20
54	w	309	CHL	C3C-C4C-NC	-2.47	108.62	114.65
50	b	839	CLA	C12-C11-C10	-2.47	102.22	113.28
46	7	301	LMG	C4-C3-C2	-2.47	106.50	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	812	CLA	C12-C11-C10	-2.46	102.24	113.28
50	a	814	CLA	C1-C2-C3	2.46	130.23	126.20
45	F	804	A1H1M	C13-C33-C31	2.46	115.18	110.01
50	y	310	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
50	a	847	CLA	C1B-NB-C4B	2.45	108.58	106.29
50	z	307	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
50	b	811	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
43	b	817	BCR	C29-C30-C25	2.45	114.00	110.44
50	x	306	CLA	C12-C11-C10	-2.45	102.30	113.28
50	b	841	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
50	a	819	CLA	C12-C11-C10	-2.45	102.31	113.28
50	x	316	CLA	O2A-CGA-CBA	2.45	121.73	114.00
46	x	315	LMG	O1-C7-C8	-2.45	104.87	110.82
50	b	801	CLA	C1-C2-C3	2.45	130.20	126.20
50	w	306	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
43	a	830	BCR	C29-C30-C25	2.44	113.99	110.44
50	a	838	CLA	C12-C11-C10	-2.44	102.32	113.28
50	x	307	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
50	a	837	CLA	C12-C11-C10	-2.44	102.33	113.28
43	a	828	BCR	C2-C1-C6	2.44	113.99	110.44
50	b	844	CLA	C12-C11-C10	-2.44	102.34	113.28
50	a	852	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
46	j	105	LMG	O1-C7-C8	-2.44	104.89	110.82
50	l	306	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
50	a	818	CLA	C1-C2-C3	2.44	130.19	126.20
50	h	201	CLA	O2A-CGA-CBA	2.44	121.34	112.14
54	w	304	CHL	C3C-C4C-NC	-2.44	108.70	114.65
50	a	854	CLA	C12-C11-C10	-2.44	102.37	113.28
54	x	319	CHL	CHA-C1A-C2A	-2.43	127.59	133.31
50	b	839	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
43	w	301	BCR	C29-C30-C25	2.43	113.97	110.44
50	a	826	CLA	O2A-CGA-CBA	2.43	121.68	114.00
43	a	831	BCR	C29-C30-C25	2.43	113.97	110.44
52	a	808	CL0	C4A-C3A-C2A	-2.43	100.54	103.91
43	b	816	BCR	C37-C22-C23	2.43	121.80	118.09
45	F	804	A1H1M	O26-C25-C27	-2.43	104.66	110.38
50	b	822	CLA	C1-C2-C3	2.42	130.17	126.20
50	a	823	CLA	C1-C2-C3	2.42	130.17	126.20
50	b	833	CLA	C12-C11-C10	-2.42	102.42	113.28
50	x	303	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
54	w	311	CHL	C1-O2A-CGA	2.42	121.56	113.06
50	a	846	CLA	O1D-CGD-CBD	-2.42	119.74	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	f	303	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
50	z	310	CLA	CMA-C3A-C2A	-2.42	110.68	116.23
50	b	805	CLA	C1-C2-C3	2.42	130.16	126.20
50	a	842	CLA	C1-C2-C3	2.42	130.16	126.20
54	z	304	CHL	C3C-C4C-NC	-2.42	108.75	114.65
50	b	809	CLA	C1-C2-C3	2.41	130.15	126.20
50	a	844	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
54	x	319	CHL	C3C-C4C-NC	-2.41	108.75	114.65
50	w	303	CLA	O2A-CGA-CBA	2.41	121.62	114.00
43	y	301	BCR	C2-C1-C6	2.41	113.94	110.44
50	x	312	CLA	C12-C11-C10	-2.41	102.48	113.28
48	j	106	SQD	O6-C44-C45	-2.41	104.96	110.82
50	a	858	CLA	C12-C11-C10	-2.41	102.48	113.28
50	x	309	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
50	x	318	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
43	x	314	BCR	C37-C22-C23	2.41	121.76	118.09
50	a	811	CLA	CHD-C1D-ND	-2.41	121.42	124.80
50	a	836	CLA	C1-C2-C3	2.41	130.14	126.20
43	f	304	BCR	C37-C22-C23	2.40	121.76	118.09
50	a	854	CLA	C1-C2-C3	2.40	130.13	126.20
50	a	841	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
54	x	301	CHL	CHA-C1A-C2A	-2.40	127.67	133.31
50	a	802	CLA	C12-C11-C10	-2.40	102.52	113.28
43	b	818	BCR	C29-C30-C25	2.40	113.92	110.44
50	w	308	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
43	b	819	BCR	C2-C1-C6	2.40	113.92	110.44
50	a	842	CLA	C12-C11-C10	-2.39	102.55	113.28
50	b	840	CLA	C12-C11-C10	-2.39	102.55	113.28
46	z	314	LMG	O1-C7-C8	-2.39	105.00	110.82
50	a	801	CLA	C12-C11-C10	-2.39	102.55	113.28
50	b	843	CLA	C12-C11-C10	-2.39	102.55	113.28
45	5	302	A1H1M	O19-C20-O21	-2.39	104.40	110.69
50	x	303	CLA	C3B-C4B-NB	-2.39	108.40	110.53
55	z	321	LUT	C26-C27-C28	-2.39	120.86	124.58
54	x	301	CHL	C4C-CHD-C1D	2.39	124.61	116.07
43	a	831	BCR	C37-C22-C23	2.39	121.74	118.09
50	b	804	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
50	b	825	CLA	C4-C3-C5	-2.39	111.08	115.23
45	5	302	A1H1M	C20-O21-C22	2.39	118.38	113.72
50	w	310	CLA	C1-C2-C3	2.38	130.10	126.20
50	a	846	CLA	C12-C11-C10	-2.38	102.60	113.28
50	b	846	CLA	C12-C11-C10	-2.38	102.60	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	x	311	CHL	CAA-C2A-C3A	-2.38	104.34	112.49
50	b	803	CLA	C12-C11-C10	-2.38	102.61	113.28
50	b	806	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
50	b	804	CLA	CHD-C1D-ND	-2.38	121.45	124.80
50	b	837	CLA	C12-C11-C10	-2.38	102.62	113.28
50	b	822	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
50	a	815	CLA	CHD-C1D-ND	-2.38	121.46	124.80
46	F	802	LMG	O1-C7-C8	-2.38	105.04	110.82
46	H	401	LMG	O1-C7-C8	-2.38	105.04	110.82
46	x	315	LMG	C1-C2-C3	-2.37	105.02	110.01
43	w	301	BCR	C21-C20-C19	-2.37	116.33	123.20
50	x	302	CLA	CMA-C3A-C2A	-2.37	110.79	116.23
50	a	839	CLA	CHD-C1D-ND	-2.37	121.47	124.80
50	y	305	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
50	b	805	CLA	C12-C11-C10	-2.37	102.66	113.28
50	a	811	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
50	a	858	CLA	CHD-C1D-ND	-2.37	121.47	124.80
54	z	312	CHL	O2D-CGD-O1D	-2.37	119.24	123.85
50	w	307	CLA	O2A-CGA-CBA	2.37	121.48	114.00
43	f	304	BCR	C2-C1-C6	2.37	113.88	110.44
46	f	306	LMG	O1-C7-C8	-2.37	105.06	110.82
50	z	308	CLA	O2A-CGA-CBA	2.37	121.48	114.00
50	b	813	CLA	CHD-C1D-ND	-2.37	121.47	124.80
50	a	809	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
50	z	303	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
50	b	812	CLA	C12-C11-C10	-2.37	102.67	113.28
50	x	306	CLA	C1-C2-C3	2.36	130.07	126.20
50	b	807	CLA	CHD-C1D-ND	-2.36	121.48	124.80
50	l	306	CLA	C12-C11-C10	-2.36	102.70	113.28
50	b	811	CLA	O2A-CGA-CBA	2.36	121.45	114.00
50	x	307	CLA	C12-C11-C10	-2.36	102.71	113.28
46	B	605	LMG	C1-C2-C3	-2.36	105.05	110.01
50	b	828	CLA	C12-C11-C10	-2.35	102.73	113.28
50	a	845	CLA	C12-C11-C10	-2.35	102.73	113.28
50	a	843	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
50	a	843	CLA	CHD-C1D-ND	-2.35	121.49	124.80
50	b	808	CLA	CHD-C1D-ND	-2.35	121.50	124.80
50	b	823	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
43	b	831	BCR	C16-C15-C14	-2.35	118.71	123.52
50	y	314	CLA	C12-C11-C10	-2.35	102.76	113.28
50	a	840	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
47	A	405	PQ9	C6-C5-C4	2.35	120.08	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	854	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
50	b	812	CLA	CHD-C1D-ND	-2.34	121.50	124.80
50	z	307	CLA	C12-C11-C10	-2.34	102.77	113.28
43	j	101	BCR	C29-C30-C25	2.34	113.84	110.44
50	b	815	CLA	C12-C11-C10	-2.34	102.80	113.28
50	a	854	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
50	a	852	CLA	C1-C2-C3	2.34	130.02	126.20
54	w	311	CHL	CHA-C1A-C2A	-2.34	127.82	133.31
50	b	824	CLA	C12-C11-C10	-2.33	102.82	113.28
50	y	308	CLA	C12-C11-C10	-2.33	102.82	113.28
50	z	305	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
50	a	848	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
50	y	305	CLA	O2A-CGA-CBA	2.33	121.36	114.00
50	f	301	CLA	C1-C2-C3	2.33	130.01	126.20
50	a	853	CLA	C12-C11-C10	-2.33	102.84	113.28
50	b	847	CLA	C12-C11-C10	-2.33	102.84	113.28
50	b	834	CLA	O2A-CGA-CBA	2.33	121.35	114.00
50	a	833	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
50	b	828	CLA	C1-C2-C3	2.33	130.01	126.20
50	w	308	CLA	C12-C11-C10	-2.33	102.86	113.28
50	b	806	CLA	C1-C2-C3	2.32	130.01	126.20
50	b	842	CLA	O1D-CGD-CBD	-2.32	119.93	124.52
50	b	824	CLA	C1-C2-C3	2.32	130.00	126.20
50	k	204	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
50	b	833	CLA	C1-C2-C3	2.32	130.00	126.20
50	z	316	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
50	a	855	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
45	5	302	A1H1M	O26-C25-C27	-2.32	104.91	110.38
50	a	812	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
50	y	302	CLA	C4-C3-C5	-2.32	111.21	115.23
50	b	836	CLA	C12-C11-C10	-2.32	102.90	113.28
50	w	302	CLA	C1-C2-C3	2.31	130.51	126.76
50	g	201	CLA	CHD-C1D-ND	-2.31	121.55	124.80
50	y	313	CLA	CHD-C1D-ND	-2.31	121.55	124.80
50	f	301	CLA	CHD-C1D-ND	-2.31	121.55	124.80
53	a	825	PQN	C17-C16-C15	-2.31	107.11	113.26
50	a	836	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
50	a	839	CLA	C12-C11-C10	-2.31	102.94	113.28
50	a	856	CLA	C12-C11-C10	-2.30	102.95	113.28
50	l	301	CLA	O2A-CGA-CBA	2.30	121.28	114.00
46	z	315	LMG	C1-C2-C3	-2.30	105.17	110.01
50	a	851	CLA	O1D-CGD-CBD	-2.30	119.98	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	826	CLA	C1-C2-C3	2.30	129.97	126.20
50	a	820	CLA	C12-C11-C10	-2.30	102.97	113.28
50	x	306	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
50	g	204	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
50	a	813	CLA	CHD-C1D-ND	-2.30	121.57	124.80
50	y	314	CLA	CHD-C1D-ND	-2.30	121.57	124.80
50	b	801	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
43	a	830	BCR	C20-C21-C22	-2.29	124.07	127.28
50	y	314	CLA	C4-C3-C5	-2.29	111.25	115.23
50	y	310	CLA	C12-C11-C10	-2.29	103.02	113.28
50	w	314	CLA	CHD-C1D-ND	-2.29	121.58	124.80
50	l	306	CLA	C1-C2-C3	2.29	129.95	126.20
50	a	815	CLA	C12-C11-C10	-2.29	103.02	113.28
50	a	840	CLA	CHD-C1D-ND	-2.29	121.58	124.80
50	l	305	CLA	CAA-C2A-C3A	-2.29	110.98	116.23
50	y	311	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
51	b	821	DGD	O5D-C6D-C5D	-2.29	104.27	109.42
46	F	802	LMG	O6-C1-O1	-2.29	104.64	110.04
50	a	849	CLA	CHD-C1D-ND	-2.29	121.59	124.80
50	w	306	CLA	C12-C11-C10	-2.29	103.04	113.28
43	a	828	BCR	C37-C22-C23	2.28	121.58	118.09
50	b	848	CLA	CHD-C1D-ND	-2.28	121.59	124.80
50	a	822	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
43	f	304	BCR	C16-C15-C14	-2.28	118.86	123.52
50	b	822	CLA	CHD-C1D-ND	-2.28	121.60	124.80
50	b	839	CLA	CHD-C1D-ND	-2.28	121.60	124.80
50	a	839	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
50	w	314	CLA	CED-O2D-CGD	2.28	121.08	115.92
50	b	801	CLA	C12-C11-C10	-2.28	103.08	113.28
55	w	319	LUT	C26-C27-C28	2.28	128.12	124.58
43	l	304	BCR	C37-C22-C23	2.28	121.56	118.09
50	z	306	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
50	a	853	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
50	x	304	CLA	CHD-C1D-ND	-2.27	121.60	124.80
50	b	847	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
46	7	301	LMG	O1-C7-C8	-2.27	105.29	110.82
54	z	312	CHL	OMC-CMC-C2C	-2.27	121.18	125.12
50	b	826	CLA	CHD-C1D-ND	-2.27	121.61	124.80
50	k	205	CLA	CHD-C1D-ND	-2.27	121.61	124.80
45	F	804	A1H1M	O28-C27-C29	-2.27	105.03	110.38
43	f	304	BCR	C16-C17-C18	-2.27	124.10	127.28
50	a	814	CLA	C12-C11-C10	-2.27	103.12	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	802	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
50	f	303	CLA	CAA-C2A-C3A	-2.26	111.04	116.23
50	a	833	CLA	C12-C11-C10	-2.26	103.13	113.28
50	b	813	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
50	a	821	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
50	w	303	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
50	z	302	CLA	C1-C2-C3	2.26	129.90	126.20
50	x	312	CLA	CHD-C1D-ND	-2.26	121.63	124.80
50	a	821	CLA	C1-C2-C3	2.26	129.89	126.20
50	b	845	CLA	CHD-C1D-ND	-2.26	121.63	124.80
50	a	852	CLA	O1D-CGD-CBD	-2.25	120.07	124.52
50	w	310	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
46	H	401	LMG	C1-C2-C3	-2.25	105.27	110.01
50	b	807	CLA	C12-C11-C10	-2.25	103.19	113.28
50	y	313	CLA	C12-C11-C10	-2.25	103.21	113.28
50	b	808	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
50	a	811	CLA	C12-C11-C10	-2.25	103.22	113.28
43	z	318	BCR	C29-C30-C25	2.24	113.70	110.44
50	a	849	CLA	C12-C11-C10	-2.24	103.22	113.28
50	w	315	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
55	w	320	LUT	C26-C27-C28	-2.24	121.09	124.58
50	x	303	CLA	CED-O2D-CGD	2.24	121.00	115.92
50	a	857	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
50	b	846	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
54	z	304	CHL	OMC-CMC-C2C	-2.24	121.22	125.12
50	a	846	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
50	a	821	CLA	CHD-C1D-ND	-2.24	121.65	124.80
54	x	319	CHL	O2A-CGA-O1A	-2.24	118.02	123.63
50	y	308	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
50	a	823	CLA	CHD-C1D-ND	-2.24	121.66	124.80
50	a	842	CLA	CHD-C1D-ND	-2.24	121.66	124.80
43	a	810	BCR	C8-C9-C10	2.23	122.52	119.01
50	b	834	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
54	z	312	CHL	C4C-CHD-C1D	2.23	124.05	116.07
50	w	315	CLA	CHD-C1D-ND	-2.23	121.66	124.80
50	a	835	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
43	x	314	BCR	C2-C1-C6	2.23	113.68	110.44
54	w	304	CHL	O2A-CGA-CBA	2.23	121.05	114.00
50	b	810	CLA	C1-C2-C3	2.23	130.37	126.76
50	b	806	CLA	CHD-C1D-ND	-2.23	121.67	124.80
50	a	844	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
50	a	848	CLA	C4-C3-C5	-2.23	111.36	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	x	310	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
50	b	812	CLA	C4-C3-C5	-2.22	111.37	115.23
50	a	838	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
50	y	310	CLA	CHD-C1D-ND	-2.22	121.67	124.80
50	k	205	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
50	a	838	CLA	C1-C2-C3	2.22	129.83	126.20
50	b	814	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
50	b	832	CLA	CHD-C1D-ND	-2.22	121.69	124.80
50	w	307	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
50	z	302	CLA	CBA-CAA-C2A	2.21	120.38	113.79
48	F	805	SQD	C4-C3-C2	-2.21	106.94	110.83
50	a	818	CLA	C2A-C1A-CHA	2.21	127.70	123.87
50	a	850	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
54	w	304	CHL	O2D-CGD-O1D	-2.21	119.54	123.85
50	a	822	CLA	C1-C2-C3	2.21	129.82	126.20
48	w	318	SQD	O47-C7-O49	-2.21	118.54	123.70
50	a	817	CLA	CAA-C2A-C3A	-2.21	111.16	116.23
50	a	851	CLA	CHD-C1D-ND	-2.21	121.69	124.80
50	b	838	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
46	w	312	LMG	C1-C2-C3	-2.21	105.37	110.01
50	z	306	CLA	C4-C3-C5	-2.21	111.40	115.23
50	z	310	CLA	CAA-C2A-C3A	-2.21	111.17	116.23
43	b	831	BCR	C3-C4-C5	-2.20	110.12	114.06
50	w	316	CLA	CMD-C2D-C1D	2.20	128.61	124.73
50	z	302	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
50	f	301	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
50	w	316	CLA	C4D-CHA-C1A	2.20	123.87	121.24
50	f	301	CLA	C12-C11-C10	-2.20	102.56	113.23
43	l	303	BCR	C21-C20-C19	-2.20	116.83	123.20
50	a	818	CLA	CHD-C1D-ND	-2.20	121.71	124.80
50	a	816	CLA	CHD-C1D-ND	-2.20	121.71	124.80
50	y	306	CLA	CAA-C2A-C3A	-2.20	111.19	116.23
50	b	851	CLA	CHD-C1D-ND	-2.20	121.71	124.80
55	w	319	LUT	C28-C29-C30	2.20	122.46	119.01
50	b	838	CLA	C1-C2-C3	2.19	129.79	126.20
50	y	311	CLA	CHD-C1D-ND	-2.19	121.72	124.80
50	b	837	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
48	F	805	SQD	C1-O5-C5	2.19	118.00	113.72
50	x	303	CLA	C2D-C1D-ND	2.19	112.29	110.13
50	a	824	CLA	CHD-C1D-ND	-2.19	121.72	124.80
50	a	824	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
52	a	808	CL0	C4C-C3C-C2C	-2.19	104.72	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	833	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
50	a	850	CLA	CHD-C1D-ND	-2.19	121.72	124.80
50	b	825	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
50	a	824	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
50	a	820	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
43	b	820	BCR	C37-C22-C23	2.19	121.43	118.09
50	b	811	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
50	b	840	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
50	y	309	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
50	b	832	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
50	y	307	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
50	b	828	CLA	CHD-C1D-ND	-2.18	121.73	124.80
50	a	809	CLA	C12-C11-C10	-2.18	102.65	113.23
45	F	804	A1H1M	O32-C31-C33	-2.18	105.23	110.38
50	l	301	CLA	CHD-C1D-ND	-2.18	121.73	124.80
54	z	312	CHL	CHA-C1A-C2A	-2.18	128.19	133.31
43	a	829	BCR	C24-C23-C22	-2.18	123.01	126.23
46	j	104	LMG	C1-C2-C3	-2.18	105.43	110.01
50	x	303	CLA	C12-C11-C10	-2.18	102.67	113.23
50	w	305	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
50	k	204	CLA	C12-C11-C10	-2.18	102.68	113.23
50	b	832	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
50	x	304	CLA	C4D-CHA-C1A	2.17	123.84	121.24
50	a	849	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
50	b	803	CLA	CHD-C4C-C3C	2.17	127.94	124.77
50	b	844	CLA	CHD-C1D-ND	-2.17	121.75	124.80
50	x	302	CLA	CED-O2D-CGD	2.17	120.84	115.92
50	y	304	CLA	CBA-CAA-C2A	2.17	118.02	113.41
50	a	822	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
50	a	833	CLA	CHD-C1D-ND	-2.17	121.75	124.80
50	y	302	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
50	a	809	CLA	CHD-C1D-ND	-2.17	121.75	124.80
50	a	818	CLA	C4-C3-C5	-2.17	111.46	115.23
45	5	302	A1H1M	O21-C22-C25	2.17	113.61	109.70
50	w	308	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
50	x	303	CLA	CMD-C2D-C1D	2.16	128.54	124.73
50	a	820	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
43	a	827	BCR	C21-C20-C19	-2.16	119.53	124.65
50	a	845	CLA	C4-C3-C5	-2.16	111.47	115.23
50	a	856	CLA	CHD-C1D-ND	-2.16	121.76	124.80
50	a	838	CLA	CHD-C1D-ND	-2.16	121.76	124.80
50	z	311	CLA	O1D-CGD-CBD	-2.16	120.25	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	842	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
50	a	801	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
50	a	815	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
50	a	837	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
50	b	845	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
50	f	302	CLA	CHD-C1D-ND	-2.15	121.77	124.80
50	a	833	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
50	b	809	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
50	x	316	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
50	g	203	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
45	5	302	A1H1M	O12-C13-C33	2.15	113.38	108.09
50	a	841	CLA	C1-C2-C3	2.15	129.71	126.20
50	a	844	CLA	C12-C11-C10	-2.14	102.83	113.23
50	a	855	CLA	CMD-C2D-C1D	2.14	128.50	124.73
50	b	836	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
50	b	838	CLA	CHD-C1D-ND	-2.14	121.79	124.80
50	z	303	CLA	CAA-C2A-C3A	-2.14	111.31	116.23
50	x	307	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
50	w	310	CLA	CHD-C1D-ND	-2.14	121.79	124.80
50	a	854	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
50	a	837	CLA	CHD-C1D-ND	-2.14	121.79	124.80
50	x	307	CLA	CHD-C1D-ND	-2.14	121.79	124.80
50	z	310	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
50	w	306	CLA	CHD-C1D-ND	-2.14	121.79	124.80
50	b	833	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
50	a	858	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
50	b	809	CLA	CHD-C1D-ND	-2.14	121.80	124.80
52	a	808	CL0	C2C-C1C-NC	2.14	116.50	110.46
46	D	601	LMG	C1-C2-C3	-2.14	105.52	110.01
50	b	836	CLA	C4-C3-C5	-2.14	111.52	115.23
50	w	310	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
43	b	819	BCR	C15-C16-C17	-2.14	119.15	123.52
50	a	853	CLA	CHD-C1D-ND	-2.13	121.80	124.80
50	b	826	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
50	w	314	CLA	CMD-C2D-C1D	2.13	128.48	124.73
50	a	835	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
50	y	306	CLA	CHD-C1D-ND	-2.13	121.84	124.84
50	x	308	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
50	w	310	CLA	CMC-C2C-C3C	2.13	131.91	126.15
50	l	306	CLA	CHD-C1D-ND	-2.13	121.81	124.80
50	a	847	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
50	b	805	CLA	CHD-C1D-ND	-2.13	121.81	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	848	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
50	b	849	CLA	CHD-C1D-ND	-2.13	121.81	124.80
43	a	827	BCR	C30-C25-C26	-2.12	119.73	122.64
43	f	304	BCR	C29-C30-C25	2.12	113.53	110.44
50	b	842	CLA	CMD-C2D-C1D	2.12	128.47	124.73
50	b	844	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
50	a	848	CLA	CHD-C1D-ND	-2.12	121.81	124.80
50	a	846	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
54	x	305	CHL	O2A-CGA-CBA	2.12	120.71	114.00
50	z	310	CLA	CMD-C2D-C1D	2.12	128.47	124.73
50	b	807	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
50	j	102	CLA	CHD-C1D-ND	-2.12	121.82	124.80
50	b	838	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
50	b	843	CLA	CHD-C1D-ND	-2.12	121.82	124.80
50	l	305	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
50	x	306	CLA	CMD-C2D-C1D	2.12	128.46	124.73
43	b	818	BCR	C37-C22-C23	2.12	121.33	118.09
50	b	823	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
48	w	318	SQD	O47-C45-C44	-2.12	100.75	108.34
43	k	201	BCR	C20-C21-C22	-2.12	124.31	127.28
50	z	305	CLA	C1-C2-C3	2.11	130.18	126.76
43	b	831	BCR	C28-C27-C26	-2.11	110.29	114.06
55	x	321	LUT	C39-C29-C28	-2.11	114.86	118.09
43	k	202	BCR	C37-C22-C23	2.11	121.31	118.09
46	f	306	LMG	C1-C2-C3	-2.11	105.57	110.01
43	b	850	BCR	C16-C15-C14	-2.11	119.20	123.52
50	a	856	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
50	b	842	CLA	C12-C11-C10	-2.11	103.00	113.23
50	x	302	CLA	CMD-C2D-C1D	2.11	128.44	124.73
50	x	306	CLA	CHD-C1D-ND	-2.10	121.84	124.80
50	x	313	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
50	x	312	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
50	b	803	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
50	a	844	CLA	CMD-C2D-C1D	2.10	128.43	124.73
50	a	856	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
50	y	312	CLA	CHD-C1D-ND	-2.10	121.84	124.80
50	z	303	CLA	CHD-C1D-ND	-2.10	121.85	124.80
50	x	318	CLA	CHD-C1D-ND	-2.10	121.88	124.84
50	w	308	CLA	C1-C2-C3	2.10	129.63	126.20
50	w	302	CLA	CHD-C1D-ND	-2.10	121.85	124.80
53	b	827	PQN	C10-C1-C2	-2.10	116.06	118.97
50	g	201	CLA	O1D-CGD-CBD	-2.10	120.38	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	y	314	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
50	x	309	CLA	CHD-C1D-ND	-2.10	121.85	124.80
50	y	306	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
50	l	305	CLA	CHD-C1D-ND	-2.10	121.85	124.80
43	a	829	BCR	C16-C17-C18	-2.10	124.34	127.28
50	x	303	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
50	y	313	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
50	a	845	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
50	w	302	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
50	z	316	CLA	CHD-C1D-ND	-2.09	121.86	124.80
50	w	316	CLA	C1-C2-C3	2.09	130.15	126.76
45	F	804	A1H1M	O34-C33-C31	-2.09	105.45	110.38
53	a	825	PQN	C10-C1-C2	-2.09	116.07	118.97
50	b	812	CLA	CMD-C2D-C1D	2.09	128.41	124.73
43	b	817	BCR	C1-C6-C5	-2.09	119.78	122.64
50	a	814	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
50	a	838	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
50	b	834	CLA	CHD-C1D-ND	-2.09	121.87	124.80
50	b	803	CLA	C2C-C1C-NC	-2.08	107.80	109.98
50	b	825	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
50	x	302	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
50	b	804	CLA	CAA-C2A-C3A	-2.08	111.46	116.23
50	x	306	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
50	w	303	CLA	CMD-C2D-C1D	2.08	128.39	124.73
50	y	303	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
50	y	312	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
50	z	306	CLA	CED-O2D-CGD	2.08	120.62	115.92
50	a	855	CLA	CHD-C1D-ND	-2.08	121.88	124.80
43	k	201	BCR	C33-C5-C4	-2.07	109.17	113.60
50	x	303	CLA	CHD-C1D-ND	-2.07	121.89	124.80
50	a	853	CLA	C1-C2-C3	2.07	129.59	126.20
50	z	309	CLA	CED-O2D-CGD	2.07	120.61	115.92
50	a	826	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
50	b	824	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
43	b	820	BCR	C21-C20-C19	-2.07	117.20	123.20
50	b	825	CLA	CHD-C1D-ND	-2.07	121.89	124.80
50	w	306	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
43	l	304	BCR	C28-C27-C26	-2.07	110.37	114.06
50	b	822	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
50	b	801	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
54	x	319	CHL	O2D-CGD-O1D	-2.07	119.83	123.85
50	b	802	CLA	CHD-C1D-ND	-2.07	121.89	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	w	314	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
50	a	812	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
43	k	201	BCR	C28-C27-C26	-2.06	110.37	114.06
50	b	815	CLA	CMD-C2D-C1D	2.06	128.36	124.73
50	z	306	CLA	C2C-C1C-NC	-2.06	107.81	109.98
50	k	205	CLA	CMD-C2D-C1D	2.06	128.36	124.73
50	a	850	CLA	C2A-C1A-CHA	2.06	127.45	123.87
50	g	203	CLA	CHD-C1D-ND	-2.06	121.90	124.80
50	b	809	CLA	C4-C3-C5	-2.06	111.65	115.23
50	b	810	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
50	b	825	CLA	C12-C11-C10	-2.06	104.04	113.28
50	x	313	CLA	CED-O2D-CGD	2.06	120.59	115.92
50	w	308	CLA	C2C-C1C-NC	-2.06	107.82	109.98
50	x	312	CLA	C4-C3-C5	-2.06	111.66	115.23
43	b	816	BCR	C21-C20-C19	-2.06	117.24	123.20
50	a	811	CLA	CMD-C2D-C1D	2.06	128.35	124.73
50	a	836	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
50	l	306	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
50	a	853	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
50	f	301	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
50	a	854	CLA	CHD-C1D-ND	-2.05	121.91	124.80
50	y	302	CLA	CHD-C1D-ND	-2.05	121.91	124.80
54	x	305	CHL	O2A-CGA-O1A	-2.05	118.05	123.33
50	a	809	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
50	b	847	CLA	C3C-C4C-NC	-2.05	107.80	110.43
43	k	201	BCR	C3-C4-C5	-2.05	110.40	114.06
50	b	839	CLA	CMD-C2D-C1D	2.05	128.34	124.73
50	b	836	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
50	a	834	CLA	C12-C11-C10	-2.05	104.09	113.28
50	b	814	CLA	CMD-C2D-C1D	2.05	128.34	124.73
50	b	813	CLA	CMD-C2D-C1D	2.05	128.34	124.73
50	a	835	CLA	C2A-C1A-CHA	2.05	127.42	123.87
50	a	812	CLA	CHD-C1D-ND	-2.05	121.92	124.80
50	b	805	CLA	CMD-C2D-C1D	2.05	128.33	124.73
55	y	316	LUT	C36-C21-C26	2.05	112.64	109.55
50	a	818	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
50	b	812	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
50	a	809	CLA	O2D-CGD-O1D	-2.05	119.87	123.85
43	a	830	BCR	C37-C22-C23	2.05	121.21	118.09
50	y	310	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
43	b	817	BCR	C21-C20-C19	-2.04	117.28	123.20
50	j	102	CLA	O1D-CGD-CBD	-2.04	120.49	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	a	826	CLA	CHD-C1D-ND	-2.04	121.93	124.80
50	b	812	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
54	x	301	CHL	OMC-CMC-C2C	-2.04	121.57	125.12
50	f	303	CLA	CHD-C1D-ND	-2.04	121.93	124.80
50	a	839	CLA	CMD-C2D-C1D	2.04	128.32	124.73
43	b	831	BCR	C16-C17-C18	-2.04	124.42	127.28
43	b	816	BCR	C11-C10-C9	2.04	130.14	127.28
50	x	310	CLA	CHD-C1D-ND	-2.04	121.93	124.80
50	b	843	CLA	C4-C3-C5	-2.04	111.69	115.23
50	a	813	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
50	a	823	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
50	z	302	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
50	a	819	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
50	a	849	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
50	a	802	CLA	CHD-C1D-ND	-2.03	121.94	124.80
43	l	302	BCR	C37-C22-C23	2.03	121.19	118.09
45	5	302	A1H1M	C37-C07-C08	-2.03	107.97	112.46
50	a	842	CLA	C4-C3-C5	-2.03	111.70	115.23
46	B	605	LMG	O1-C7-C8	-2.03	105.88	110.82
50	y	314	CLA	CED-O2D-CGD	2.03	120.53	115.92
50	b	805	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
50	f	302	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
50	b	851	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
50	b	849	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
50	z	305	CLA	CMD-C2D-C1D	2.03	128.30	124.73
50	a	847	CLA	C1C-NC-C4C	2.03	108.43	107.03
50	y	303	CLA	CHD-C1D-ND	-2.03	121.95	124.80
50	x	308	CLA	C1-C2-C3	2.03	130.04	126.76
50	b	848	CLA	CMD-C2D-C1D	2.03	128.30	124.73
50	b	805	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
50	b	828	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
50	b	844	CLA	CHB-C1B-NB	2.03	127.09	124.05
50	j	102	CLA	CMD-C2D-C1D	2.02	128.29	124.73
43	a	829	BCR	C20-C21-C22	-2.02	124.44	127.28
50	k	203	CLA	CHD-C1D-ND	-2.02	121.95	124.80
50	k	204	CLA	CMD-C2D-C1D	2.02	128.29	124.73
50	a	814	CLA	CMD-C2D-C1D	2.02	128.29	124.73
50	a	833	CLA	CHB-C1B-NB	2.02	127.08	124.05
50	g	203	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
50	a	819	CLA	CHD-C1D-ND	-2.02	121.96	124.80
50	b	824	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
50	h	201	CLA	CED-O2D-CGD	2.02	120.49	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	x	305	CHL	O2D-CGD-O1D	-2.02	119.92	123.85
50	k	205	CLA	CED-O2D-CGD	2.02	120.49	115.92
50	w	308	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
50	a	841	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
50	b	804	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
50	x	308	CLA	CHD-C1D-ND	-2.02	121.97	124.80
50	b	846	CLA	CHD-C1D-ND	-2.01	121.97	124.80
50	b	843	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
50	b	845	CLA	C4D-CHA-C1A	2.01	123.65	121.24
50	a	848	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
50	a	843	CLA	CED-O2D-CGD	2.01	120.48	115.92
50	a	822	CLA	CHD-C1D-ND	-2.01	121.97	124.80
51	b	821	DGD	O1G-C1G-C2G	-2.01	102.59	108.40
50	a	838	CLA	CMD-C2D-C1D	2.01	128.27	124.73
53	b	827	PQN	C17-C16-C15	-2.01	107.90	113.26
50	b	814	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
50	b	826	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
50	a	849	CLA	CMD-C2D-C1D	2.01	128.27	124.73
50	y	302	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
43	i	101	BCR	C10-C11-C12	-2.01	117.38	123.20
50	x	308	CLA	CMD-C2D-C1D	2.01	128.26	124.73
50	a	847	CLA	CHD-C1D-ND	-2.01	121.98	124.80
50	b	806	CLA	CMD-C2D-C1D	2.01	128.26	124.73
50	b	823	CLA	CHD-C1D-ND	-2.01	121.98	124.80
50	x	308	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
50	a	857	CLA	CHD-C1D-ND	-2.00	121.98	124.80
50	z	310	CLA	CHD-C1D-ND	-2.00	121.98	124.80
50	y	302	CLA	C2A-C1A-CHA	2.00	127.34	123.87
46	D	601	LMG	O6-C1-O1	-2.00	105.31	110.04
50	z	319	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
50	a	813	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
50	a	820	CLA	CHB-C1B-NB	2.00	127.05	124.05
50	b	815	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
45	F	804	A1H1M	C05-C06-C07	2.00	116.71	112.29
50	a	802	CLA	O2D-CGD-O1D	-2.00	119.95	123.85

All (174) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
50	a	801	CLA	ND
50	a	802	CLA	ND
50	a	809	CLA	ND

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Mol	Chain	Res	Type	Atom
50	a	811	CLA	ND
50	a	812	CLA	ND
50	a	813	CLA	ND
50	a	814	CLA	ND
50	a	815	CLA	ND
50	a	816	CLA	ND
50	a	817	CLA	ND
50	a	818	CLA	ND
50	a	819	CLA	ND
50	a	820	CLA	ND
50	a	821	CLA	ND
50	a	822	CLA	ND
50	a	823	CLA	ND
50	a	824	CLA	ND
50	a	826	CLA	ND
50	a	833	CLA	ND
50	a	834	CLA	ND
50	a	835	CLA	ND
50	a	836	CLA	ND
50	a	837	CLA	ND
50	a	838	CLA	ND
50	a	839	CLA	ND
50	a	840	CLA	ND
50	a	841	CLA	ND
50	a	842	CLA	ND
50	a	843	CLA	ND
50	a	844	CLA	ND
50	a	845	CLA	ND
50	a	846	CLA	ND
50	a	847	CLA	ND
50	a	848	CLA	ND
50	a	849	CLA	ND
50	a	850	CLA	ND
50	a	851	CLA	ND
50	a	852	CLA	ND
50	a	853	CLA	ND
50	a	854	CLA	ND
50	a	855	CLA	ND
50	a	856	CLA	ND
50	a	857	CLA	ND
50	a	858	CLA	ND
50	b	801	CLA	ND

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Mol	Chain	Res	Type	Atom
50	b	802	CLA	ND
50	b	803	CLA	ND
50	b	804	CLA	ND
50	b	805	CLA	ND
50	b	806	CLA	ND
50	b	807	CLA	ND
50	b	808	CLA	ND
50	b	809	CLA	ND
50	b	810	CLA	ND
50	b	811	CLA	ND
50	b	812	CLA	ND
50	b	813	CLA	ND
50	b	814	CLA	ND
50	b	815	CLA	ND
50	b	822	CLA	ND
50	b	823	CLA	ND
50	b	824	CLA	ND
50	b	825	CLA	ND
50	b	826	CLA	ND
50	b	828	CLA	ND
50	b	832	CLA	ND
50	b	833	CLA	ND
50	b	834	CLA	ND
50	b	835	CLA	ND
50	b	836	CLA	ND
50	b	837	CLA	ND
50	b	838	CLA	ND
50	b	839	CLA	ND
50	b	840	CLA	ND
50	b	841	CLA	ND
50	b	842	CLA	ND
50	b	843	CLA	ND
50	b	844	CLA	ND
50	b	845	CLA	ND
50	b	846	CLA	ND
50	b	847	CLA	ND
50	b	848	CLA	ND
50	b	849	CLA	ND
50	b	851	CLA	ND
50	f	301	CLA	ND
50	f	302	CLA	ND
50	f	303	CLA	ND

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Mol	Chain	Res	Type	Atom
50	g	201	CLA	ND
50	g	203	CLA	ND
50	g	204	CLA	ND
50	h	201	CLA	ND
50	j	102	CLA	ND
50	k	203	CLA	ND
50	k	204	CLA	ND
50	k	205	CLA	ND
50	l	301	CLA	ND
50	l	305	CLA	ND
50	l	306	CLA	ND
50	w	302	CLA	ND
50	w	303	CLA	ND
50	w	305	CLA	ND
50	w	306	CLA	ND
50	w	307	CLA	ND
50	w	308	CLA	ND
50	w	310	CLA	ND
50	w	314	CLA	ND
50	w	315	CLA	ND
50	w	316	CLA	ND
50	x	302	CLA	ND
50	x	303	CLA	ND
50	x	304	CLA	ND
50	x	306	CLA	ND
50	x	307	CLA	ND
50	x	308	CLA	ND
50	x	309	CLA	ND
50	x	310	CLA	ND
50	x	312	CLA	ND
50	x	313	CLA	ND
50	x	316	CLA	ND
50	x	318	CLA	ND
50	y	302	CLA	ND
50	y	303	CLA	ND
50	y	304	CLA	ND
50	y	305	CLA	ND
50	y	306	CLA	ND
50	y	307	CLA	ND
50	y	308	CLA	ND
50	y	309	CLA	ND
50	y	310	CLA	ND

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Mol	Chain	Res	Type	Atom
50	y	311	CLA	ND
50	y	312	CLA	ND
50	y	313	CLA	ND
50	y	314	CLA	ND
50	z	302	CLA	ND
50	z	303	CLA	ND
50	z	305	CLA	ND
50	z	306	CLA	ND
50	z	307	CLA	ND
50	z	308	CLA	ND
50	z	309	CLA	ND
50	z	310	CLA	ND
50	z	311	CLA	ND
50	z	316	CLA	ND
50	z	319	CLA	ND
52	a	808	CL0	ND
52	a	808	CL0	NA
52	a	808	CL0	NC
54	w	304	CHL	ND
54	w	304	CHL	NA
54	w	304	CHL	NC
54	w	309	CHL	ND
54	w	309	CHL	NA
54	w	309	CHL	NC
54	w	311	CHL	ND
54	w	311	CHL	NA
54	w	311	CHL	NC
54	x	301	CHL	ND
54	x	301	CHL	NA
54	x	301	CHL	NC
54	x	305	CHL	ND
54	x	305	CHL	NA
54	x	305	CHL	NC
54	x	311	CHL	ND
54	x	311	CHL	NA
54	x	311	CHL	NC
54	x	319	CHL	ND
54	x	319	CHL	NA
54	x	319	CHL	NC
54	z	304	CHL	ND
54	z	304	CHL	NA
54	z	304	CHL	NC

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Mol	Chain	Res	Type	Atom
54	z	312	CHL	ND
54	z	312	CHL	NA
54	z	312	CHL	NC

All (2336) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	4	101	BCR	C5-C6-C7-C8
43	4	101	BCR	C21-C22-C23-C24
43	a	803	BCR	C5-C6-C7-C8
43	a	803	BCR	C7-C8-C9-C10
43	a	803	BCR	C7-C8-C9-C34
43	a	810	BCR	C11-C12-C13-C14
43	a	810	BCR	C11-C12-C13-C35
43	a	810	BCR	C17-C18-C19-C20
43	a	810	BCR	C36-C18-C19-C20
43	a	830	BCR	C21-C22-C23-C24
43	a	830	BCR	C37-C22-C23-C24
43	a	830	BCR	C23-C24-C25-C26
43	a	831	BCR	C7-C8-C9-C10
43	a	831	BCR	C7-C8-C9-C34
43	a	831	BCR	C21-C22-C23-C24
43	b	816	BCR	C7-C8-C9-C10
43	b	816	BCR	C7-C8-C9-C34
43	b	816	BCR	C9-C10-C11-C12
43	b	817	BCR	C9-C10-C11-C12
43	b	818	BCR	C7-C8-C9-C10
43	b	819	BCR	C1-C6-C7-C8
43	b	819	BCR	C5-C6-C7-C8
43	b	819	BCR	C7-C8-C9-C10
43	b	820	BCR	C21-C22-C23-C24
43	b	820	BCR	C37-C22-C23-C24
43	b	831	BCR	C17-C18-C19-C20
43	b	850	BCR	C21-C22-C23-C24
43	b	850	BCR	C37-C22-C23-C24
43	g	202	BCR	C17-C18-C19-C20
43	g	202	BCR	C36-C18-C19-C20
43	i	101	BCR	C21-C22-C23-C24
43	i	101	BCR	C23-C24-C25-C26
43	j	101	BCR	C11-C12-C13-C14
43	j	101	BCR	C19-C20-C21-C22
43	j	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
43	j	101	BCR	C37-C22-C23-C24
43	j	103	BCR	C17-C18-C19-C20
43	j	103	BCR	C36-C18-C19-C20
43	j	103	BCR	C23-C24-C25-C26
43	k	201	BCR	C17-C18-C19-C20
43	k	201	BCR	C36-C18-C19-C20
43	l	302	BCR	C7-C8-C9-C10
43	l	302	BCR	C7-C8-C9-C34
43	l	302	BCR	C23-C24-C25-C26
43	l	303	BCR	C21-C22-C23-C24
43	l	303	BCR	C37-C22-C23-C24
43	x	314	BCR	C5-C6-C7-C8
43	x	314	BCR	C7-C8-C9-C10
43	x	314	BCR	C11-C12-C13-C14
43	x	314	BCR	C11-C12-C13-C35
43	x	314	BCR	C17-C18-C19-C20
43	x	314	BCR	C36-C18-C19-C20
43	x	314	BCR	C23-C24-C25-C26
43	y	301	BCR	C5-C6-C7-C8
43	y	301	BCR	C21-C22-C23-C24
43	z	318	BCR	C13-C14-C15-C16
44	5	301	PGT	C1-O3P-P-O1P
44	5	301	PGT	C1-O3P-P-O4P
44	A	401	PGT	C32-C31-O2-C2
44	A	401	PGT	O31-C31-O2-C2
44	A	401	PGT	C4-O4P-P-O3P
44	A	401	PGT	C5-C4-O4P-P
44	A	403	PGT	C32-C31-O2-C2
44	A	403	PGT	C4-O4P-P-O3P
44	A	403	PGT	C4-O4P-P-O1P
44	A	404	PGT	C32-C31-O2-C2
44	A	404	PGT	C1-O3P-P-O1P
44	B	601	PGT	C32-C31-O2-C2
44	B	601	PGT	C1-O3P-P-O4P
44	B	602	PGT	C32-C31-O2-C2
44	B	602	PGT	O31-C31-O2-C2
44	B	602	PGT	C1-O3P-P-O4P
44	B	603	PGT	C4-O4P-P-O3P
44	B	603	PGT	C4-O4P-P-O1P
44	B	603	PGT	C4-O4P-P-O2P
44	B	606	PGT	C32-C31-O2-C2
44	B	606	PGT	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
44	B	606	PGT	C1-O3P-P-O1P
44	B	606	PGT	C1-O3P-P-O4P
44	B	606	PGT	C4-O4P-P-O3P
44	B	606	PGT	C4-O4P-P-O1P
44	B	606	PGT	C5-C4-O4P-P
44	D	602	PGT	O3P-C1-C2-O2
44	F	803	PGT	C32-C31-O2-C2
44	F	803	PGT	O31-C31-O2-C2
44	F	803	PGT	C4-O4P-P-O3P
44	F	803	PGT	C5-C4-O4P-P
44	I	203	PGT	C1-O3P-P-O1P
44	I	203	PGT	C1-O3P-P-O4P
44	N	301	PGT	C1-O3P-P-O1P
44	N	301	PGT	C1-O3P-P-O4P
44	N	301	PGT	C4-O4P-P-O1P
44	a	805	PGT	C1-O3P-P-O1P
44	a	805	PGT	C1-O3P-P-O2P
44	a	805	PGT	C1-O3P-P-O4P
44	a	806	PGT	C32-C31-O2-C2
44	a	806	PGT	C1-O3P-P-O1P
44	a	806	PGT	C1-O3P-P-O2P
44	a	806	PGT	C1-O3P-P-O4P
44	a	806	PGT	C4-O4P-P-O3P
44	a	806	PGT	C4-O4P-P-O1P
44	a	807	PGT	C1-O3P-P-O2P
44	a	807	PGT	C1-O3P-P-O4P
44	a	807	PGT	C4-O4P-P-O3P
44	a	807	PGT	C5-C4-O4P-P
44	b	829	PGT	C32-C31-O2-C2
44	b	829	PGT	C1-O3P-P-O1P
44	b	830	PGT	C1-O3P-P-O2P
44	b	830	PGT	C1-O3P-P-O4P
44	b	830	PGT	C4-O4P-P-O3P
44	f	305	PGT	O31-C31-O2-C2
44	z	301	PGT	C2-C1-O3P-P
44	z	301	PGT	C1-O3P-P-O2P
44	z	301	PGT	C1-O3P-P-O4P
44	z	301	PGT	C4-O4P-P-O3P
44	z	301	PGT	C5-C4-O4P-P
44	z	313	PGT	C32-C31-O2-C2
44	z	317	PGT	C1-O3P-P-O4P
45	F	804	A1H1M	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
45	F	804	A1H1M	C06-C07-C08-C36
46	7	301	LMG	C11-C10-O7-C8
46	B	605	LMG	O1-C7-C8-O7
46	B	605	LMG	O9-C10-O7-C8
46	B	605	LMG	C11-C10-O7-C8
46	D	601	LMG	O9-C10-O7-C8
46	j	105	LMG	O9-C10-O7-C8
46	w	312	LMG	O9-C10-O7-C8
46	w	312	LMG	C11-C10-O7-C8
46	z	314	LMG	O7-C8-C9-O8
47	A	405	PQ9	C2-C11-C12-C13
47	A	405	PQ9	C25-C26-C27-C28
48	B	604	SQD	O5-C1-O6-C44
48	B	604	SQD	O5-C5-C6-S
48	a	859	SQD	O5-C1-O6-C44
48	w	318	SQD	O49-C7-O47-C45
48	w	318	SQD	C8-C7-O47-C45
50	a	801	CLA	CAD-CBD-CGD-O2D
50	a	809	CLA	C1-C2-C3-C5
50	a	811	CLA	C1A-C2A-CAA-CBA
50	a	811	CLA	C3A-C2A-CAA-CBA
50	a	812	CLA	C4B-C3B-CAB-CBB
50	a	812	CLA	CBD-CGD-O2D-CED
50	a	812	CLA	C1-C2-C3-C4
50	a	812	CLA	C1-C2-C3-C5
50	a	813	CLA	CHA-CBD-CGD-O1D
50	a	813	CLA	CHA-CBD-CGD-O2D
50	a	815	CLA	CHA-CBD-CGD-O1D
50	a	815	CLA	CHA-CBD-CGD-O2D
50	a	816	CLA	CBD-CGD-O2D-CED
50	a	818	CLA	C3A-C2A-CAA-CBA
50	a	818	CLA	C2B-C3B-CAB-CBB
50	a	818	CLA	C4B-C3B-CAB-CBB
50	a	819	CLA	C2B-C3B-CAB-CBB
50	a	819	CLA	C4B-C3B-CAB-CBB
50	a	819	CLA	CAD-CBD-CGD-O2D
50	a	821	CLA	CBD-CGD-O2D-CED
50	a	822	CLA	C2-C3-C5-C6
50	a	822	CLA	C4-C3-C5-C6
50	a	824	CLA	C1-C2-C3-C5
50	a	826	CLA	C3A-C2A-CAA-CBA
50	a	826	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
50	a	826	CLA	C4B-C3B-CAB-CBB
50	a	826	CLA	CAD-CBD-CGD-O2D
50	a	826	CLA	CBD-CGD-O2D-CED
50	a	833	CLA	C3A-C2A-CAA-CBA
50	a	833	CLA	CHA-CBD-CGD-O1D
50	a	833	CLA	C1-C2-C3-C4
50	a	833	CLA	C1-C2-C3-C5
50	a	835	CLA	C4B-C3B-CAB-CBB
50	a	835	CLA	C1-C2-C3-C4
50	a	835	CLA	C1-C2-C3-C5
50	a	836	CLA	C11-C10-C8-C7
50	a	837	CLA	C1A-C2A-CAA-CBA
50	a	837	CLA	C3A-C2A-CAA-CBA
50	a	837	CLA	CBD-CGD-O2D-CED
50	a	838	CLA	C3A-C2A-CAA-CBA
50	a	838	CLA	C2B-C3B-CAB-CBB
50	a	838	CLA	C4B-C3B-CAB-CBB
50	a	838	CLA	C1-C2-C3-C5
50	a	839	CLA	C2B-C3B-CAB-CBB
50	a	839	CLA	C4B-C3B-CAB-CBB
50	a	839	CLA	CBD-CGD-O2D-CED
50	a	840	CLA	CBD-CGD-O2D-CED
50	a	841	CLA	C2B-C3B-CAB-CBB
50	a	841	CLA	C4B-C3B-CAB-CBB
50	a	842	CLA	C1A-C2A-CAA-CBA
50	a	842	CLA	C3A-C2A-CAA-CBA
50	a	842	CLA	C2B-C3B-CAB-CBB
50	a	842	CLA	C4B-C3B-CAB-CBB
50	a	842	CLA	C1-C2-C3-C4
50	a	842	CLA	C1-C2-C3-C5
50	a	843	CLA	CBD-CGD-O2D-CED
50	a	845	CLA	C2B-C3B-CAB-CBB
50	a	845	CLA	C4B-C3B-CAB-CBB
50	a	845	CLA	C1-C2-C3-C5
50	a	847	CLA	C2A-C1A-CHA-C4D
50	a	847	CLA	C2B-C3B-CAB-CBB
50	a	847	CLA	C4B-C3B-CAB-CBB
50	a	849	CLA	C1A-C2A-CAA-CBA
50	a	849	CLA	CBD-CGD-O2D-CED
50	a	849	CLA	C1-C2-C3-C4
50	a	849	CLA	C1-C2-C3-C5
50	a	850	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
50	a	852	CLA	CAD-CBD-CGD-O1D
50	a	852	CLA	CAD-CBD-CGD-O2D
50	a	854	CLA	C2B-C3B-CAB-CBB
50	a	854	CLA	C4B-C3B-CAB-CBB
50	a	855	CLA	CBD-CGD-O2D-CED
50	a	856	CLA	C2B-C3B-CAB-CBB
50	a	856	CLA	C4B-C3B-CAB-CBB
50	a	856	CLA	CBD-CGD-O2D-CED
50	a	856	CLA	C1-C2-C3-C5
50	a	858	CLA	C4B-C3B-CAB-CBB
50	b	801	CLA	CBD-CGD-O2D-CED
50	b	802	CLA	C1A-C2A-CAA-CBA
50	b	803	CLA	C1A-C2A-CAA-CBA
50	b	803	CLA	C3A-C2A-CAA-CBA
50	b	803	CLA	C11-C12-C13-C14
50	b	805	CLA	CBA-CGA-O2A-C1
50	b	805	CLA	O1A-CGA-O2A-C1
50	b	805	CLA	CHA-CBD-CGD-O1D
50	b	807	CLA	C1A-C2A-CAA-CBA
50	b	807	CLA	C4B-C3B-CAB-CBB
50	b	807	CLA	CBD-CGD-O2D-CED
50	b	807	CLA	O1D-CGD-O2D-CED
50	b	808	CLA	CHA-CBD-CGD-O2D
50	b	809	CLA	C1-C2-C3-C5
50	b	810	CLA	C1A-C2A-CAA-CBA
50	b	810	CLA	C3A-C2A-CAA-CBA
50	b	812	CLA	C2B-C3B-CAB-CBB
50	b	812	CLA	C4B-C3B-CAB-CBB
50	b	812	CLA	C1-C2-C3-C4
50	b	812	CLA	C1-C2-C3-C5
50	b	812	CLA	C11-C10-C8-C9
50	b	814	CLA	C2B-C3B-CAB-CBB
50	b	814	CLA	C4B-C3B-CAB-CBB
50	b	815	CLA	C2B-C3B-CAB-CBB
50	b	815	CLA	C4B-C3B-CAB-CBB
50	b	822	CLA	C4B-C3B-CAB-CBB
50	b	822	CLA	CHA-CBD-CGD-O1D
50	b	822	CLA	CHA-CBD-CGD-O2D
50	b	823	CLA	C1A-C2A-CAA-CBA
50	b	824	CLA	C11-C10-C8-C9
50	b	825	CLA	C1-C2-C3-C5
50	b	826	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
50	b	826	CLA	C3A-C2A-CAA-CBA
50	b	826	CLA	C4-C3-C5-C6
50	b	828	CLA	C1-C2-C3-C4
50	b	832	CLA	CBA-CGA-O2A-C1
50	b	832	CLA	O1A-CGA-O2A-C1
50	b	833	CLA	C2B-C3B-CAB-CBB
50	b	833	CLA	C4B-C3B-CAB-CBB
50	b	833	CLA	C11-C12-C13-C14
50	b	835	CLA	C2B-C3B-CAB-CBB
50	b	835	CLA	C4B-C3B-CAB-CBB
50	b	836	CLA	C11-C12-C13-C14
50	b	837	CLA	C3A-C2A-CAA-CBA
50	b	839	CLA	C2B-C3B-CAB-CBB
50	b	839	CLA	C4B-C3B-CAB-CBB
50	b	839	CLA	CHA-CBD-CGD-O1D
50	b	839	CLA	CHA-CBD-CGD-O2D
50	b	840	CLA	C1-C2-C3-C4
50	b	840	CLA	C1-C2-C3-C5
50	b	841	CLA	C1A-C2A-CAA-CBA
50	b	841	CLA	CBD-CGD-O2D-CED
50	b	842	CLA	C1A-C2A-CAA-CBA
50	b	842	CLA	O1A-CGA-O2A-C1
50	b	842	CLA	CHA-CBD-CGD-O1D
50	b	842	CLA	CHA-CBD-CGD-O2D
50	b	842	CLA	C11-C10-C8-C9
50	b	843	CLA	CHA-CBD-CGD-O1D
50	b	843	CLA	CHA-CBD-CGD-O2D
50	b	844	CLA	C1A-C2A-CAA-CBA
50	b	844	CLA	C2B-C3B-CAB-CBB
50	b	844	CLA	C4B-C3B-CAB-CBB
50	b	844	CLA	CBD-CGD-O2D-CED
50	b	844	CLA	C1-C2-C3-C4
50	b	844	CLA	C1-C2-C3-C5
50	b	845	CLA	C1A-C2A-CAA-CBA
50	b	845	CLA	C3A-C2A-CAA-CBA
50	b	846	CLA	C3A-C2A-CAA-CBA
50	b	847	CLA	O1A-CGA-O2A-C1
50	b	847	CLA	C2-C1-O2A-CGA
50	b	847	CLA	CBD-CGD-O2D-CED
50	b	849	CLA	C1A-C2A-CAA-CBA
50	b	851	CLA	C2B-C3B-CAB-CBB
50	b	851	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
50	f	301	CLA	C1A-C2A-CAA-CBA
50	f	303	CLA	CBD-CGD-O2D-CED
50	g	201	CLA	CBA-CGA-O2A-C1
50	g	201	CLA	O1A-CGA-O2A-C1
50	g	201	CLA	CBD-CGD-O2D-CED
50	g	203	CLA	CBD-CGD-O2D-CED
50	g	204	CLA	C2A-CAA-CBA-CGA
50	g	204	CLA	CBD-CGD-O2D-CED
50	h	201	CLA	C3A-C2A-CAA-CBA
50	h	201	CLA	CBD-CGD-O2D-CED
50	k	205	CLA	CAD-CBD-CGD-O2D
50	k	205	CLA	CBD-CGD-O2D-CED
50	l	306	CLA	C1A-C2A-CAA-CBA
50	l	306	CLA	C3A-C2A-CAA-CBA
50	l	306	CLA	C2B-C3B-CAB-CBB
50	l	306	CLA	C4B-C3B-CAB-CBB
50	w	302	CLA	C1A-C2A-CAA-CBA
50	w	302	CLA	C3A-C2A-CAA-CBA
50	w	302	CLA	C1-C2-C3-C5
50	w	303	CLA	C3A-C2A-CAA-CBA
50	w	305	CLA	C1-C2-C3-C5
50	w	306	CLA	CHA-CBD-CGD-O2D
50	w	306	CLA	C11-C10-C8-C7
50	w	307	CLA	C1A-C2A-CAA-CBA
50	w	307	CLA	C3A-C2A-CAA-CBA
50	w	307	CLA	CBD-CGD-O2D-CED
50	w	307	CLA	O1D-CGD-O2D-CED
50	w	308	CLA	C3A-C2A-CAA-CBA
50	w	310	CLA	C1A-C2A-CAA-CBA
50	w	310	CLA	C1-C2-C3-C5
50	w	314	CLA	C1A-C2A-CAA-CBA
50	w	314	CLA	C3A-C2A-CAA-CBA
50	w	314	CLA	CAA-CBA-CGA-O1A
50	w	314	CLA	CAD-CBD-CGD-O1D
50	w	314	CLA	CAD-CBD-CGD-O2D
50	w	314	CLA	CBD-CGD-O2D-CED
50	w	315	CLA	CBD-CGD-O2D-CED
50	w	315	CLA	O1D-CGD-O2D-CED
50	w	316	CLA	C1A-C2A-CAA-CBA
50	w	316	CLA	C3A-C2A-CAA-CBA
50	w	316	CLA	CBD-CGD-O2D-CED
50	w	316	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
50	x	302	CLA	CBD-CGD-O2D-CED
50	x	303	CLA	C1A-C2A-CAA-CBA
50	x	303	CLA	CBD-CGD-O2D-CED
50	x	306	CLA	C1-C2-C3-C5
50	x	307	CLA	CHA-CBD-CGD-O2D
50	x	308	CLA	C2B-C3B-CAB-CBB
50	x	308	CLA	C4B-C3B-CAB-CBB
50	x	309	CLA	C1A-C2A-CAA-CBA
50	x	310	CLA	C3A-C2A-CAA-CBA
50	x	312	CLA	C3A-C2A-CAA-CBA
50	x	313	CLA	O1A-CGA-O2A-C1
50	x	313	CLA	CBD-CGD-O2D-CED
50	x	316	CLA	CAD-CBD-CGD-O2D
50	x	318	CLA	C1A-C2A-CAA-CBA
50	y	302	CLA	C1-C2-C3-C5
50	y	303	CLA	CBA-CGA-O2A-C1
50	y	303	CLA	O1A-CGA-O2A-C1
50	y	306	CLA	CBD-CGD-O2D-CED
50	y	306	CLA	O1D-CGD-O2D-CED
50	y	307	CLA	C1A-C2A-CAA-CBA
50	y	307	CLA	C3A-C2A-CAA-CBA
50	y	307	CLA	CBD-CGD-O2D-CED
50	y	309	CLA	C1A-C2A-CAA-CBA
50	y	310	CLA	C2B-C3B-CAB-CBB
50	y	310	CLA	C4B-C3B-CAB-CBB
50	y	310	CLA	CHA-CBD-CGD-O2D
50	y	311	CLA	C1A-C2A-CAA-CBA
50	y	312	CLA	C1-C2-C3-C5
50	y	314	CLA	C2-C1-O2A-CGA
50	y	314	CLA	C2B-C3B-CAB-CBB
50	y	314	CLA	C4B-C3B-CAB-CBB
50	y	314	CLA	CHA-CBD-CGD-O1D
50	y	314	CLA	CHA-CBD-CGD-O2D
50	y	314	CLA	C1-C2-C3-C4
50	y	314	CLA	C1-C2-C3-C5
50	z	302	CLA	CBD-CGD-O2D-CED
50	z	303	CLA	CBD-CGD-O2D-CED
50	z	305	CLA	C1-C2-C3-C5
50	z	306	CLA	C1A-C2A-CAA-CBA
50	z	306	CLA	C3A-C2A-CAA-CBA
50	z	306	CLA	C1-C2-C3-C5
50	z	307	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
50	z	307	CLA	C4B-C3B-CAB-CBB
50	z	307	CLA	CHA-CBD-CGD-O2D
50	z	310	CLA	CAD-CBD-CGD-O1D
50	z	310	CLA	CAD-CBD-CGD-O2D
50	z	310	CLA	CBD-CGD-O2D-CED
50	z	311	CLA	CHA-CBD-CGD-O1D
51	a	804	DGD	C2D-C1D-O3G-C3G
51	a	804	DGD	O6D-C1D-O3G-C3G
51	b	821	DGD	C2B-C1B-O2G-C2G
51	b	821	DGD	O2G-C2G-C3G-O3G
51	x	317	DGD	O1B-C1B-O2G-C2G
51	x	317	DGD	O6D-C1D-O3G-C3G
54	w	304	CHL	C1C-C2C-CMC-OMC
54	w	304	CHL	C3C-C2C-CMC-OMC
54	w	309	CHL	C3A-C2A-CAA-CBA
54	w	311	CHL	C1A-C2A-CAA-CBA
54	w	311	CHL	CBD-CGD-O2D-CED
54	x	301	CHL	C1A-C2A-CAA-CBA
54	x	301	CHL	CBD-CGD-O2D-CED
54	x	311	CHL	CBD-CGD-O2D-CED
54	x	319	CHL	C3A-C2A-CAA-CBA
54	z	304	CHL	C1C-C2C-CMC-OMC
54	z	312	CHL	C1C-C2C-CMC-OMC
54	z	312	CHL	C3C-C2C-CMC-OMC
54	z	312	CHL	CBD-CGD-O2D-CED
55	w	319	LUT	C21-C26-C27-C28
55	w	319	LUT	C25-C26-C27-C28
55	w	319	LUT	C27-C28-C29-C30
55	w	319	LUT	C27-C28-C29-C39
55	x	321	LUT	C7-C8-C9-C10
55	x	321	LUT	C7-C8-C9-C19
55	x	321	LUT	C21-C26-C27-C28
55	x	321	LUT	C25-C26-C27-C28
55	y	316	LUT	C21-C26-C27-C28
55	y	316	LUT	C25-C26-C27-C28
55	y	316	LUT	C27-C28-C29-C30
55	y	316	LUT	C27-C28-C29-C39
50	w	310	CLA	C4C-C3C-CAC-CBC
50	b	848	CLA	O1D-CGD-O2D-CED
50	f	303	CLA	O1D-CGD-O2D-CED
50	h	201	CLA	O1D-CGD-O2D-CED
50	l	301	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
50	w	314	CLA	O1D-CGD-O2D-CED
50	x	303	CLA	O1D-CGD-O2D-CED
54	w	309	CHL	O1D-CGD-O2D-CED
50	a	821	CLA	O1D-CGD-O2D-CED
50	k	205	CLA	O1D-CGD-O2D-CED
50	x	313	CLA	O1D-CGD-O2D-CED
50	z	302	CLA	O1D-CGD-O2D-CED
50	z	309	CLA	O1D-CGD-O2D-CED
54	x	301	CHL	O1D-CGD-O2D-CED
54	x	311	CHL	O1D-CGD-O2D-CED
50	a	802	CLA	CBD-CGD-O2D-CED
50	a	811	CLA	CBD-CGD-O2D-CED
50	a	824	CLA	CBD-CGD-O2D-CED
50	b	802	CLA	CBD-CGD-O2D-CED
50	b	805	CLA	CBD-CGD-O2D-CED
50	b	808	CLA	CBD-CGD-O2D-CED
50	b	838	CLA	CBD-CGD-O2D-CED
50	b	845	CLA	CBD-CGD-O2D-CED
50	b	848	CLA	CBD-CGD-O2D-CED
50	f	301	CLA	CBD-CGD-O2D-CED
50	k	203	CLA	CBD-CGD-O2D-CED
50	l	301	CLA	CBD-CGD-O2D-CED
50	w	302	CLA	CBD-CGD-O2D-CED
50	w	306	CLA	CBD-CGD-O2D-CED
50	w	308	CLA	CBD-CGD-O2D-CED
50	x	306	CLA	CBD-CGD-O2D-CED
50	x	307	CLA	CBD-CGD-O2D-CED
50	y	310	CLA	CBD-CGD-O2D-CED
50	y	312	CLA	CBD-CGD-O2D-CED
50	z	307	CLA	CBD-CGD-O2D-CED
50	z	308	CLA	CBD-CGD-O2D-CED
50	z	309	CLA	CBD-CGD-O2D-CED
54	w	309	CHL	CBD-CGD-O2D-CED
54	z	304	CHL	CBD-CGD-O2D-CED
44	B	602	PGT	O11-C11-O3-C3
44	a	805	PGT	O11-C11-O3-C3
44	b	830	PGT	O11-C11-O3-C3
44	z	301	PGT	O11-C11-O3-C3
48	w	318	SQD	O10-C23-O48-C46
50	a	809	CLA	O1A-CGA-O2A-C1
50	a	814	CLA	O1A-CGA-O2A-C1
50	a	857	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
50	b	838	CLA	O1A-CGA-O2A-C1
50	x	306	CLA	O1A-CGA-O2A-C1
50	x	308	CLA	O1A-CGA-O2A-C1
50	w	310	CLA	C2C-C3C-CAC-CBC
50	a	812	CLA	O1D-CGD-O2D-CED
50	g	201	CLA	O1D-CGD-O2D-CED
50	b	801	CLA	O1D-CGD-O2D-CED
50	f	301	CLA	O1D-CGD-O2D-CED
50	g	203	CLA	O1D-CGD-O2D-CED
50	x	302	CLA	O1D-CGD-O2D-CED
54	z	304	CHL	O1D-CGD-O2D-CED
54	z	312	CHL	O1D-CGD-O2D-CED
44	a	805	PGT	C12-C11-O3-C3
44	a	806	PGT	C12-C11-O3-C3
44	z	301	PGT	C12-C11-O3-C3
48	w	318	SQD	C24-C23-O48-C46
50	a	809	CLA	CBA-CGA-O2A-C1
50	a	815	CLA	CBA-CGA-O2A-C1
50	a	823	CLA	CBA-CGA-O2A-C1
50	a	857	CLA	CBA-CGA-O2A-C1
50	w	302	CLA	CBA-CGA-O2A-C1
54	x	319	CHL	CBD-CGD-O2D-CED
44	5	301	PGT	O11-C11-O3-C3
44	A	401	PGT	O11-C11-O3-C3
44	A	404	PGT	O11-C11-O3-C3
44	B	601	PGT	O11-C11-O3-C3
44	I	203	PGT	O11-C11-O3-C3
44	a	806	PGT	O11-C11-O3-C3
44	b	829	PGT	O11-C11-O3-C3
46	7	301	LMG	O10-C28-O8-C9
46	D	601	LMG	O10-C28-O8-C9
46	j	104	LMG	O10-C28-O8-C9
46	z	315	LMG	O10-C28-O8-C9
50	a	801	CLA	O1A-CGA-O2A-C1
50	a	815	CLA	O1A-CGA-O2A-C1
50	a	823	CLA	O1A-CGA-O2A-C1
50	a	849	CLA	O1A-CGA-O2A-C1
50	b	815	CLA	O1A-CGA-O2A-C1
50	b	828	CLA	O1A-CGA-O2A-C1
50	b	836	CLA	O1A-CGA-O2A-C1
50	w	302	CLA	O1A-CGA-O2A-C1
50	w	316	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
50	x	312	CLA	O1A-CGA-O2A-C1
50	y	314	CLA	O1A-CGA-O2A-C1
51	a	804	DGD	O1A-C1A-O1G-C1G
50	a	839	CLA	C15-C16-C17-C18
50	b	845	CLA	O1D-CGD-O2D-CED
50	y	312	CLA	O1D-CGD-O2D-CED
45	5	302	A1H1M	O14-C13-O12-C11
45	F	804	A1H1M	C33-C13-O12-C11
50	b	805	CLA	O1D-CGD-O2D-CED
50	w	302	CLA	O1D-CGD-O2D-CED
50	x	306	CLA	O1D-CGD-O2D-CED
50	z	308	CLA	O1D-CGD-O2D-CED
50	a	839	CLA	O1A-CGA-O2A-C1
50	w	308	CLA	O1A-CGA-O2A-C1
44	A	403	PGT	O31-C31-O2-C2
44	A	404	PGT	O31-C31-O2-C2
44	B	601	PGT	O31-C31-O2-C2
44	B	606	PGT	O31-C31-O2-C2
44	b	829	PGT	O31-C31-O2-C2
44	z	313	PGT	O31-C31-O2-C2
46	7	301	LMG	O9-C10-O7-C8
51	b	821	DGD	O1B-C1B-O2G-C2G
50	a	851	CLA	CBA-CGA-O2A-C1
50	a	851	CLA	O1A-CGA-O2A-C1
45	5	302	A1H1M	C25-C22-C23-O24
50	a	811	CLA	C3-C5-C6-C7
50	a	836	CLA	C3-C5-C6-C7
50	f	301	CLA	C3-C5-C6-C7
53	b	827	PQN	C13-C15-C16-C17
47	A	405	PQ9	C20-C21-C22-C23
44	A	401	PGT	C12-C11-O3-C3
44	B	601	PGT	C12-C11-O3-C3
44	B	602	PGT	C12-C11-O3-C3
44	I	203	PGT	C12-C11-O3-C3
44	b	829	PGT	C12-C11-O3-C3
44	b	830	PGT	C12-C11-O3-C3
46	7	301	LMG	C29-C28-O8-C9
46	D	601	LMG	C29-C28-O8-C9
46	j	104	LMG	C29-C28-O8-C9
50	a	801	CLA	CBA-CGA-O2A-C1
50	a	821	CLA	CBA-CGA-O2A-C1
50	a	833	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
50	a	841	CLA	CBA-CGA-O2A-C1
50	a	842	CLA	CBA-CGA-O2A-C1
50	a	849	CLA	CBA-CGA-O2A-C1
50	b	842	CLA	CBA-CGA-O2A-C1
50	x	308	CLA	CBA-CGA-O2A-C1
50	x	312	CLA	CBA-CGA-O2A-C1
50	x	313	CLA	CBA-CGA-O2A-C1
51	a	804	DGD	C2A-C1A-O1G-C1G
50	a	815	CLA	CBD-CGD-O2D-CED
50	a	836	CLA	CBD-CGD-O2D-CED
50	a	845	CLA	CBD-CGD-O2D-CED
50	a	853	CLA	CBD-CGD-O2D-CED
50	a	857	CLA	CBD-CGD-O2D-CED
50	b	803	CLA	CBD-CGD-O2D-CED
50	b	806	CLA	CBD-CGD-O2D-CED
50	b	813	CLA	CBD-CGD-O2D-CED
50	b	823	CLA	CBD-CGD-O2D-CED
50	b	834	CLA	CBD-CGD-O2D-CED
50	x	318	CLA	CBD-CGD-O2D-CED
50	y	303	CLA	CBD-CGD-O2D-CED
50	y	308	CLA	CBD-CGD-O2D-CED
50	z	311	CLA	CBD-CGD-O2D-CED
44	f	305	PGT	C32-C31-O2-C2
46	D	601	LMG	C11-C10-O7-C8
46	j	105	LMG	C11-C10-O7-C8
51	x	317	DGD	C2B-C1B-O2G-C2G
45	F	804	A1H1M	O14-C13-O12-C11
50	a	811	CLA	O1D-CGD-O2D-CED
50	a	824	CLA	O1D-CGD-O2D-CED
50	a	826	CLA	O1D-CGD-O2D-CED
50	b	803	CLA	O1D-CGD-O2D-CED
50	b	847	CLA	O1D-CGD-O2D-CED
50	k	203	CLA	O1D-CGD-O2D-CED
50	b	802	CLA	O1D-CGD-O2D-CED
50	a	820	CLA	C4-C3-C5-C6
50	a	833	CLA	C4-C3-C5-C6
50	a	844	CLA	C4-C3-C5-C6
50	a	846	CLA	C4-C3-C5-C6
50	a	849	CLA	C4-C3-C5-C6
50	b	822	CLA	C4-C3-C5-C6
50	b	828	CLA	C4-C3-C5-C6
50	b	832	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
50	b	844	CLA	C4-C3-C5-C6
50	l	306	CLA	C4-C3-C5-C6
50	x	307	CLA	C4-C3-C5-C6
50	y	313	CLA	C4-C3-C5-C6
50	a	820	CLA	C2-C3-C5-C6
50	a	846	CLA	C2-C3-C5-C6
50	b	823	CLA	C2-C3-C5-C6
50	b	828	CLA	C2-C3-C5-C6
50	b	844	CLA	C2-C3-C5-C6
50	l	306	CLA	C2-C3-C5-C6
50	x	307	CLA	C2-C3-C5-C6
50	y	313	CLA	C2-C3-C5-C6
50	h	201	CLA	CBA-CGA-O2A-C1
50	a	811	CLA	C2A-CAA-CBA-CGA
50	b	839	CLA	C2A-CAA-CBA-CGA
50	b	845	CLA	C2A-CAA-CBA-CGA
50	g	201	CLA	C2A-CAA-CBA-CGA
50	w	303	CLA	C2A-CAA-CBA-CGA
50	a	841	CLA	O1A-CGA-O2A-C1
50	b	801	CLA	C3-C5-C6-C7
50	b	802	CLA	C3-C5-C6-C7
50	b	805	CLA	C3-C5-C6-C7
50	b	847	CLA	C3-C5-C6-C7
50	y	308	CLA	C3-C5-C6-C7
44	5	301	PGT	C12-C11-O3-C3
44	A	404	PGT	C12-C11-O3-C3
46	z	315	LMG	C29-C28-O8-C9
50	a	839	CLA	CBA-CGA-O2A-C1
50	a	843	CLA	CBA-CGA-O2A-C1
50	a	848	CLA	CBA-CGA-O2A-C1
50	b	802	CLA	CBA-CGA-O2A-C1
50	b	815	CLA	CBA-CGA-O2A-C1
50	b	828	CLA	CBA-CGA-O2A-C1
50	b	836	CLA	CBA-CGA-O2A-C1
50	b	846	CLA	CBA-CGA-O2A-C1
50	l	306	CLA	CBA-CGA-O2A-C1
50	w	308	CLA	CBA-CGA-O2A-C1
50	w	316	CLA	CBA-CGA-O2A-C1
50	x	306	CLA	CBA-CGA-O2A-C1
46	w	312	LMG	O6-C5-C6-O5
43	a	810	BCR	C15-C16-C17-C18
43	b	819	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
43	g	202	BCR	C19-C20-C21-C22
43	k	201	BCR	C13-C14-C15-C16
50	a	812	CLA	O1A-CGA-O2A-C1
50	a	833	CLA	O1A-CGA-O2A-C1
50	a	842	CLA	O1A-CGA-O2A-C1
50	a	843	CLA	O1A-CGA-O2A-C1
50	b	802	CLA	O1A-CGA-O2A-C1
50	b	840	CLA	O1A-CGA-O2A-C1
50	b	841	CLA	O1A-CGA-O2A-C1
50	k	204	CLA	O1A-CGA-O2A-C1
50	w	310	CLA	O1A-CGA-O2A-C1
50	z	305	CLA	O1A-CGA-O2A-C1
44	a	806	PGT	O31-C31-O2-C2
50	a	816	CLA	O1D-CGD-O2D-CED
50	a	849	CLA	O1D-CGD-O2D-CED
50	a	837	CLA	O1D-CGD-O2D-CED
50	a	839	CLA	O1D-CGD-O2D-CED
50	z	310	CLA	O1D-CGD-O2D-CED
50	a	814	CLA	C3-C5-C6-C7
50	z	306	CLA	C3-C5-C6-C7
53	a	825	PQN	C13-C15-C16-C17
50	b	851	CLA	CBD-CGD-O2D-CED
50	j	102	CLA	CBD-CGD-O2D-CED
54	w	304	CHL	CBD-CGD-O2D-CED
44	A	403	PGT	C13-C14-C15-C16
44	L	201	PGT	C12-C11-O3-C3
44	z	317	PGT	C12-C11-O3-C3
50	a	814	CLA	CBA-CGA-O2A-C1
50	b	838	CLA	CBA-CGA-O2A-C1
50	b	840	CLA	CBA-CGA-O2A-C1
50	b	847	CLA	CBA-CGA-O2A-C1
50	a	834	CLA	O1A-CGA-O2A-C1
50	a	845	CLA	O1A-CGA-O2A-C1
50	w	306	CLA	O1D-CGD-O2D-CED
54	w	311	CHL	O1D-CGD-O2D-CED
50	b	826	CLA	CBD-CGD-O2D-CED
46	B	605	LMG	O6-C5-C6-O5
46	D	601	LMG	O6-C5-C6-O5
46	w	312	LMG	C4-C5-C6-O5
50	a	843	CLA	O1D-CGD-O2D-CED
50	a	812	CLA	C3-C5-C6-C7
50	a	835	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
50	a	841	CLA	CBD-CGD-O2D-CED
50	y	314	CLA	CBA-CGA-O2A-C1
50	a	833	CLA	C2-C3-C5-C6
50	b	826	CLA	C2-C3-C5-C6
50	b	832	CLA	C2-C3-C5-C6
50	w	308	CLA	C2-C3-C5-C6
50	b	823	CLA	O1A-CGA-O2A-C1
47	A	405	PQ9	C13-C15-C16-C17
50	a	814	CLA	CBD-CGD-O2D-CED
50	a	833	CLA	CBD-CGD-O2D-CED
50	b	835	CLA	CBD-CGD-O2D-CED
50	w	310	CLA	CBD-CGD-O2D-CED
46	F	802	LMG	O6-C5-C6-O5
46	H	401	LMG	O6-C5-C6-O5
50	b	823	CLA	C2A-CAA-CBA-CGA
50	f	301	CLA	C2A-CAA-CBA-CGA
50	k	204	CLA	C2A-CAA-CBA-CGA
50	w	307	CLA	C2A-CAA-CBA-CGA
50	x	304	CLA	C2A-CAA-CBA-CGA
50	z	306	CLA	C2A-CAA-CBA-CGA
44	z	317	PGT	O11-C11-O3-C3
50	a	821	CLA	O1A-CGA-O2A-C1
50	b	846	CLA	O1A-CGA-O2A-C1
46	j	105	LMG	O6-C1-O1-C7
51	a	804	DGD	O6E-C1E-O5D-C6D
44	B	606	PGT	C12-C11-O3-C3
50	k	204	CLA	CBA-CGA-O2A-C1
50	z	305	CLA	CBA-CGA-O2A-C1
50	a	818	CLA	CBD-CGD-O2D-CED
50	b	822	CLA	CBD-CGD-O2D-CED
50	x	308	CLA	CBD-CGD-O2D-CED
50	z	306	CLA	CBD-CGD-O2D-CED
45	5	302	A1H1M	O21-C22-C23-O24
44	L	201	PGT	O11-C11-O3-C3
50	a	802	CLA	O1A-CGA-O2A-C1
45	5	302	A1H1M	O14-C15-C16-O17
45	F	804	A1H1M	O14-C15-C16-O17
44	A	403	PGT	C36-C37-C38-C39
44	D	602	PGT	C32-C31-O2-C2
44	B	606	PGT	O11-C11-O3-C3
50	a	848	CLA	O1A-CGA-O2A-C1
44	A	403	PGT	O4P-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
44	z	313	PGT	O4P-C4-C5-C6
44	B	603	PGT	C12-C11-O3-C3
44	F	803	PGT	C12-C11-O3-C3
44	N	301	PGT	C12-C11-O3-C3
50	a	802	CLA	CBA-CGA-O2A-C1
50	a	812	CLA	CBA-CGA-O2A-C1
50	a	834	CLA	CBA-CGA-O2A-C1
50	a	837	CLA	CBA-CGA-O2A-C1
50	a	845	CLA	CBA-CGA-O2A-C1
50	a	846	CLA	CBA-CGA-O2A-C1
50	b	807	CLA	CBA-CGA-O2A-C1
50	b	809	CLA	CBA-CGA-O2A-C1
50	b	841	CLA	CBA-CGA-O2A-C1
50	b	849	CLA	CBA-CGA-O2A-C1
50	w	310	CLA	CBA-CGA-O2A-C1
50	b	845	CLA	C10-C11-C12-C13
51	a	804	DGD	O6E-C5E-C6E-O5E
50	b	814	CLA	CBD-CGD-O2D-CED
50	b	843	CLA	CBD-CGD-O2D-CED
46	F	802	LMG	C4-C5-C6-O5
46	B	605	LMG	C29-C30-C31-C32
50	z	303	CLA	O1D-CGD-O2D-CED
50	w	308	CLA	C4-C3-C5-C6
50	b	822	CLA	C2-C3-C5-C6
50	a	844	CLA	C3-C5-C6-C7
50	a	814	CLA	C6-C7-C8-C9
50	a	815	CLA	C14-C13-C15-C16
50	a	820	CLA	C11-C10-C8-C9
50	a	820	CLA	C14-C13-C15-C16
50	a	835	CLA	C6-C7-C8-C9
50	a	839	CLA	C11-C12-C13-C14
50	a	842	CLA	C14-C13-C15-C16
50	a	843	CLA	C14-C13-C15-C16
50	a	849	CLA	C11-C10-C8-C9
50	a	858	CLA	C11-C12-C13-C14
50	b	803	CLA	C14-C13-C15-C16
50	b	807	CLA	C11-C12-C13-C14
50	b	807	CLA	C14-C13-C15-C16
50	b	812	CLA	C11-C12-C13-C14
50	b	825	CLA	C11-C10-C8-C9
50	b	837	CLA	C11-C10-C8-C9
50	b	837	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
50	b	843	CLA	C11-C12-C13-C14
50	b	843	CLA	C14-C13-C15-C16
50	b	845	CLA	C6-C7-C8-C9
50	b	846	CLA	C11-C12-C13-C14
50	w	306	CLA	C6-C7-C8-C9
50	w	306	CLA	C11-C12-C13-C14
50	w	310	CLA	C14-C13-C15-C16
50	x	312	CLA	C11-C10-C8-C9
50	a	855	CLA	O1D-CGD-O2D-CED
50	b	844	CLA	O1D-CGD-O2D-CED
46	j	105	LMG	C2-C1-O1-C7
51	a	804	DGD	C2E-C1E-O5D-C6D
44	A	403	PGT	O4P-C4-C5-O5
44	B	601	PGT	O4P-C4-C5-O5
44	z	301	PGT	O4P-C4-C5-O5
50	y	307	CLA	O1D-CGD-O2D-CED
46	B	605	LMG	C4-C5-C6-O5
50	g	204	CLA	O1D-CGD-O2D-CED
43	4	101	BCR	C7-C8-C9-C34
43	4	101	BCR	C37-C22-C23-C24
43	a	829	BCR	C7-C8-C9-C34
43	a	831	BCR	C37-C22-C23-C24
43	b	818	BCR	C7-C8-C9-C34
43	b	819	BCR	C7-C8-C9-C34
43	b	831	BCR	C36-C18-C19-C20
43	b	831	BCR	C37-C22-C23-C24
43	g	202	BCR	C37-C22-C23-C24
43	i	101	BCR	C37-C22-C23-C24
43	j	101	BCR	C11-C12-C13-C35
43	j	103	BCR	C37-C22-C23-C24
43	l	302	BCR	C37-C22-C23-C24
43	x	314	BCR	C7-C8-C9-C34
43	y	301	BCR	C37-C22-C23-C24
55	x	321	LUT	C27-C28-C29-C39
55	z	320	LUT	C27-C28-C29-C39
43	4	101	BCR	C7-C8-C9-C10
43	a	829	BCR	C7-C8-C9-C10
43	b	831	BCR	C21-C22-C23-C24
43	g	202	BCR	C21-C22-C23-C24
43	j	103	BCR	C21-C22-C23-C24
43	l	302	BCR	C21-C22-C23-C24
55	x	321	LUT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
45	F	804	A1H1M	C18-C15-C16-O17
50	a	839	CLA	C2A-CAA-CBA-CGA
50	x	313	CLA	C2A-CAA-CBA-CGA
50	x	318	CLA	C2A-CAA-CBA-CGA
44	z	301	PGT	C31-C32-C33-C34
44	B	603	PGT	O11-C11-O3-C3
44	N	301	PGT	O11-C11-O3-C3
50	a	837	CLA	O1A-CGA-O2A-C1
50	l	306	CLA	O1A-CGA-O2A-C1
46	j	105	LMG	C29-C28-O8-C9
50	b	823	CLA	CBA-CGA-O2A-C1
50	a	801	CLA	C15-C16-C17-C18
46	z	314	LMG	C10-C11-C12-C13
50	x	308	CLA	O1D-CGD-O2D-CED
51	b	821	DGD	C4E-C5E-C6E-O5E
50	a	834	CLA	C15-C16-C17-C18
50	a	846	CLA	C15-C16-C17-C18
50	a	857	CLA	C5-C6-C7-C8
50	b	802	CLA	C10-C11-C12-C13
50	b	824	CLA	C8-C10-C11-C12
50	b	825	CLA	C10-C11-C12-C13
50	b	825	CLA	C15-C16-C17-C18
50	b	841	CLA	C5-C6-C7-C8
50	b	845	CLA	C15-C16-C17-C18
50	w	308	CLA	C10-C11-C12-C13
50	a	814	CLA	C11-C10-C8-C7
50	a	814	CLA	C12-C13-C15-C16
50	a	843	CLA	C11-C12-C13-C15
50	b	802	CLA	C12-C13-C15-C16
50	x	307	CLA	C11-C10-C8-C7
50	y	314	CLA	C11-C12-C13-C15
50	a	822	CLA	CBA-CGA-O2A-C1
50	a	843	CLA	C13-C15-C16-C17
50	b	846	CLA	C10-C11-C12-C13
46	H	401	LMG	C4-C5-C6-O5
44	A	403	PGT	C31-C32-C33-C34
46	7	301	LMG	C10-C11-C12-C13
43	x	314	BCR	C19-C20-C21-C22
50	l	306	CLA	C3-C5-C6-C7
50	x	312	CLA	C3-C5-C6-C7
50	y	313	CLA	C3-C5-C6-C7
50	a	815	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
50	b	815	CLA	C5-C6-C7-C8
50	b	828	CLA	C8-C10-C11-C12
50	w	310	CLA	C13-C15-C16-C17
50	x	307	CLA	C8-C10-C11-C12
44	B	601	PGT	C31-C32-C33-C34
44	B	603	PGT	C11-C12-C13-C14
44	b	830	PGT	C11-C12-C13-C14
44	z	313	PGT	C31-C32-C33-C34
46	x	315	LMG	C28-C29-C30-C31
51	x	317	DGD	C1B-C2B-C3B-C4B
50	a	811	CLA	O1A-CGA-O2A-C1
50	a	820	CLA	C5-C6-C7-C8
50	a	824	CLA	C5-C6-C7-C8
50	a	833	CLA	C10-C11-C12-C13
50	y	308	CLA	C10-C11-C12-C13
53	a	825	PQN	C18-C20-C21-C22
50	a	802	CLA	C2A-CAA-CBA-CGA
50	a	812	CLA	C2A-CAA-CBA-CGA
50	a	837	CLA	C2A-CAA-CBA-CGA
50	a	844	CLA	C2A-CAA-CBA-CGA
50	a	848	CLA	C2A-CAA-CBA-CGA
50	a	857	CLA	C2A-CAA-CBA-CGA
50	b	809	CLA	C2A-CAA-CBA-CGA
50	b	810	CLA	C2A-CAA-CBA-CGA
50	b	822	CLA	C2A-CAA-CBA-CGA
50	b	838	CLA	C2A-CAA-CBA-CGA
50	g	203	CLA	C2A-CAA-CBA-CGA
50	h	201	CLA	C2A-CAA-CBA-CGA
50	l	306	CLA	C2A-CAA-CBA-CGA
50	w	316	CLA	C2A-CAA-CBA-CGA
50	y	312	CLA	C2A-CAA-CBA-CGA
50	z	316	CLA	C2A-CAA-CBA-CGA
50	a	840	CLA	O1D-CGD-O2D-CED
50	a	819	CLA	C10-C11-C12-C13
50	a	820	CLA	C15-C16-C17-C18
50	a	836	CLA	C5-C6-C7-C8
50	a	853	CLA	C10-C11-C12-C13
50	a	856	CLA	C15-C16-C17-C18
50	b	807	CLA	C13-C15-C16-C17
50	b	837	CLA	C10-C11-C12-C13
50	b	842	CLA	C5-C6-C7-C8
46	j	104	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
46	j	105	LMG	O6-C5-C6-O5
44	z	301	PGT	C11-C12-C13-C14
44	F	803	PGT	O11-C11-O3-C3
50	a	819	CLA	O1A-CGA-O2A-C1
50	a	835	CLA	O1A-CGA-O2A-C1
50	a	844	CLA	O1A-CGA-O2A-C1
50	b	801	CLA	O1A-CGA-O2A-C1
51	b	821	DGD	O6E-C5E-C6E-O5E
46	D	601	LMG	C4-C5-C6-O5
50	a	811	CLA	C15-C16-C17-C18
50	a	812	CLA	C5-C6-C7-C8
50	a	814	CLA	C5-C6-C7-C8
50	a	814	CLA	C13-C15-C16-C17
50	a	833	CLA	C15-C16-C17-C18
50	a	836	CLA	C10-C11-C12-C13
50	a	837	CLA	C15-C16-C17-C18
50	a	849	CLA	C5-C6-C7-C8
50	a	857	CLA	C15-C16-C17-C18
50	a	858	CLA	C15-C16-C17-C18
50	b	815	CLA	C15-C16-C17-C18
50	b	824	CLA	C10-C11-C12-C13
50	b	837	CLA	C5-C6-C7-C8
50	b	840	CLA	C5-C6-C7-C8
50	b	840	CLA	C10-C11-C12-C13
50	b	840	CLA	C15-C16-C17-C18
50	b	843	CLA	C15-C16-C17-C18
50	l	306	CLA	C10-C11-C12-C13
50	w	306	CLA	C10-C11-C12-C13
50	w	308	CLA	C5-C6-C7-C8
53	a	825	PQN	C15-C16-C17-C18
51	b	821	DGD	C9B-CAB-CBB-CCB
45	5	302	A1H1M	C01-C02-C03-C04
50	b	842	CLA	C8-C10-C11-C12
44	b	829	PGT	C11-C12-C13-C14
50	a	836	CLA	C15-C16-C17-C18
50	b	809	CLA	C8-C10-C11-C12
50	b	839	CLA	C10-C11-C12-C13
50	w	310	CLA	C10-C11-C12-C13
44	D	602	PGT	O31-C31-O2-C2
50	x	309	CLA	O1D-CGD-O2D-CED
50	a	819	CLA	C8-C10-C11-C12
50	a	837	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
50	b	833	CLA	C5-C6-C7-C8
50	x	303	CLA	C5-C6-C7-C8
51	a	804	DGD	C9B-CAB-CBB-CCB
50	a	846	CLA	O1D-CGD-O2D-CED
50	a	856	CLA	O1D-CGD-O2D-CED
50	b	838	CLA	O1D-CGD-O2D-CED
51	x	317	DGD	C4D-C5D-C6D-O5D
50	a	846	CLA	C10-C11-C12-C13
50	b	803	CLA	C10-C11-C12-C13
50	b	833	CLA	C10-C11-C12-C13
50	w	308	CLA	C15-C16-C17-C18
50	a	820	CLA	CBA-CGA-O2A-C1
50	b	837	CLA	CBA-CGA-O2A-C1
50	f	301	CLA	CBA-CGA-O2A-C1
45	5	302	A1H1M	C18-C15-C16-O17
46	j	105	LMG	O10-C28-O8-C9
50	b	809	CLA	O1A-CGA-O2A-C1
50	y	310	CLA	C13-C15-C16-C17
50	b	825	CLA	C3-C5-C6-C7
43	a	803	BCR	C15-C16-C17-C18
50	b	812	CLA	C8-C10-C11-C12
50	x	312	CLA	C15-C16-C17-C18
51	a	804	DGD	CAA-CBA-CCA-CDA
44	z	301	PGT	O4P-C4-C5-C6
50	a	833	CLA	C2A-CAA-CBA-CGA
50	x	308	CLA	C2A-CAA-CBA-CGA
46	f	306	LMG	C29-C28-O8-C9
50	a	811	CLA	CBA-CGA-O2A-C1
50	b	803	CLA	CBA-CGA-O2A-C1
50	w	305	CLA	CBA-CGA-O2A-C1
50	a	820	CLA	C13-C15-C16-C17
50	a	842	CLA	C8-C10-C11-C12
50	a	846	CLA	C5-C6-C7-C8
50	a	850	CLA	C15-C16-C17-C18
50	b	824	CLA	C5-C6-C7-C8
50	b	836	CLA	C5-C6-C7-C8
50	b	836	CLA	C10-C11-C12-C13
50	b	839	CLA	C13-C15-C16-C17
50	w	306	CLA	C8-C10-C11-C12
50	w	308	CLA	C8-C10-C11-C12
50	x	306	CLA	C10-C11-C12-C13
50	y	308	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
51	x	317	DGD	O6D-C5D-C6D-O5D
50	a	821	CLA	C15-C16-C17-C18
50	b	837	CLA	C15-C16-C17-C18
50	b	840	CLA	C13-C15-C16-C17
50	x	312	CLA	C10-C11-C12-C13
50	y	313	CLA	C10-C11-C12-C13
53	b	827	PQN	C20-C21-C22-C23
50	b	841	CLA	O1D-CGD-O2D-CED
50	a	801	CLA	C13-C15-C16-C17
50	a	820	CLA	C8-C10-C11-C12
50	a	845	CLA	C8-C10-C11-C12
50	a	858	CLA	C10-C11-C12-C13
50	b	815	CLA	C13-C15-C16-C17
50	y	310	CLA	C10-C11-C12-C13
50	y	314	CLA	C10-C11-C12-C13
50	b	813	CLA	C2A-CAA-CBA-CGA
50	b	839	CLA	C4-C3-C5-C6
50	a	854	CLA	C10-C11-C12-C13
50	b	803	CLA	C15-C16-C17-C18
50	b	849	CLA	C1-C2-C3-C5
50	w	302	CLA	C1-C2-C3-C4
50	x	308	CLA	C1-C2-C3-C5
50	z	305	CLA	C1-C2-C3-C4
44	N	301	PGT	C32-C31-O2-C2
50	a	839	CLA	C14-C13-C15-C16
50	a	845	CLA	O1D-CGD-O2D-CED
44	N	301	PGT	O31-C31-O2-C2
50	b	805	CLA	C5-C6-C7-C8
50	b	814	CLA	C10-C11-C12-C13
50	a	833	CLA	C5-C6-C7-C8
43	j	101	BCR	C36-C18-C19-C20
43	k	202	BCR	C36-C18-C19-C20
43	l	303	BCR	C36-C18-C19-C20
43	l	304	BCR	C36-C18-C19-C20
43	z	318	BCR	C11-C12-C13-C35
43	j	101	BCR	C17-C18-C19-C20
43	z	318	BCR	C11-C12-C13-C14
46	f	306	LMG	O10-C28-O8-C9
50	a	815	CLA	C2A-CAA-CBA-CGA
50	b	832	CLA	C2A-CAA-CBA-CGA
50	w	308	CLA	C2A-CAA-CBA-CGA
50	y	303	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
50	a	843	CLA	C15-C16-C17-C18
50	a	854	CLA	C15-C16-C17-C18
53	a	825	PQN	C23-C25-C26-C27
44	L	201	PGT	C11-C12-C13-C14
51	a	804	DGD	C1A-C2A-C3A-C4A
54	x	305	CHL	O1D-CGD-O2D-CED
45	F	804	A1H1M	O21-C20-O19-C18
50	a	814	CLA	C16-C17-C18-C19
50	a	819	CLA	C11-C12-C13-C14
50	a	842	CLA	C16-C17-C18-C20
50	a	843	CLA	C16-C17-C18-C19
50	a	843	CLA	C16-C17-C18-C20
50	b	826	CLA	C6-C7-C8-C9
50	b	828	CLA	C11-C12-C13-C14
50	y	313	CLA	C16-C17-C18-C19
50	z	302	CLA	C6-C7-C8-C9
50	b	807	CLA	C10-C11-C12-C13
52	a	808	CL0	CAA-CBA-CGA-O2A
50	a	847	CLA	CMA-C3A-C4A-CHB
50	b	846	CLA	O1D-CGD-O2D-CED
54	x	319	CHL	O1D-CGD-O2D-CED
50	b	844	CLA	C15-C16-C17-C18
50	a	814	CLA	C16-C17-C18-C20
50	b	825	CLA	C16-C17-C18-C20
50	b	828	CLA	C11-C12-C13-C15
50	y	313	CLA	C16-C17-C18-C20
50	z	302	CLA	C6-C7-C8-C10
50	z	307	CLA	C11-C12-C13-C14
50	b	849	CLA	O1A-CGA-O2A-C1
44	L	201	PGT	C38-C39-C40-C41
44	z	301	PGT	C35-C36-C37-C38
50	x	316	CLA	O1D-CGD-O2D-CED
50	a	838	CLA	CBA-CGA-O2A-C1
44	5	301	PGT	C37-C38-C39-C40
44	A	403	PGT	C34-C35-C36-C37
44	z	317	PGT	C15-C16-C17-C18
50	b	835	CLA	C10-C11-C12-C13
52	a	808	CL0	C2-C1-O2A-CGA
50	w	314	CLA	C2A-CAA-CBA-CGA
50	w	308	CLA	O1D-CGD-O2D-CED
50	y	303	CLA	O1D-CGD-O2D-CED
50	a	834	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
50	a	813	CLA	C4B-C3B-CAB-CBB
50	a	815	CLA	C4B-C3B-CAB-CBB
50	a	822	CLA	C4B-C3B-CAB-CBB
50	a	824	CLA	C4B-C3B-CAB-CBB
50	b	849	CLA	C4B-C3B-CAB-CBB
44	A	402	PGT	C31-C32-C33-C34
50	a	839	CLA	C16-C17-C18-C19
50	a	842	CLA	C16-C17-C18-C19
50	a	845	CLA	C16-C17-C18-C19
50	b	825	CLA	C16-C17-C18-C19
50	b	826	CLA	C6-C7-C8-C10
50	a	818	CLA	O1D-CGD-O2D-CED
50	a	858	CLA	C2A-CAA-CBA-CGA
50	w	302	CLA	C2A-CAA-CBA-CGA
51	a	804	DGD	C8A-C9A-CAA-CBA
50	b	846	CLA	C8-C10-C11-C12
44	a	805	PGT	C32-C31-O2-C2
46	x	315	LMG	C11-C10-O7-C8
50	a	821	CLA	C10-C11-C12-C13
50	a	812	CLA	C11-C12-C13-C15
51	a	804	DGD	CAB-CBB-CCB-CDB
50	a	819	CLA	CBA-CGA-O2A-C1
53	a	825	PQN	C20-C21-C22-C23
46	f	306	LMG	C11-C12-C13-C14
50	a	836	CLA	C3A-C2A-CAA-CBA
50	b	802	CLA	C3A-C2A-CAA-CBA
50	b	805	CLA	C3A-C2A-CAA-CBA
50	b	808	CLA	C3A-C2A-CAA-CBA
50	b	823	CLA	C3A-C2A-CAA-CBA
50	b	834	CLA	C3A-C2A-CAA-CBA
50	b	839	CLA	C3A-C2A-CAA-CBA
50	b	840	CLA	C3A-C2A-CAA-CBA
50	b	844	CLA	C3A-C2A-CAA-CBA
50	b	849	CLA	C3A-C2A-CAA-CBA
50	f	301	CLA	C3A-C2A-CAA-CBA
50	g	204	CLA	C3A-C2A-CAA-CBA
50	x	304	CLA	C3A-C2A-CAA-CBA
50	x	318	CLA	C3A-C2A-CAA-CBA
50	y	311	CLA	C3A-C2A-CAA-CBA
50	z	302	CLA	C3A-C2A-CAA-CBA
54	w	311	CHL	C3A-C2A-CAA-CBA
50	a	847	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
43	a	827	BCR	C21-C22-C23-C24
50	a	847	CLA	CBD-CGD-O2D-CED
45	F	804	A1H1M	C37-C07-C08-C09
45	F	804	A1H1M	C37-C07-C08-C36
54	z	312	CHL	C8-C10-C11-C12
50	y	310	CLA	O1D-CGD-O2D-CED
50	a	839	CLA	C16-C17-C18-C20
50	a	845	CLA	C16-C17-C18-C20
44	B	601	PGT	O4P-C4-C5-C6
44	z	317	PGT	O4P-C4-C5-C6
50	a	802	CLA	O1D-CGD-O2D-CED
51	x	317	DGD	O1G-C1G-C2G-C3G
44	z	317	PGT	C17-C18-C19-C20
46	H	401	LMG	C30-C31-C32-C33
46	w	312	LMG	C29-C30-C31-C32
50	w	308	CLA	C3-C5-C6-C7
46	j	105	LMG	C10-C11-C12-C13
50	b	805	CLA	C15-C16-C17-C18
44	A	403	PGT	C35-C36-C37-C38
44	L	201	PGT	C13-C14-C15-C16
44	f	305	PGT	C34-C35-C36-C37
50	b	807	CLA	O1A-CGA-O2A-C1
46	w	312	LMG	C15-C16-C17-C18
50	x	312	CLA	C2C-C3C-CAC-CBC
51	a	804	DGD	C4E-C5E-C6E-O5E
51	b	821	DGD	CEB-CFB-CGB-CHB
43	4	101	BCR	C1-C6-C7-C8
43	4	101	BCR	C23-C24-C25-C26
43	a	803	BCR	C1-C6-C7-C8
43	a	810	BCR	C5-C6-C7-C8
43	b	816	BCR	C5-C6-C7-C8
43	i	101	BCR	C23-C24-C25-C30
43	j	103	BCR	C23-C24-C25-C30
43	l	302	BCR	C23-C24-C25-C30
43	l	303	BCR	C5-C6-C7-C8
43	w	301	BCR	C23-C24-C25-C26
43	x	314	BCR	C1-C6-C7-C8
43	x	314	BCR	C23-C24-C25-C30
43	y	301	BCR	C1-C6-C7-C8
50	a	813	CLA	C2B-C3B-CAB-CBB
50	a	815	CLA	C2B-C3B-CAB-CBB
50	a	824	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
50	a	835	CLA	C2B-C3B-CAB-CBB
50	a	858	CLA	C2B-C3B-CAB-CBB
50	b	807	CLA	C2B-C3B-CAB-CBB
50	b	822	CLA	C2B-C3B-CAB-CBB
55	z	320	LUT	C1-C6-C7-C8
55	z	320	LUT	C5-C6-C7-C8
50	b	832	CLA	CBD-CGD-O2D-CED
50	h	201	CLA	O1A-CGA-O2A-C1
51	x	317	DGD	C2A-C1A-O1G-C1G
50	b	843	CLA	C3-C5-C6-C7
50	z	319	CLA	O1D-CGD-O2D-CED
44	b	830	PGT	C35-C36-C37-C38
46	D	601	LMG	C30-C31-C32-C33
50	a	818	CLA	C2A-CAA-CBA-CGA
50	x	312	CLA	C2A-CAA-CBA-CGA
50	y	311	CLA	C2A-CAA-CBA-CGA
50	a	814	CLA	C8-C10-C11-C12
50	b	805	CLA	C10-C11-C12-C13
46	B	605	LMG	C32-C33-C34-C35
51	a	804	DGD	C3A-C4A-C5A-C6A
44	a	805	PGT	O31-C31-O2-C2
50	a	811	CLA	C4-C3-C5-C6
50	b	824	CLA	C4-C3-C5-C6
53	b	827	PQN	C14-C13-C15-C16
52	a	808	CL0	C16-C17-C18-C19
44	a	807	PGT	C32-C33-C34-C35
50	z	307	CLA	O1D-CGD-O2D-CED
46	H	401	LMG	C29-C28-O8-C9
50	a	835	CLA	CBA-CGA-O2A-C1
50	b	801	CLA	CBA-CGA-O2A-C1
50	a	845	CLA	C11-C10-C8-C9
50	b	815	CLA	C14-C13-C15-C16
50	b	825	CLA	C11-C12-C13-C14
44	A	402	PGT	C12-C13-C14-C15
44	A	404	PGT	C16-C17-C18-C19
46	x	315	LMG	C31-C32-C33-C34
50	b	828	CLA	C5-C6-C7-C8
50	y	302	CLA	C5-C6-C7-C8
50	b	811	CLA	O1D-CGD-O2D-CED
44	B	606	PGT	C13-C14-C15-C16
46	B	605	LMG	C2-C1-O1-C7
46	j	104	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
48	B	604	SQD	C2-C1-O6-C44
48	a	859	SQD	C2-C1-O6-C44
51	a	804	DGD	C4B-C5B-C6B-C7B
50	b	809	CLA	C10-C11-C12-C13
50	a	815	CLA	C16-C17-C18-C19
50	b	801	CLA	C16-C17-C18-C20
44	w	313	PGT	C32-C31-O2-C2
46	z	314	LMG	C11-C10-O7-C8
51	a	804	DGD	C2B-C1B-O2G-C2G
44	w	313	PGT	O31-C31-O2-C2
46	x	315	LMG	O9-C10-O7-C8
50	a	838	CLA	C8-C10-C11-C12
50	a	838	CLA	C10-C11-C12-C13
50	b	839	CLA	C8-C10-C11-C12
50	b	847	CLA	C10-C11-C12-C13
55	w	320	LUT	C7-C8-C9-C19
44	A	402	PGT	C11-C12-C13-C14
50	a	821	CLA	C3-C5-C6-C7
46	7	301	LMG	C8-C7-O1-C1
50	a	838	CLA	C13-C15-C16-C17
50	b	844	CLA	C2A-CAA-CBA-CGA
50	a	815	CLA	C16-C17-C18-C20
52	a	808	CL0	C16-C17-C18-C20
50	a	857	CLA	C4-C3-C5-C6
50	b	845	CLA	C4-C3-C5-C6
46	H	401	LMG	C29-C30-C31-C32
51	a	804	DGD	C5B-C6B-C7B-C8B
50	b	808	CLA	O1D-CGD-O2D-CED
50	a	846	CLA	C13-C15-C16-C17
50	b	825	CLA	C13-C15-C16-C17
50	b	835	CLA	C8-C10-C11-C12
50	b	844	CLA	C8-C10-C11-C12
51	b	821	DGD	C6B-C7B-C8B-C9B
50	a	801	CLA	C10-C11-C12-C13
50	a	811	CLA	C8-C10-C11-C12
50	a	849	CLA	C10-C11-C12-C13
50	a	854	CLA	C13-C15-C16-C17
50	b	828	CLA	C10-C11-C12-C13
44	z	313	PGT	C11-C12-C13-C14
46	z	314	LMG	O9-C10-O7-C8
51	a	804	DGD	O1B-C1B-O2G-C2G
45	5	302	A1H1M	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
44	B	603	PGT	O3P-C1-C2-O2
50	b	843	CLA	C13-C15-C16-C17
50	l	306	CLA	C5-C6-C7-C8
50	a	818	CLA	C10-C11-C12-C13
50	b	805	CLA	C8-C10-C11-C12
51	x	317	DGD	C5A-C6A-C7A-C8A
44	D	602	PGT	C12-C13-C14-C15
44	D	602	PGT	C13-C14-C15-C16
46	j	104	LMG	C29-C30-C31-C32
50	a	853	CLA	C15-C16-C17-C18
46	x	315	LMG	C29-C30-C31-C32
50	b	842	CLA	C4-C3-C5-C6
50	f	301	CLA	C2-C3-C5-C6
44	w	313	PGT	C15-C16-C17-C18
50	a	809	CLA	C2A-CAA-CBA-CGA
50	a	845	CLA	C2A-CAA-CBA-CGA
50	a	853	CLA	C2A-CAA-CBA-CGA
50	b	805	CLA	C2A-CAA-CBA-CGA
50	w	310	CLA	C2A-CAA-CBA-CGA
50	f	302	CLA	O1D-CGD-O2D-CED
50	z	306	CLA	CBA-CGA-O2A-C1
50	w	310	CLA	C15-C16-C17-C18
46	H	401	LMG	C11-C10-O7-C8
44	A	403	PGT	C14-C15-C16-C17
44	b	830	PGT	C36-C37-C38-C39
51	b	821	DGD	C6A-C7A-C8A-C9A
51	x	317	DGD	O1A-C1A-O1G-C1G
46	B	605	LMG	C31-C32-C33-C34
50	a	818	CLA	C1A-C2A-CAA-CBA
50	a	826	CLA	C1A-C2A-CAA-CBA
50	a	833	CLA	C1A-C2A-CAA-CBA
50	a	836	CLA	C1A-C2A-CAA-CBA
50	a	838	CLA	C1A-C2A-CAA-CBA
50	a	852	CLA	C1A-C2A-CAA-CBA
50	b	805	CLA	C1A-C2A-CAA-CBA
50	b	808	CLA	C1A-C2A-CAA-CBA
50	b	834	CLA	C1A-C2A-CAA-CBA
50	b	835	CLA	C1A-C2A-CAA-CBA
50	b	837	CLA	C1A-C2A-CAA-CBA
50	b	838	CLA	C1A-C2A-CAA-CBA
50	b	840	CLA	C1A-C2A-CAA-CBA
50	b	846	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
50	g	204	CLA	C1A-C2A-CAA-CBA
50	h	201	CLA	C1A-C2A-CAA-CBA
50	w	303	CLA	C1A-C2A-CAA-CBA
50	w	305	CLA	C1A-C2A-CAA-CBA
50	w	308	CLA	C1A-C2A-CAA-CBA
50	x	304	CLA	C1A-C2A-CAA-CBA
50	x	310	CLA	C1A-C2A-CAA-CBA
50	x	312	CLA	C1A-C2A-CAA-CBA
50	y	305	CLA	C1A-C2A-CAA-CBA
50	z	302	CLA	C1A-C2A-CAA-CBA
50	z	305	CLA	C1A-C2A-CAA-CBA
50	a	821	CLA	C11-C12-C13-C15
50	b	824	CLA	O1A-CGA-O2A-C1
50	z	302	CLA	O1A-CGA-O2A-C1
44	b	830	PGT	C37-C38-C39-C40
44	A	403	PGT	O3P-C1-C2-C3
44	D	602	PGT	O3P-C1-C2-C3
44	B	603	PGT	C35-C36-C37-C38
50	a	858	CLA	C11-C10-C8-C7
50	b	803	CLA	C11-C12-C13-C15
50	b	807	CLA	C11-C10-C8-C7
50	b	814	CLA	C11-C10-C8-C7
50	b	839	CLA	C6-C7-C8-C10
50	b	845	CLA	C11-C12-C13-C15
50	b	845	CLA	C12-C13-C15-C16
50	k	204	CLA	C11-C10-C8-C7
50	y	313	CLA	C6-C7-C8-C10
50	w	305	CLA	O1A-CGA-O2A-C1
54	x	319	CHL	O1A-CGA-O2A-C1
50	y	309	CLA	C3A-C2A-CAA-CBA
50	b	814	CLA	C8-C10-C11-C12
50	b	824	CLA	C15-C16-C17-C18
50	b	843	CLA	C8-C10-C11-C12
50	a	814	CLA	C4-C3-C5-C6
50	a	836	CLA	C4-C3-C5-C6
46	H	401	LMG	O10-C28-O8-C9
50	y	314	CLA	C13-C15-C16-C17
50	a	856	CLA	C2A-CAA-CBA-CGA
50	a	834	CLA	C11-C12-C13-C14
50	a	842	CLA	C11-C12-C13-C14
50	a	845	CLA	C14-C13-C15-C16
50	b	801	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
50	b	839	CLA	C6-C7-C8-C9
50	b	839	CLA	C11-C10-C8-C9
50	b	842	CLA	C6-C7-C8-C9
50	b	843	CLA	C6-C7-C8-C9
50	b	845	CLA	C11-C12-C13-C14
50	b	846	CLA	C6-C7-C8-C9
50	x	307	CLA	C11-C10-C8-C9
50	y	308	CLA	C6-C7-C8-C9
50	y	313	CLA	C6-C7-C8-C9
50	z	311	CLA	CBA-CGA-O2A-C1
50	x	307	CLA	O1D-CGD-O2D-CED
50	z	311	CLA	O1D-CGD-O2D-CED
44	f	305	PGT	C35-C36-C37-C38
44	z	317	PGT	C16-C17-C18-C19
46	w	312	LMG	C2-C1-O1-C7
48	F	801	SQD	C2-C1-O6-C44
51	x	317	DGD	C2D-C1D-O3G-C3G
50	y	310	CLA	C15-C16-C17-C18
46	z	314	LMG	C7-C8-C9-O8
48	w	317	SQD	O6-C44-C45-C46
51	a	804	DGD	C1G-C2G-C3G-O3G
46	w	312	LMG	C31-C32-C33-C34
51	x	317	DGD	C3B-C4B-C5B-C6B
46	D	601	LMG	C13-C14-C15-C16
54	w	304	CHL	CHA-CBD-CGD-O2D
54	x	305	CHL	CHA-CBD-CGD-O1D
44	5	301	PGT	C39-C40-C41-C42
46	z	314	LMG	C30-C31-C32-C33
44	N	301	PGT	C11-C12-C13-C14
50	b	814	CLA	C4-C3-C5-C6
50	a	811	CLA	C2-C3-C5-C6
54	z	312	CHL	C2-C3-C5-C6
50	b	826	CLA	C5-C6-C7-C8
43	a	830	BCR	C36-C18-C19-C20
44	z	317	PGT	C34-C35-C36-C37
43	z	318	BCR	C21-C22-C23-C24
50	a	820	CLA	C10-C11-C12-C13
50	a	823	CLA	C2A-CAA-CBA-CGA
46	x	315	LMG	C34-C35-C36-C37
44	A	403	PGT	C11-C12-C13-C14
50	b	833	CLA	O1A-CGA-O2A-C1
50	a	813	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
44	B	606	PGT	C3-C2-O2-C31
50	a	801	CLA	O2A-C1-C2-C3
50	a	819	CLA	O2A-C1-C2-C3
50	a	842	CLA	O2A-C1-C2-C3
50	a	857	CLA	O2A-C1-C2-C3
50	b	802	CLA	O2A-C1-C2-C3
50	b	809	CLA	O2A-C1-C2-C3
50	b	844	CLA	O2A-C1-C2-C3
50	x	307	CLA	C5-C6-C7-C8
44	A	404	PGT	C36-C37-C38-C39
44	z	317	PGT	C12-C13-C14-C15
46	7	301	LMG	C31-C32-C33-C34
48	j	106	SQD	C33-C34-C35-C36
51	a	804	DGD	CBA-CCA-CDA-CEA
51	a	804	DGD	CEB-CFB-CGB-CHB
51	b	821	DGD	C4B-C5B-C6B-C7B
54	x	311	CHL	C3C-C2C-CMC-OMC
54	z	304	CHL	C3C-C2C-CMC-OMC
50	a	841	CLA	C3-C5-C6-C7
44	A	402	PGT	O3P-C1-C2-O2
44	a	805	PGT	O3P-C1-C2-O2
50	b	807	CLA	C8-C10-C11-C12
54	w	311	CHL	C2-C1-O2A-CGA
50	b	822	CLA	C10-C11-C12-C13
46	z	314	LMG	C33-C34-C35-C36
50	b	838	CLA	C4-C3-C5-C6
50	b	840	CLA	C4-C3-C5-C6
50	b	814	CLA	C2-C3-C5-C6
44	A	401	PGT	C35-C36-C37-C38
44	b	830	PGT	C15-C16-C17-C18
44	B	606	PGT	O2-C2-C3-O3
46	D	601	LMG	O7-C8-C9-O8
46	z	314	LMG	O1-C7-C8-O7
46	z	315	LMG	O7-C8-C9-O8
44	b	830	PGT	O4P-C4-C5-O5
46	j	104	LMG	C30-C31-C32-C33
45	F	804	A1H1M	C29-C20-O19-C18
50	b	837	CLA	O1A-CGA-O2A-C1
51	x	317	DGD	C4B-C5B-C6B-C7B
48	F	805	SQD	O47-C7-C8-C9
48	a	859	SQD	O47-C7-C8-C9
48	w	317	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
50	b	840	CLA	C2A-CAA-CBA-CGA
50	a	851	CLA	O1D-CGD-O2D-CED
44	a	807	PGT	C42-C43-C44-C45
44	a	807	PGT	C38-C39-C40-C41
50	y	313	CLA	CBA-CGA-O2A-C1
46	z	315	LMG	C30-C31-C32-C33
44	A	402	PGT	C32-C33-C34-C35
50	b	844	CLA	C3-C5-C6-C7
46	z	314	LMG	C34-C35-C36-C37
44	b	830	PGT	C32-C33-C34-C35
44	a	806	PGT	C16-C17-C18-C19
50	a	837	CLA	C8-C10-C11-C12
53	b	827	PQN	C18-C20-C21-C22
46	B	605	LMG	O8-C28-C29-C30
50	a	836	CLA	C2-C3-C5-C6
50	a	844	CLA	CBA-CGA-O2A-C1
50	b	839	CLA	CBA-CGA-O2A-C1
51	b	821	DGD	CFB-CGB-CHB-CIB
46	z	314	LMG	C13-C14-C15-C16
50	a	812	CLA	C11-C10-C8-C9
50	a	812	CLA	C11-C12-C13-C14
50	a	824	CLA	C11-C12-C13-C14
50	a	857	CLA	C14-C13-C15-C16
50	b	801	CLA	C11-C10-C8-C9
50	b	802	CLA	C6-C7-C8-C9
50	b	802	CLA	C14-C13-C15-C16
50	b	807	CLA	C11-C10-C8-C9
50	b	814	CLA	C11-C10-C8-C9
50	b	833	CLA	C11-C10-C8-C9
50	b	835	CLA	C11-C10-C8-C9
50	k	204	CLA	C11-C10-C8-C9
46	j	105	LMG	C12-C13-C14-C15
50	a	818	CLA	C5-C6-C7-C8
44	I	203	PGT	C5-C4-O4P-P
50	y	311	CLA	C4B-C3B-CAB-CBB
51	a	804	DGD	CFA-CGA-CHA-CIA
50	a	826	CLA	C2A-CAA-CBA-CGA
50	b	815	CLA	C2A-CAA-CBA-CGA
50	b	825	CLA	C2A-CAA-CBA-CGA
44	b	829	PGT	C12-C13-C14-C15
51	x	317	DGD	C7A-C8A-C9A-CAA
44	B	606	PGT	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
44	z	317	PGT	C14-C15-C16-C17
46	w	312	LMG	C34-C35-C36-C37
50	a	811	CLA	C6-C7-C8-C10
50	a	812	CLA	C11-C10-C8-C7
50	a	820	CLA	C12-C13-C15-C16
50	a	834	CLA	C11-C12-C13-C15
50	a	842	CLA	C11-C12-C13-C15
50	a	845	CLA	C12-C13-C15-C16
50	a	849	CLA	C11-C10-C8-C7
50	a	850	CLA	C11-C10-C8-C7
50	a	857	CLA	C12-C13-C15-C16
50	b	801	CLA	C11-C10-C8-C7
50	b	805	CLA	C11-C12-C13-C15
50	b	805	CLA	C12-C13-C15-C16
50	b	812	CLA	C11-C10-C8-C7
50	b	824	CLA	C11-C12-C13-C15
50	b	825	CLA	C11-C10-C8-C7
50	b	833	CLA	C11-C10-C8-C7
50	b	833	CLA	C11-C12-C13-C15
50	b	835	CLA	C11-C10-C8-C7
50	b	836	CLA	C11-C12-C13-C15
50	b	836	CLA	C12-C13-C15-C16
50	b	839	CLA	C11-C12-C13-C15
50	b	842	CLA	C6-C7-C8-C10
50	b	842	CLA	C11-C10-C8-C7
50	b	843	CLA	C6-C7-C8-C10
50	b	846	CLA	C6-C7-C8-C10
50	b	846	CLA	C11-C12-C13-C15
50	b	846	CLA	C12-C13-C15-C16
50	x	312	CLA	C11-C12-C13-C15
50	y	310	CLA	C12-C13-C15-C16
50	b	807	CLA	C15-C16-C17-C18
50	a	822	CLA	O1A-CGA-O2A-C1
50	y	314	CLA	C5-C6-C7-C8
45	F	804	A1H1M	C35-C11-O12-C13
44	B	602	PGT	C12-C13-C14-C15
44	D	602	PGT	C16-C17-C18-C19
50	a	813	CLA	C4-C3-C5-C6
50	a	848	CLA	C3A-C2A-CAA-CBA
50	b	809	CLA	C3A-C2A-CAA-CBA
50	b	841	CLA	C3A-C2A-CAA-CBA
50	y	313	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
54	z	312	CHL	C4-C3-C5-C6
50	a	813	CLA	C2-C3-C5-C6
53	b	827	PQN	C12-C13-C15-C16
50	x	312	CLA	C4C-C3C-CAC-CBC
46	B	605	LMG	O6-C1-O1-C7
51	b	821	DGD	CCB-CDB-CEB-CFB
43	a	810	BCR	C19-C20-C21-C22
43	k	201	BCR	C19-C20-C21-C22
43	z	318	BCR	C9-C10-C11-C12
50	b	801	CLA	C16-C17-C18-C19
55	w	319	LUT	C11-C12-C13-C20
51	a	804	DGD	CFB-CGB-CHB-CIB
43	k	202	BCR	C17-C18-C19-C20
44	B	601	PGT	C11-C12-C13-C14
44	B	606	PGT	O4P-C4-C5-C6
44	I	203	PGT	C1-C2-C3-O3
46	B	605	LMG	O1-C7-C8-C9
46	B	605	LMG	C7-C8-C9-O8
46	j	104	LMG	O1-C7-C8-C9
48	B	604	SQD	O6-C44-C45-C46
48	j	106	SQD	O6-C44-C45-C46
51	b	821	DGD	O1G-C1G-C2G-C3G
50	b	842	CLA	C3-C5-C6-C7
44	B	602	PGT	C11-C12-C13-C14
50	b	842	CLA	C1-C2-C3-C4
46	j	105	LMG	C32-C33-C34-C35
50	f	301	CLA	C4-C3-C5-C6
50	a	846	CLA	O1A-CGA-O2A-C1
44	A	403	PGT	O3P-C1-C2-O2
44	B	606	PGT	O3P-C1-C2-O2
43	a	830	BCR	C23-C24-C25-C30
43	l	304	BCR	C1-C6-C7-C8
43	l	304	BCR	C5-C6-C7-C8
50	y	311	CLA	C2B-C3B-CAB-CBB
44	b	830	PGT	C32-C31-O2-C2
51	b	821	DGD	CAB-CBB-CCB-CDB
44	b	829	PGT	C2-C1-O3P-P
44	z	313	PGT	C2-C1-O3P-P
48	j	106	SQD	C30-C31-C32-C33
50	a	834	CLA	C8-C10-C11-C12
50	b	846	CLA	C15-C16-C17-C18
44	b	829	PGT	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
51	x	317	DGD	C6A-C7A-C8A-C9A
50	a	819	CLA	C11-C12-C13-C15
46	B	605	LMG	O7-C8-C9-O8
46	f	306	LMG	O7-C8-C9-O8
46	j	104	LMG	O1-C7-C8-O7
46	w	312	LMG	O7-C8-C9-O8
46	x	315	LMG	O7-C8-C9-O8
48	w	317	SQD	O6-C44-C45-O47
51	x	317	DGD	O1G-C1G-C2G-O2G
46	j	105	LMG	C11-C12-C13-C14
46	j	105	LMG	C29-C30-C31-C32
44	b	829	PGT	C32-C33-C34-C35
50	a	835	CLA	C10-C11-C12-C13
50	a	812	CLA	C12-C13-C15-C16
44	5	301	PGT	C31-C32-C33-C34
44	f	305	PGT	C31-C32-C33-C34
46	7	301	LMG	C28-C29-C30-C31
50	b	844	CLA	O1A-CGA-O2A-C1
50	b	805	CLA	C2-C3-C5-C6
50	b	833	CLA	C2-C3-C5-C6
50	x	306	CLA	C2-C3-C5-C6
50	y	314	CLA	C2-C3-C5-C6
44	A	403	PGT	C39-C40-C41-C42
50	a	813	CLA	C1-C2-C3-C5
50	a	815	CLA	C1-C2-C3-C5
50	a	818	CLA	C1-C2-C3-C5
50	a	821	CLA	C1-C2-C3-C5
50	a	822	CLA	C1-C2-C3-C5
50	a	823	CLA	C1-C2-C3-C5
50	a	858	CLA	C1-C2-C3-C5
50	b	807	CLA	C1-C2-C3-C5
50	b	814	CLA	C1-C2-C3-C5
50	b	823	CLA	C1-C2-C3-C5
50	b	826	CLA	C1-C2-C3-C5
50	b	832	CLA	C1-C2-C3-C5
50	b	836	CLA	C1-C2-C3-C5
50	b	837	CLA	C1-C2-C3-C5
50	b	838	CLA	C1-C2-C3-C5
50	b	845	CLA	C1-C2-C3-C5
50	w	306	CLA	C1-C2-C3-C5
50	x	312	CLA	C1-C2-C3-C5
50	z	302	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
50	b	824	CLA	C3-C5-C6-C7
50	a	811	CLA	C6-C7-C8-C9
50	a	814	CLA	C14-C13-C15-C16
50	a	838	CLA	C11-C10-C8-C9
50	a	858	CLA	C11-C10-C8-C9
50	b	805	CLA	C14-C13-C15-C16
50	b	839	CLA	C11-C12-C13-C14
50	b	844	CLA	C6-C7-C8-C9
50	b	846	CLA	C14-C13-C15-C16
50	y	310	CLA	C14-C13-C15-C16
45	5	302	A1H1M	C02-C03-C04-C38
50	g	201	CLA	O2A-C1-C2-C3
50	a	811	CLA	C10-C11-C12-C13
44	a	806	PGT	C15-C16-C17-C18
50	b	809	CLA	C5-C6-C7-C8
44	N	301	PGT	C12-C13-C14-C15
44	B	601	PGT	C14-C15-C16-C17
46	x	315	LMG	C17-C18-C19-C20
50	b	806	CLA	C2-C3-C5-C6
50	a	850	CLA	C16-C17-C18-C20
51	a	804	DGD	C6B-C7B-C8B-C9B
50	b	845	CLA	C5-C6-C7-C8
46	H	401	LMG	O9-C10-O7-C8
50	a	836	CLA	CBA-CGA-O2A-C1
50	a	824	CLA	C10-C11-C12-C13
50	b	802	CLA	C15-C16-C17-C18
50	b	845	CLA	C8-C10-C11-C12
44	N	301	PGT	O3P-C1-C2-C3
50	z	307	CLA	C11-C12-C13-C15
43	b	817	BCR	C37-C22-C23-C24
43	z	318	BCR	C37-C22-C23-C24
55	x	320	LUT	C11-C12-C13-C20
50	a	838	CLA	C11-C10-C8-C7
50	a	839	CLA	C11-C12-C13-C15
50	a	842	CLA	C11-C10-C8-C7
50	a	846	CLA	C11-C10-C8-C7
50	a	846	CLA	C12-C13-C15-C16
50	a	858	CLA	C12-C13-C15-C16
50	b	801	CLA	C6-C7-C8-C10
50	b	802	CLA	C6-C7-C8-C10
50	b	844	CLA	C6-C7-C8-C10
50	b	844	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
50	w	308	CLA	C12-C13-C15-C16
50	y	308	CLA	C12-C13-C15-C16
53	a	825	PQN	C21-C22-C23-C25
45	F	804	A1H1M	C01-C02-C03-C04
50	b	801	CLA	C10-C11-C12-C13
50	b	833	CLA	C8-C10-C11-C12
43	a	830	BCR	C17-C18-C19-C20
43	l	303	BCR	C17-C18-C19-C20
43	l	304	BCR	C17-C18-C19-C20
44	I	203	PGT	C43-C44-C45-C46
50	a	802	CLA	C5-C6-C7-C8
50	a	842	CLA	C2A-CAA-CBA-CGA
50	b	811	CLA	C2A-CAA-CBA-CGA
50	b	802	CLA	C16-C17-C18-C19
50	w	310	CLA	CAA-CBA-CGA-O2A
50	b	803	CLA	O1A-CGA-O2A-C1
50	g	203	CLA	C2-C3-C5-C6
50	a	824	CLA	C3-C5-C6-C7
50	y	302	CLA	C3-C5-C6-C7
45	5	302	A1H1M	C37-C07-C08-C36
50	a	812	CLA	O2A-C1-C2-C3
50	b	803	CLA	O2A-C1-C2-C3
50	b	822	CLA	O2A-C1-C2-C3
50	b	826	CLA	O2A-C1-C2-C3
50	a	858	CLA	C16-C17-C18-C19
50	y	308	CLA	C16-C17-C18-C20
44	z	313	PGT	C33-C34-C35-C36
51	x	317	DGD	C4A-C5A-C6A-C7A
44	L	201	PGT	O3P-C1-C2-O2
46	j	104	LMG	O6-C1-O1-C7
44	a	807	PGT	C35-C36-C37-C38
44	B	606	PGT	C1-C2-C3-O3
44	w	313	PGT	C1-C2-C3-O3
46	7	301	LMG	C7-C8-C9-O8
46	f	306	LMG	C7-C8-C9-O8
46	w	312	LMG	C7-C8-C9-O8
46	x	315	LMG	C7-C8-C9-O8
46	z	314	LMG	O1-C7-C8-C9
51	b	821	DGD	C1G-C2G-C3G-O3G
46	F	802	LMG	C11-C10-O7-C8
50	w	307	CLA	C2C-C3C-CAC-CBC
50	b	806	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
46	7	301	LMG	O7-C8-C9-O8
46	j	105	LMG	O1-C7-C8-O7
46	w	312	LMG	O1-C7-C8-O7
48	B	604	SQD	O6-C44-C45-O47
50	a	814	CLA	C11-C10-C8-C9
50	a	842	CLA	C11-C10-C8-C9
50	b	801	CLA	C6-C7-C8-C9
50	b	805	CLA	C11-C12-C13-C14
50	b	836	CLA	C14-C13-C15-C16
50	w	306	CLA	C14-C13-C15-C16
50	y	308	CLA	C14-C13-C15-C16
53	a	825	PQN	C21-C22-C23-C24
54	z	312	CHL	C11-C10-C8-C9
50	a	836	CLA	C16-C17-C18-C19
44	b	830	PGT	O31-C31-O2-C2
44	L	201	PGT	C32-C33-C34-C35
50	a	811	CLA	C5-C6-C7-C8
50	y	314	CLA	C15-C16-C17-C18
44	L	201	PGT	C14-C15-C16-C17
46	7	301	LMG	C35-C36-C37-C38
50	a	801	CLA	C2-C1-O2A-CGA
50	l	306	CLA	C11-C12-C13-C14
50	b	843	CLA	O1D-CGD-O2D-CED
46	j	105	LMG	C34-C35-C36-C37
50	a	836	CLA	O1D-CGD-O2D-CED
51	b	821	DGD	C8A-C9A-CAA-CBA
44	z	301	PGT	C18-C19-C20-C21
51	x	317	DGD	C3A-C4A-C5A-C6A
46	x	315	LMG	C14-C15-C16-C17
50	a	842	CLA	C3-C5-C6-C7
50	b	803	CLA	C2C-C3C-CAC-CBC
48	j	106	SQD	C4-C5-C6-S
54	z	312	CHL	C4C-C3C-CAC-CBC
50	b	834	CLA	O1D-CGD-O2D-CED
46	w	312	LMG	C30-C31-C32-C33
44	f	305	PGT	C32-C33-C34-C35
50	a	850	CLA	C16-C17-C18-C19
50	b	847	CLA	C11-C12-C13-C15
50	a	820	CLA	C4B-C3B-CAB-CBB
50	a	848	CLA	C1A-C2A-CAA-CBA
50	a	851	CLA	C1A-C2A-CAA-CBA
50	b	809	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
50	b	839	CLA	C1A-C2A-CAA-CBA
50	b	842	CLA	C4B-C3B-CAB-CBB
50	w	302	CLA	C4B-C3B-CAB-CBB
50	w	306	CLA	C4B-C3B-CAB-CBB
50	x	307	CLA	C4B-C3B-CAB-CBB
50	x	312	CLA	C4B-C3B-CAB-CBB
50	z	308	CLA	C4B-C3B-CAB-CBB
50	j	102	CLA	O1D-CGD-O2D-CED
55	z	320	LUT	C27-C28-C29-C30
50	a	821	CLA	C2A-CAA-CBA-CGA
46	j	104	LMG	C13-C14-C15-C16
50	x	310	CLA	C2A-CAA-CBA-CGA
44	B	601	PGT	O3P-C1-C2-C3
44	B	603	PGT	O3P-C1-C2-C3
44	L	201	PGT	O3P-C1-C2-C3
44	a	805	PGT	O3P-C1-C2-C3
46	F	802	LMG	O9-C10-O7-C8
50	a	852	CLA	C2-C3-C5-C6
50	a	801	CLA	C11-C12-C13-C15
50	a	814	CLA	C6-C7-C8-C10
50	a	844	CLA	C11-C10-C8-C7
50	a	854	CLA	C11-C12-C13-C15
50	a	858	CLA	C11-C12-C13-C15
50	b	801	CLA	C12-C13-C15-C16
50	b	837	CLA	C6-C7-C8-C10
50	b	837	CLA	C12-C13-C15-C16
50	x	303	CLA	C6-C7-C8-C10
50	y	313	CLA	C11-C12-C13-C15
53	b	827	PQN	C22-C23-C25-C26
46	7	301	LMG	C34-C35-C36-C37
46	D	601	LMG	C12-C13-C14-C15
50	a	811	CLA	C16-C17-C18-C19
50	y	308	CLA	C16-C17-C18-C19
50	a	816	CLA	C3A-C2A-CAA-CBA
51	b	821	DGD	C7B-C8B-C9B-CAB
50	a	841	CLA	C5-C6-C7-C8
44	5	301	PGT	C5-C4-O4P-P
44	D	602	PGT	C5-C4-O4P-P
50	a	849	CLA	C3A-C2A-CAA-CBA
50	a	823	CLA	C6-C7-C8-C10
50	a	846	CLA	C16-C17-C18-C19
44	B	601	PGT	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
44	N	301	PGT	O3P-C1-C2-O2
44	z	317	PGT	O3P-C1-C2-O2
46	f	306	LMG	C11-C10-O7-C8
50	z	311	CLA	C2A-CAA-CBA-CGA
50	a	846	CLA	C11-C10-C8-C9
50	a	846	CLA	C14-C13-C15-C16
50	a	858	CLA	C14-C13-C15-C16
50	w	308	CLA	C14-C13-C15-C16
50	b	832	CLA	C5-C6-C7-C8
50	a	815	CLA	C13-C15-C16-C17
43	k	201	BCR	C15-C16-C17-C18
44	b	829	PGT	C39-C40-C41-C42
50	g	201	CLA	C1-C2-C3-C4
54	x	319	CHL	C1-C2-C3-C4
44	A	404	PGT	C17-C18-C19-C20
51	x	317	DGD	C8A-C9A-CAA-CBA
44	I	203	PGT	O2-C2-C3-O3
44	z	301	PGT	O2-C2-C3-O3
46	j	105	LMG	O7-C8-C9-O8
51	b	821	DGD	O1G-C1G-C2G-O2G
50	b	814	CLA	C13-C15-C16-C17
44	I	203	PGT	C14-C15-C16-C17
50	a	836	CLA	C16-C17-C18-C20
46	j	105	LMG	O1-C7-C8-C9
46	j	105	LMG	C7-C8-C9-O8
46	w	312	LMG	O1-C7-C8-C9
51	x	317	DGD	C1G-C2G-C3G-O3G
44	a	805	PGT	C14-C15-C16-C17
50	a	839	CLA	CAD-CBD-CGD-O2D
50	a	847	CLA	C2A-C1A-CHA-CBD
50	y	309	CLA	CAD-CBD-CGD-O2D
54	w	309	CHL	C1A-C2A-CAA-CBA
54	z	304	CHL	CAD-CBD-CGD-O2D
50	a	815	CLA	O1D-CGD-O2D-CED
44	L	201	PGT	C42-C43-C44-C45
50	f	301	CLA	O1A-CGA-O2A-C1
51	b	821	DGD	C1B-C2B-C3B-C4B
44	5	301	PGT	C1-O3P-P-O2P
44	A	401	PGT	C4-O4P-P-O1P
44	A	403	PGT	C4-O4P-P-O2P
44	A	404	PGT	C1-O3P-P-O4P
44	A	404	PGT	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
44	B	601	PGT	C1-O3P-P-O1P
44	B	602	PGT	C1-O3P-P-O1P
44	B	602	PGT	C4-O4P-P-O1P
44	F	803	PGT	C4-O4P-P-O1P
44	I	203	PGT	C1-O3P-P-O2P
44	N	301	PGT	C4-O4P-P-O3P
44	N	301	PGT	C4-O4P-P-O2P
44	a	806	PGT	C4-O4P-P-O2P
44	a	807	PGT	C1-O3P-P-O1P
44	a	807	PGT	C4-O4P-P-O1P
44	b	829	PGT	C1-O3P-P-O4P
44	b	830	PGT	C4-O4P-P-O1P
44	w	313	PGT	C1-O3P-P-O2P
44	w	313	PGT	C4-O4P-P-O1P
44	z	301	PGT	C4-O4P-P-O1P
44	z	313	PGT	C4-O4P-P-O1P
44	z	317	PGT	C1-O3P-P-O1P
50	a	801	CLA	CAD-CBD-CGD-O1D
50	a	814	CLA	CHA-CBD-CGD-O1D
50	a	819	CLA	CAD-CBD-CGD-O1D
50	a	826	CLA	CAD-CBD-CGD-O1D
50	a	835	CLA	CAD-CBD-CGD-O1D
50	a	838	CLA	CAD-CBD-CGD-O1D
50	a	839	CLA	CAD-CBD-CGD-O1D
50	a	847	CLA	CHA-CBD-CGD-O1D
50	b	801	CLA	CHA-CBD-CGD-O1D
50	b	805	CLA	CHA-CBD-CGD-O2D
50	b	808	CLA	CHA-CBD-CGD-O1D
50	b	824	CLA	CAD-CBD-CGD-O1D
50	b	832	CLA	CAD-CBD-CGD-O1D
50	b	840	CLA	CHA-CBD-CGD-O2D
50	k	205	CLA	CAD-CBD-CGD-O1D
50	l	306	CLA	CHA-CBD-CGD-O2D
50	x	316	CLA	CAD-CBD-CGD-O1D
50	z	307	CLA	CHA-CBD-CGD-O1D
50	z	311	CLA	CHA-CBD-CGD-O2D
54	x	311	CHL	CHA-CBD-CGD-O1D
54	x	311	CHL	CHA-CBD-CGD-O2D
54	z	304	CHL	CAD-CBD-CGD-O1D
54	z	312	CHL	CHA-CBD-CGD-O2D
50	a	858	CLA	C16-C17-C18-C20
50	a	820	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
50	a	822	CLA	C2B-C3B-CAB-CBB
50	b	842	CLA	C2B-C3B-CAB-CBB
50	b	849	CLA	C2B-C3B-CAB-CBB
44	A	402	PGT	C2-C1-O3P-P
44	N	301	PGT	C2-C1-O3P-P
44	a	805	PGT	C2-C1-O3P-P
51	x	317	DGD	C2A-C3A-C4A-C5A
50	b	847	CLA	C5-C6-C7-C8
44	a	805	PGT	C32-C33-C34-C35
44	z	317	PGT	O4P-C4-C5-O5
44	D	602	PGT	C3-C2-O2-C31
44	N	301	PGT	C3-C2-O2-C31
43	a	810	BCR	C10-C11-C12-C13
43	a	810	BCR	C18-C19-C20-C21
43	z	318	BCR	C10-C11-C12-C13
44	A	404	PGT	C21-C22-C23-C24
50	a	811	CLA	C16-C17-C18-C20
50	a	823	CLA	C6-C7-C8-C9
50	b	833	CLA	C15-C16-C17-C18
46	x	315	LMG	C4-C5-C6-O5
52	a	808	CL0	CBA-CGA-O2A-C1
44	A	402	PGT	O3P-C1-C2-C3
50	a	811	CLA	C11-C12-C13-C14
50	a	833	CLA	C11-C12-C13-C14
50	a	843	CLA	C11-C12-C13-C14
50	b	824	CLA	C11-C12-C13-C14
50	b	844	CLA	C14-C13-C15-C16
50	l	306	CLA	C11-C10-C8-C9
50	x	312	CLA	C11-C12-C13-C14
50	y	314	CLA	C11-C12-C13-C14
50	b	837	CLA	C11-C10-C8-C7
50	x	312	CLA	C11-C10-C8-C7
46	f	306	LMG	O9-C10-O7-C8
46	x	315	LMG	O6-C1-O1-C7
51	b	821	DGD	O6D-C1D-O3G-C3G
44	b	829	PGT	C38-C39-C40-C41
44	A	404	PGT	C32-C33-C34-C35
50	y	303	CLA	C6-C7-C8-C10
44	F	803	PGT	C2-C1-O3P-P
48	j	106	SQD	O6-C44-C45-O47
51	a	804	DGD	O2G-C2G-C3G-O3G
50	b	824	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
50	y	303	CLA	C6-C7-C8-C9
44	A	402	PGT	C38-C39-C40-C41
50	a	849	CLA	CAA-CBA-CGA-O2A
45	F	804	A1H1M	C02-C03-C04-C05
50	x	306	CLA	C2A-CAA-CBA-CGA
50	a	818	CLA	CBA-CGA-O2A-C1
44	f	305	PGT	C15-C16-C17-C18
50	x	312	CLA	C16-C17-C18-C20
50	b	843	CLA	C2-C3-C5-C6
50	a	854	CLA	C5-C6-C7-C8
50	b	806	CLA	O1D-CGD-O2D-CED
44	B	603	PGT	C17-C18-C19-C20
55	z	320	LUT	C7-C8-C9-C19
50	x	306	CLA	C11-C12-C13-C15
50	b	849	CLA	O1D-CGD-O2D-CED
44	b	829	PGT	C41-C42-C43-C44
50	a	835	CLA	C2A-CAA-CBA-CGA
50	a	843	CLA	C2A-CAA-CBA-CGA
50	b	801	CLA	C2A-CAA-CBA-CGA
50	b	803	CLA	C2A-CAA-CBA-CGA
50	b	842	CLA	C2A-CAA-CBA-CGA
50	x	316	CLA	C2A-CAA-CBA-CGA
43	l	302	BCR	C13-C14-C15-C16
50	b	802	CLA	C16-C17-C18-C20
51	b	821	DGD	C3A-C4A-C5A-C6A
50	a	843	CLA	C4-C3-C5-C6
50	y	314	CLA	C4-C3-C5-C6
50	b	825	CLA	C8-C10-C11-C12
50	b	842	CLA	C2-C3-C5-C6
50	a	853	CLA	O1D-CGD-O2D-CED
44	5	301	PGT	C33-C34-C35-C36
48	F	805	SQD	O49-C7-C8-C9
50	a	801	CLA	C11-C12-C13-C14
50	a	838	CLA	C14-C13-C15-C16
50	a	844	CLA	C11-C10-C8-C9
50	b	837	CLA	C6-C7-C8-C9
50	y	313	CLA	C11-C12-C13-C14
50	x	307	CLA	CBA-CGA-O2A-C1
44	I	203	PGT	C2-C1-O3P-P
50	y	308	CLA	O1A-CGA-O2A-C1
50	b	805	CLA	C4B-C3B-CAB-CBB
50	b	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
50	b	840	CLA	C16-C17-C18-C19
48	a	859	SQD	O49-C7-C8-C9
53	b	827	PQN	C15-C16-C17-C18
44	B	603	PGT	C36-C37-C38-C39
44	z	301	PGT	C37-C38-C39-C40
48	w	317	SQD	O49-C7-C8-C9
50	a	843	CLA	C12-C13-C15-C16
50	a	850	CLA	C11-C12-C13-C15
50	b	824	CLA	C12-C13-C15-C16
50	w	310	CLA	C11-C12-C13-C15
50	w	310	CLA	C12-C13-C15-C16
44	I	203	PGT	C11-C12-C13-C14
44	A	402	PGT	C12-C11-O3-C3
50	x	306	CLA	C11-C12-C13-C14
50	x	312	CLA	C16-C17-C18-C19
44	F	803	PGT	C13-C14-C15-C16
50	a	854	CLA	O1A-CGA-O2A-C1
50	z	319	CLA	CBD-CGD-O2D-CED
44	b	829	PGT	C17-C18-C19-C20
51	a	804	DGD	C4A-C5A-C6A-C7A
46	f	306	LMG	O1-C7-C8-O7
50	a	824	CLA	C4-C3-C5-C6
50	b	828	CLA	C3A-C2A-CAA-CBA
50	b	836	CLA	C4-C3-C5-C6
50	b	842	CLA	C3A-C2A-CAA-CBA
50	b	847	CLA	C3A-C2A-CAA-CBA
50	x	303	CLA	C3A-C2A-CAA-CBA
50	y	312	CLA	C3A-C2A-CAA-CBA
50	z	308	CLA	C3A-C2A-CAA-CBA
46	w	312	LMG	C14-C15-C16-C17
44	B	603	PGT	C12-C13-C14-C15
51	x	317	DGD	C2B-C3B-C4B-C5B
43	a	810	BCR	C16-C17-C18-C36
43	a	831	BCR	C11-C10-C9-C34
43	a	831	BCR	C35-C13-C14-C15
43	b	818	BCR	C11-C10-C9-C34
43	b	818	BCR	C20-C21-C22-C37
43	f	304	BCR	C35-C13-C14-C15
43	l	304	BCR	C11-C10-C9-C34
46	D	601	LMG	O6-C1-O1-C7
50	a	850	CLA	C5-C6-C7-C8
44	z	317	PGT	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
44	a	807	PGT	C21-C22-C23-C24
43	l	304	BCR	C9-C10-C11-C12
50	b	802	CLA	C5-C6-C7-C8
43	b	816	BCR	C37-C22-C23-C24
44	A	404	PGT	C5-C4-O4P-P
44	L	201	PGT	C2-C1-O3P-P
50	b	807	CLA	C4-C3-C5-C6
50	y	308	CLA	O1D-CGD-O2D-CED
48	j	106	SQD	C31-C32-C33-C34
44	A	403	PGT	C38-C39-C40-C41
46	z	315	LMG	C7-C8-C9-O8
50	w	310	CLA	C8-C10-C11-C12
54	w	304	CHL	CAA-CBA-CGA-O1A
50	a	836	CLA	C11-C10-C8-C9
50	a	843	CLA	C11-C10-C8-C9
50	a	850	CLA	C11-C12-C13-C14
50	a	850	CLA	C14-C13-C15-C16
50	a	854	CLA	C14-C13-C15-C16
50	b	802	CLA	C11-C12-C13-C14
50	b	824	CLA	C14-C13-C15-C16
50	b	840	CLA	C11-C10-C8-C9
50	x	303	CLA	C6-C7-C8-C9
50	y	313	CLA	C11-C10-C8-C9
53	b	827	PQN	C24-C23-C25-C26
44	a	807	PGT	C34-C35-C36-C37
51	a	804	DGD	CEA-CFA-CGA-CHA
44	A	401	PGT	C3-C2-O2-C31
48	F	805	SQD	C44-C45-O47-C7
50	b	809	CLA	C1-C2-C3-C4
50	w	310	CLA	C1-C2-C3-C4
50	y	312	CLA	C1-C2-C3-C4
50	z	306	CLA	C1-C2-C3-C4
54	x	305	CHL	C1A-C2A-CAA-CBA
44	A	404	PGT	C22-C23-C24-C25
50	y	310	CLA	C2-C3-C5-C6
46	j	105	LMG	C31-C32-C33-C34
50	a	824	CLA	C2A-CAA-CBA-CGA
46	B	605	LMG	O10-C28-C29-C30
43	a	810	BCR	C16-C17-C18-C19
43	a	831	BCR	C11-C10-C9-C8
43	a	831	BCR	C12-C13-C14-C15
43	b	818	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
43	b	818	BCR	C20-C21-C22-C23
43	f	304	BCR	C12-C13-C14-C15
43	l	304	BCR	C11-C10-C9-C8
50	b	833	CLA	C1A-C2A-CAA-CBA
50	b	836	CLA	C1A-C2A-CAA-CBA
50	l	301	CLA	C1A-C2A-CAA-CBA
50	y	313	CLA	C1A-C2A-CAA-CBA
50	a	857	CLA	O1D-CGD-O2D-CED
44	f	305	PGT	O3P-C1-C2-O2
44	z	313	PGT	O3P-C1-C2-O2
50	a	850	CLA	C3-C5-C6-C7
51	a	804	DGD	C9A-CAA-CBA-CCA
50	a	853	CLA	C8-C10-C11-C12
43	a	827	BCR	C5-C6-C7-C8
43	g	202	BCR	C23-C24-C25-C26
43	i	101	BCR	C5-C6-C7-C8
43	j	101	BCR	C23-C24-C25-C26
43	j	103	BCR	C1-C6-C7-C8
43	j	103	BCR	C5-C6-C7-C8
43	w	301	BCR	C5-C6-C7-C8
43	w	301	BCR	C23-C24-C25-C30
43	y	301	BCR	C23-C24-C25-C26
43	z	318	BCR	C23-C24-C25-C26
50	b	805	CLA	C2B-C3B-CAB-CBB
50	w	302	CLA	C2B-C3B-CAB-CBB
50	w	306	CLA	C2B-C3B-CAB-CBB
50	x	307	CLA	C2B-C3B-CAB-CBB
50	x	312	CLA	C2B-C3B-CAB-CBB
50	z	308	CLA	C2B-C3B-CAB-CBB
44	B	603	PGT	C18-C19-C20-C21
50	a	812	CLA	C14-C13-C15-C16
50	b	843	CLA	C16-C17-C18-C20
44	5	301	PGT	C35-C36-C37-C38
50	a	847	CLA	NB-C1B-CHB-C4A
50	a	856	CLA	O2A-C1-C2-C3
50	a	811	CLA	C11-C12-C13-C15
50	a	824	CLA	C6-C7-C8-C10
50	a	833	CLA	C11-C12-C13-C15
50	a	838	CLA	C12-C13-C15-C16
50	a	853	CLA	C11-C12-C13-C15
50	b	805	CLA	C11-C10-C8-C7
50	b	845	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
50	a	814	CLA	C2A-CAA-CBA-CGA
50	a	820	CLA	C2A-CAA-CBA-CGA
50	b	846	CLA	C2A-CAA-CBA-CGA
51	a	804	DGD	O1G-C1G-C2G-O2G
48	w	317	SQD	C11-C10-C9-C8
43	k	202	BCR	C37-C22-C23-C24
55	z	320	LUT	C11-C12-C13-C20
44	w	313	PGT	C33-C34-C35-C36
50	a	834	CLA	C4-C3-C5-C6
50	b	823	CLA	C4-C3-C5-C6
50	a	850	CLA	CAA-CBA-CGA-O2A
44	A	402	PGT	O11-C11-O3-C3
50	z	311	CLA	O1A-CGA-O2A-C1
50	b	842	CLA	C1-C2-C3-C5
50	w	302	CLA	C2-C1-O2A-CGA
54	x	319	CHL	C2-C1-O2A-CGA
50	a	835	CLA	C5-C6-C7-C8
50	b	844	CLA	C10-C11-C12-C13
44	b	829	PGT	C15-C16-C17-C18
44	a	807	PGT	C33-C34-C35-C36
50	b	843	CLA	C16-C17-C18-C19
50	b	823	CLA	O1D-CGD-O2D-CED
50	a	820	CLA	O1A-CGA-O2A-C1
50	b	839	CLA	O1A-CGA-O2A-C1
50	a	842	CLA	C4-C3-C5-C6
50	a	850	CLA	C4-C3-C5-C6
44	I	203	PGT	C41-C42-C43-C44
50	a	844	CLA	C2-C3-C5-C6
50	a	849	CLA	C2-C3-C5-C6
50	l	301	CLA	CAA-CBA-CGA-O1A
50	l	301	CLA	CAA-CBA-CGA-O2A
50	w	306	CLA	O1A-CGA-O2A-C1
44	5	301	PGT	C32-C33-C34-C35
50	b	848	CLA	C1A-C2A-CAA-CBA
50	b	837	CLA	CAA-CBA-CGA-O2A
50	a	818	CLA	C11-C12-C13-C14
50	b	828	CLA	O1D-CGD-O2D-CED
50	a	854	CLA	C4-C3-C5-C6
50	a	847	CLA	C2A-C3A-C4A-CHB
44	B	603	PGT	C44-C45-C46-C47
50	y	313	CLA	O1A-CGA-O2A-C1
45	5	302	A1H1M	C37-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
44	D	602	PGT	C15-C16-C17-C18
50	b	846	CLA	C16-C17-C18-C19
46	z	315	LMG	O9-C10-O7-C8
54	w	309	CHL	CHA-CBD-CGD-O1D
54	x	301	CHL	CHA-CBD-CGD-O1D
54	x	305	CHL	CHA-CBD-CGD-O2D
46	x	315	LMG	O1-C7-C8-O7
46	B	605	LMG	C34-C35-C36-C37
50	a	819	CLA	C3-C5-C6-C7
50	b	803	CLA	C5-C6-C7-C8
50	a	849	CLA	C6-C7-C8-C10
44	B	603	PGT	C33-C34-C35-C36
50	b	845	CLA	C13-C15-C16-C17
46	x	315	LMG	C15-C16-C17-C18
50	w	308	CLA	C16-C17-C18-C20
44	z	313	PGT	O4P-C4-C5-O5
50	b	843	CLA	C11-C10-C8-C9
50	w	306	CLA	C11-C10-C8-C9
48	B	604	SQD	C45-C44-O6-C1
51	x	317	DGD	C5D-C6D-O5D-C1E
50	b	811	CLA	CAA-CBA-CGA-O2A
50	x	307	CLA	C2A-CAA-CBA-CGA
50	a	823	CLA	C2-C1-O2A-CGA
50	a	854	CLA	C2-C1-O2A-CGA
50	b	807	CLA	C2-C1-O2A-CGA
50	b	825	CLA	C2-C1-O2A-CGA
50	w	316	CLA	C2-C1-O2A-CGA
44	B	603	PGT	C14-C15-C16-C17
46	x	315	LMG	O6-C5-C6-O5
50	b	814	CLA	C15-C16-C17-C18
50	z	307	CLA	C10-C11-C12-C13
44	B	606	PGT	C17-C18-C19-C20
50	a	853	CLA	C3A-C2A-CAA-CBA
50	b	813	CLA	C3A-C2A-CAA-CBA
50	b	833	CLA	C3A-C2A-CAA-CBA
50	b	815	CLA	C2-C3-C5-C6
44	B	601	PGT	C15-C16-C17-C18
54	w	304	CHL	CAA-CBA-CGA-O2A
46	x	315	LMG	C21-C22-C23-C24
51	a	804	DGD	CCB-CDB-CEB-CFB
51	x	317	DGD	C2G-C1G-O1G-C1A
44	5	301	PGT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
48	a	859	SQD	C46-C45-O47-C7
48	w	318	SQD	C46-C45-O47-C7
50	a	846	CLA	O2A-C1-C2-C3
50	b	810	CLA	O2A-C1-C2-C3
50	b	841	CLA	O2A-C1-C2-C3
51	a	804	DGD	C1G-C2G-O2G-C1B
50	b	809	CLA	CAA-CBA-CGA-O2A
50	y	313	CLA	C15-C16-C17-C18
44	z	317	PGT	C19-C20-C21-C22
50	a	826	CLA	CAA-CBA-CGA-O2A
50	b	801	CLA	C2-C3-C5-C6
50	a	847	CLA	C2A-CAA-CBA-CGA
50	y	303	CLA	C3-C5-C6-C7
46	7	301	LMG	C29-C30-C31-C32
46	D	601	LMG	C7-C8-C9-O8
44	B	602	PGT	C15-C16-C17-C18
44	I	203	PGT	C34-C35-C36-C37
43	i	101	BCR	C13-C14-C15-C16
50	a	853	CLA	C16-C17-C18-C19
50	w	308	CLA	C16-C17-C18-C19
44	w	313	PGT	C18-C19-C20-C21
50	y	311	CLA	O1A-CGA-O2A-C1
46	H	401	LMG	O7-C10-C11-C12
50	b	842	CLA	CAA-CBA-CGA-O2A
44	b	830	PGT	C12-C13-C14-C15
44	a	806	PGT	O2-C2-C3-O3
50	a	854	CLA	C11-C12-C13-C14
50	a	853	CLA	C16-C17-C18-C20
50	l	306	CLA	C11-C12-C13-C15
44	f	305	PGT	O3P-C1-C2-C3
50	y	305	CLA	CAA-CBA-CGA-O2A
43	b	817	BCR	C21-C22-C23-C24
50	y	308	CLA	C8-C10-C11-C12
44	a	807	PGT	C15-C16-C17-C18
46	z	314	LMG	C32-C33-C34-C35
50	b	833	CLA	C16-C17-C18-C20
50	b	828	CLA	C2A-CAA-CBA-CGA
50	a	801	CLA	C11-C10-C8-C7
50	a	815	CLA	C12-C13-C15-C16
50	a	820	CLA	C11-C10-C8-C7
50	a	835	CLA	C6-C7-C8-C10
50	a	842	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
50	a	857	CLA	C11-C12-C13-C15
50	b	803	CLA	C12-C13-C15-C16
50	b	812	CLA	C11-C12-C13-C15
50	b	814	CLA	C12-C13-C15-C16
50	b	824	CLA	C11-C10-C8-C7
50	b	843	CLA	C11-C10-C8-C7
50	b	843	CLA	C12-C13-C15-C16
50	w	306	CLA	C11-C12-C13-C15
50	w	308	CLA	C11-C10-C8-C7
50	y	313	CLA	C11-C10-C8-C7
43	4	101	BCR	C23-C24-C25-C30
43	a	827	BCR	C1-C6-C7-C8
43	a	830	BCR	C5-C6-C7-C8
43	j	101	BCR	C5-C6-C7-C8
43	j	101	BCR	C23-C24-C25-C30
43	l	302	BCR	C5-C6-C7-C8
43	l	303	BCR	C1-C6-C7-C8
50	b	825	CLA	C2B-C3B-CAB-CBB
50	b	826	CLA	O1D-CGD-O2D-CED
44	5	301	PGT	O31-C31-O2-C2
51	a	804	DGD	C7B-C8B-C9B-CAB
50	x	303	CLA	CBA-CGA-O2A-C1
50	k	204	CLA	C8-C10-C11-C12
44	B	606	PGT	O3-C11-C12-C13
44	z	313	PGT	O2-C31-C32-C33
50	a	854	CLA	C3-C5-C6-C7
50	b	841	CLA	CAA-CBA-CGA-O2A
50	a	843	CLA	C2-C3-C5-C6
50	w	306	CLA	C2A-CAA-CBA-CGA
44	5	301	PGT	C32-C31-O2-C2
46	z	315	LMG	C11-C10-O7-C8
44	a	807	PGT	C20-C21-C22-C23
50	a	834	CLA	CAA-CBA-CGA-O2A
50	a	852	CLA	CAA-CBA-CGA-O2A
50	y	308	CLA	C13-C15-C16-C17
48	F	801	SQD	C4-C5-C6-S
48	F	805	SQD	C4-C5-C6-S
48	w	318	SQD	C4-C5-C6-S
50	a	802	CLA	C4-C3-C5-C6
50	a	814	CLA	C2-C3-C5-C6
54	w	304	CHL	C2A-CAA-CBA-CGA
50	a	833	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
50	a	824	CLA	C6-C7-C8-C9
50	b	837	CLA	C14-C13-C15-C16
50	f	301	CLA	C11-C10-C8-C9
48	j	106	SQD	C32-C33-C34-C35
54	z	312	CHL	C2C-C3C-CAC-CBC
44	B	606	PGT	O2-C31-C32-C33
50	b	847	CLA	CAA-CBA-CGA-O2A
44	z	301	PGT	C17-C18-C19-C20
44	a	806	PGT	C1-C2-C3-O3
44	z	301	PGT	C1-C2-C3-O3
46	f	306	LMG	O1-C7-C8-C9
50	a	854	CLA	C8-C10-C11-C12
50	a	822	CLA	C1A-C2A-CAA-CBA
50	a	850	CLA	C4B-C3B-CAB-CBB
50	b	813	CLA	C1A-C2A-CAA-CBA
50	b	825	CLA	C4B-C3B-CAB-CBB
50	y	313	CLA	C4B-C3B-CAB-CBB
50	z	308	CLA	C1A-C2A-CAA-CBA
44	z	313	PGT	C32-C33-C34-C35
50	b	808	CLA	C2A-CAA-CBA-CGA
50	a	854	CLA	CAA-CBA-CGA-O2A
50	b	839	CLA	CAA-CBA-CGA-O2A
44	A	404	PGT	O2-C2-C3-O3
43	b	816	BCR	C21-C22-C23-C24
55	w	319	LUT	C11-C12-C13-C14
50	a	821	CLA	C12-C13-C15-C16
44	a	805	PGT	O2-C31-C32-C33
46	z	315	LMG	O8-C28-C29-C30
50	a	848	CLA	CAA-CBA-CGA-O2A
50	w	306	CLA	CAA-CBA-CGA-O2A
50	z	311	CLA	CAA-CBA-CGA-O2A
44	B	606	PGT	C12-C13-C14-C15
50	a	842	CLA	C2-C1-O2A-CGA
50	a	853	CLA	C2-C1-O2A-CGA
50	b	839	CLA	C2-C1-O2A-CGA
54	z	312	CHL	C2-C1-O2A-CGA
50	a	824	CLA	C12-C13-C15-C16
50	b	824	CLA	C6-C7-C8-C10
50	b	837	CLA	C11-C12-C13-C15
44	B	606	PGT	C15-C16-C17-C18
44	a	805	PGT	C11-C12-C13-C14
44	B	603	PGT	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
48	F	805	SQD	C46-C45-O47-C7
48	a	859	SQD	C44-C45-O47-C7
48	w	318	SQD	C44-C45-O47-C7
44	F	803	PGT	C12-C13-C14-C15
44	b	829	PGT	C37-C38-C39-C40
46	f	306	LMG	O7-C10-C11-C12
50	a	824	CLA	C13-C15-C16-C17
50	z	319	CLA	C3A-C2A-CAA-CBA
50	b	833	CLA	C2A-CAA-CBA-CGA
44	f	305	PGT	O3-C11-C12-C13
50	x	318	CLA	CAA-CBA-CGA-O2A
50	x	318	CLA	O1D-CGD-O2D-CED
44	B	603	PGT	C2-C1-O3P-P
50	a	835	CLA	C4-C3-C5-C6
50	a	839	CLA	C3A-C2A-CAA-CBA
50	a	850	CLA	C3A-C2A-CAA-CBA
50	b	807	CLA	C3A-C2A-CAA-CBA
50	g	201	CLA	C3A-C2A-CAA-CBA
50	w	310	CLA	C3A-C2A-CAA-CBA
53	a	825	PQN	C14-C13-C15-C16
50	b	840	CLA	C16-C17-C18-C20
46	f	306	LMG	C15-C16-C17-C18
50	b	811	CLA	CAA-CBA-CGA-O1A
44	w	313	PGT	C32-C33-C34-C35
44	b	829	PGT	O3P-C1-C2-O2
50	b	838	CLA	CAA-CBA-CGA-O1A
50	y	308	CLA	CAA-CBA-CGA-O1A
50	z	311	CLA	CAA-CBA-CGA-O1A
50	a	809	CLA	CBD-CGD-O2D-CED
50	b	802	CLA	C2A-CAA-CBA-CGA
50	b	843	CLA	C2A-CAA-CBA-CGA
50	y	302	CLA	C2A-CAA-CBA-CGA
50	a	849	CLA	C6-C7-C8-C9
46	7	301	LMG	C13-C14-C15-C16
50	a	801	CLA	CAA-CBA-CGA-O1A
50	b	832	CLA	CAA-CBA-CGA-O1A
44	F	803	PGT	C34-C35-C36-C37
50	b	802	CLA	C8-C10-C11-C12
50	b	815	CLA	C4-C3-C5-C6
50	a	834	CLA	CAA-CBA-CGA-O1A
50	g	201	CLA	CAA-CBA-CGA-O1A
44	5	301	PGT	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
46	z	314	LMG	C31-C32-C33-C34
50	a	802	CLA	C8-C10-C11-C12
48	F	805	SQD	O5-C5-C6-S
48	j	106	SQD	O5-C5-C6-S
48	w	318	SQD	O5-C5-C6-S
44	B	606	PGT	O11-C11-C12-C13
50	a	821	CLA	CAA-CBA-CGA-O1A
51	b	821	DGD	C8B-C9B-CAB-CBB
46	B	605	LMG	C35-C36-C37-C38
50	a	842	CLA	C5-C6-C7-C8
44	F	803	PGT	C20-C21-C22-C23
48	F	805	SQD	C11-C12-C13-C14
46	F	802	LMG	C29-C30-C31-C32
50	g	201	CLA	CAA-CBA-CGA-O2A
50	a	826	CLA	CAA-CBA-CGA-O1A
43	k	202	BCR	C21-C22-C23-C24
50	b	835	CLA	CBA-CGA-O2A-C1
44	z	313	PGT	O31-C31-C32-C33
50	a	814	CLA	CAA-CBA-CGA-O1A
50	b	844	CLA	CAA-CBA-CGA-O1A
50	x	313	CLA	CAA-CBA-CGA-O1A
44	b	829	PGT	C19-C20-C21-C22
46	f	306	LMG	O9-C10-C11-C12
50	a	811	CLA	CAA-CBA-CGA-O1A
50	l	306	CLA	CAA-CBA-CGA-O1A
50	b	805	CLA	CAA-CBA-CGA-O2A
50	k	204	CLA	CAA-CBA-CGA-O2A
50	y	302	CLA	O1D-CGD-O2D-CED
44	L	201	PGT	C41-C42-C43-C44
46	D	601	LMG	O1-C7-C8-C9
44	B	606	PGT	O31-C31-C32-C33
46	H	401	LMG	O9-C10-C11-C12
50	b	824	CLA	CAA-CBA-CGA-O1A
50	w	315	CLA	CAA-CBA-CGA-O1A
50	h	201	CLA	CAA-CBA-CGA-O2A
50	b	839	CLA	CAA-CBA-CGA-O1A
50	a	834	CLA	CAD-CBD-CGD-O2D
50	b	832	CLA	CAD-CBD-CGD-O2D
50	l	306	CLA	CAD-CBD-CGD-O2D
50	x	306	CLA	CAD-CBD-CGD-O2D
50	z	311	CLA	CAD-CBD-CGD-O2D
50	z	307	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
50	b	845	CLA	CAA-CBA-CGA-O2A
50	a	841	CLA	CAA-CBA-CGA-O1A
50	a	819	CLA	C5-C6-C7-C8
44	z	317	PGT	O3P-C1-C2-C3
50	a	833	CLA	C2-C1-O2A-CGA
50	a	841	CLA	C2-C1-O2A-CGA
50	x	306	CLA	C2-C1-O2A-CGA
50	x	312	CLA	C2-C1-O2A-CGA
54	x	319	CHL	CAA-CBA-CGA-O1A
44	B	601	PGT	O3-C11-C12-C13
44	w	313	PGT	O2-C31-C32-C33
50	z	307	CLA	CAA-CBA-CGA-O2A
50	a	820	CLA	C1-C2-C3-C4
50	a	845	CLA	C1-C2-C3-C4
50	b	825	CLA	C1-C2-C3-C4
50	b	832	CLA	C1-C2-C3-C4
50	l	306	CLA	C1-C2-C3-C4
50	x	303	CLA	C1-C2-C3-C4
44	B	603	PGT	C40-C41-C42-C43
50	x	308	CLA	CAA-CBA-CGA-O1A
50	z	316	CLA	CAA-CBA-CGA-O1A
50	b	826	CLA	O1A-CGA-O2A-C1
44	A	402	PGT	O3-C11-C12-C13
50	a	835	CLA	CAA-CBA-CGA-O2A
50	w	315	CLA	CAA-CBA-CGA-O2A
50	y	308	CLA	CAA-CBA-CGA-O2A
50	y	311	CLA	CAA-CBA-CGA-O2A
50	b	828	CLA	CAA-CBA-CGA-O1A
50	a	843	CLA	CAA-CBA-CGA-O2A
50	y	314	CLA	CAA-CBA-CGA-O2A
50	z	316	CLA	CAA-CBA-CGA-O2A
50	a	842	CLA	CAA-CBA-CGA-O1A
50	b	842	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

201 monomers are involved in 576 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	y	316	LUT	28	0
43	l	302	BCR	2	0
54	z	312	CHL	7	0
50	a	856	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	f	306	LMG	1	0
51	a	804	DGD	2	0
50	a	824	CLA	4	0
44	B	602	PGT	2	0
50	x	306	CLA	1	0
43	b	816	BCR	3	0
43	y	301	BCR	1	0
44	a	805	PGT	3	0
50	y	302	CLA	7	0
50	a	815	CLA	3	0
50	b	811	CLA	2	0
50	a	834	CLA	3	0
51	x	317	DGD	2	0
50	g	203	CLA	2	0
44	5	301	PGT	2	0
46	j	105	LMG	2	0
43	w	301	BCR	1	0
43	a	810	BCR	4	0
50	b	807	CLA	4	0
50	b	810	CLA	1	0
50	y	310	CLA	5	0
46	H	401	LMG	1	0
50	a	823	CLA	3	0
43	a	827	BCR	4	0
50	b	823	CLA	1	0
50	b	849	CLA	4	0
43	a	829	BCR	1	0
50	z	307	CLA	2	0
50	x	308	CLA	2	0
50	y	308	CLA	4	0
43	b	820	BCR	4	0
46	F	802	LMG	2	0
50	b	838	CLA	1	0
50	b	848	CLA	1	0
50	a	846	CLA	6	0
50	y	314	CLA	3	0
50	z	316	CLA	1	0
50	a	812	CLA	2	0
44	B	606	PGT	1	0
50	l	301	CLA	3	0
50	w	308	CLA	9	0
50	b	805	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	b	847	CLA	4	0
50	b	851	CLA	5	0
50	f	301	CLA	2	0
50	f	303	CLA	1	0
50	x	312	CLA	7	0
46	w	312	LMG	2	0
50	a	842	CLA	3	0
49	I	202	SF4	1	0
50	b	814	CLA	1	0
50	a	849	CLA	4	0
54	w	311	CHL	9	0
44	D	602	PGT	1	0
50	b	826	CLA	1	0
50	a	826	CLA	2	0
54	x	305	CHL	1	0
50	a	848	CLA	1	0
50	z	309	CLA	4	0
50	w	303	CLA	3	0
50	x	316	CLA	2	0
50	a	801	CLA	5	0
46	x	315	LMG	4	0
50	a	811	CLA	4	0
46	z	314	LMG	4	0
55	x	320	LUT	10	0
55	x	321	LUT	11	0
50	b	844	CLA	4	0
44	z	301	PGT	5	0
43	b	819	BCR	6	0
43	g	202	BCR	2	0
43	f	304	BCR	2	0
50	z	306	CLA	10	0
50	x	318	CLA	1	0
50	z	310	CLA	3	0
50	k	205	CLA	3	0
43	j	101	BCR	6	0
43	a	830	BCR	3	0
50	a	858	CLA	6	0
44	b	829	PGT	2	0
50	b	837	CLA	2	0
43	4	101	BCR	4	0
43	b	817	BCR	1	0
50	b	828	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	b	840	CLA	6	0
50	w	306	CLA	7	0
44	z	317	PGT	3	0
50	a	841	CLA	2	0
43	b	831	BCR	5	0
47	A	405	PQ9	15	0
50	b	841	CLA	3	0
54	w	304	CHL	1	0
50	x	307	CLA	3	0
53	a	825	PQN	1	0
50	a	814	CLA	5	0
50	w	316	CLA	2	0
50	z	302	CLA	3	0
54	x	311	CHL	3	0
55	y	315	LUT	32	0
50	w	307	CLA	5	0
50	a	852	CLA	1	0
50	a	843	CLA	3	0
50	b	839	CLA	2	0
43	l	303	BCR	2	0
50	a	844	CLA	3	0
50	b	803	CLA	5	0
50	b	822	CLA	3	0
50	a	833	CLA	3	0
50	a	820	CLA	5	0
50	b	804	CLA	3	0
44	a	806	PGT	1	0
55	w	319	LUT	9	0
44	A	403	PGT	2	0
44	w	313	PGT	1	0
55	w	320	LUT	21	0
46	D	601	LMG	1	0
53	b	827	PQN	3	0
50	b	836	CLA	4	0
50	w	310	CLA	4	0
43	b	818	BCR	1	0
50	a	850	CLA	2	0
43	a	803	BCR	1	0
50	a	838	CLA	8	0
43	a	831	BCR	2	0
50	w	314	CLA	1	0
44	z	313	PGT	1	0

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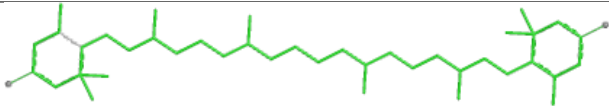
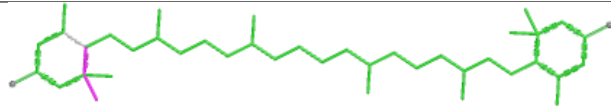
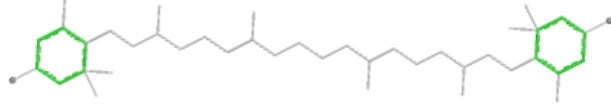
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	a	807	PGT	2	0
50	a	854	CLA	4	0
50	a	809	CLA	3	0
44	B	603	PGT	3	0
50	b	801	CLA	6	0
50	b	812	CLA	2	0
50	a	818	CLA	1	0
50	a	853	CLA	2	0
46	B	605	LMG	1	0
46	z	315	LMG	3	0
50	x	310	CLA	1	0
54	x	301	CHL	1	0
48	w	317	SQD	2	0
50	b	835	CLA	1	0
50	b	809	CLA	2	0
44	L	201	PGT	2	0
45	F	804	A1H1M	6	0
50	l	306	CLA	2	0
50	k	204	CLA	1	0
48	a	859	SQD	3	0
50	b	842	CLA	2	0
50	g	201	CLA	2	0
55	z	320	LUT	27	0
50	b	802	CLA	3	0
50	a	802	CLA	2	0
50	b	815	CLA	3	0
50	h	201	CLA	2	0
50	b	833	CLA	5	0
48	B	604	SQD	10	0
43	i	101	BCR	2	0
48	w	318	SQD	13	0
50	b	813	CLA	1	0
51	b	821	DGD	3	0
50	a	822	CLA	2	0
50	x	303	CLA	2	0
50	b	834	CLA	1	0
50	a	857	CLA	5	0
50	b	845	CLA	5	0
50	y	313	CLA	5	0
50	a	839	CLA	5	0
50	a	836	CLA	4	0
54	x	319	CHL	5	0

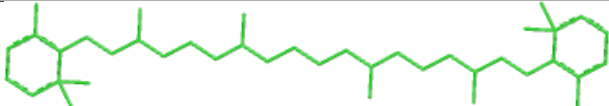
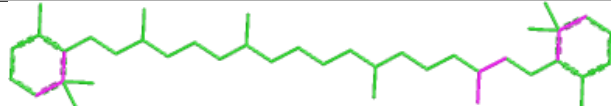
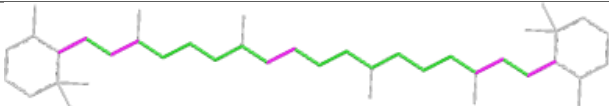
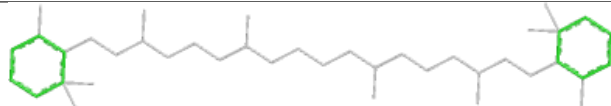
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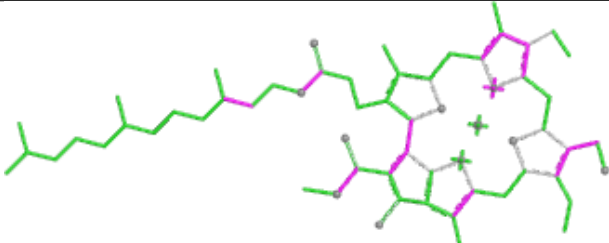
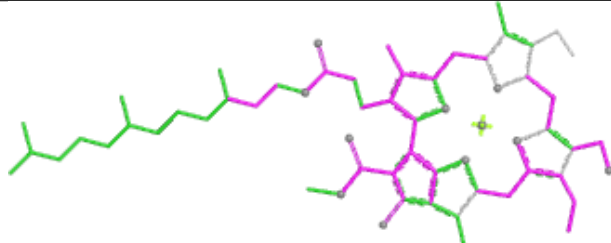
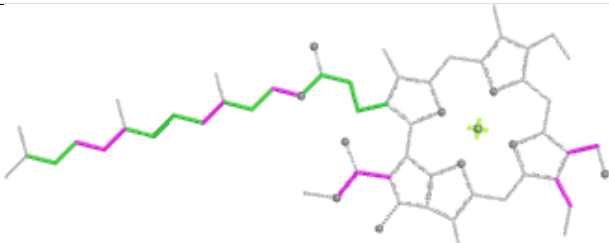
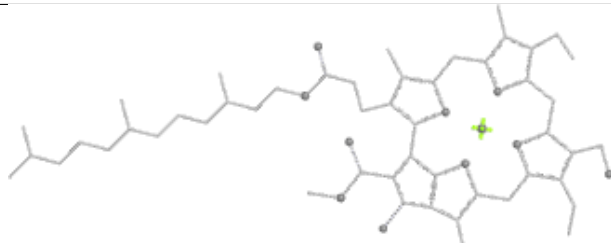
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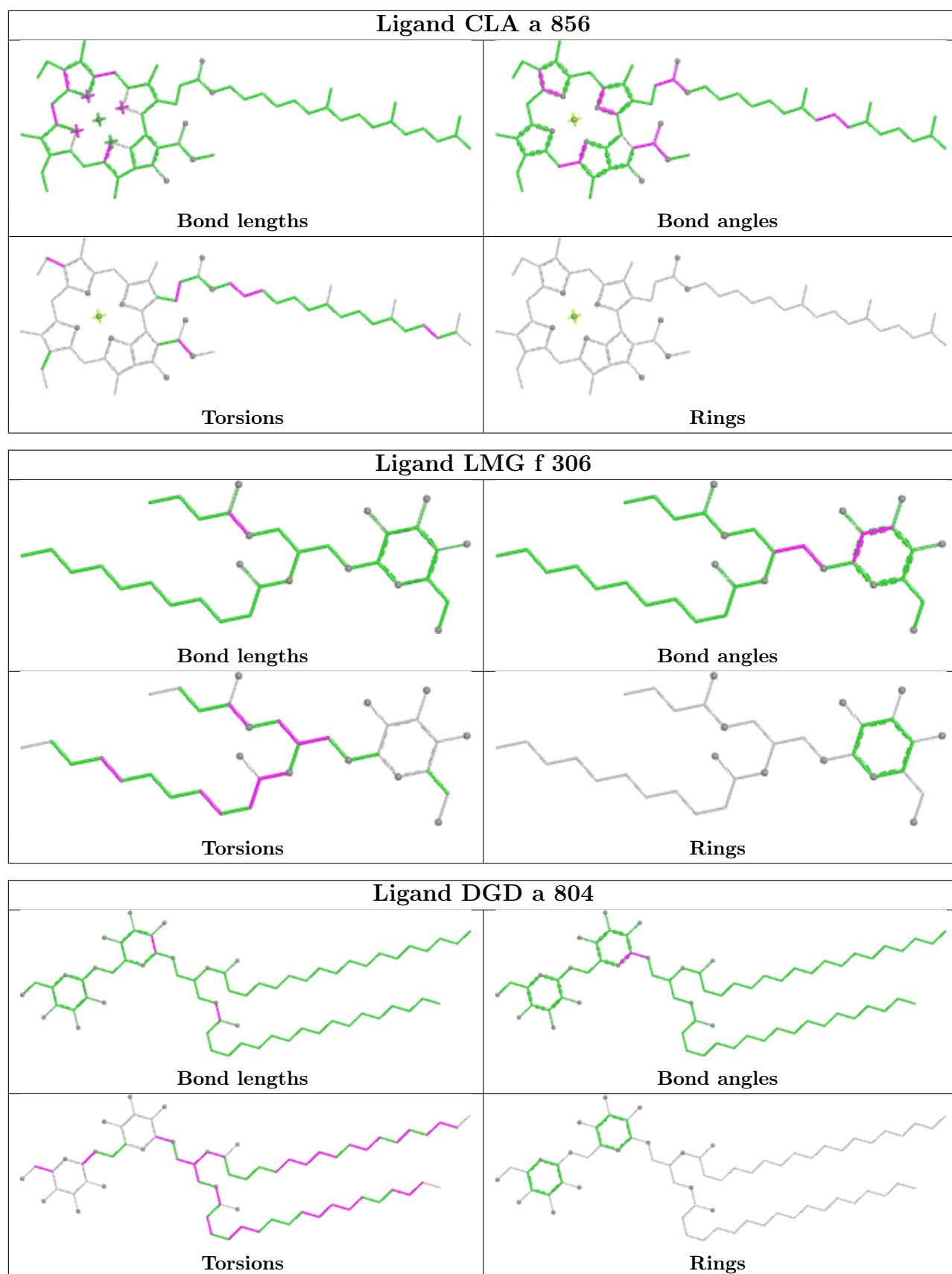
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	a	835	CLA	5	0
48	F	801	SQD	7	0
43	j	103	BCR	4	0
54	w	309	CHL	3	0
50	b	846	CLA	1	0
50	l	305	CLA	1	0
50	b	806	CLA	1	0
43	z	318	BCR	1	0
44	N	301	PGT	2	0
43	a	828	BCR	4	0
46	j	104	LMG	1	0
43	b	850	BCR	3	0
50	k	203	CLA	1	0
54	z	304	CHL	1	0
50	y	311	CLA	5	0
48	F	805	SQD	11	0
43	x	314	BCR	1	0
50	a	813	CLA	2	0
50	z	305	CLA	1	0
50	b	825	CLA	3	0
50	y	312	CLA	3	0
50	y	303	CLA	11	0
55	z	321	LUT	7	0
50	b	843	CLA	2	0
44	A	402	PGT	1	0
50	a	845	CLA	5	0
50	z	319	CLA	3	0
43	l	304	BCR	1	0
50	a	837	CLA	1	0

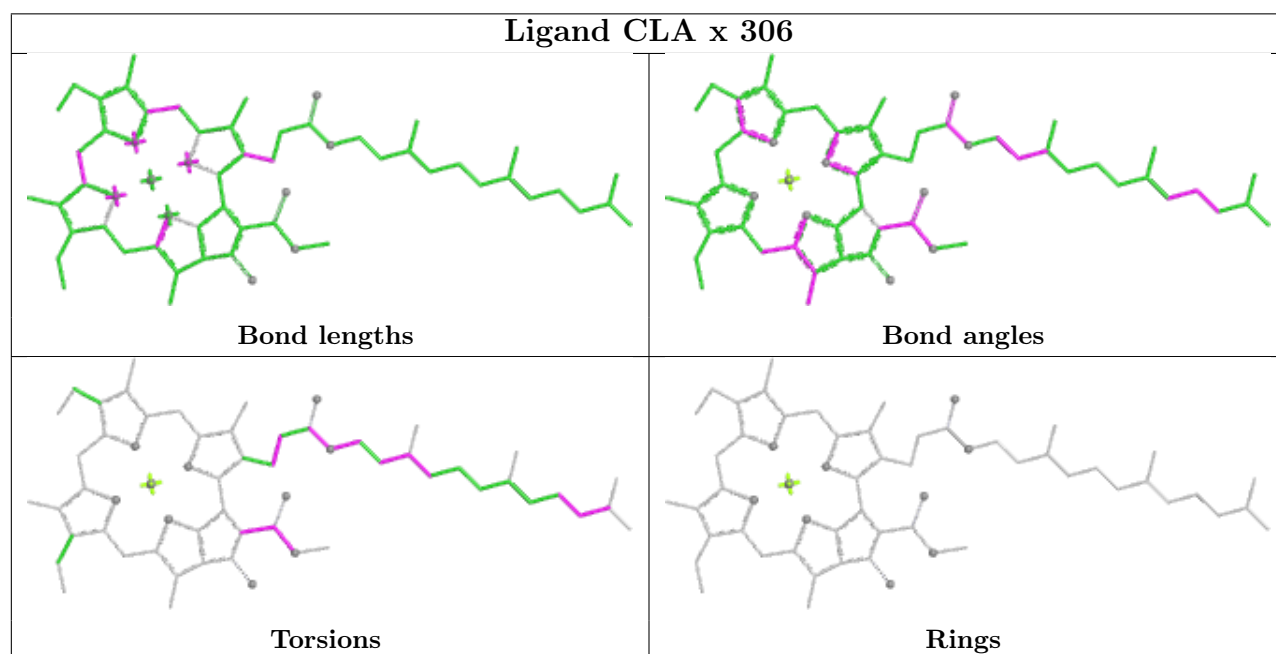
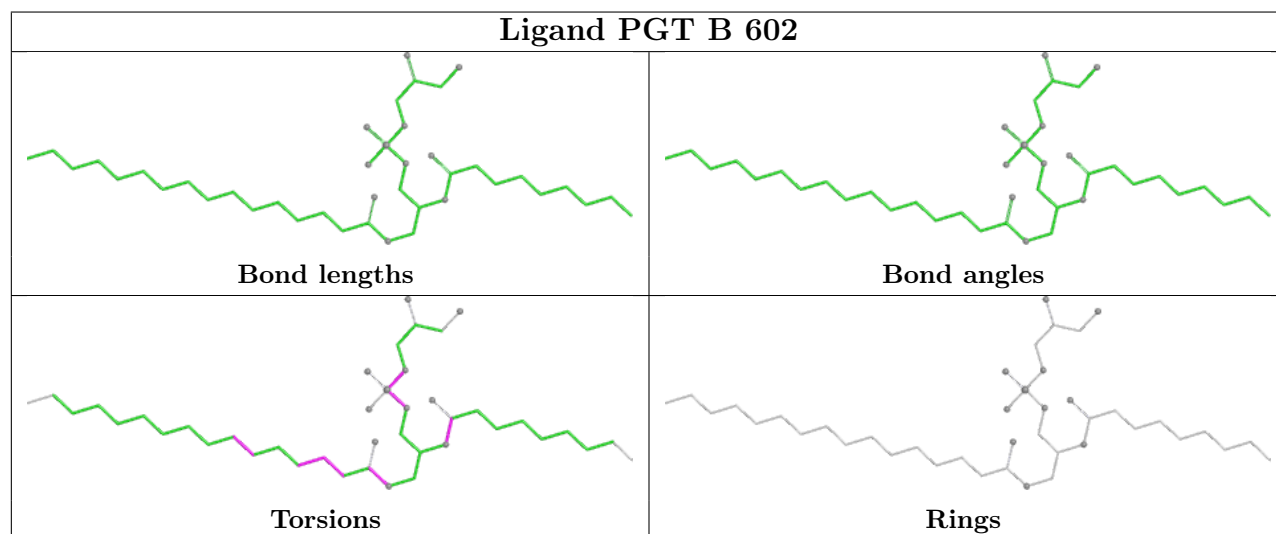
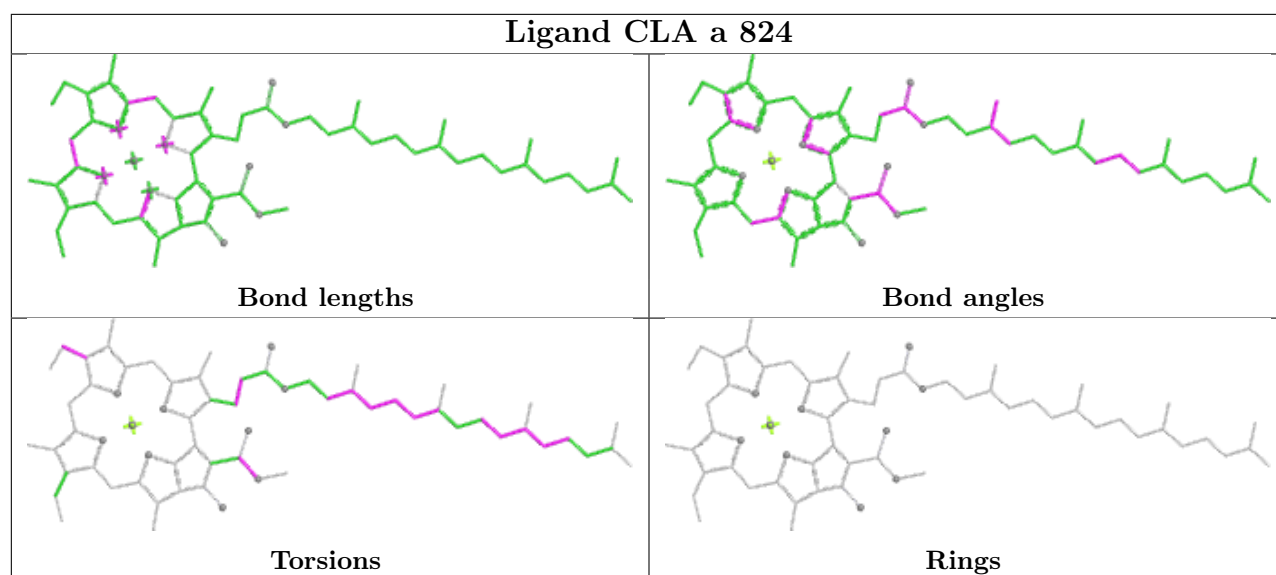
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

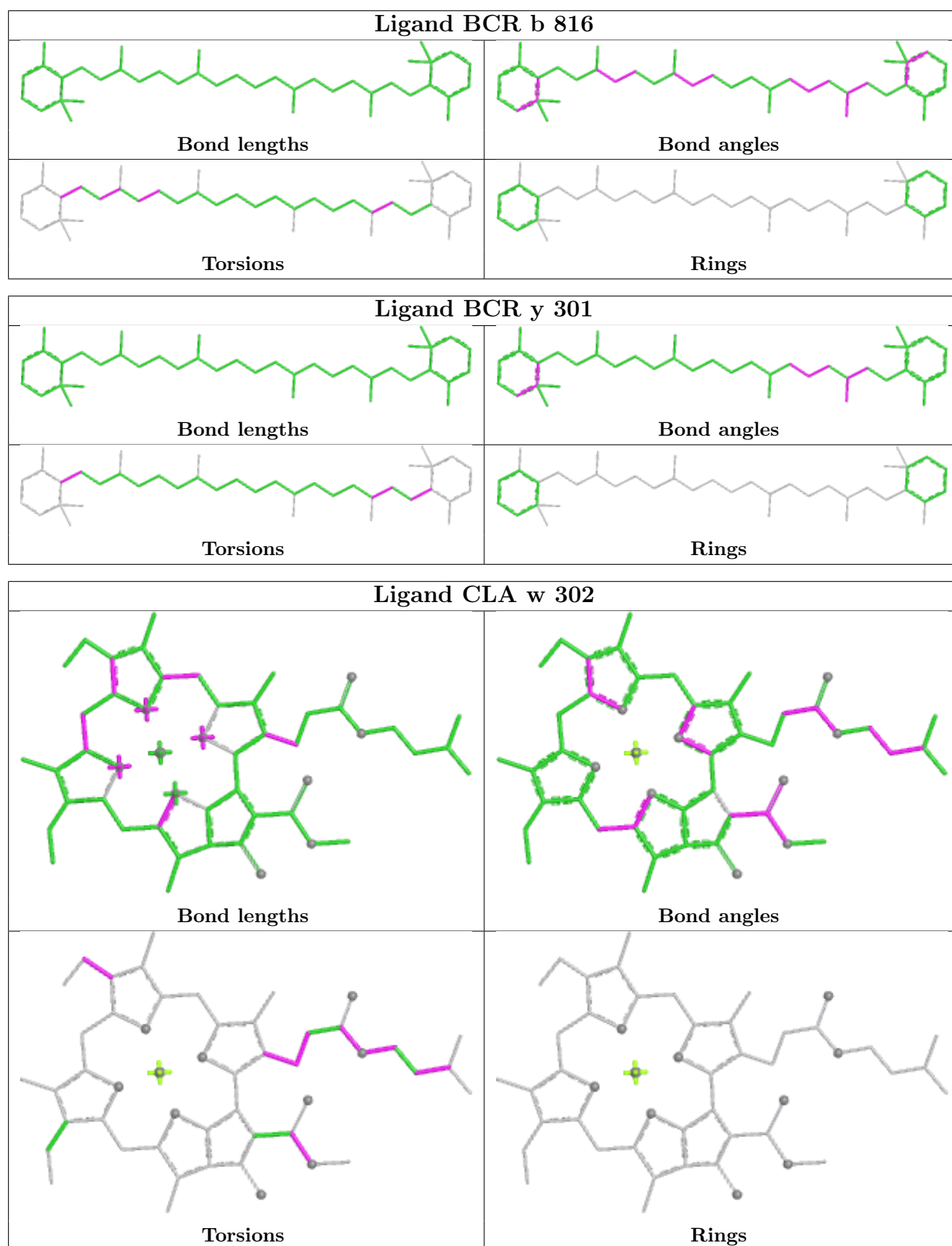
Ligand LUT y 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

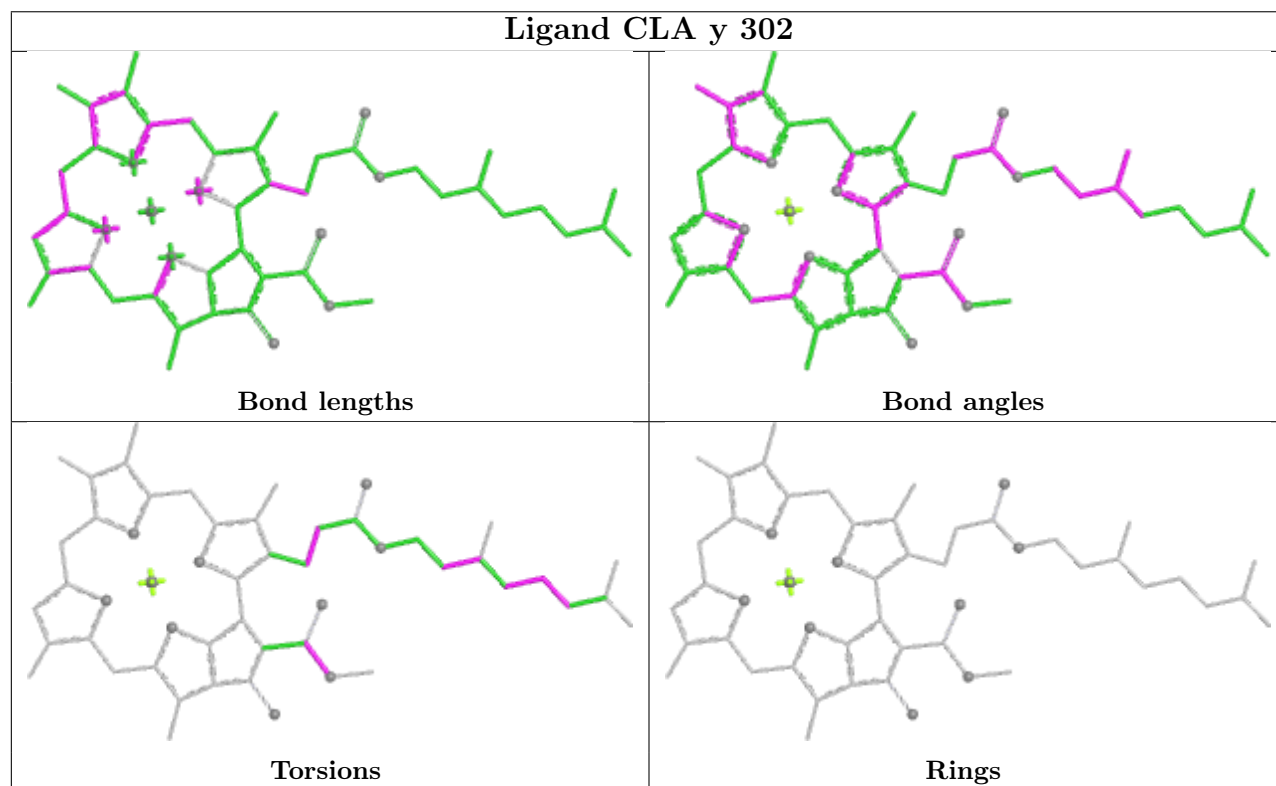
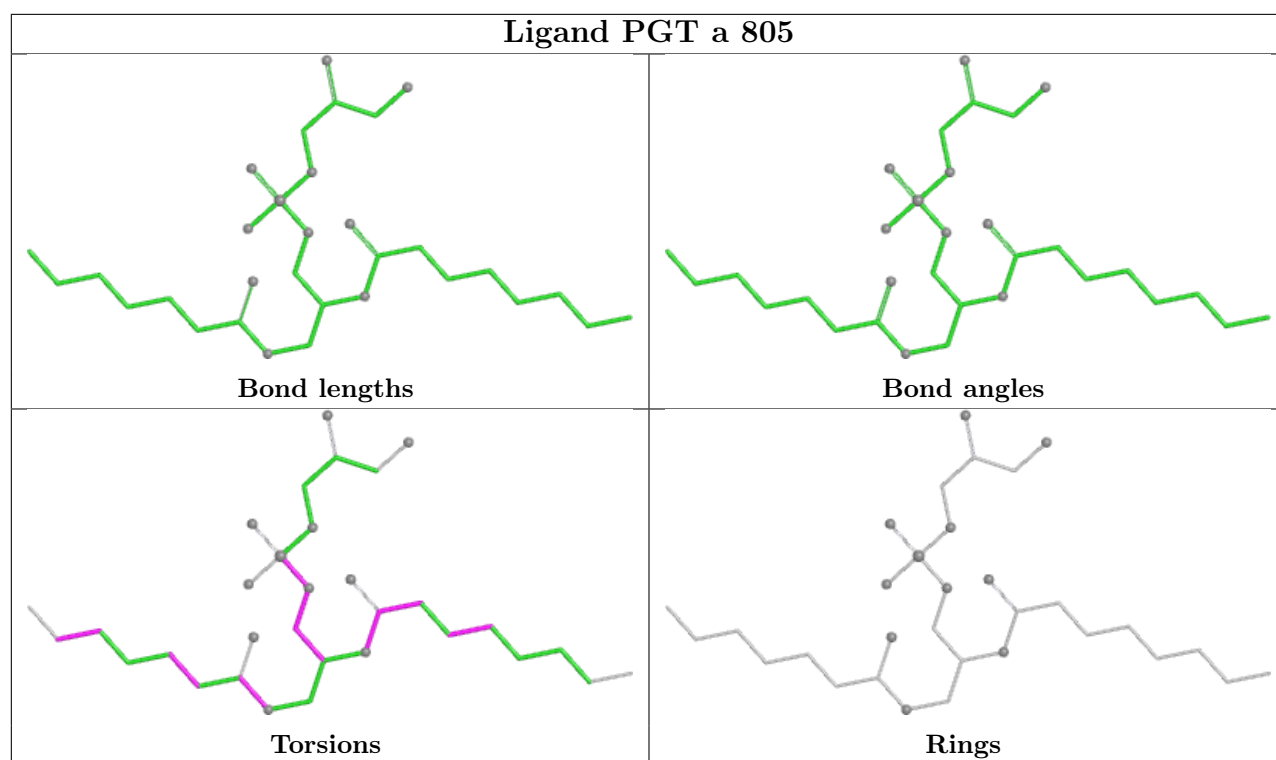
Ligand BCR l 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

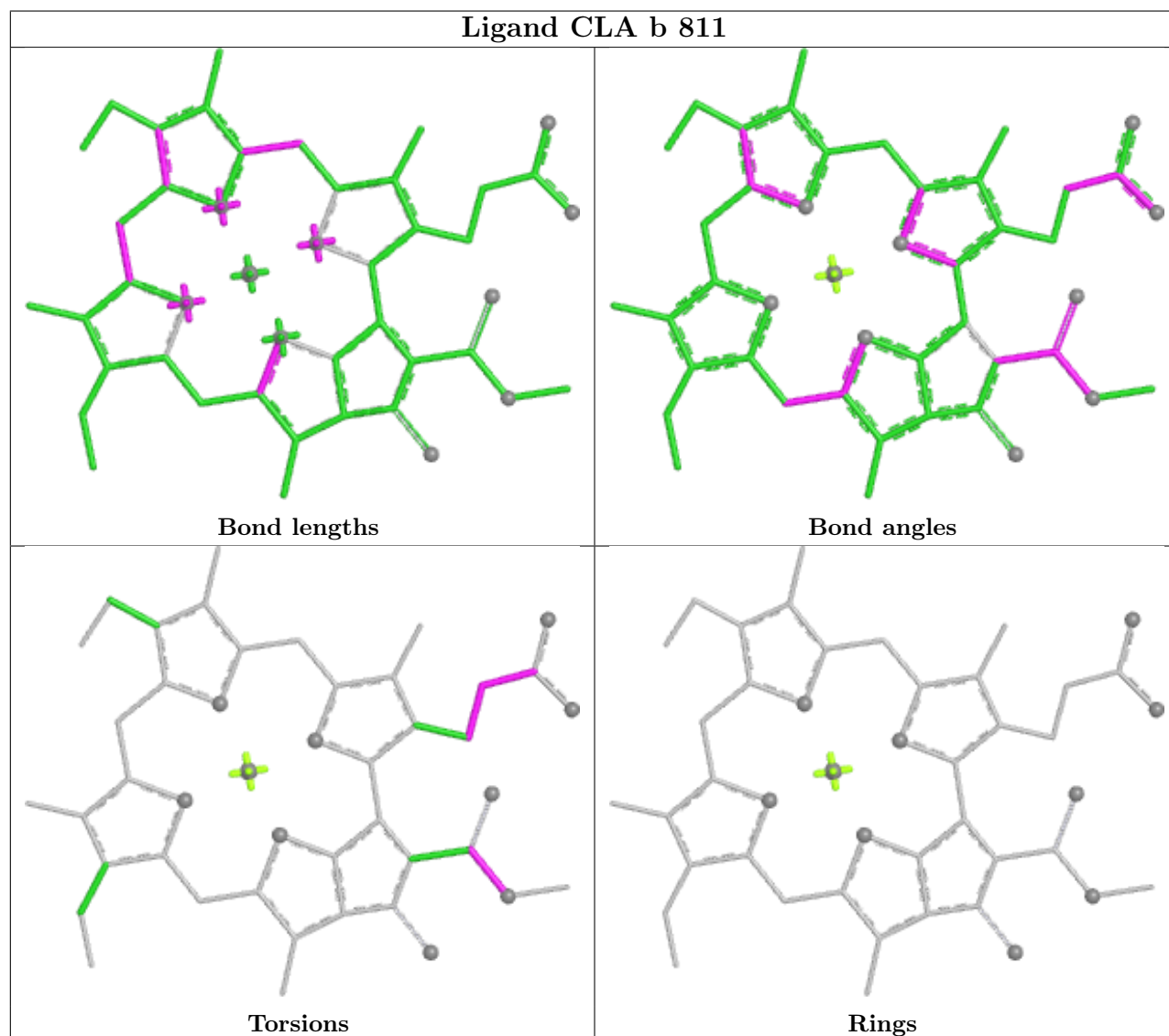
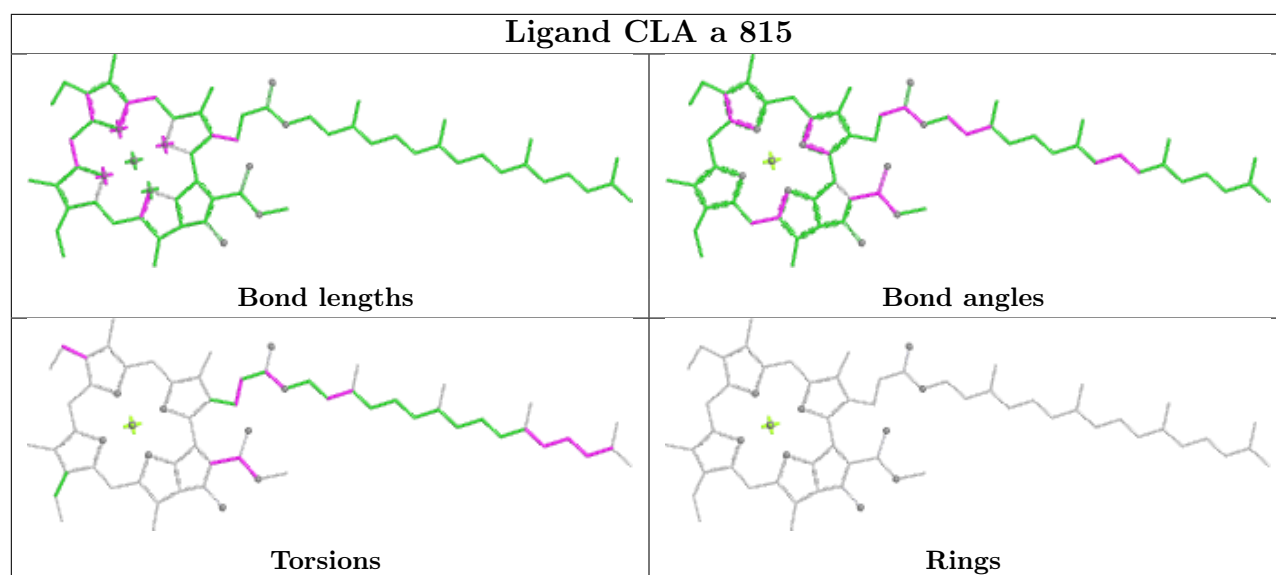
Ligand CHL z 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

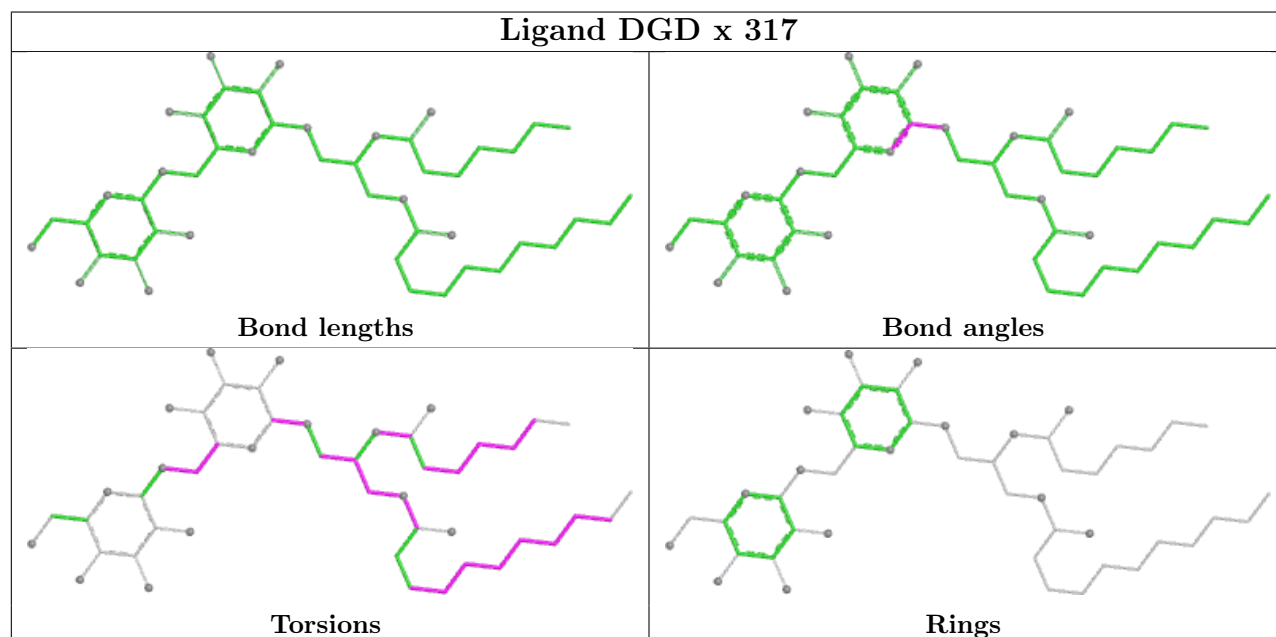
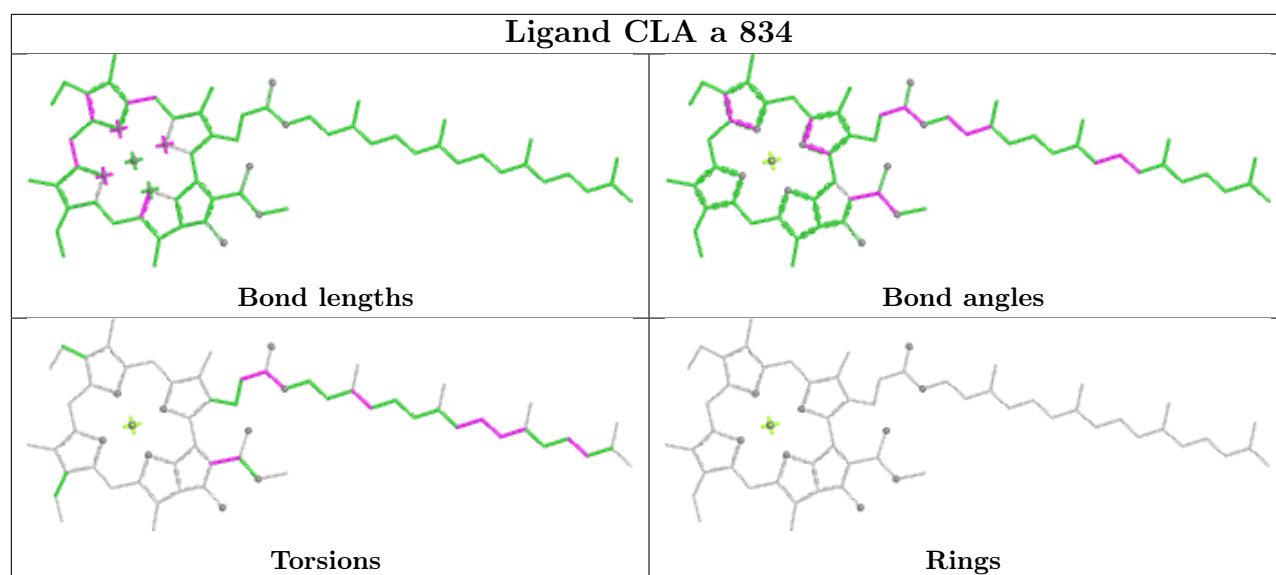


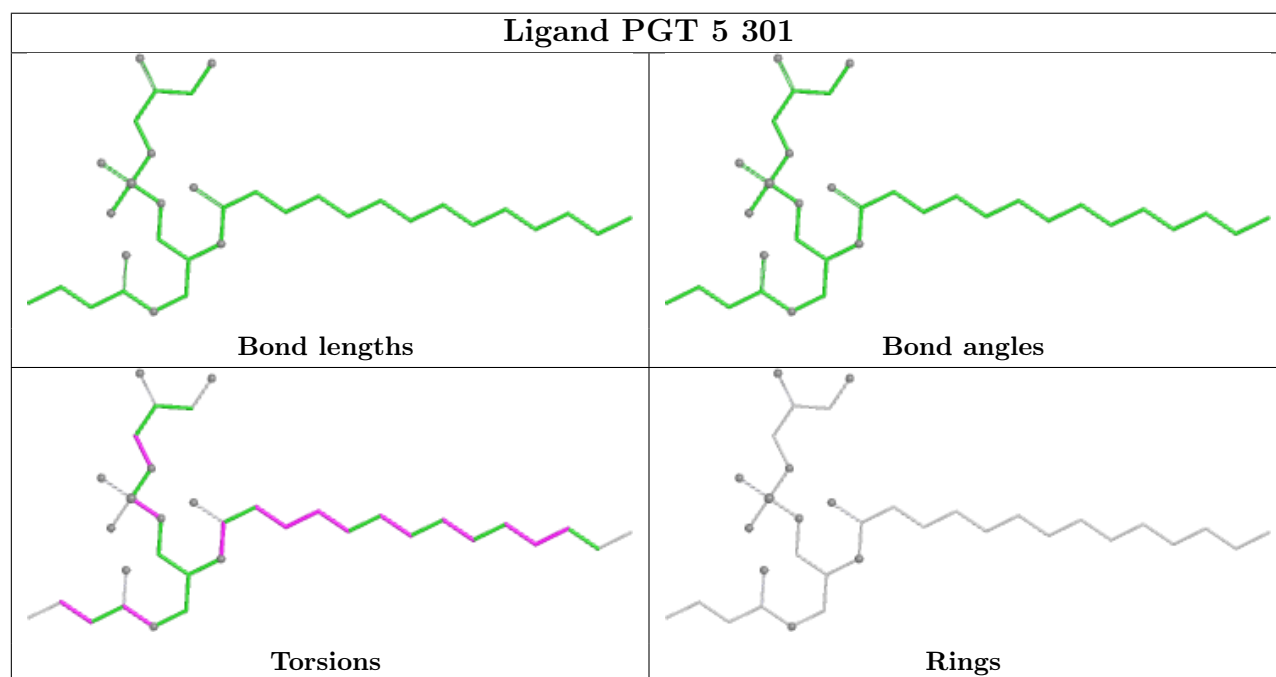
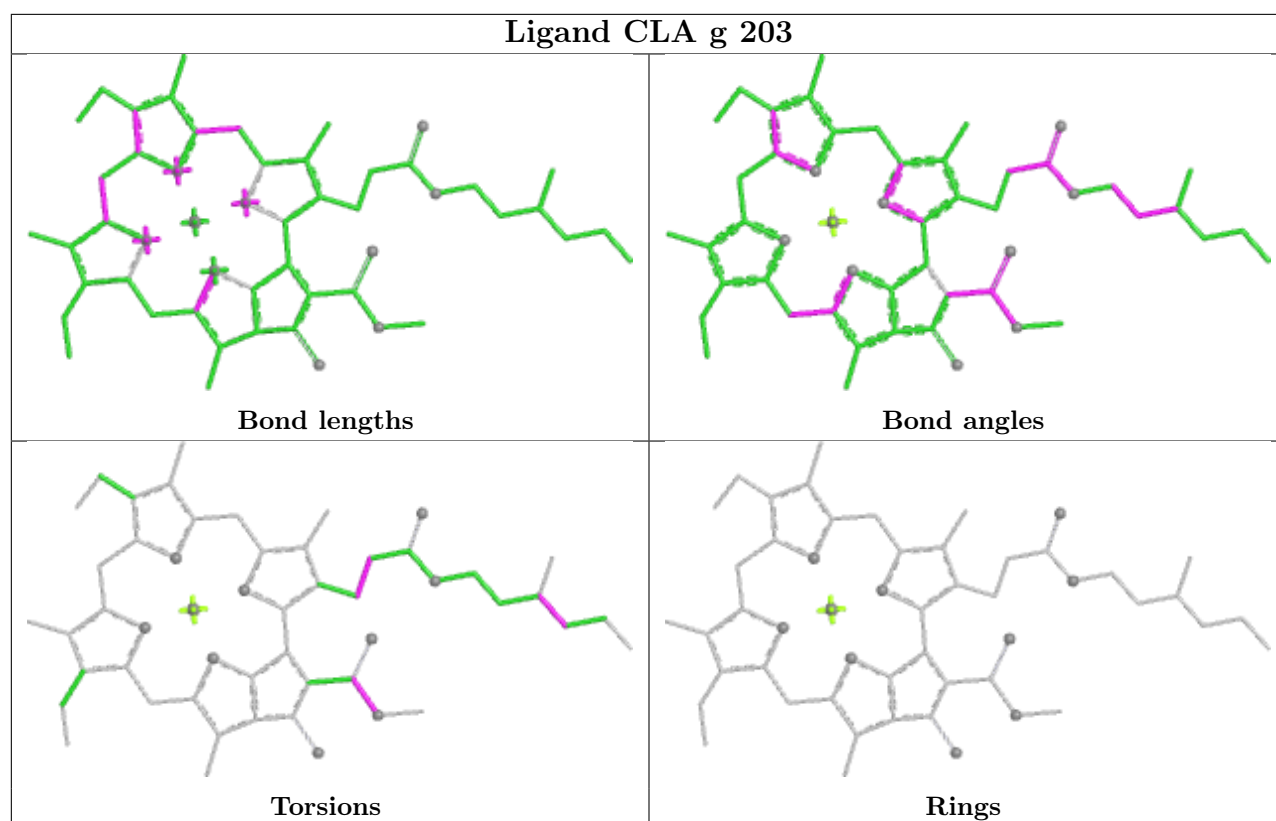


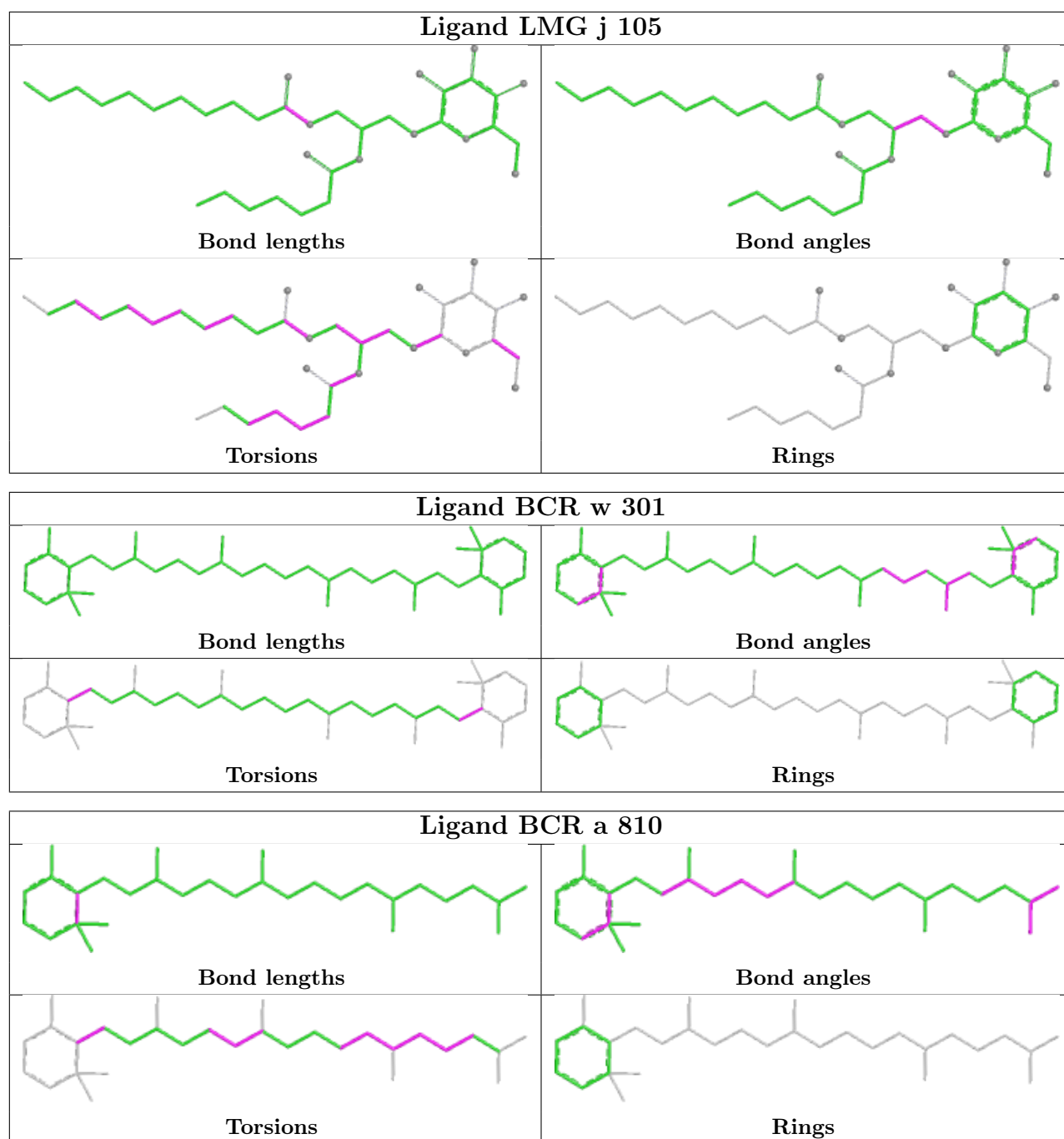


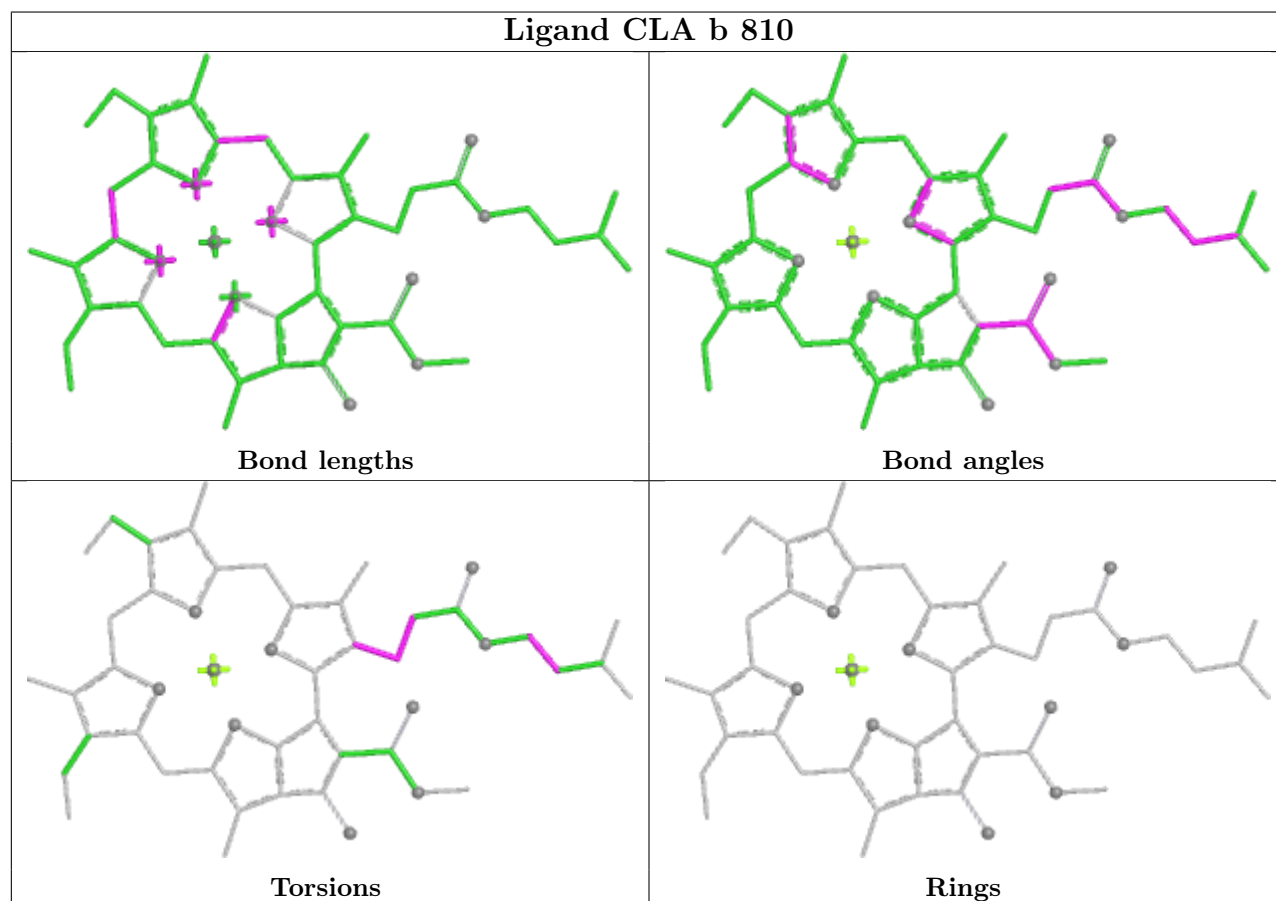
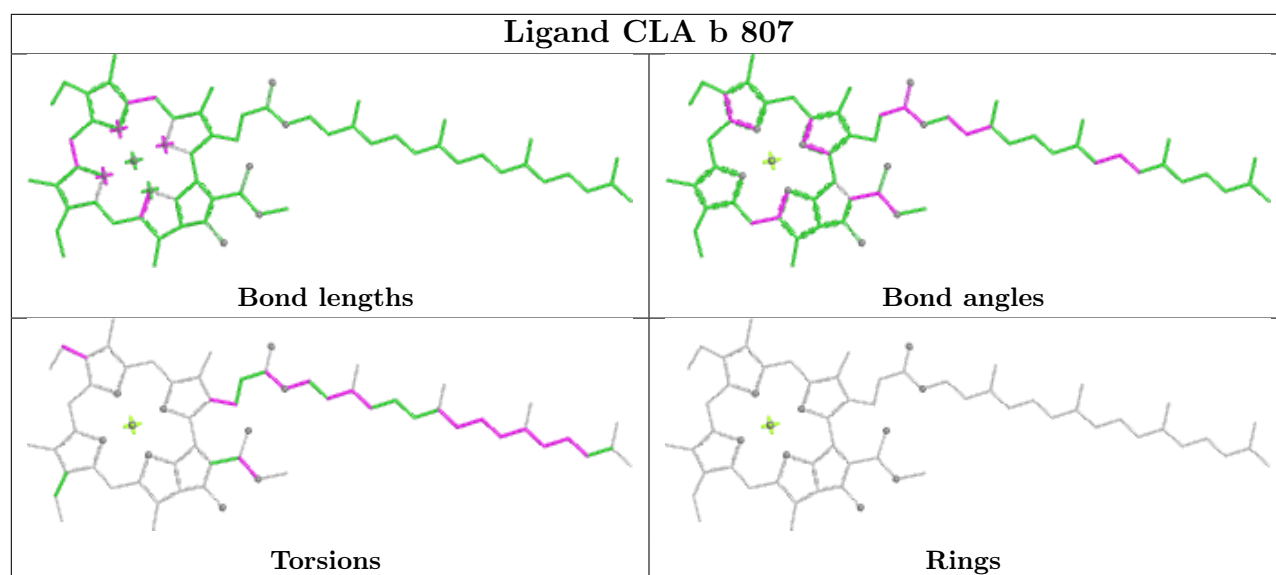


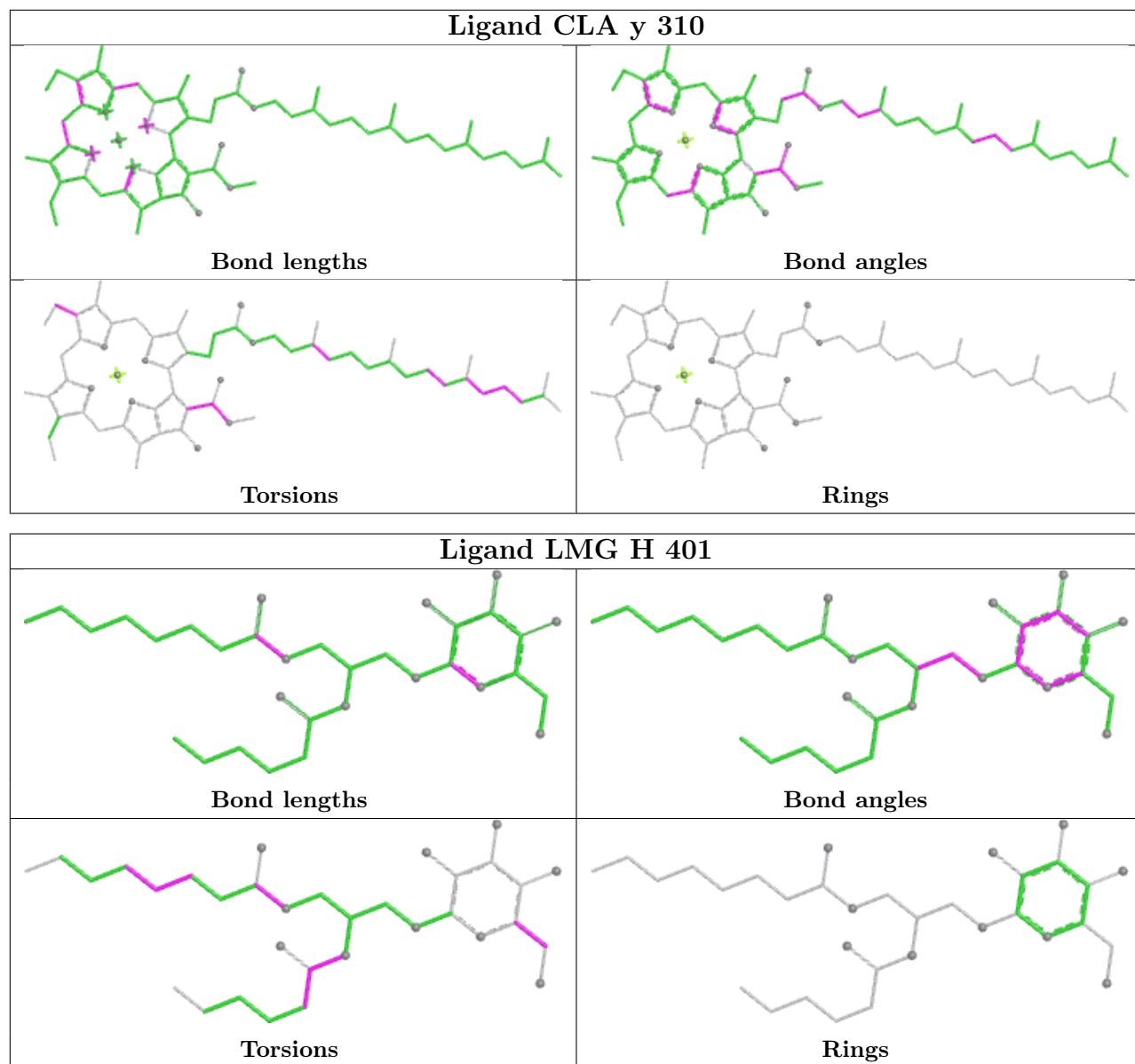


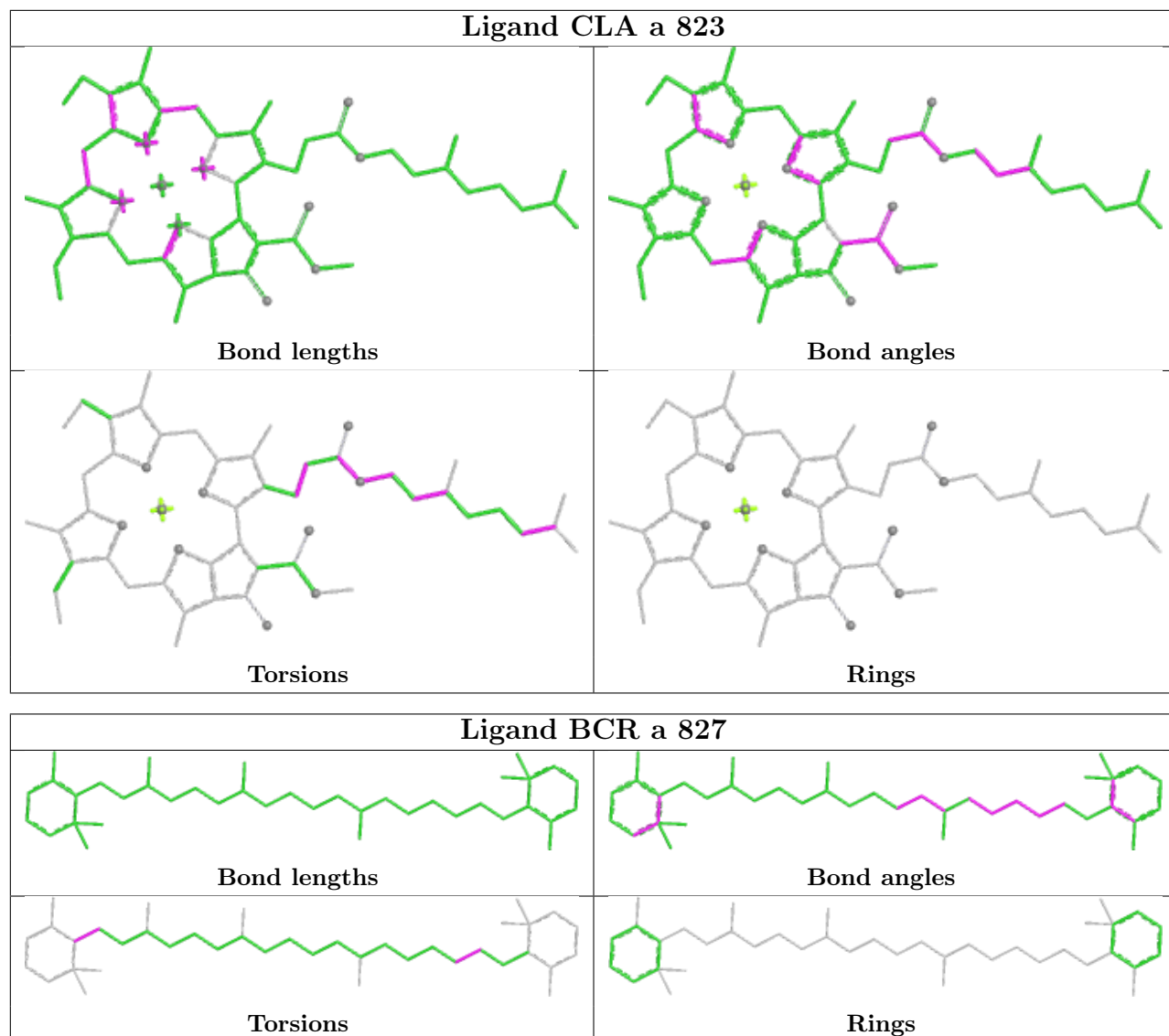




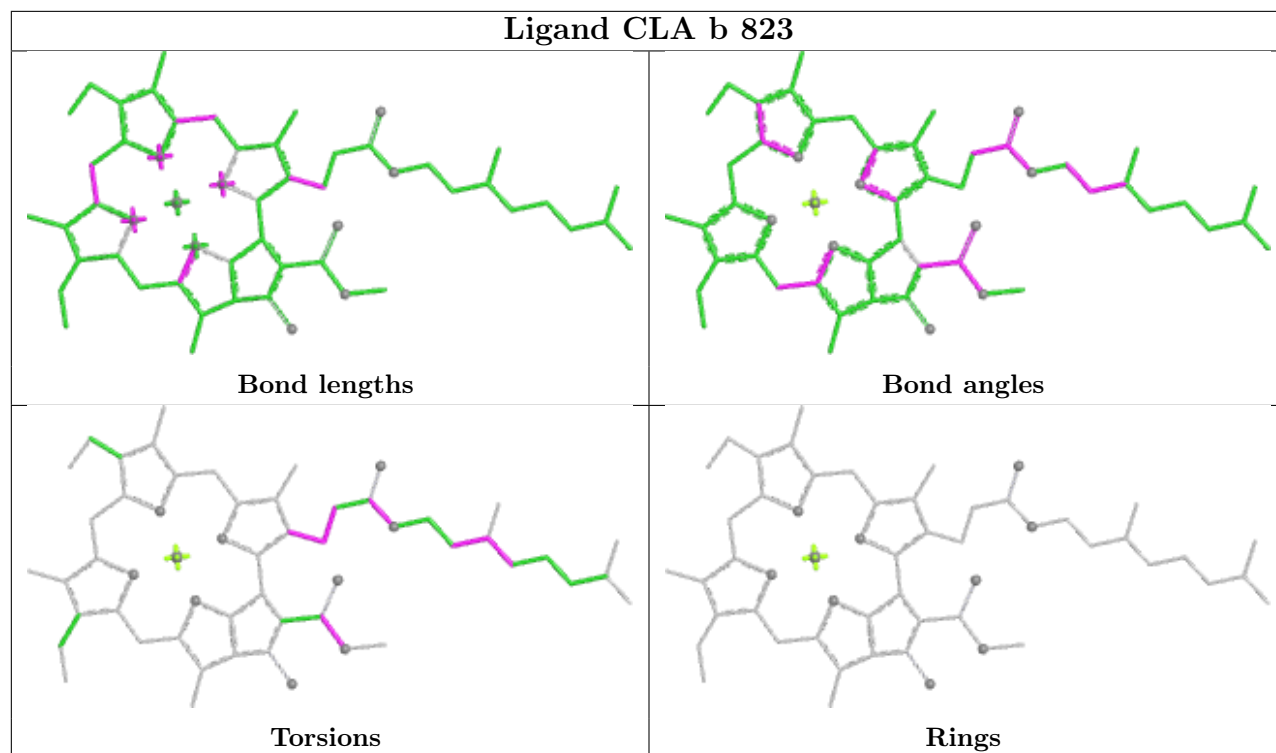




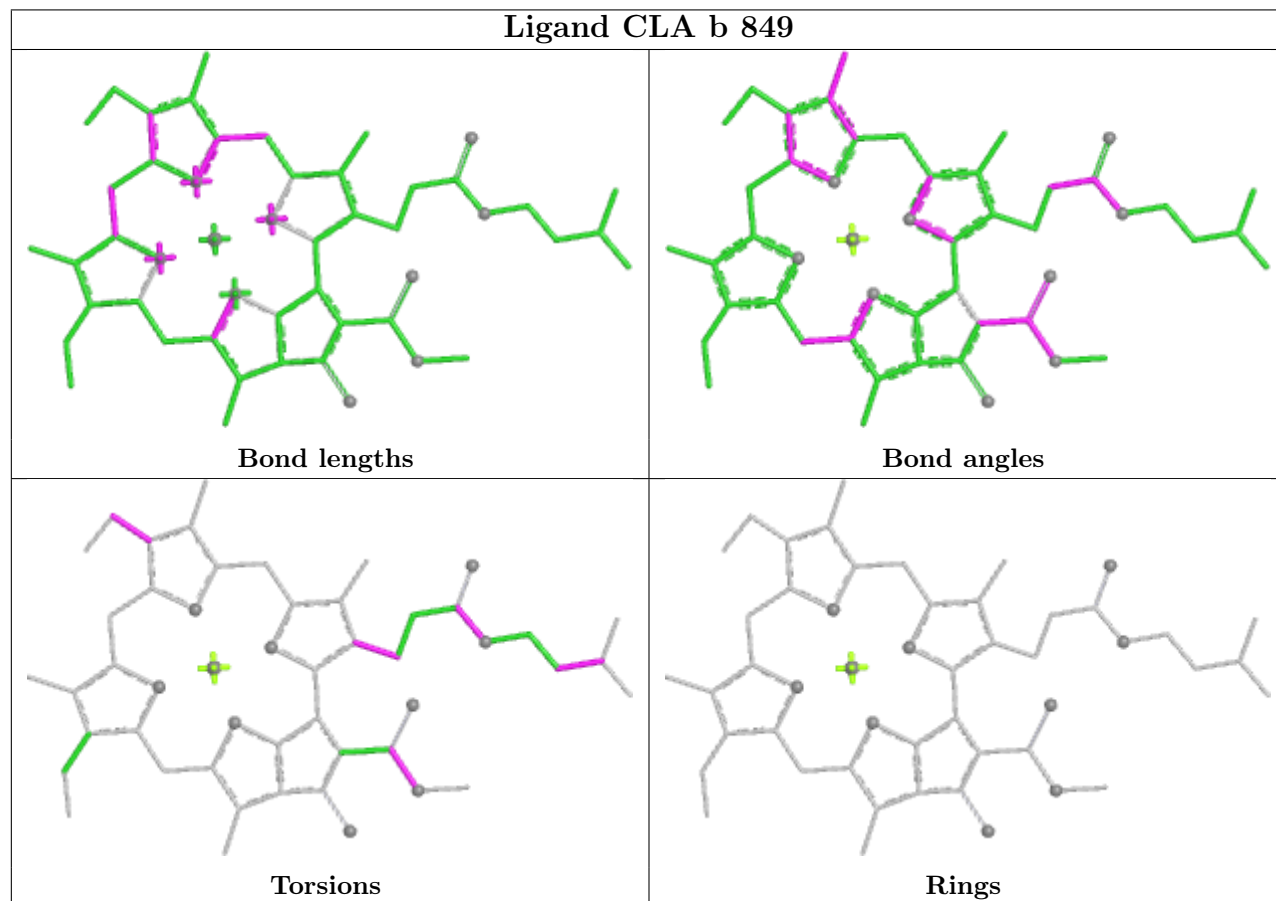


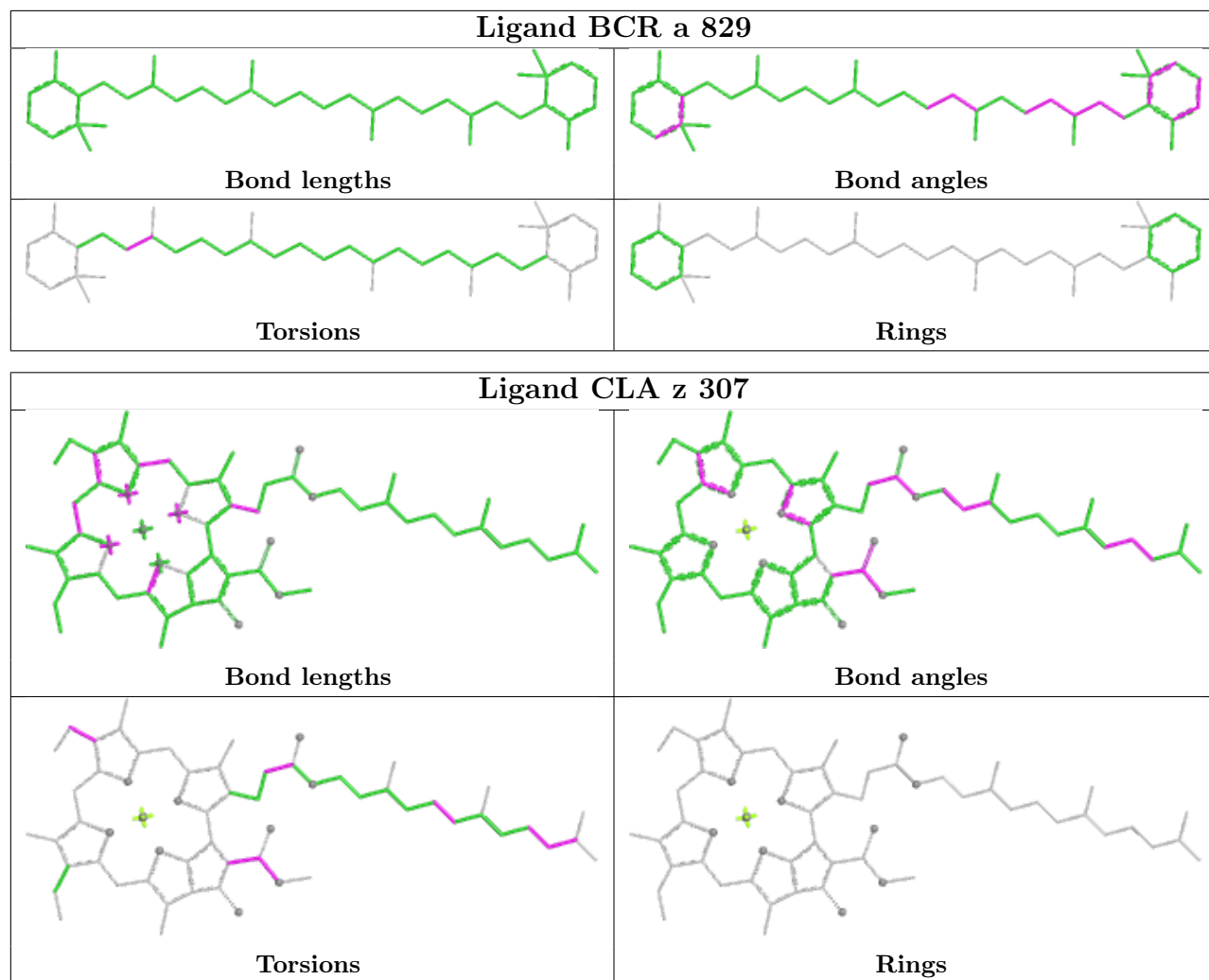


Ligand CLA b 823

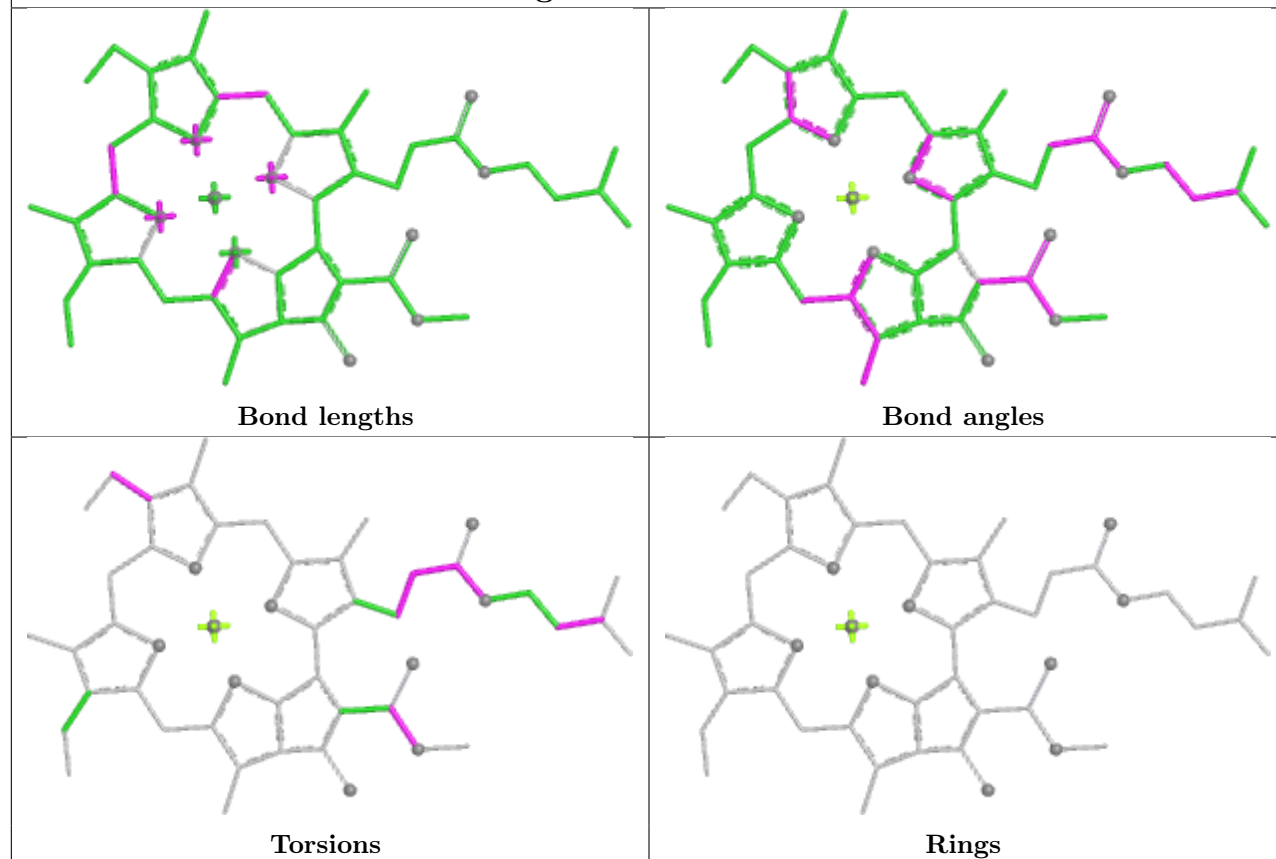


Ligand CLA b 849

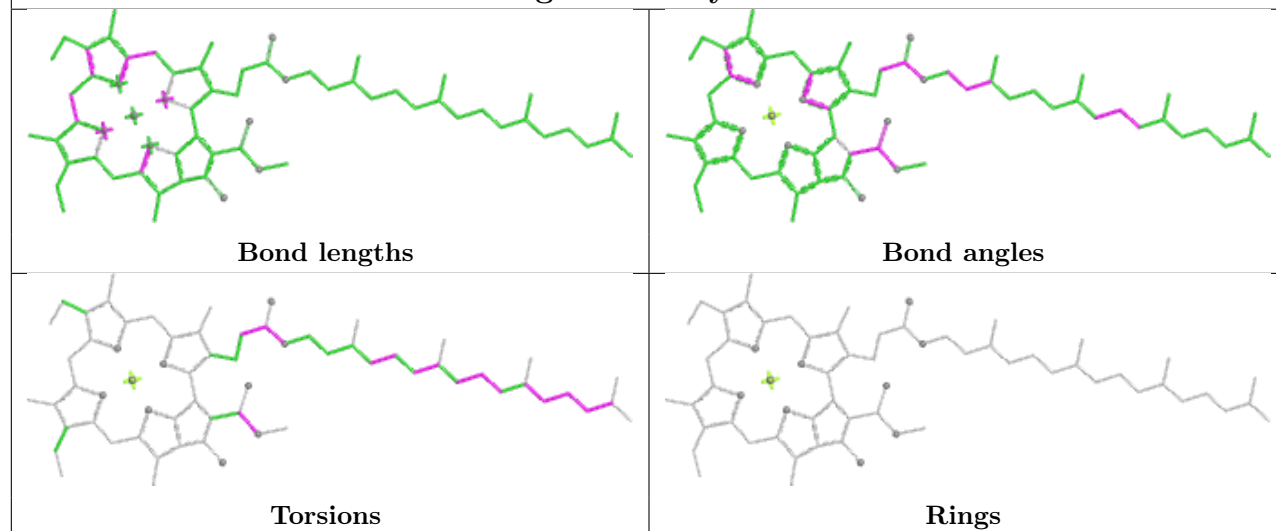


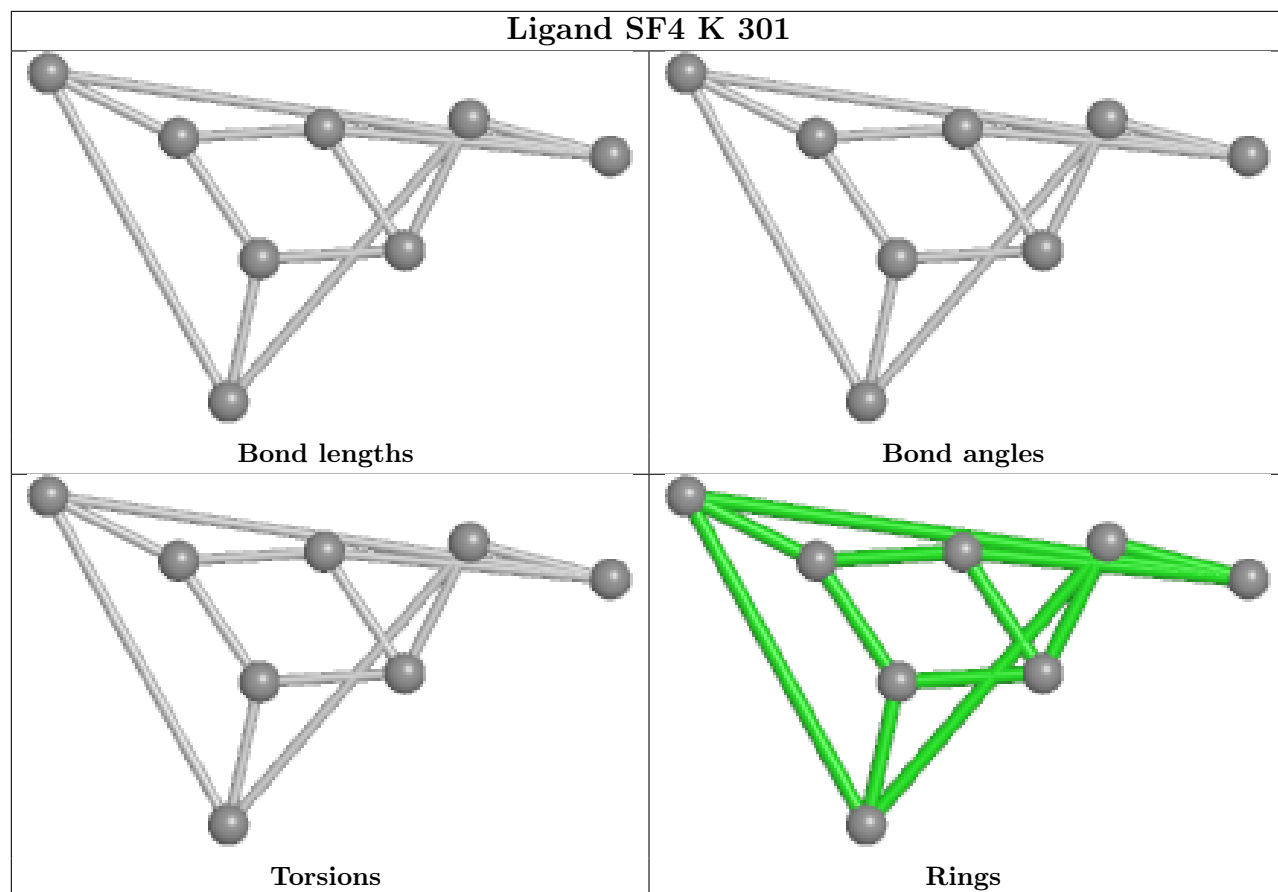


Ligand CLA x 308

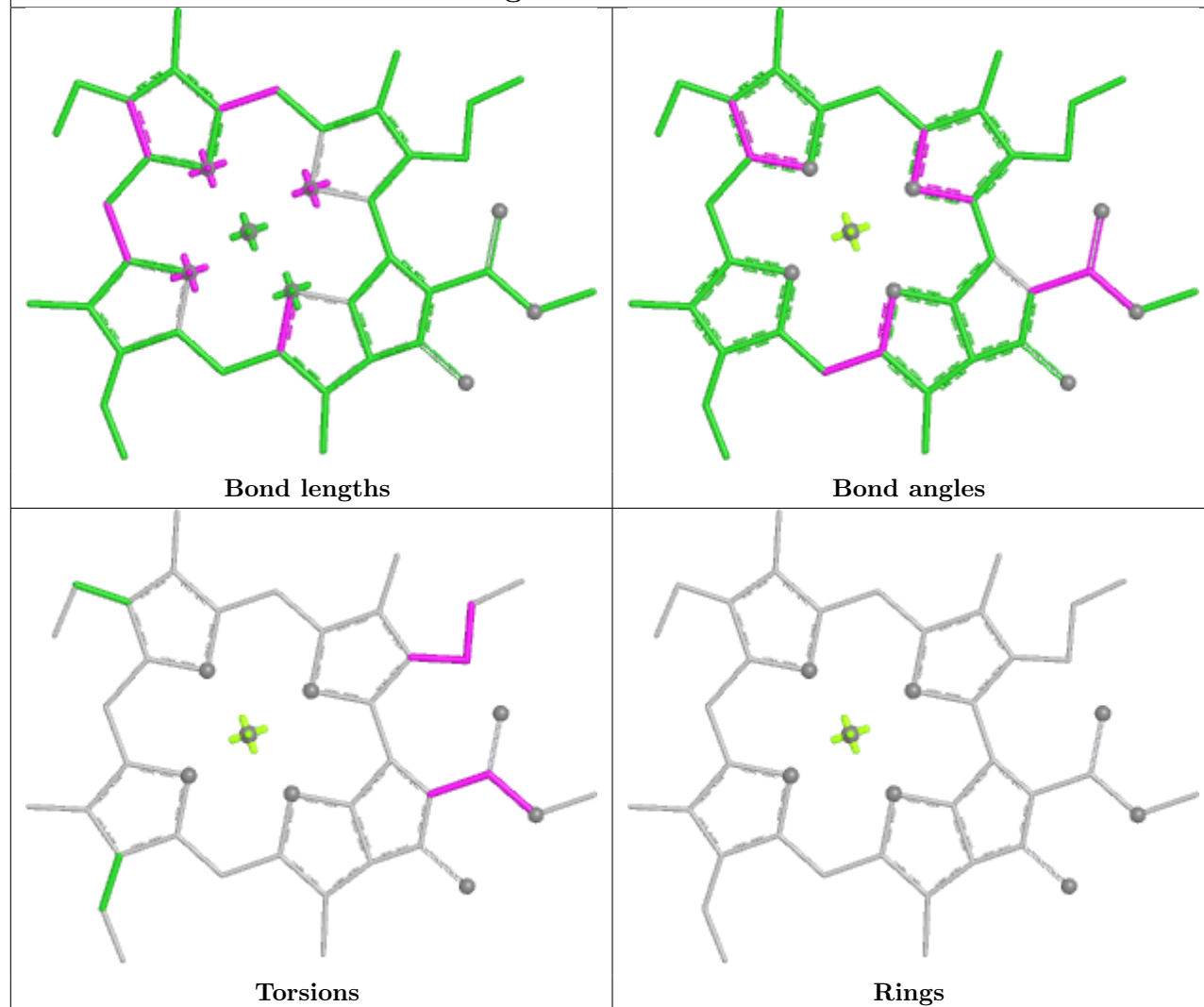


Ligand CLA y 308

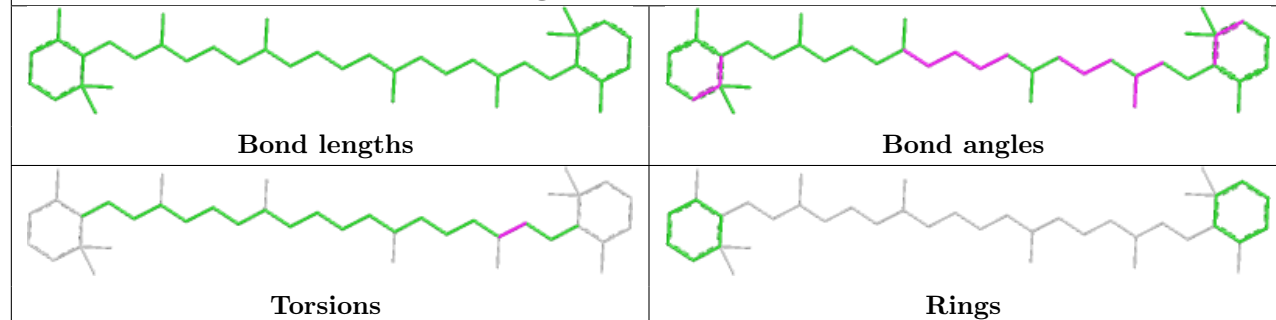


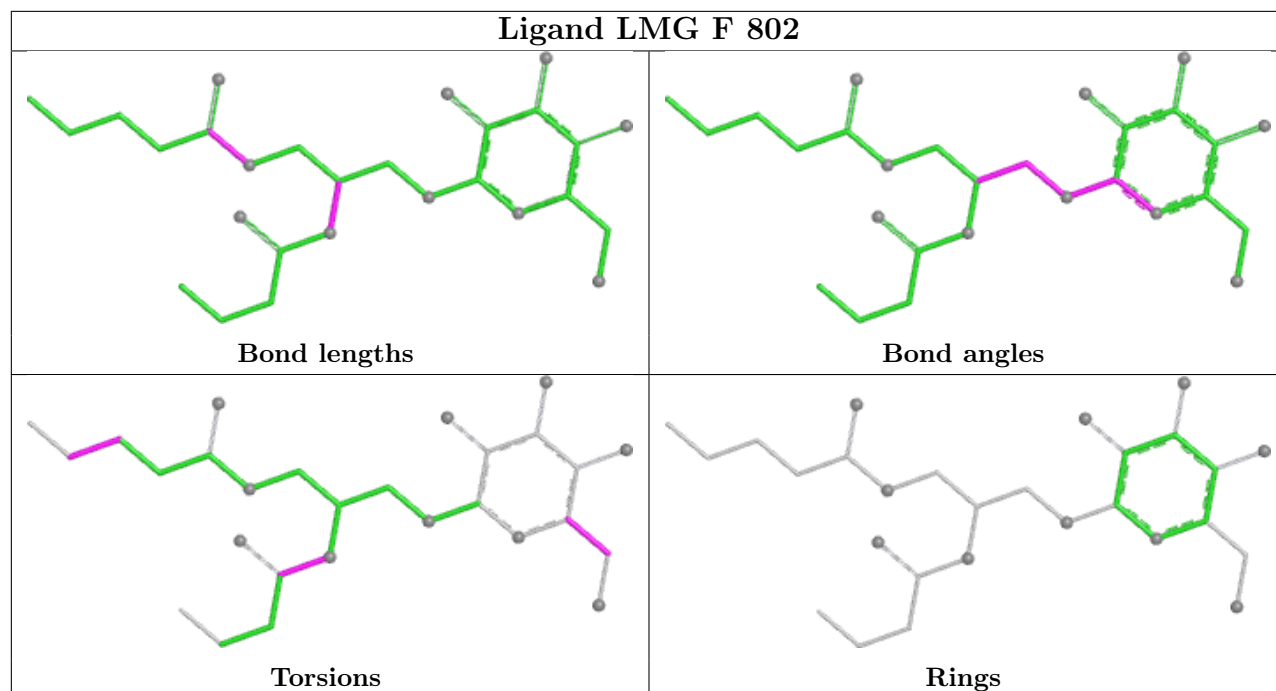


Ligand CLA b 808

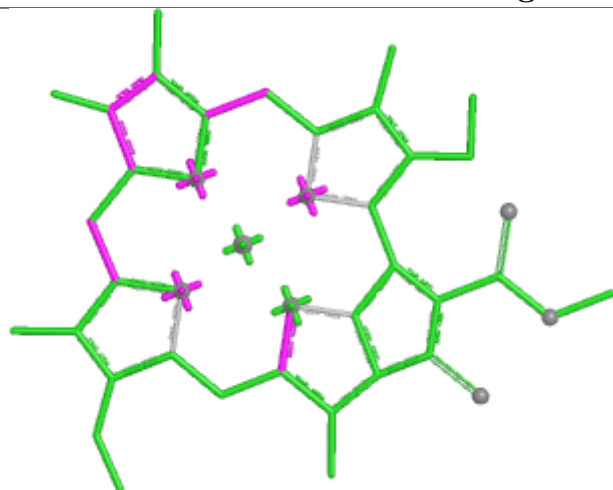


Ligand BCR b 820

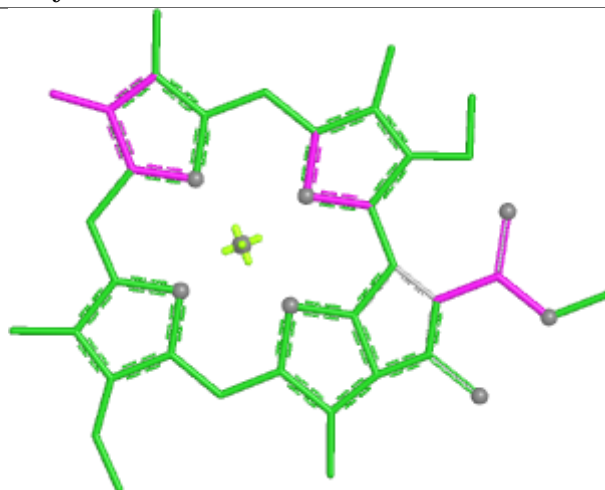




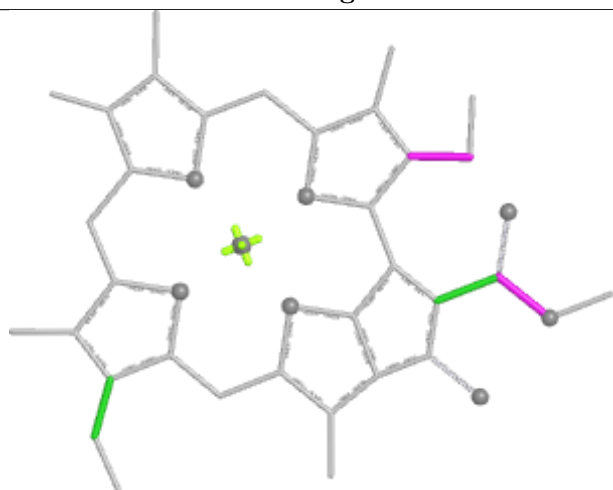
Ligand CLA y 307



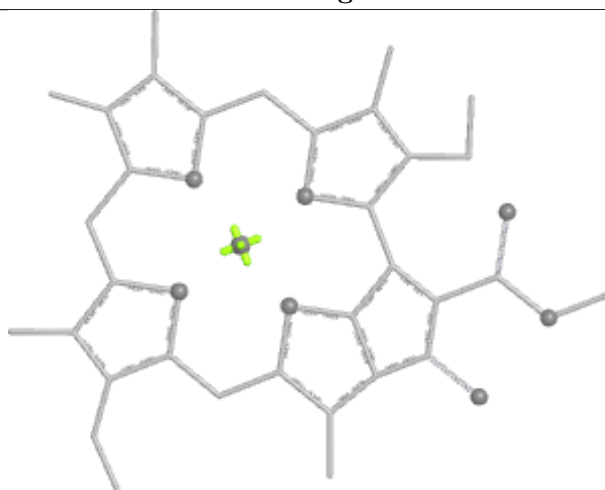
Bond lengths



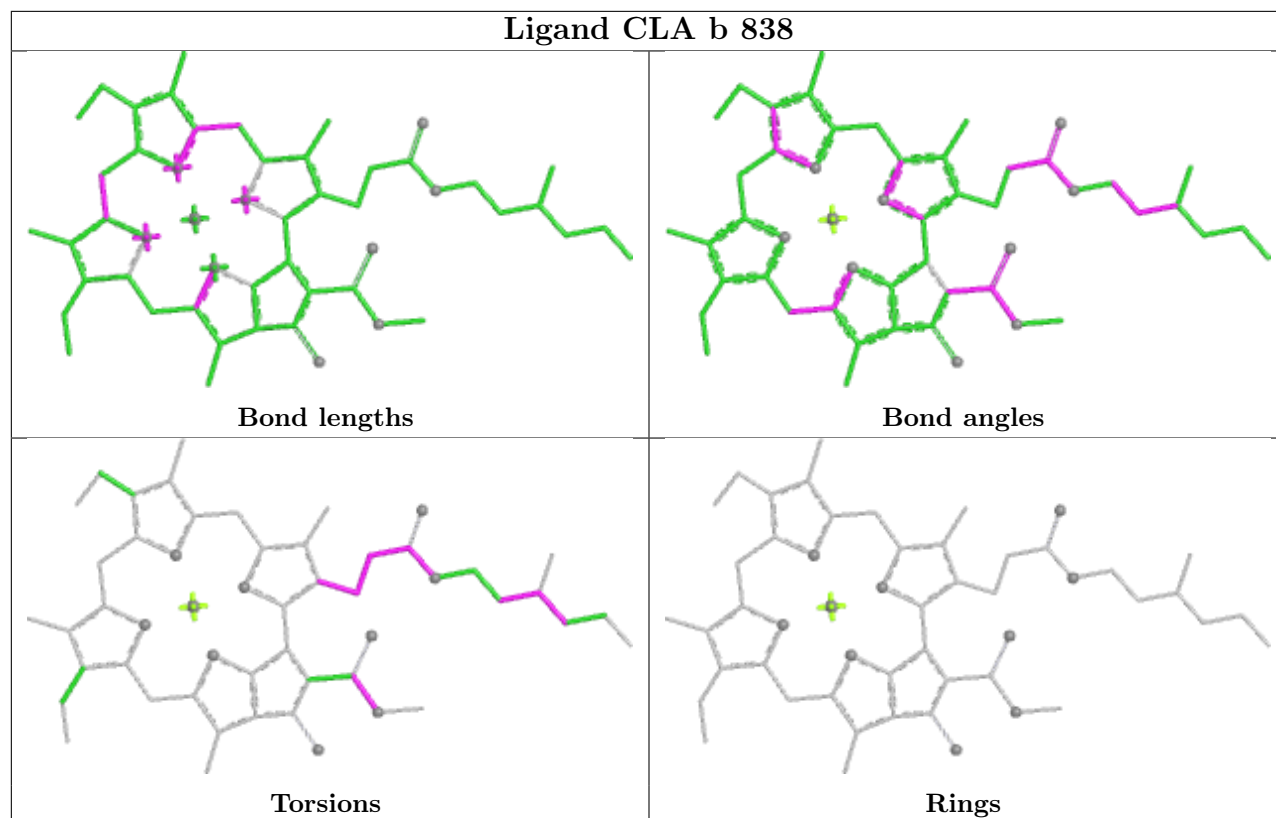
Bond angles



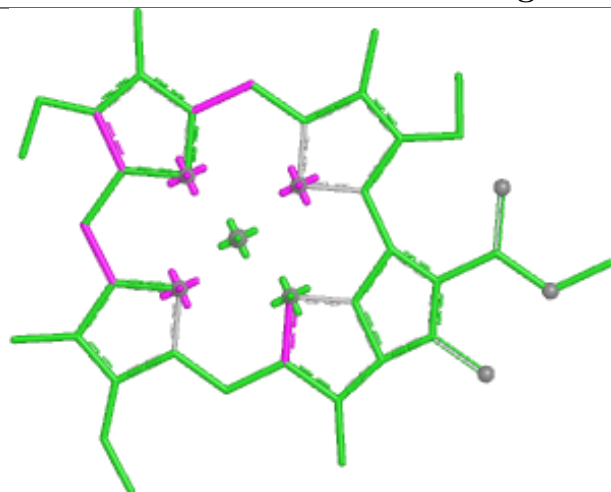
Torsions



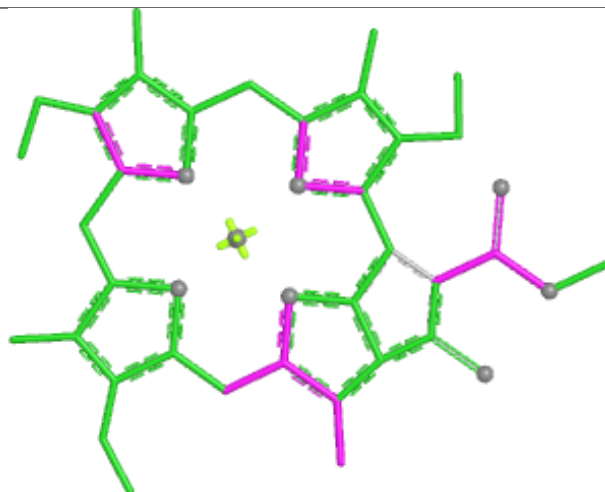
Rings



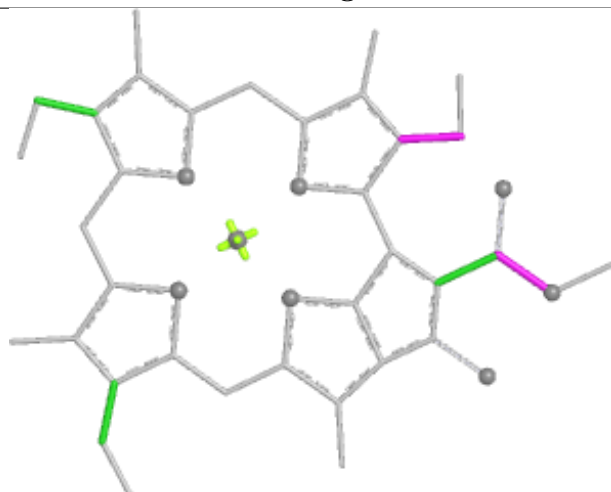
Ligand CLA b 848



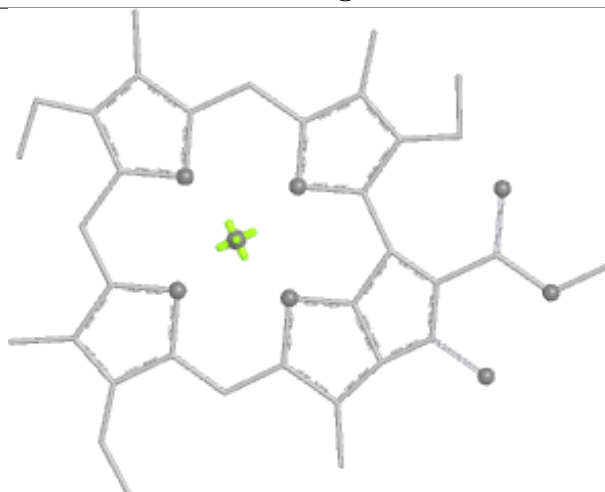
Bond lengths



Bond angles

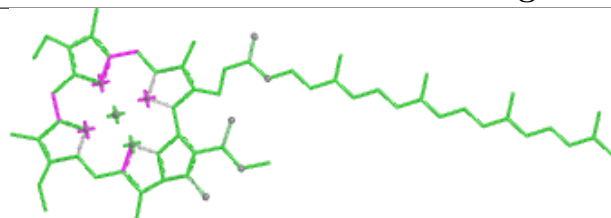


Torsions

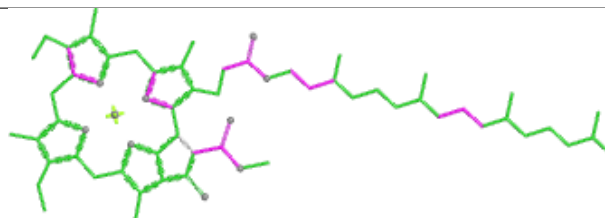


Rings

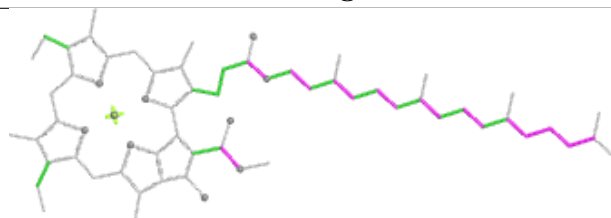
Ligand CLA a 846



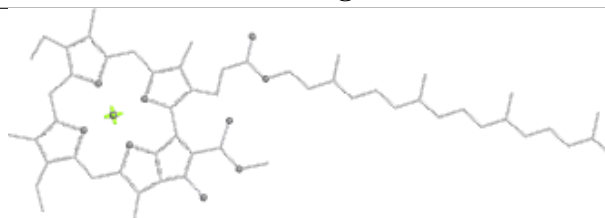
Bond lengths



Bond angles

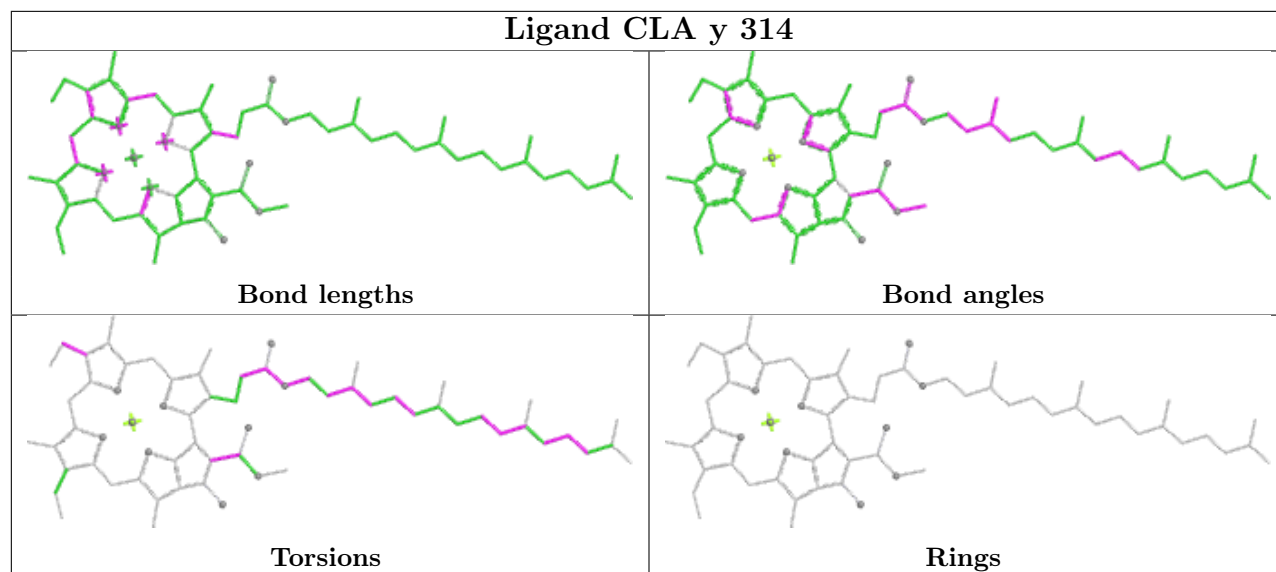


Torsions

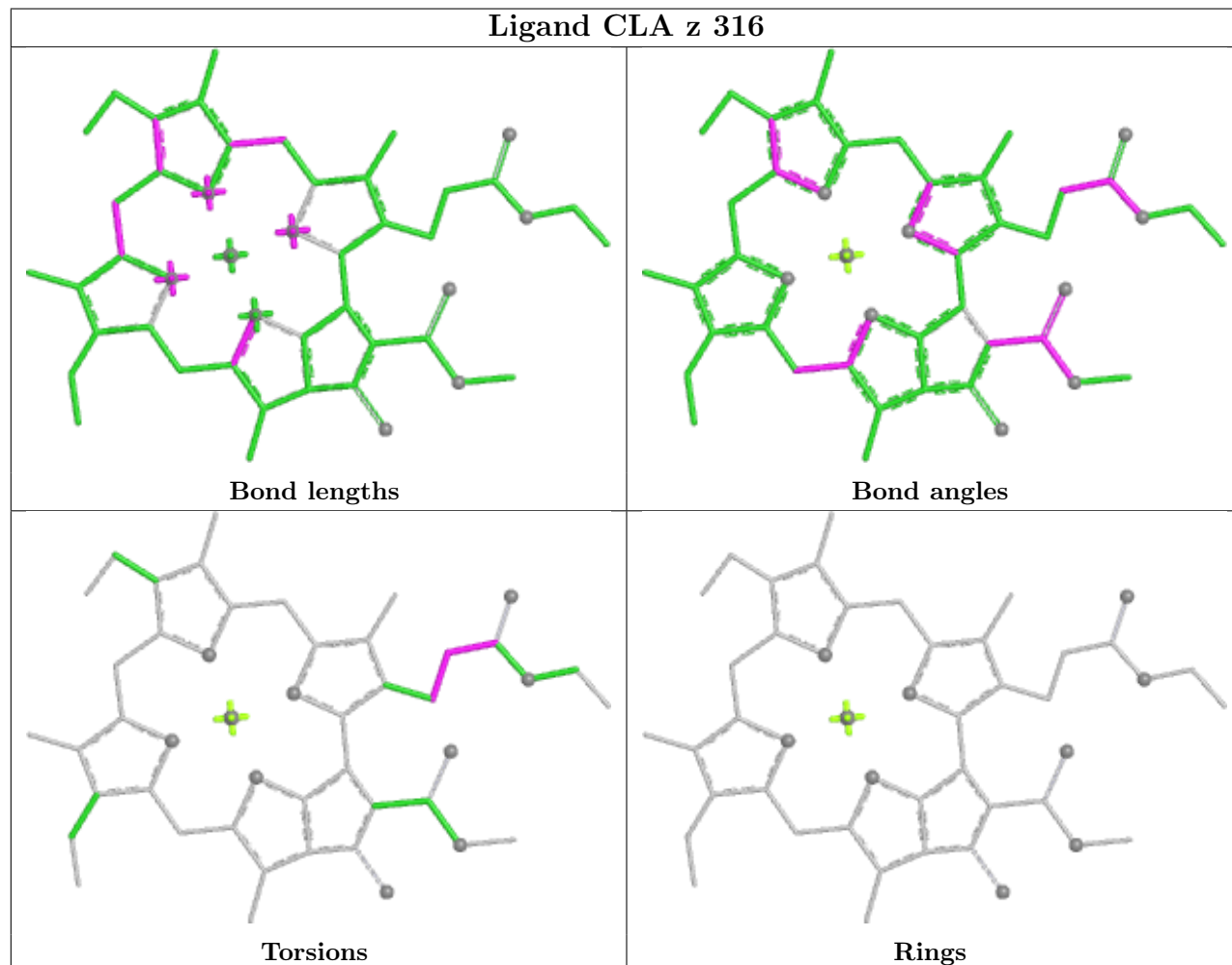


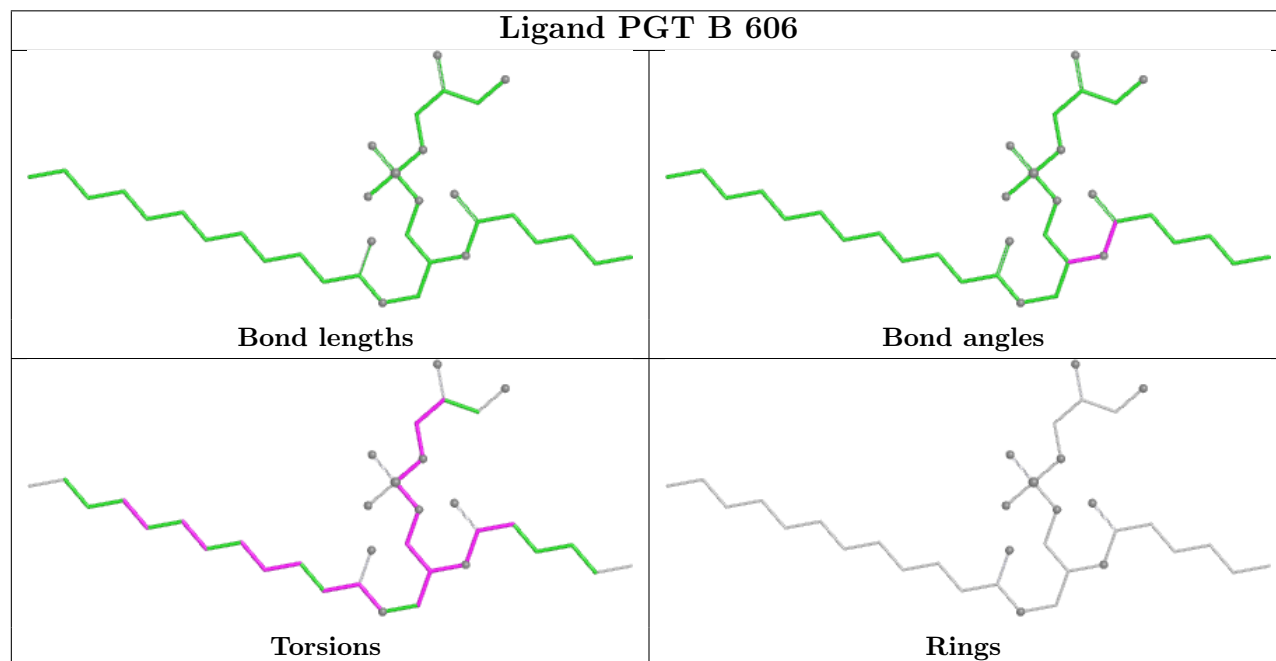
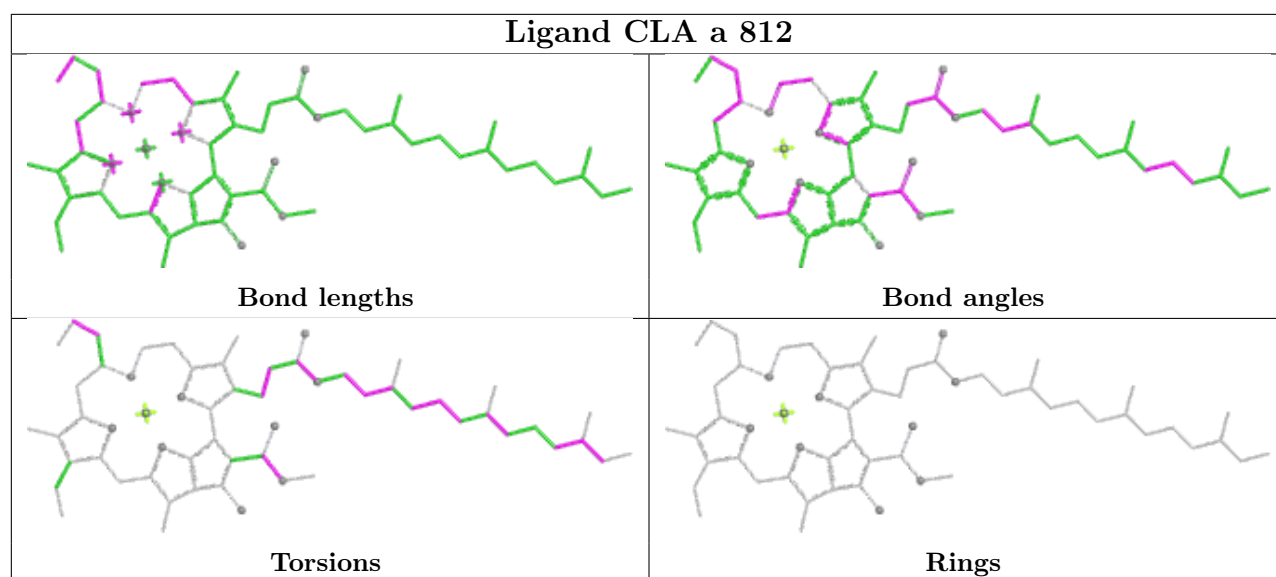
Rings

Ligand CLA y 314

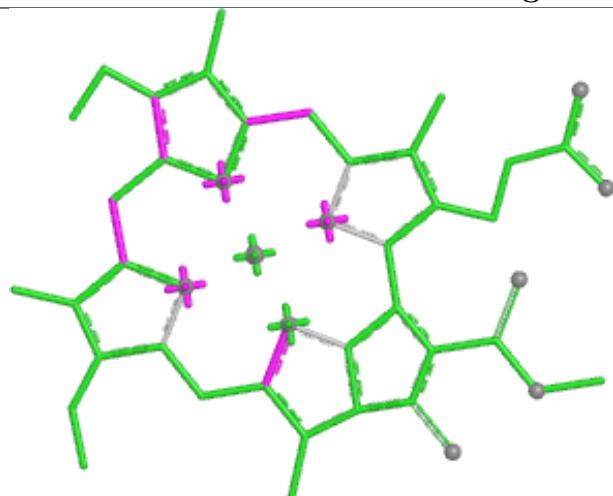


Ligand CLA z 316

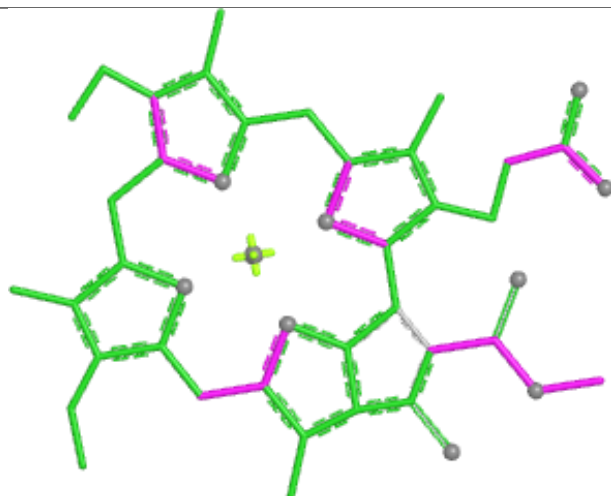




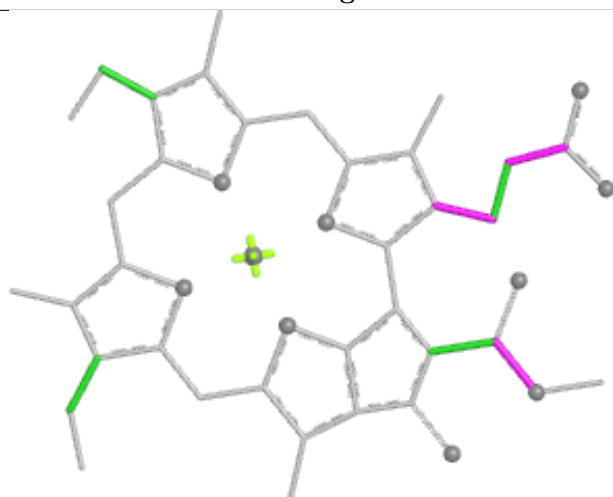
Ligand CLA l 301



Bond lengths



Bond angles

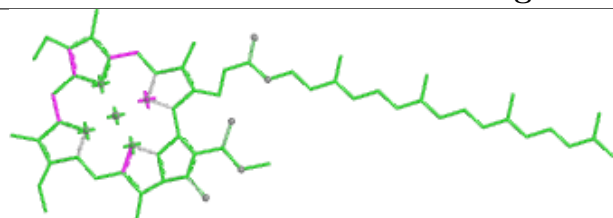


Torsions

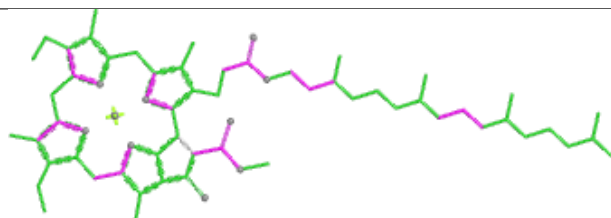


Rings

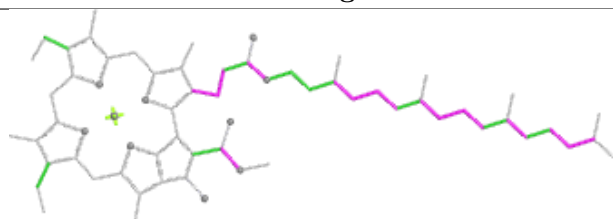
Ligand CLA w 308



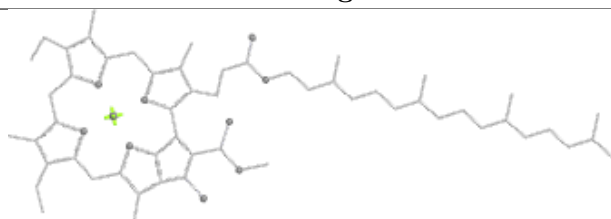
Bond lengths



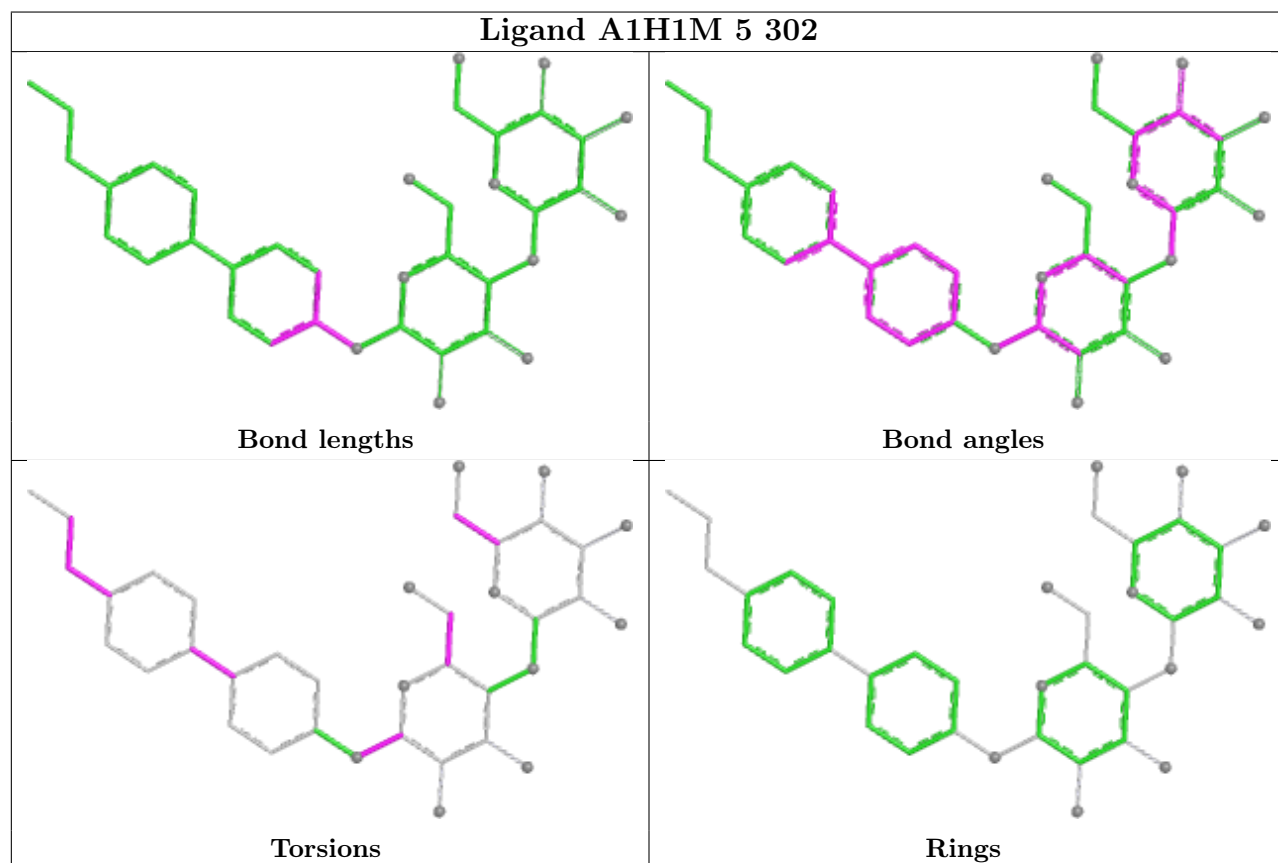
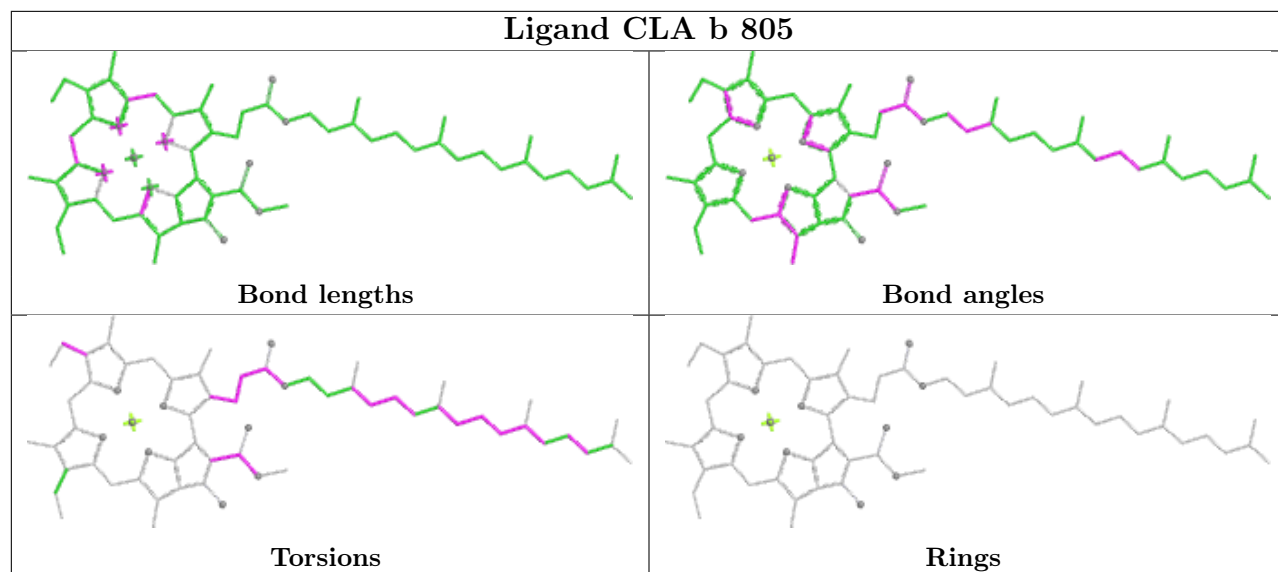
Bond angles

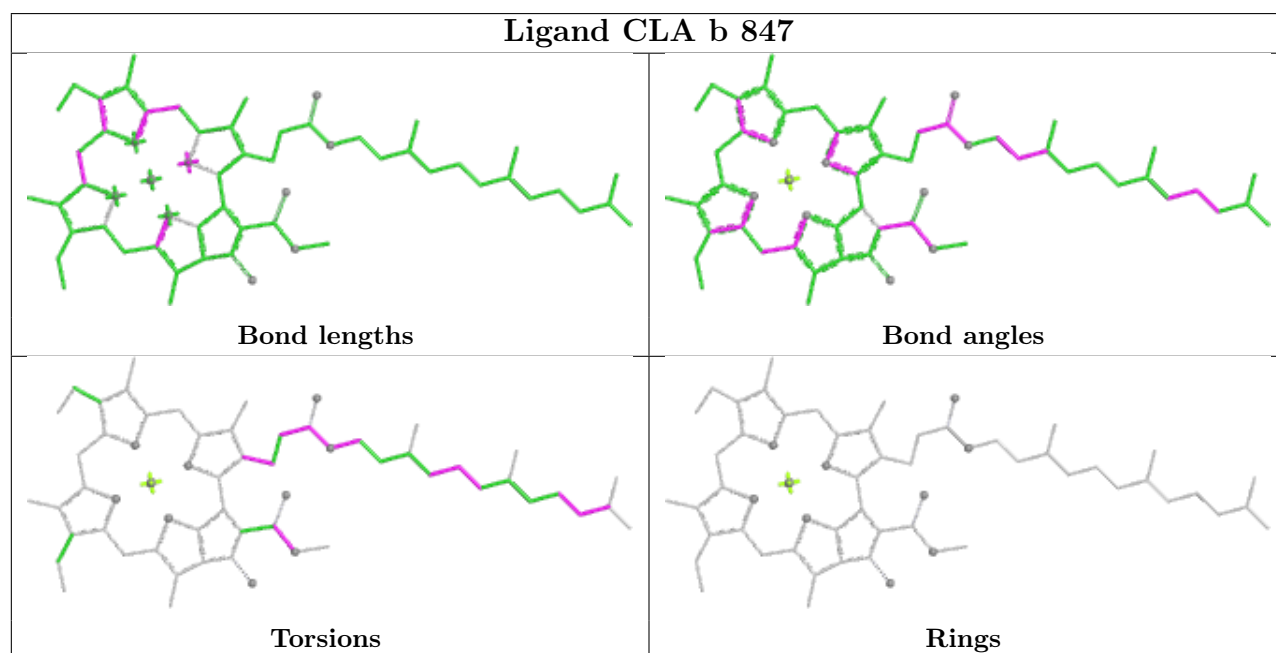
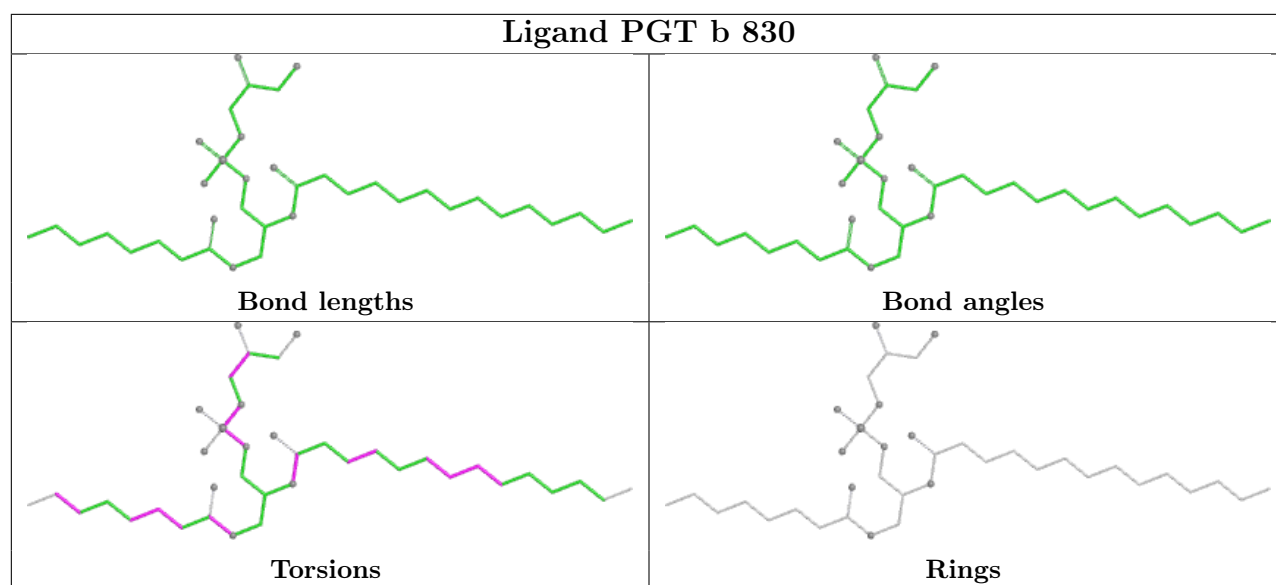


Torsions

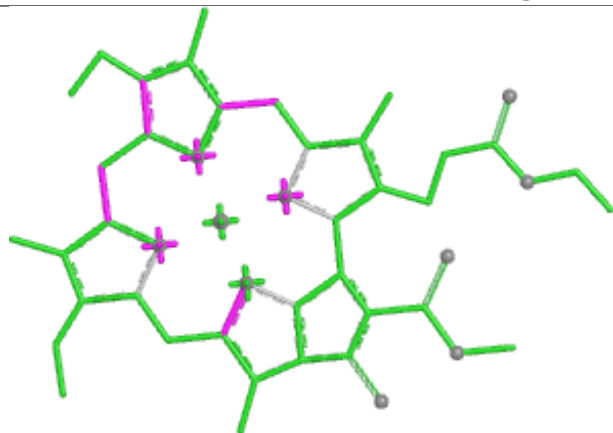


Rings

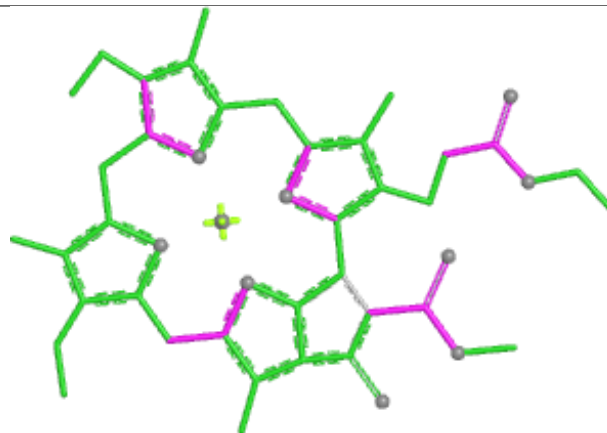




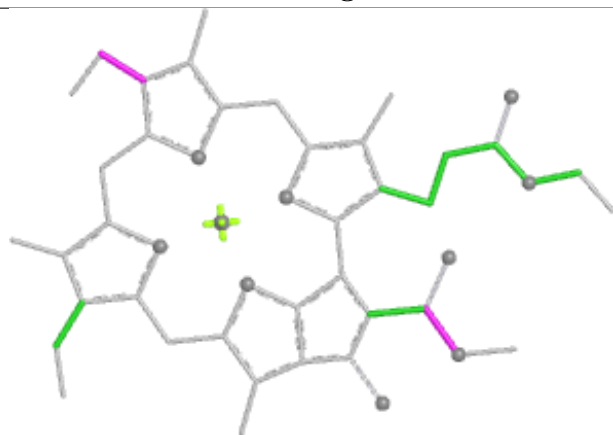
Ligand CLA b 851



Bond lengths



Bond angles

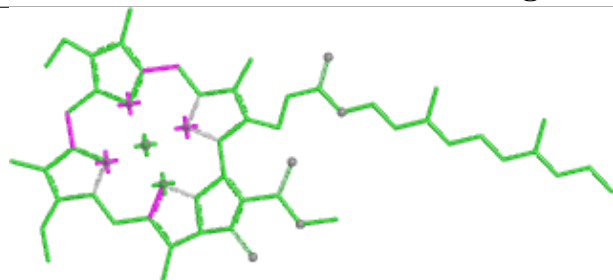


Torsions

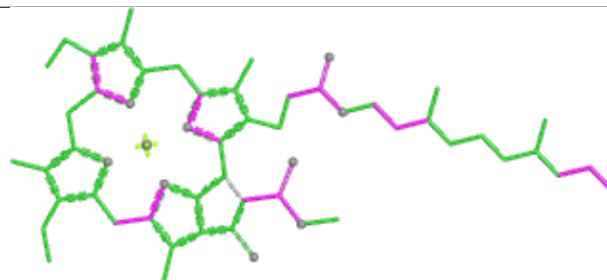


Rings

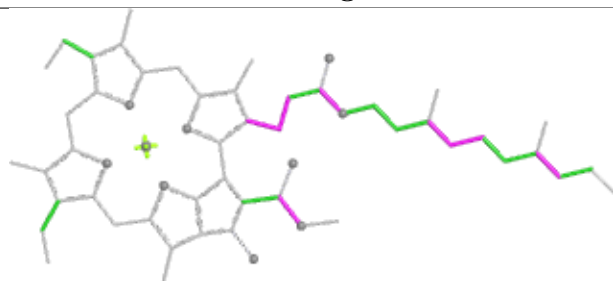
Ligand CLA f 301



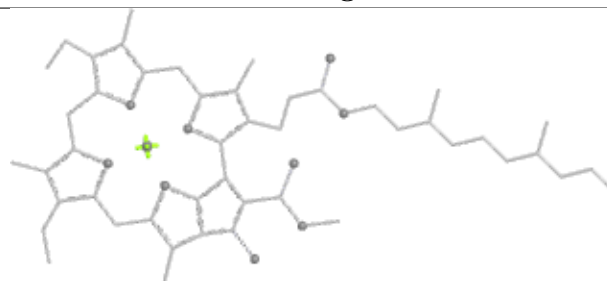
Bond lengths



Bond angles

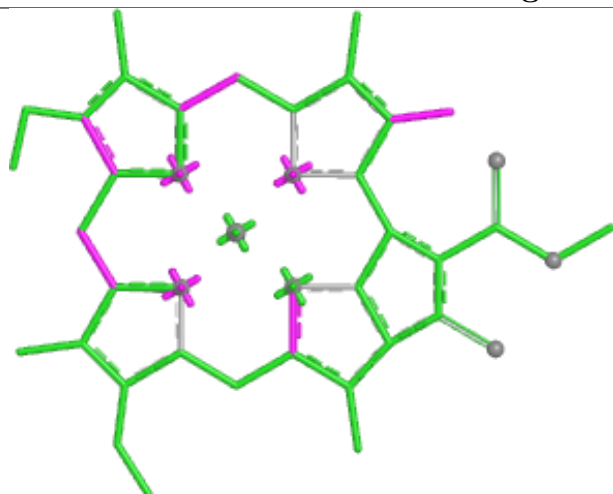


Torsions

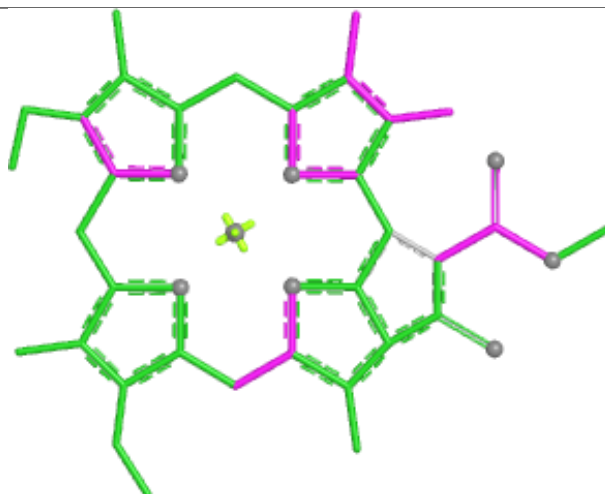


Rings

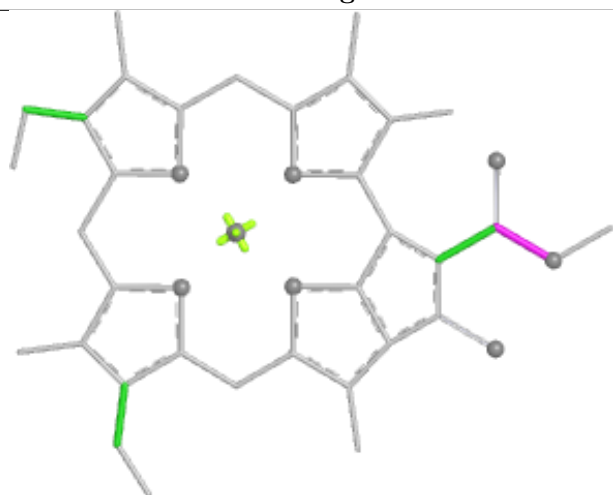
Ligand CLA f 303



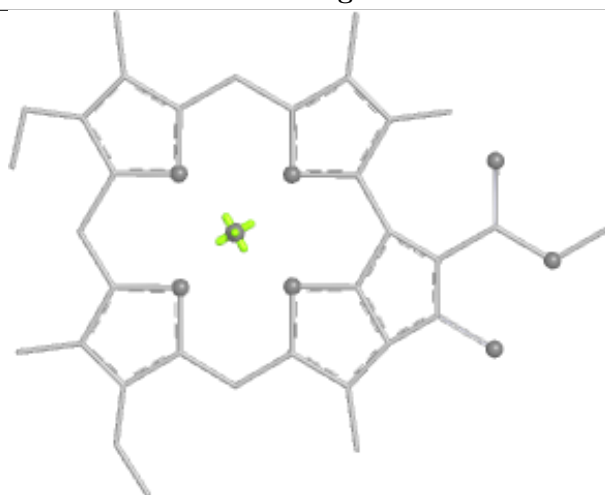
Bond lengths



Bond angles

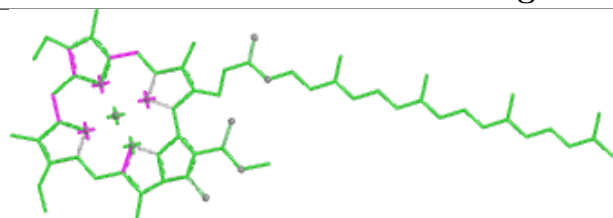


Torsions

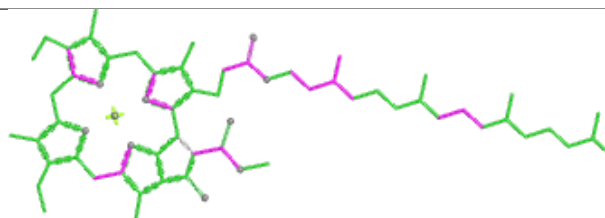


Rings

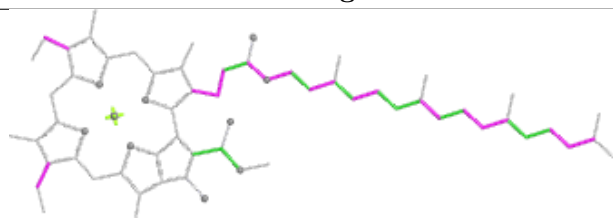
Ligand CLA x 312



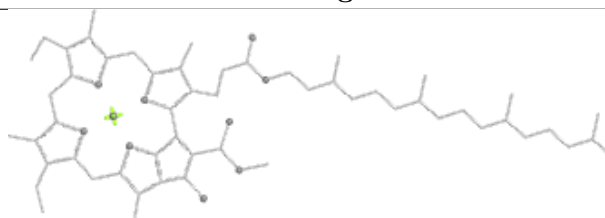
Bond lengths



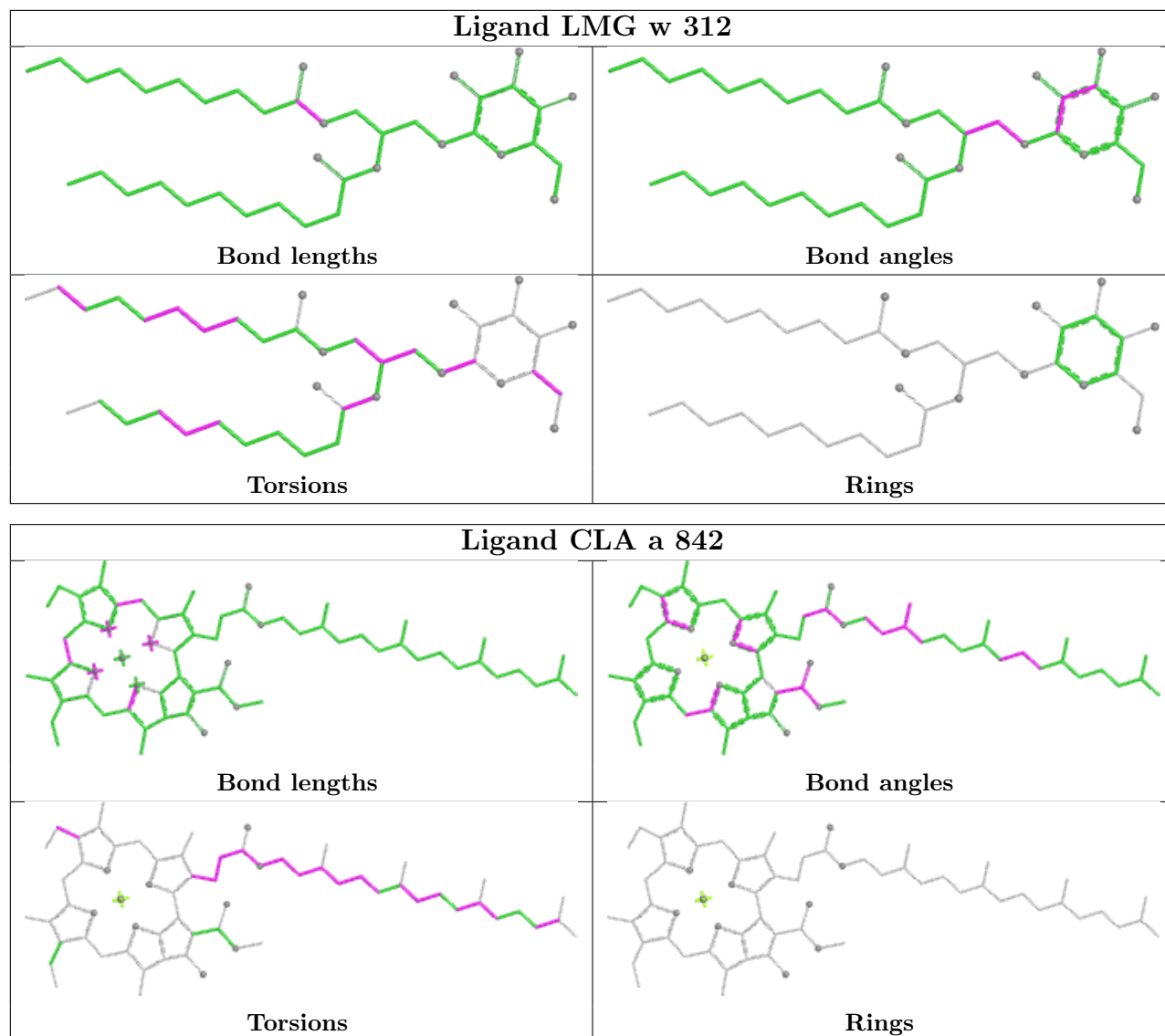
Bond angles

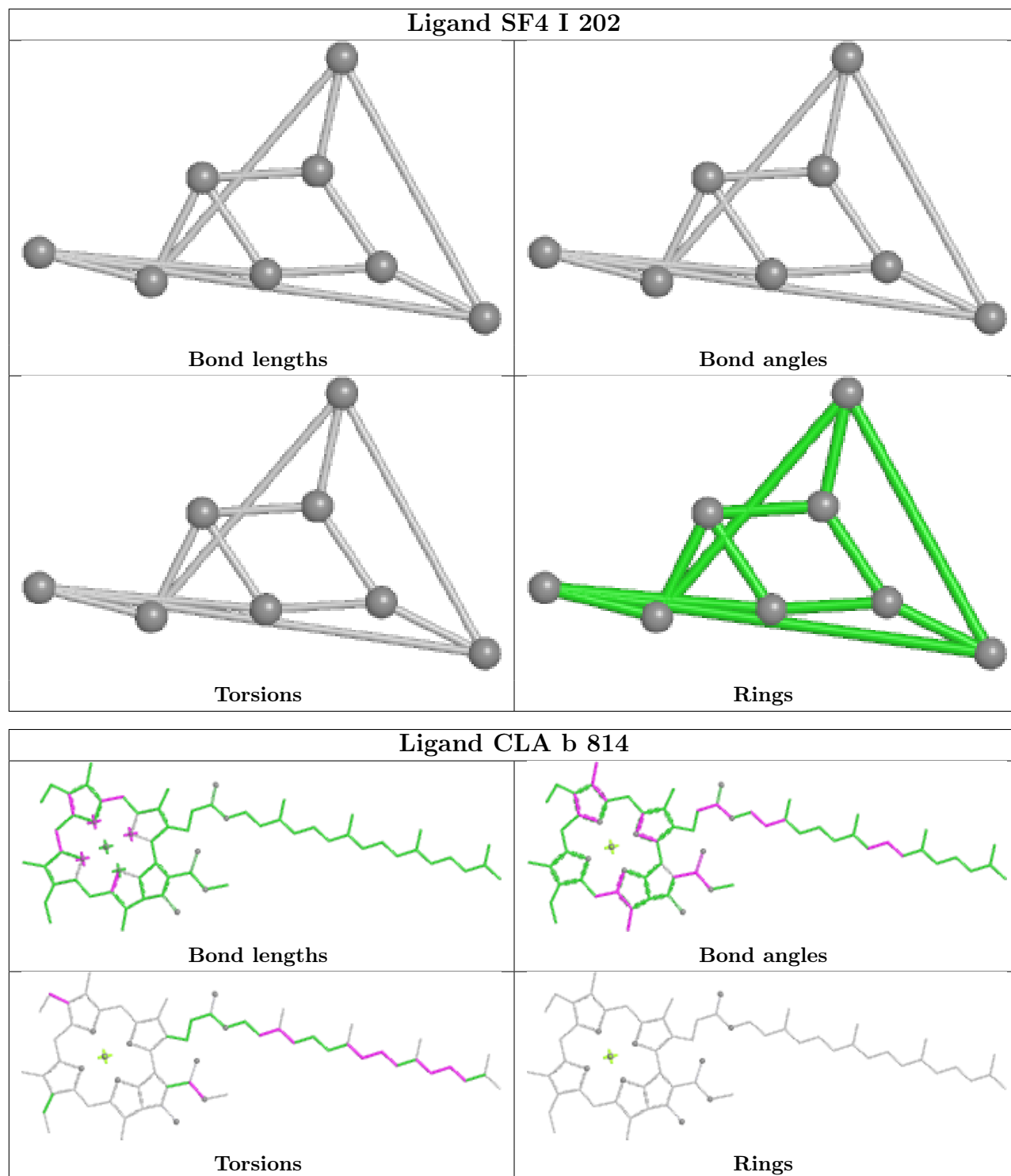


Torsions

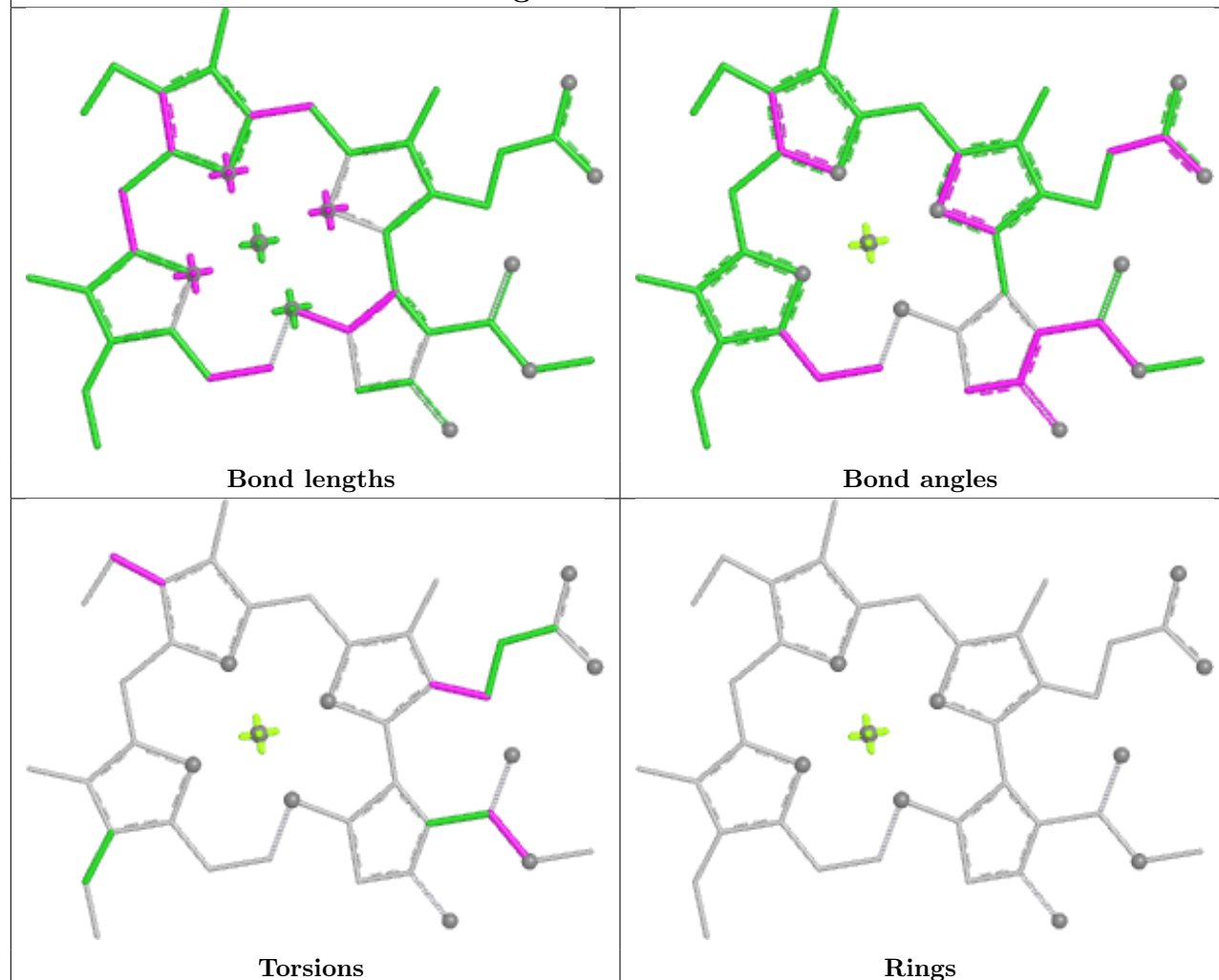


Rings

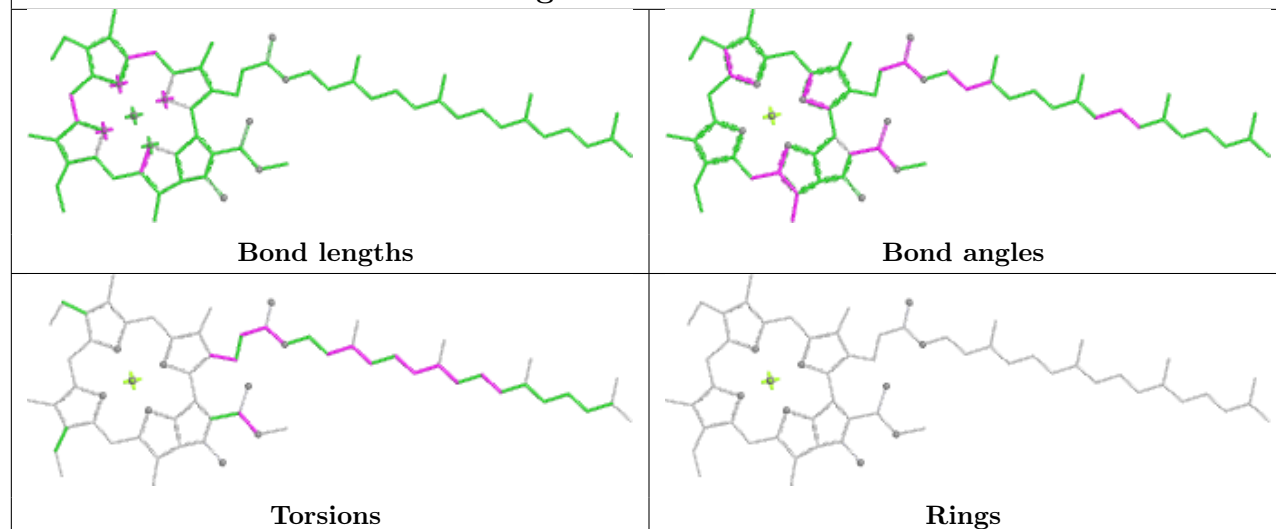


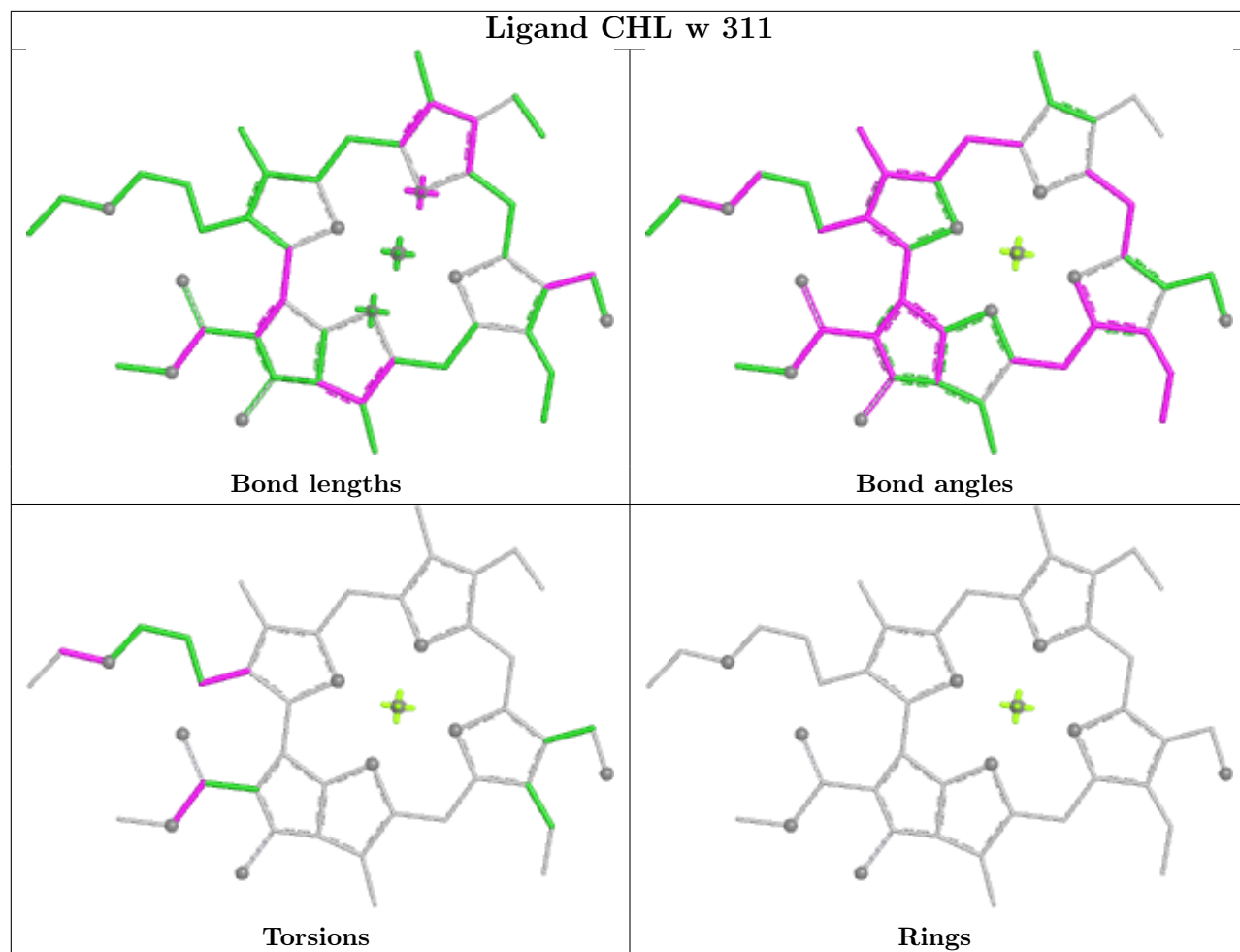


Ligand CLA z 308

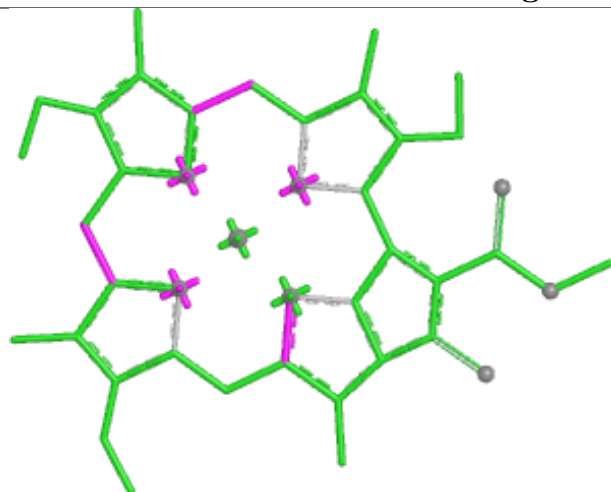


Ligand CLA a 849

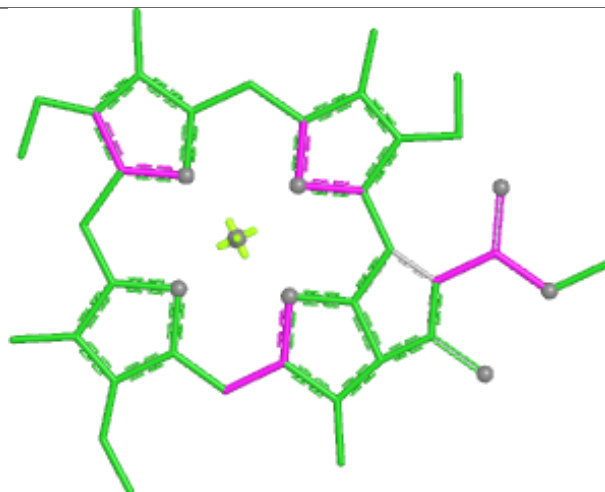




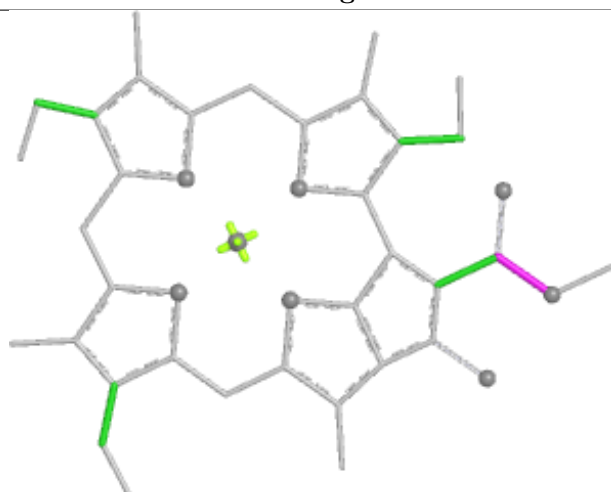
Ligand CLA f 302



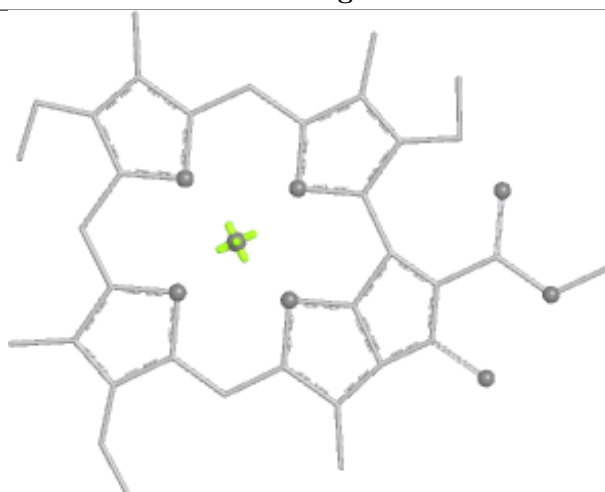
Bond lengths



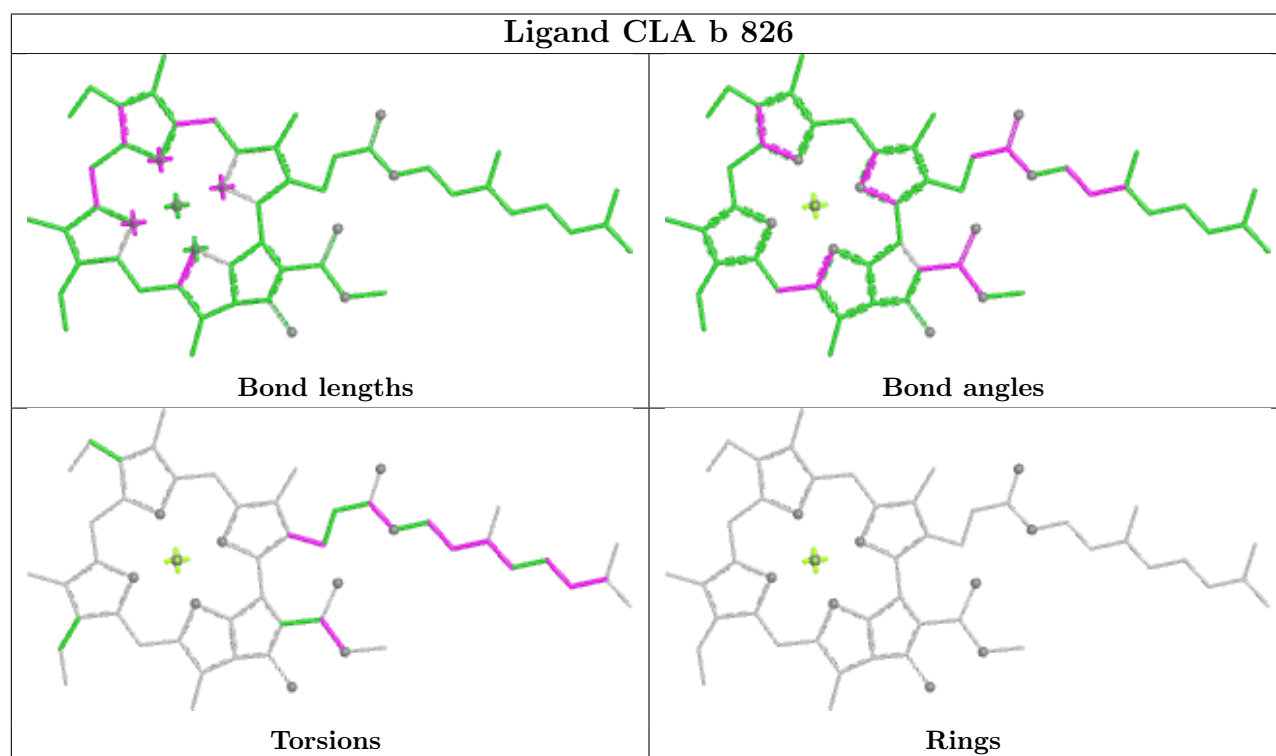
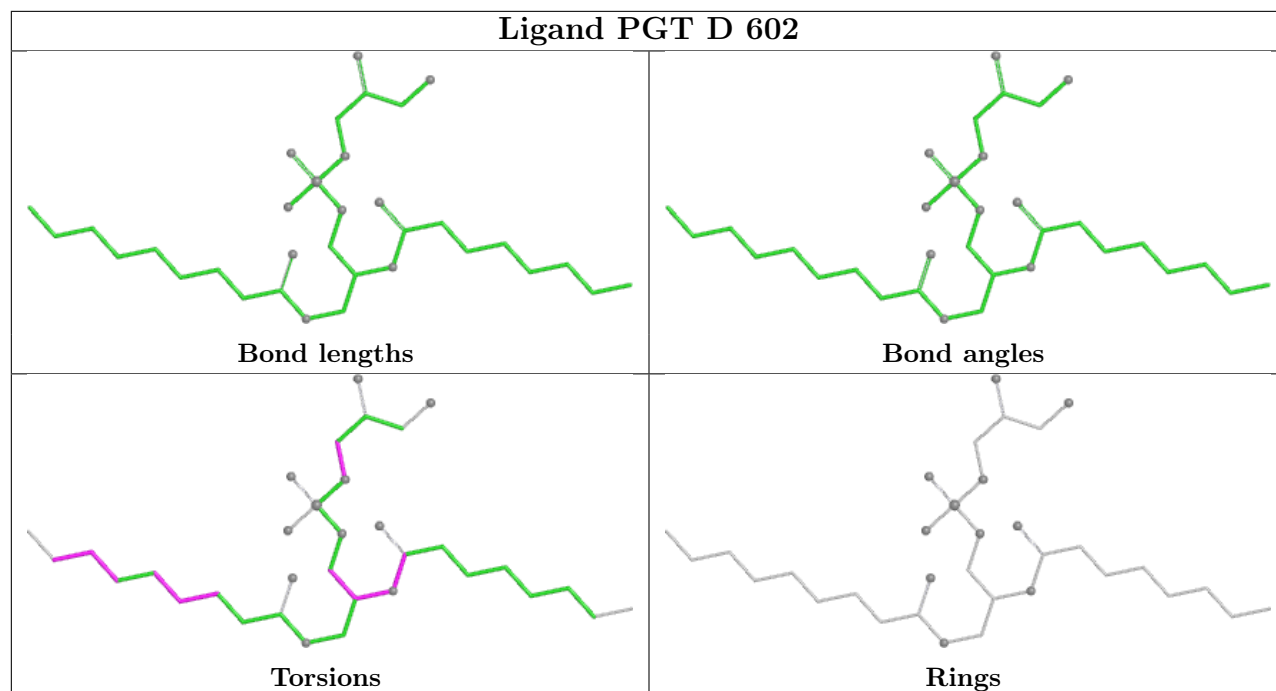
Bond angles



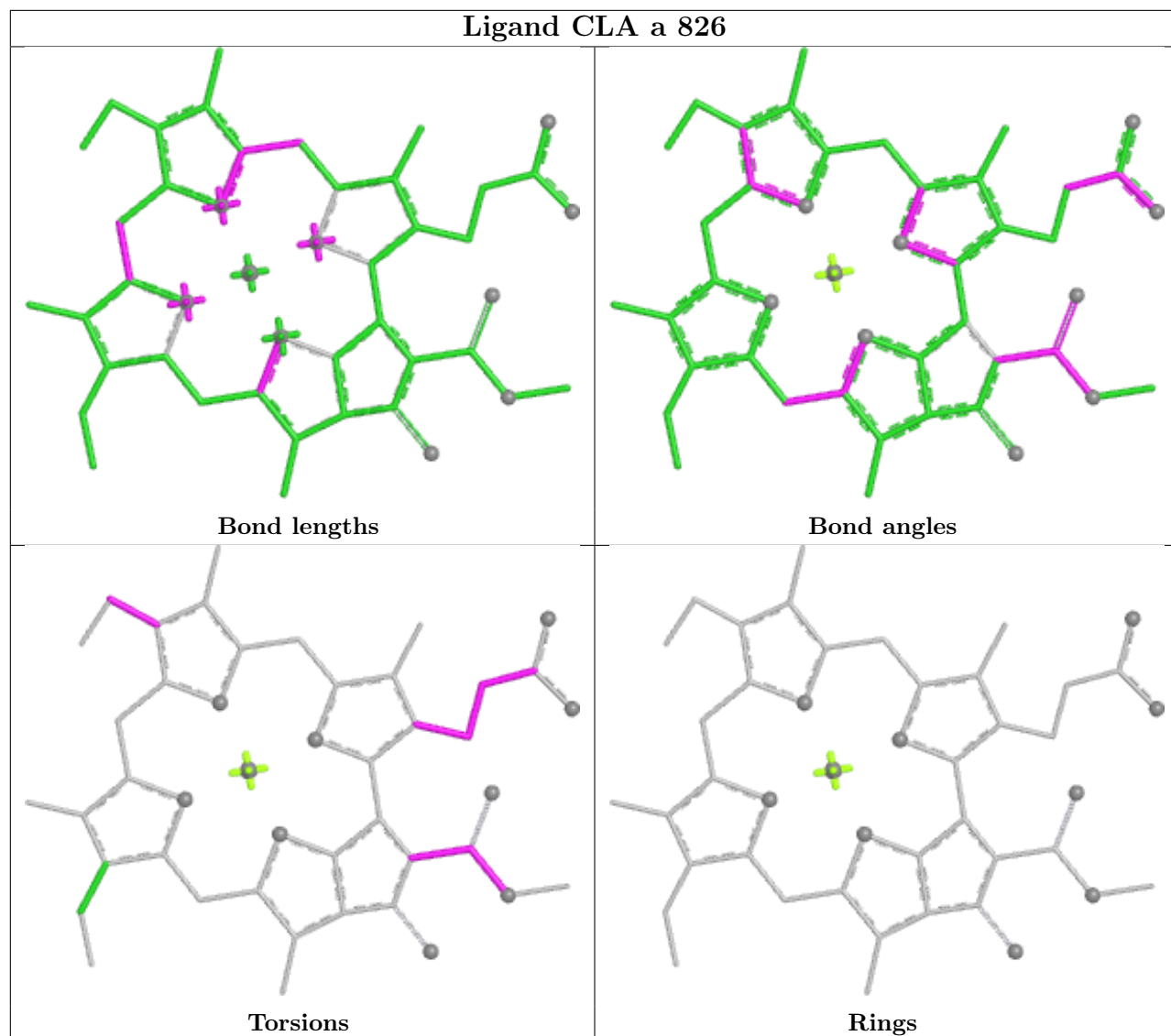
Torsions

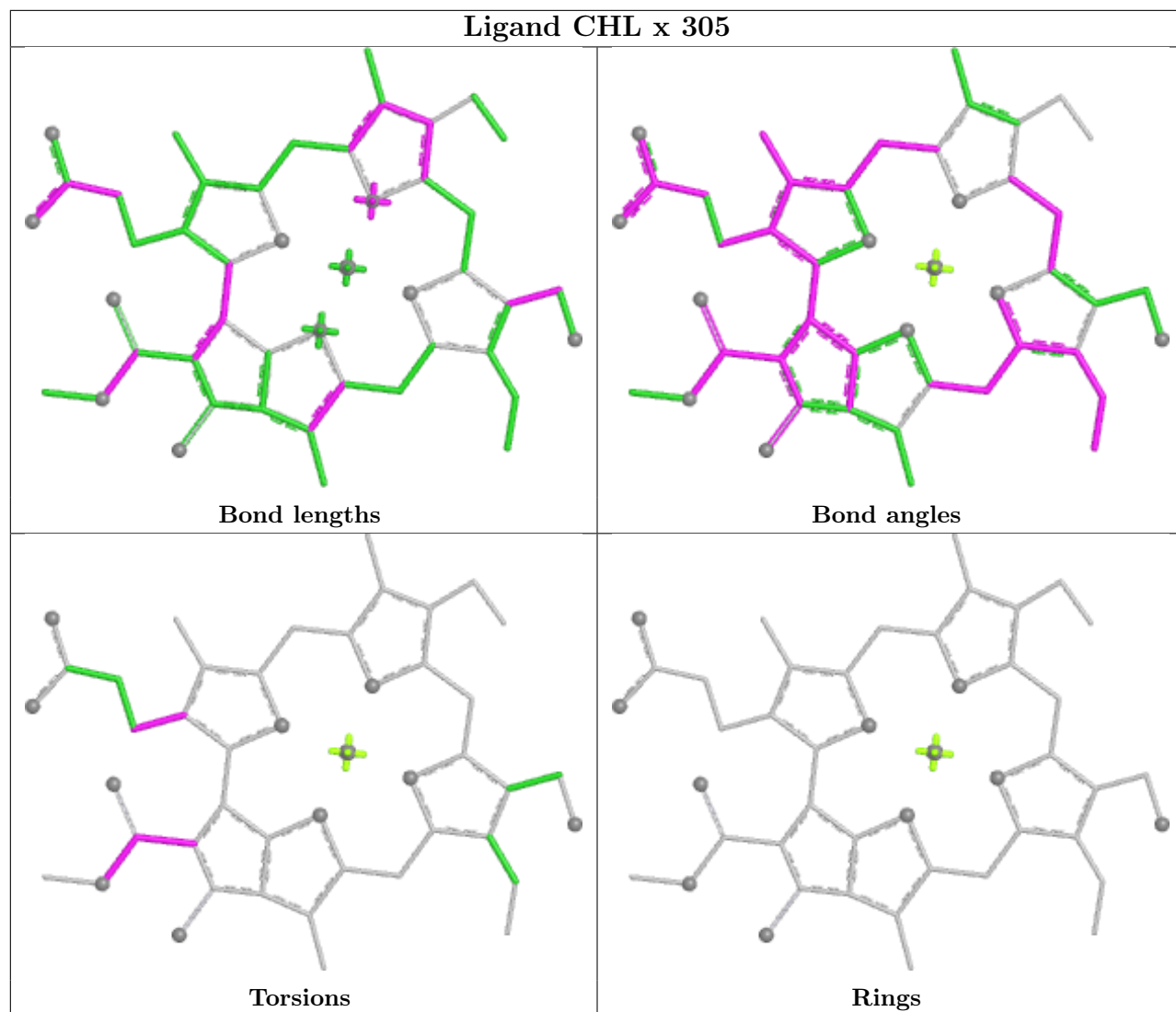


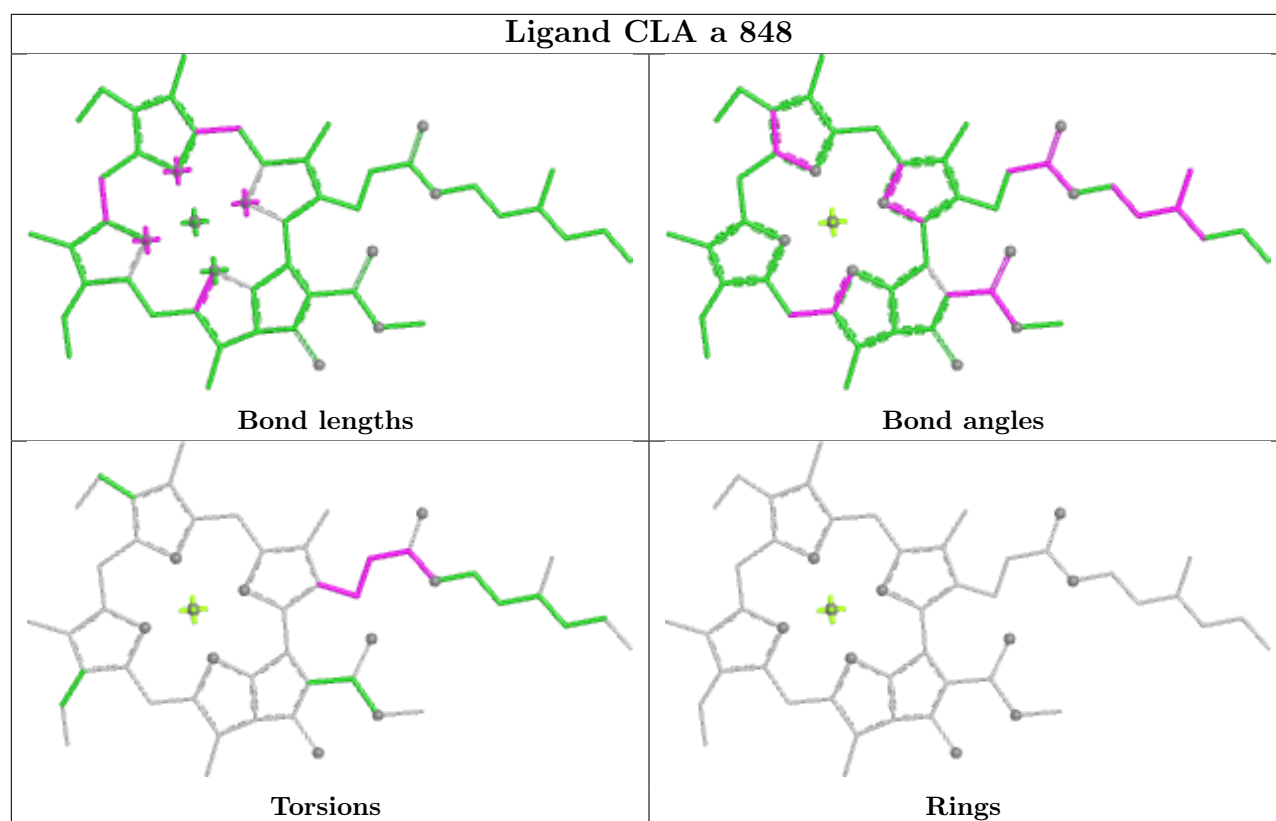
Rings



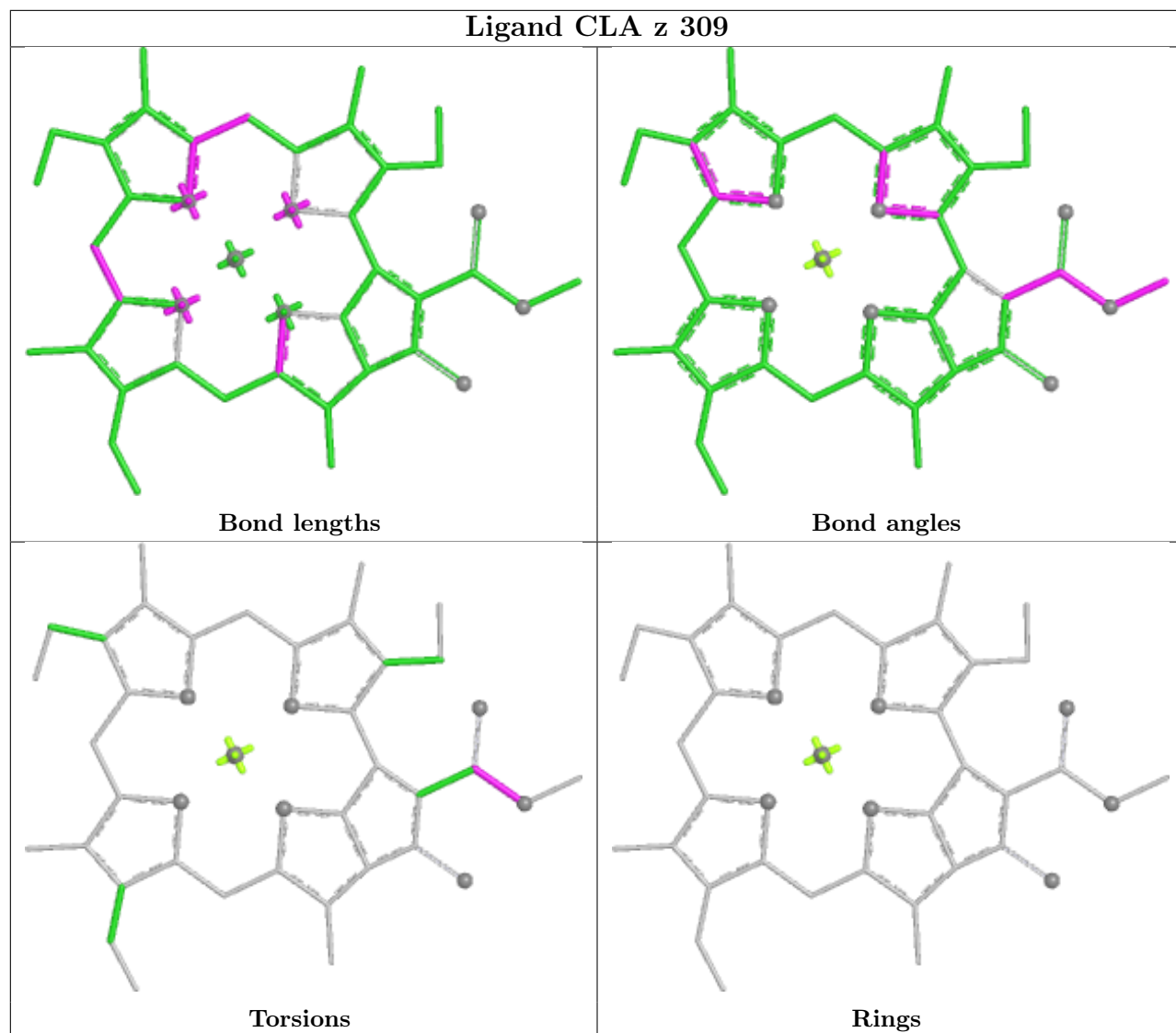
Ligand CLA a 826

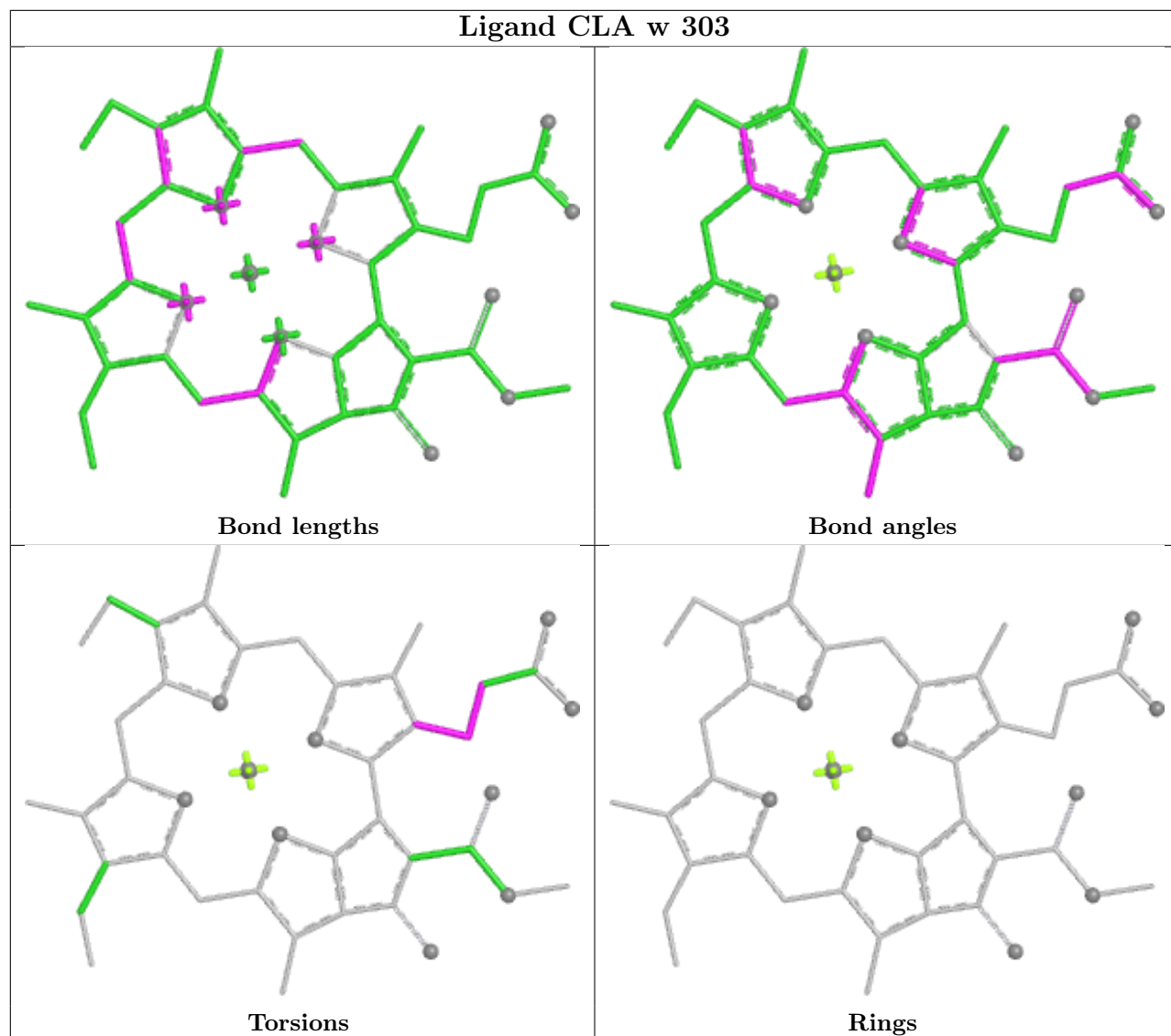




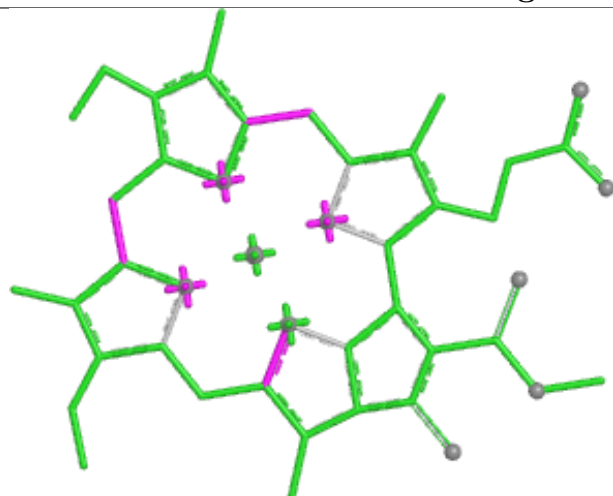


Ligand CLA z 309

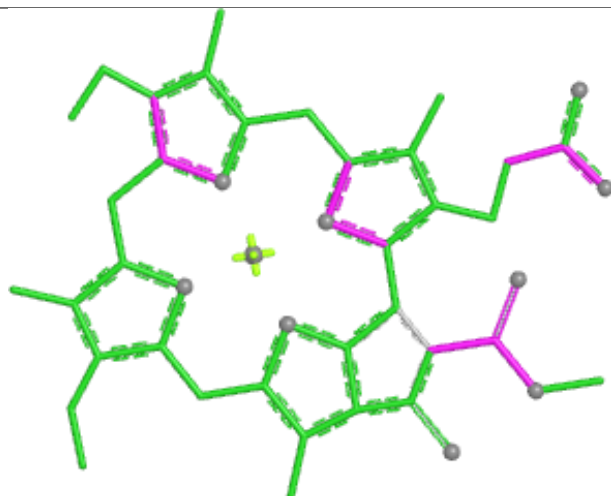




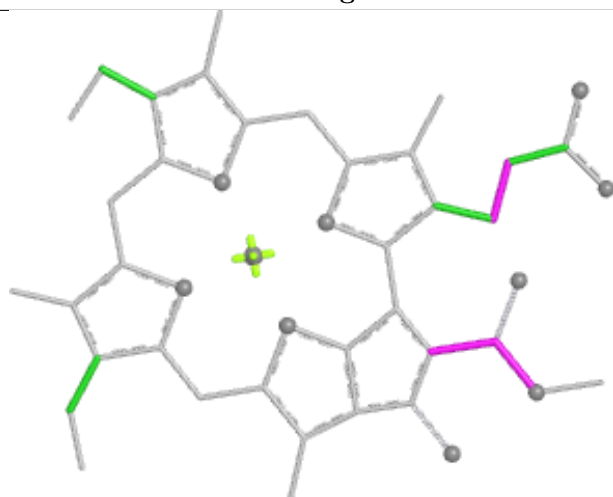
Ligand CLA x 316



Bond lengths



Bond angles

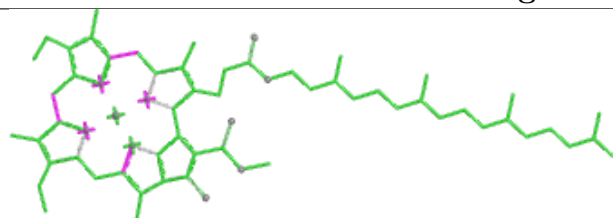


Torsions

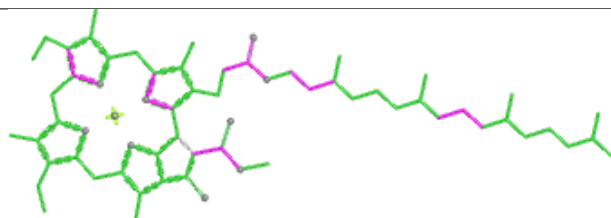


Rings

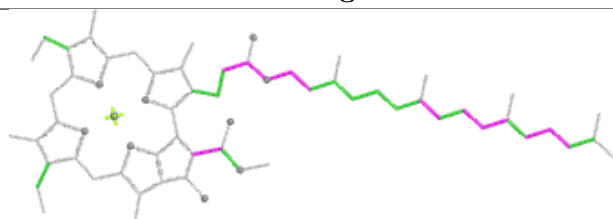
Ligand CLA a 801



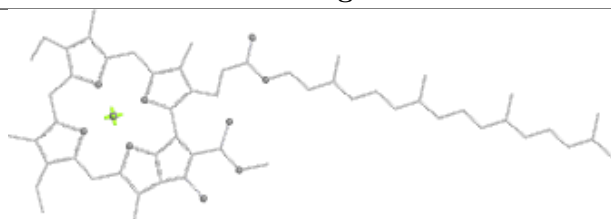
Bond lengths



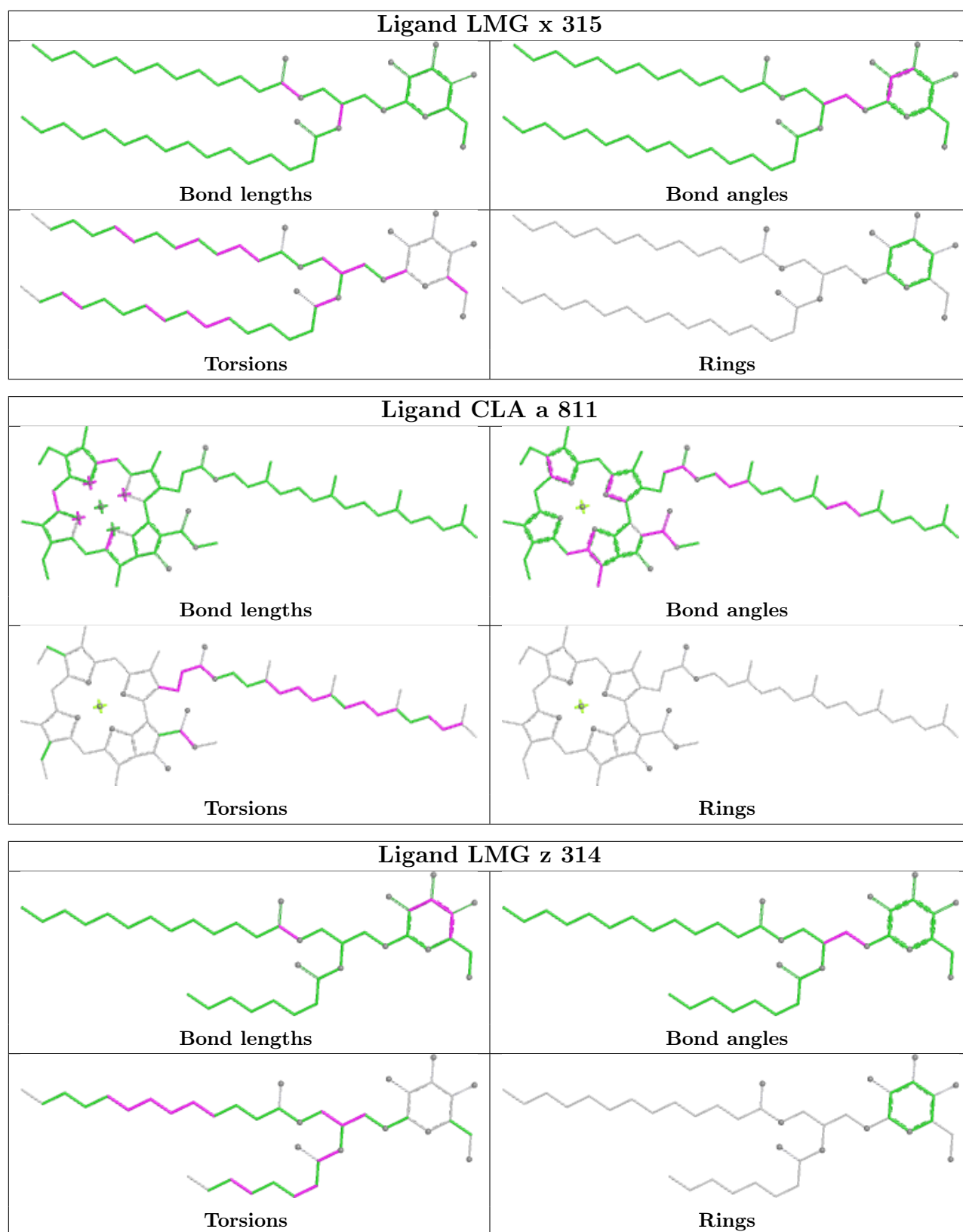
Bond angles

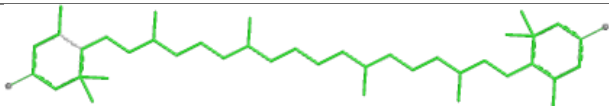
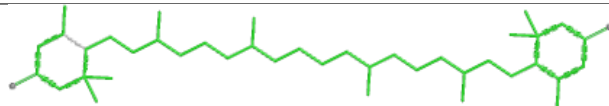
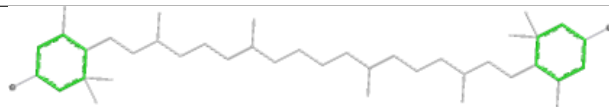


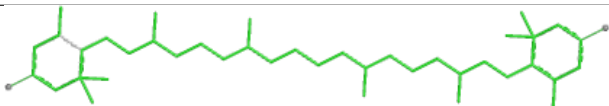
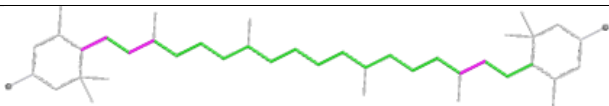
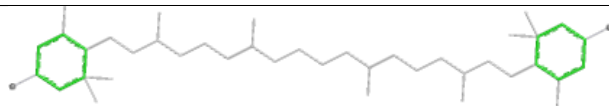
Torsions

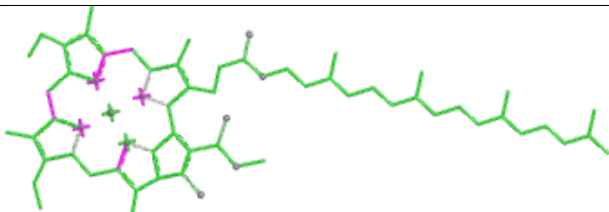
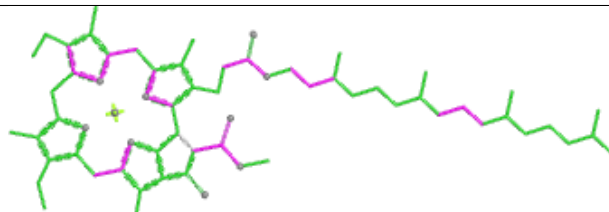
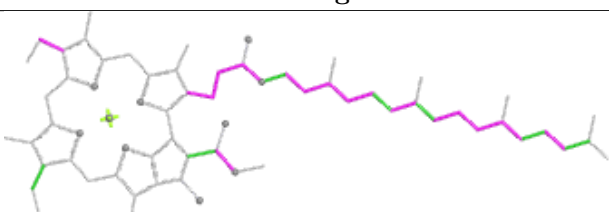
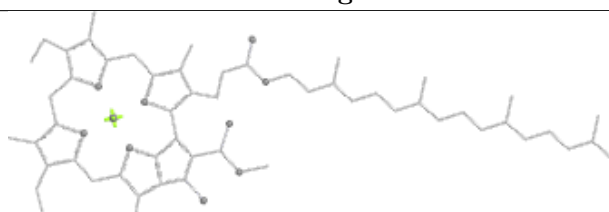


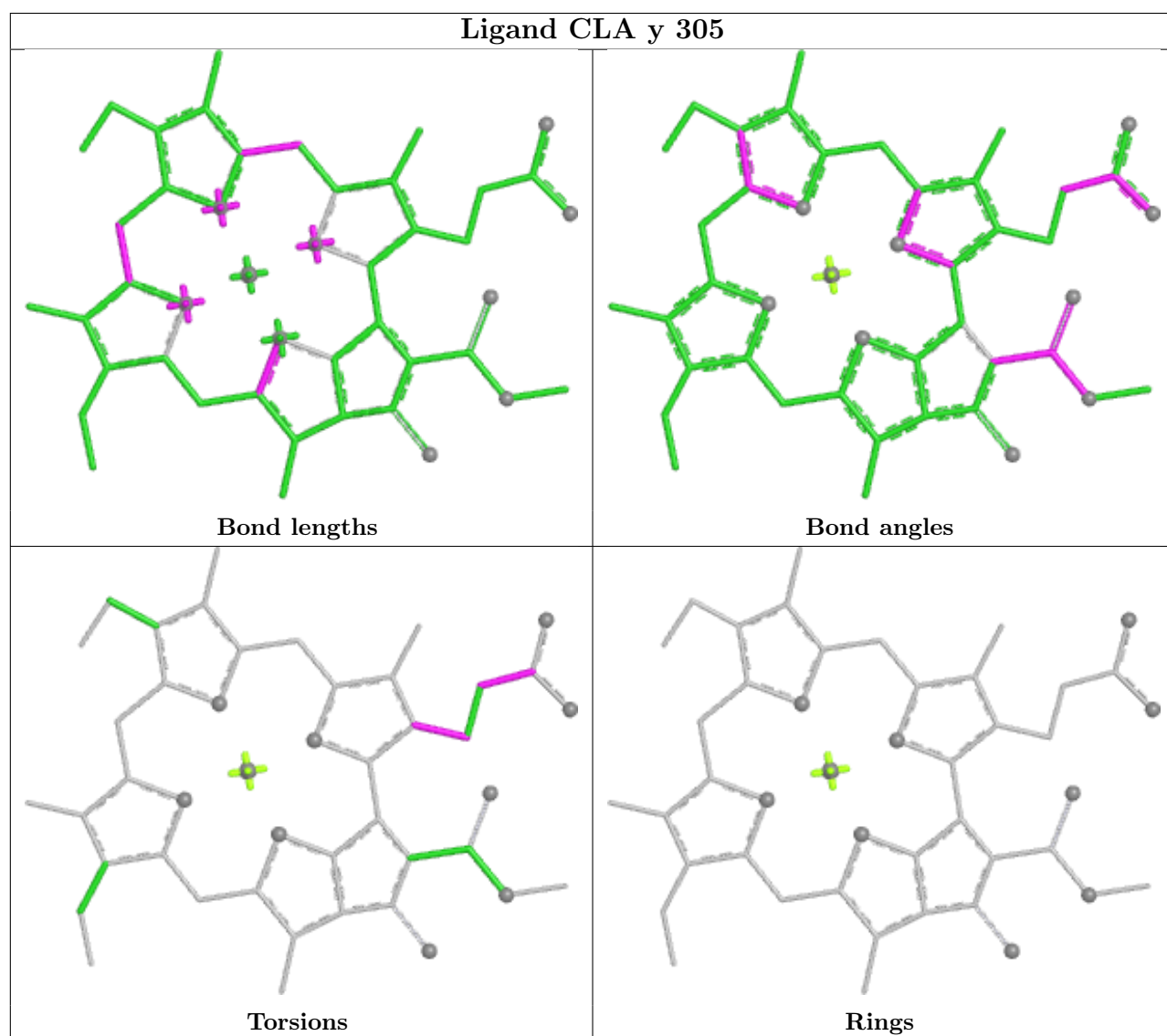
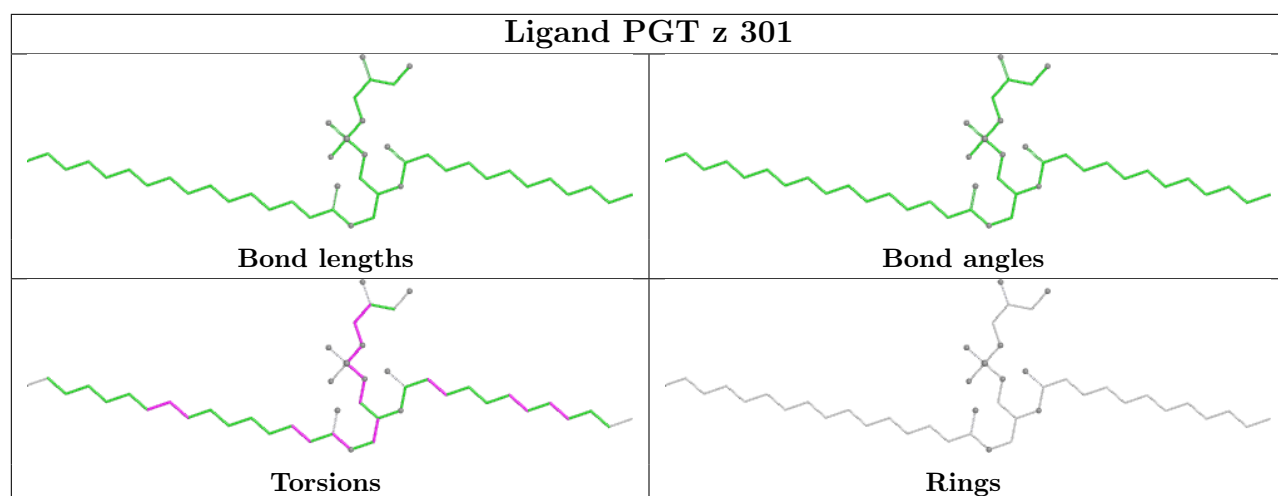
Rings

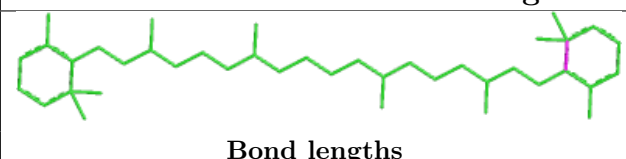
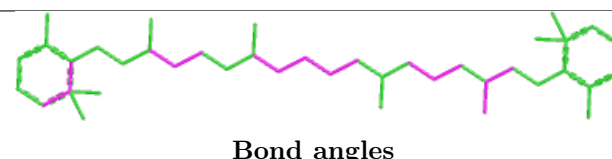
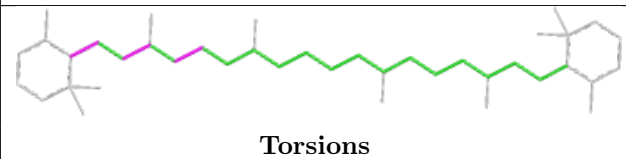
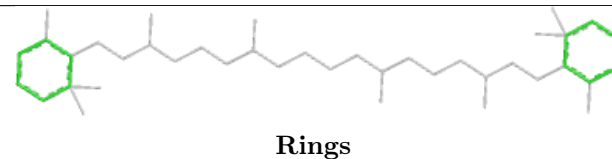


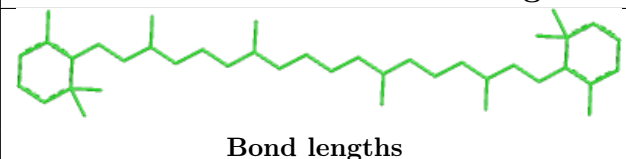
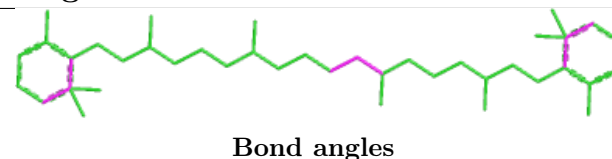
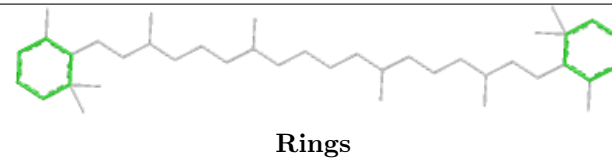
Ligand LUT x 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

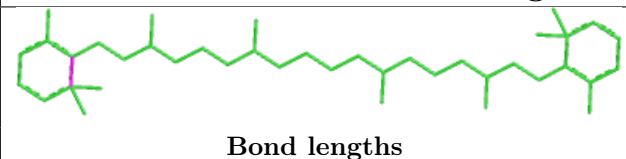
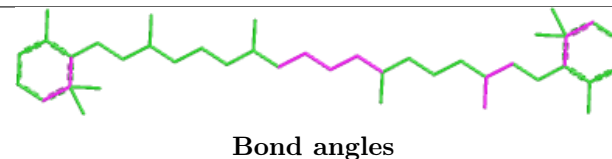
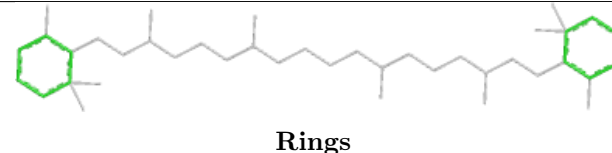
Ligand LUT x 321	
	
Bond lengths	Bond angles
	
Torsions	Rings

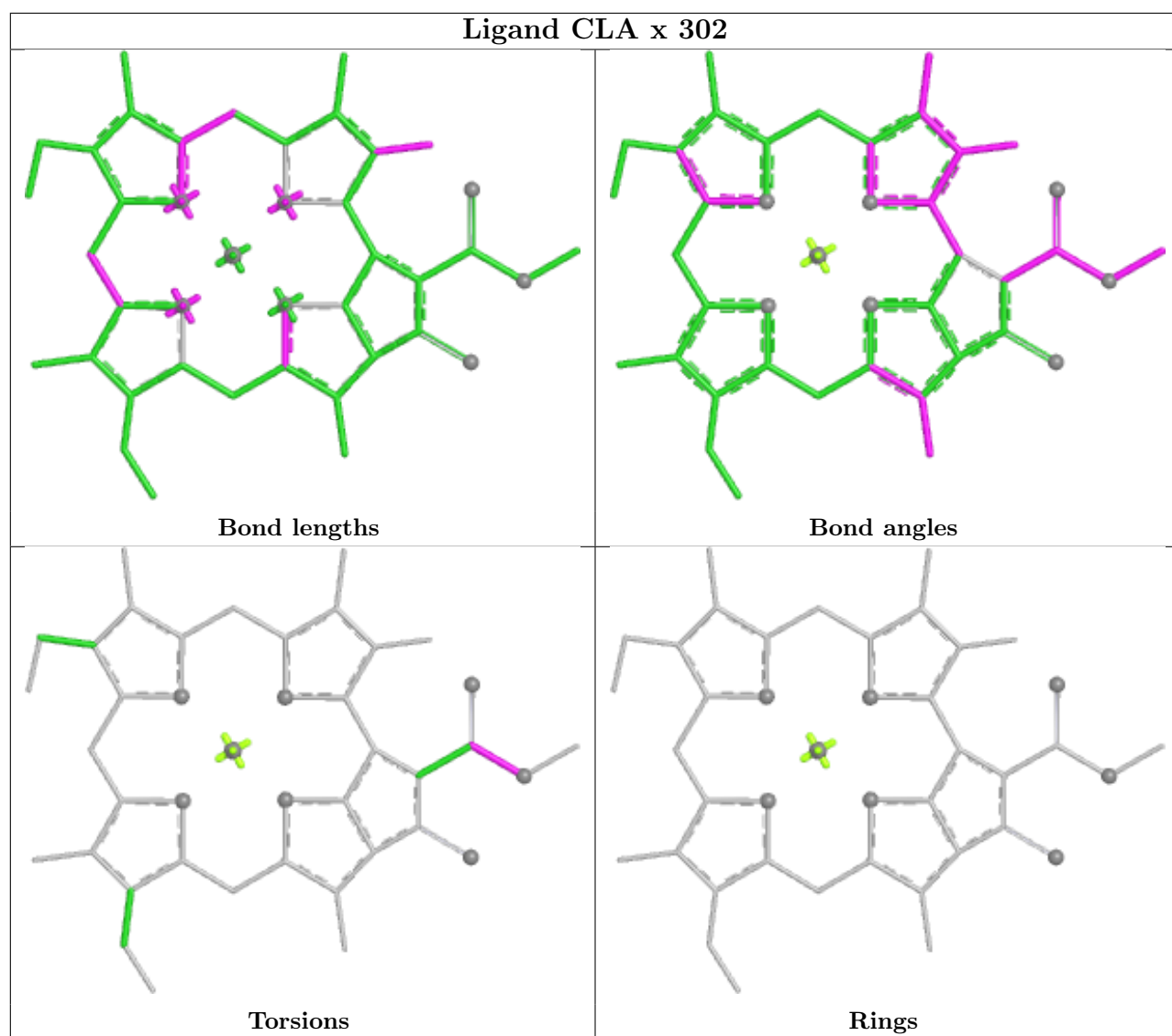
Ligand CLA b 844	
	
Bond lengths	Bond angles
	
Torsions	Rings



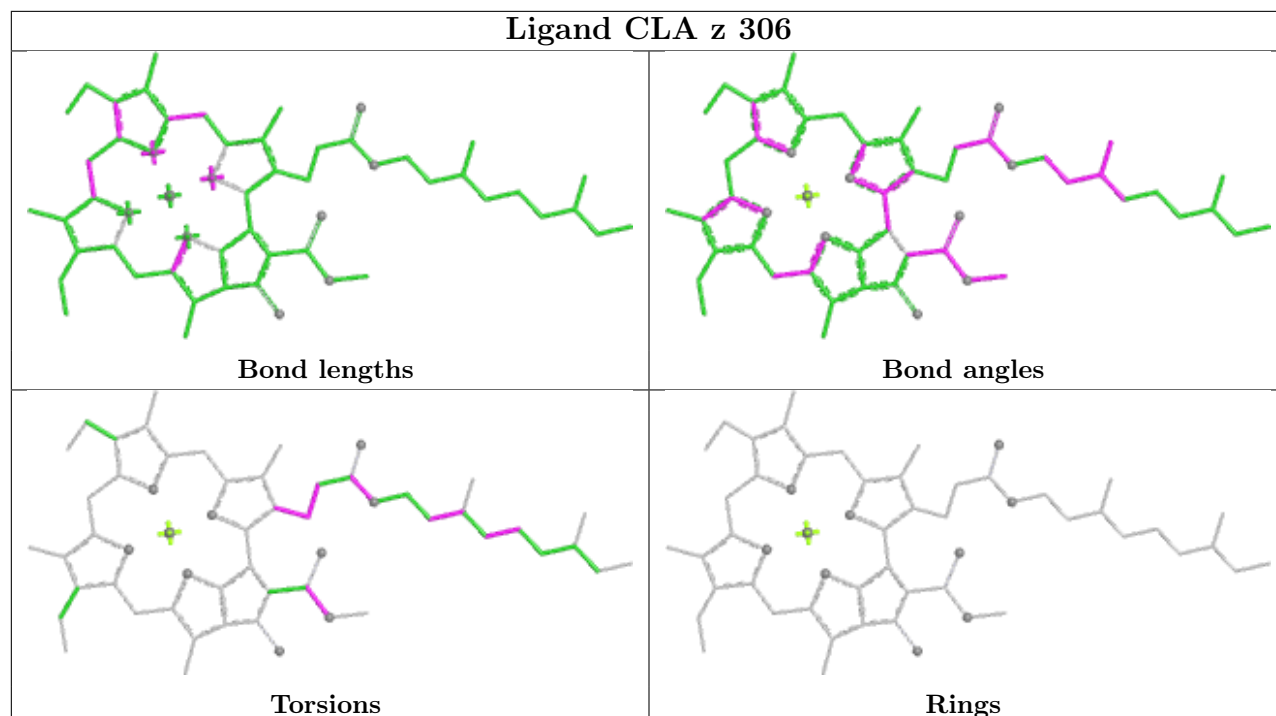
Ligand BCR b 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR g 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

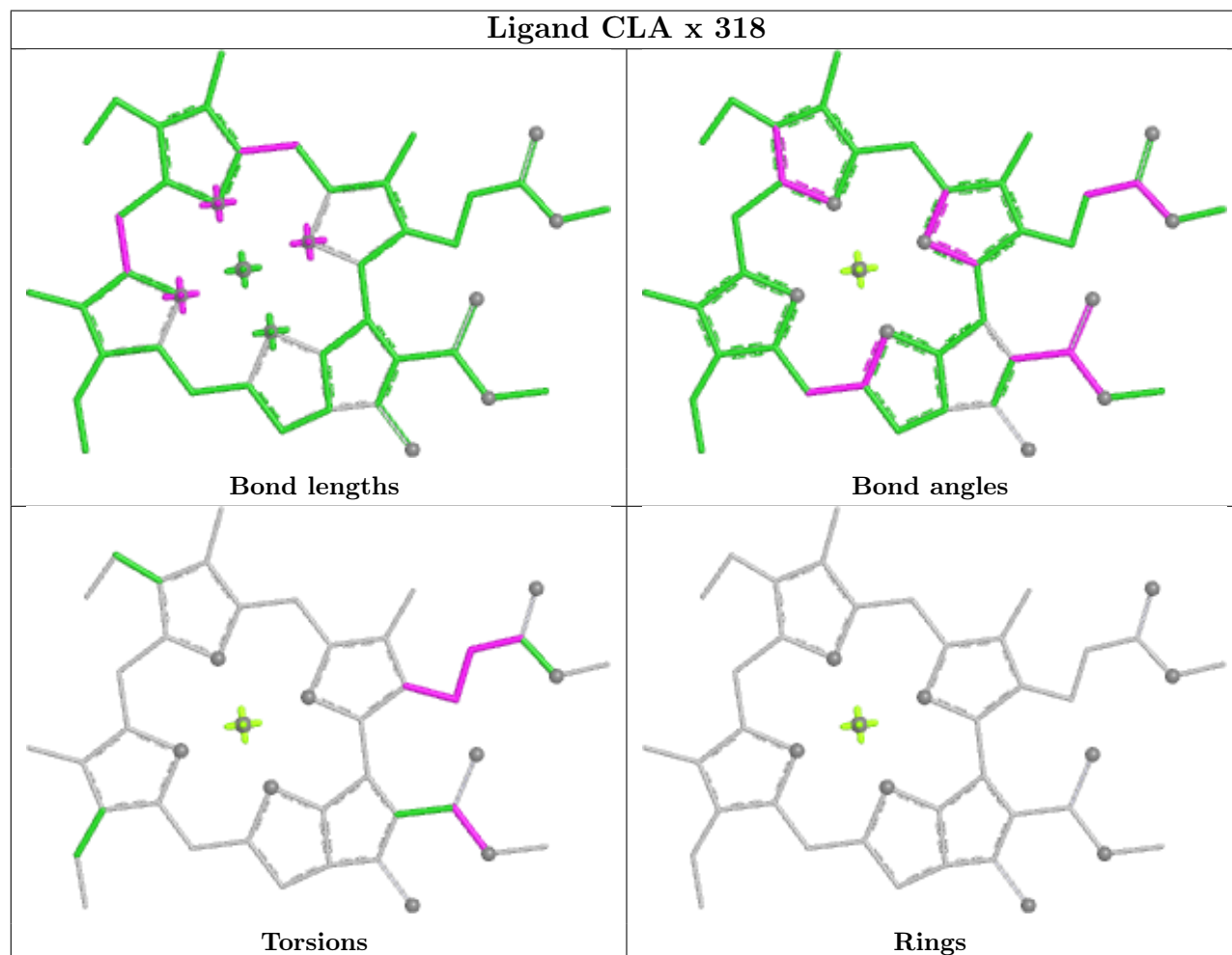
Ligand BCR f 304	
	
Bond lengths	Bond angles
	
Torsions	Rings



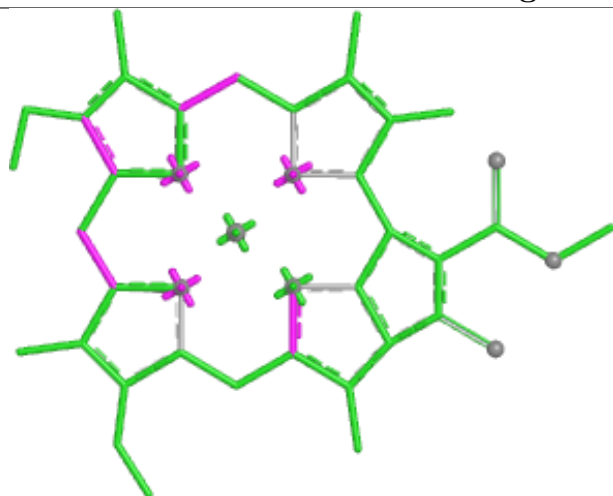
Ligand CLA z 306



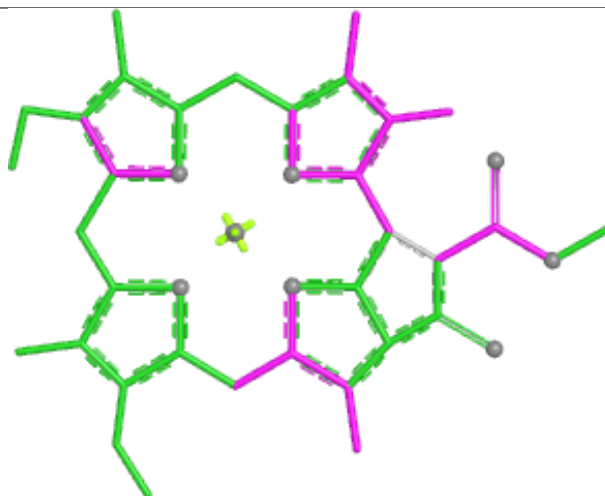
Ligand CLA x 318



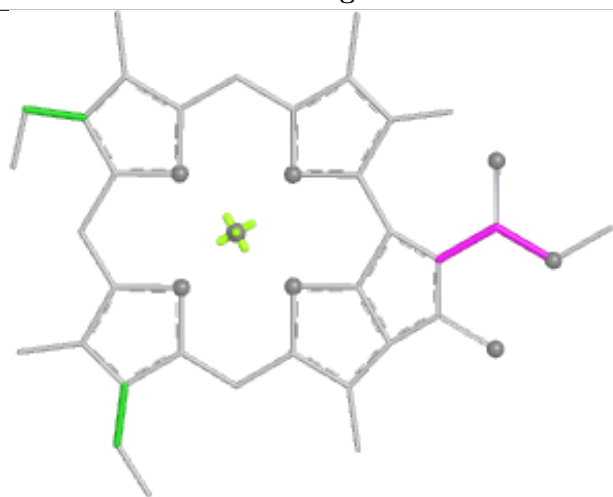
Ligand CLA z 310



Bond lengths



Bond angles

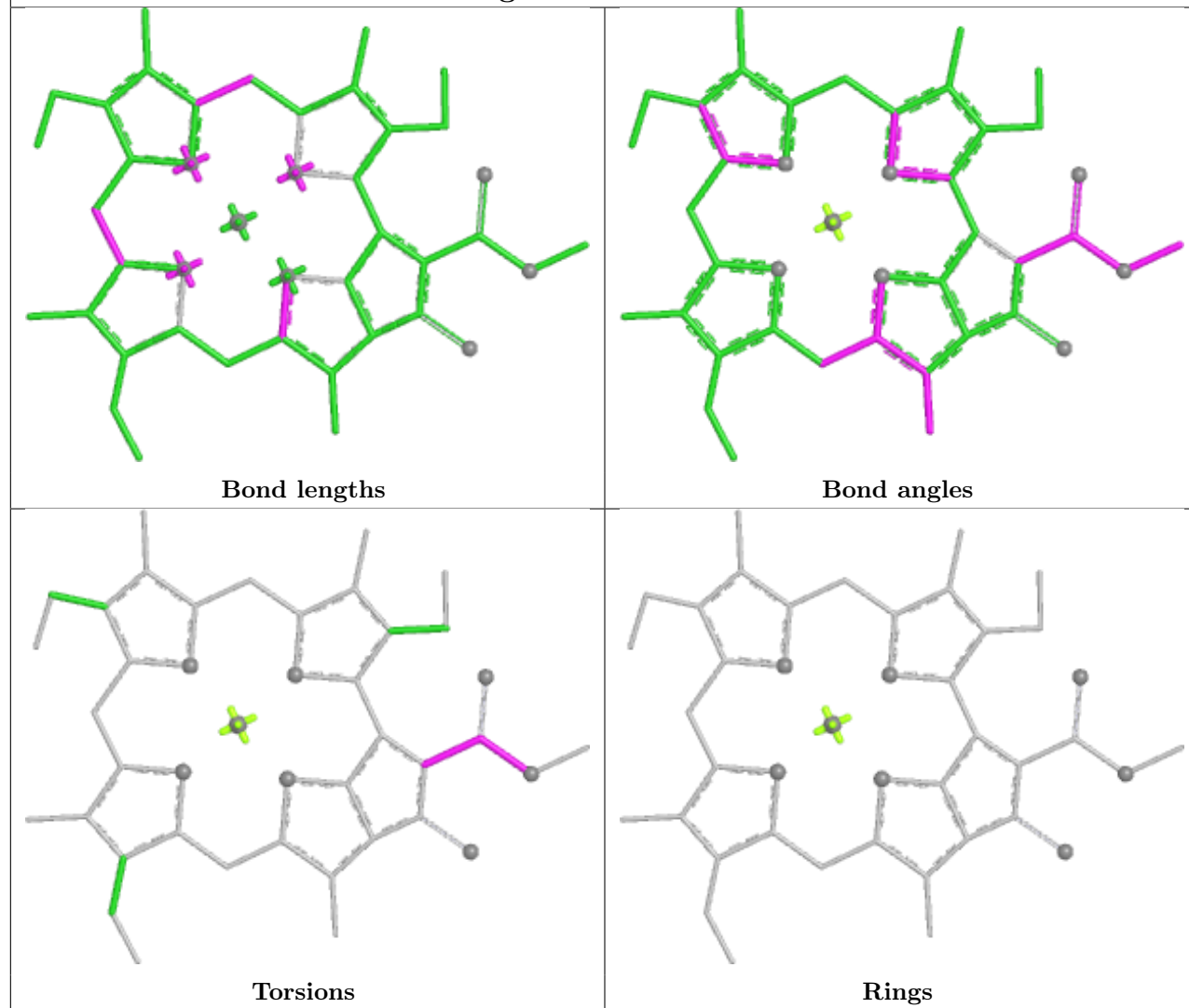


Torsions

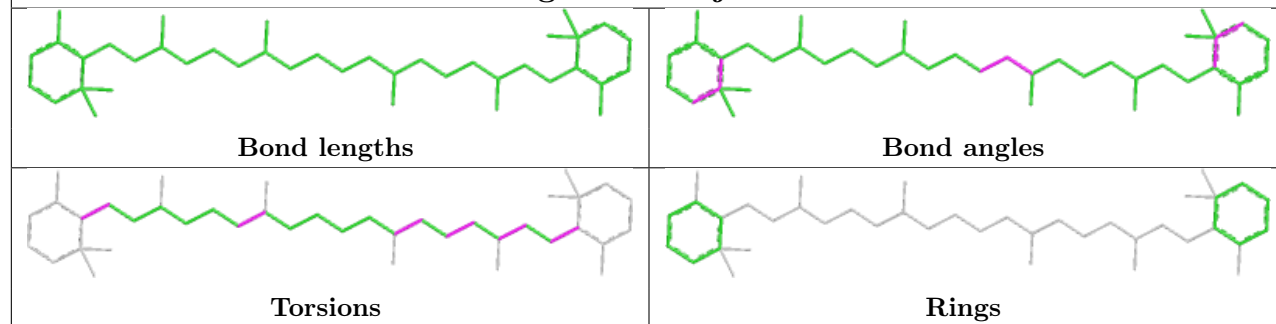


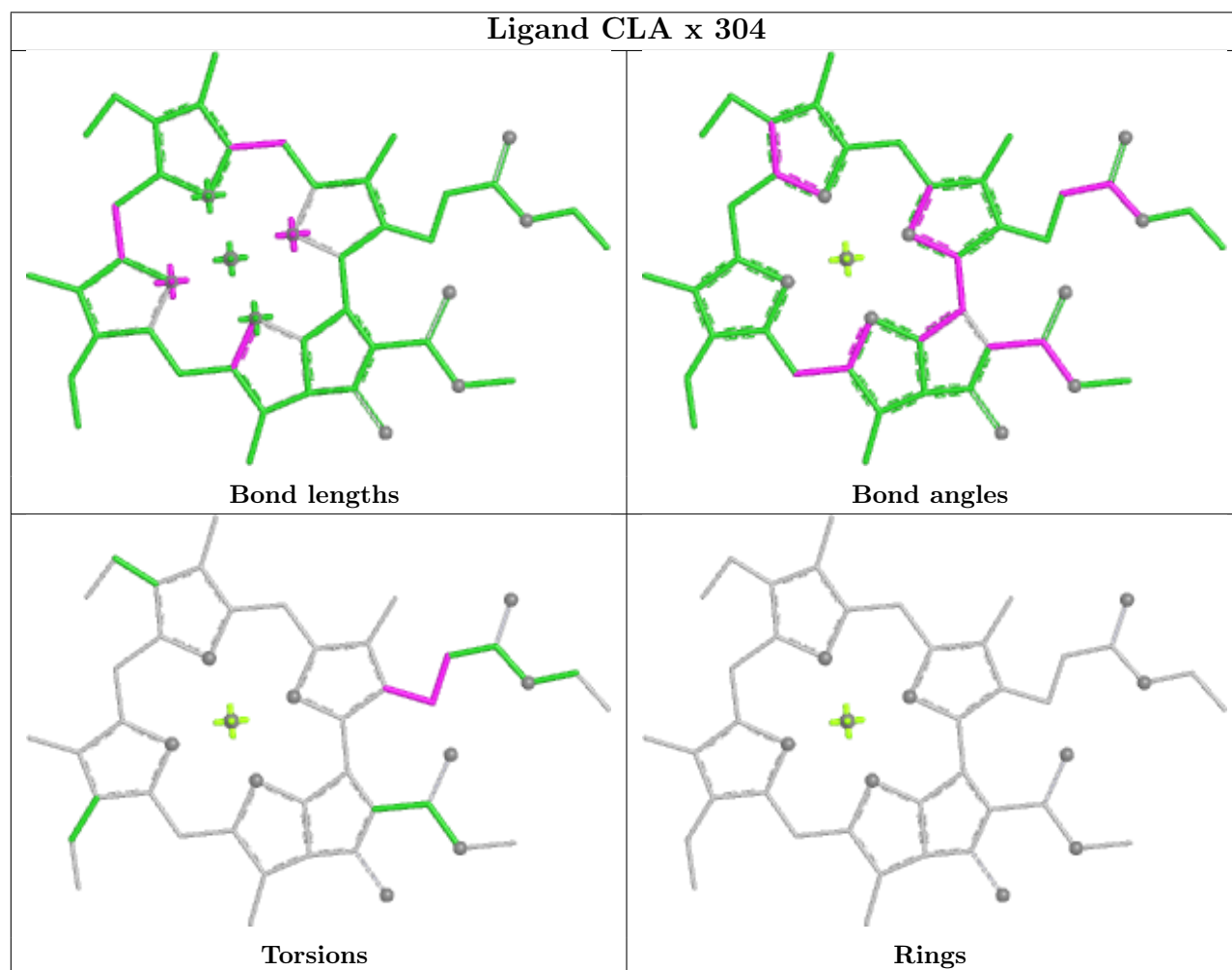
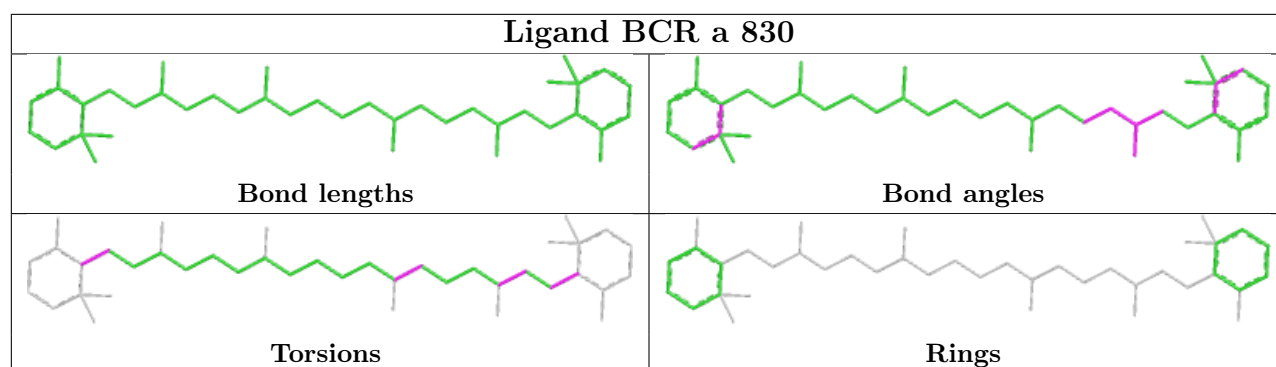
Rings

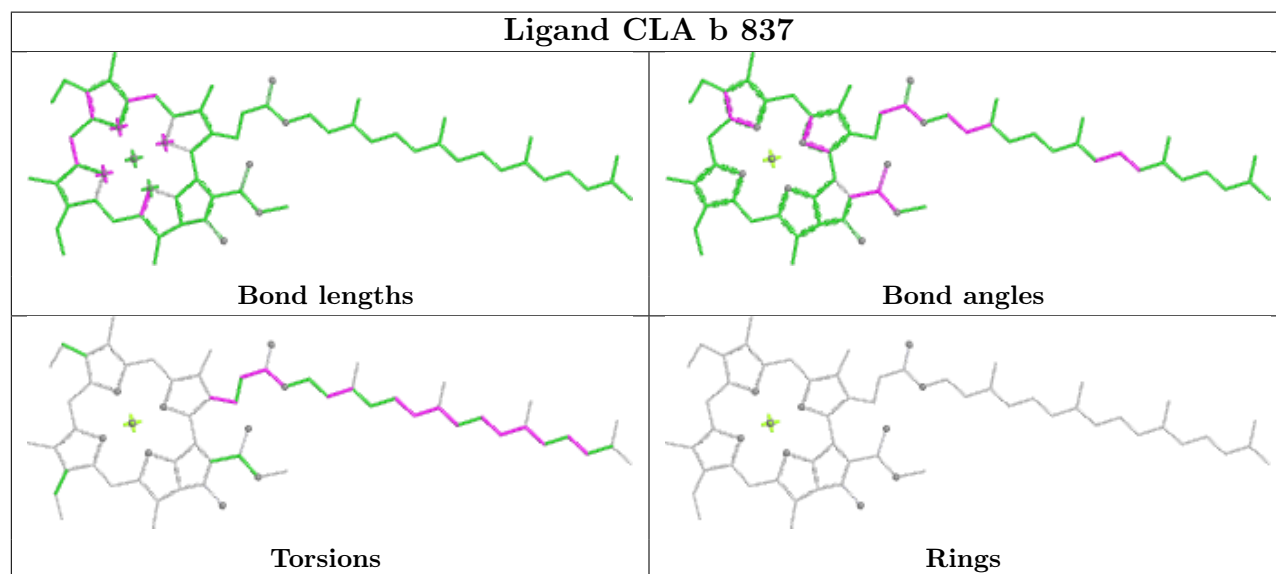
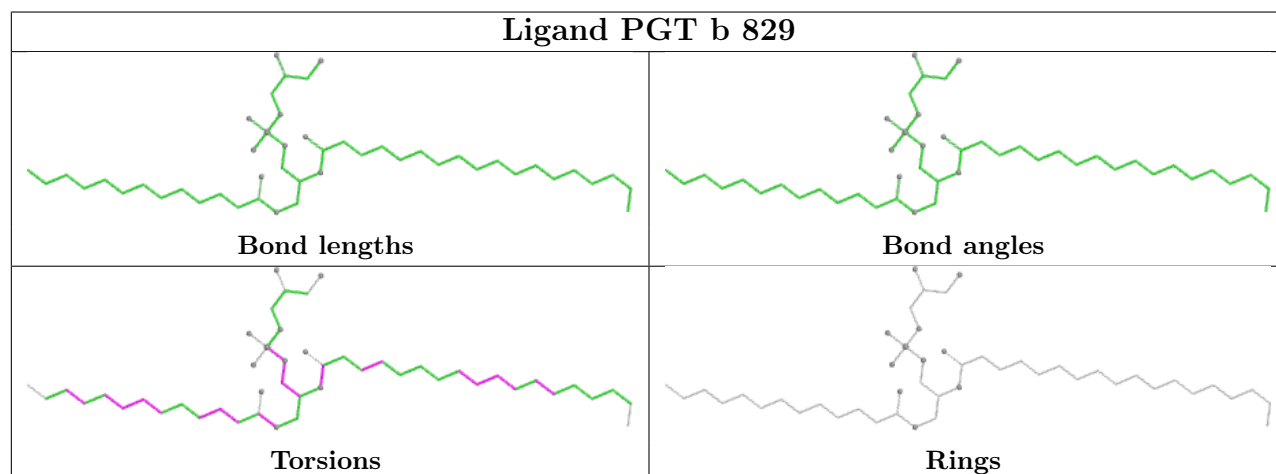
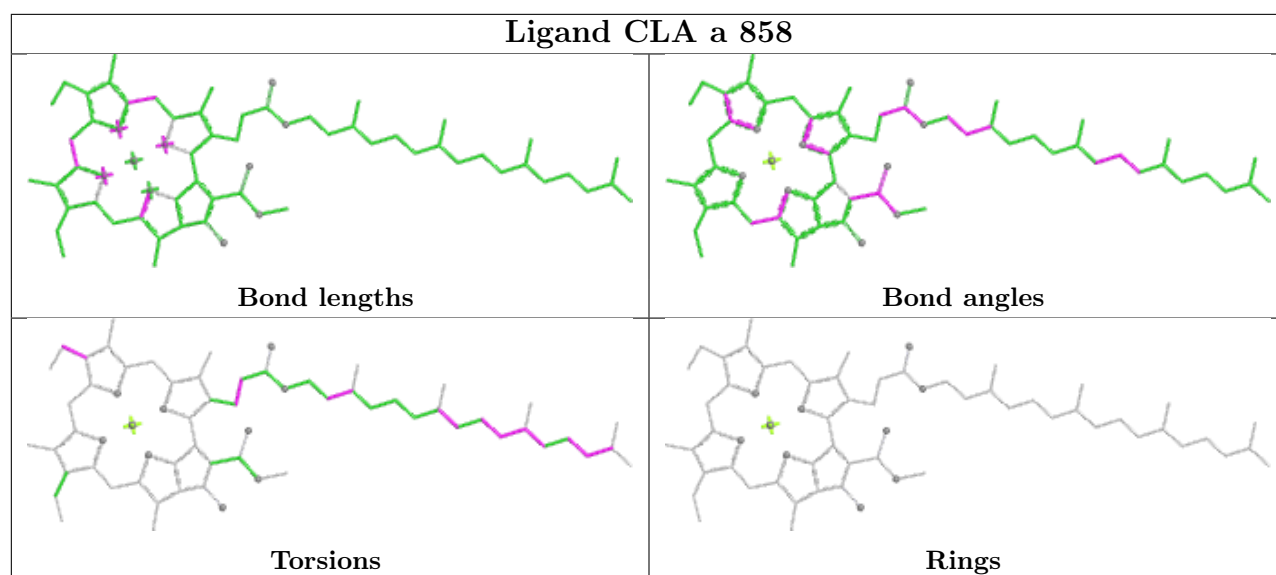
Ligand CLA k 205

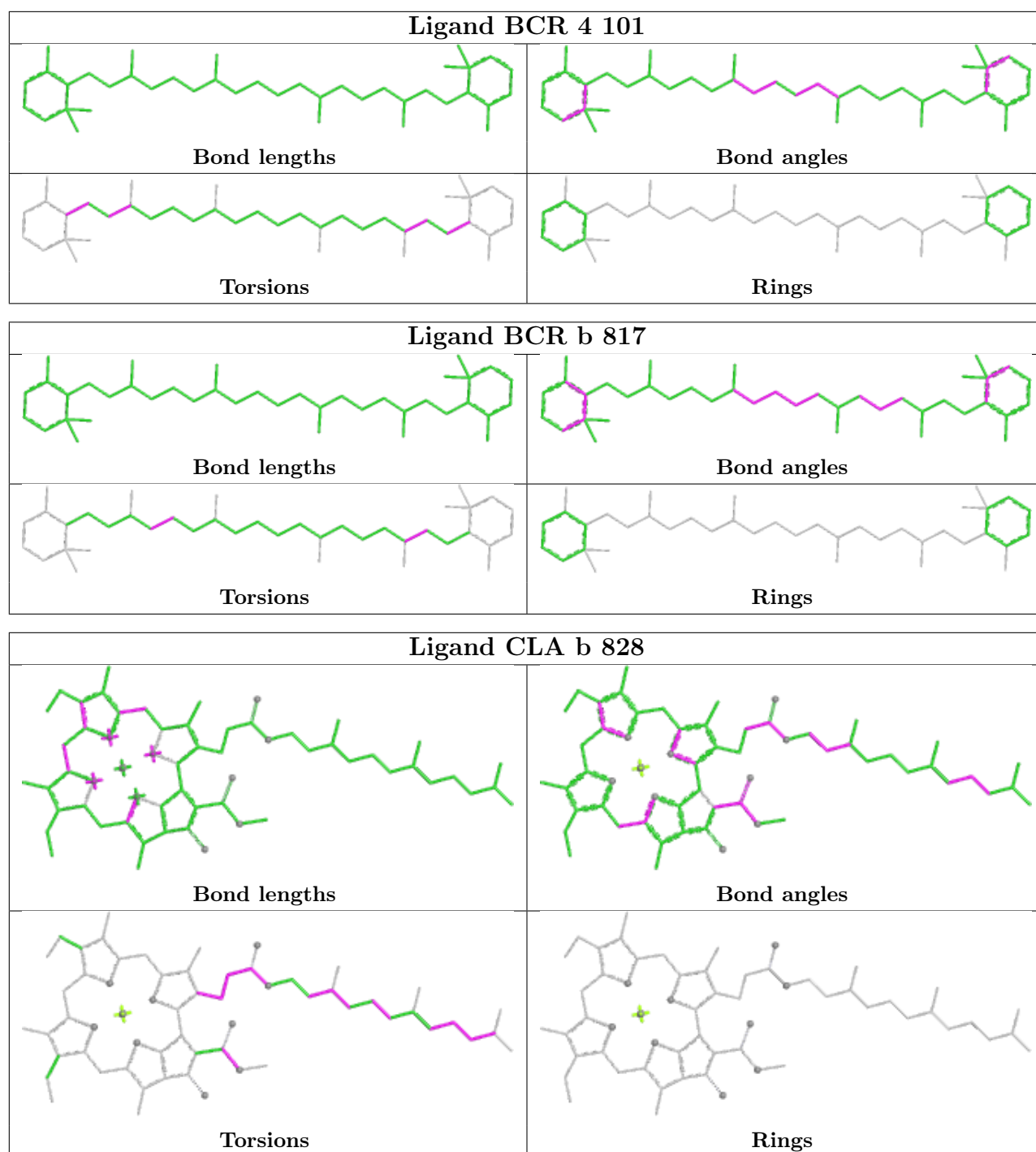


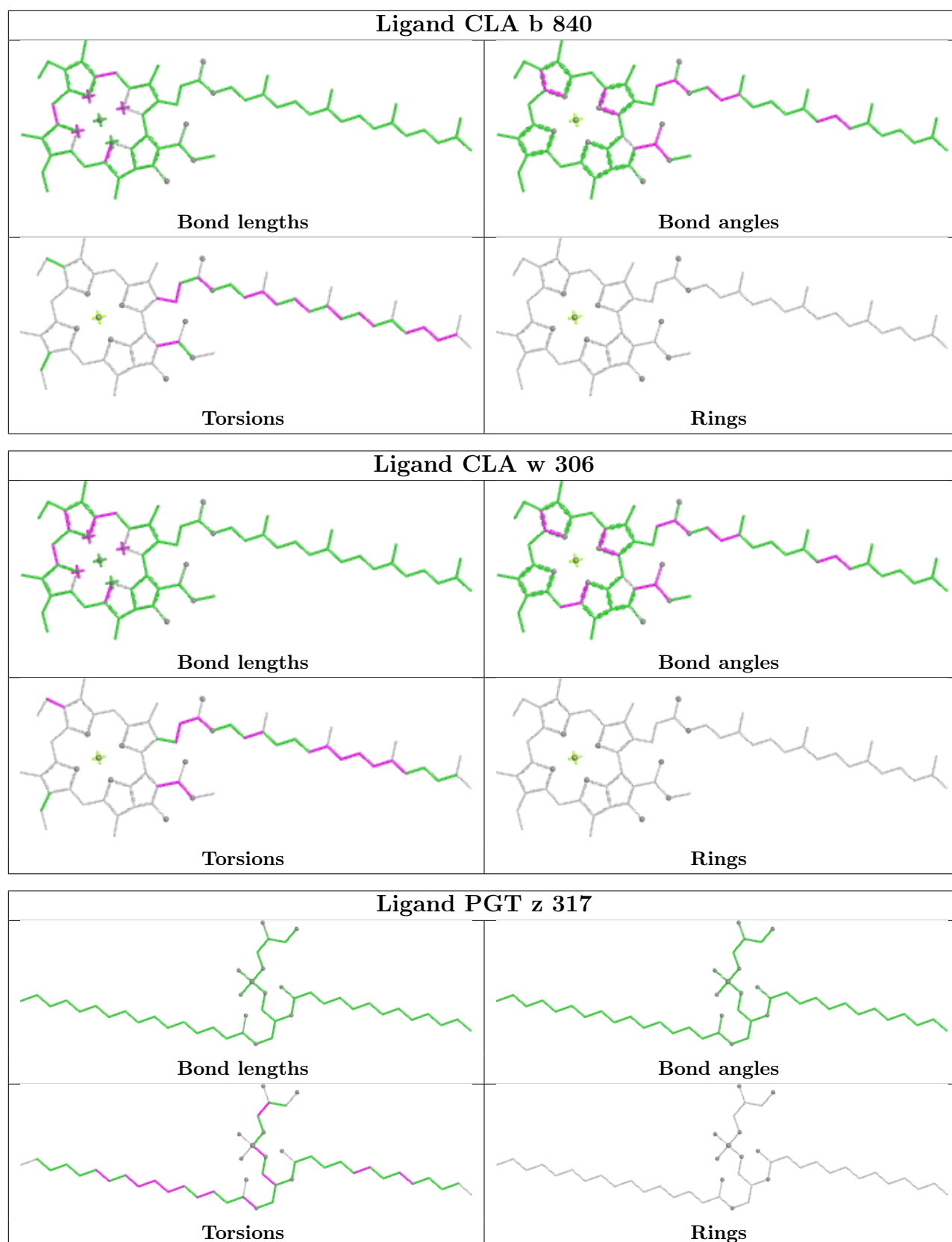
Ligand BCR j 101



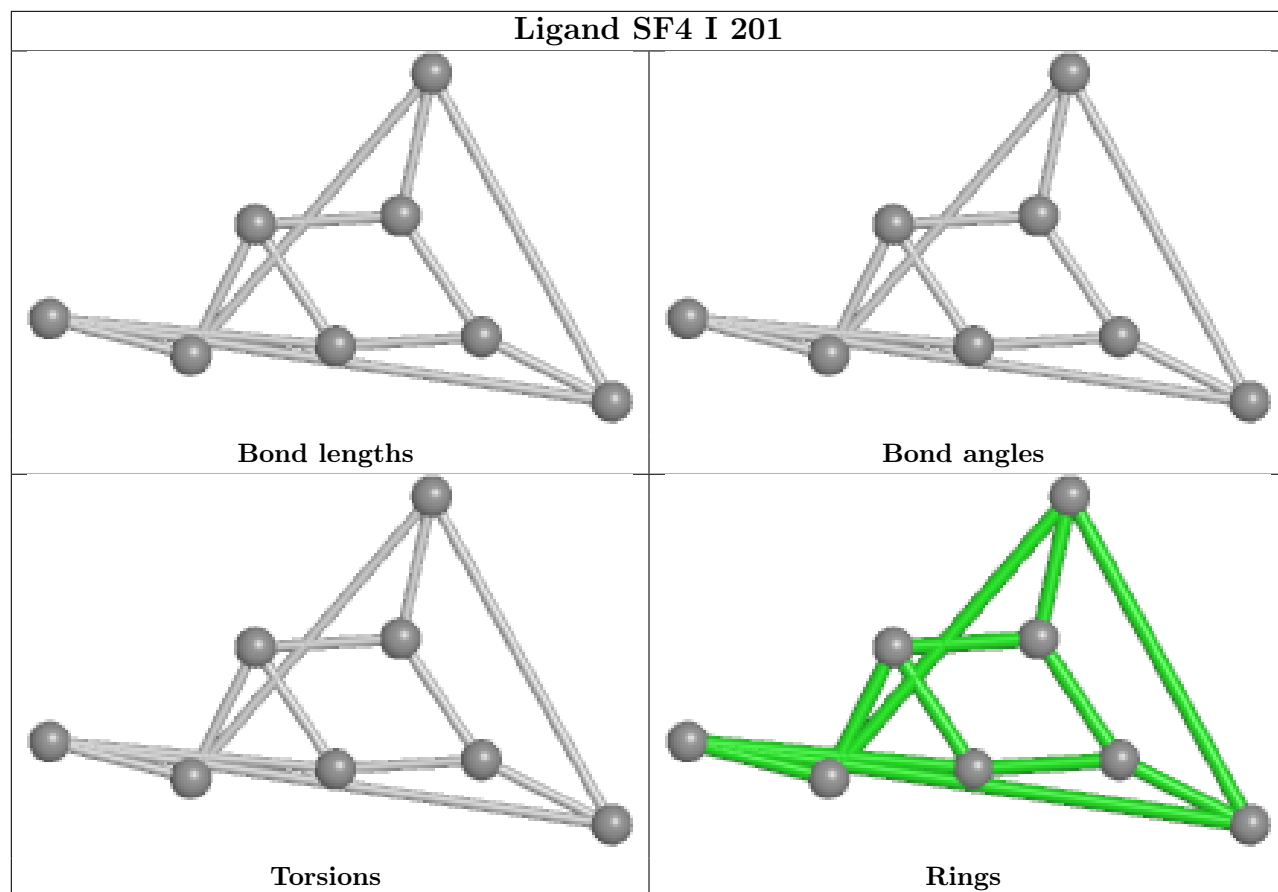




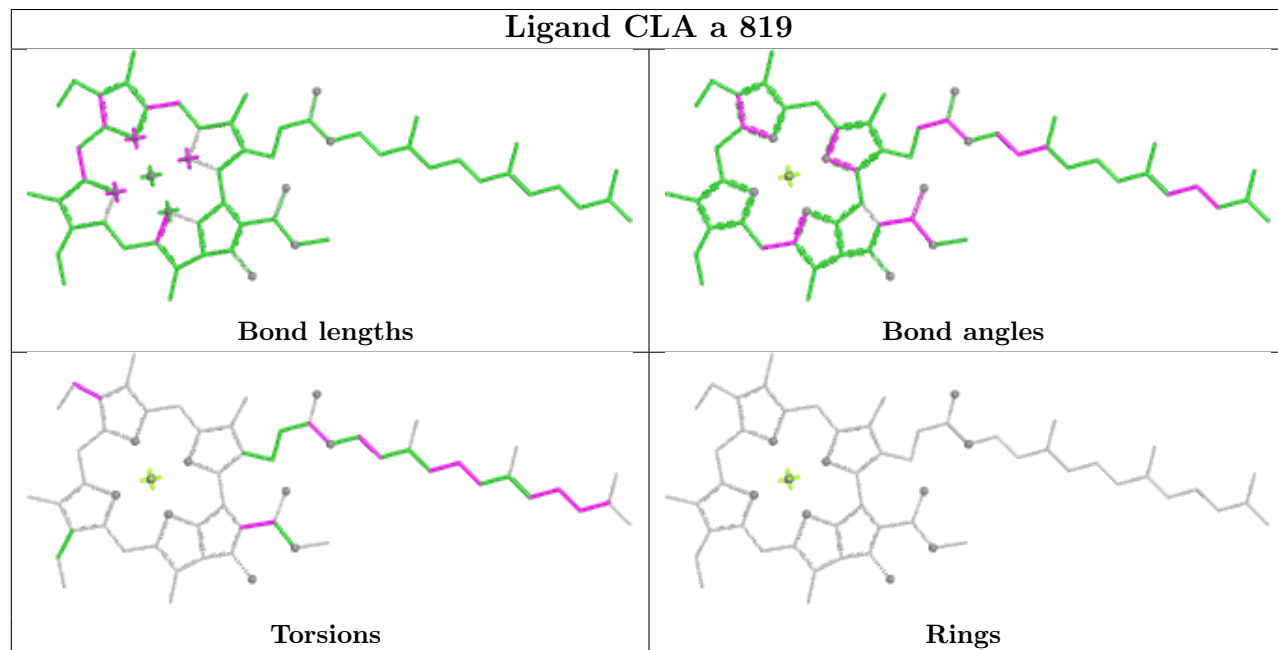


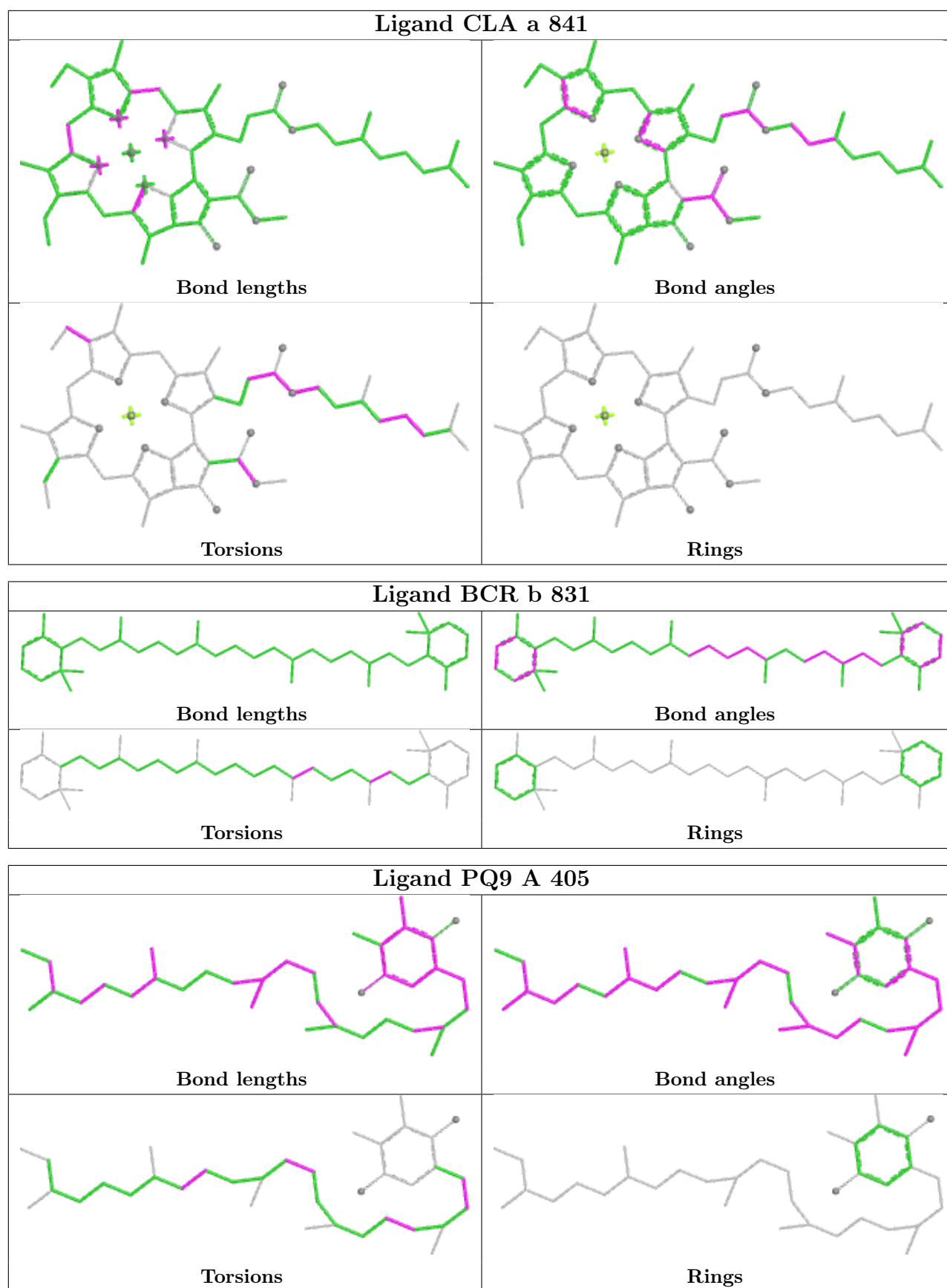


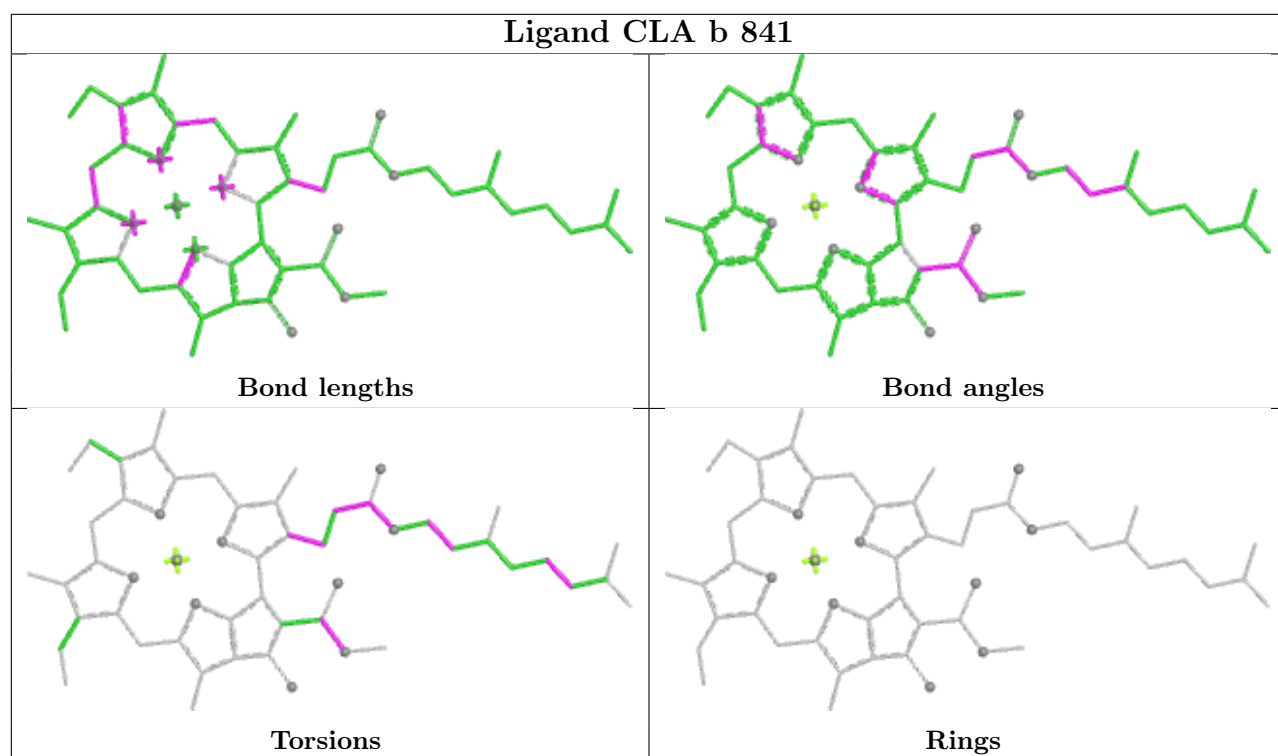
Ligand SF4 I 201



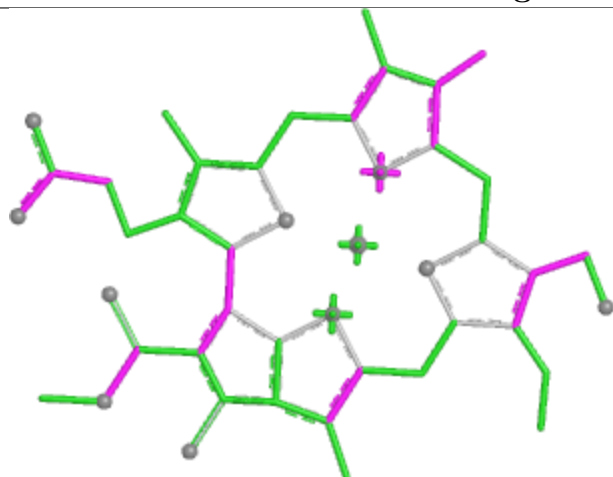
Ligand CLA a 819



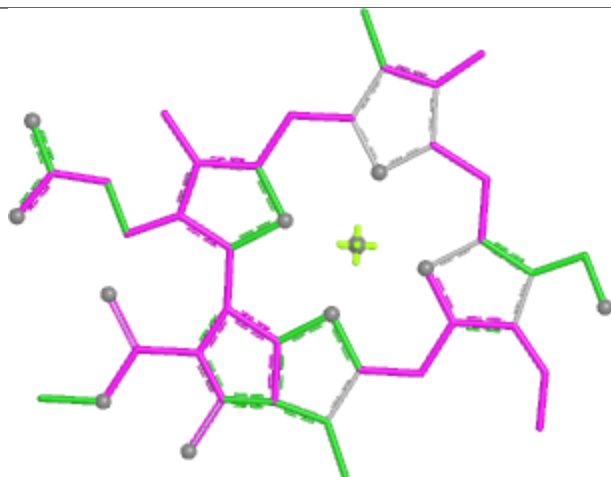




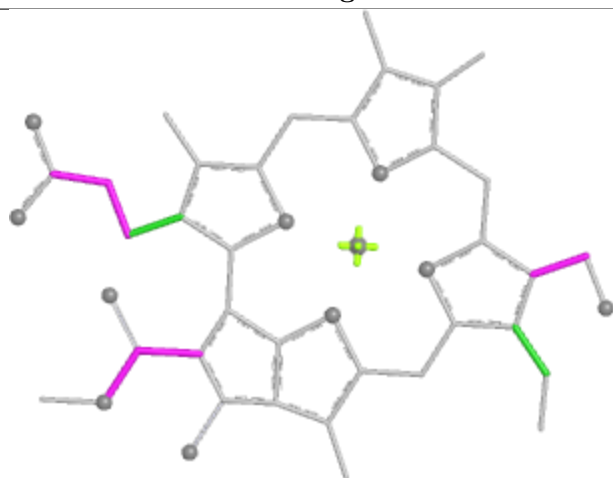
Ligand CHL w 304



Bond lengths



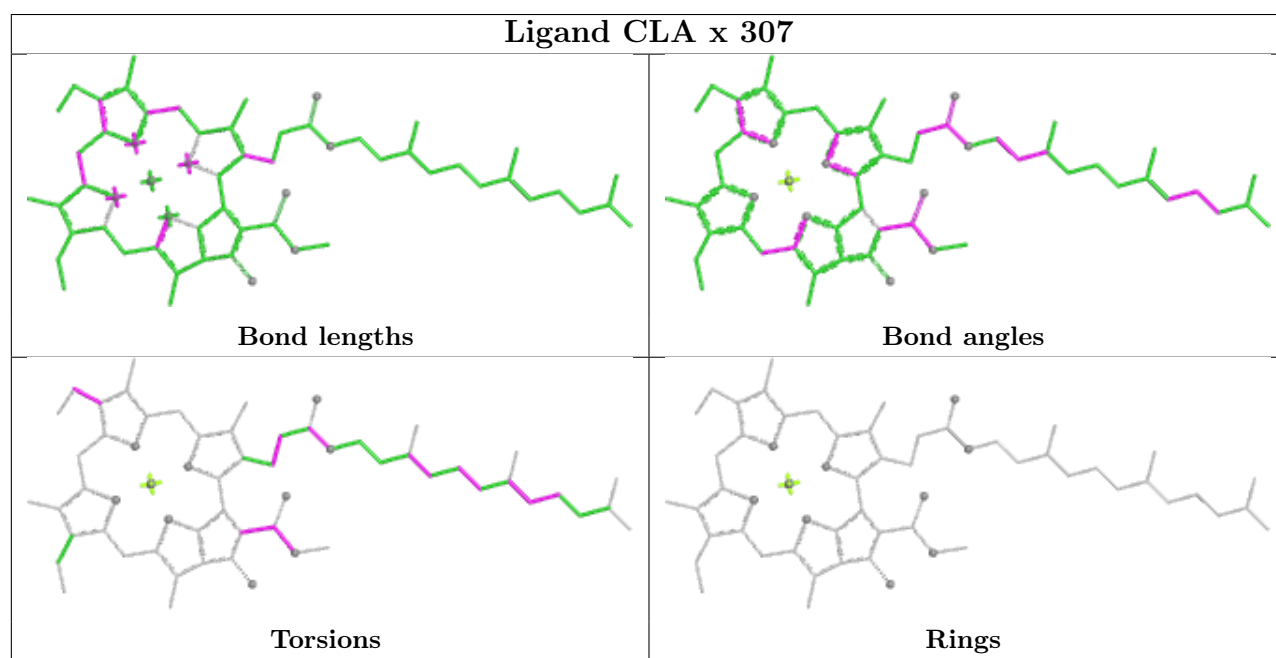
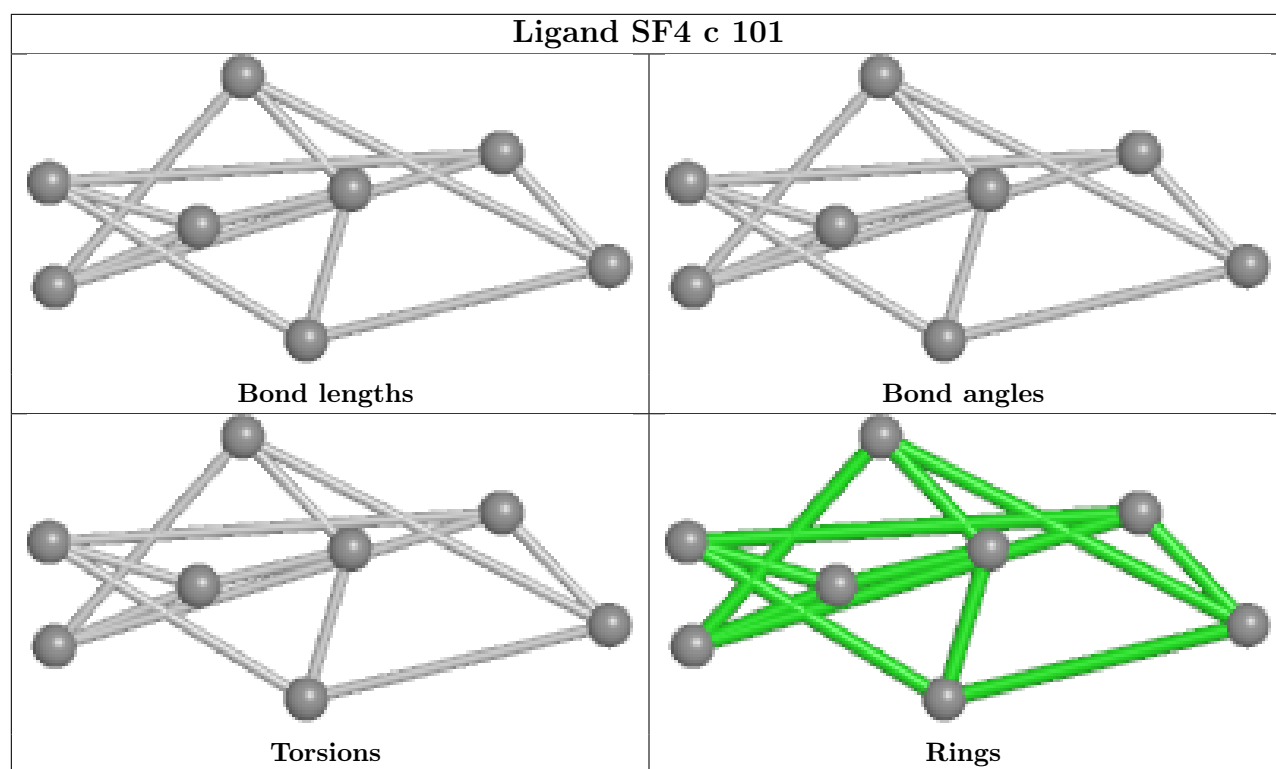
Bond angles

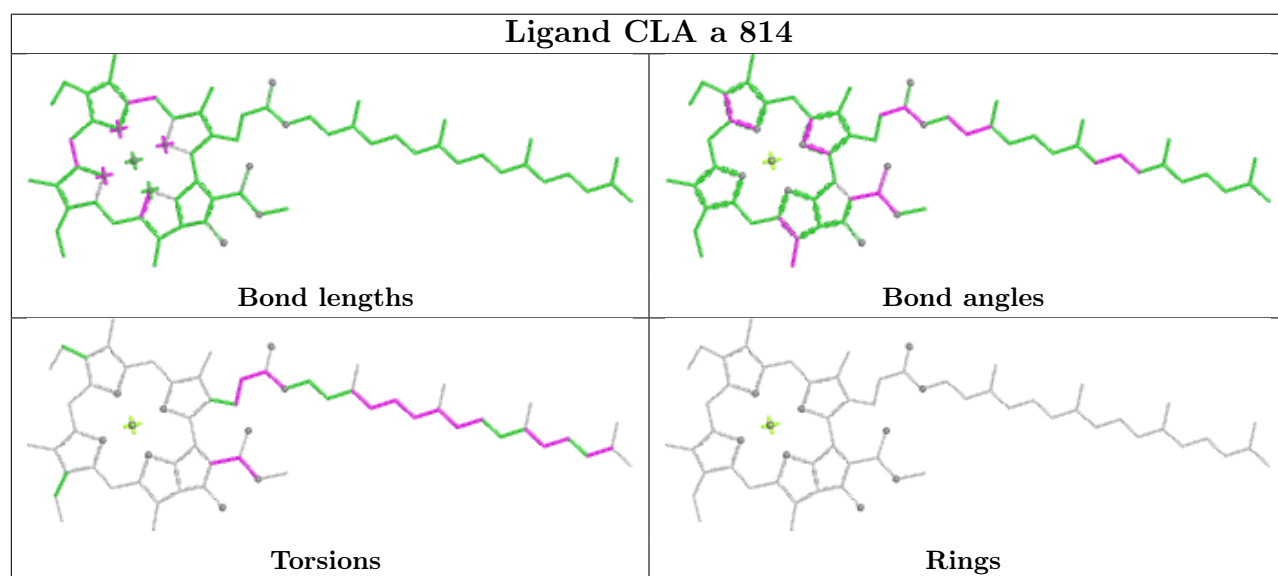
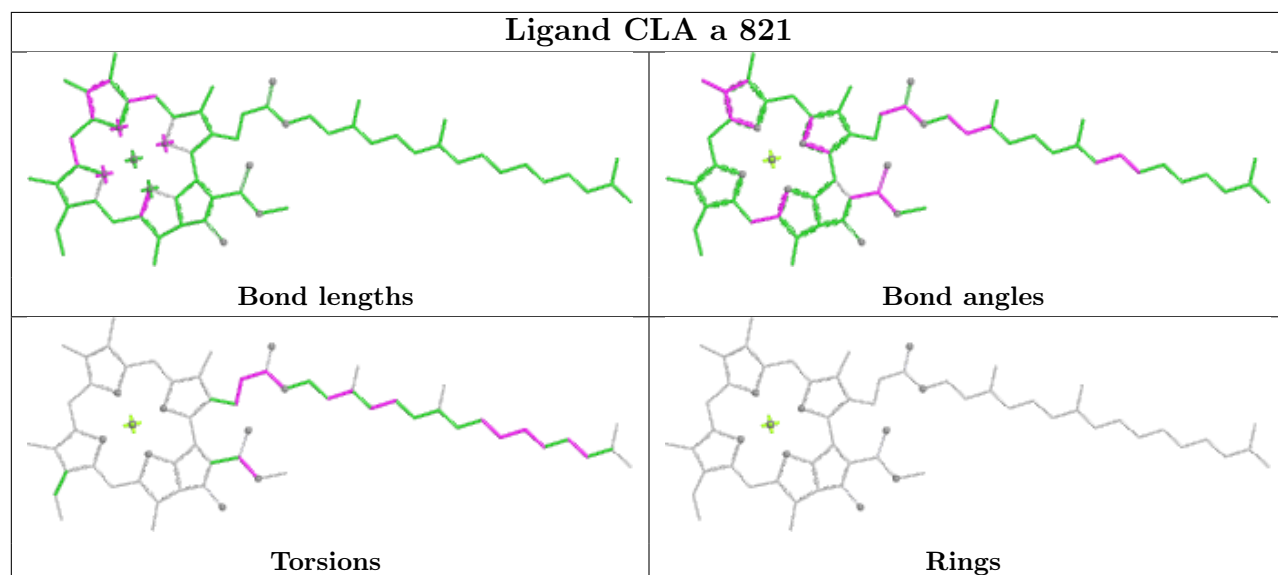
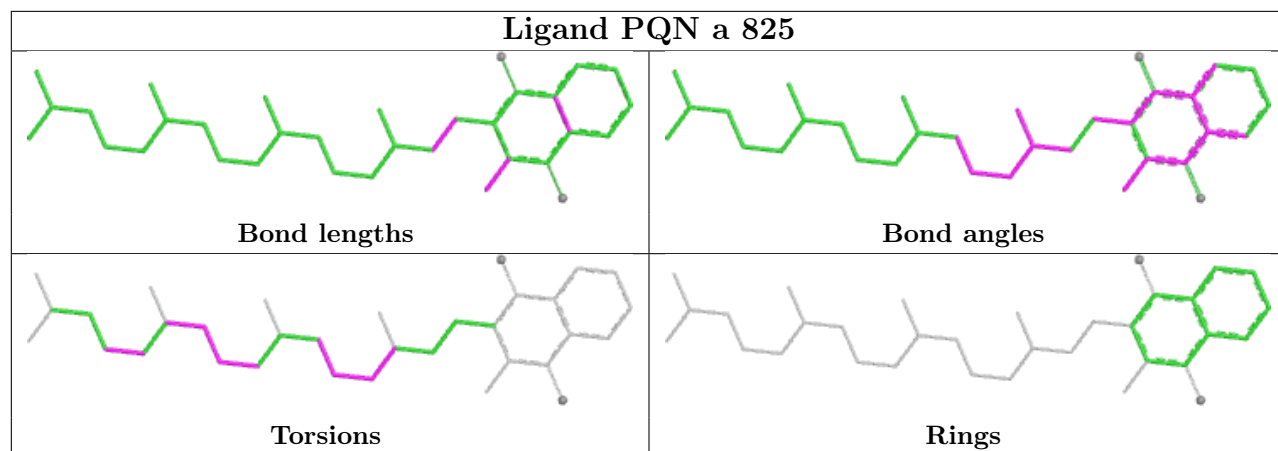


Torsions

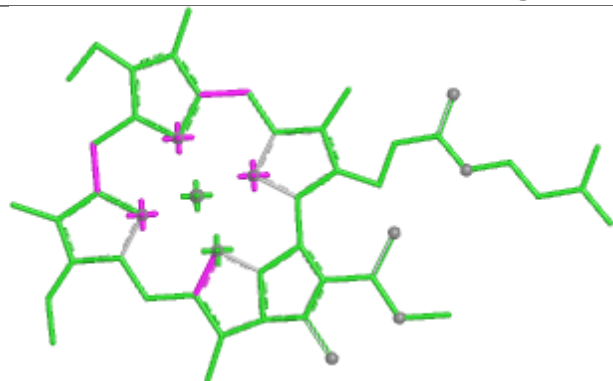


Rings

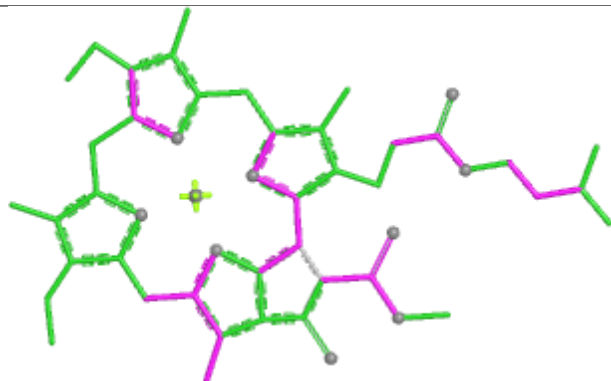




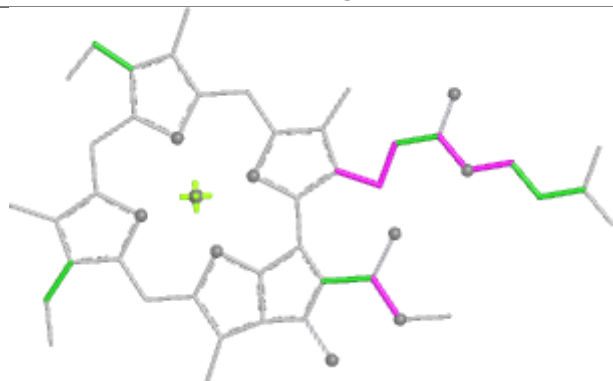
Ligand CLA w 316



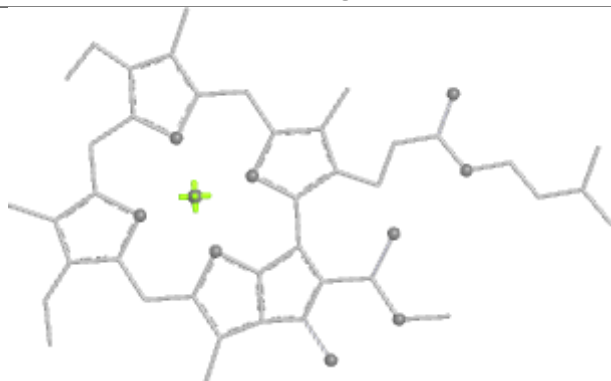
Bond lengths



Bond angles

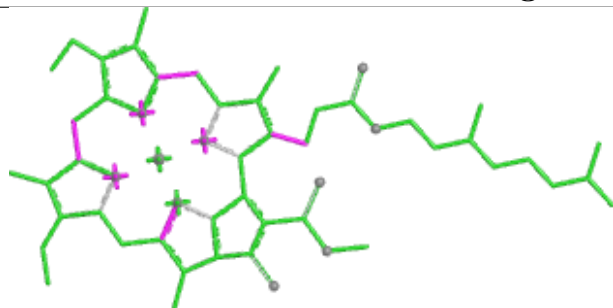


Torsions

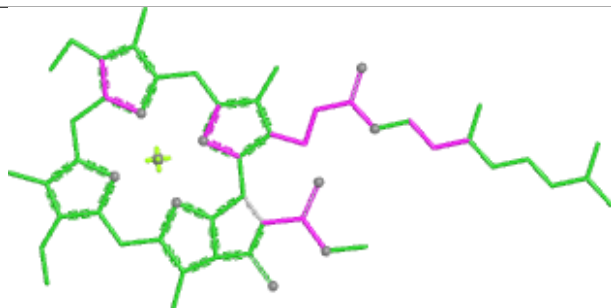


Rings

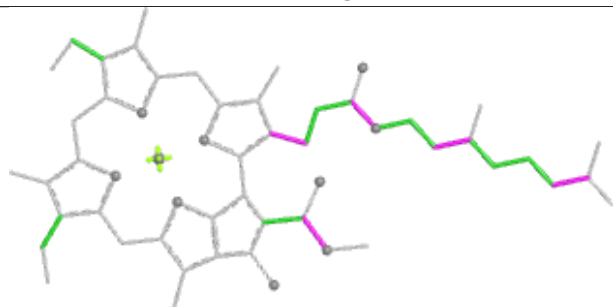
Ligand CLA z 302



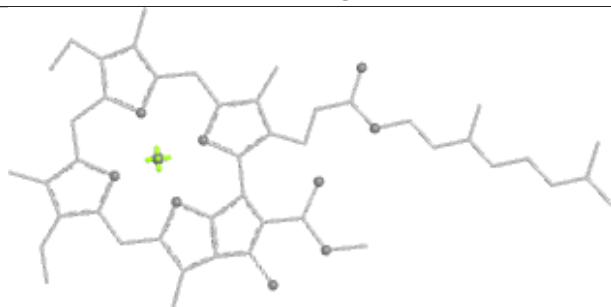
Bond lengths



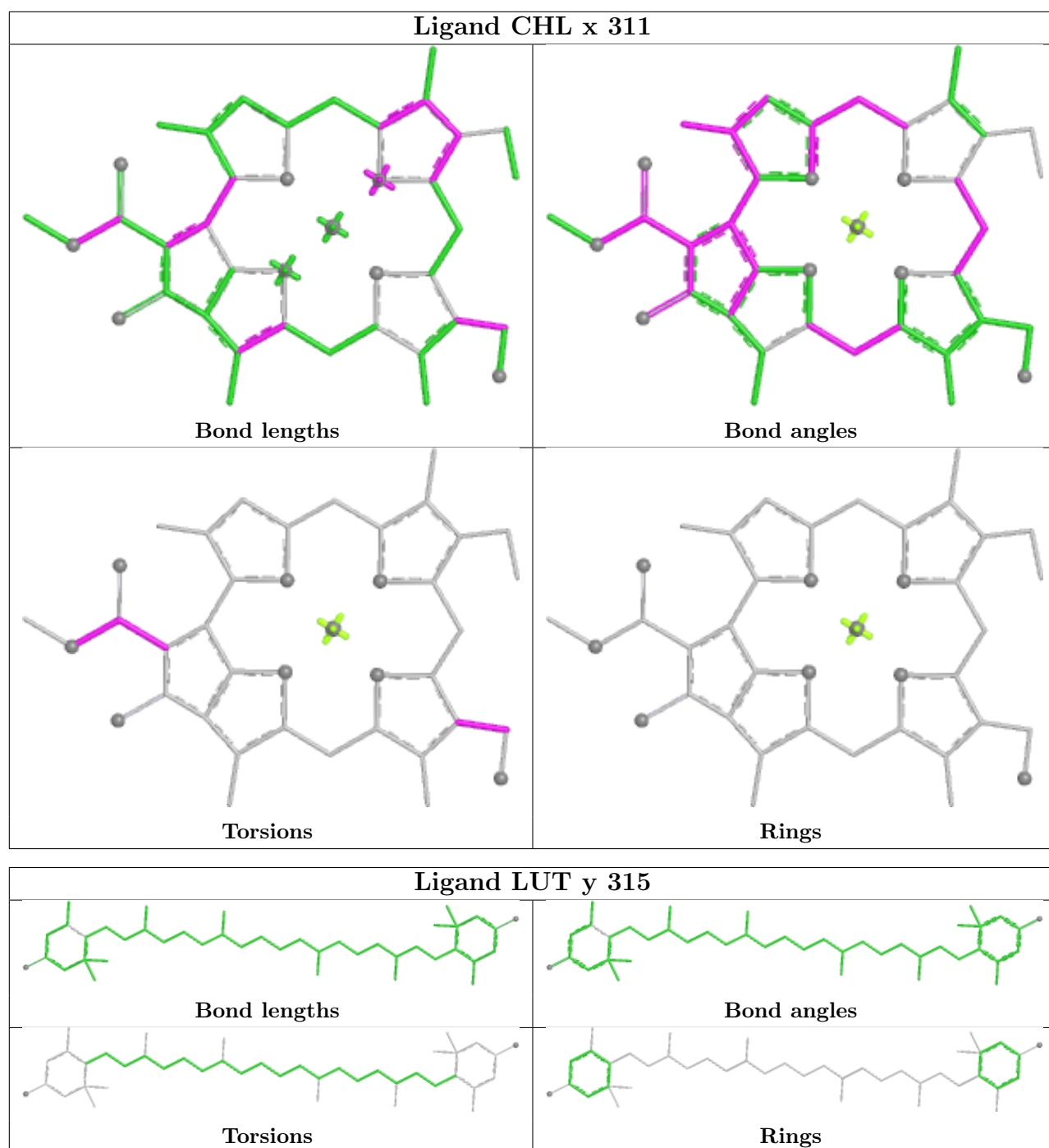
Bond angles



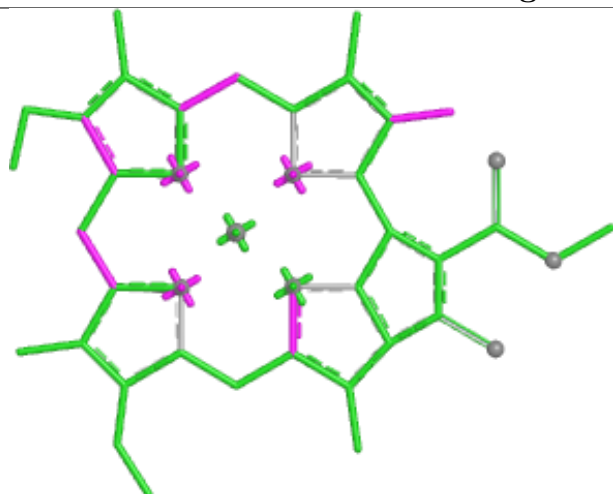
Torsions



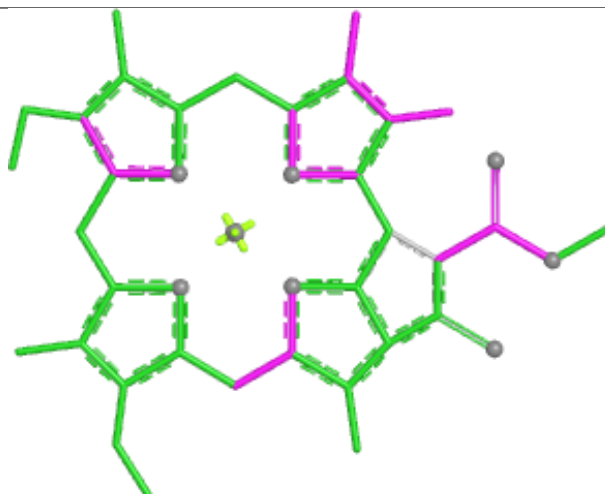
Rings



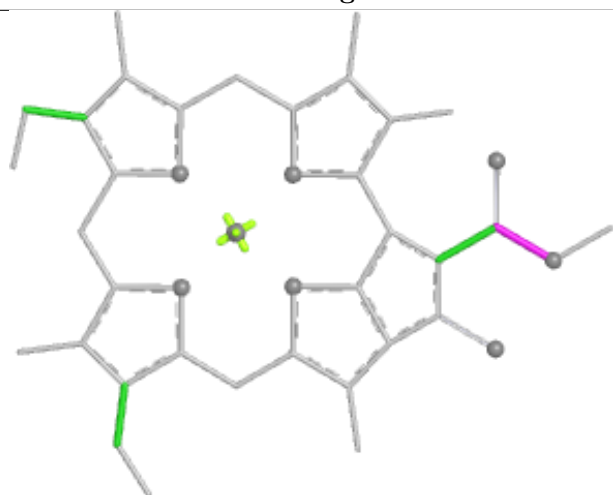
Ligand CLA z 303



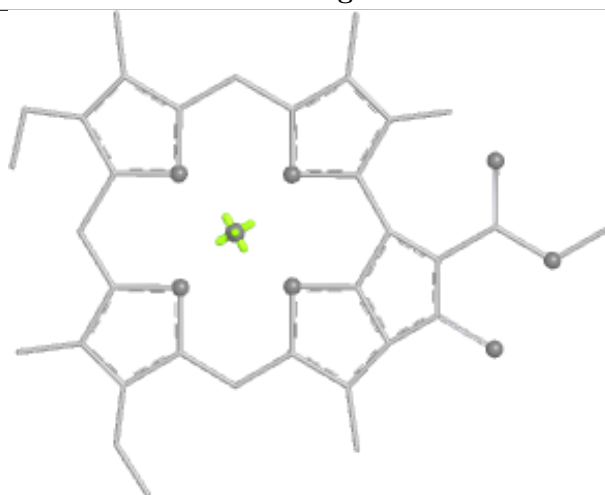
Bond lengths



Bond angles

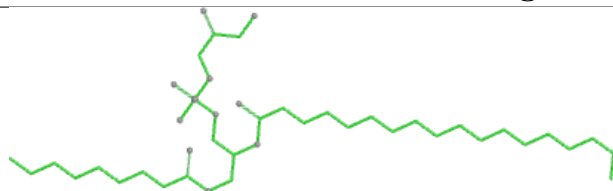


Torsions

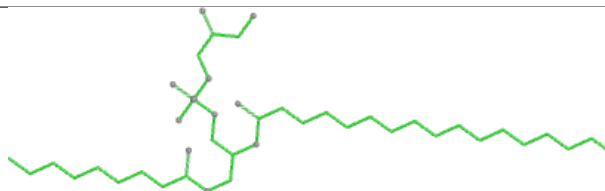


Rings

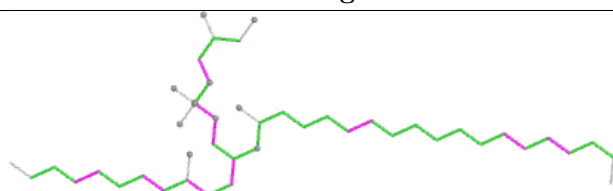
Ligand PGT I 203



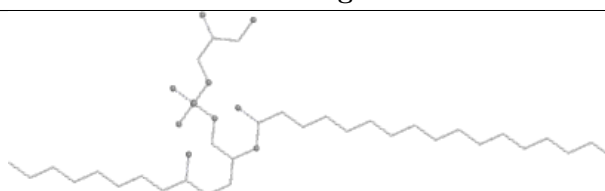
Bond lengths



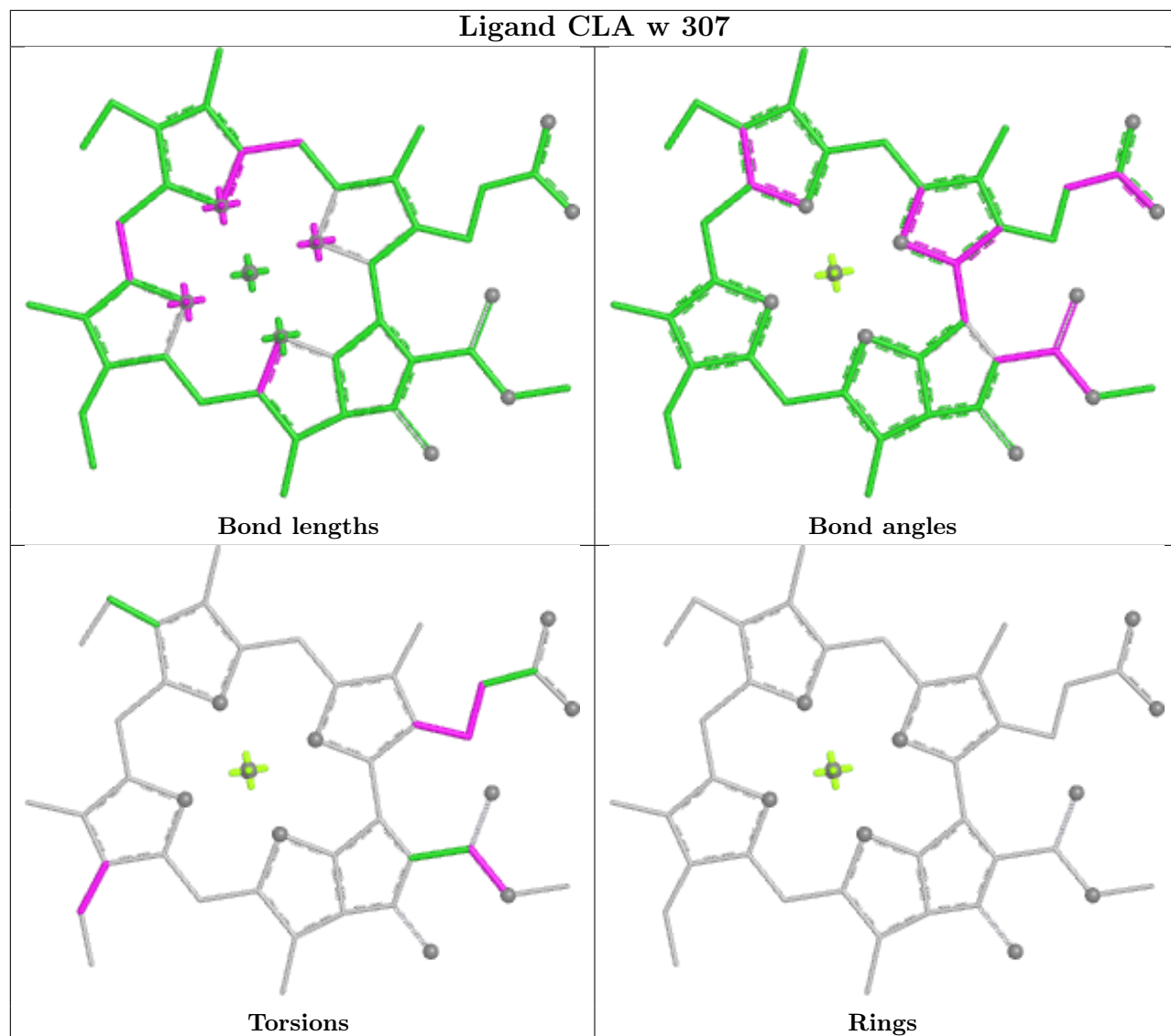
Bond angles



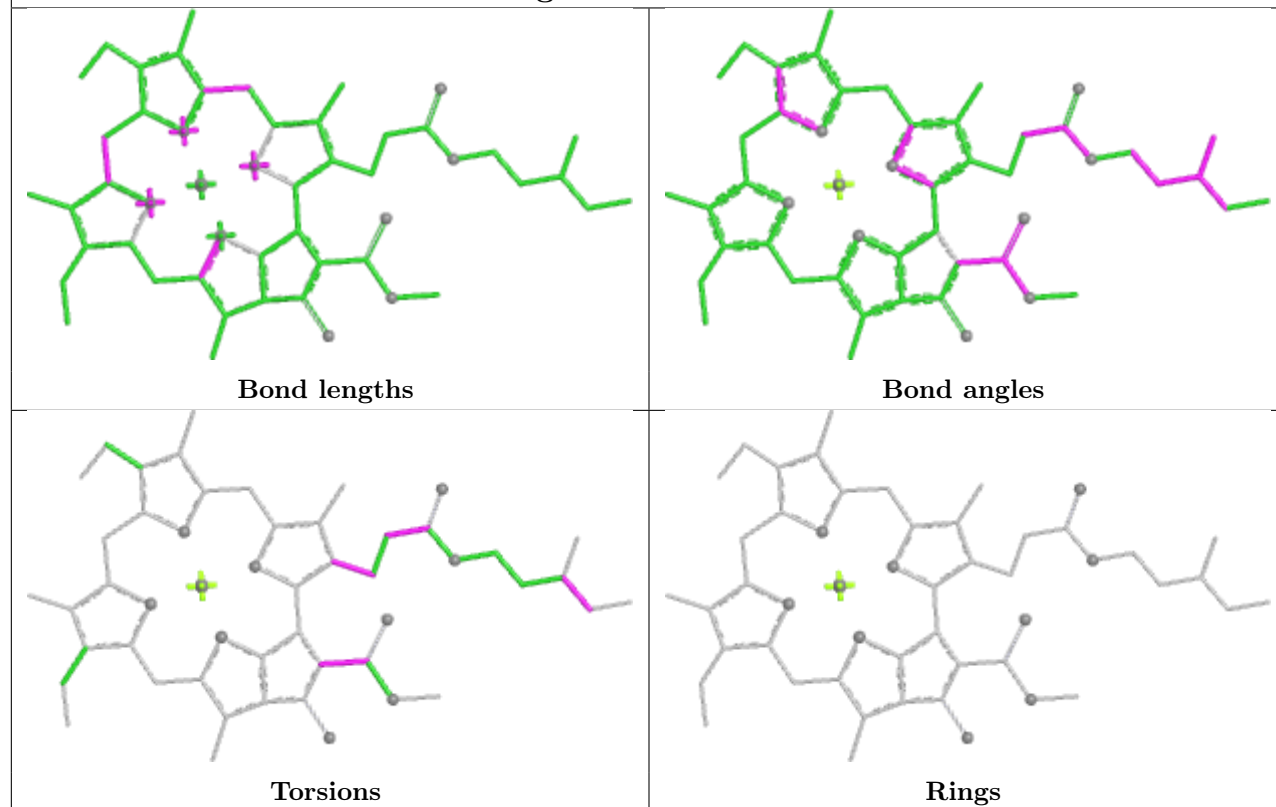
Torsions



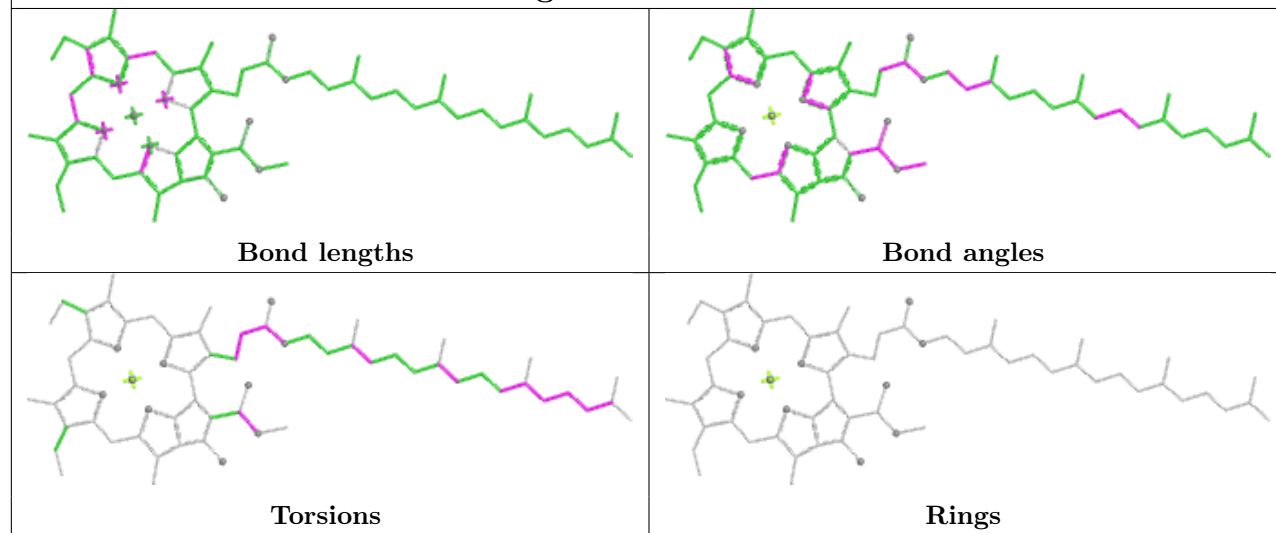
Rings

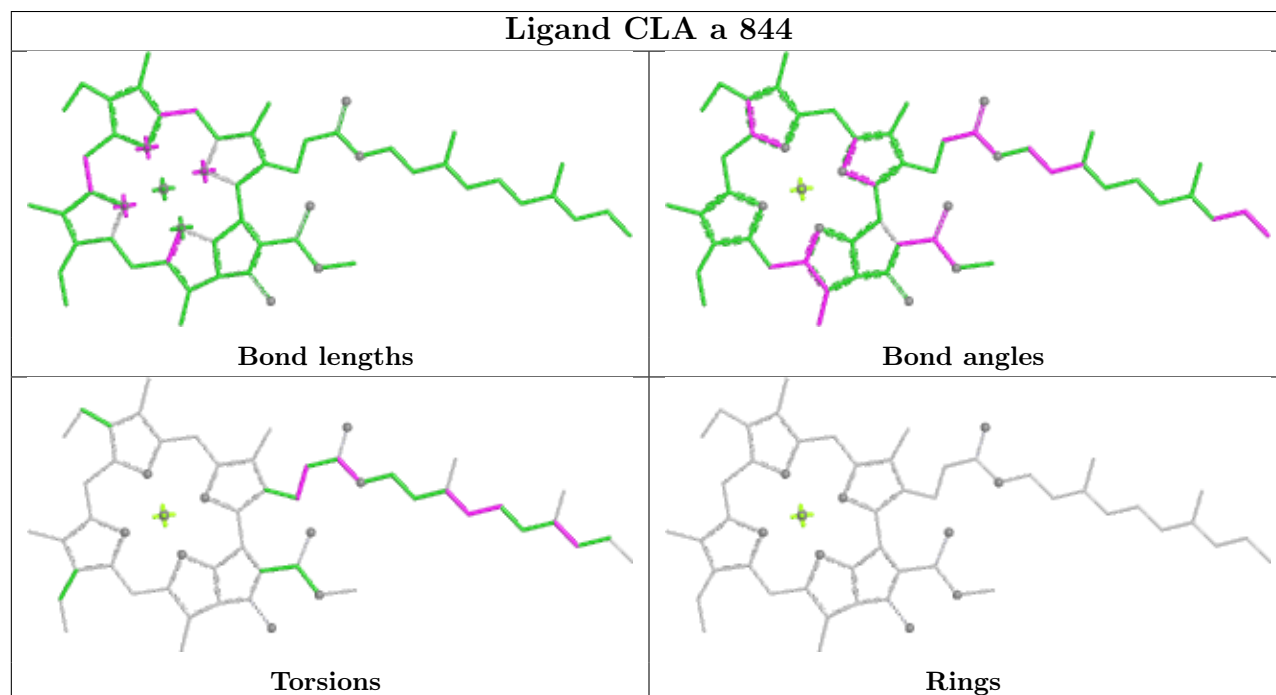
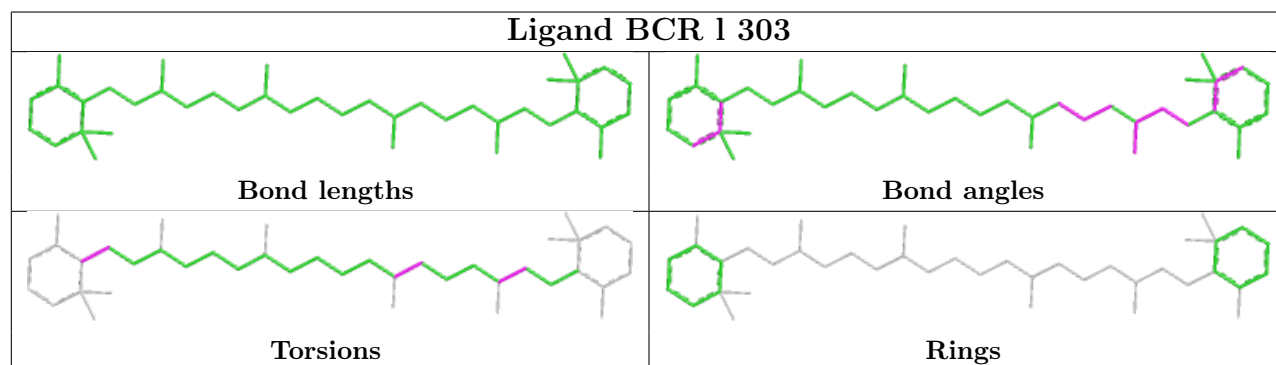
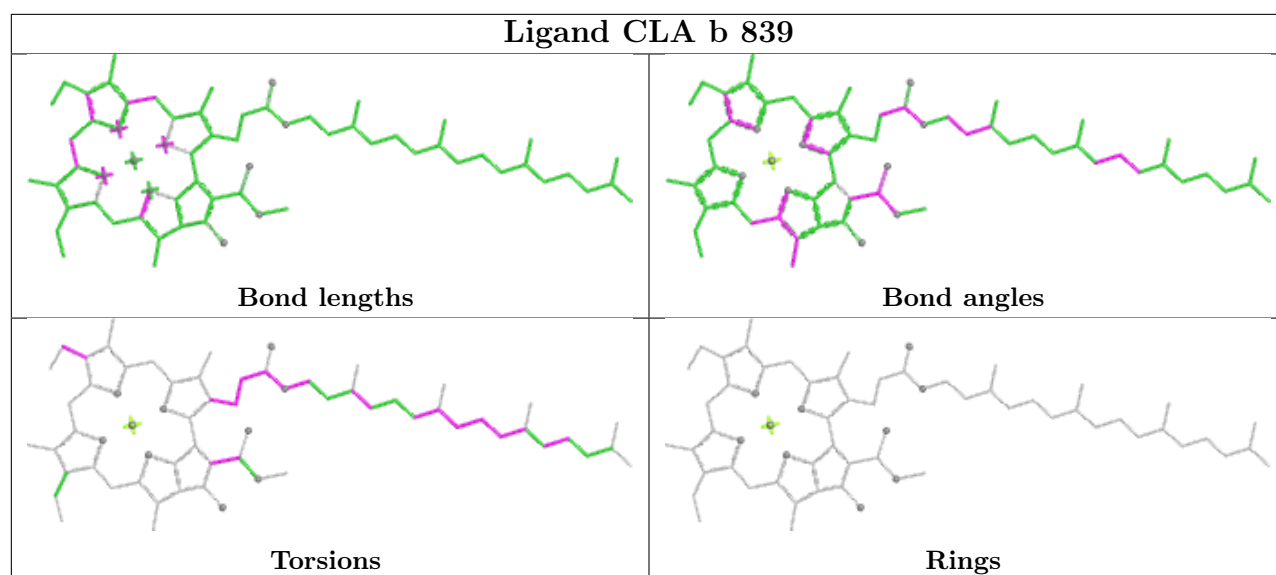


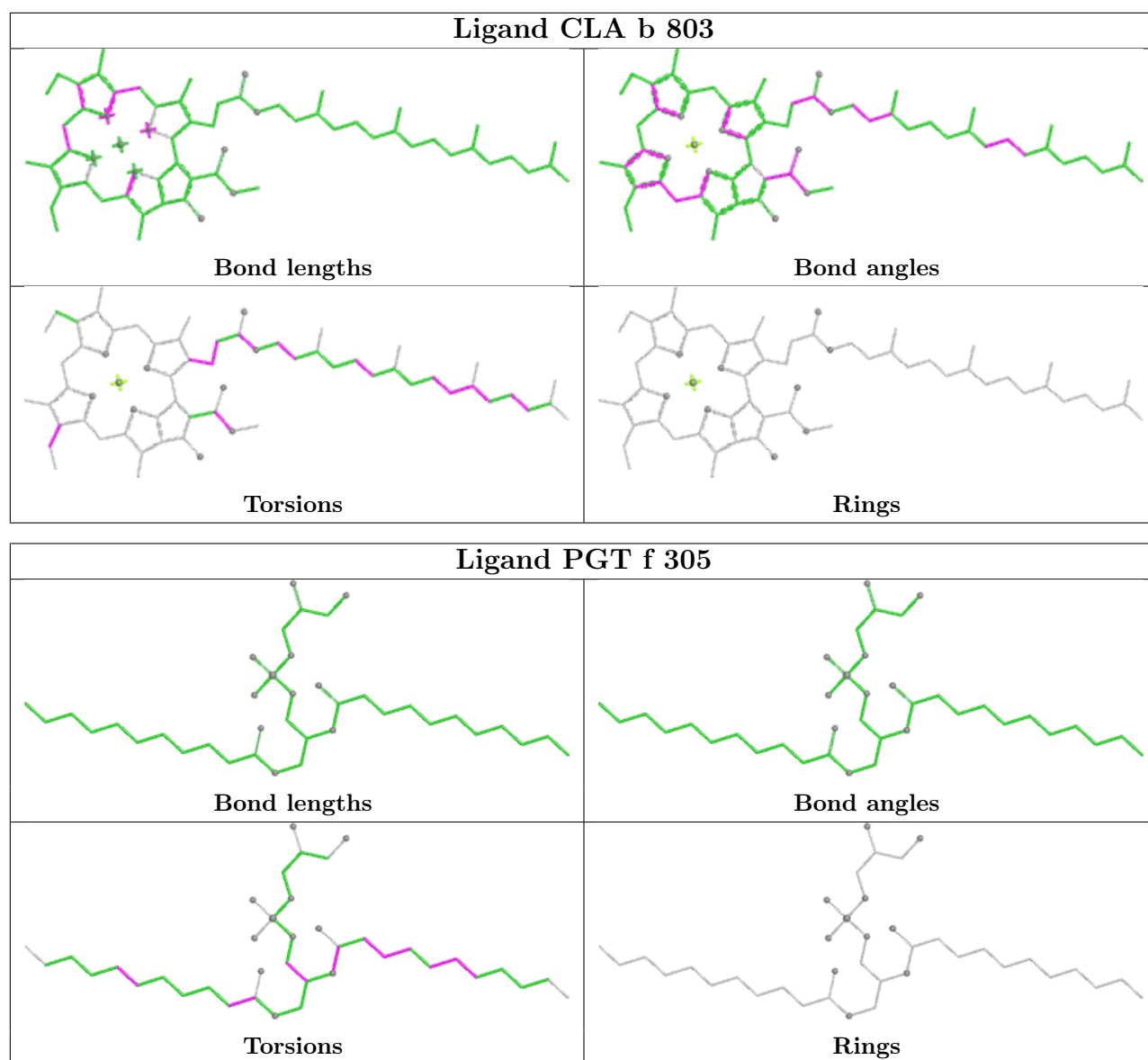
Ligand CLA a 852

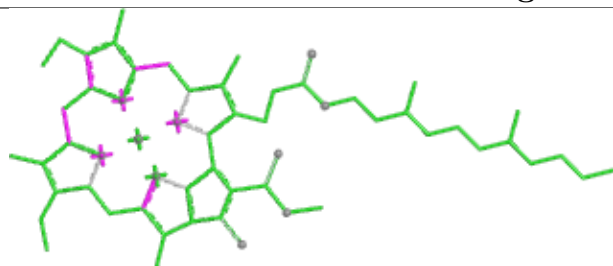


Ligand CLA a 843

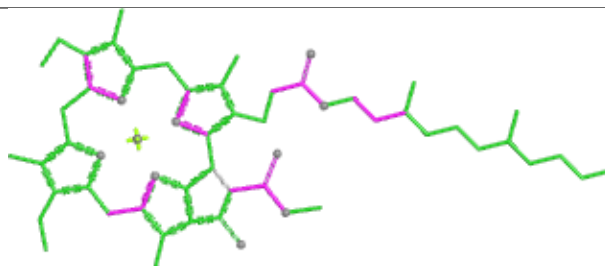




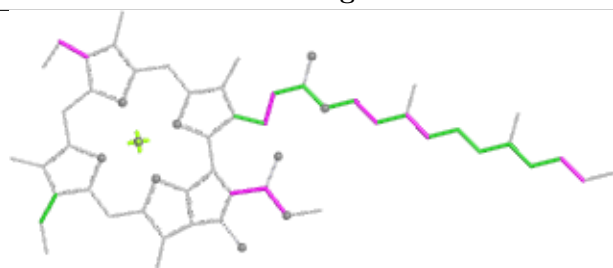


Ligand CLA b 822

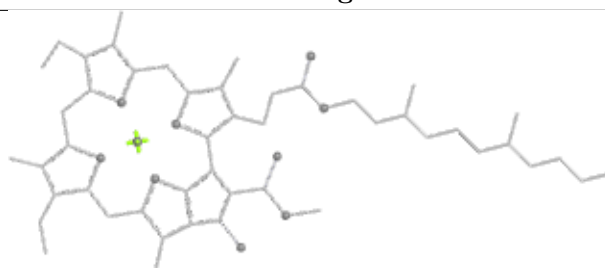
Bond lengths



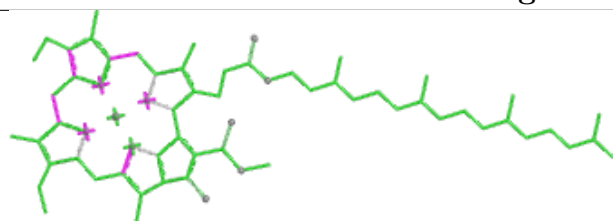
Bond angles



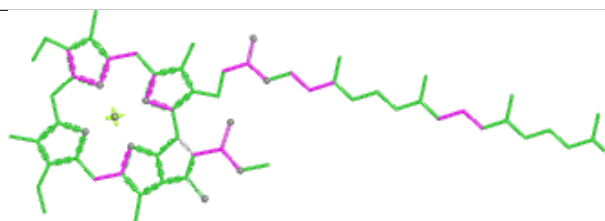
Torsions



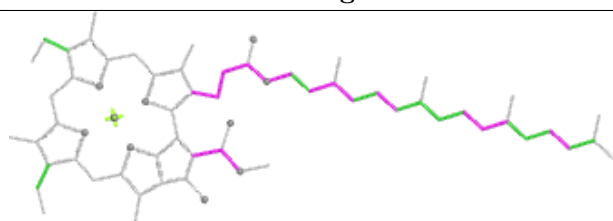
Rings

Ligand CLA a 833

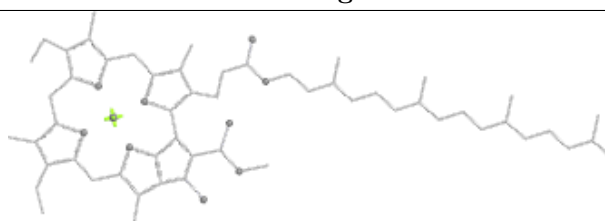
Bond lengths



Bond angles

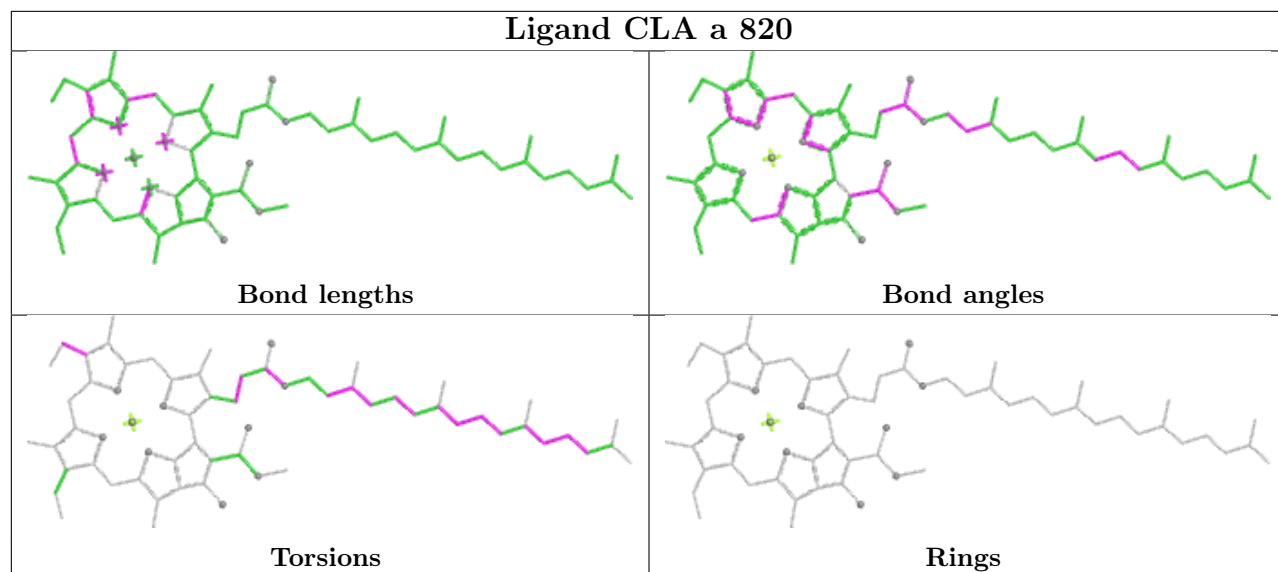


Torsions

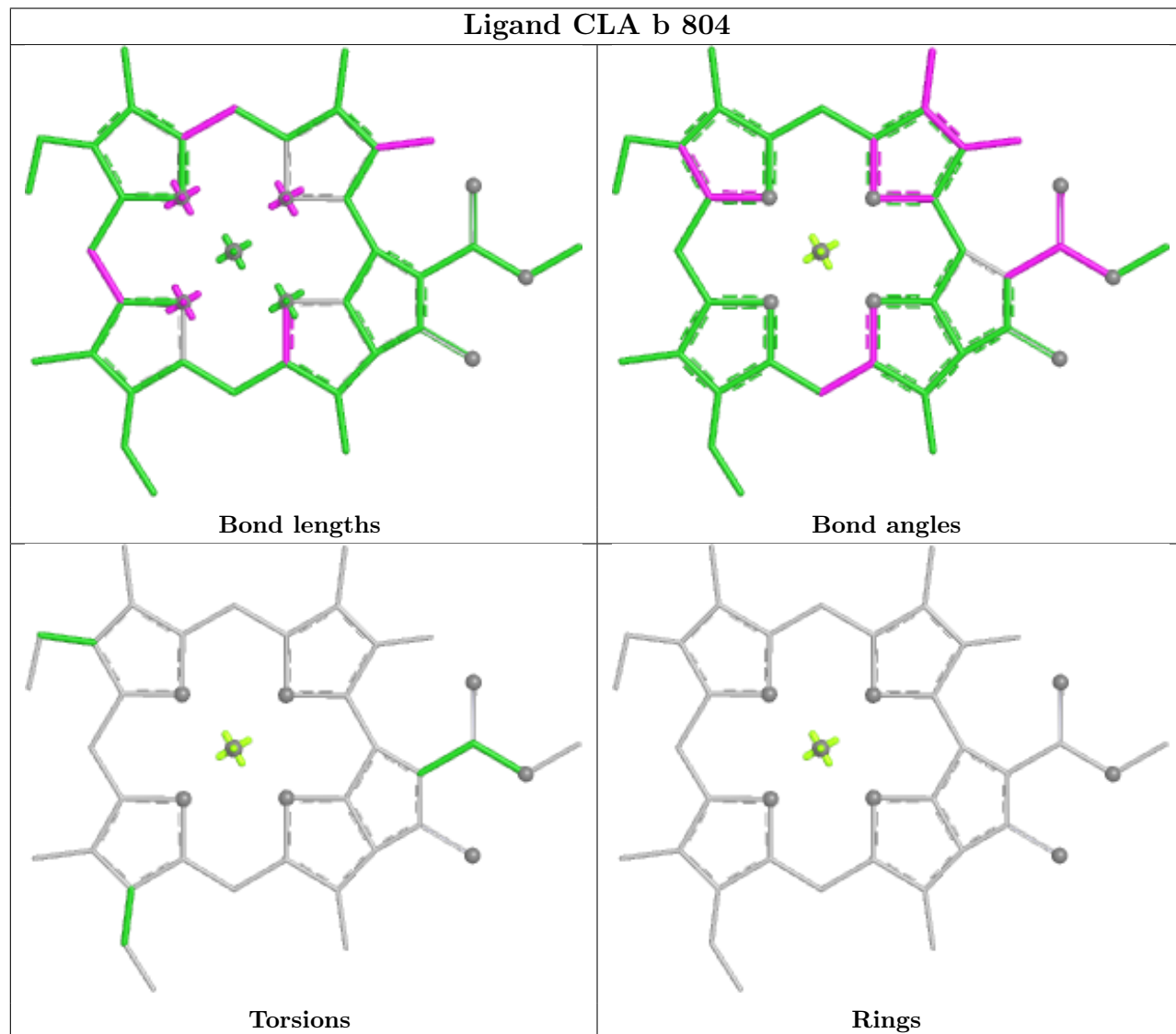


Rings

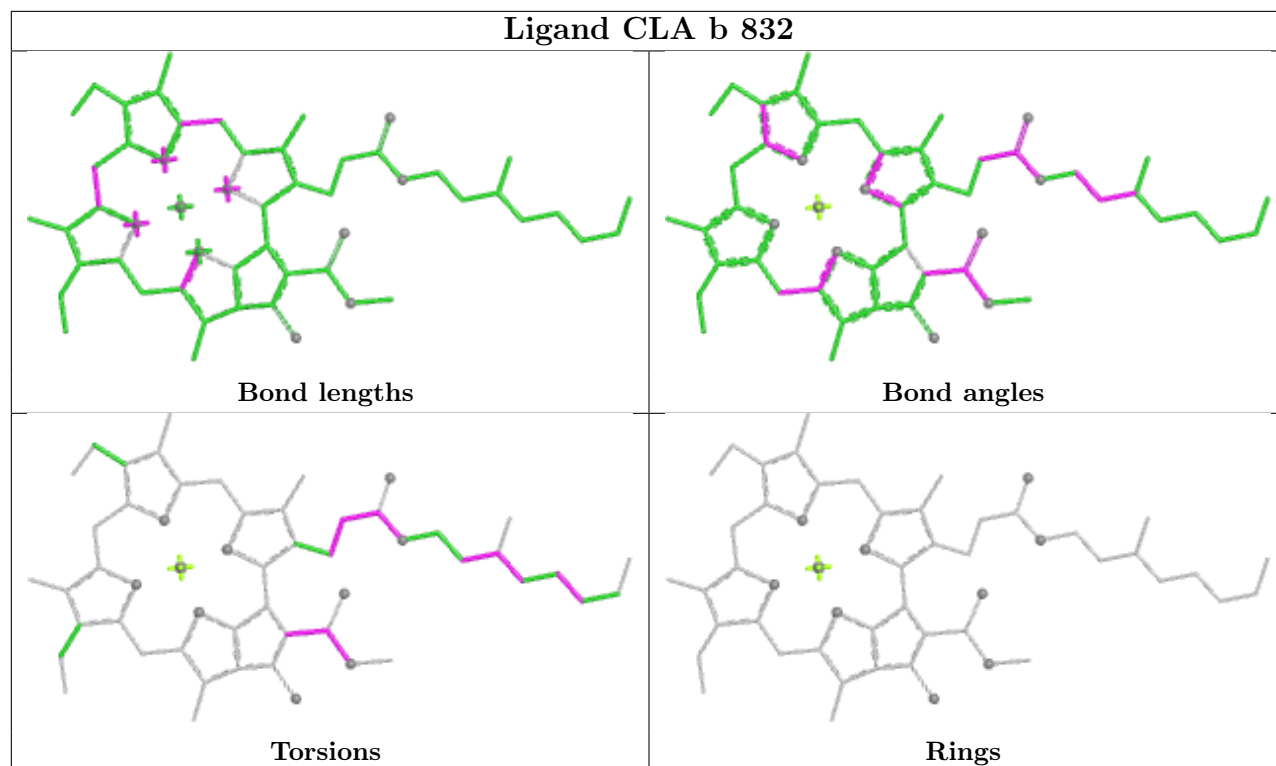
Ligand CLA a 820



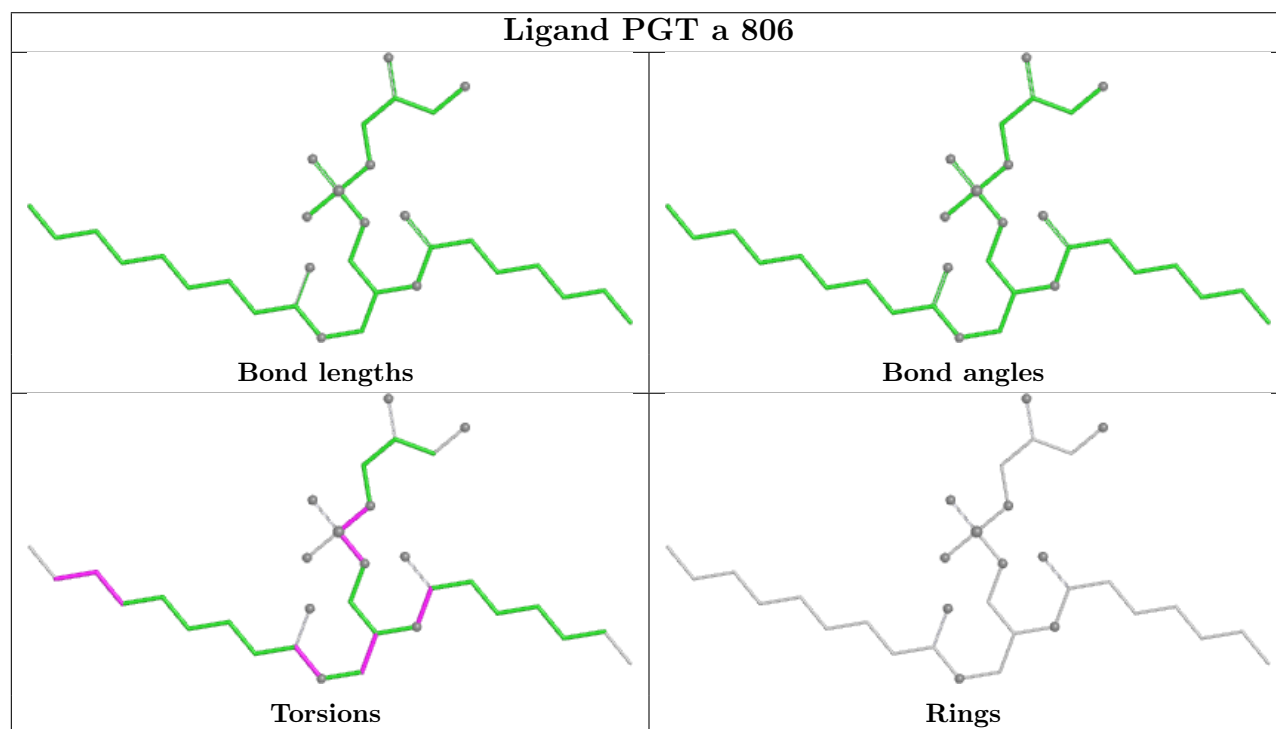
Ligand CLA b 804

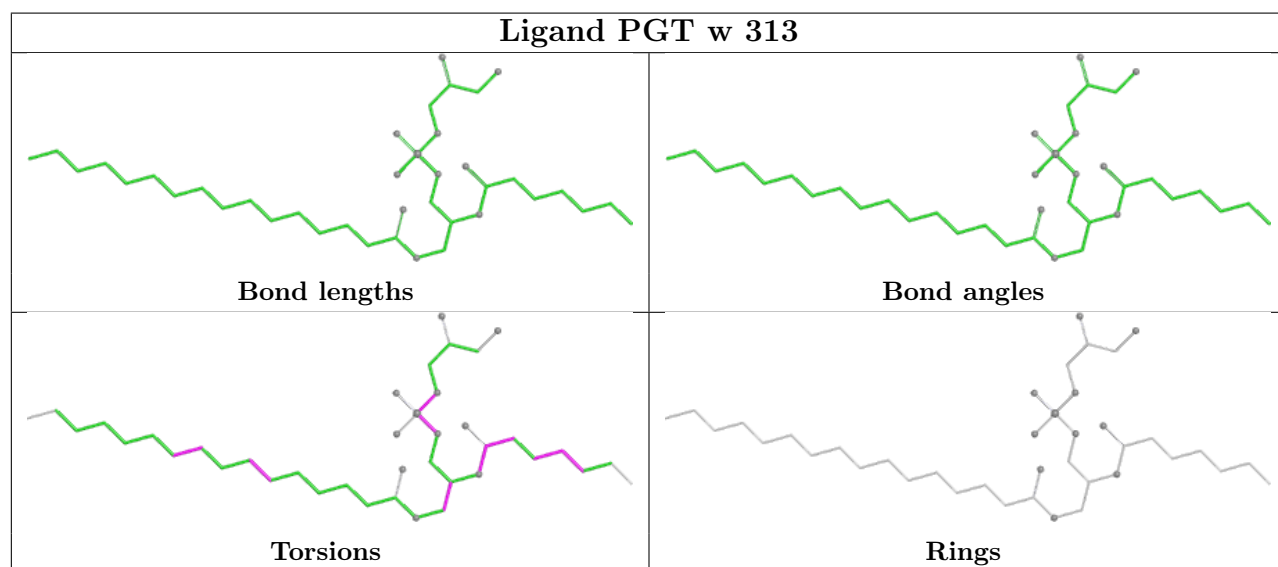
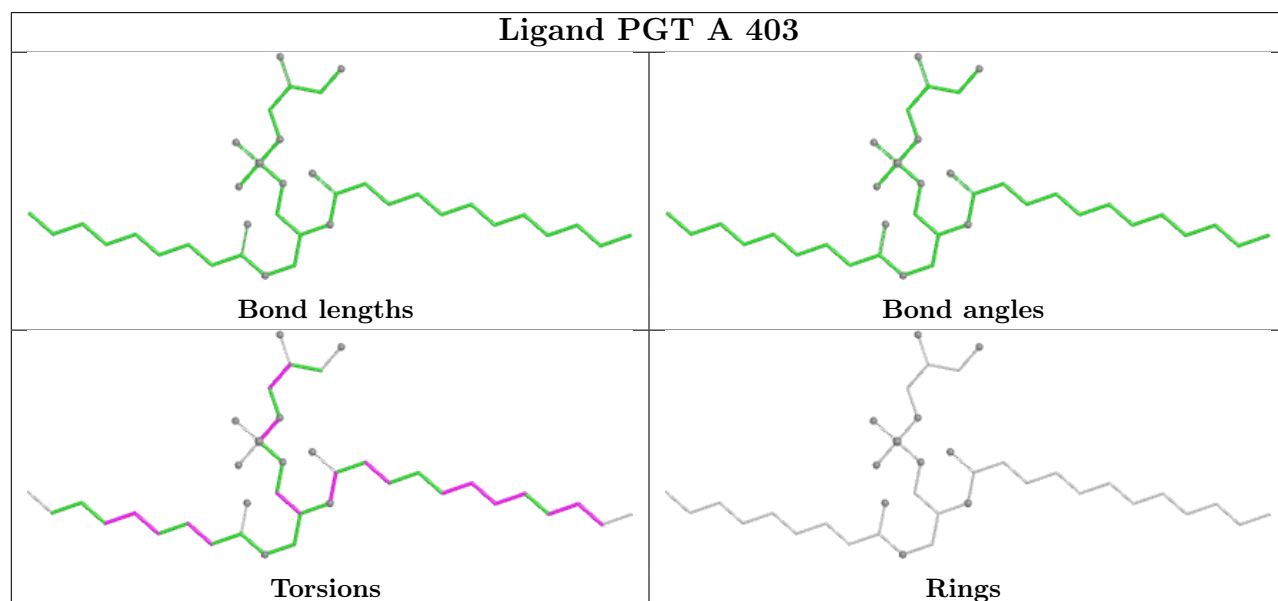
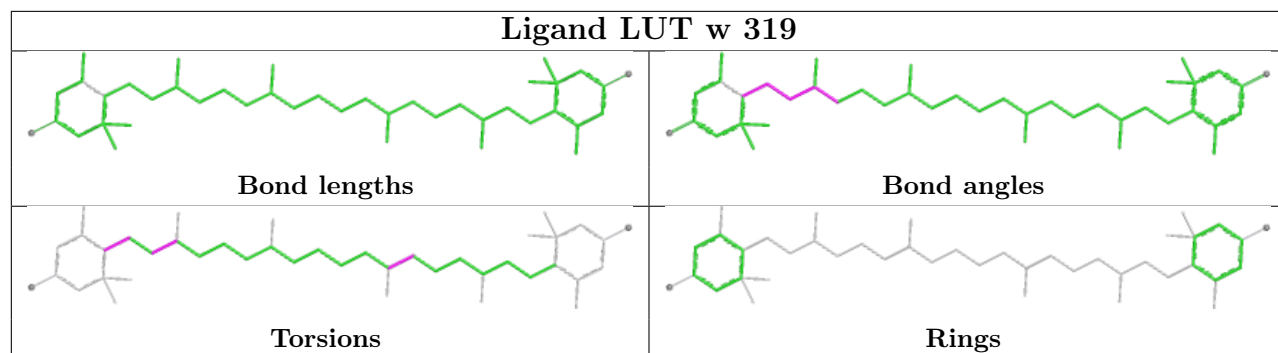


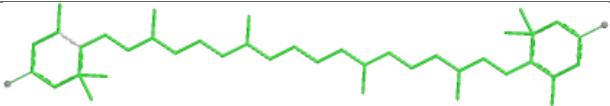
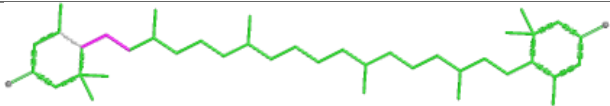
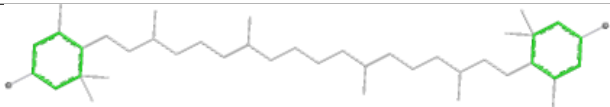
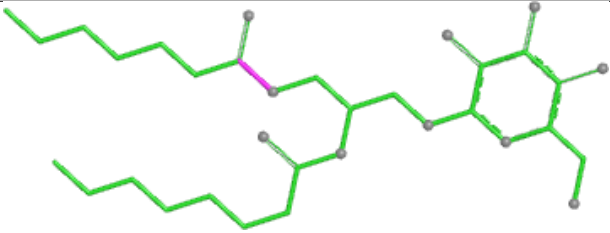
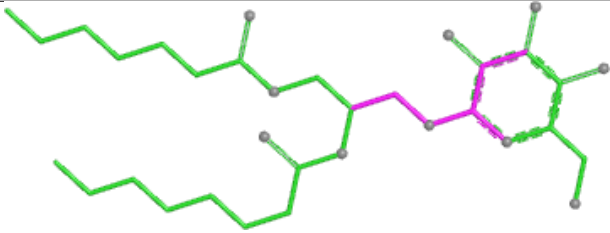
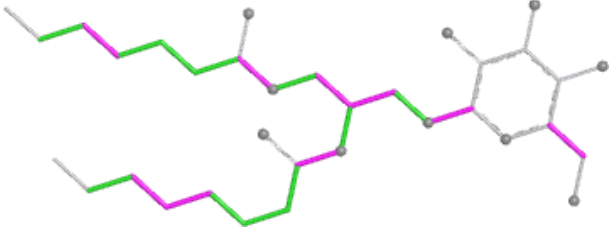
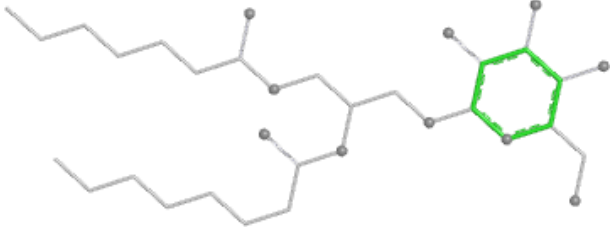
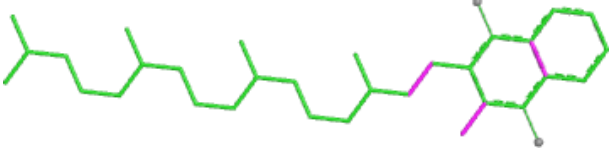
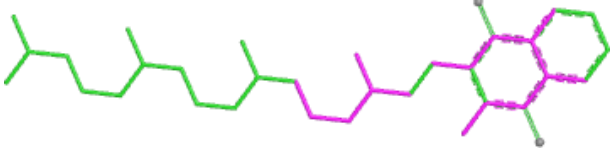
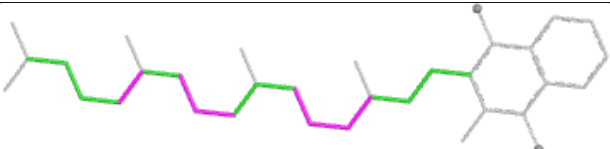
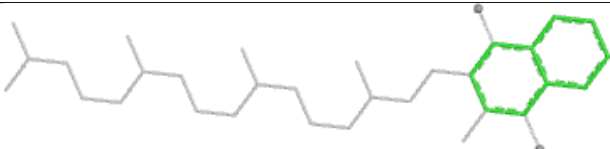
Ligand CLA b 832



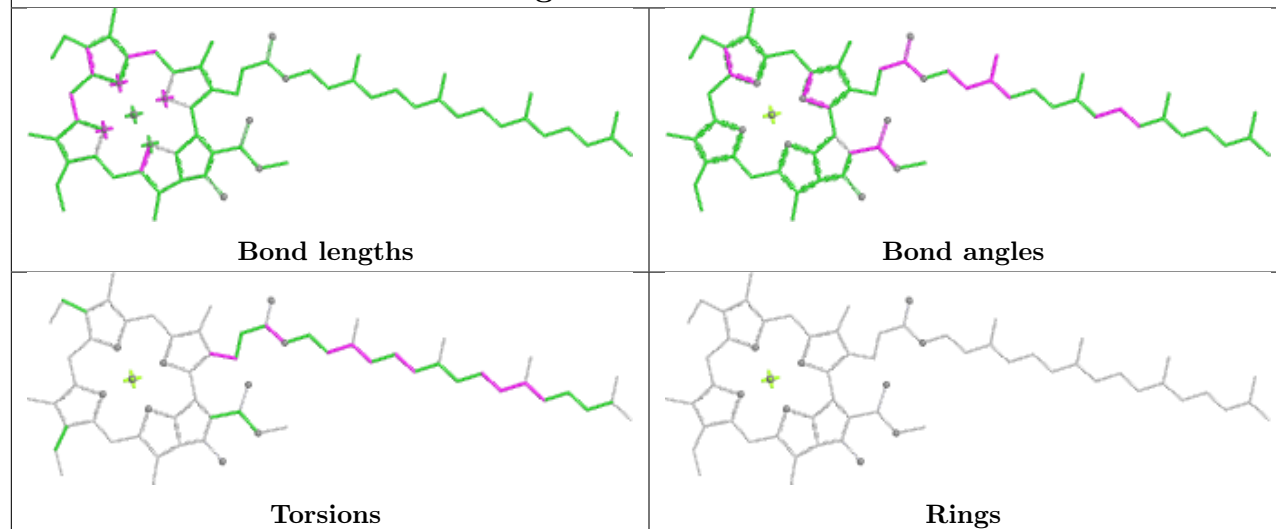
Ligand PGT a 806



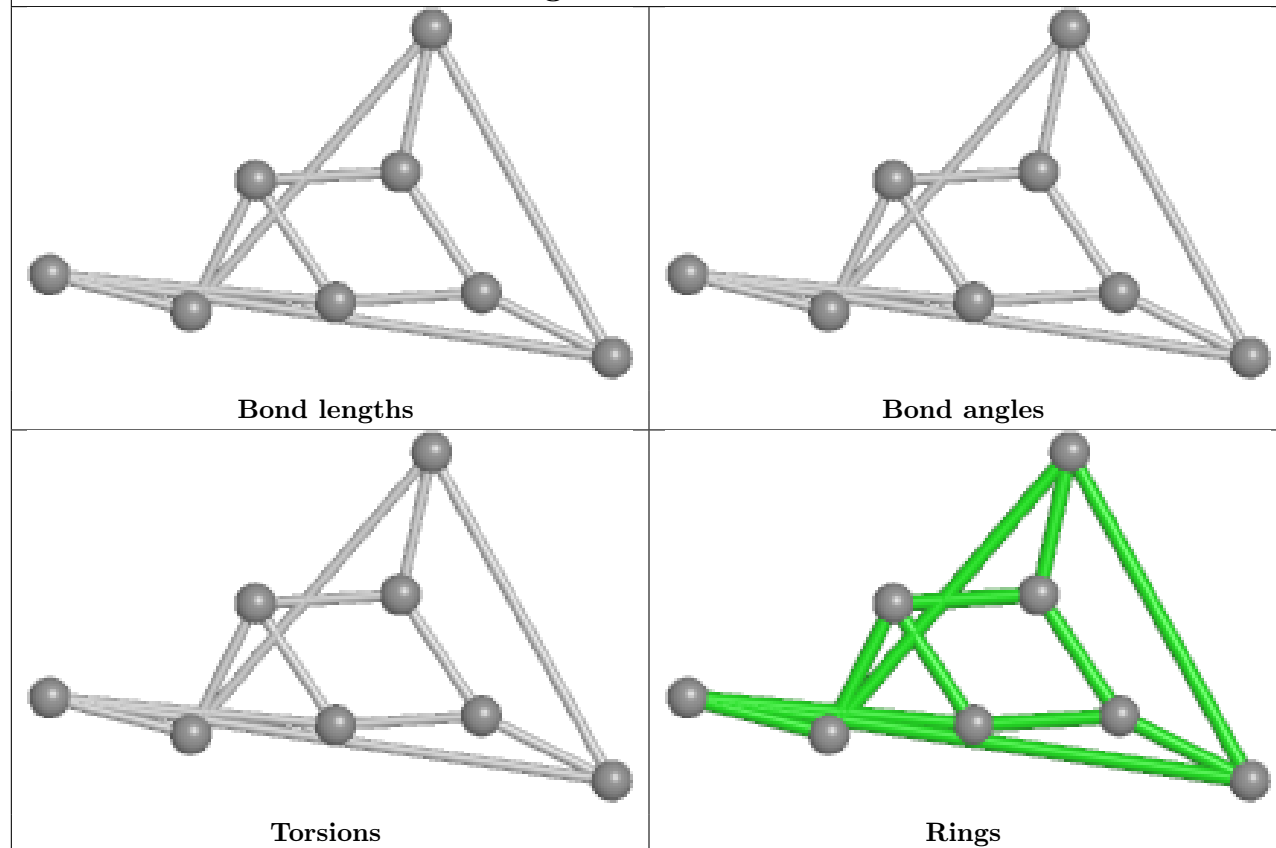


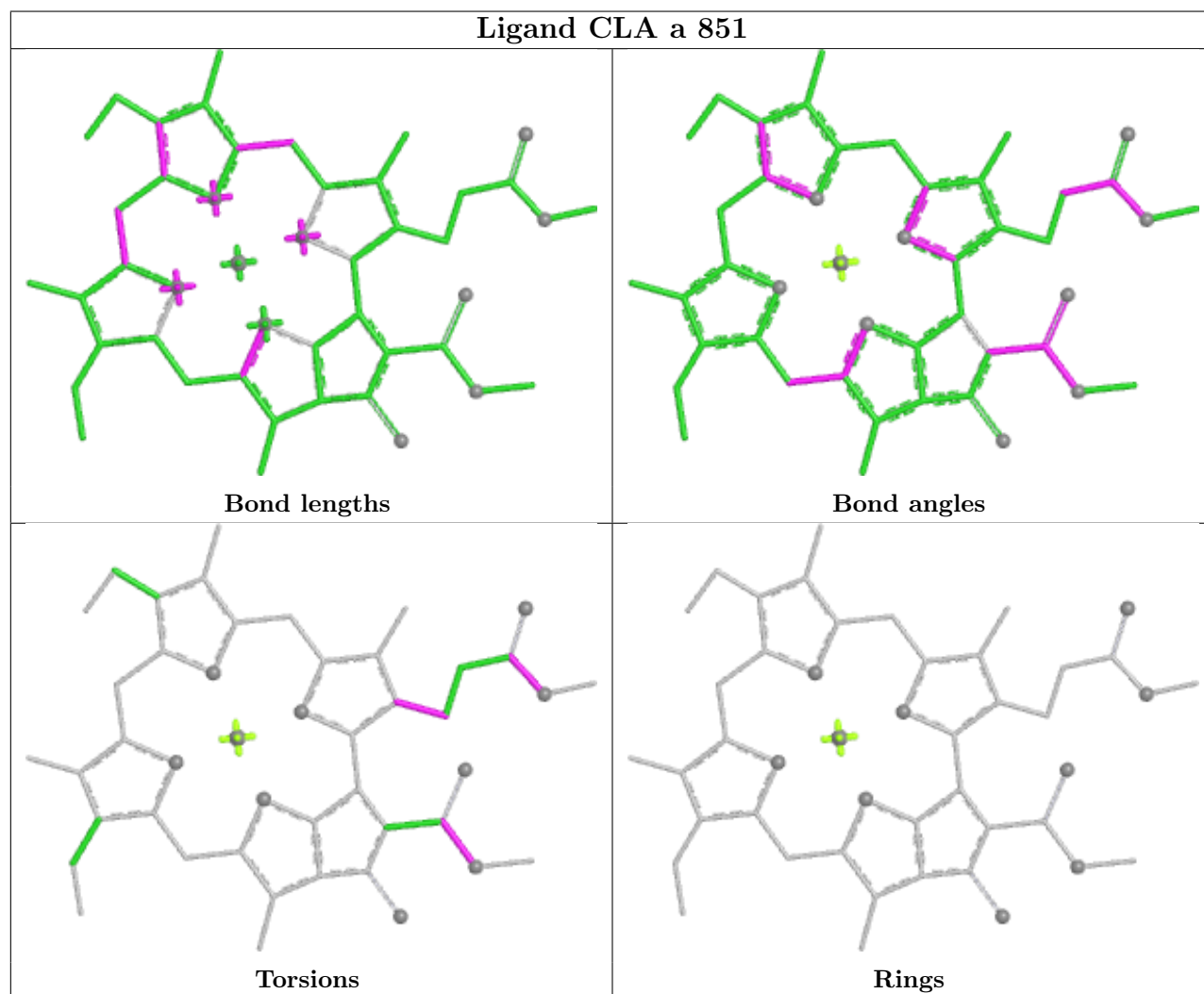
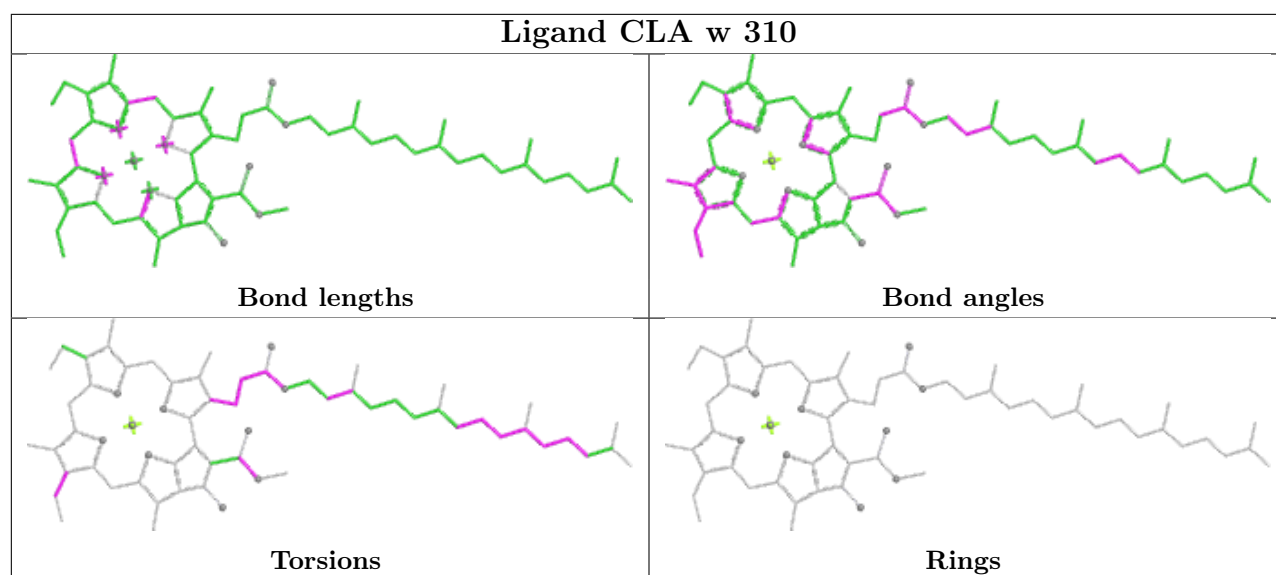
Ligand LUT w 320	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PQN b 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

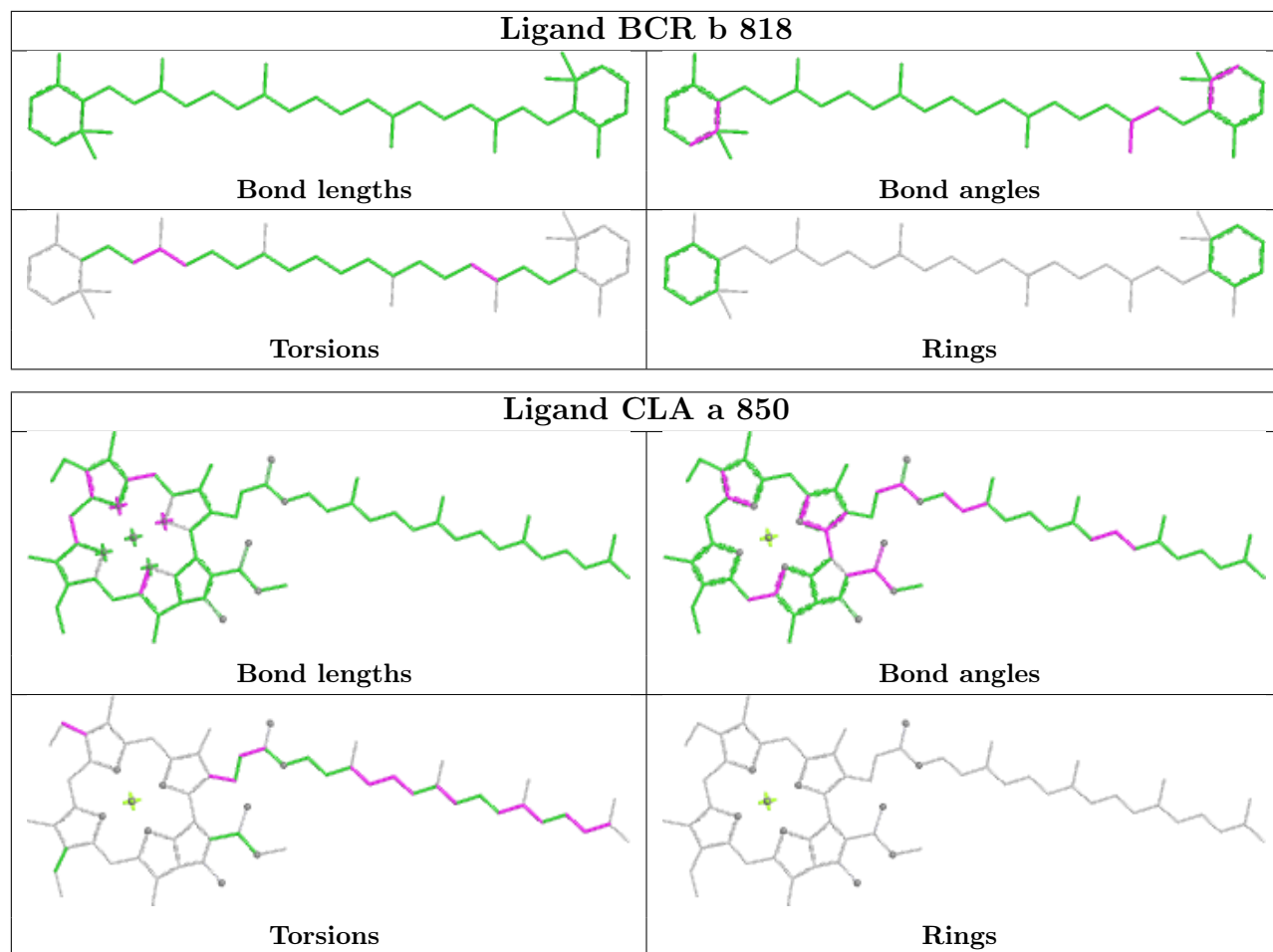
Ligand CLA b 836

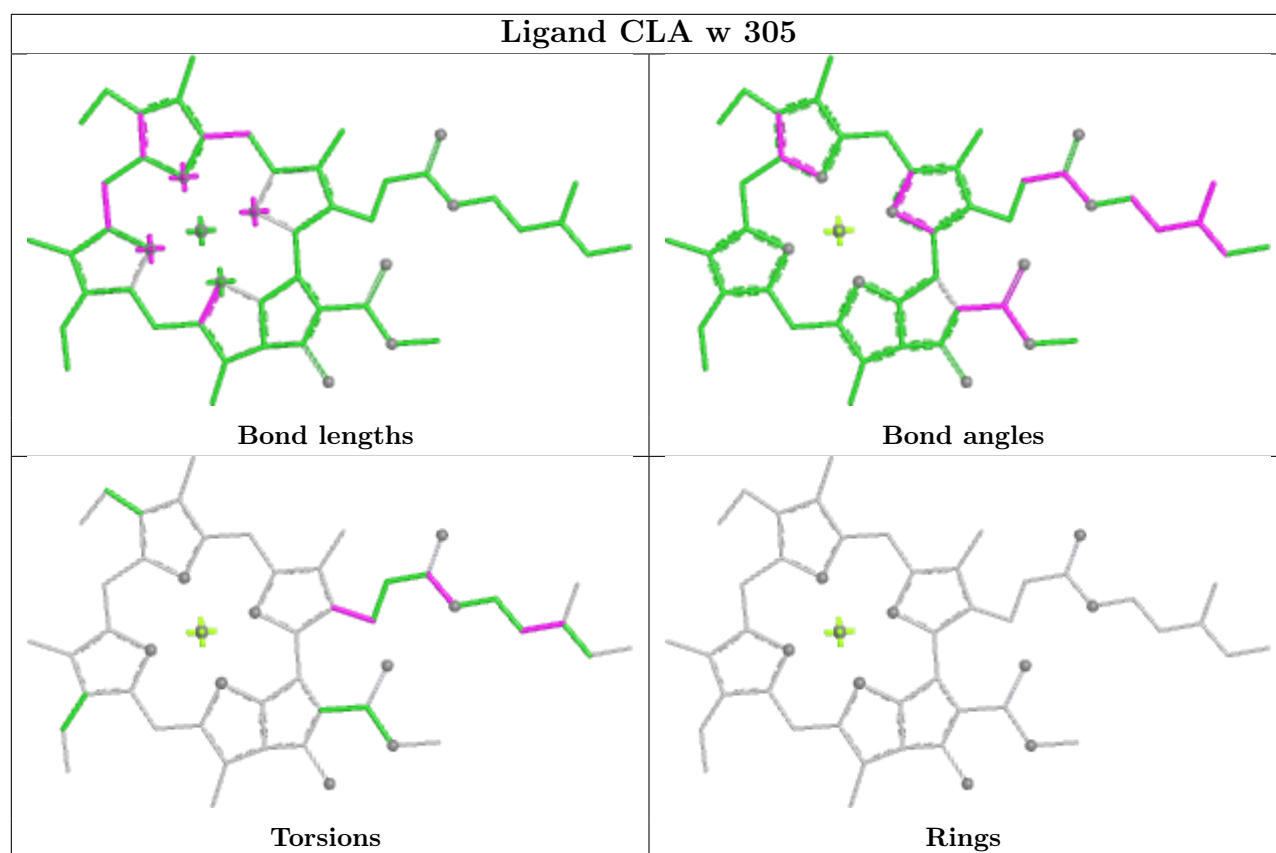


Ligand SF4 c 102

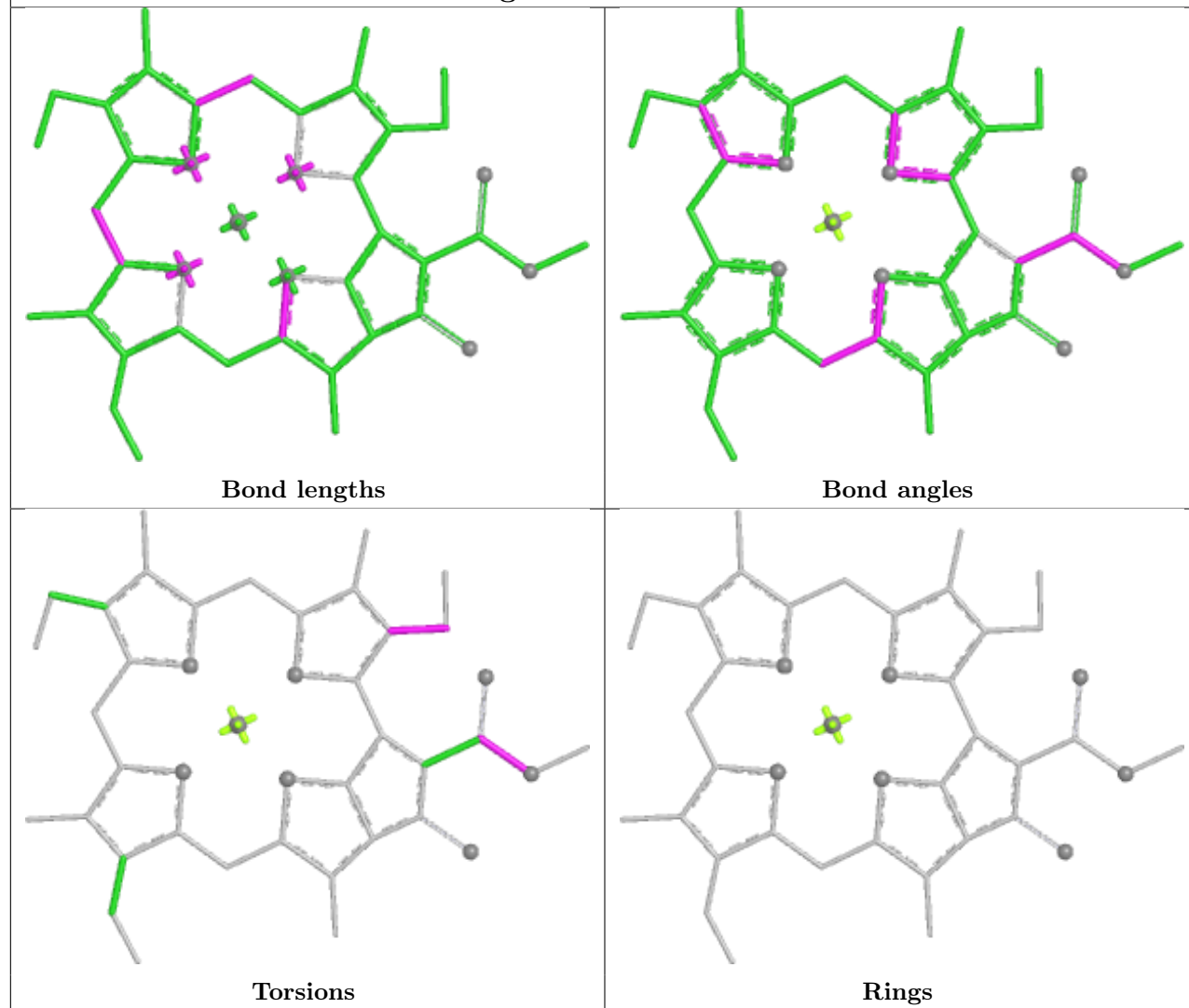




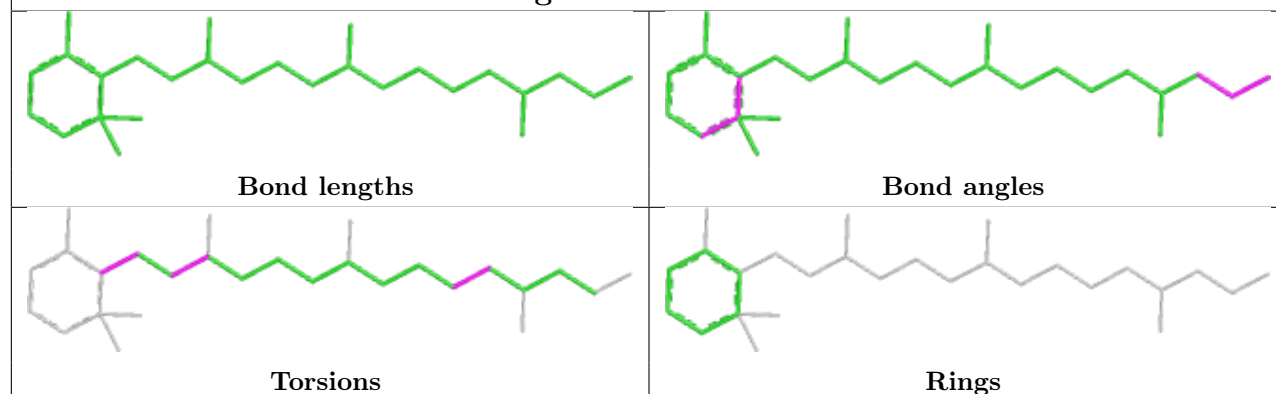




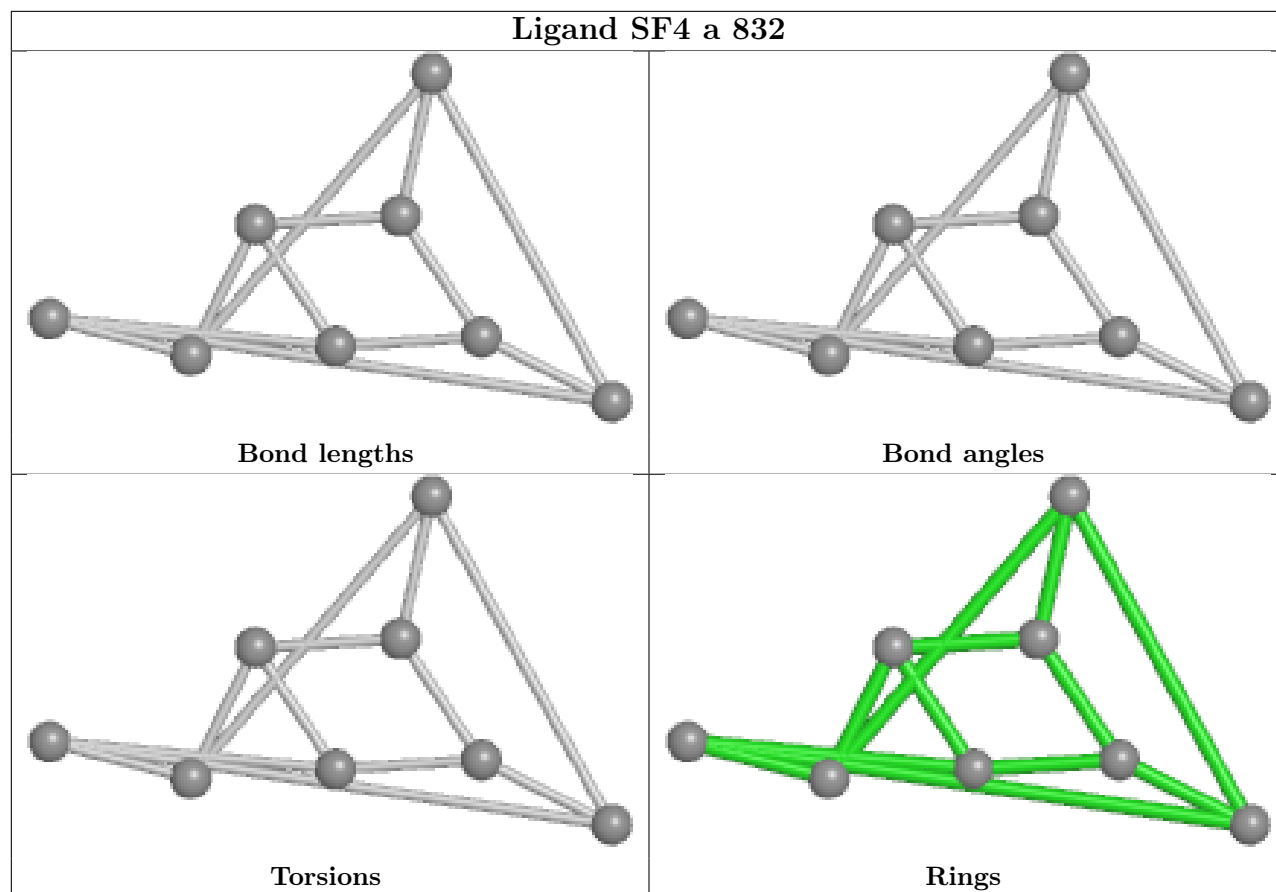
Ligand CLA a 816



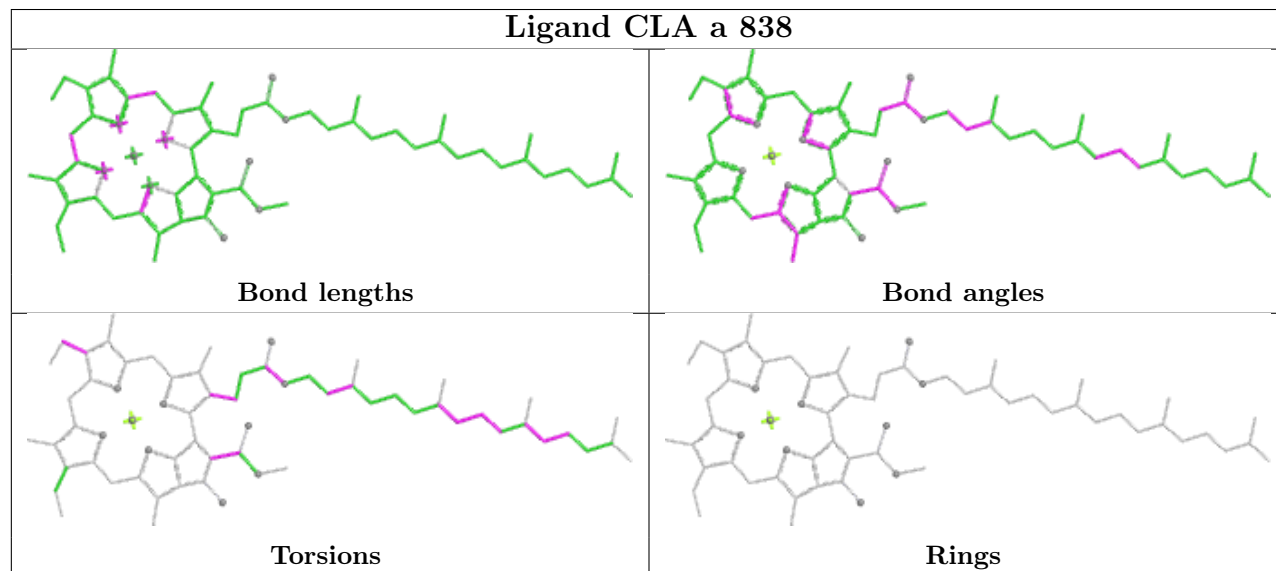
Ligand BCR a 803

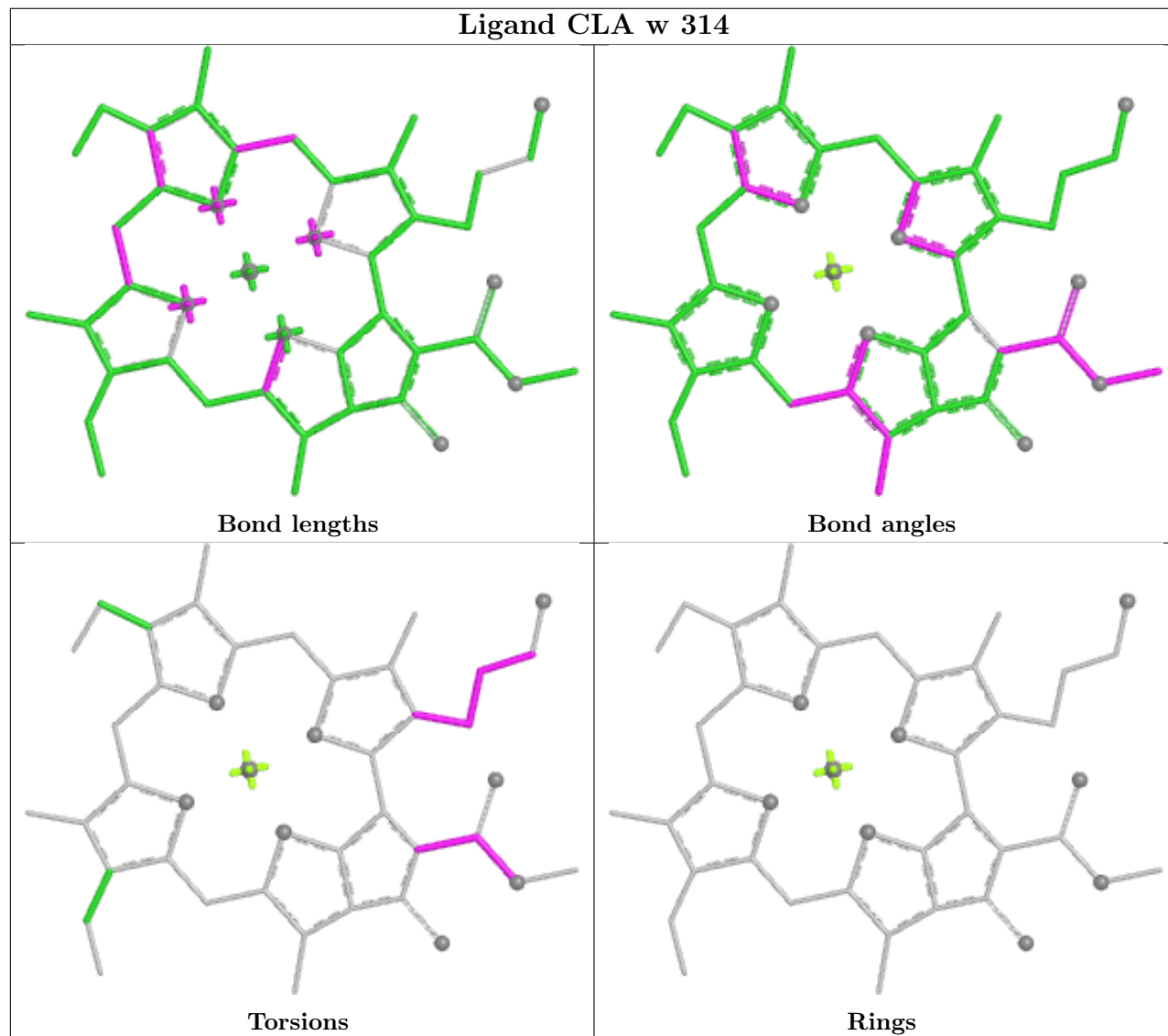
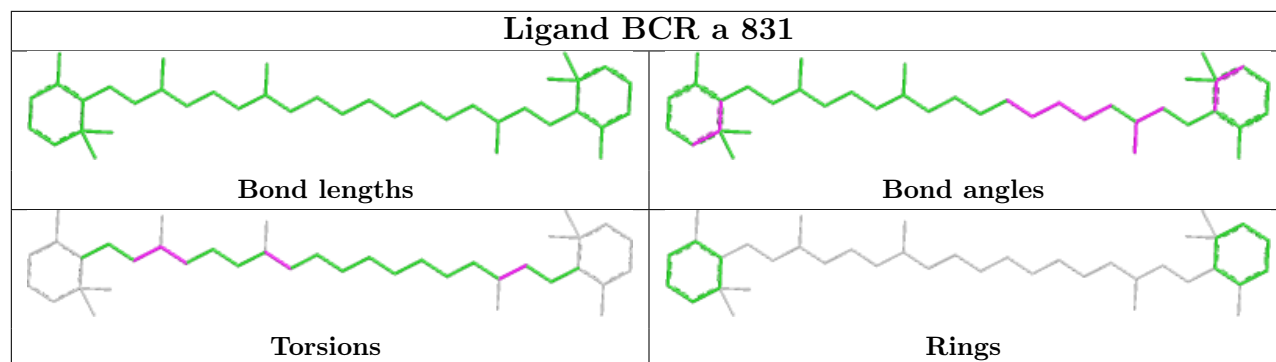


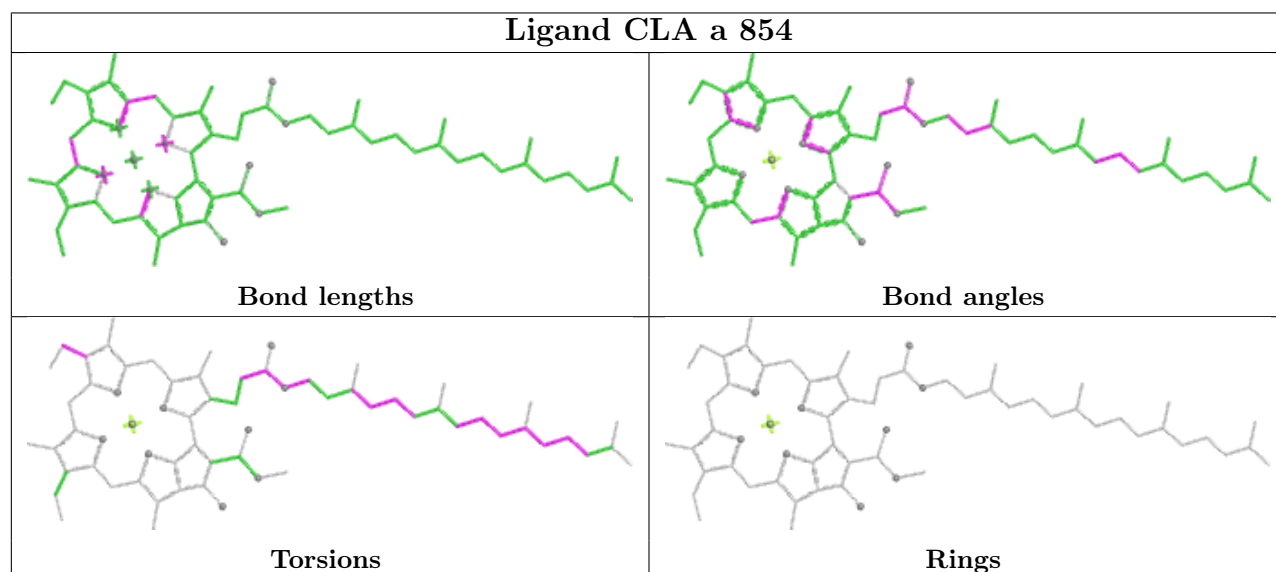
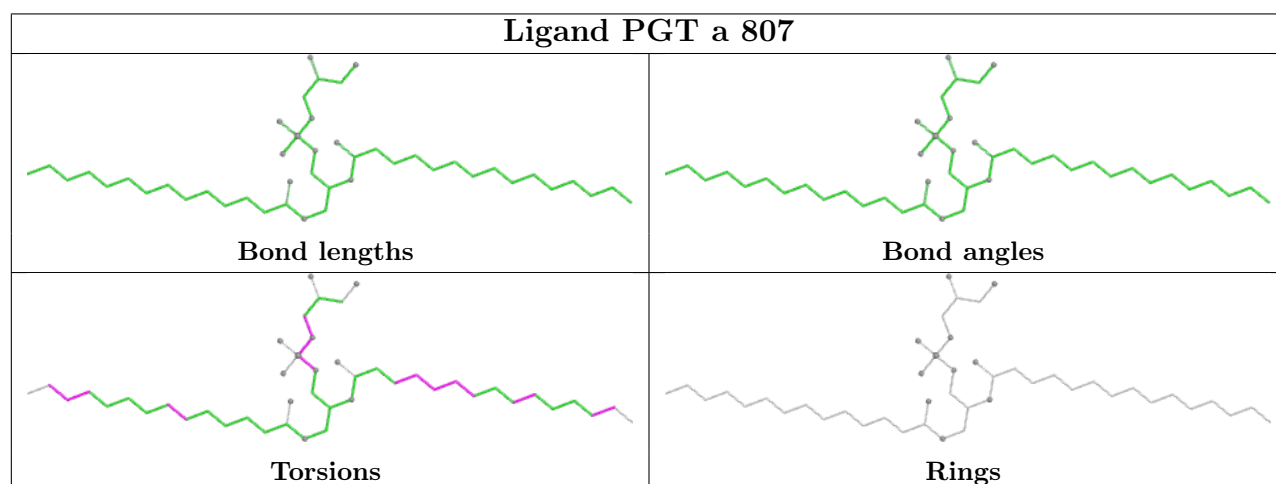
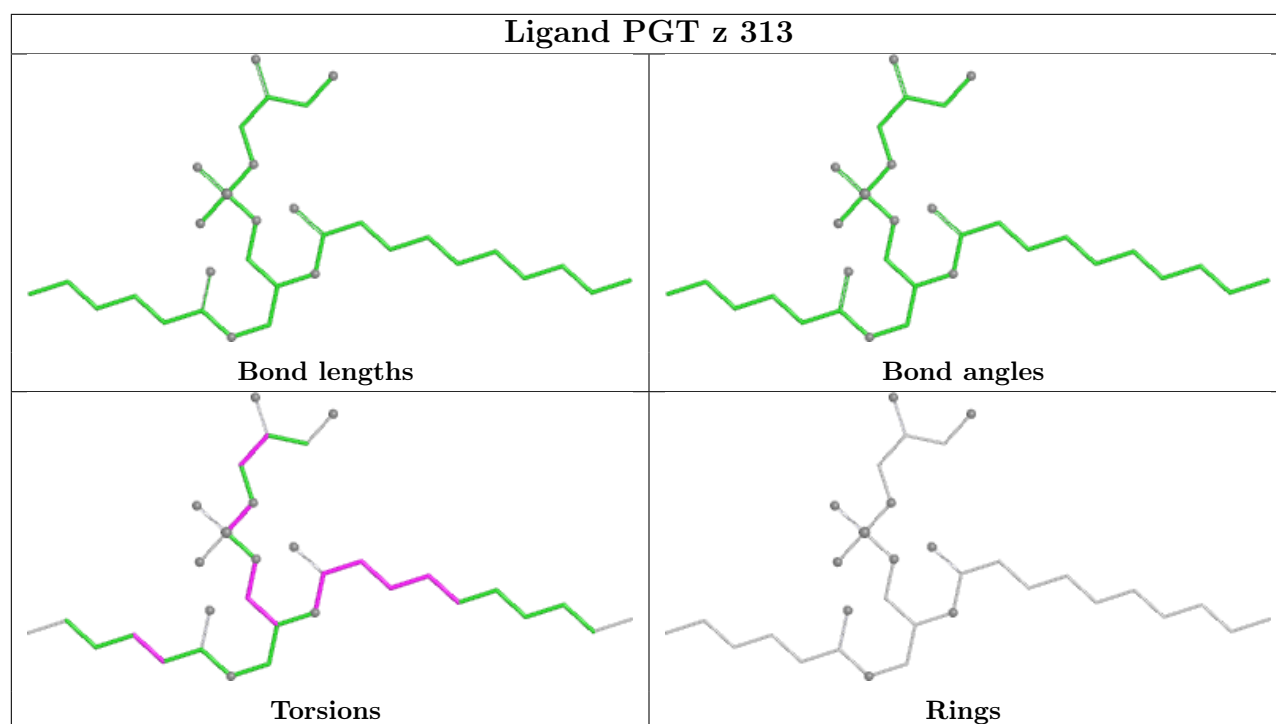
Ligand SF4 a 832

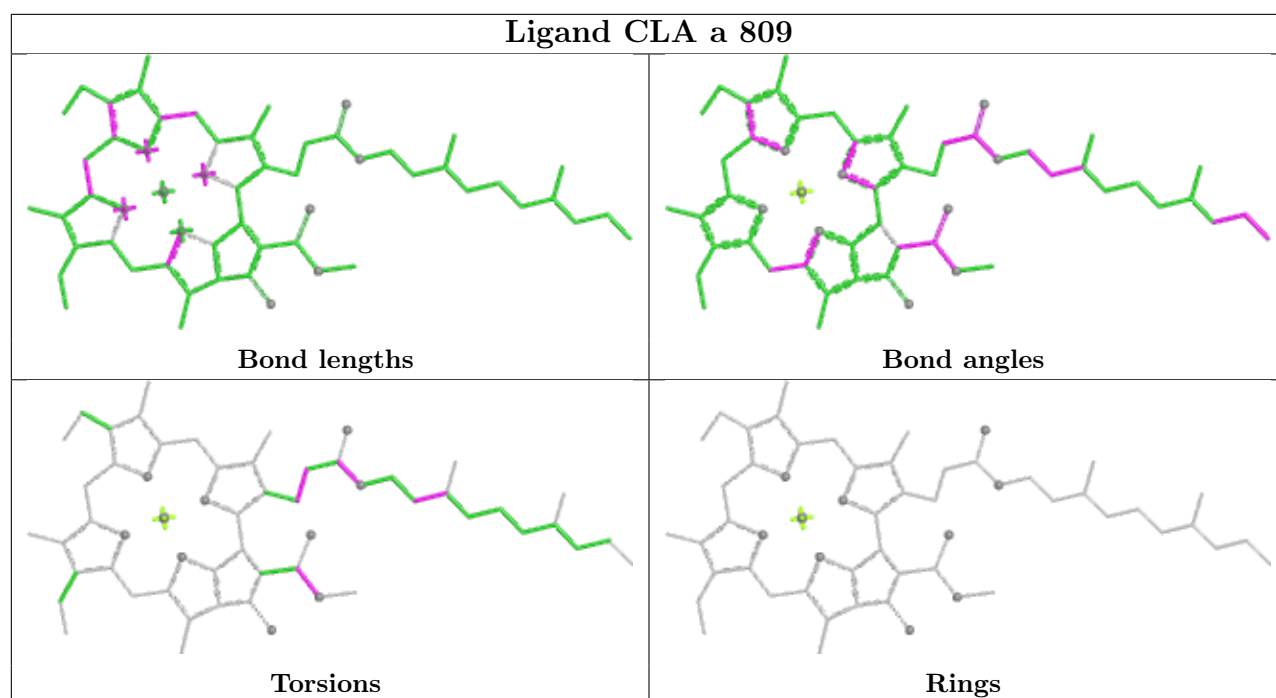


Ligand CLA a 838

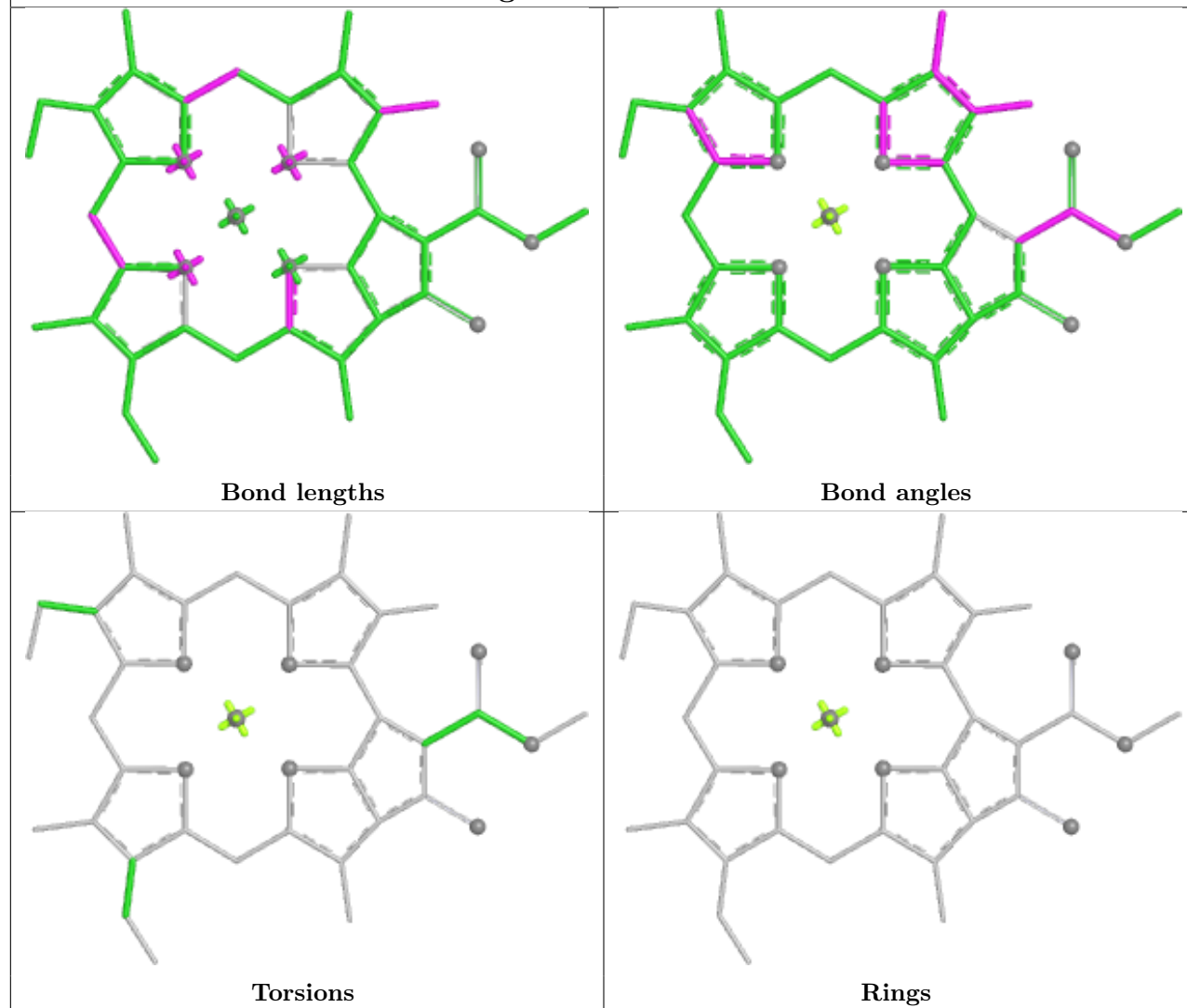




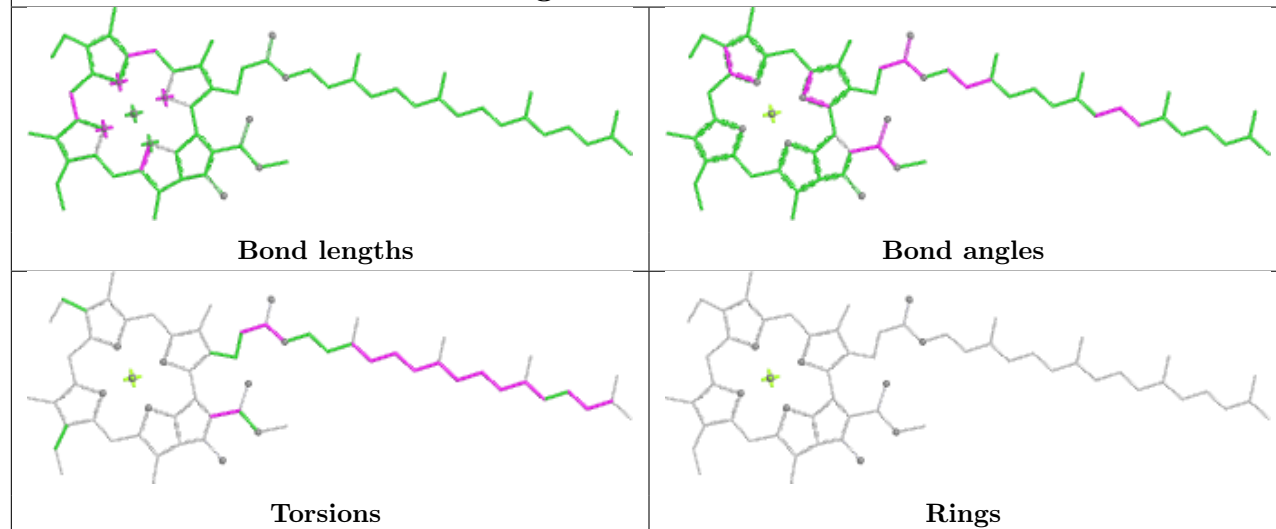


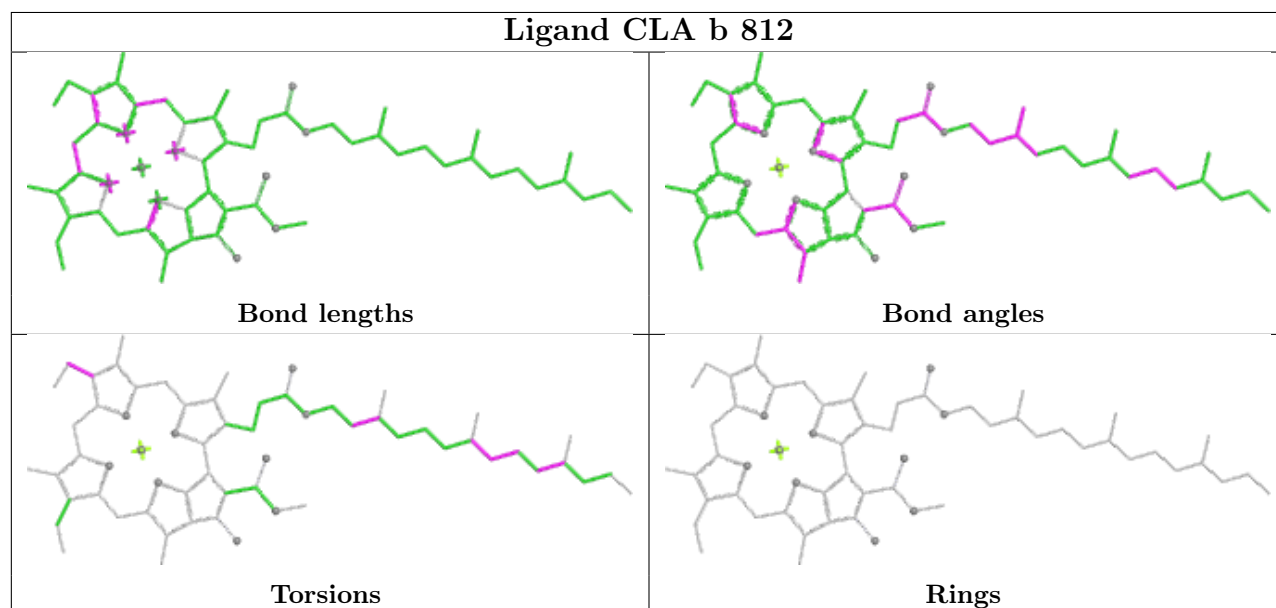
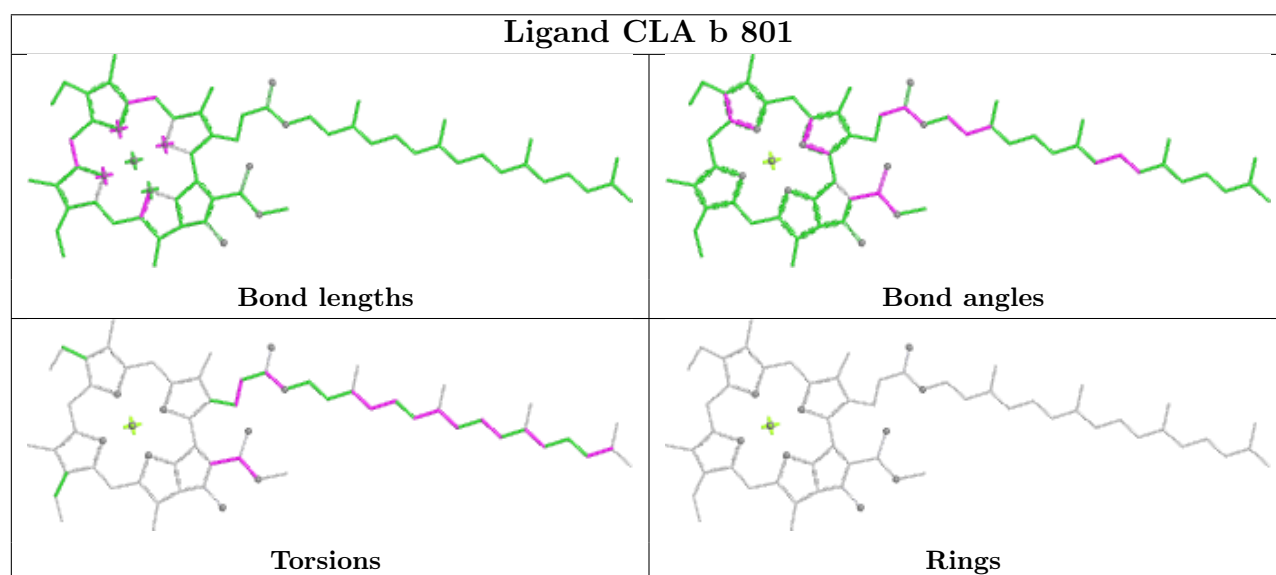
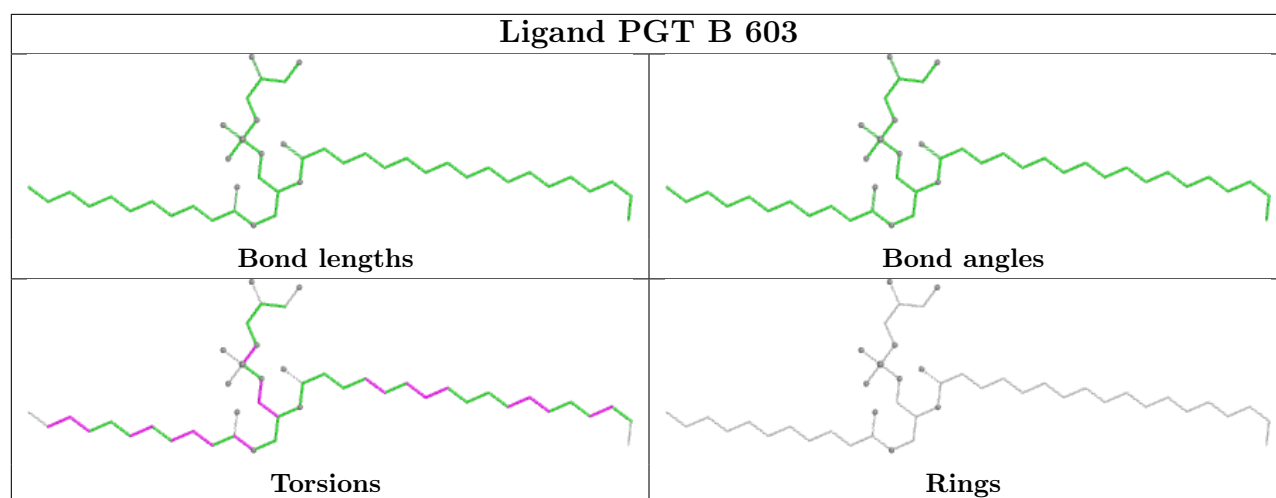


Ligand CLA a 817

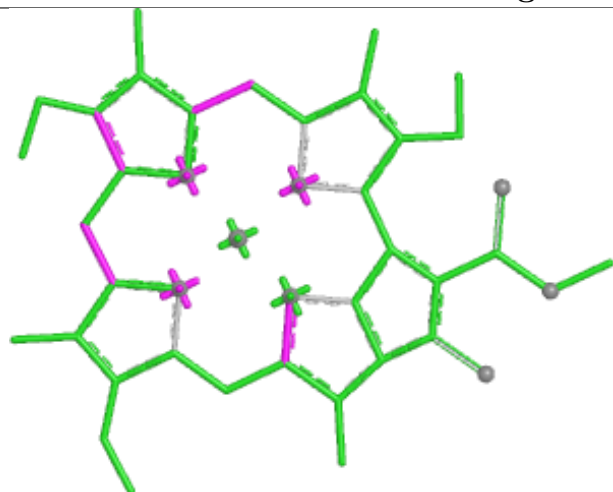


Ligand CLA b 824

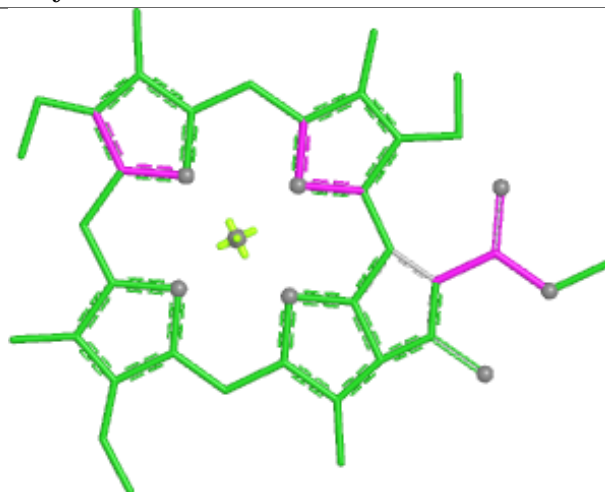




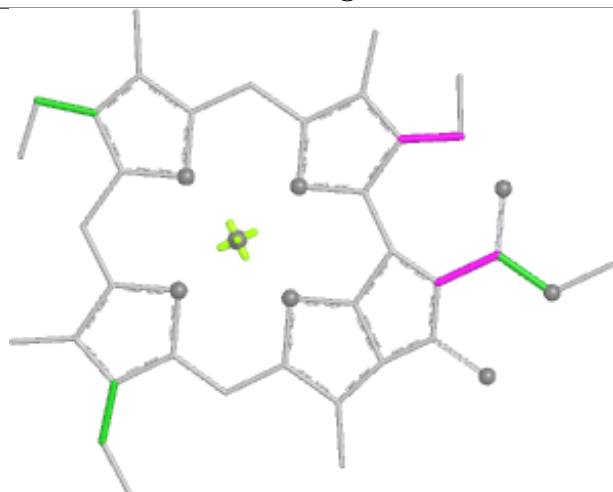
Ligand CLA y 309



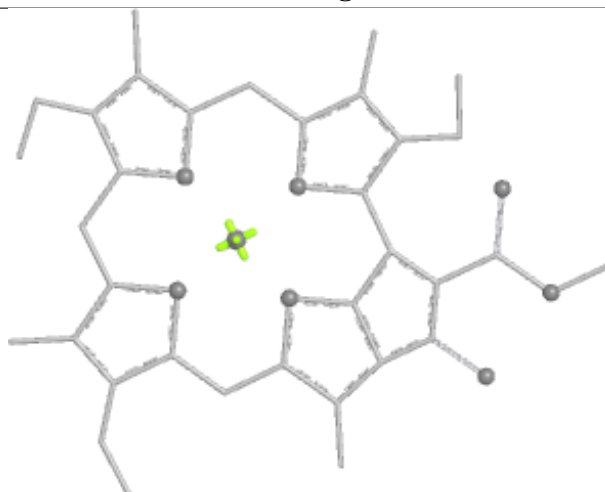
Bond lengths



Bond angles

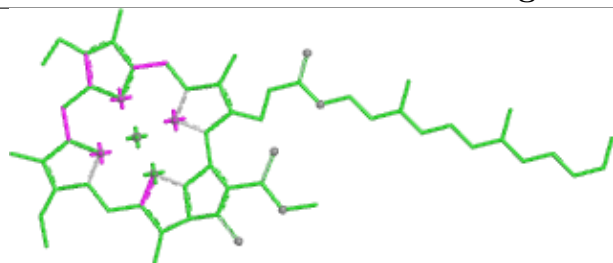


Torsions

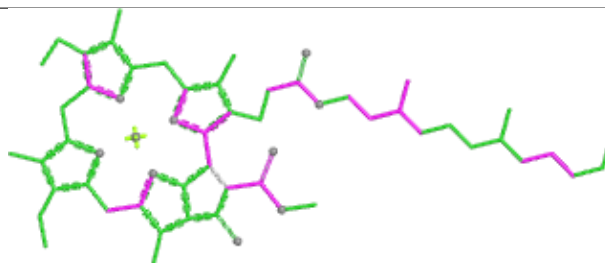


Rings

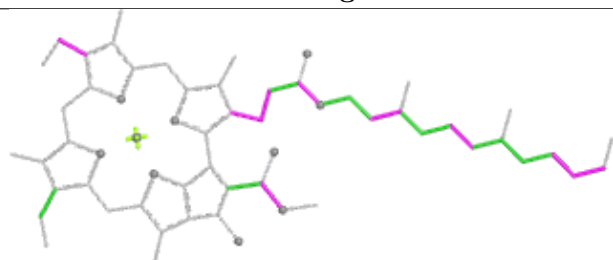
Ligand CLA a 818



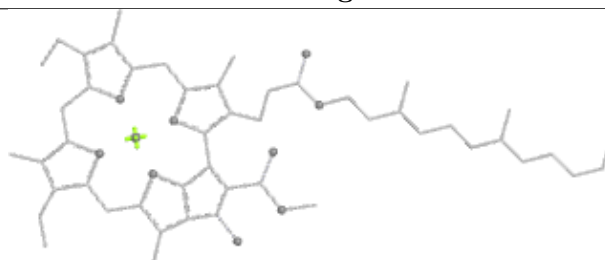
Bond lengths



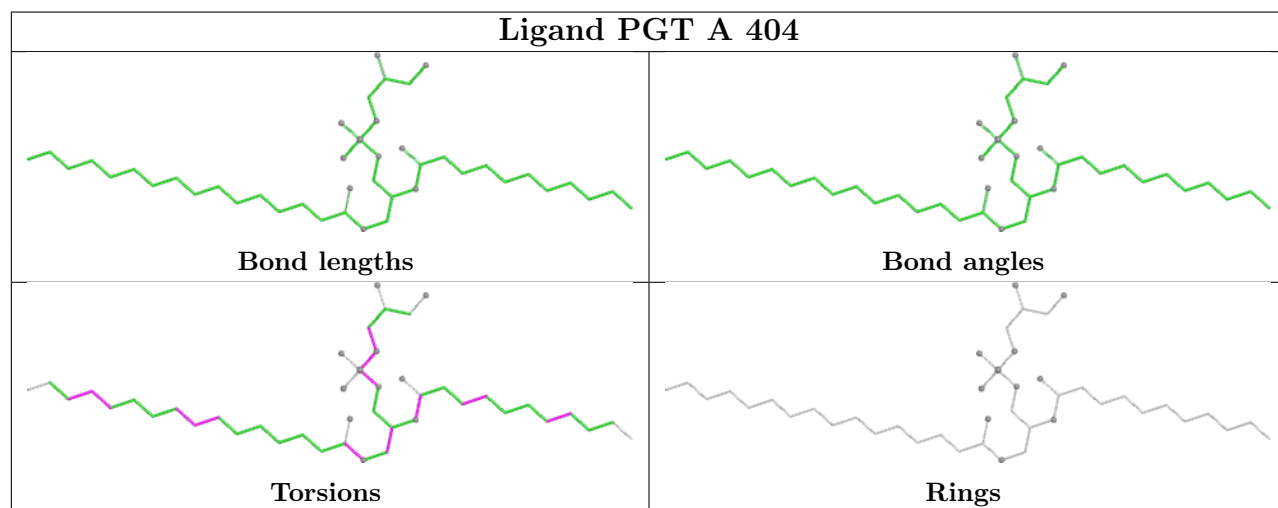
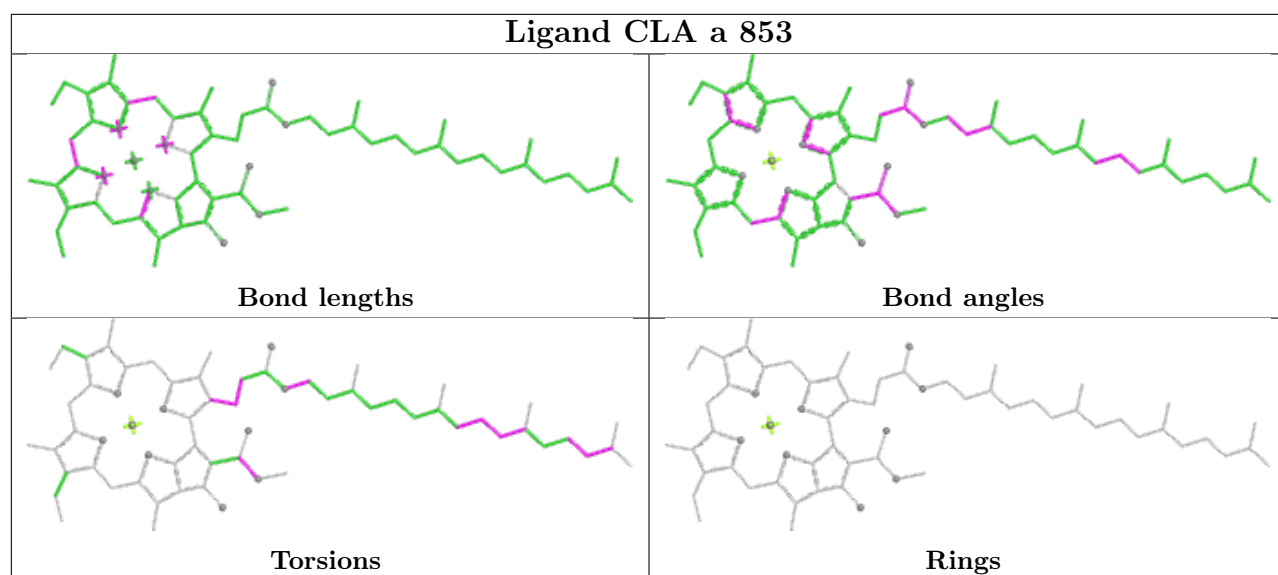
Bond angles



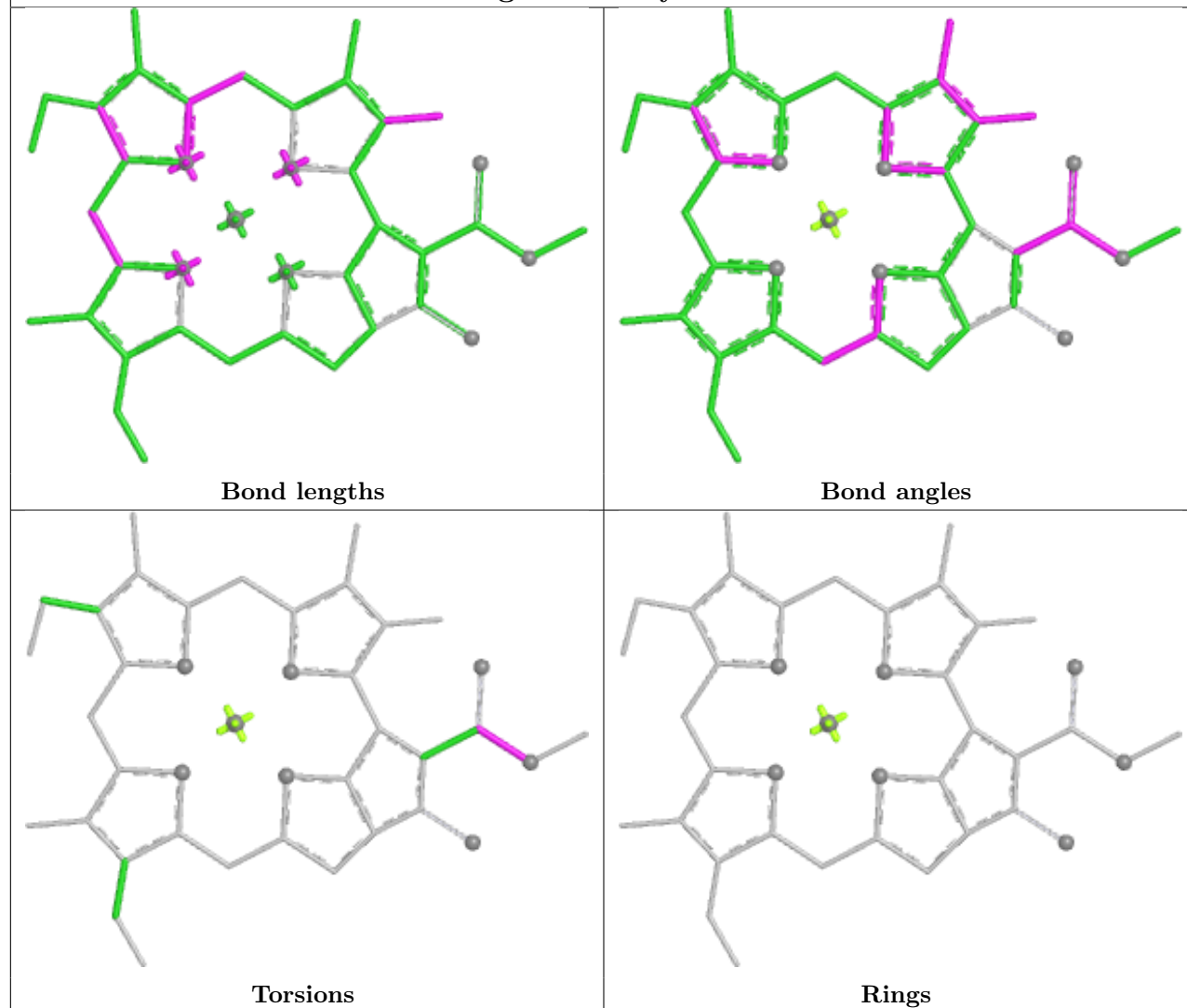
Torsions



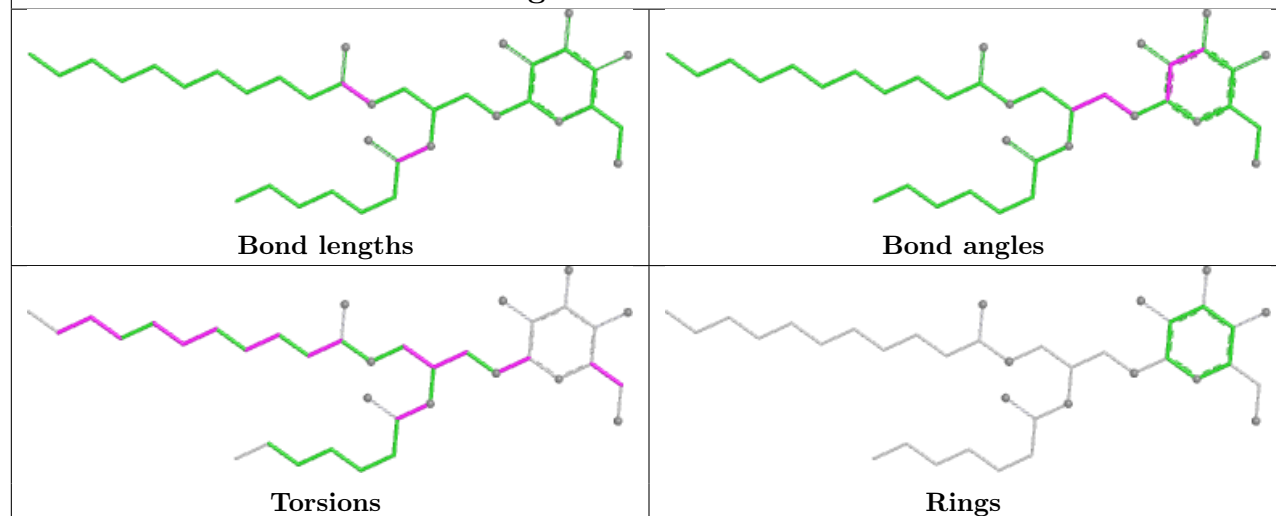
Rings

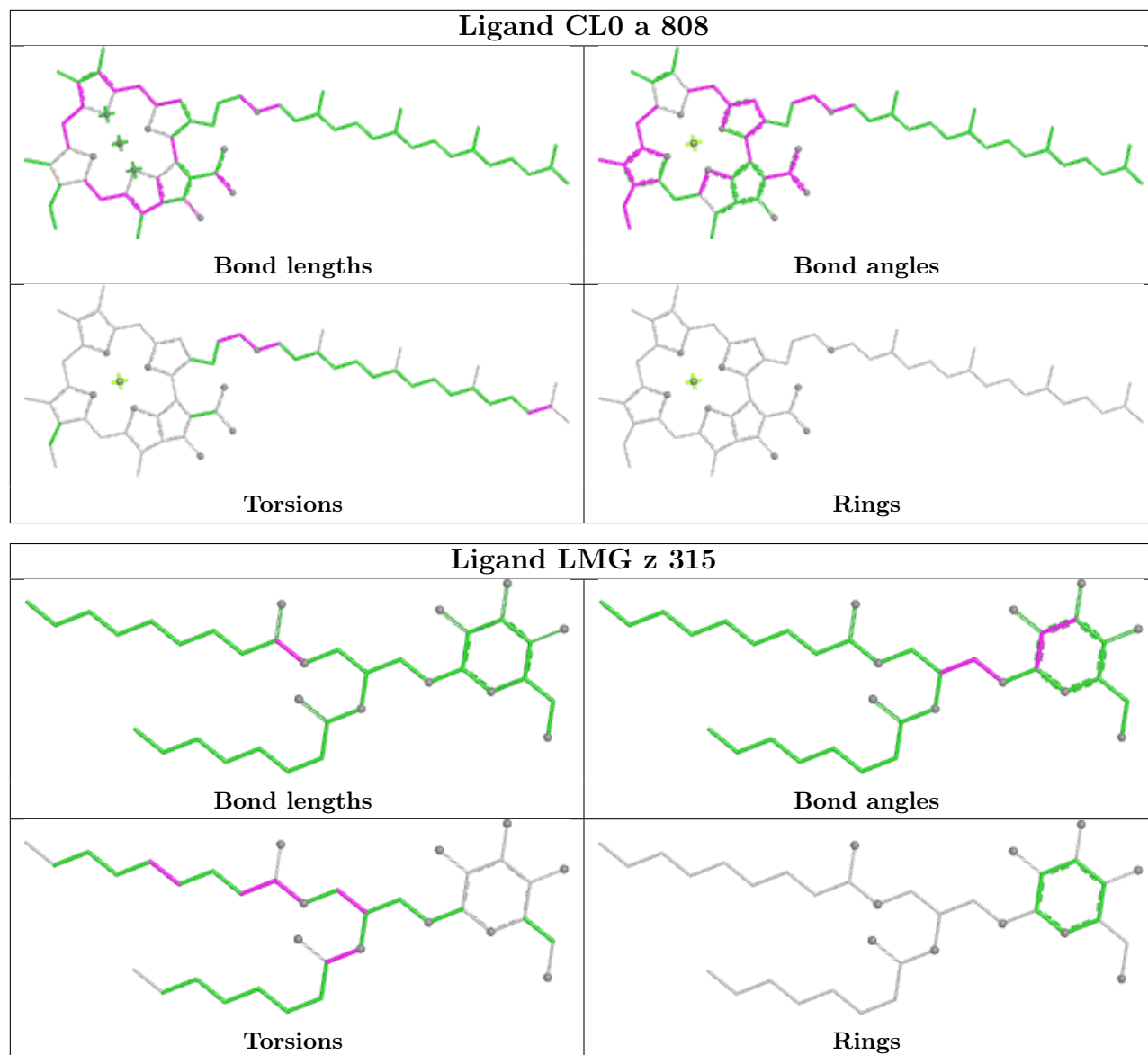


Ligand CLA y 306

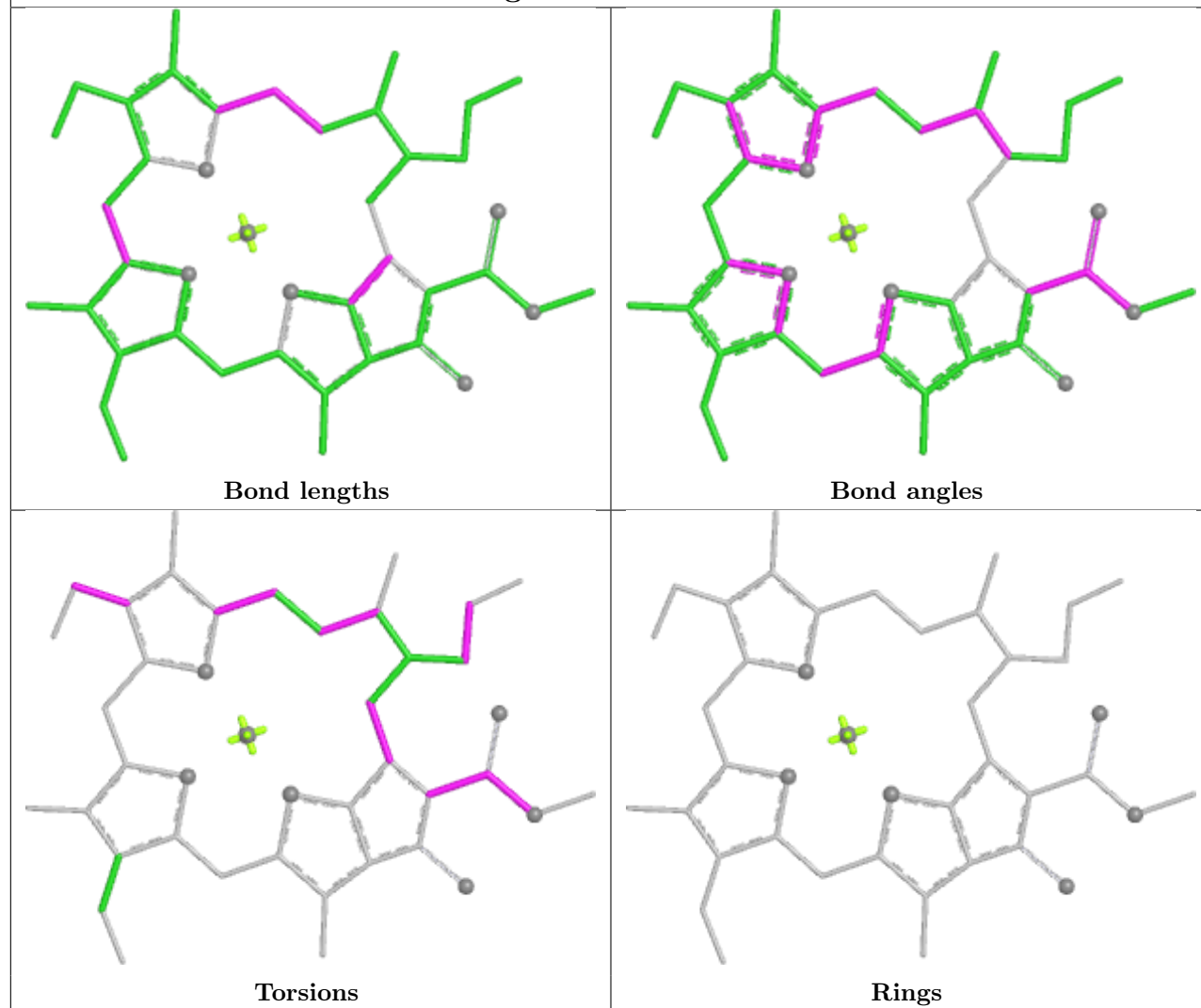


Ligand LMG B 605

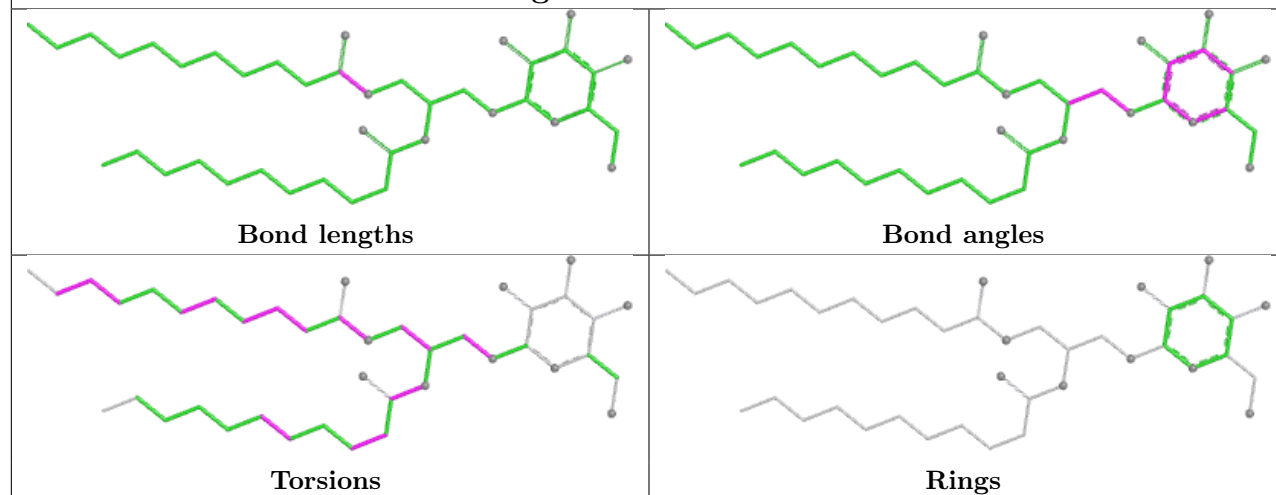


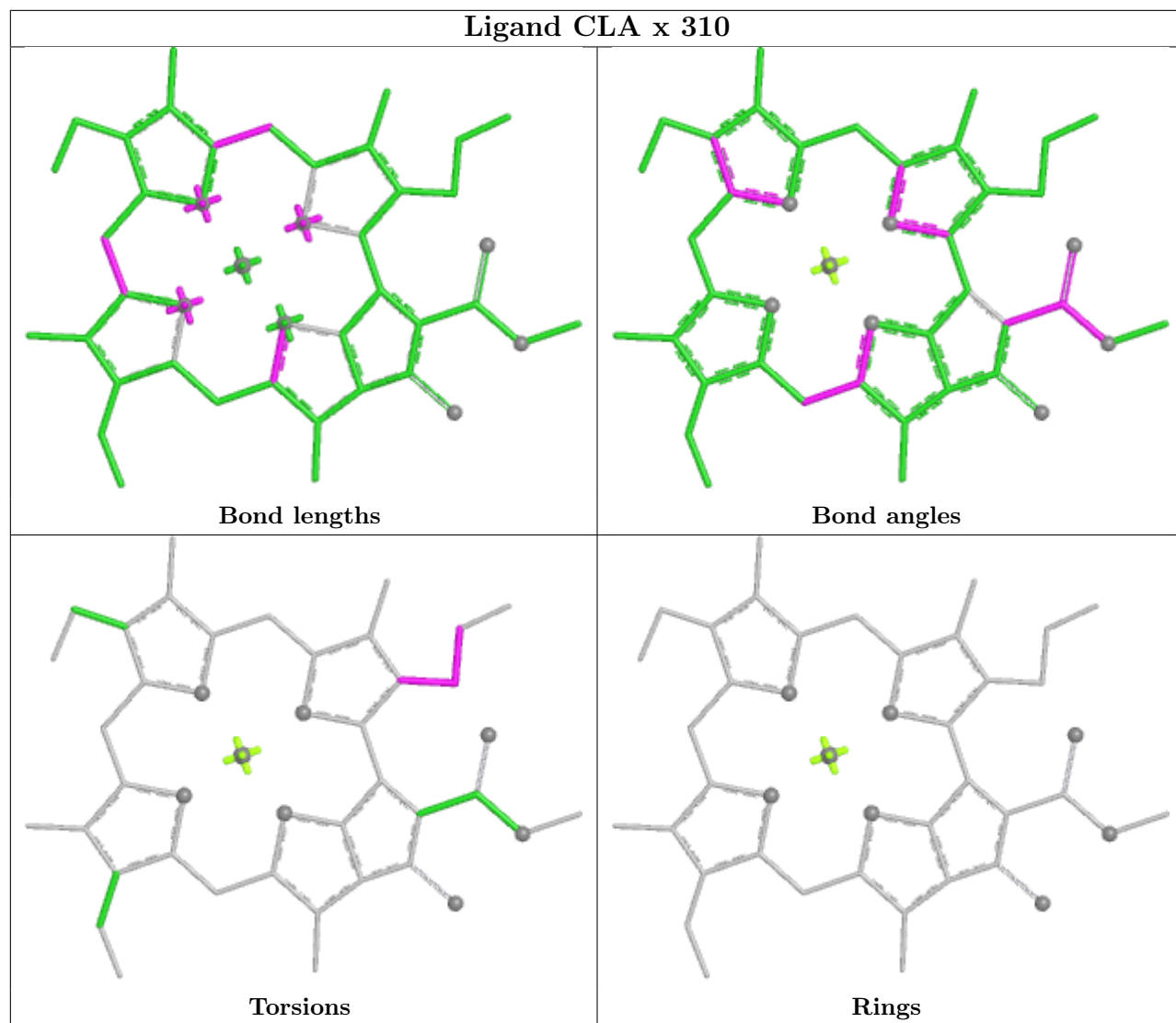


Ligand CLA a 847

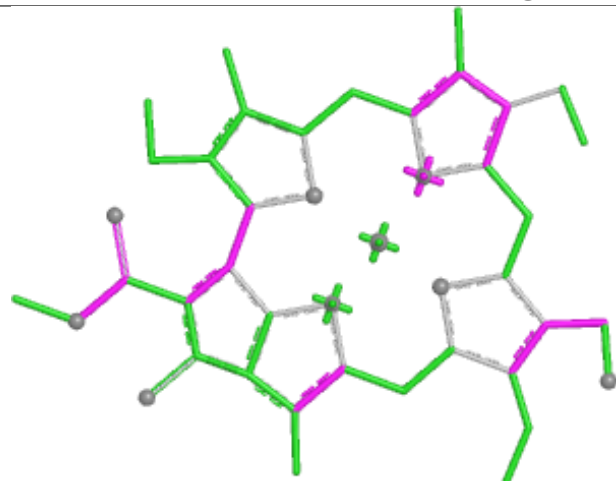


Ligand LMG 7 301

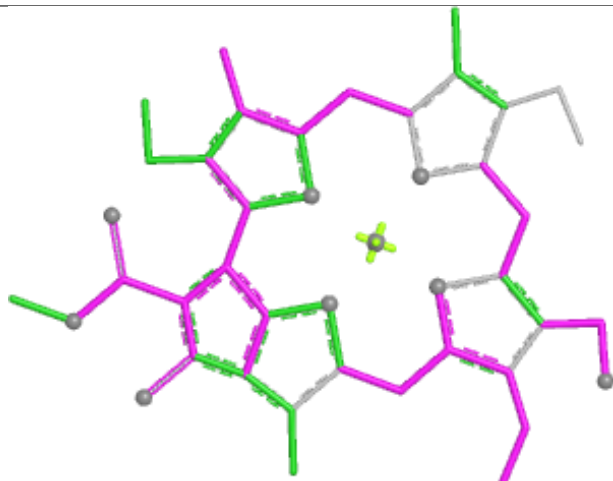




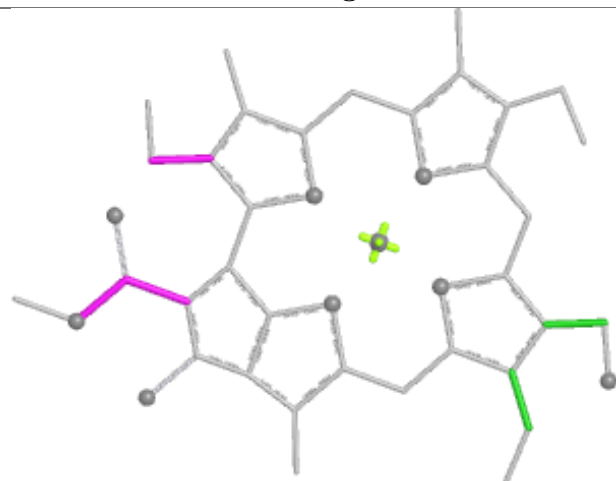
Ligand CHL x 301



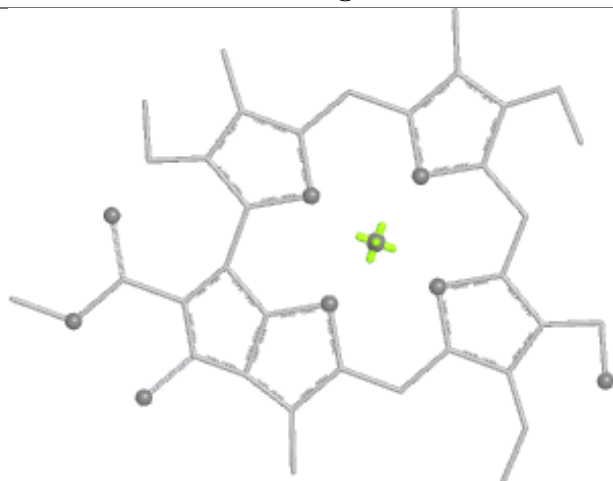
Bond lengths



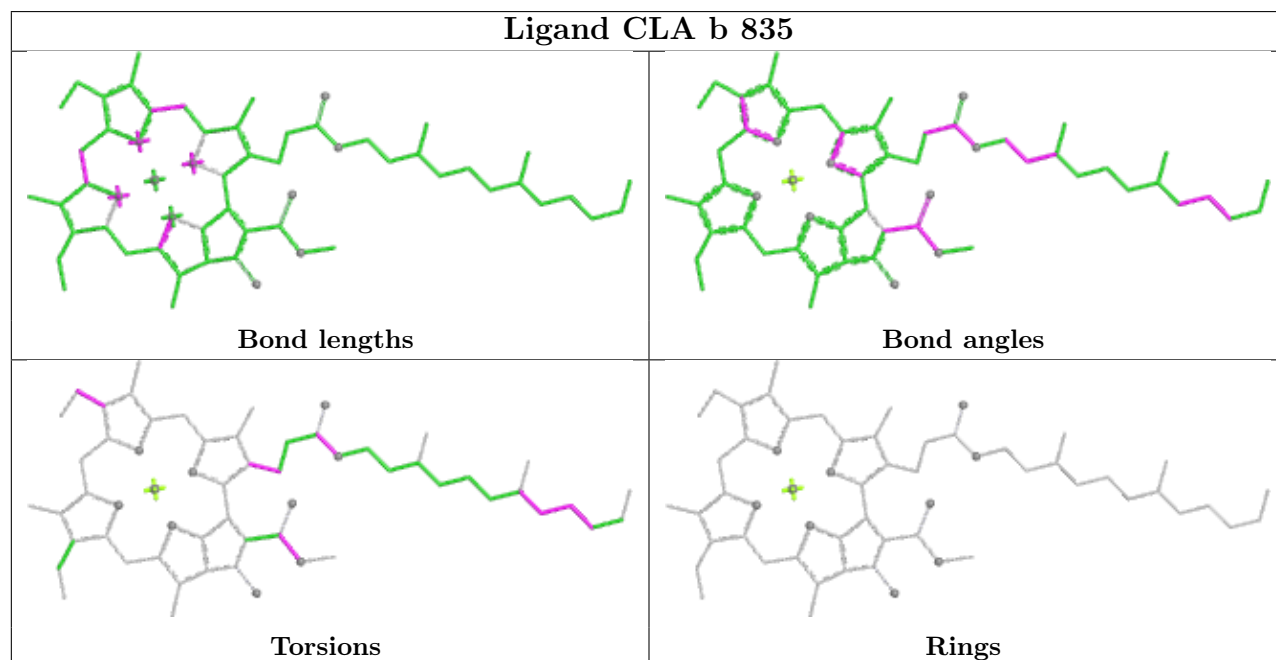
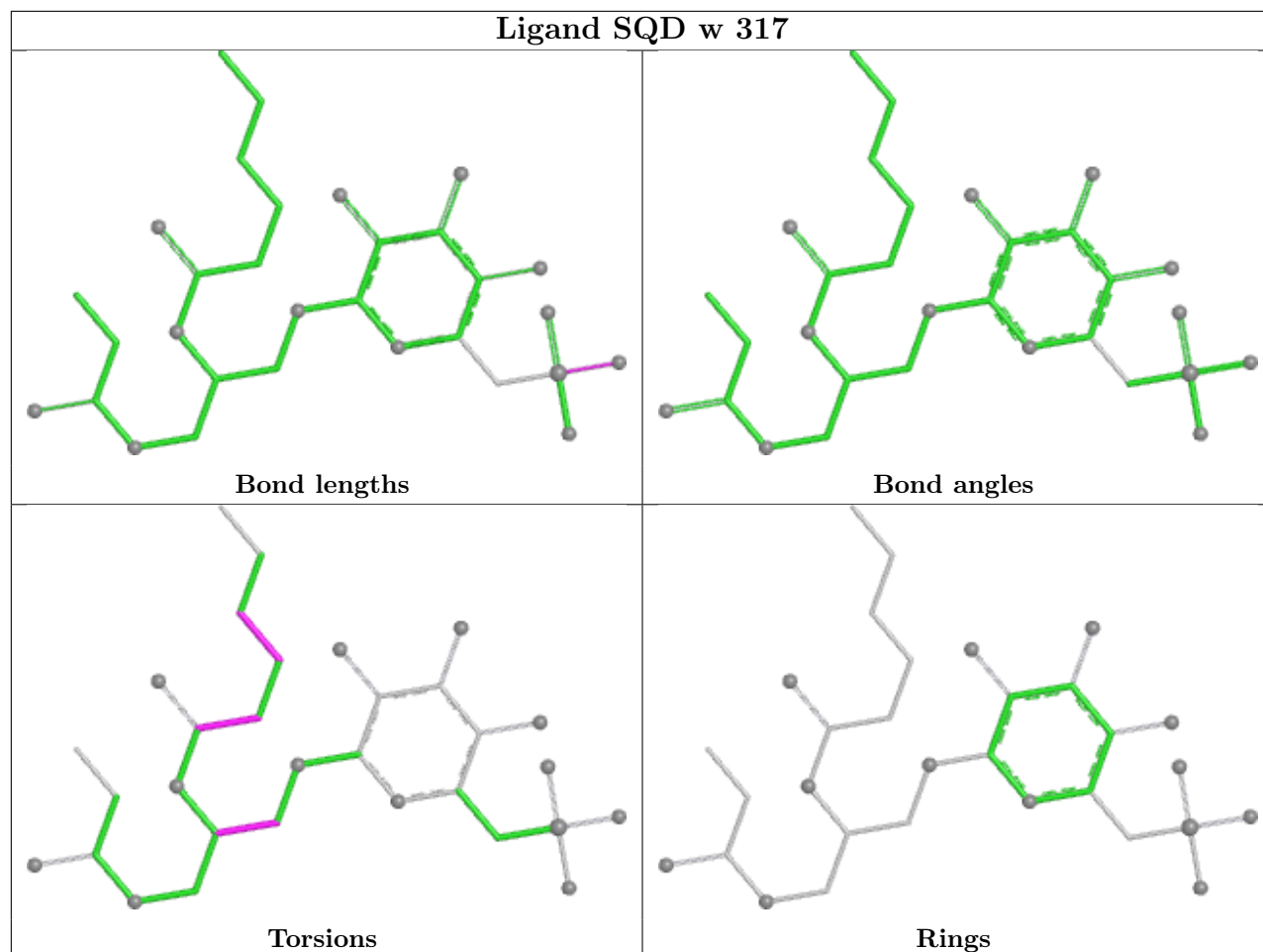
Bond angles



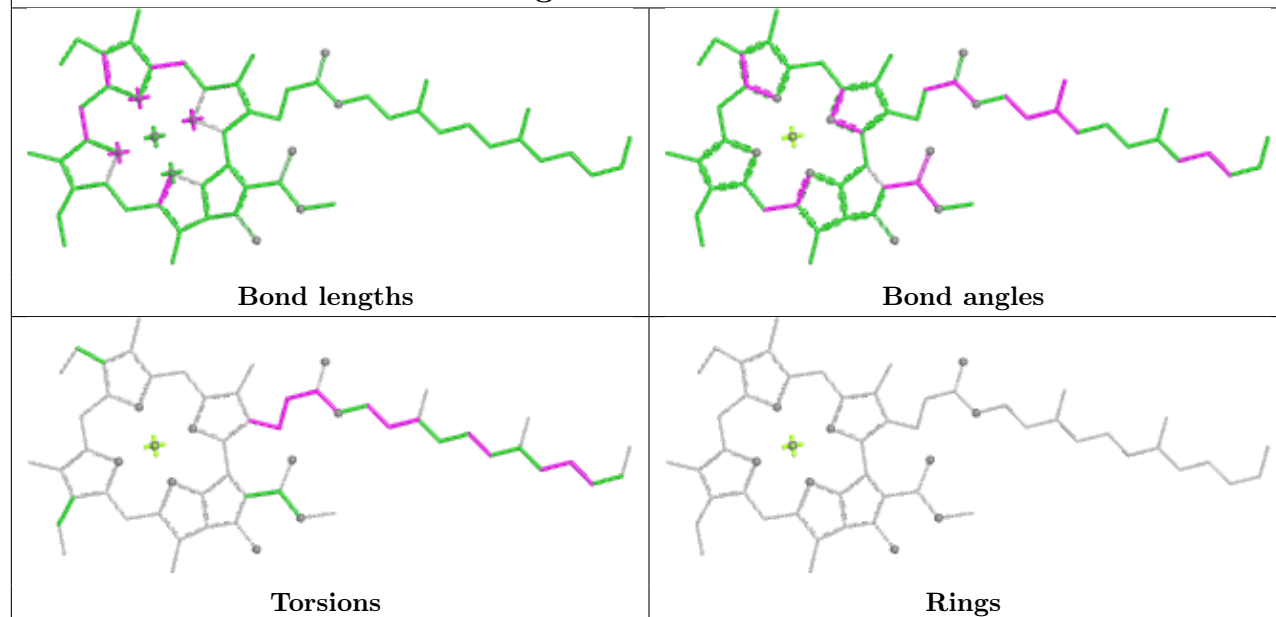
Torsions



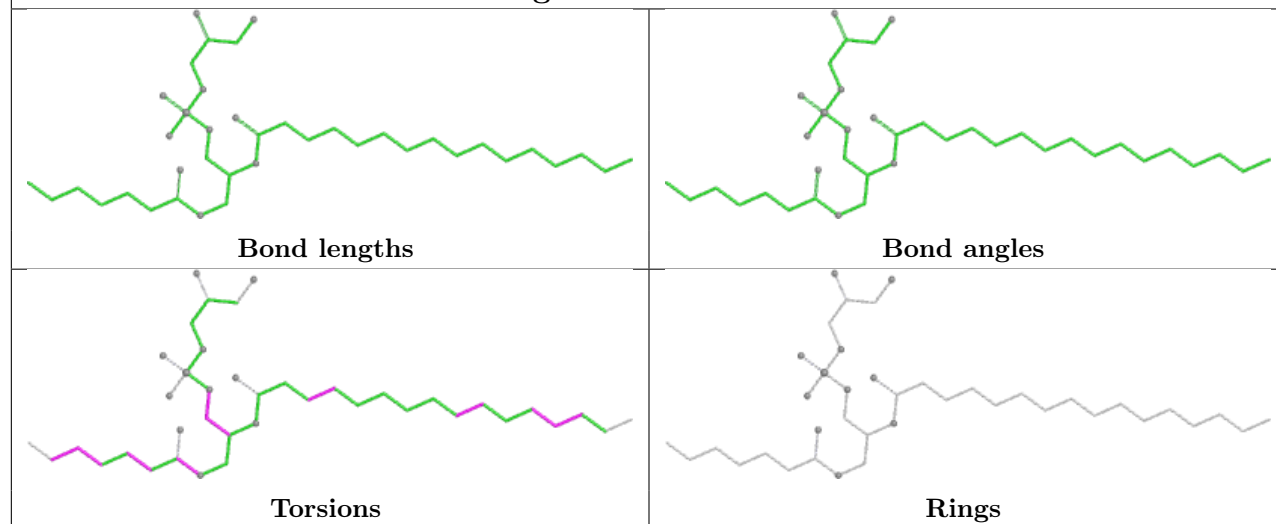
Rings

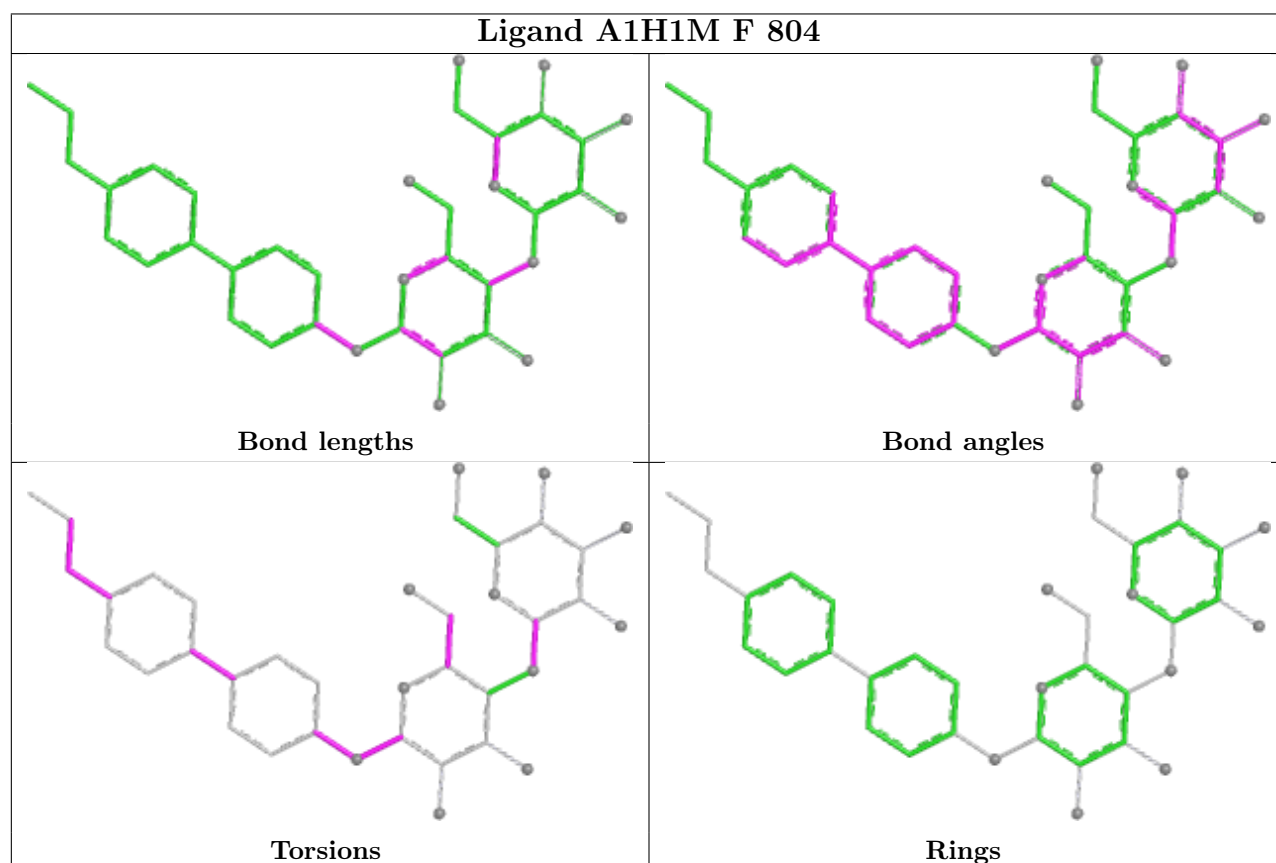
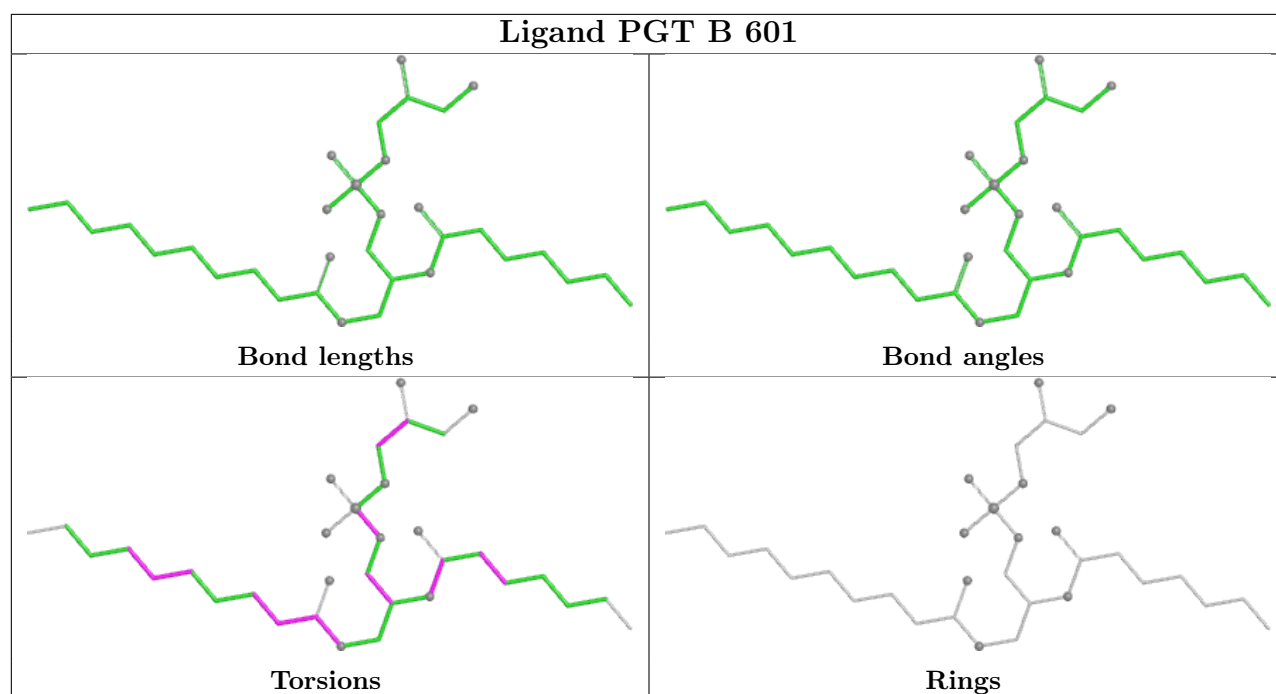


Ligand CLA b 809

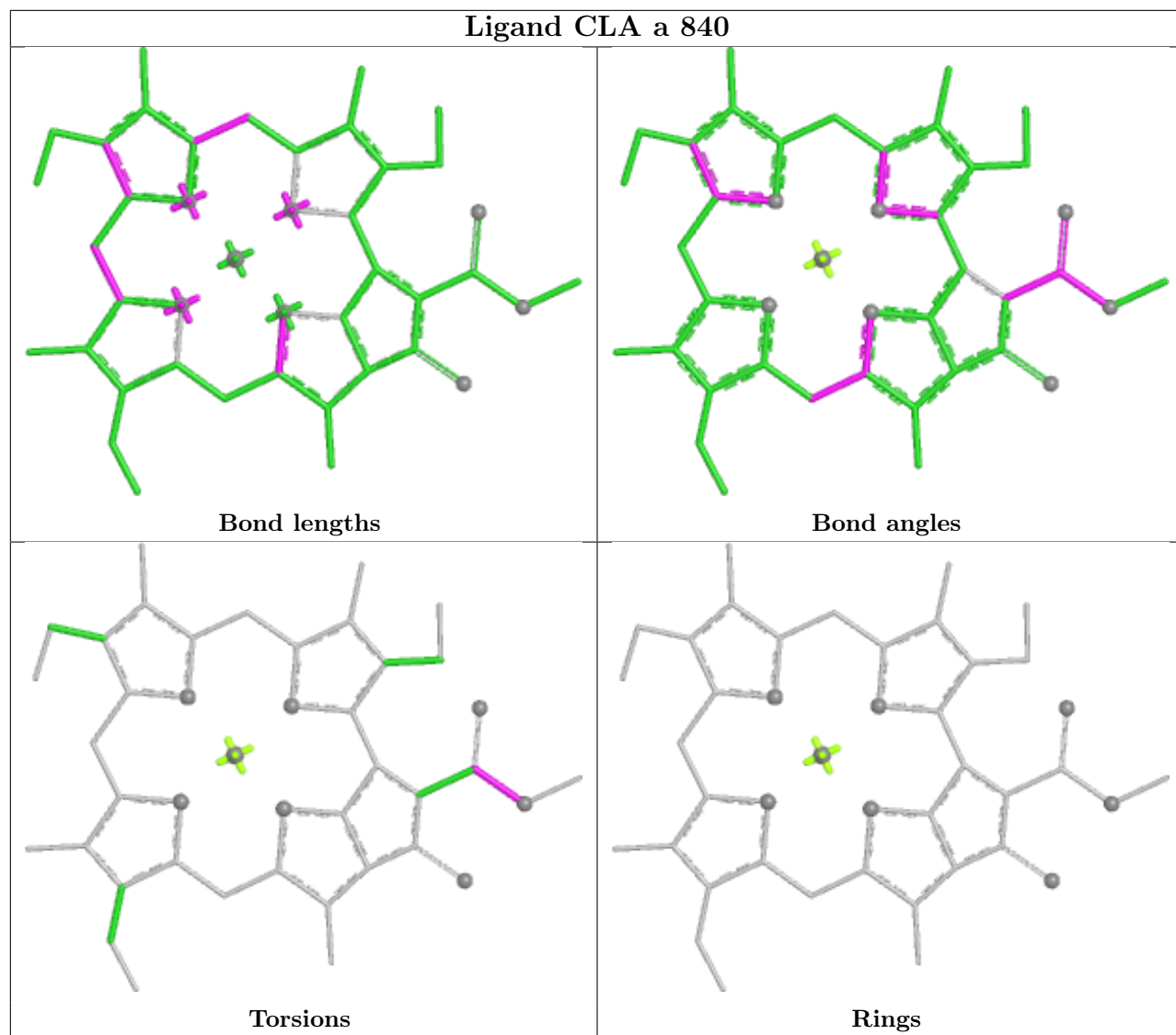


Ligand PGT L 201

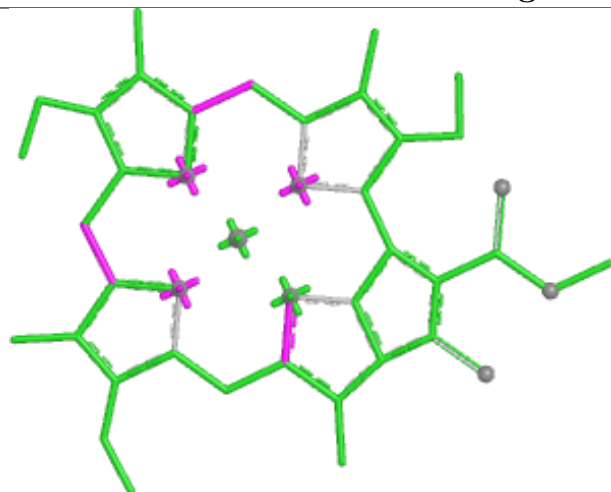




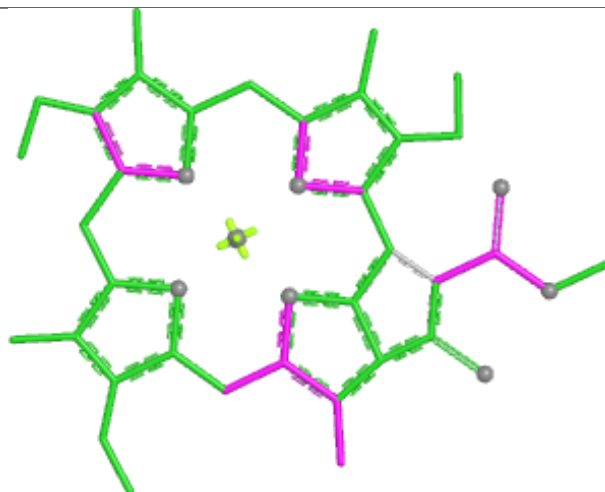
Ligand CLA a 840



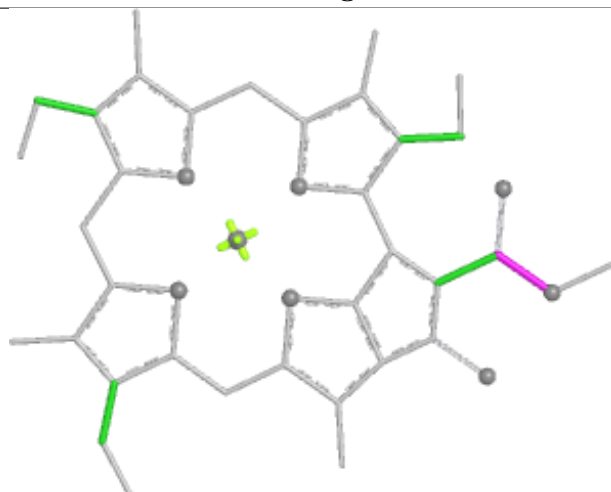
Ligand CLA a 855



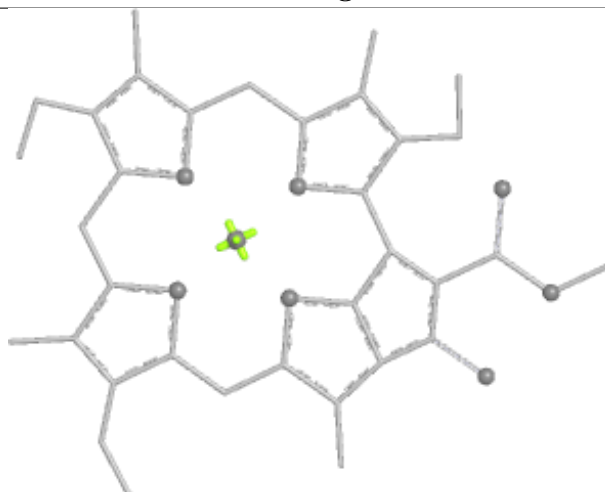
Bond lengths



Bond angles

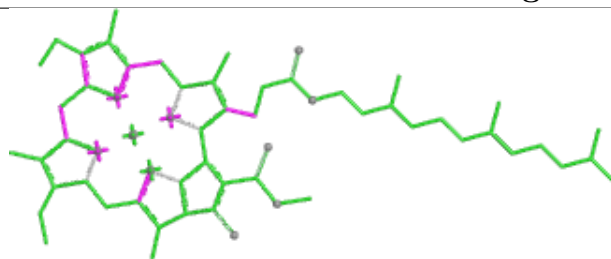


Torsions

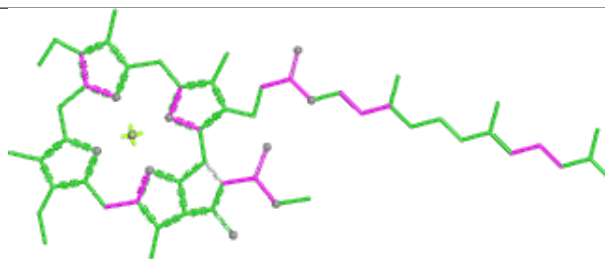


Rings

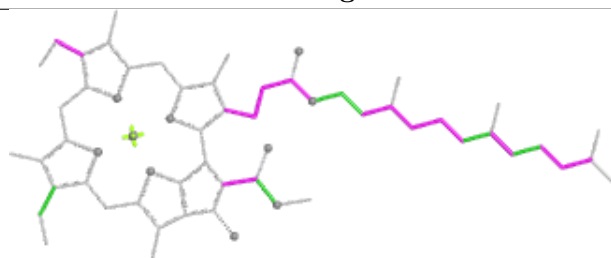
Ligand CLA l 306



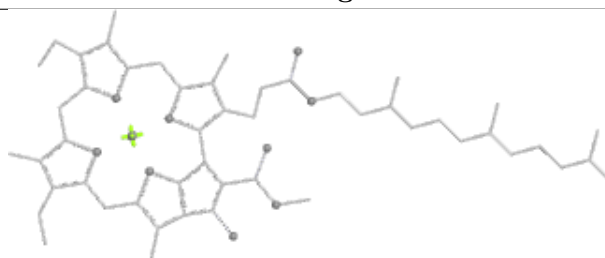
Bond lengths



Bond angles

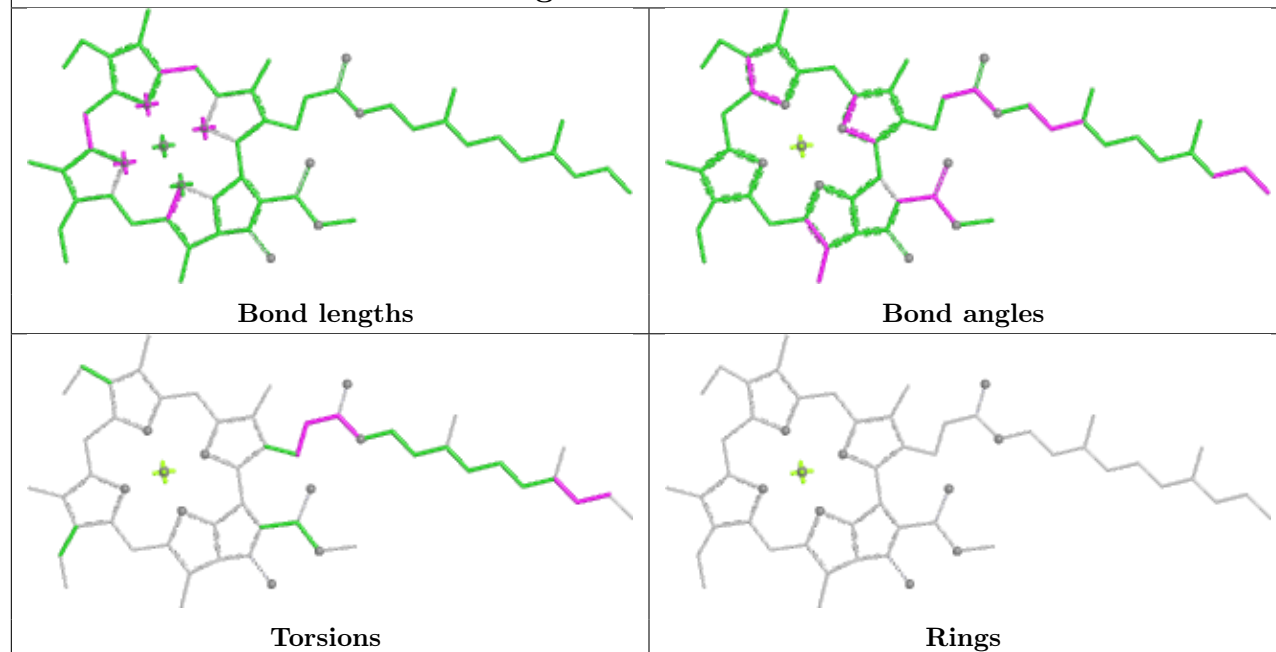


Torsions

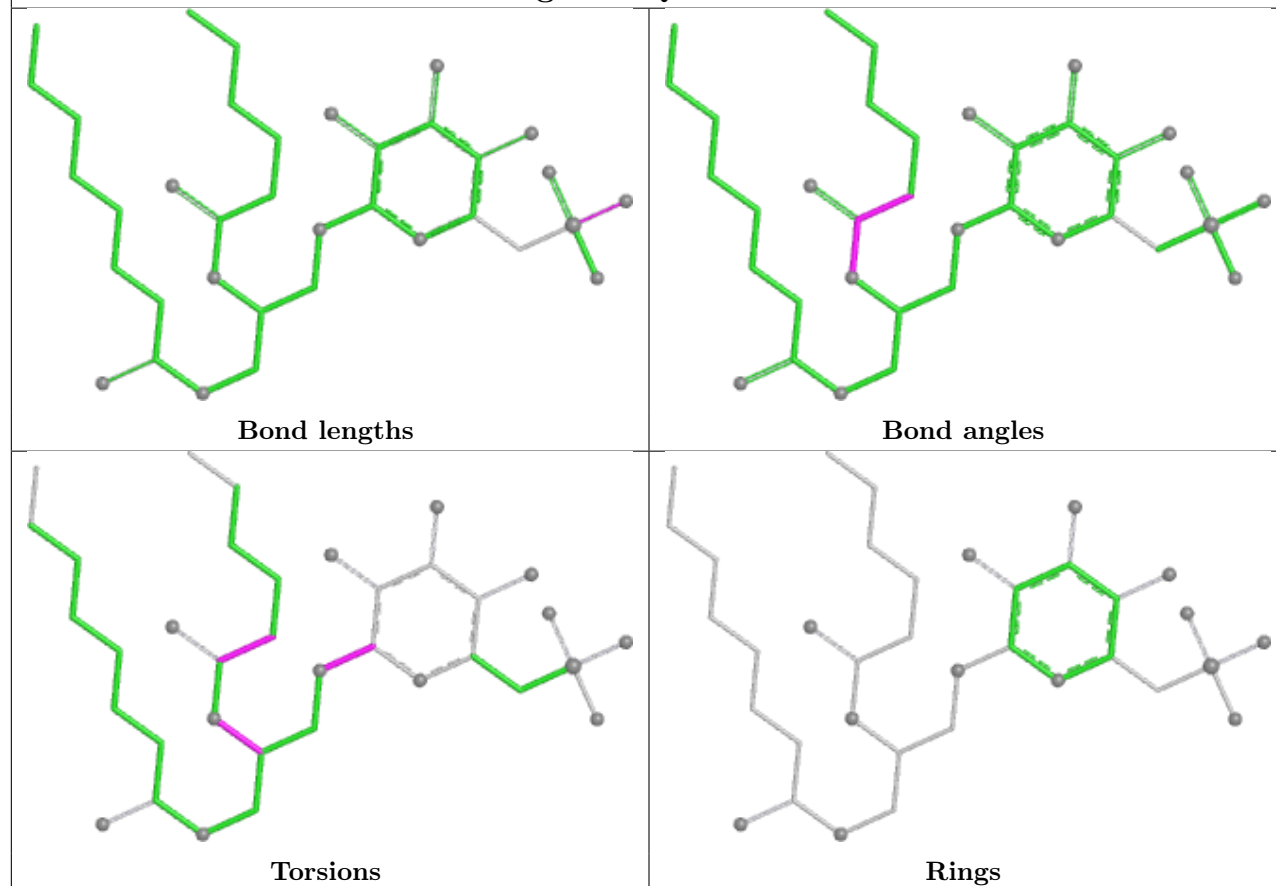


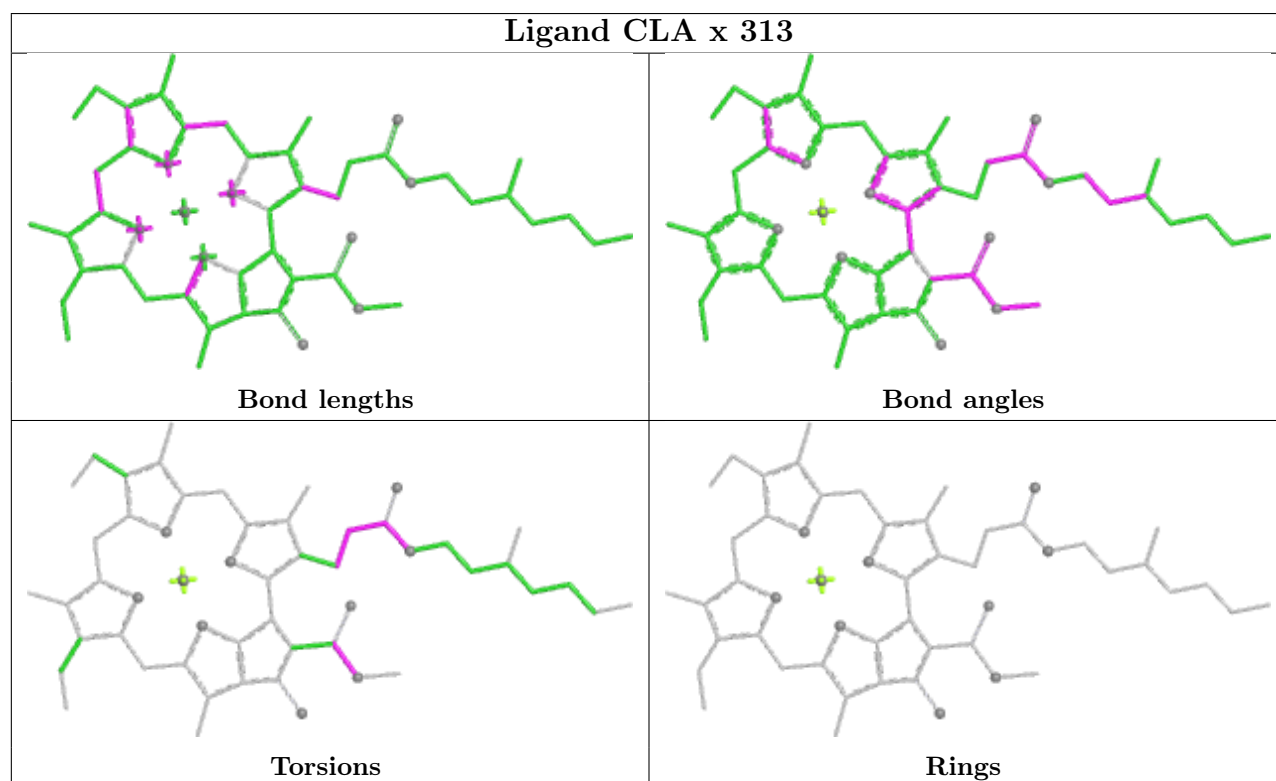
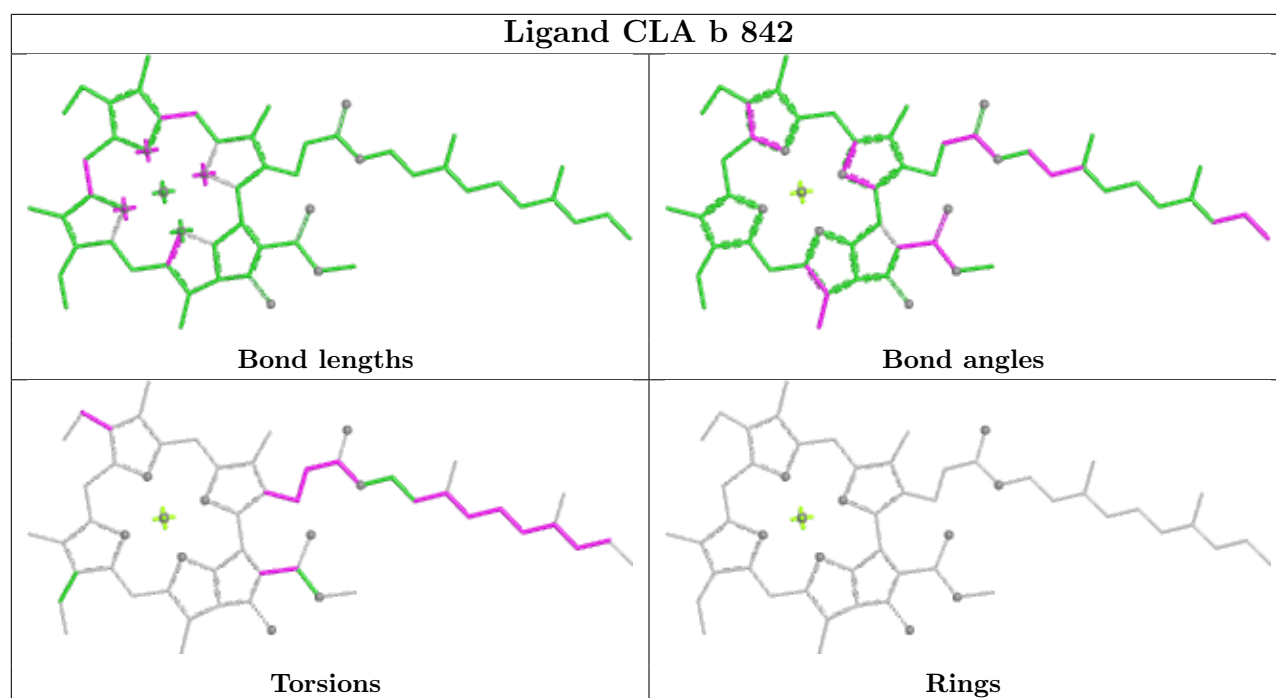
Rings

Ligand CLA k 204

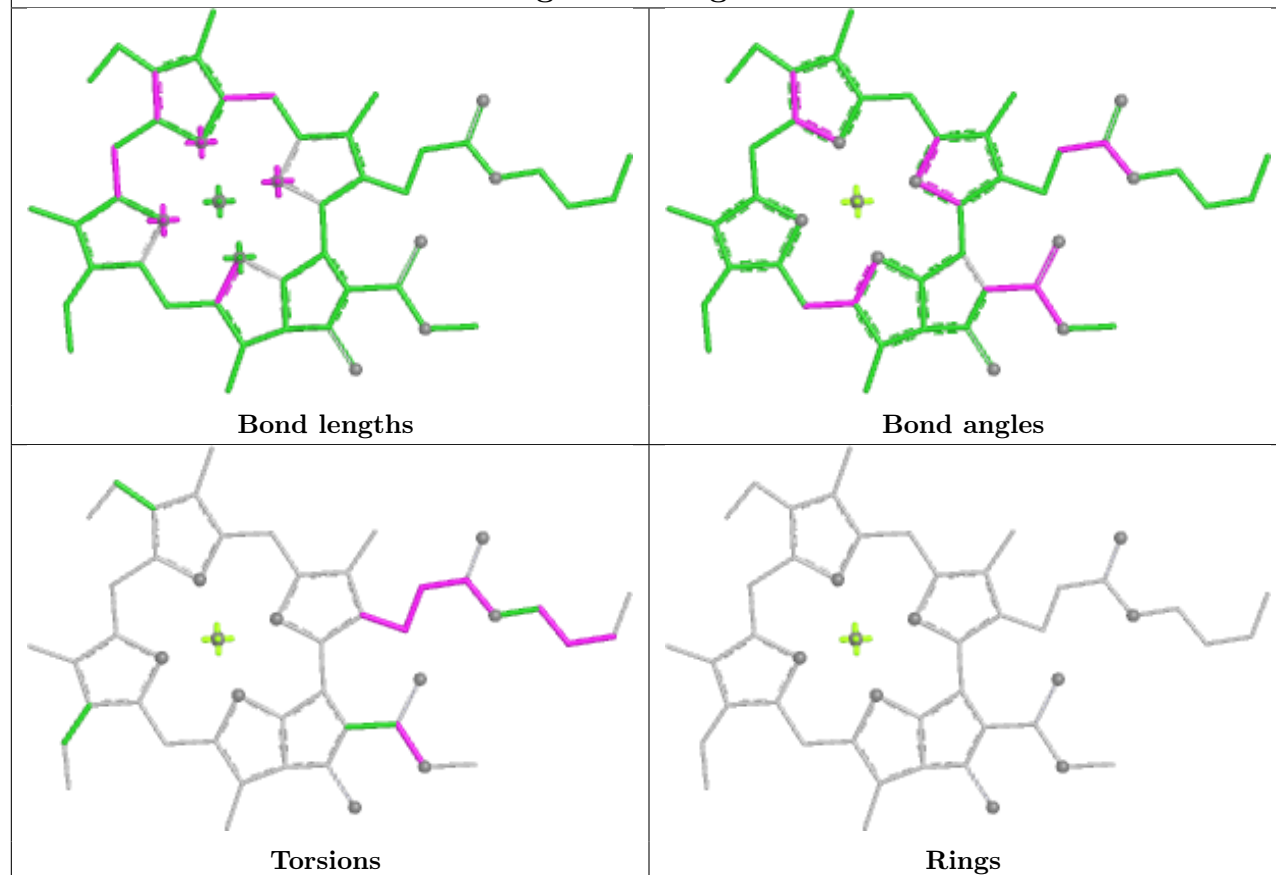


Ligand SQD a 859

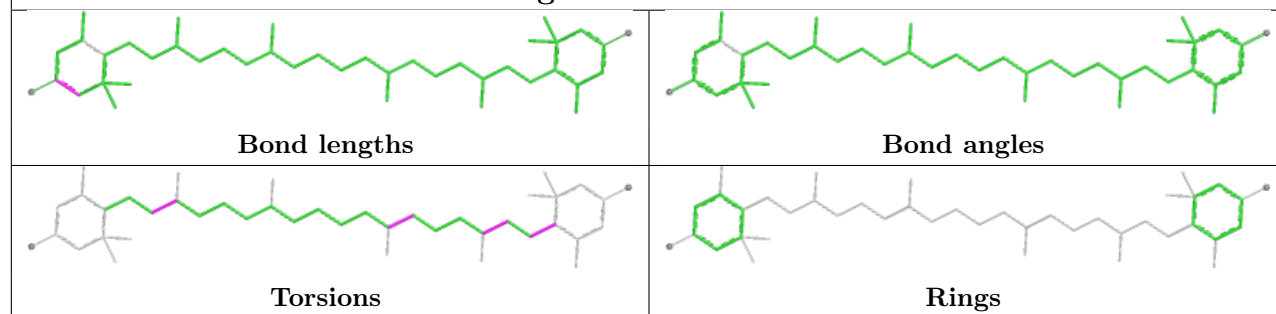


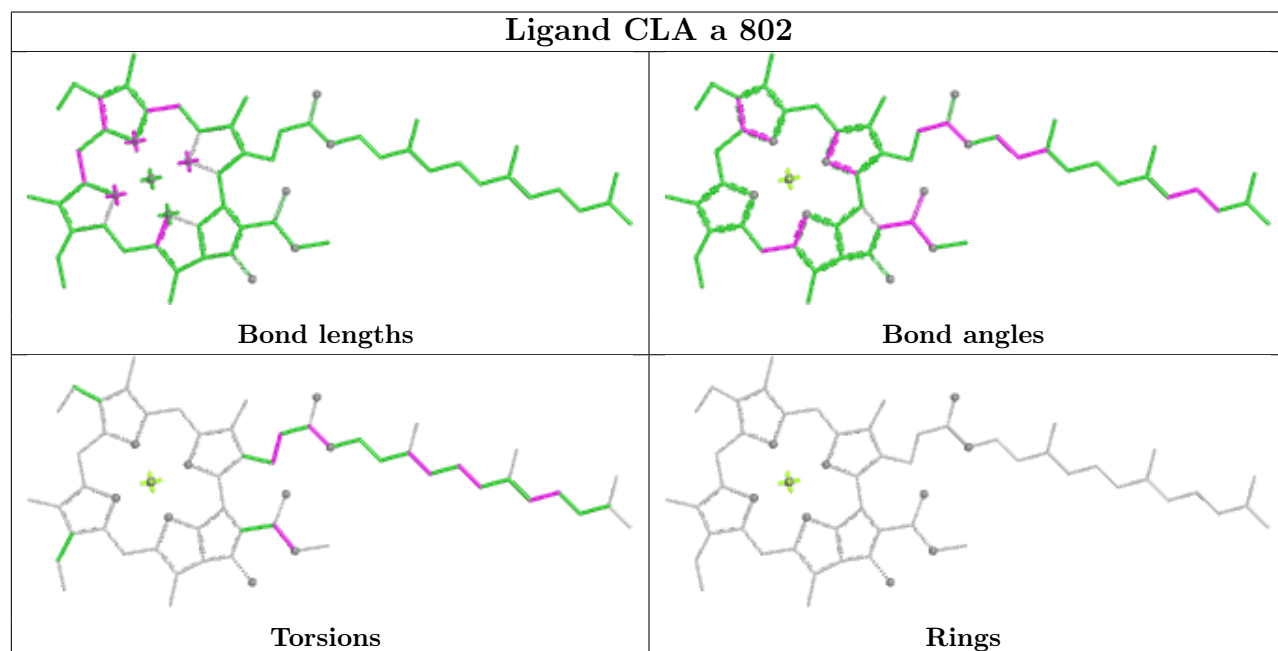
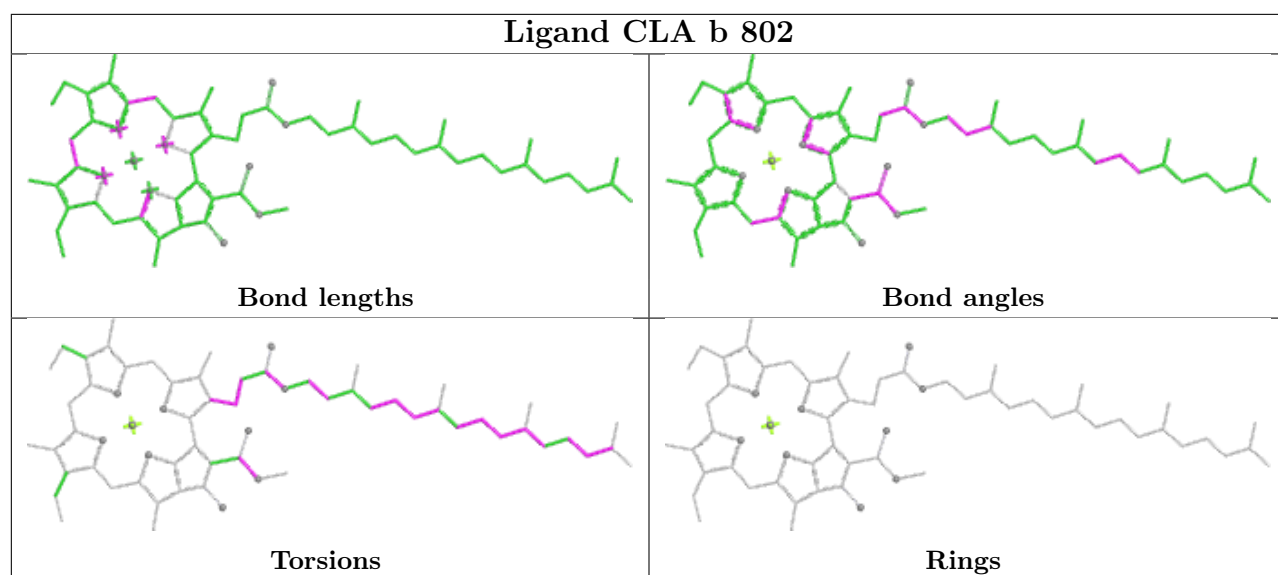


Ligand CLA g 201

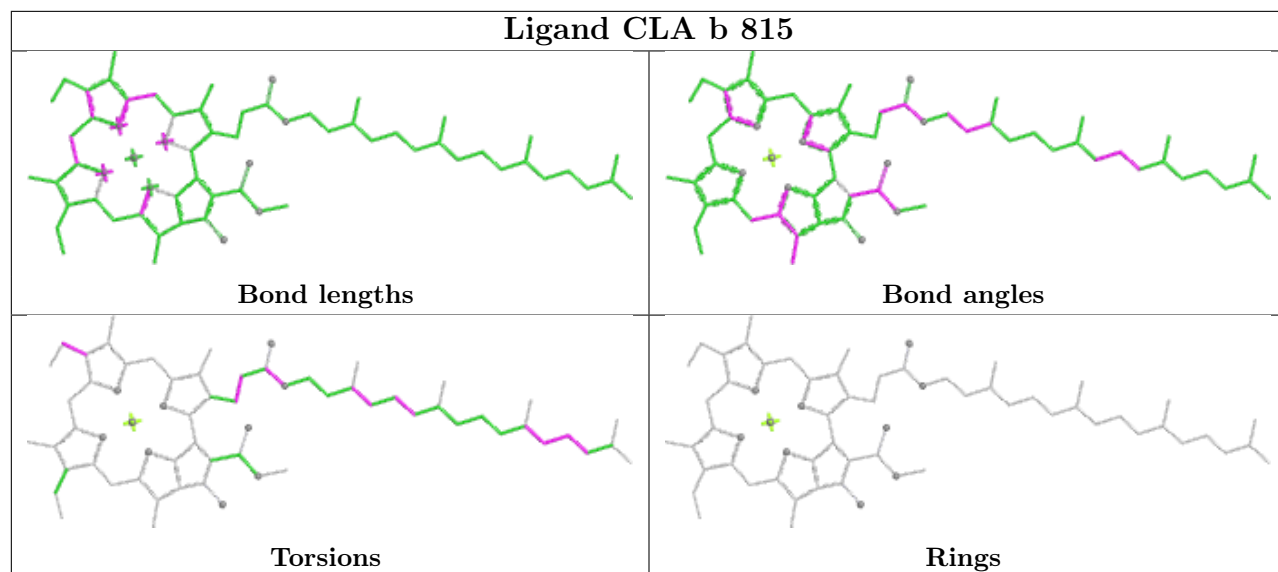


Ligand LUT z 320

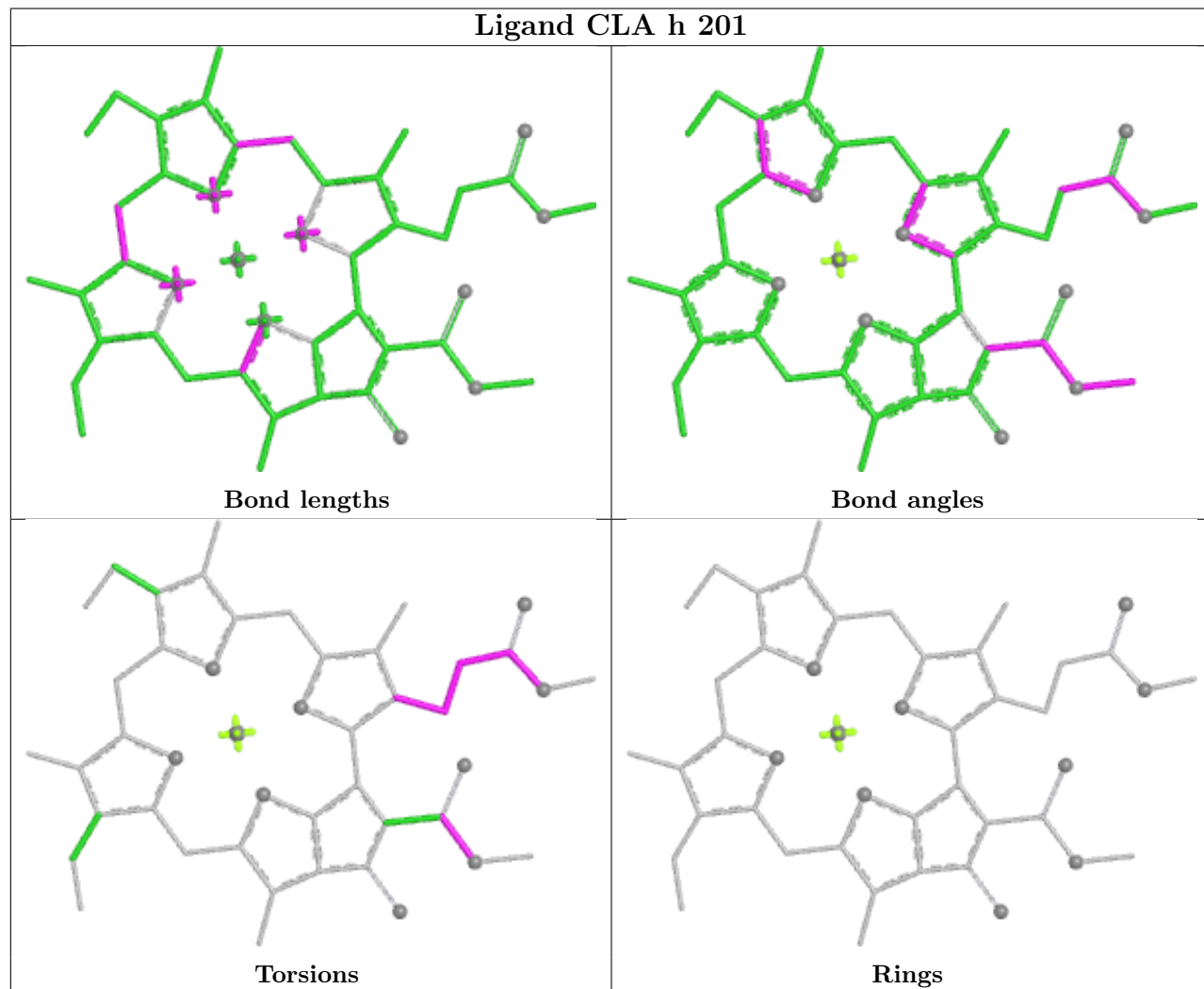


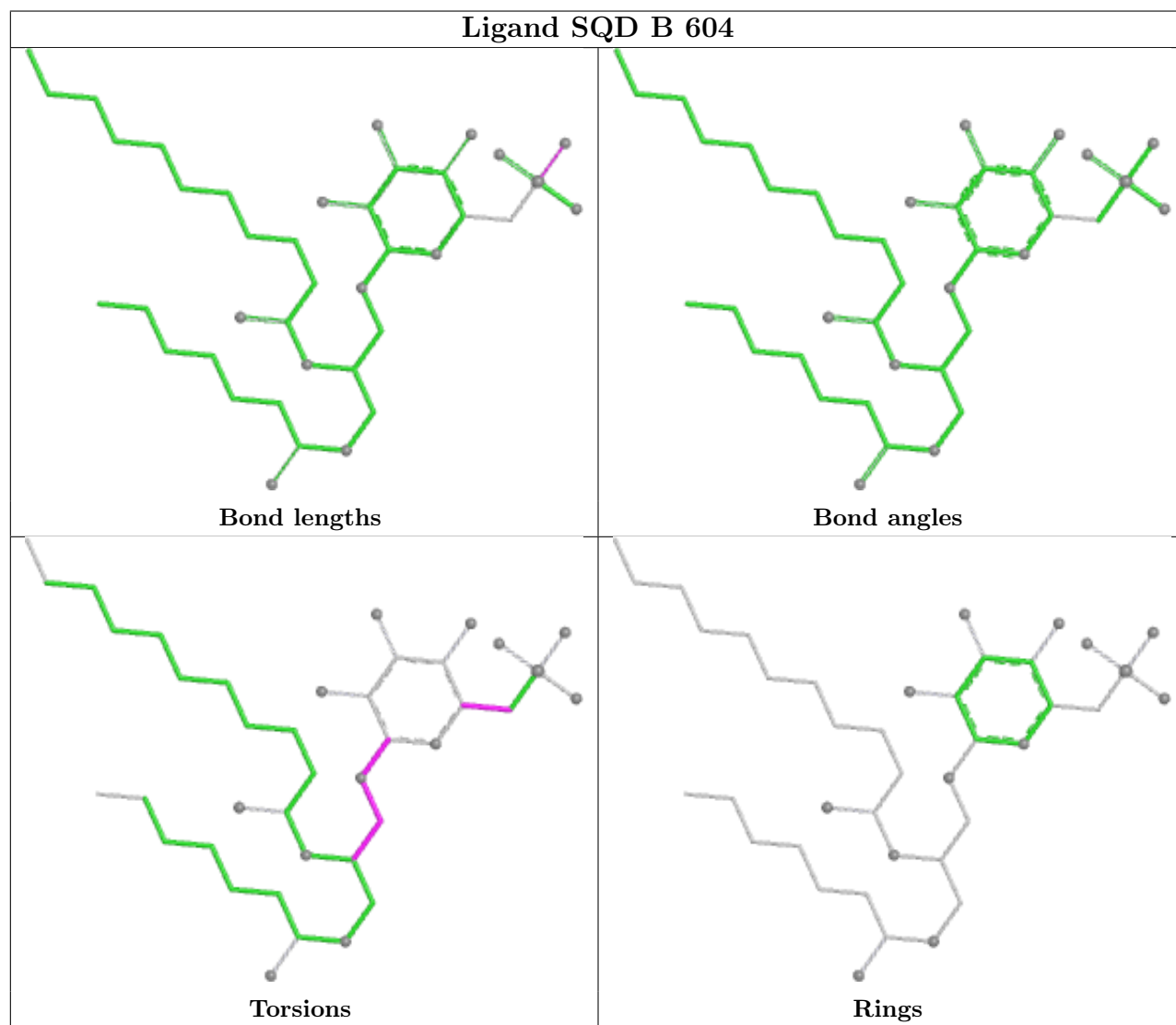
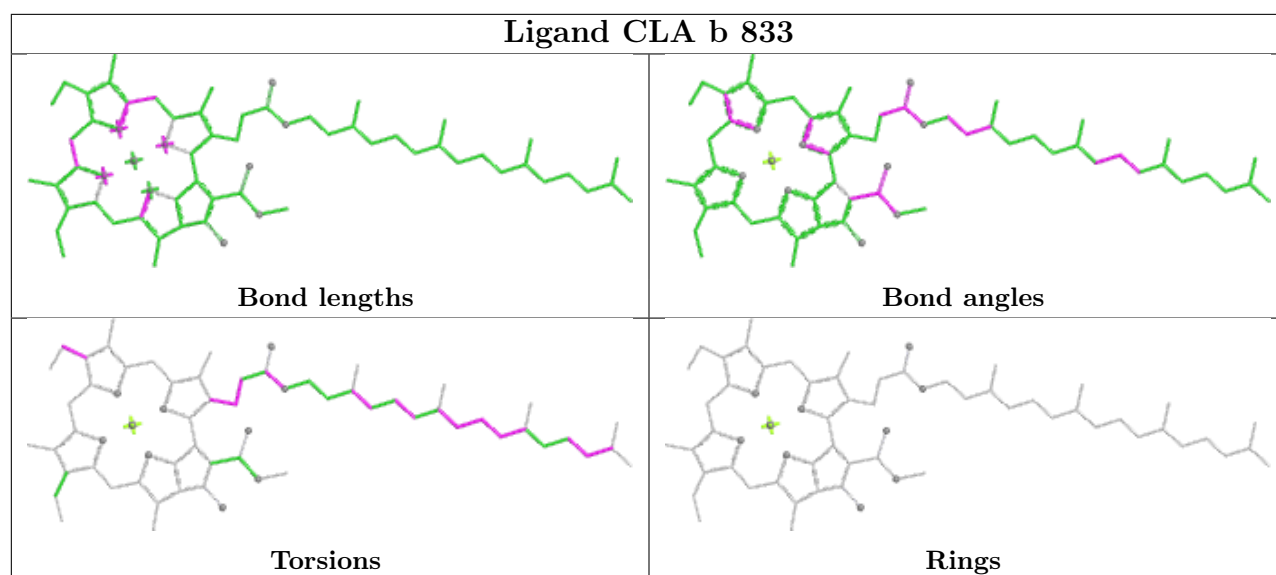


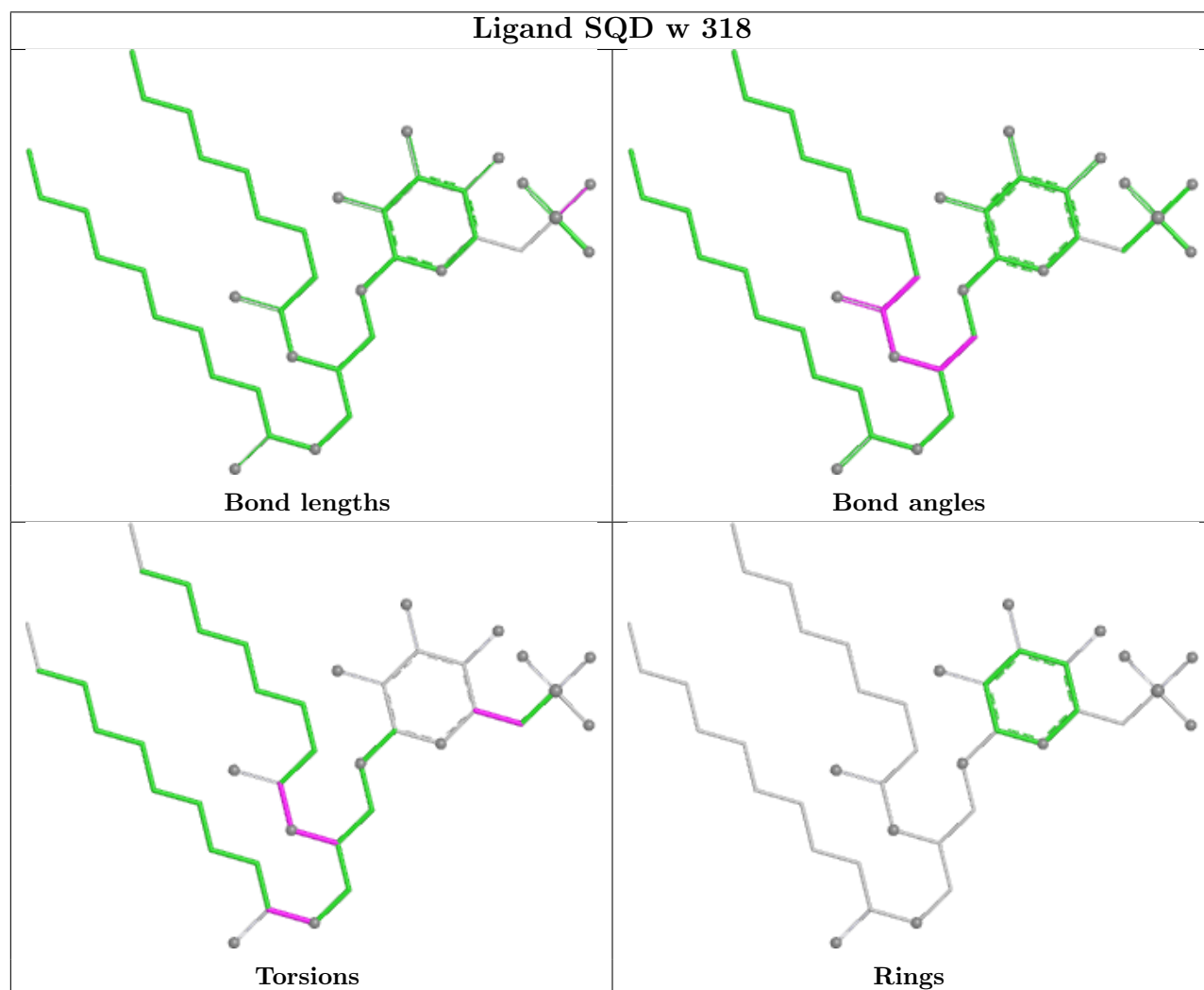
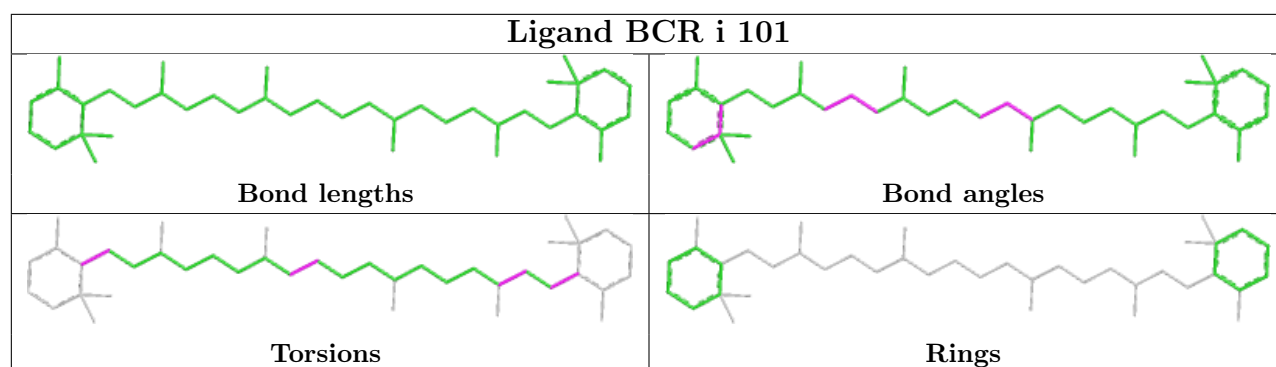
Ligand CLA b 815



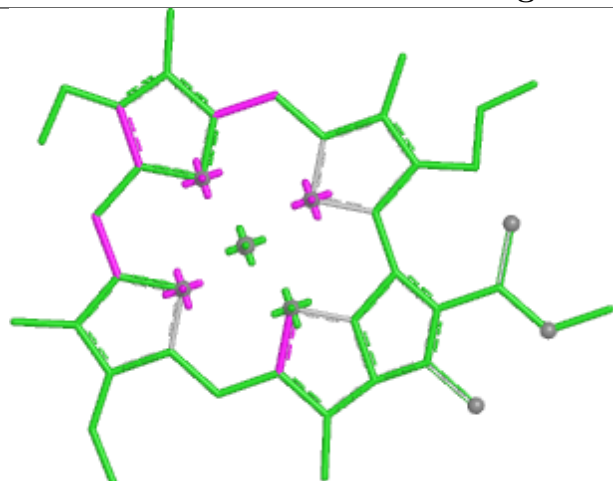
Ligand CLA h 201



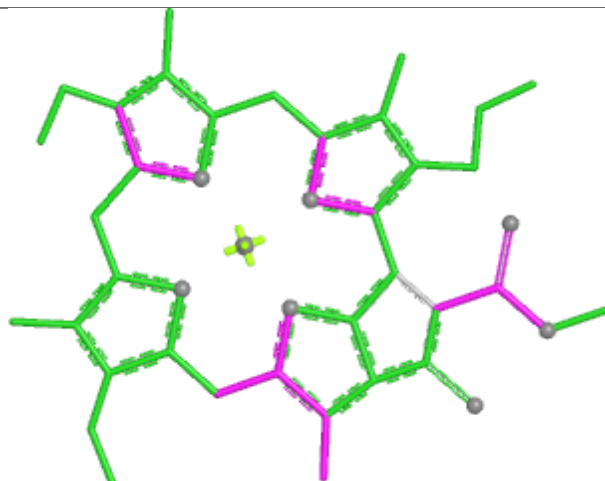




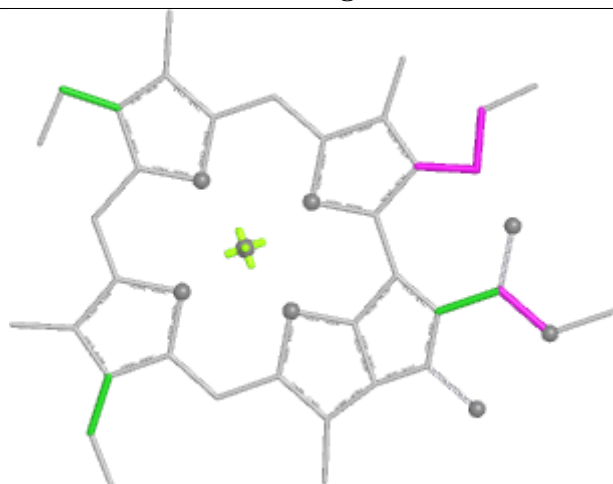
Ligand CLA b 813



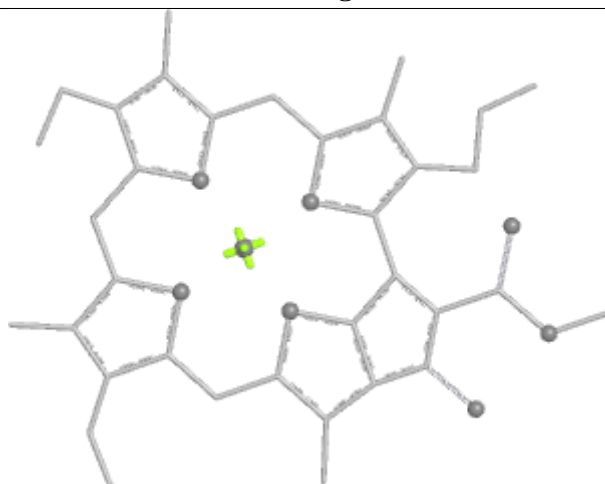
Bond lengths



Bond angles

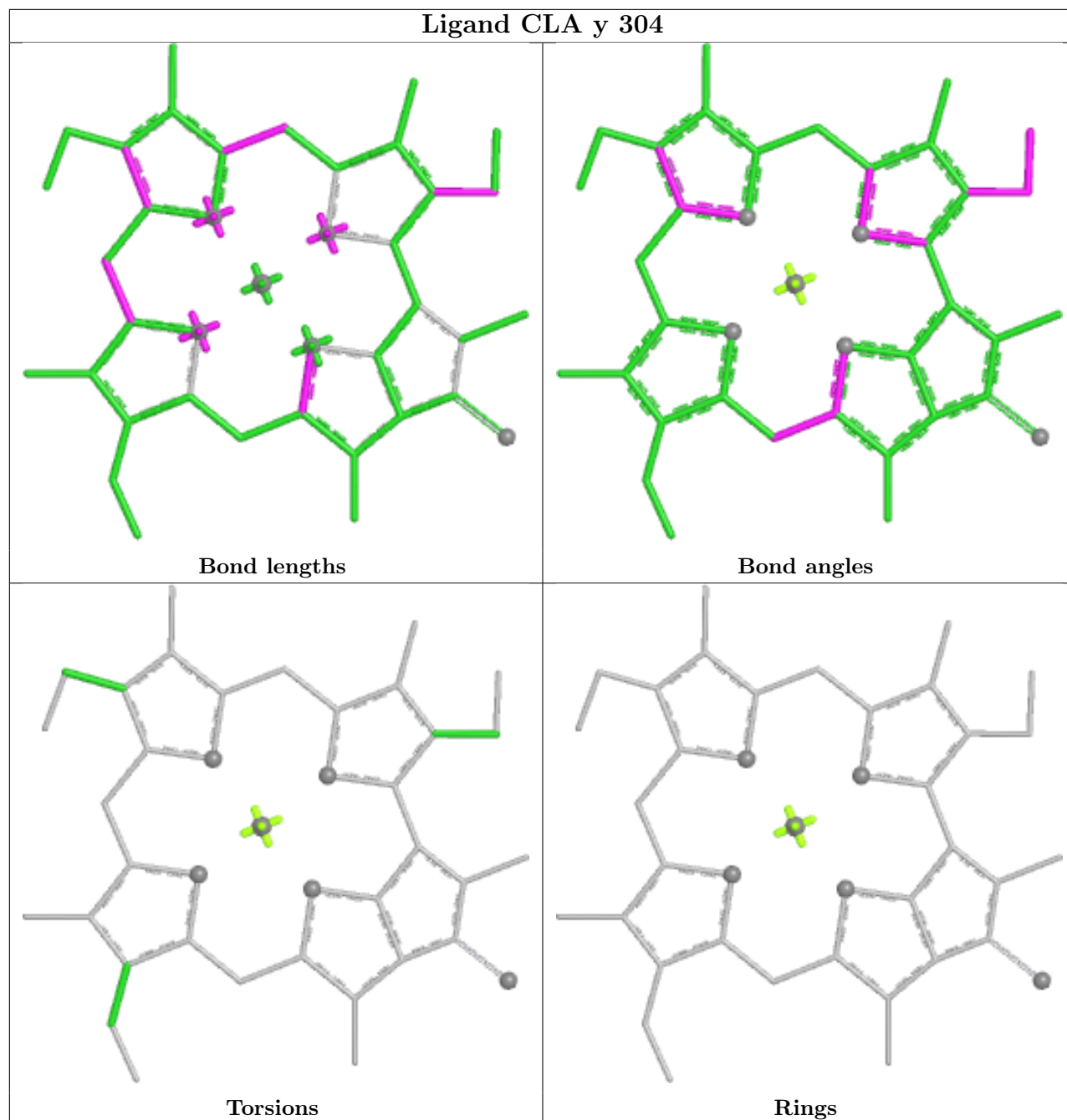


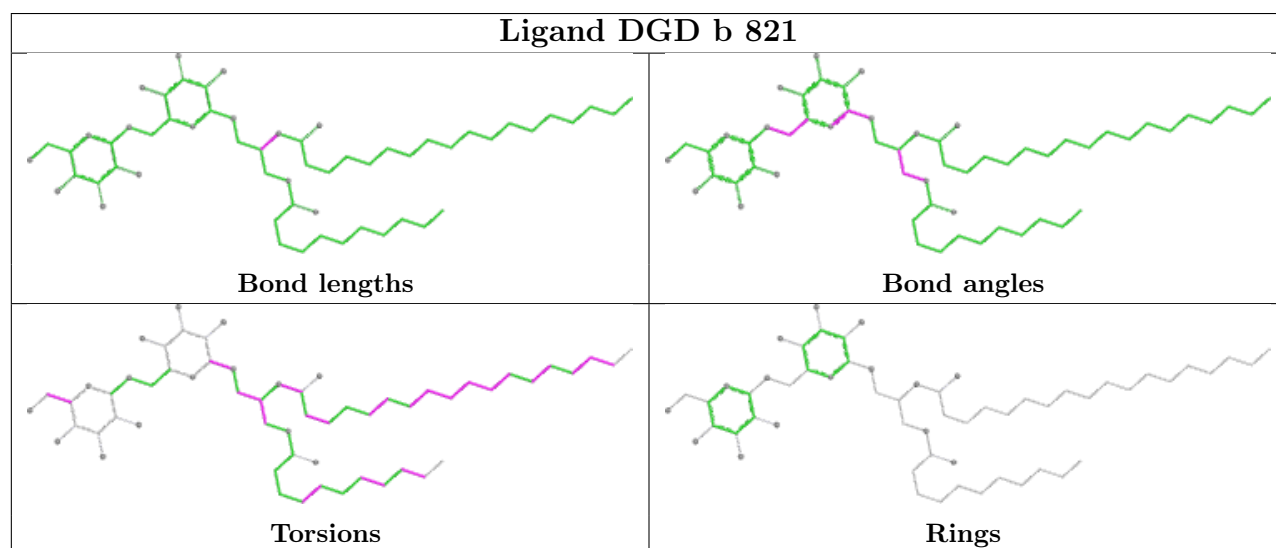
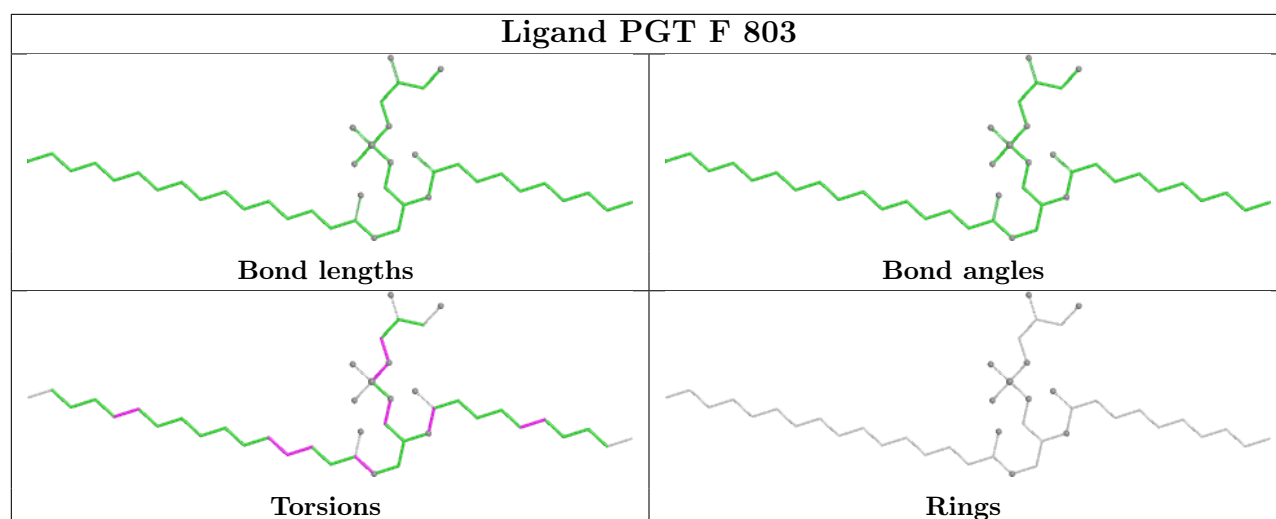
Torsions



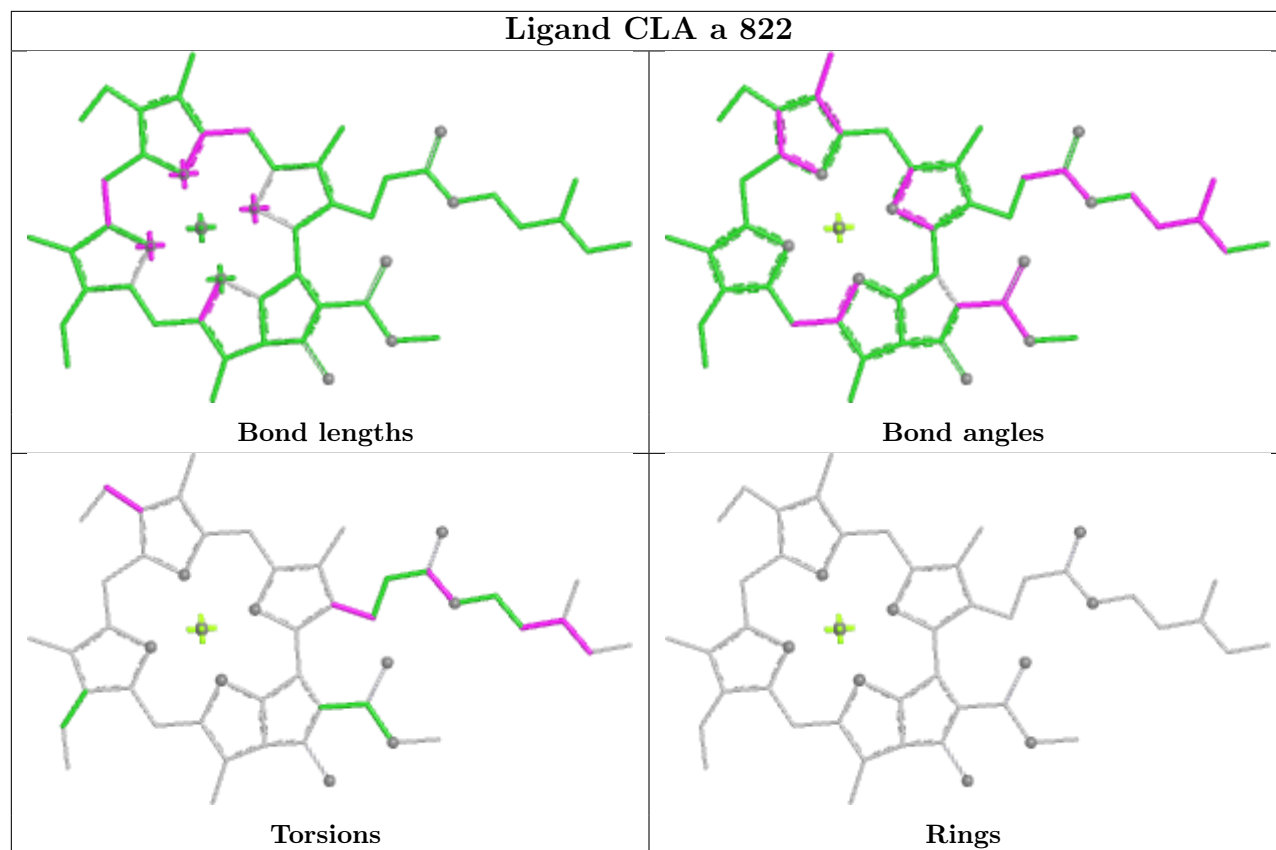
Rings

Ligand CLA y 304

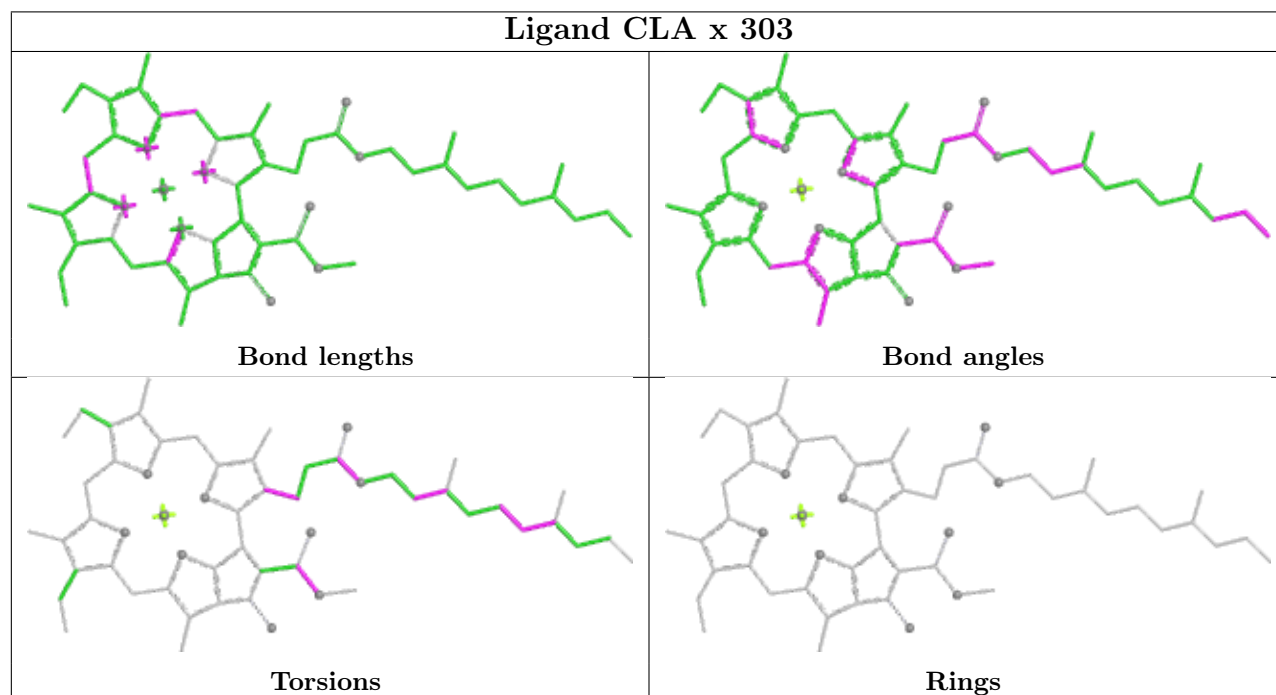




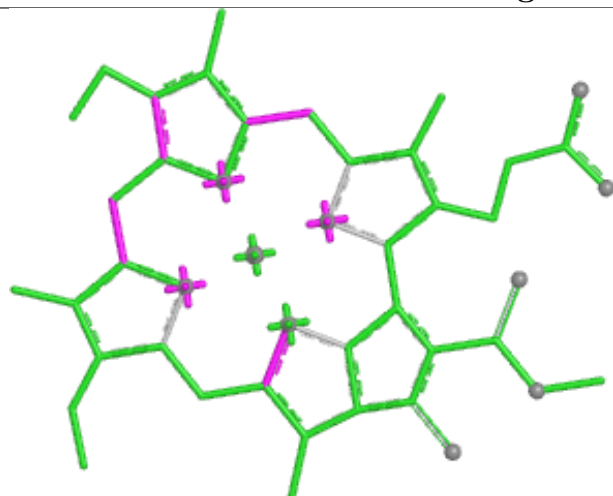
Ligand CLA a 822



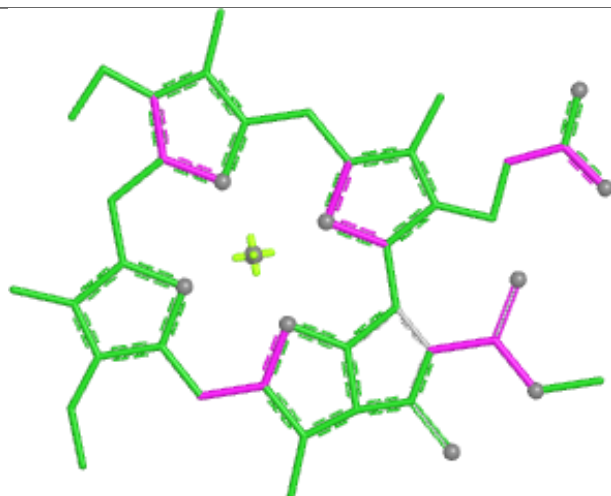
Ligand CLA x 303



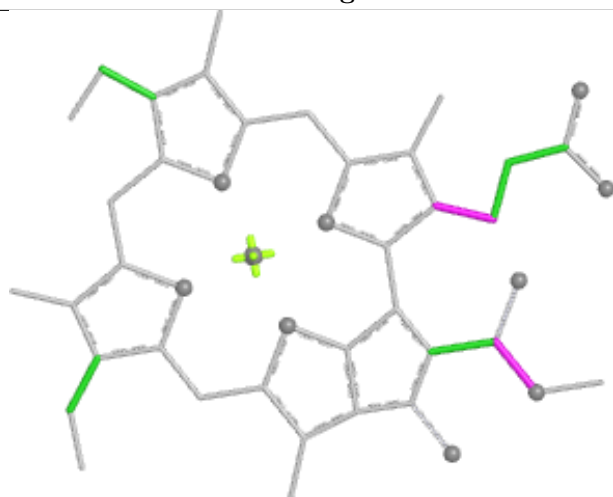
Ligand CLA b 834



Bond lengths



Bond angles

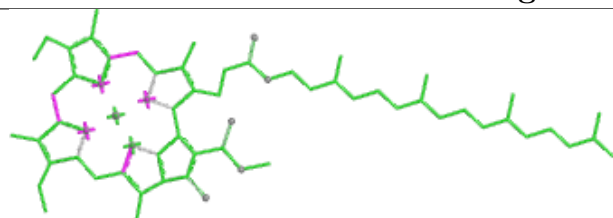


Torsions

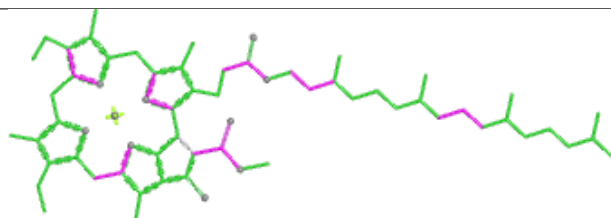


Rings

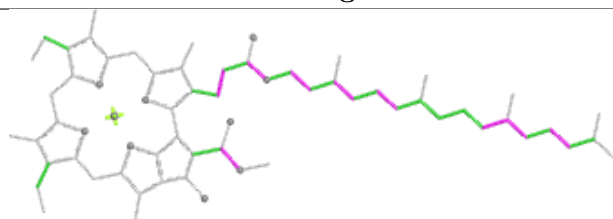
Ligand CLA a 857



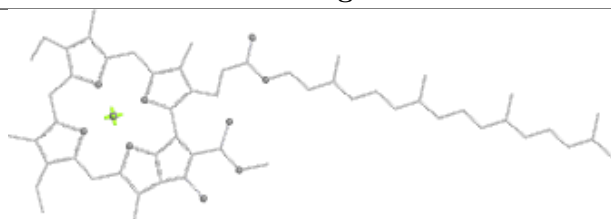
Bond lengths



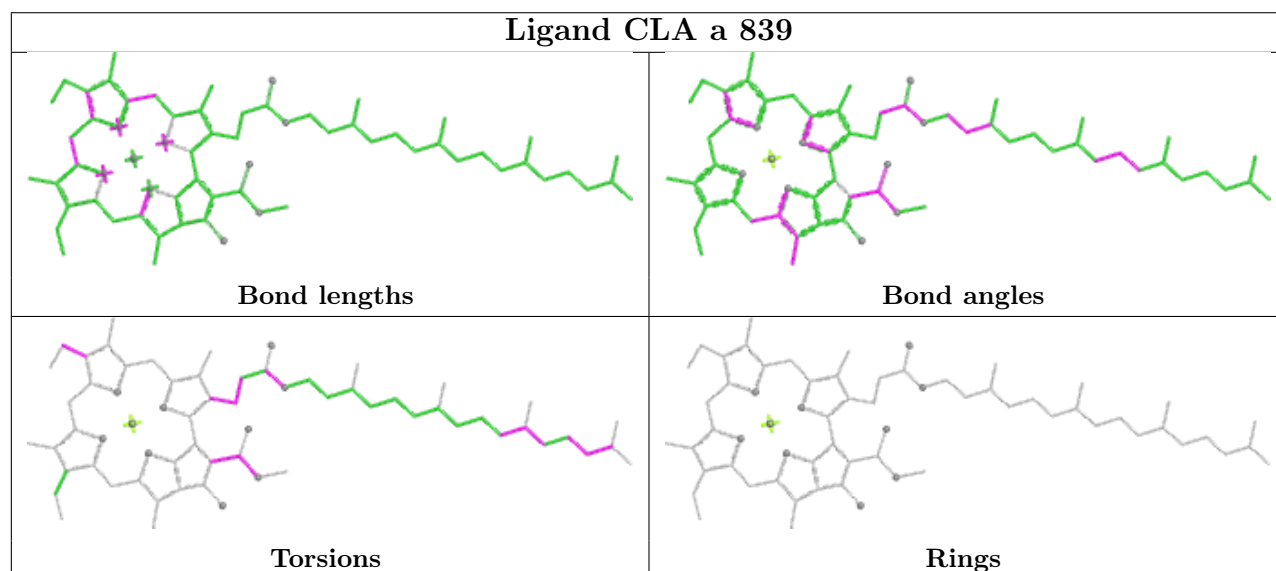
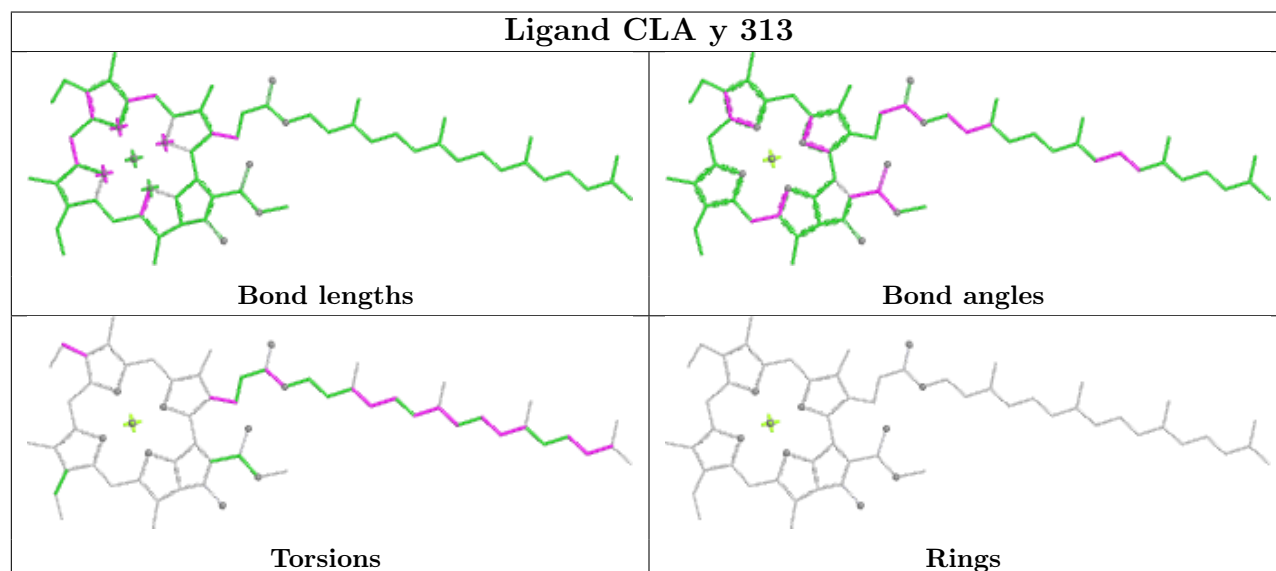
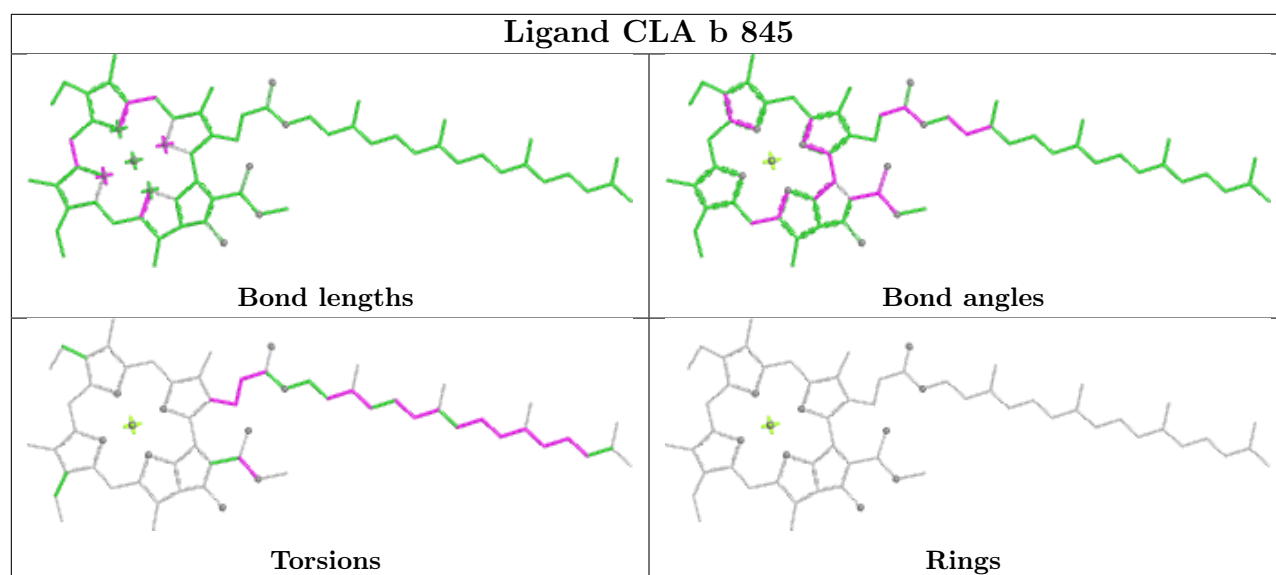
Bond angles



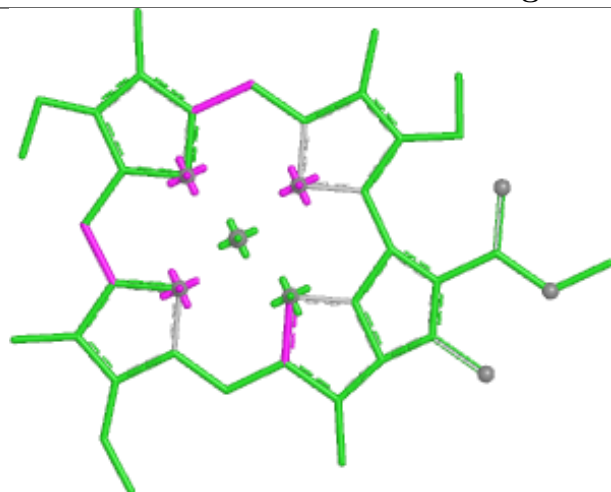
Torsions



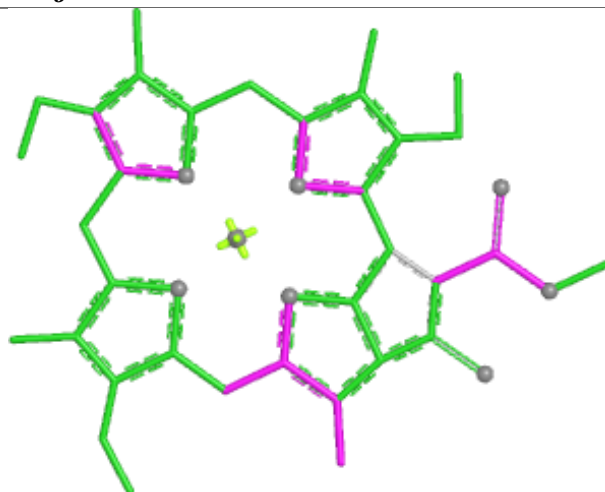
Rings



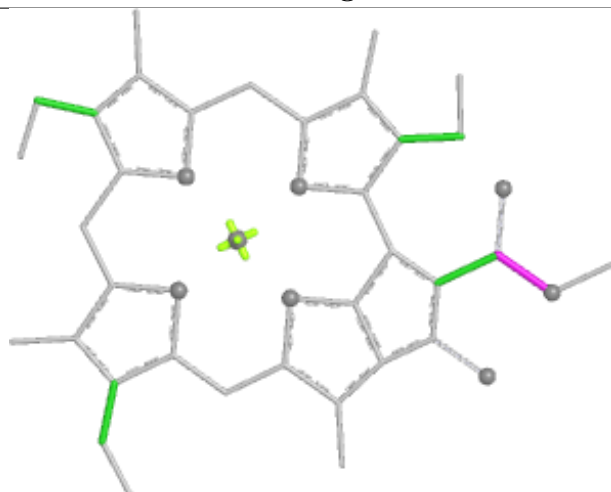
Ligand CLA j 102



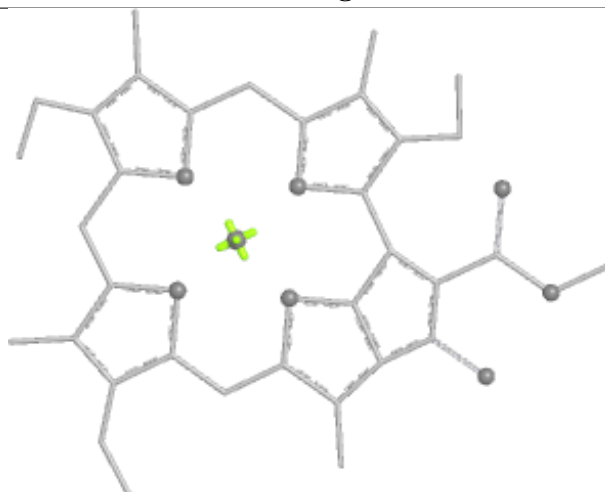
Bond lengths



Bond angles

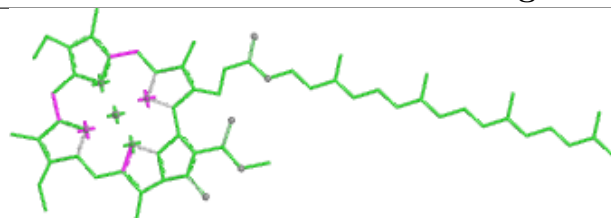


Torsions

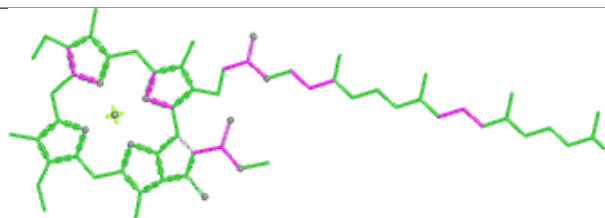


Rings

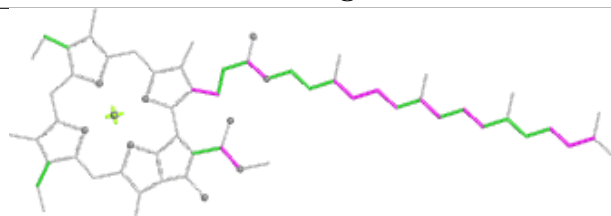
Ligand CLA a 836



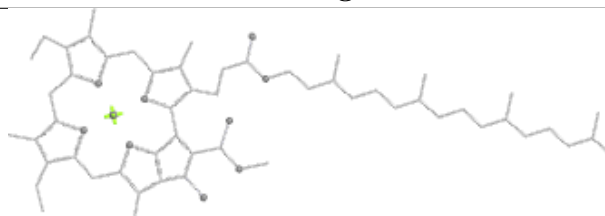
Bond lengths



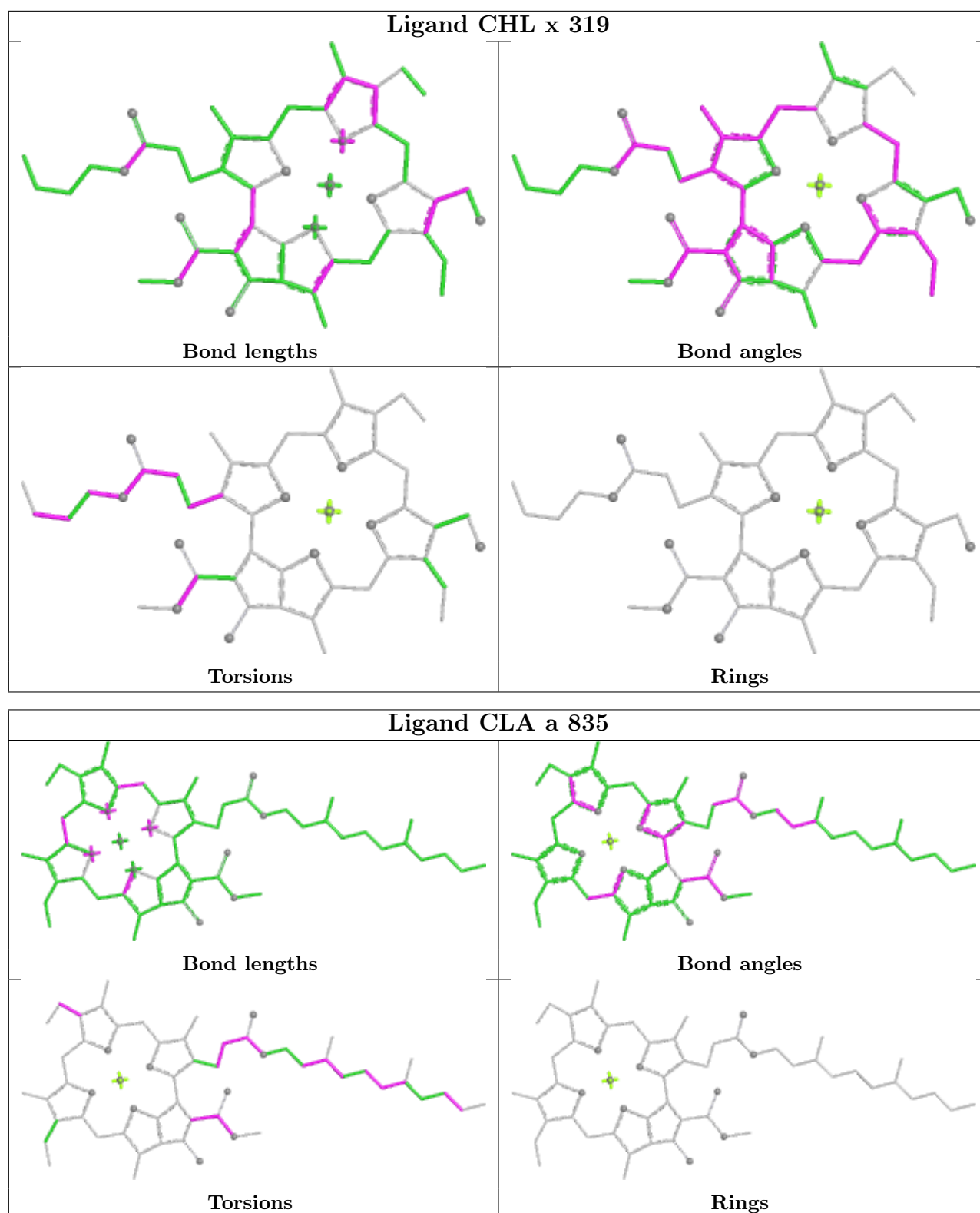
Bond angles

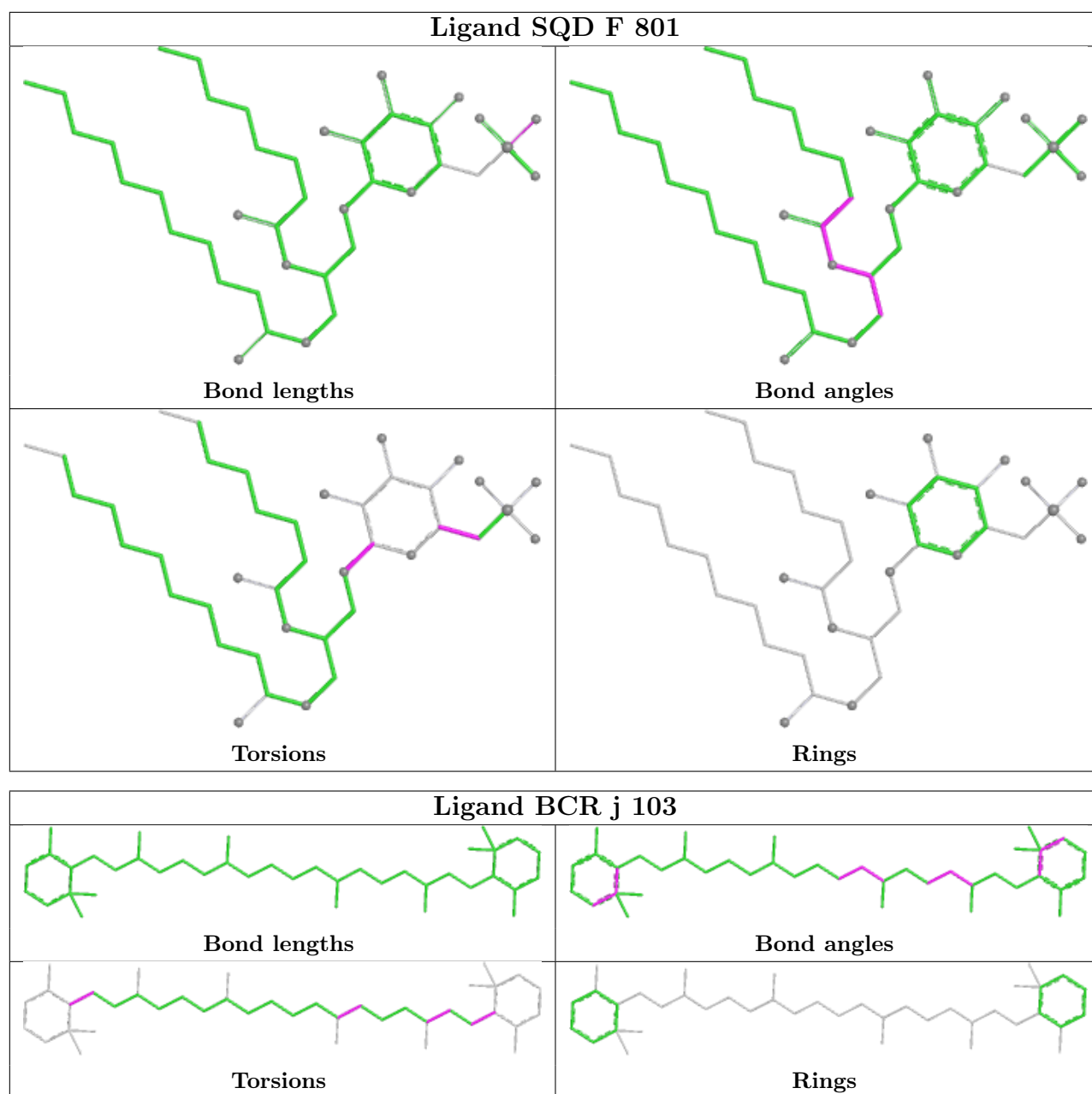


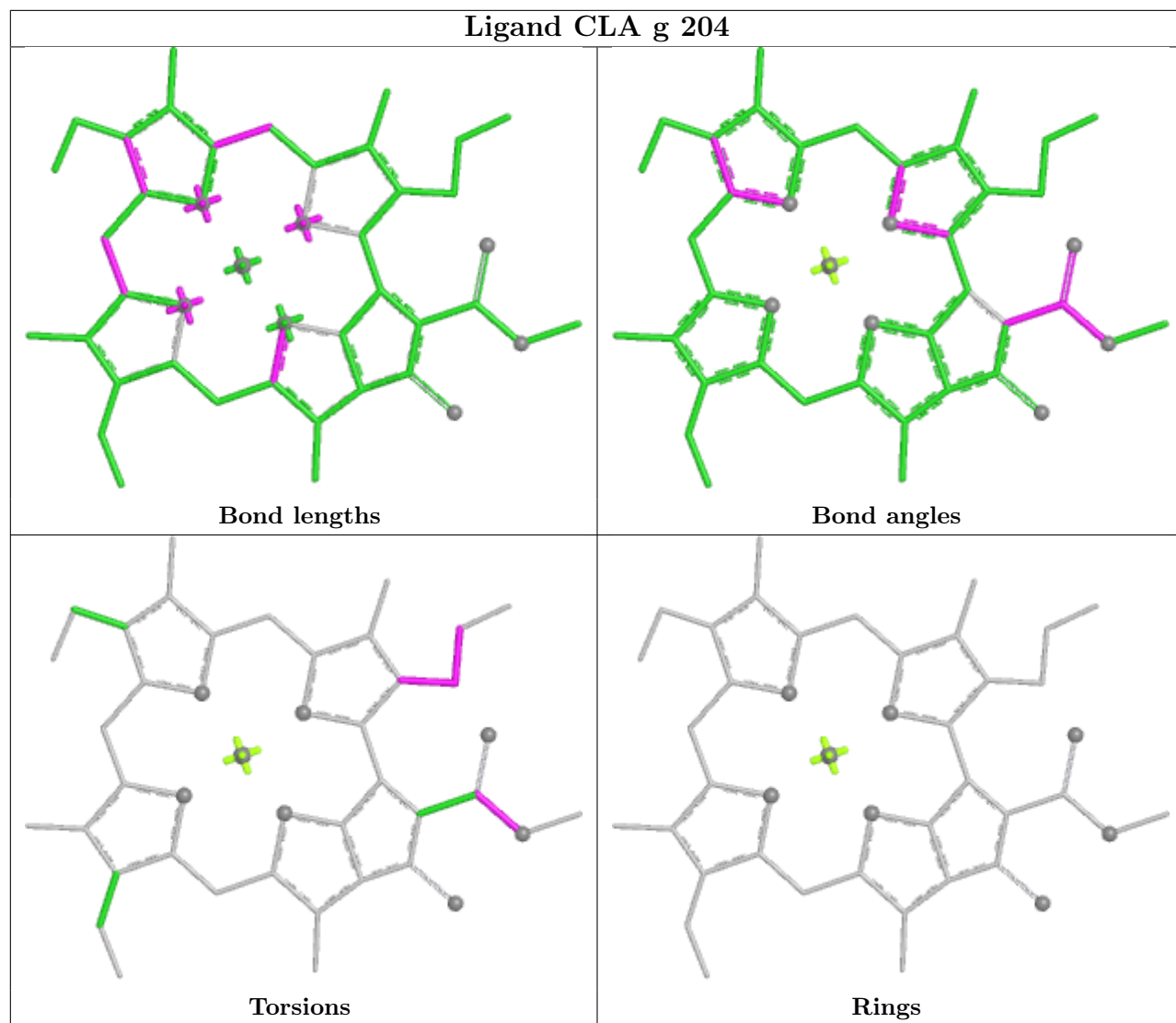
Torsions

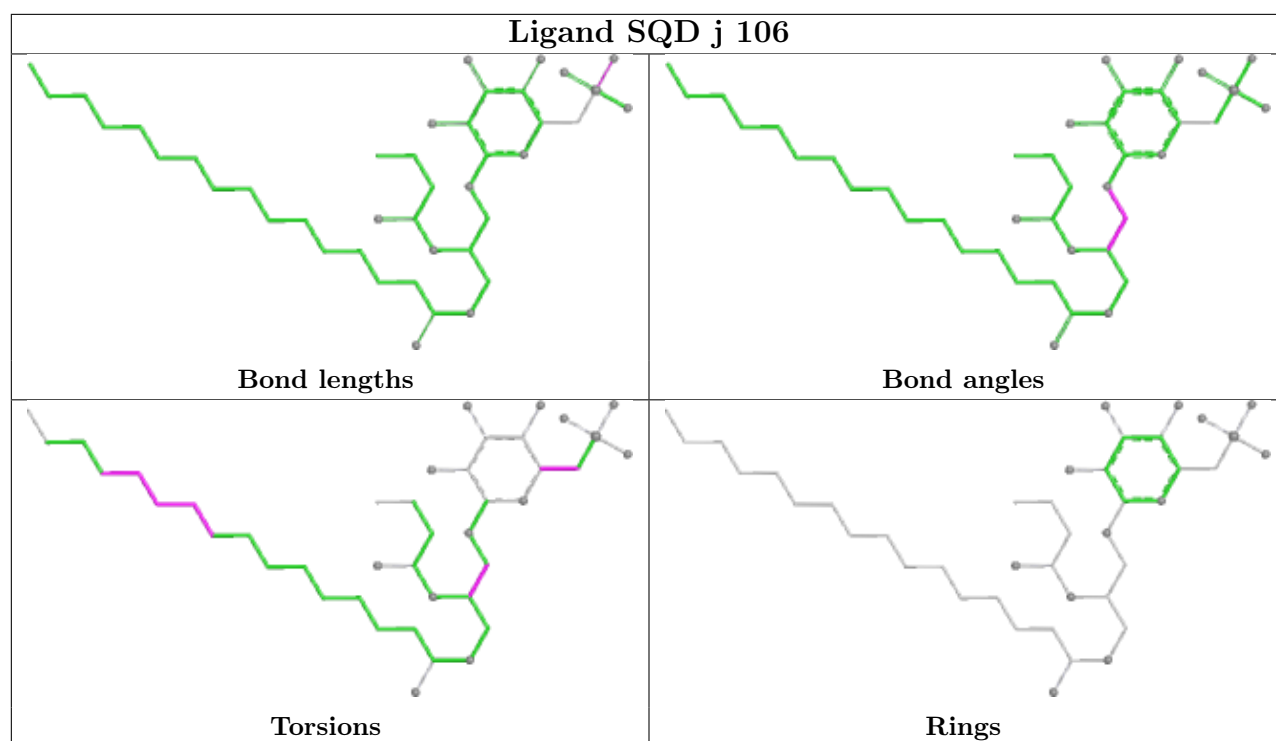


Rings

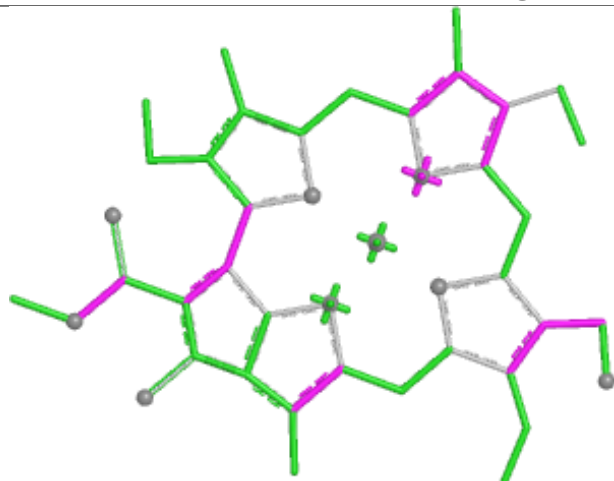




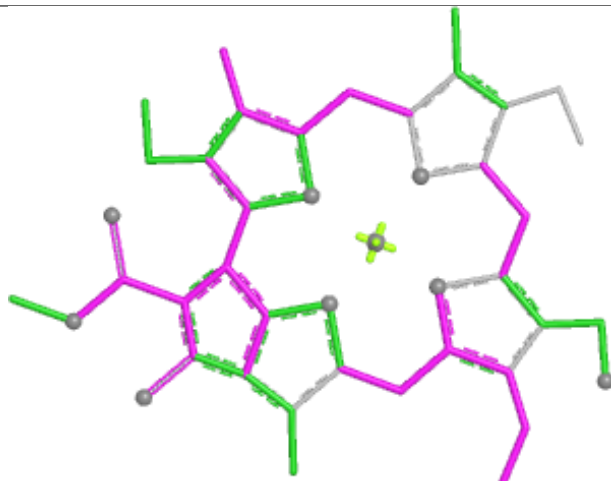




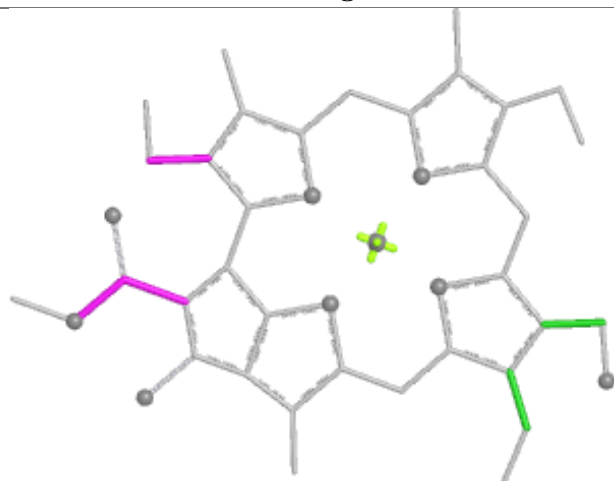
Ligand CHL w 309



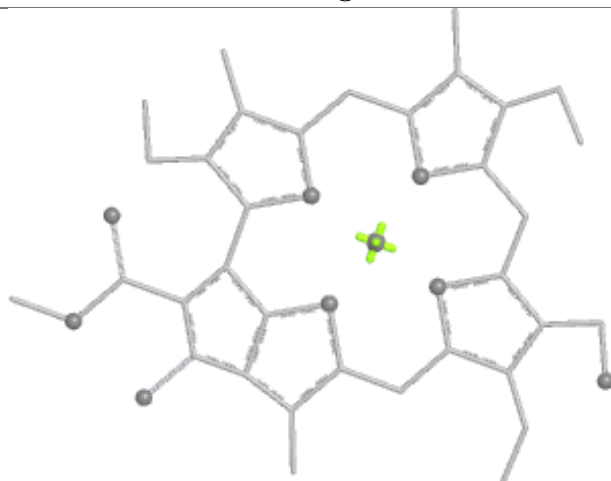
Bond lengths



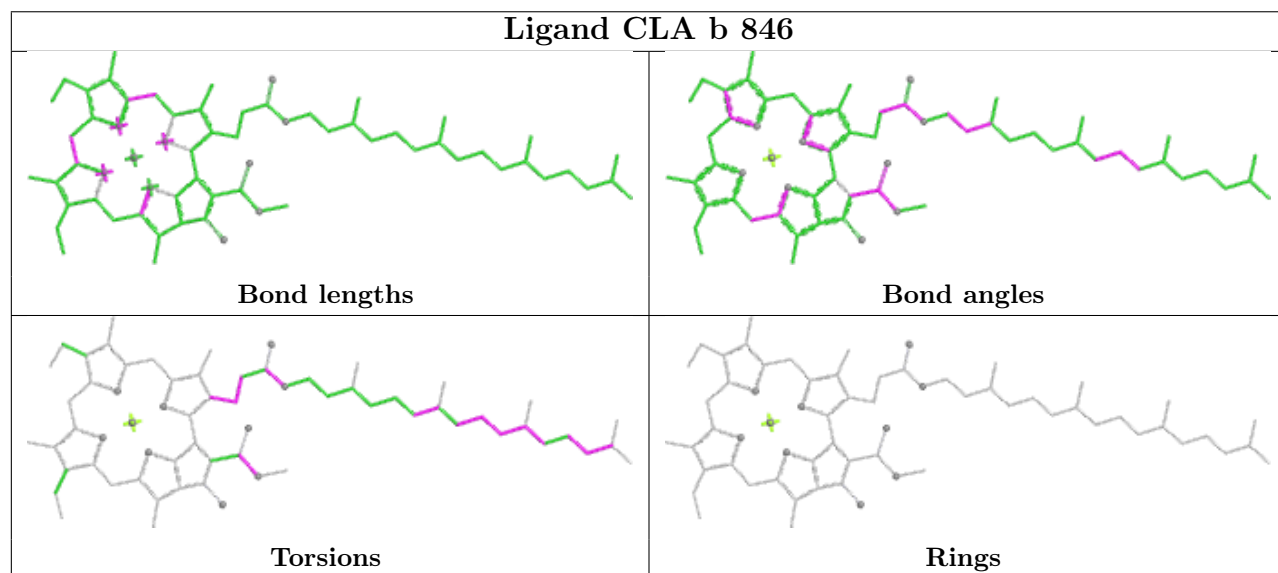
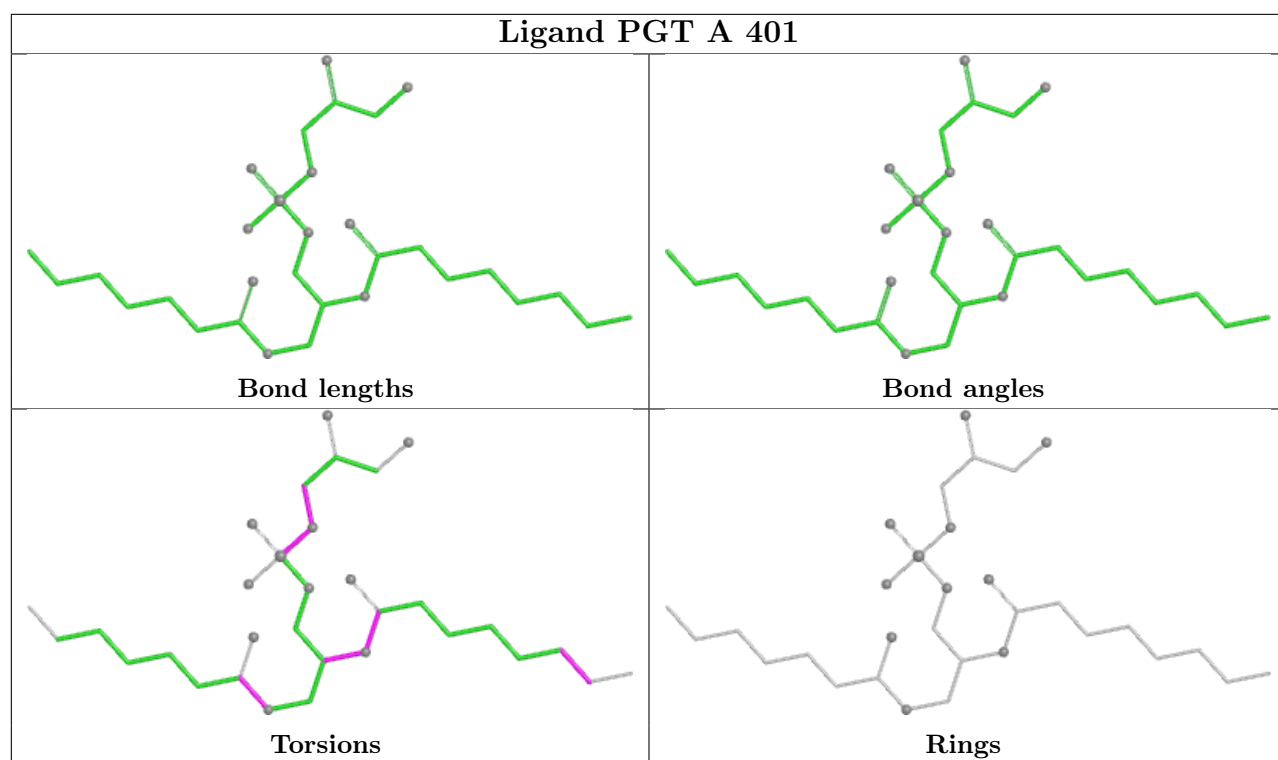
Bond angles



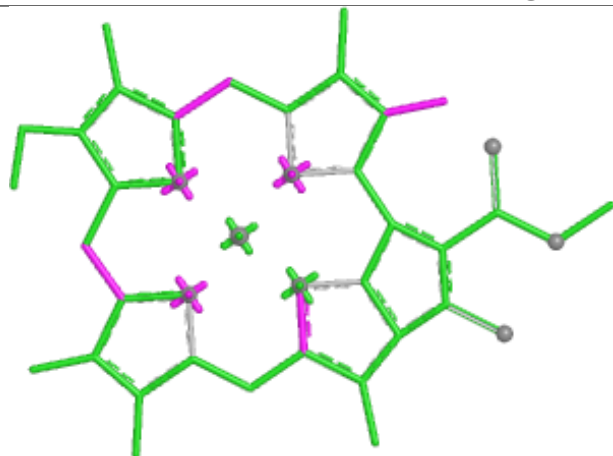
Torsions



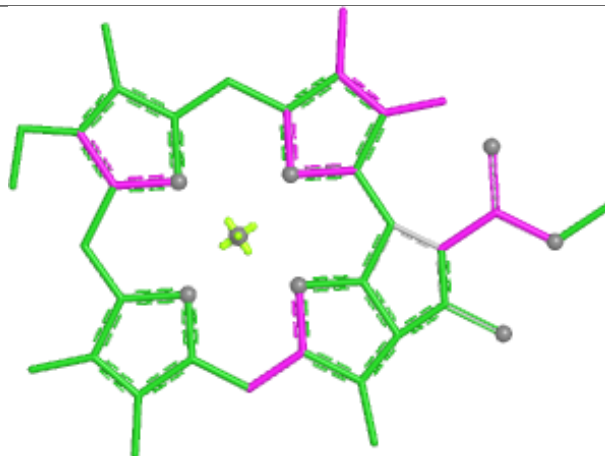
Rings



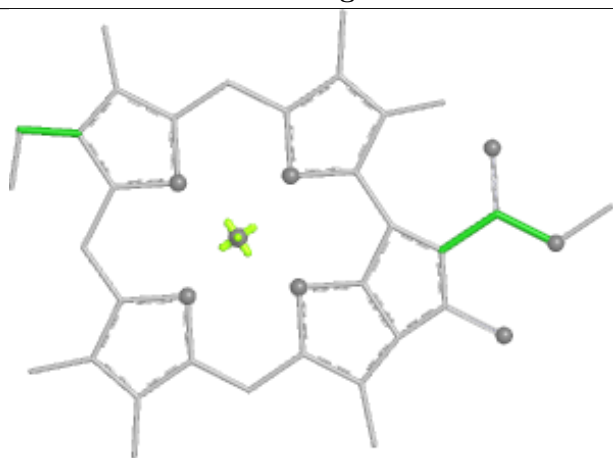
Ligand CLA 1 305



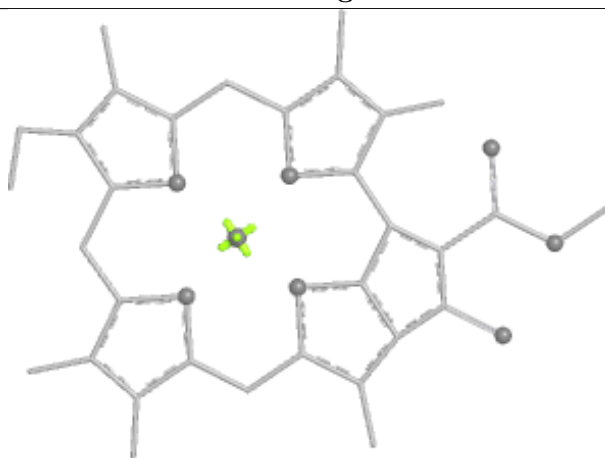
Bond lengths



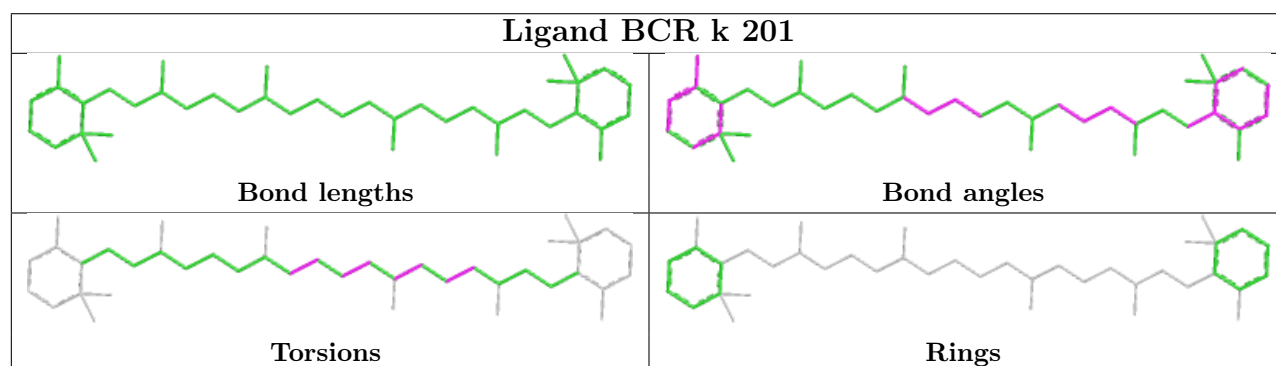
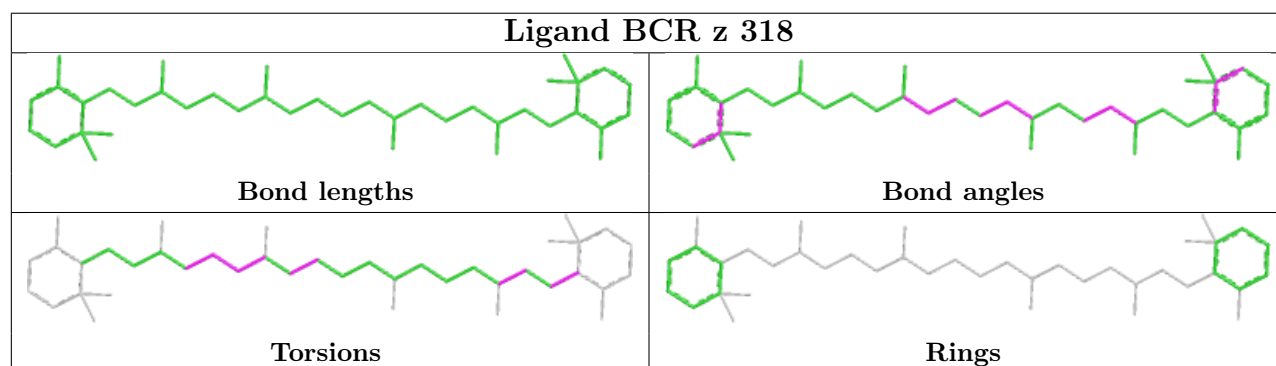
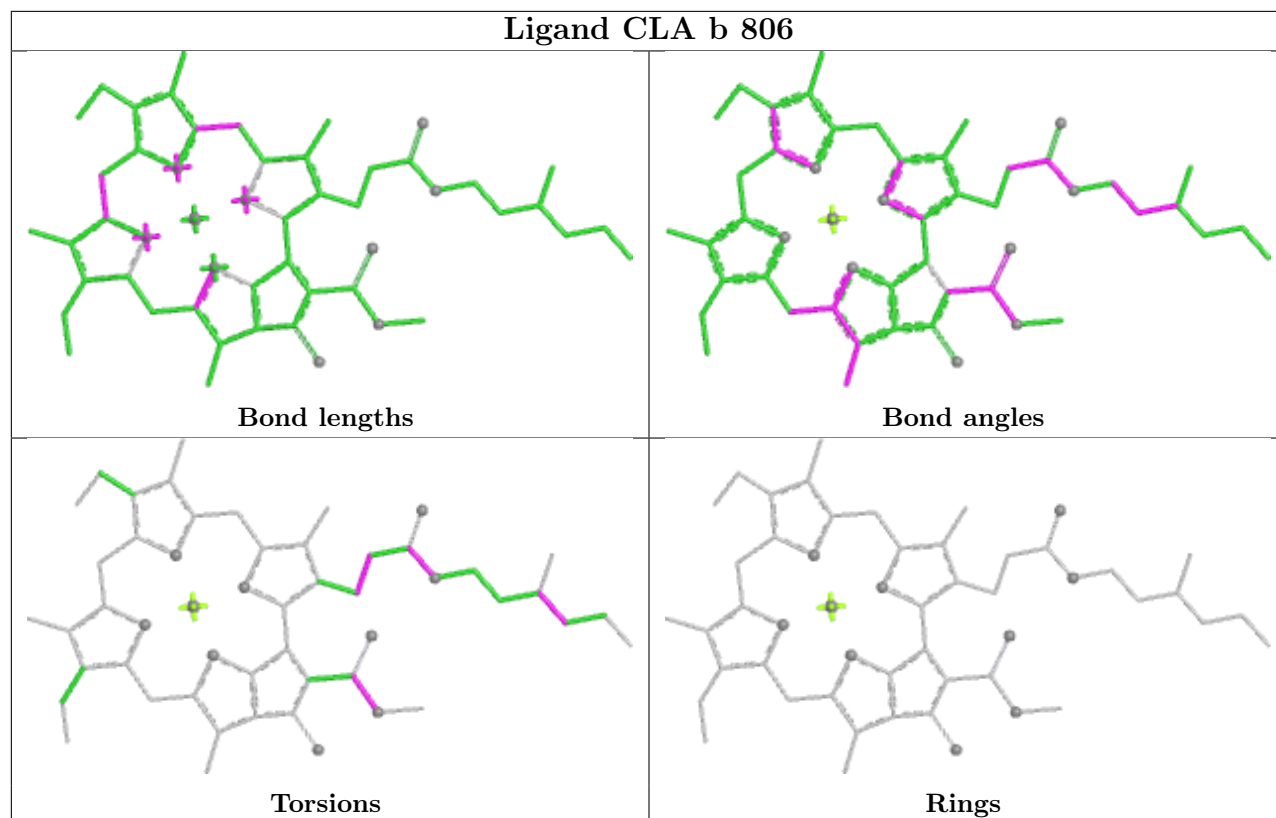
Bond angles

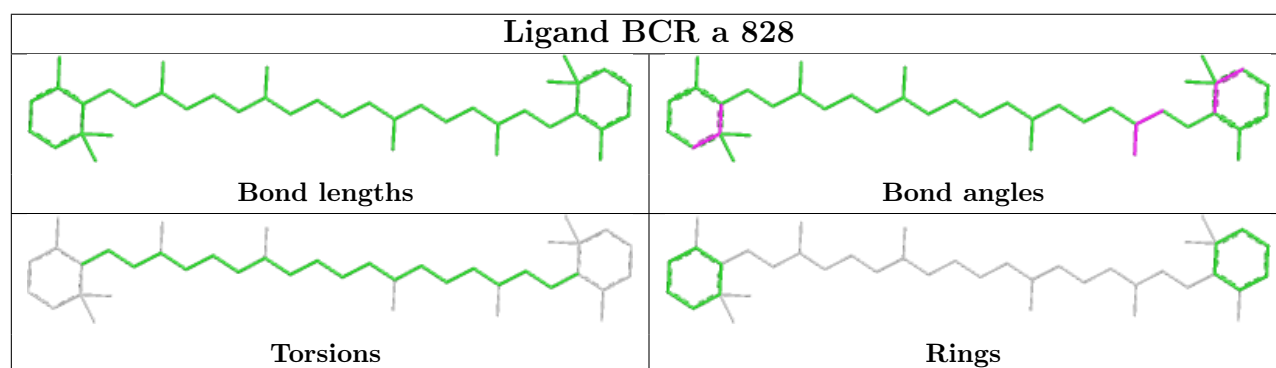
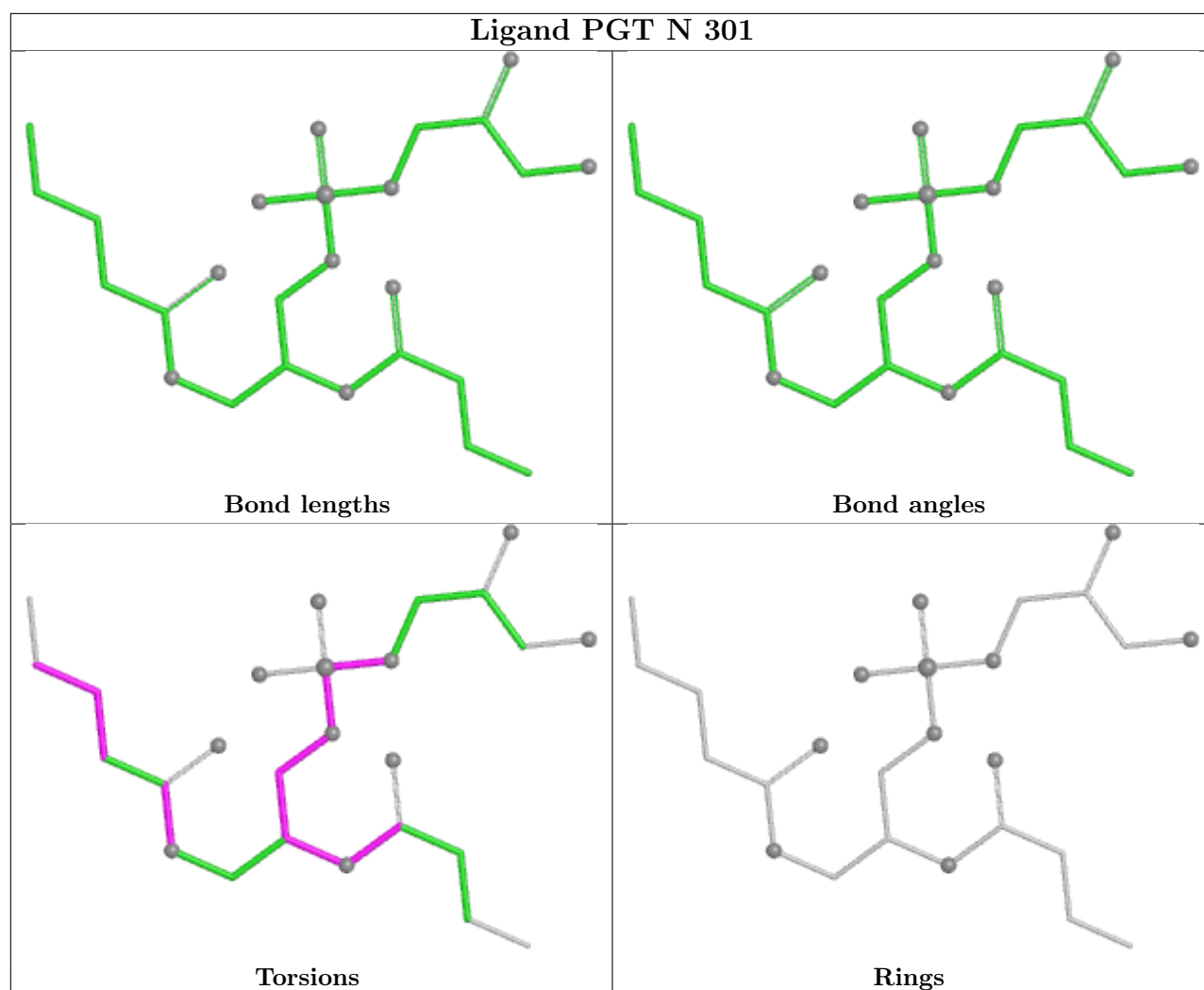


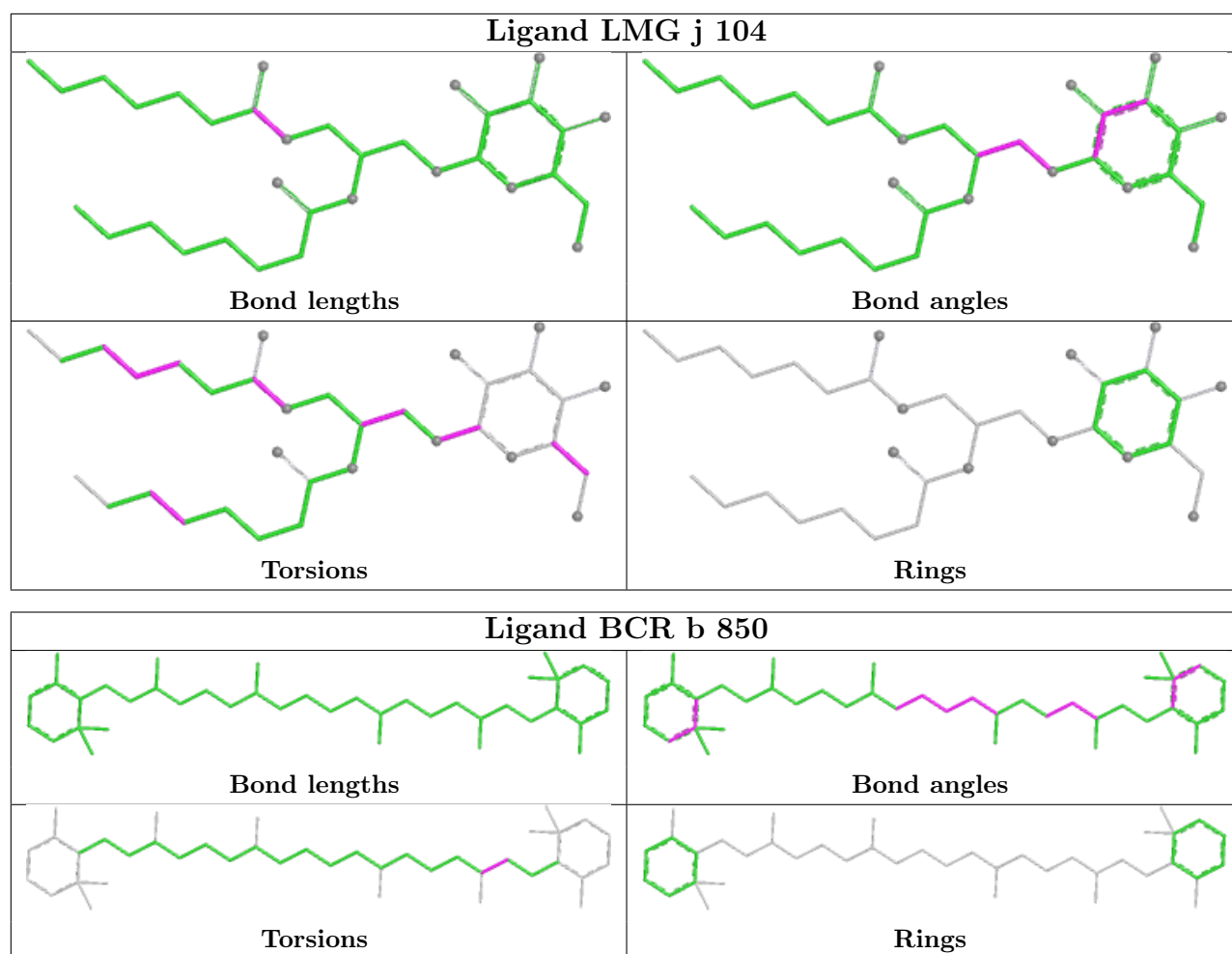
Torsions



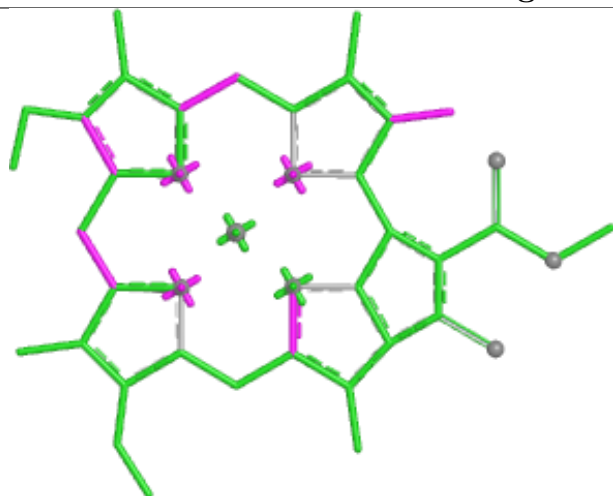
Rings



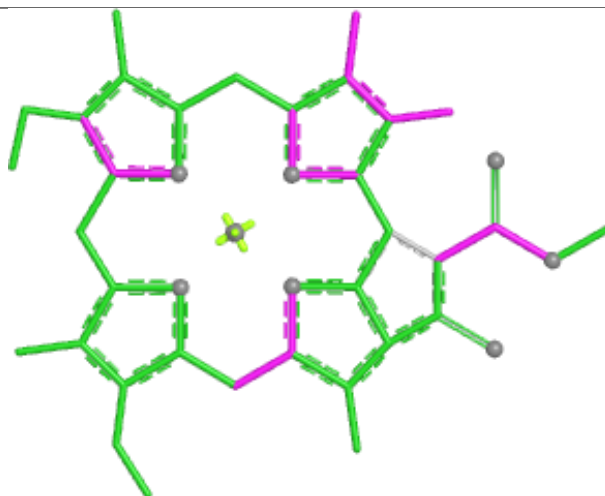




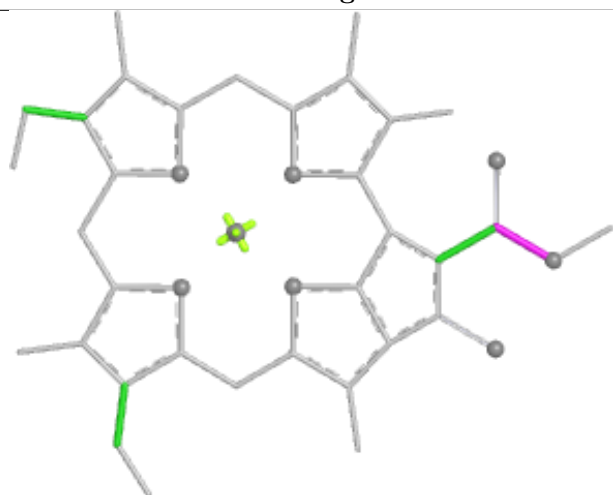
Ligand CLA k 203



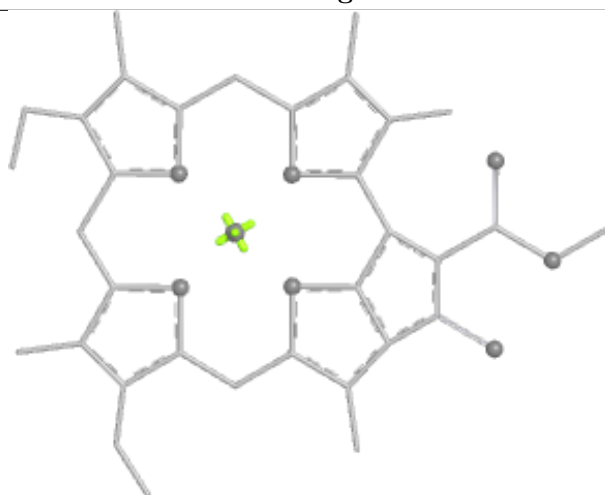
Bond lengths



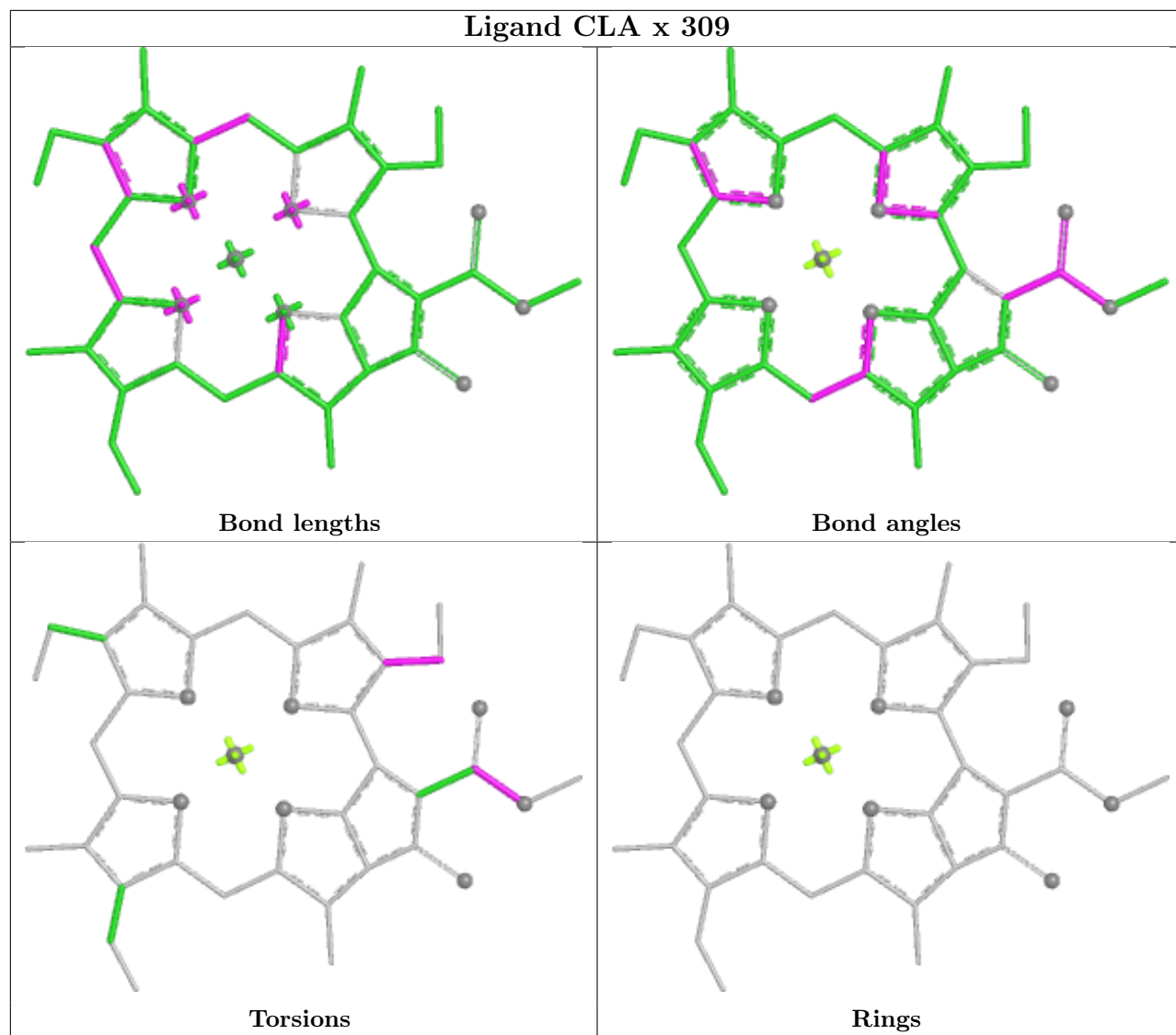
Bond angles



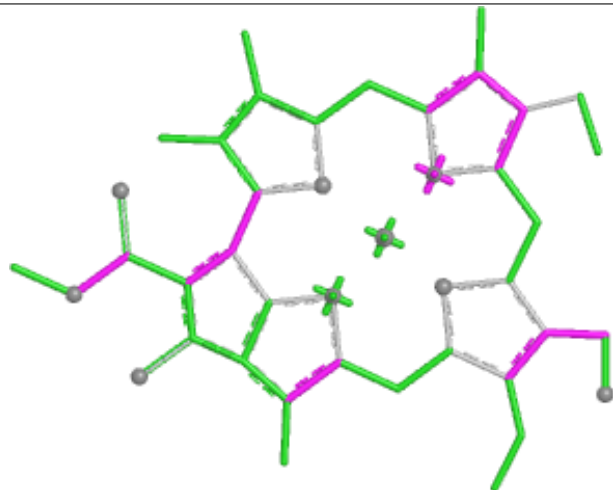
Torsions



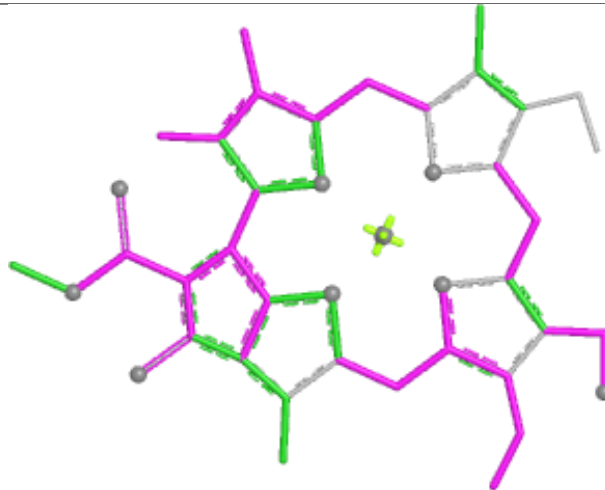
Rings



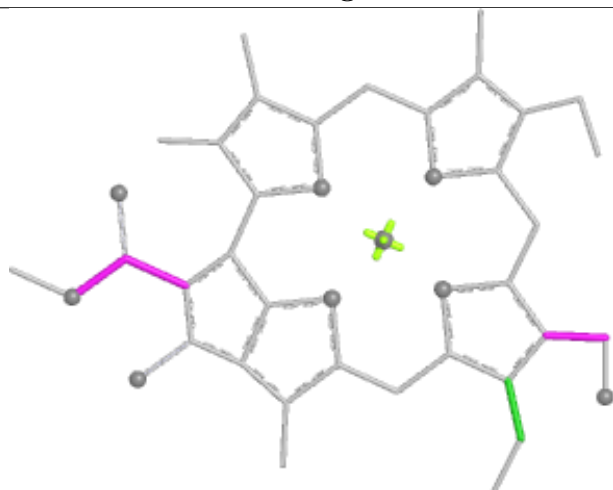
Ligand CHL z 304



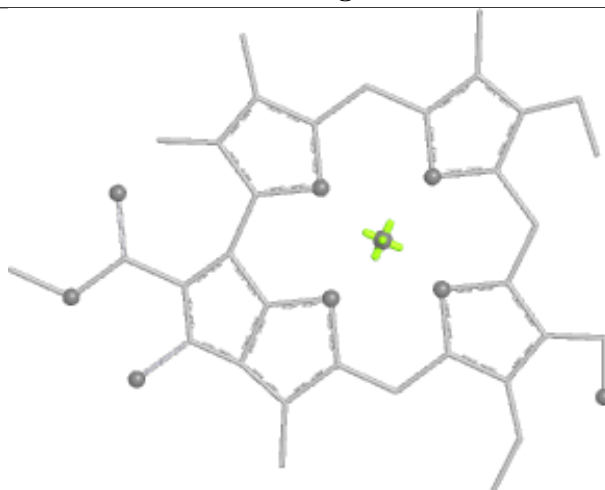
Bond lengths



Bond angles

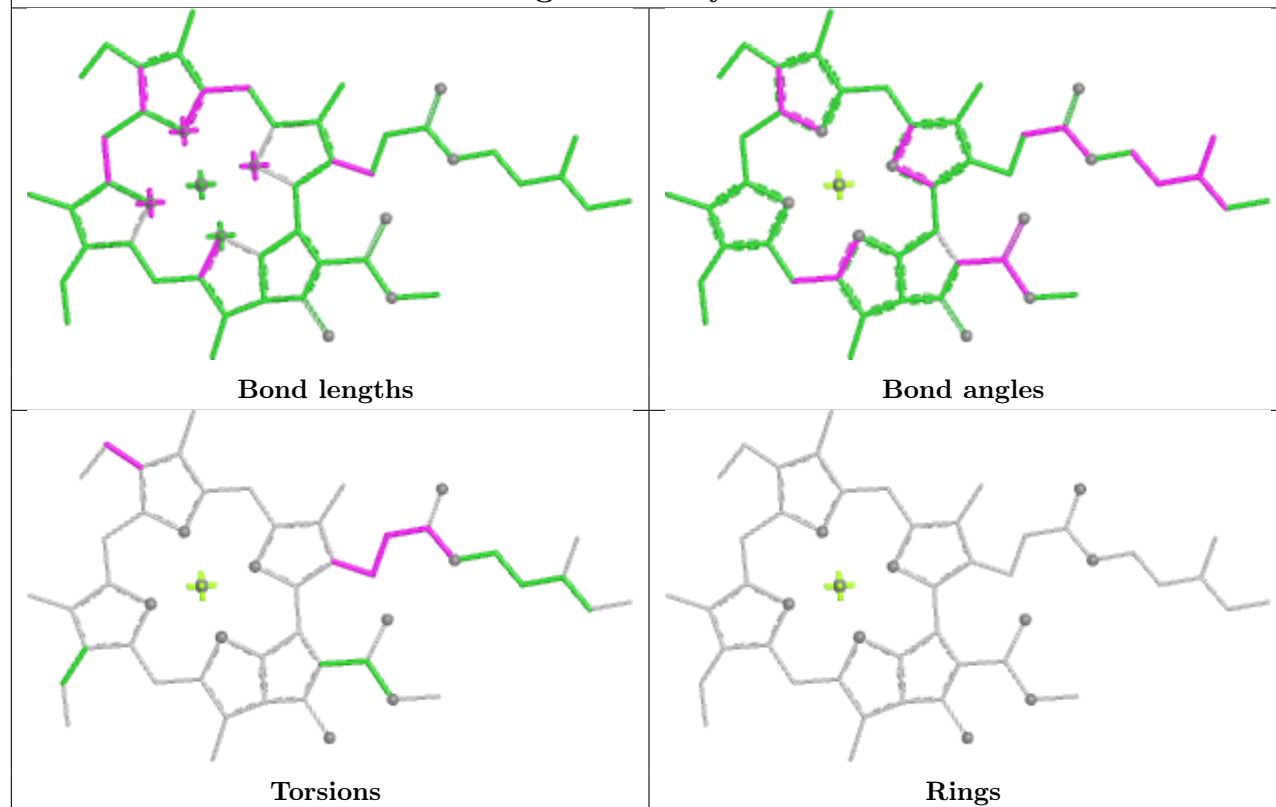


Torsions

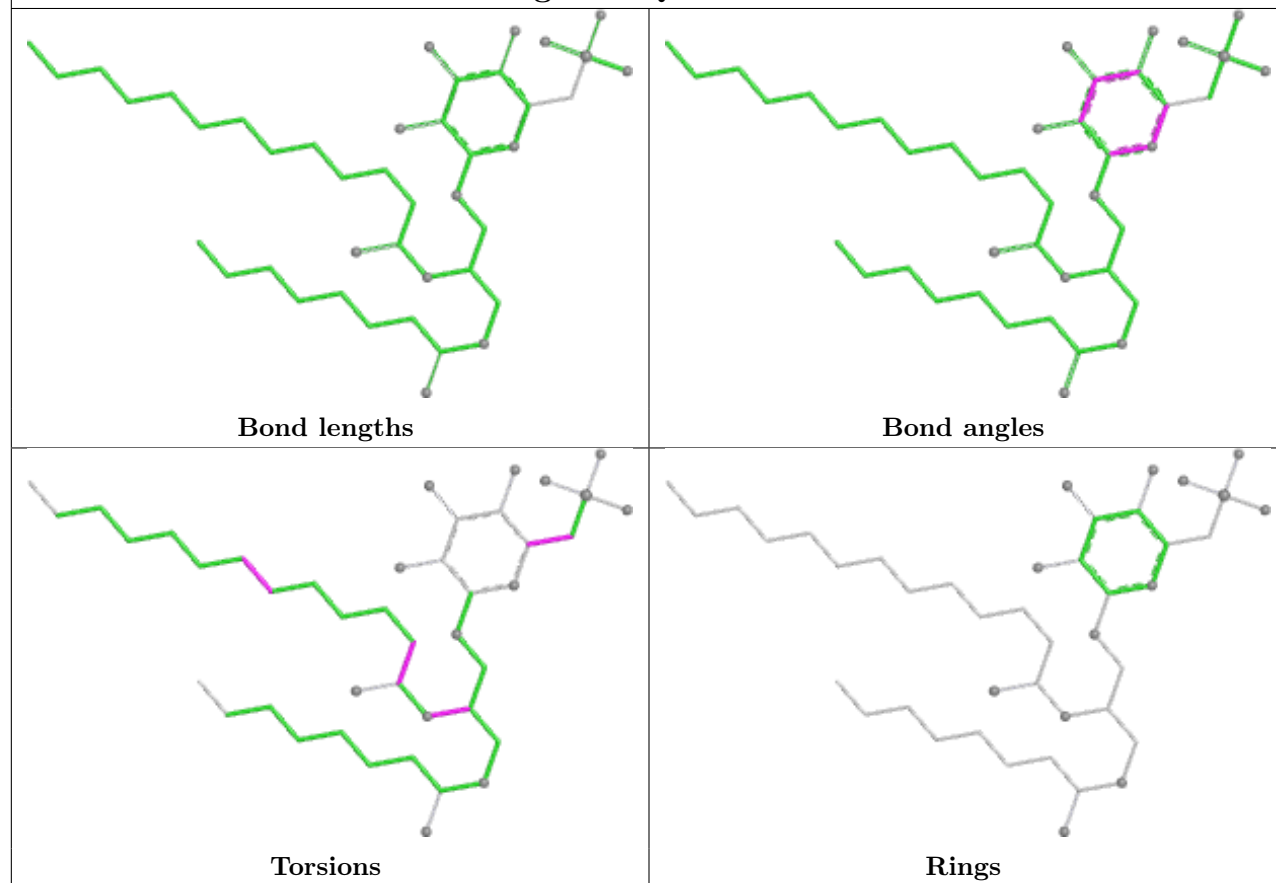


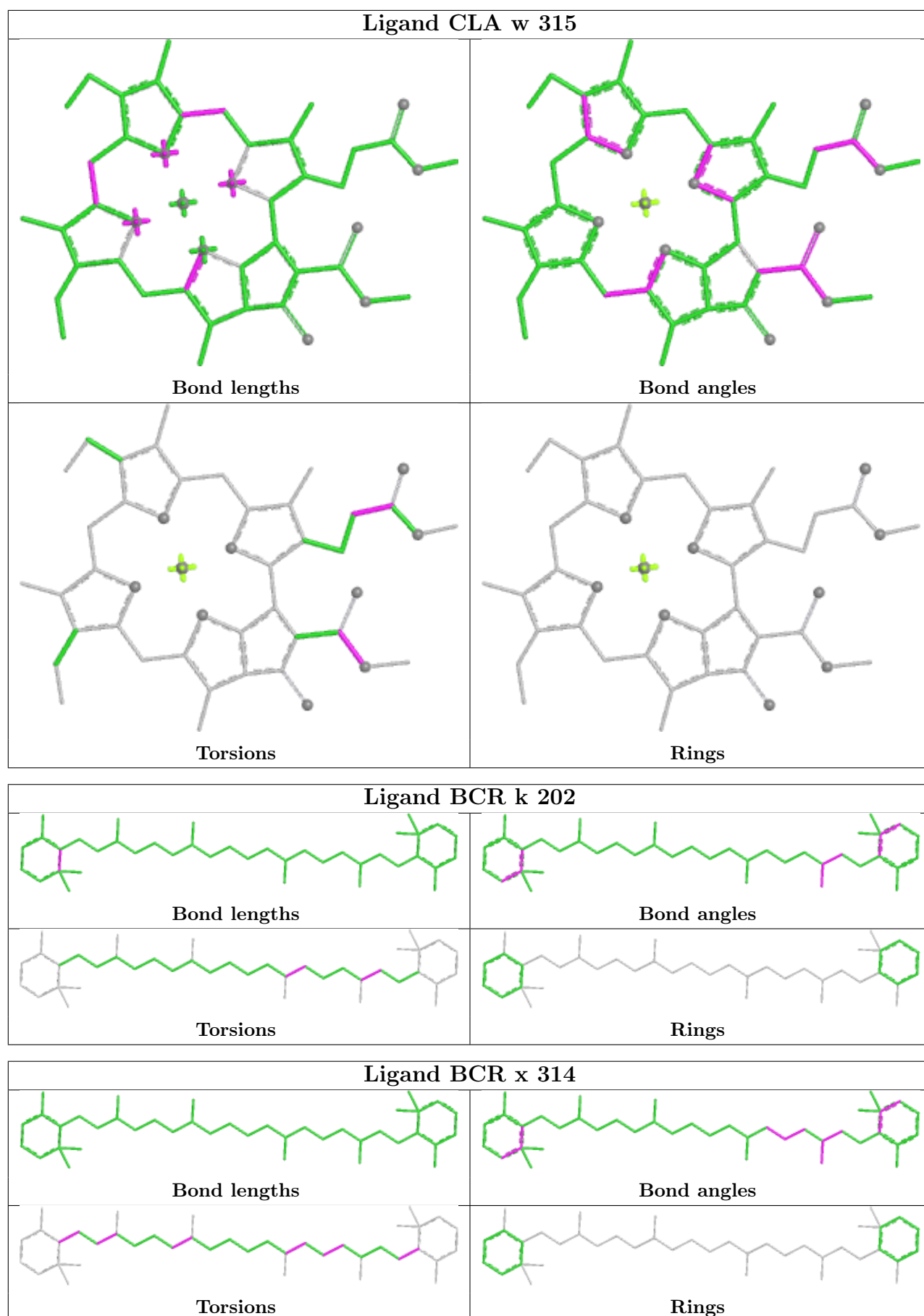
Rings

Ligand CLA y 311

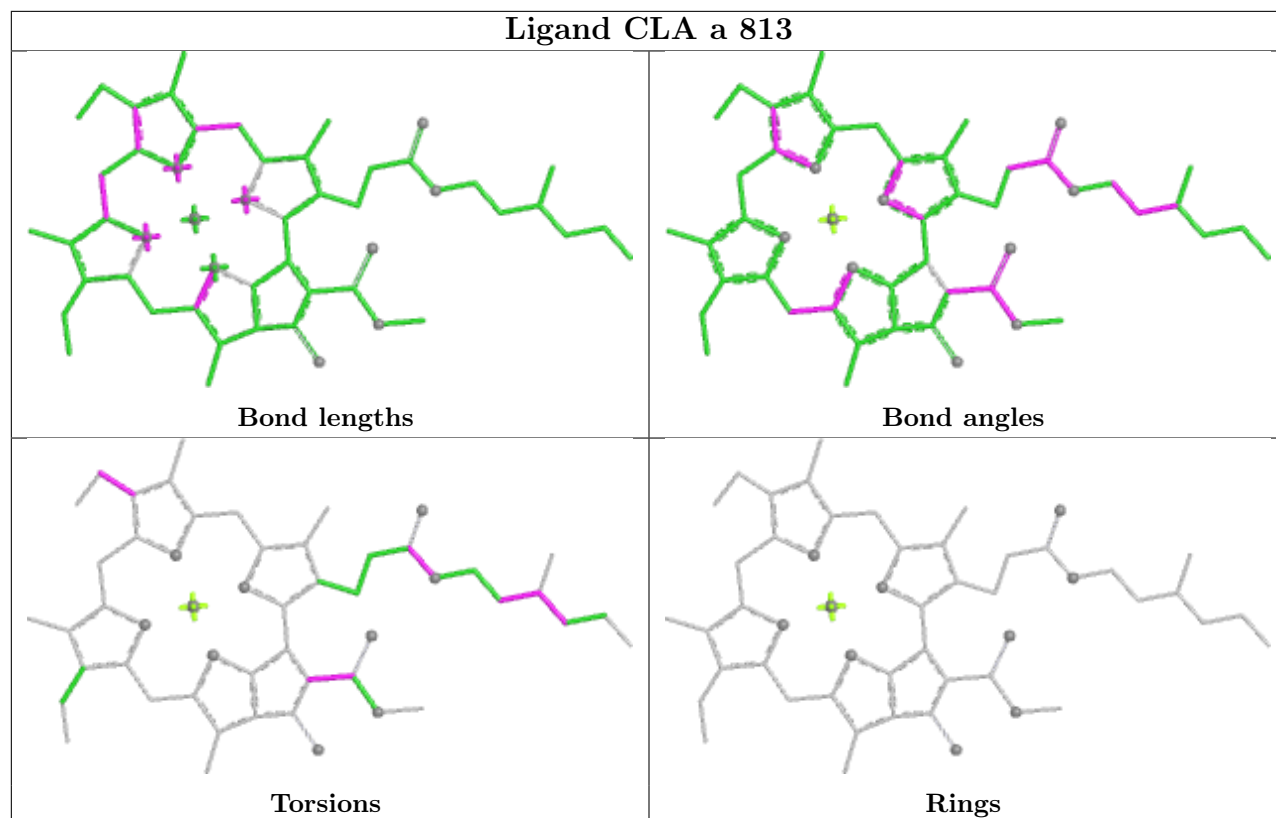


Ligand SQD F 805

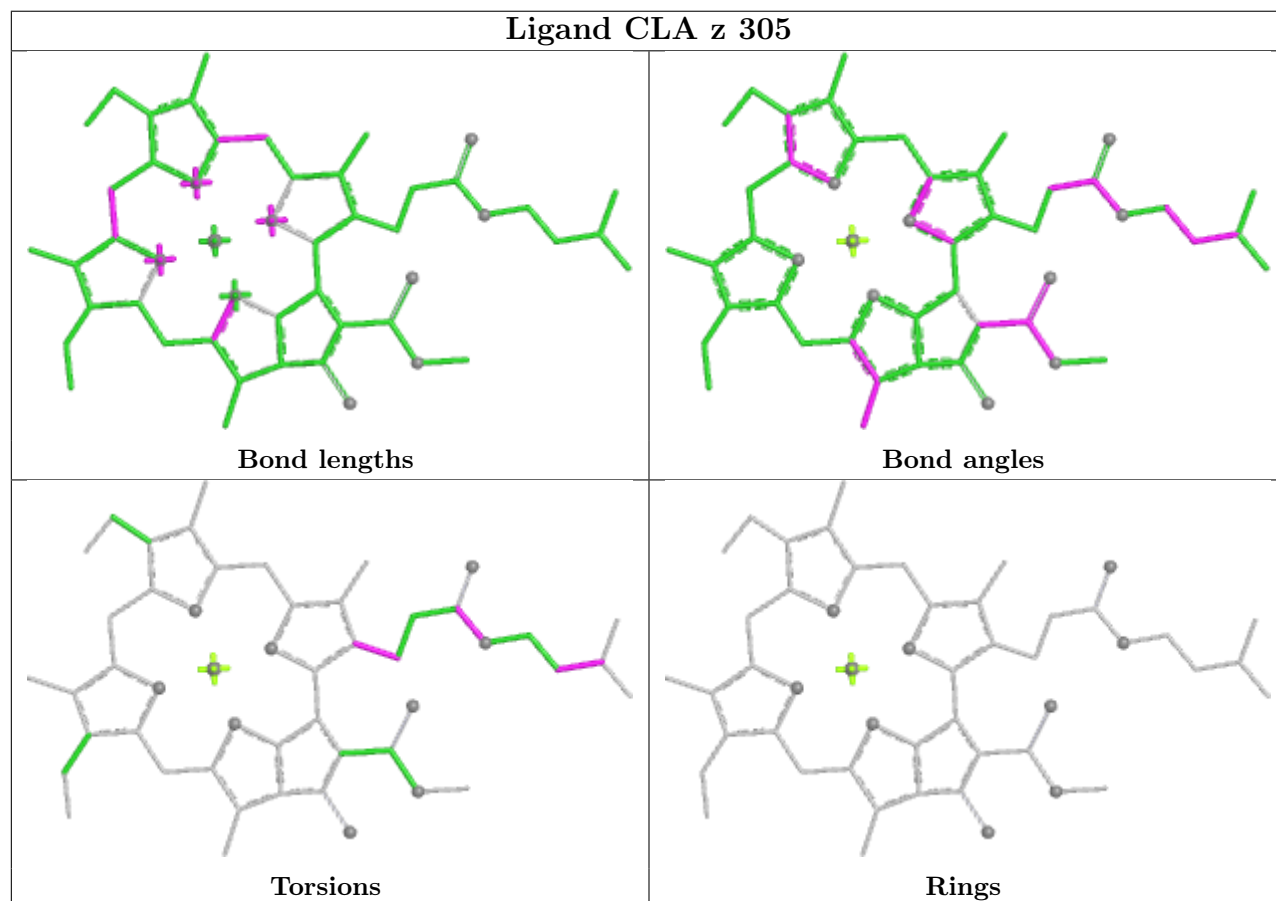


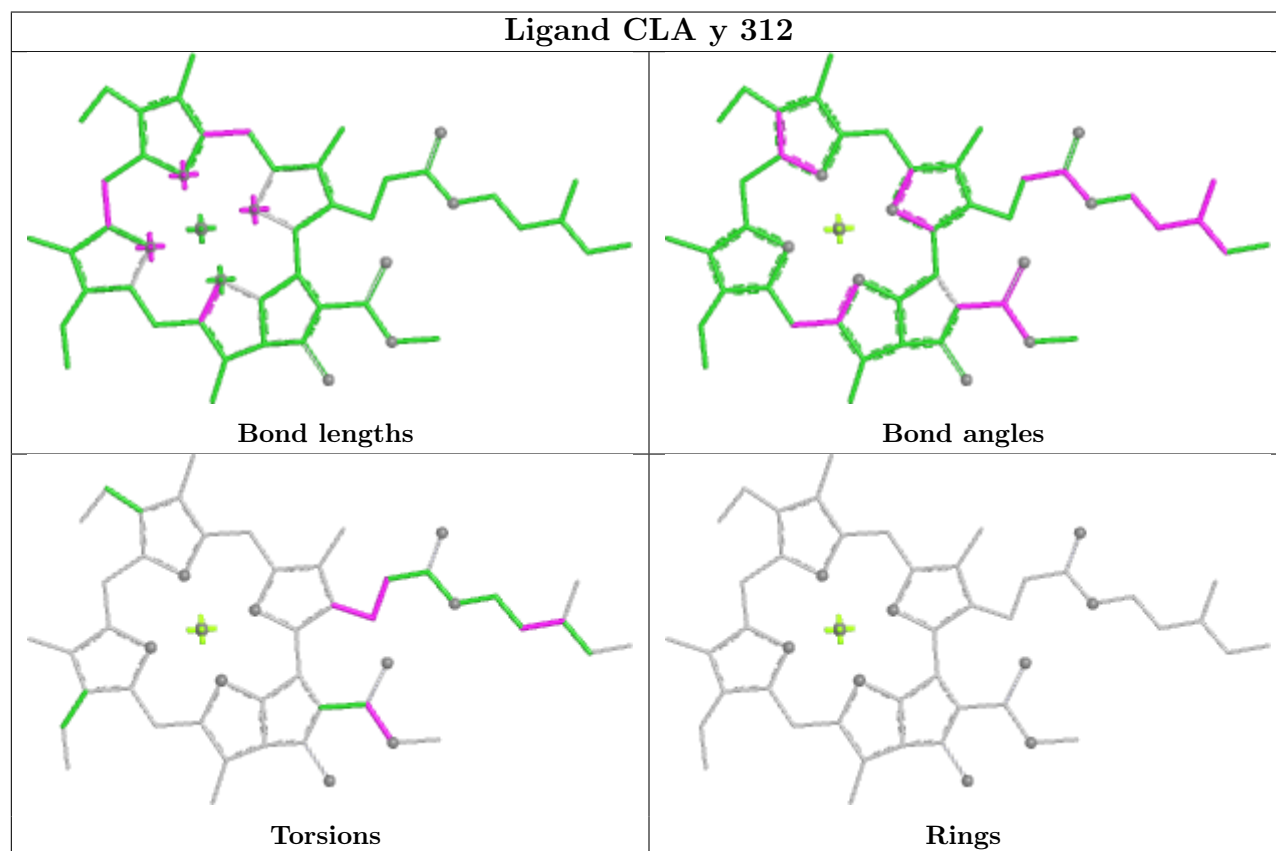
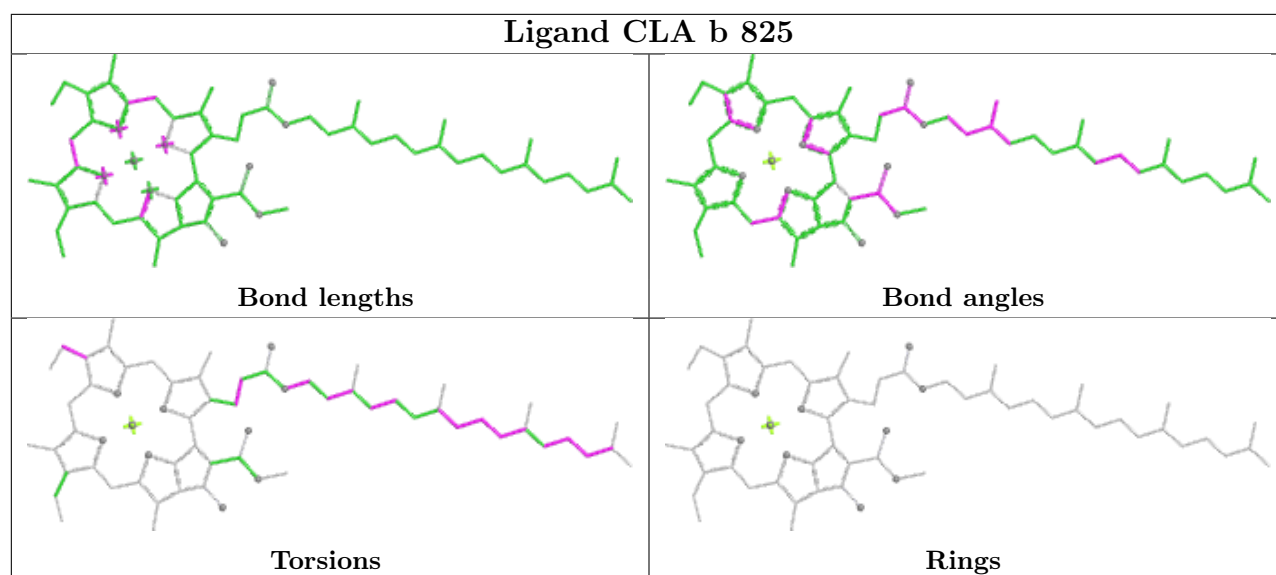


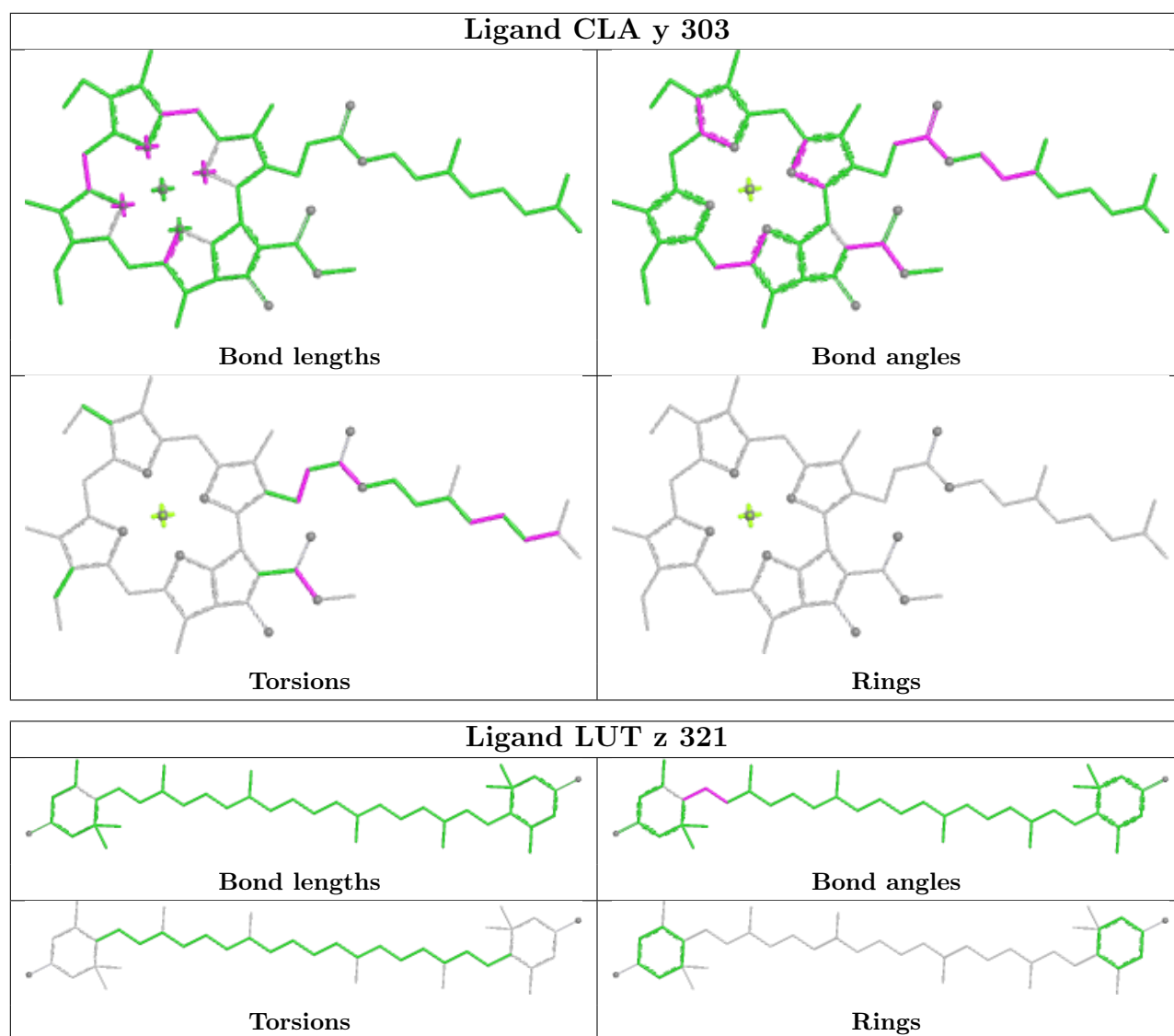
Ligand CLA a 813



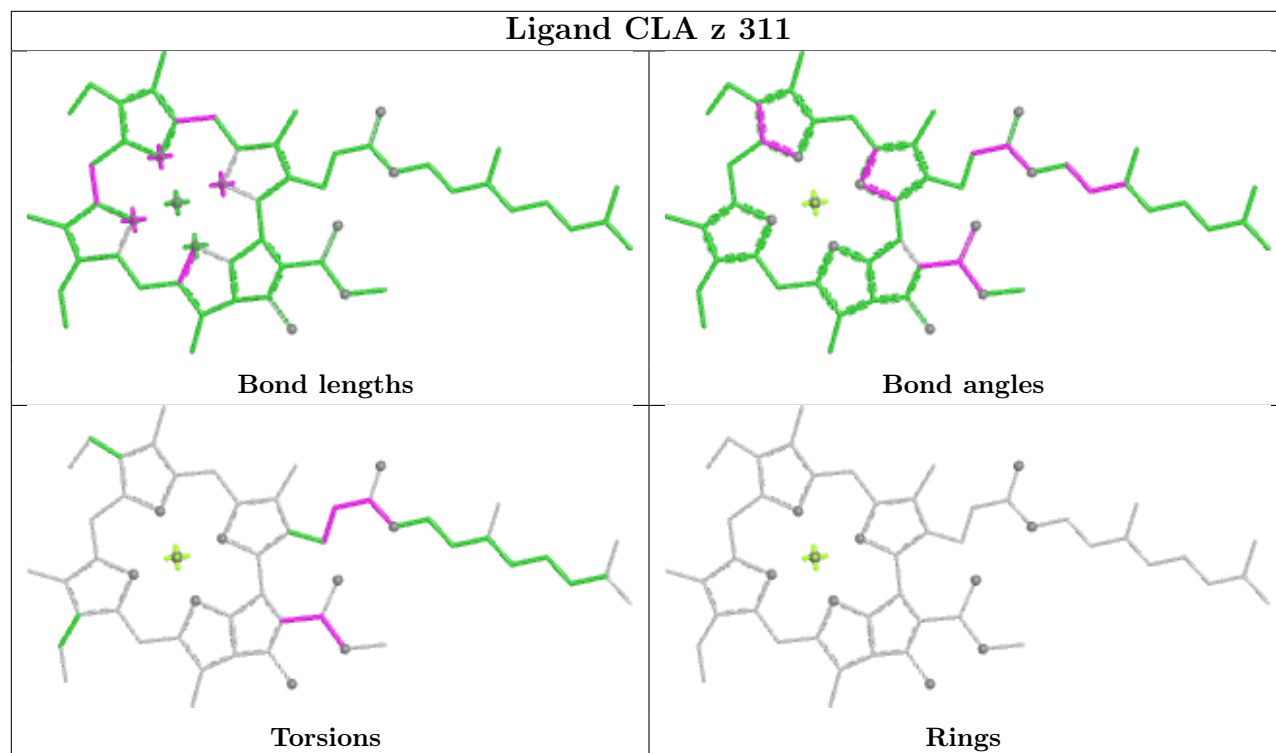
Ligand CLA z 305



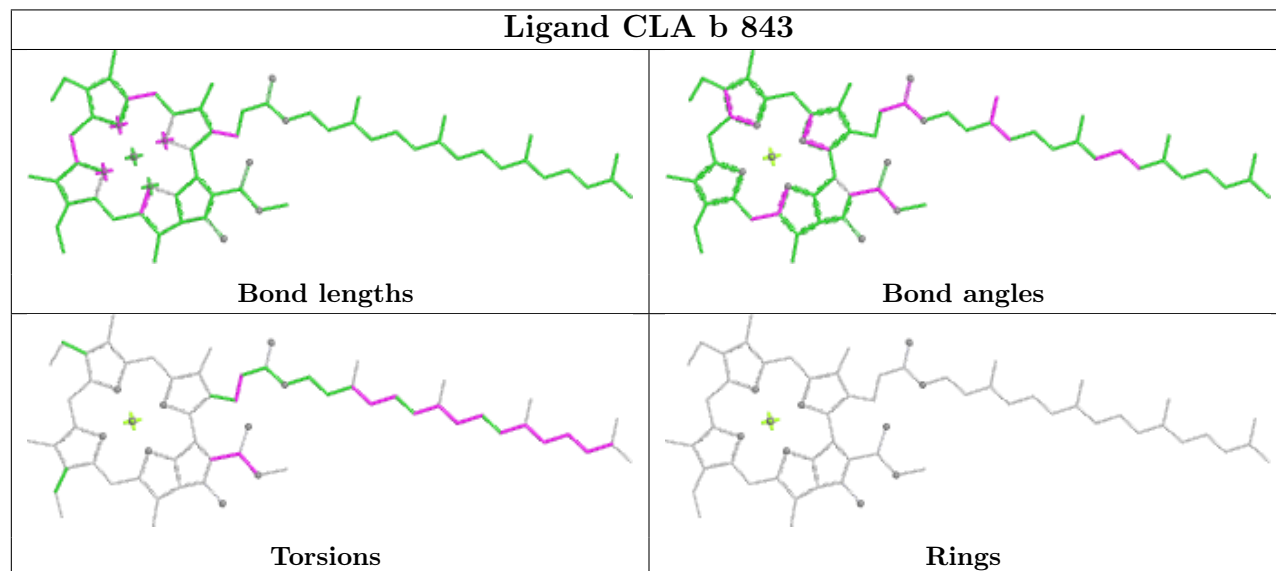


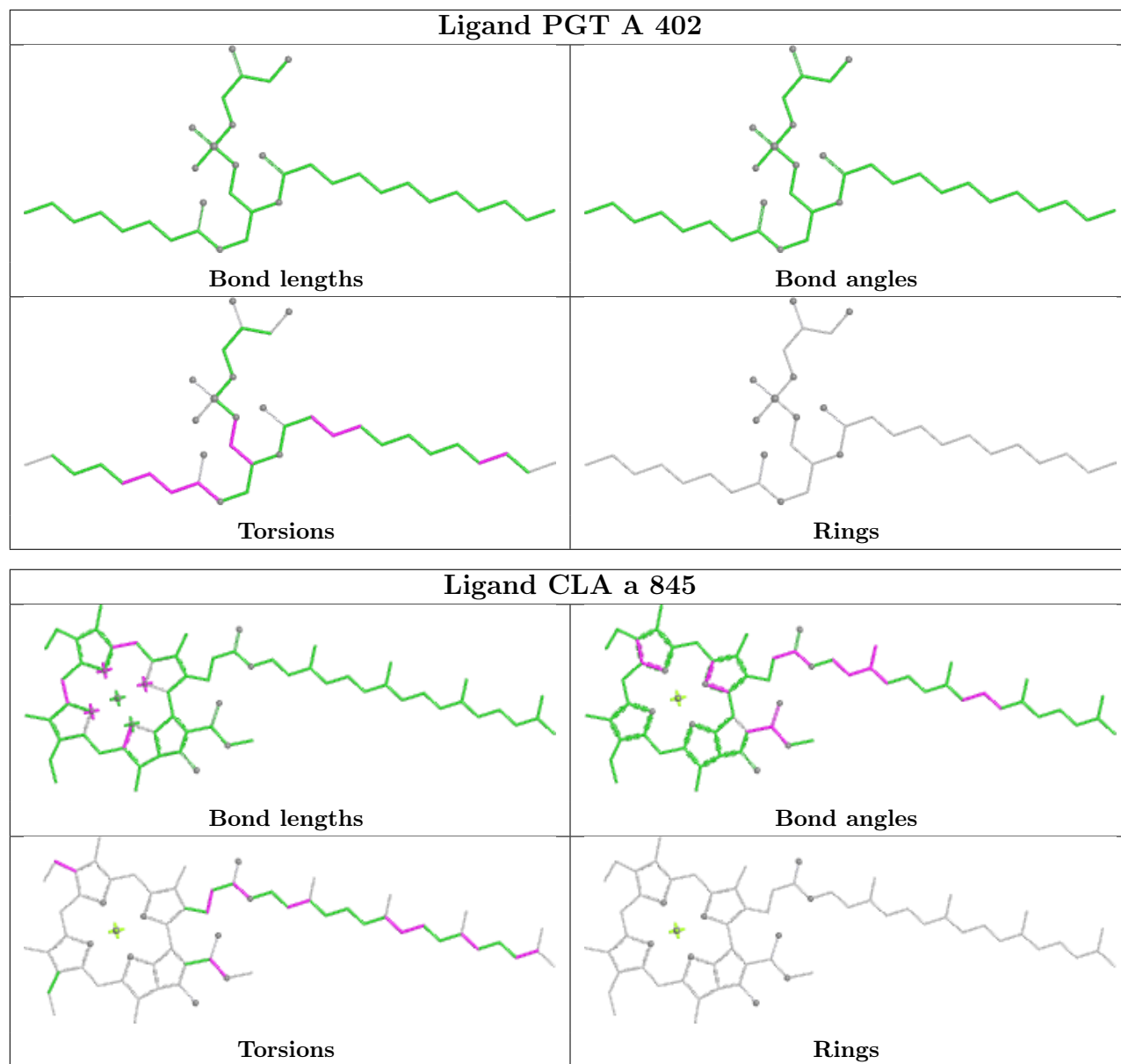


Ligand CLA z 311

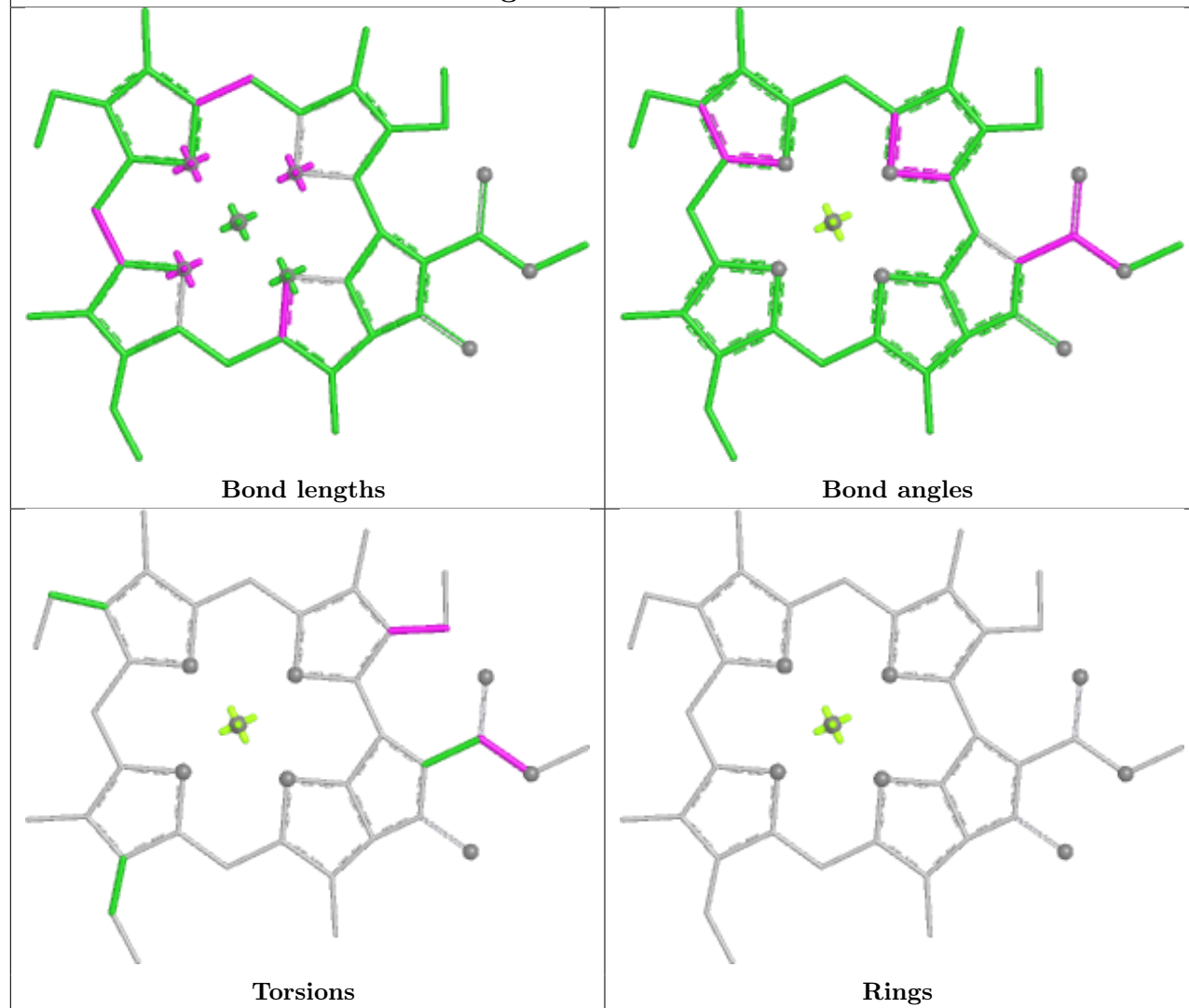


Ligand CLA b 843

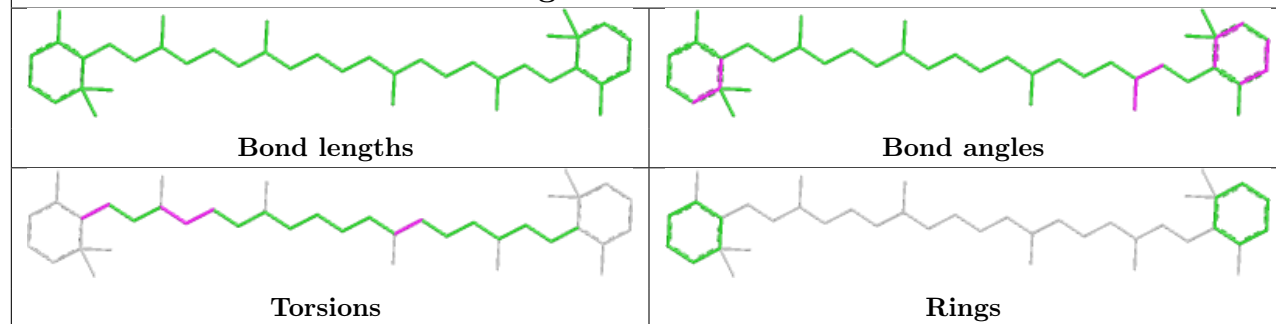


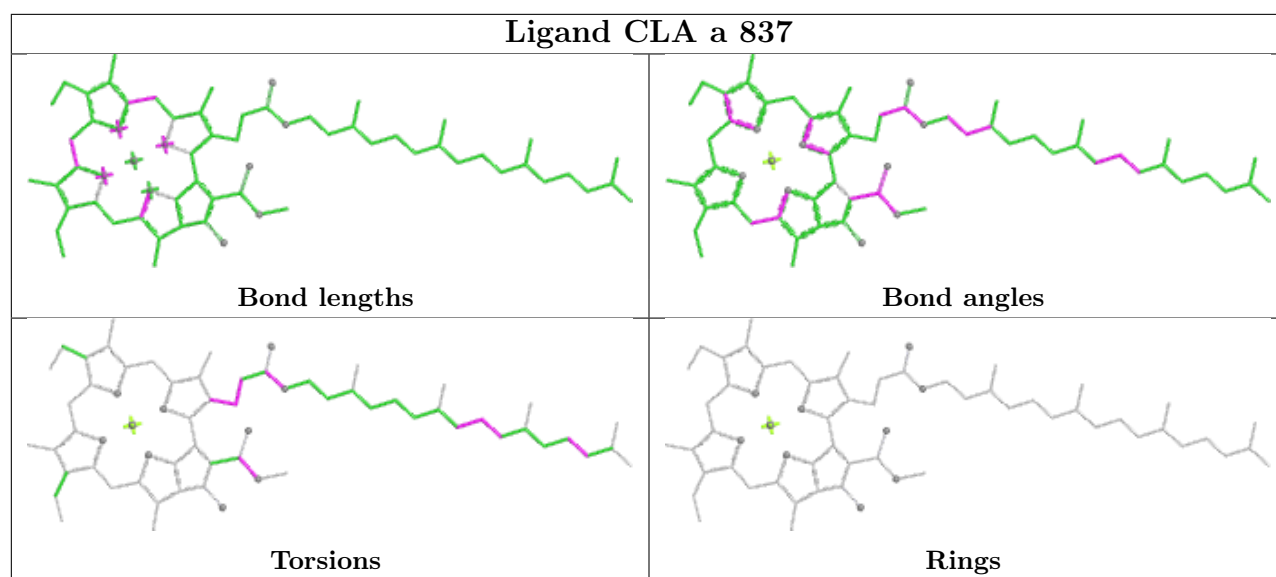


Ligand CLA z 319



Ligand BCR 1 304





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.

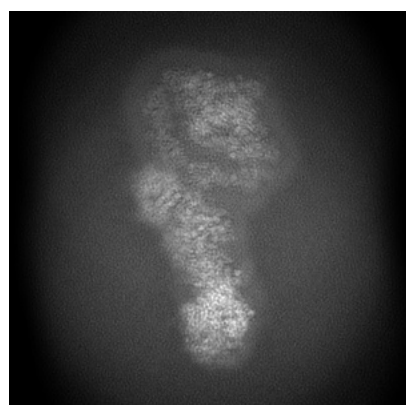
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51527. These allow visual inspection of the internal detail of the map and identification of artifacts.

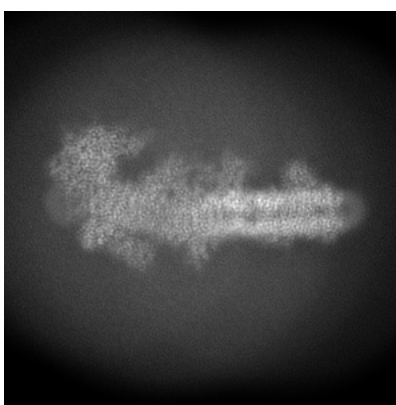
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

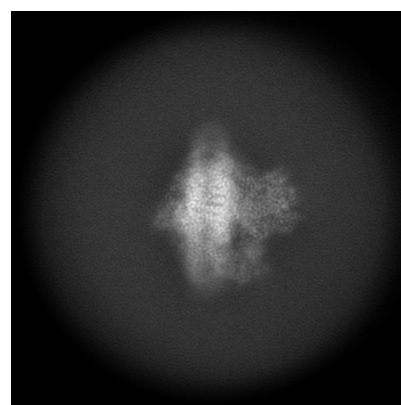
6.1.1 Primary map



X



Y

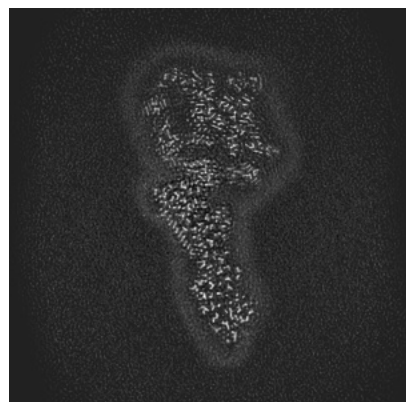


Z

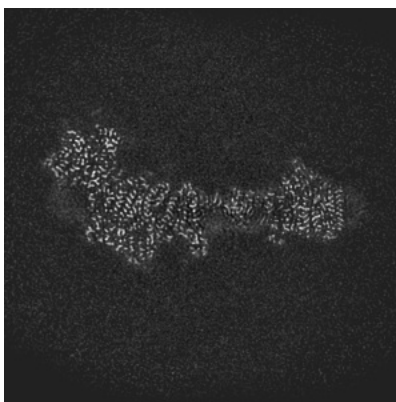
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

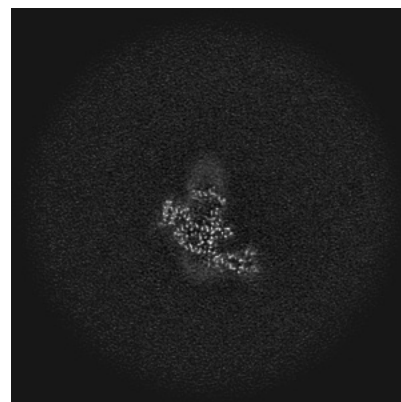
6.2.1 Primary map



X Index: 256



Y Index: 256

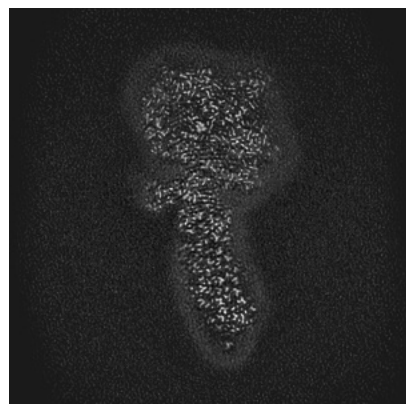


Z Index: 256

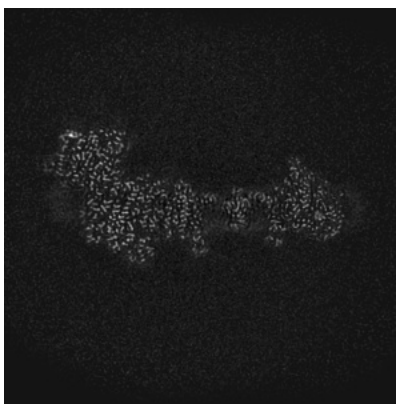
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

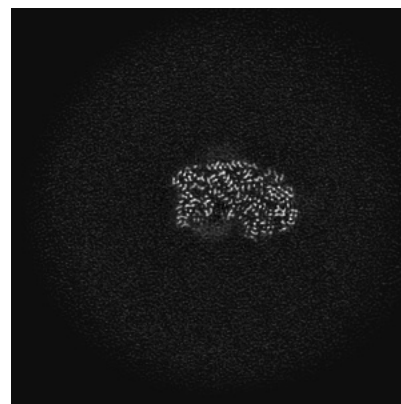
6.3.1 Primary map



X Index: 265



Y Index: 260

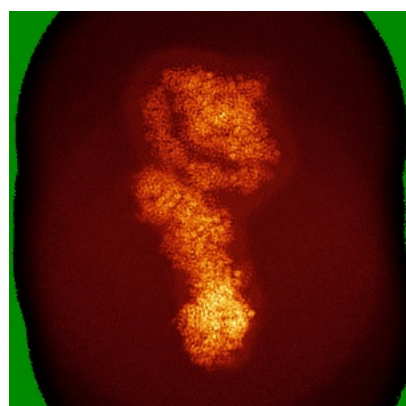


Z Index: 125

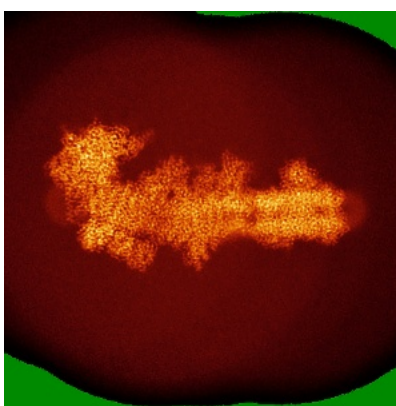
The images above show the largest variance slices of the map in three orthogonal directions.

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

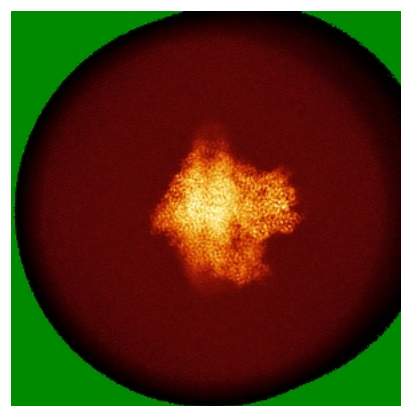
6.4.1 Primary map



X



Y

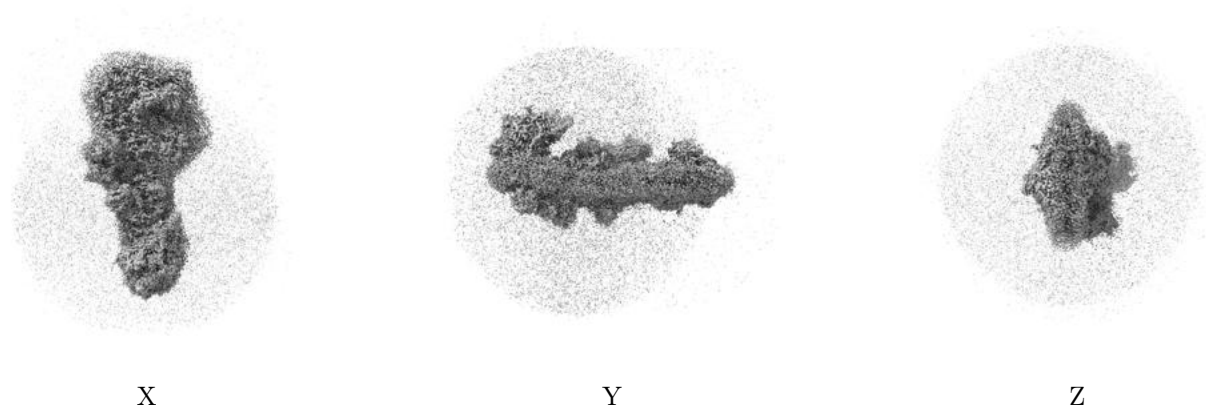


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

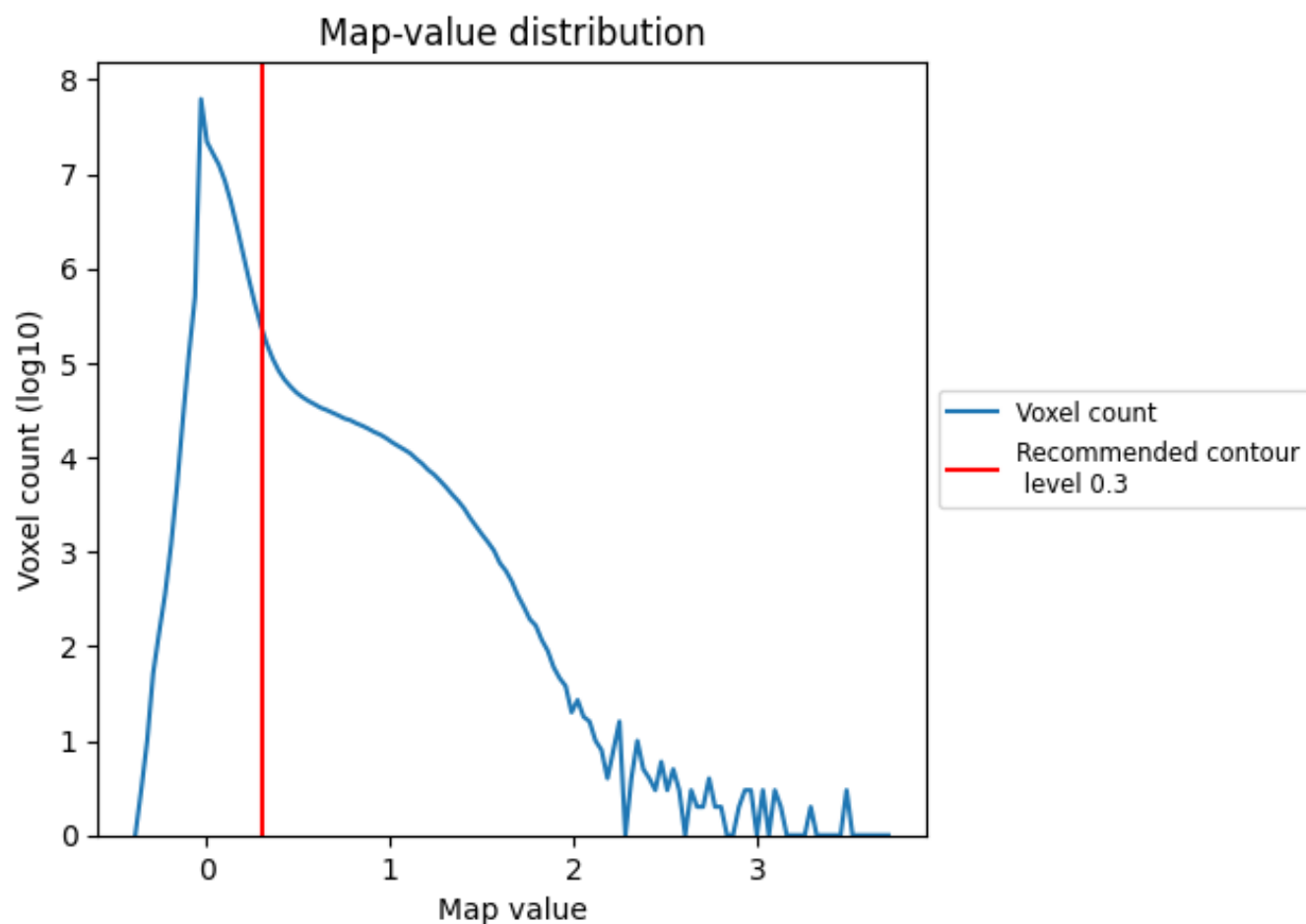
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

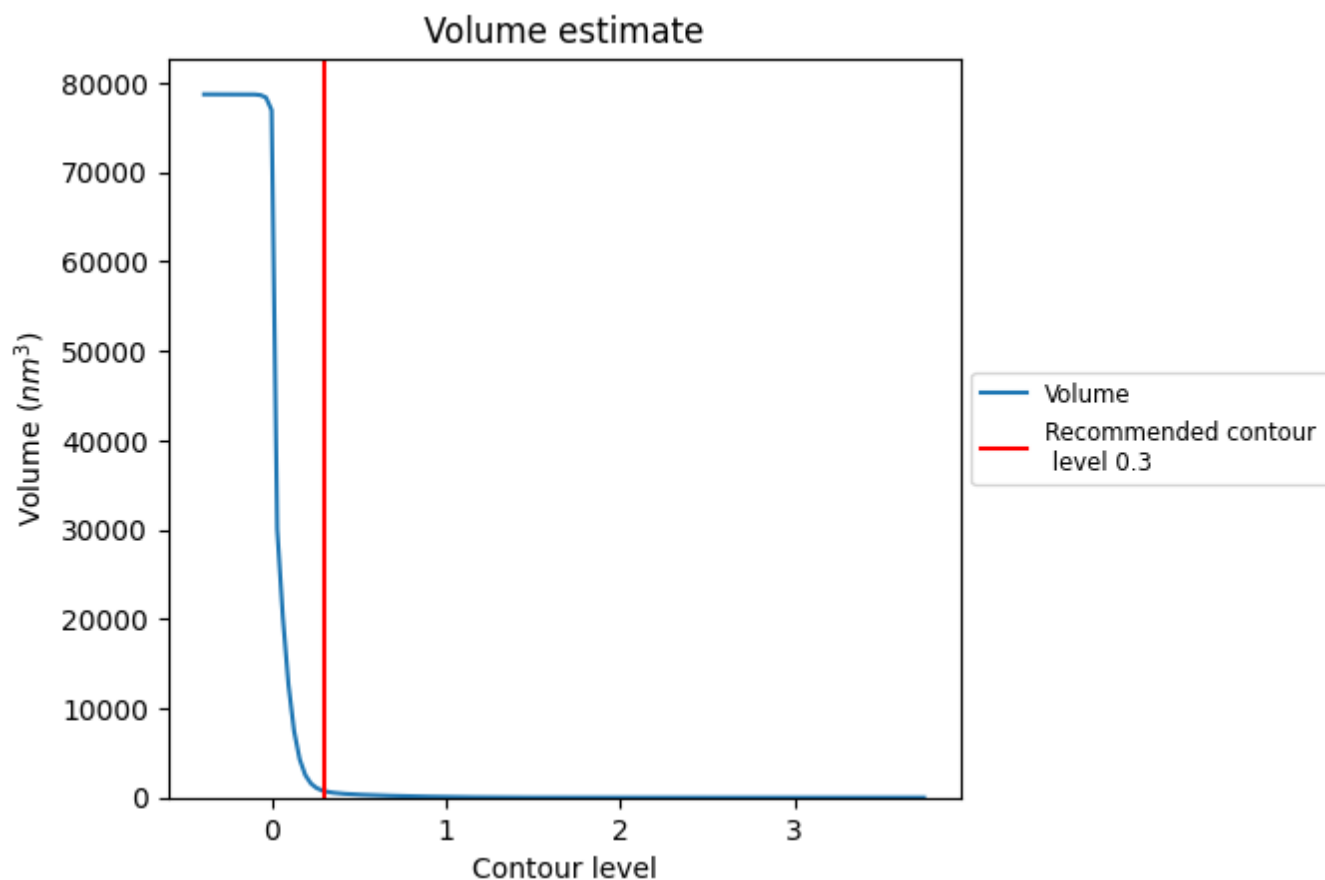
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

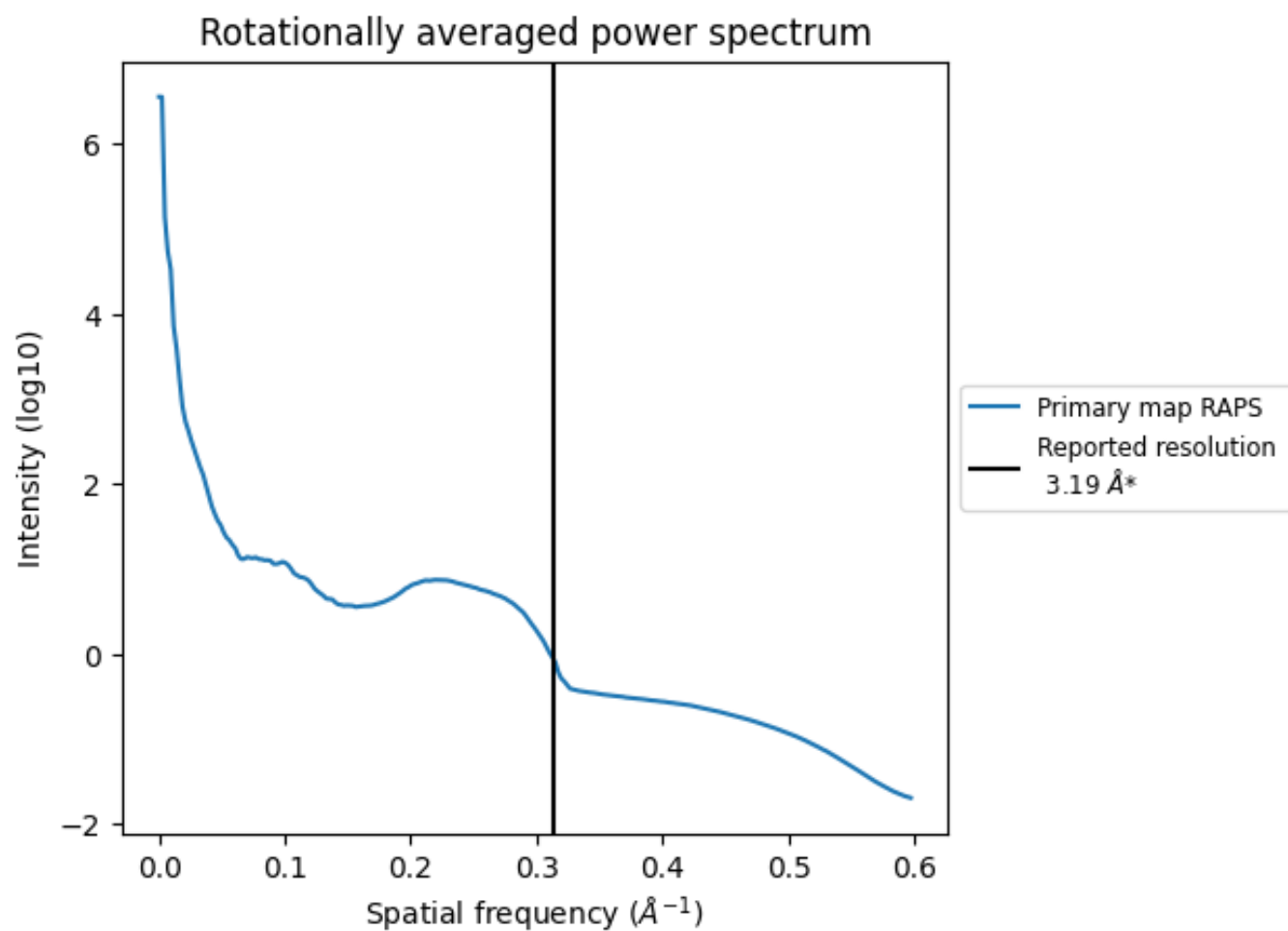
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm³; this corresponds to an approximate mass of 675 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.313 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

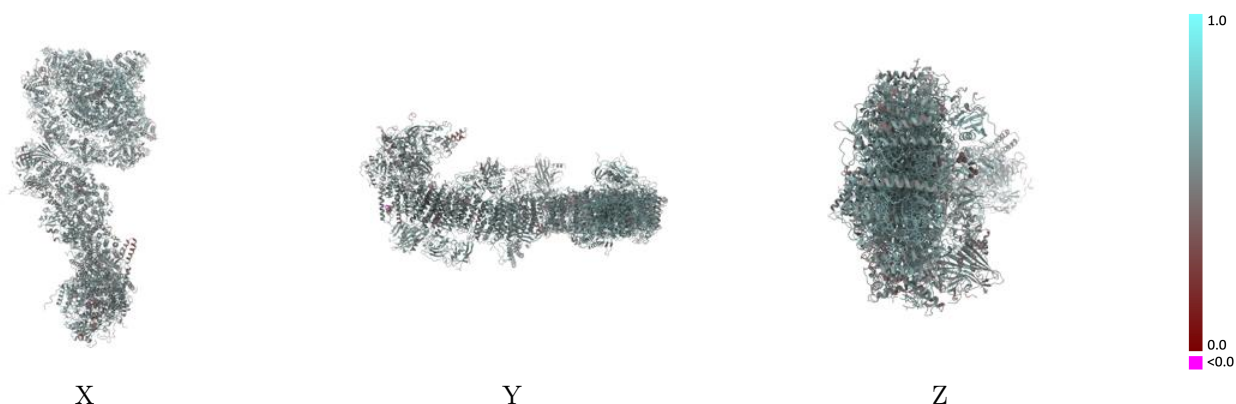
This section contains information regarding the fit between EMDB map EMD-51527 and PDB model 9GRX. Per-residue inclusion information can be found in section [3](#) on page [34](#).

9.1 Map-model overlay [i](#)



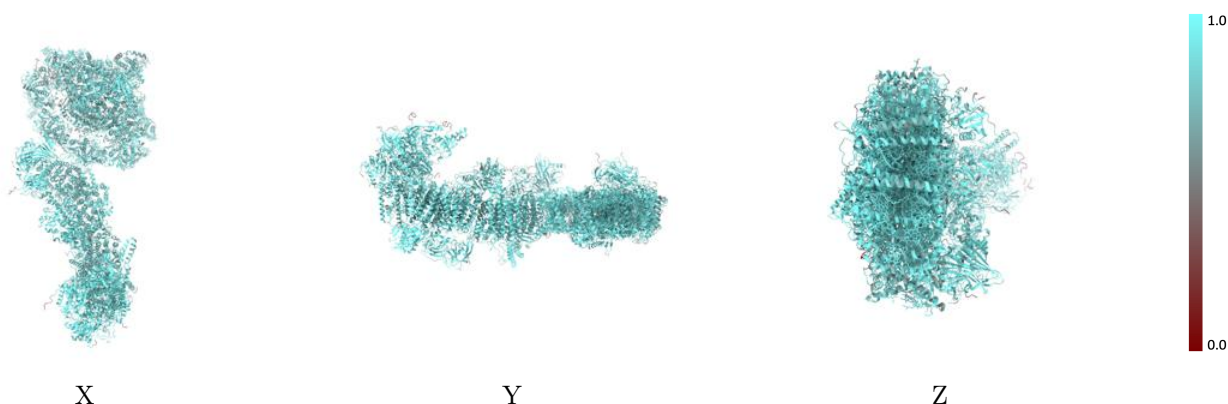
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



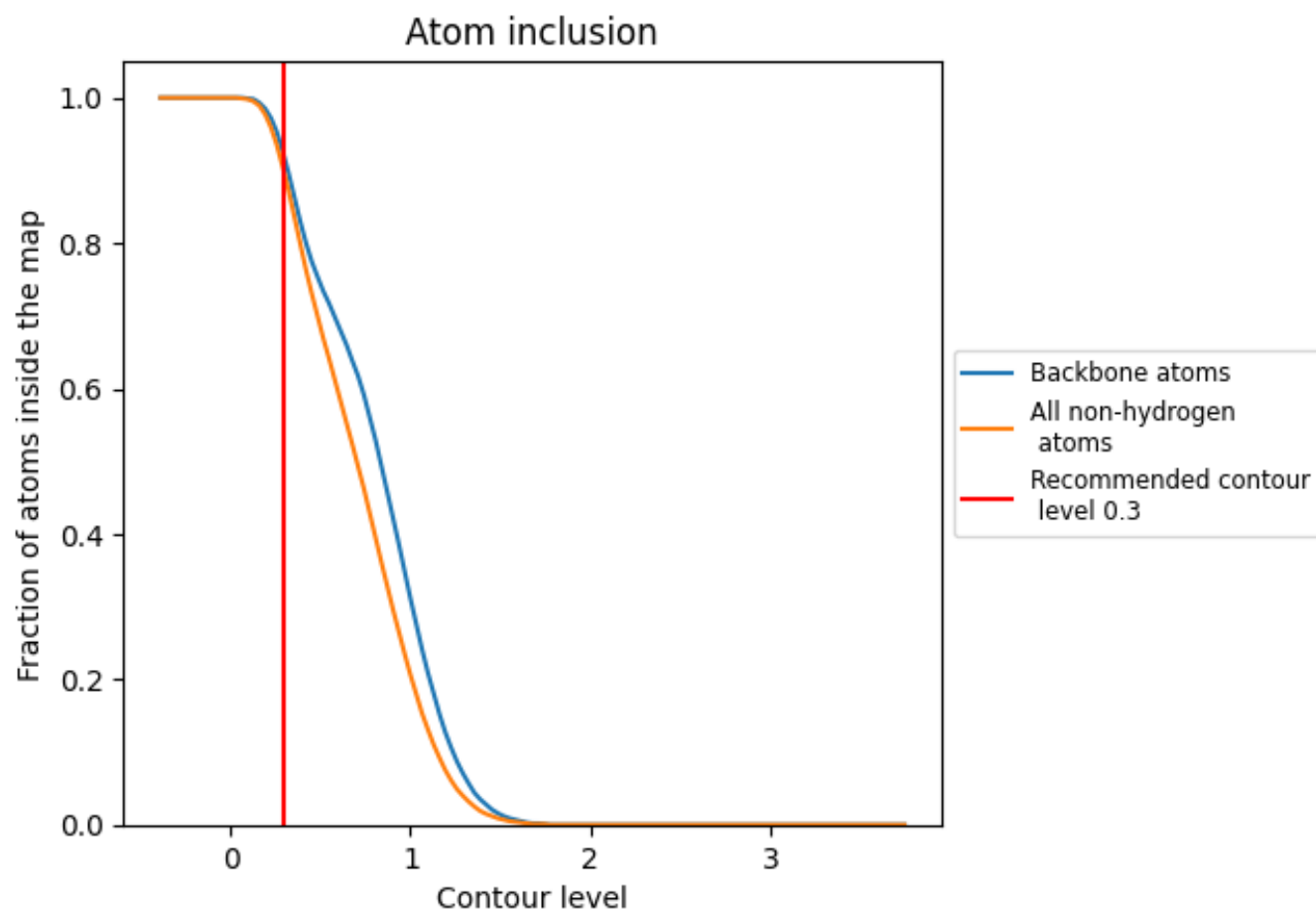
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.5410
0	 0.9360	 0.5380
1	 0.9010	 0.5310
2	 0.9130	 0.5190
3	 0.8660	 0.5090
4	 0.9060	 0.5410
5	 0.9090	 0.5360
6	 0.9370	 0.5290
7	 0.9390	 0.5360
8	 0.9580	 0.5540
9	 0.9370	 0.5460
A	 0.8730	 0.5200
B	 0.8910	 0.5230
C	 0.8800	 0.5150
D	 0.9330	 0.5510
E	 0.9290	 0.5410
F	 0.9090	 0.5240
G	 0.8980	 0.5220
H	 0.8970	 0.5250
I	 0.9000	 0.5250
J	 0.9310	 0.5430
K	 0.8970	 0.5220
L	 0.9000	 0.5250
M	 0.8910	 0.5260
N	 0.9000	 0.5150
O	 0.8800	 0.5110
U	 0.8480	 0.4840
a	 0.9150	 0.5790
b	 0.9070	 0.5780
c	 0.9210	 0.5590
d	 0.9030	 0.5710
e	 0.8230	 0.5320
f	 0.8740	 0.5640
g	 0.7850	 0.5270
h	 0.7260	 0.5120



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Chain	Atom inclusion	Q-score
i	 0.8970	 0.5740
j	 0.8510	 0.5490
k	 0.8000	 0.4920
l	 0.8070	 0.5390
w	 0.9280	 0.5470
x	 0.8710	 0.5420
y	 0.9030	 0.5330
z	 0.8010	 0.5160